Department of Earth Science and Engineering
Imperial College London

New Methods for Inferring Past Climatic Changes from Underground Temperatures

Peter Orlando Hopcroft

A thesis submitted in fulfilment of the requirements for the degree of

Doctor of Philosophy and the Diploma of Imperial College

Submitted August 2008

Examination 2nd December 2008
Declaration

The material in this thesis is entirely the result of my own independent research under the supervision of Prof. Kerry Gallagher and Prof. Christopher Pain, and is not the outcome of any collaborative work. The research was carried out in the Department of Earth Science and Engineering at Imperial College London. All published or unpublished material used in this thesis has been given full acknowledgement.

No part of this work has been previously submitted to this or any other academic institution for a degree or diploma, or any other qualification.

Name: Peter O. Hopcroft
Date: January 4th 2009
Abstract

In this thesis new methods have been developed for the recovery of past surface temperature variations from underground temperature-depth profiles. This has been undertaken from a Bayesian standpoint with an emphasis on model comparison, which allows differently parameterised inverse models (inferred past temperature histories) to be automatically constructed and compared in the light of the data and the prescribed prior information.

In the first contribution a new method for inverting temperature-depth profiles is presented which relies on trans-dimensional Bayesian sampling. The temperature histories are parameterised in terms of a variable number of linear segments over time. Relying on the natural parsimony of Bayesian inference, whereby simpler models which can adequately explain the data are preferred, the complexity or roughness of the temperature histories can be determined without the need for explicit \textit{a priori} smoothing. This method therefore allows a more objective inference of the past temperature changes.

These concepts are extended to the spatial domain in the following chapter using the method of Bayesian partition modelling. This seeks to find the posterior distribution of the number and spatial distribution of independent temperature histories given a spatially distributed ensemble of temperature-depth profiles. The results from application to 23 real boreholes in the UK are discussed in detail and show a clear preference for 8 or 9 independent (and mostly contrasting) temperature histories. It is thus concluded that the majority of these data cannot be considered as reliable sources of palaeoclimate reconstruction.

A 3D finite element heat transfer forward model is developed in the latter part of the thesis, and is used to simulate underground temperatures. This forward model is linked to
the first of the two Bayesian inverse methods described above. The effect of the reduction in average ground surface temperature with altitude is included in the forward model and inversion of the resultant profiles using a 1D forward model is shown to give significant discrepancies in the inferred temperature histories. Finally the inversion results from the Bayesian formulation are compared with those using a conventional gradient descent method.

The thesis concludes with some possibilities for future research in this field which builds upon the work presented herein.
I would like to acknowledge the support and counsel of my two supervisors Kerry Gallagher and Christopher Pain. They allowed me the independence to develop work as I felt best, but with help and invaluable advice along the way. I am grateful to Fangxin Fang who helped me with learning how to use both Fortran and Fluidity. Discussions on MCMC with fellow students John Stephenson and Karl Charvin were also of great help. Comments on this work by amongst others, Klaus Mosegaard and Malcolm Sambridge have been most helpful.

I would also like to acknowledge the support of my girlfriend Suzanne, my parents Catherine and Michael and my brother John, and finally Twajazz for all of the great jazz rehearsals and gigs we did together.

This PhD project was funded through the Environmental Mathematics and Statistics programme of NERC and EPSRC.
Acronyms

abp Years before present
BGS British Geological Survey
BPM Bayesian partition model
CET Central England temperature
FE Finite element
FSI Frequency spectrum inversion
GCM Global climate model
GST Ground surface temperature
IHFC International Heatflow Commission
MCMC Markov chain Monte Carlo
NLCG Non-linear conjugate gradient
pdf Probability density function
POD Proper orthogonal decomposition
POM Pre-observational mean
POM-SAT Pre-observational mean - surface air temperature
rj-MCMC Reversible jump Markov chain Monte Carlo
SAT Surface air temperature
SVD Singular value decomposition

$q_0$ Basal heat flux
$T_{eq}$ [Long term] equilibrium surface temperature
det Determinant
# Table of Contents

Declaration i

Abstract ii

Acknowledgements v

Acronyms vi

List of Figures x

List of Tables xiv

1 Introduction 1

1.1 Palaeoclimate ................................................. 1

1.2 Temperature reconstructions of the past millennium ................. 3

1.3 Motivation for studying borehole climatology .......................... 6

1.4 Publications resulting from the work in this thesis ................. 8

2 Borehole climatology 9

2.1 Surface air and ground temperatures .................................. 9

2.2 Temperature and rock property measurements ........................ 10

   2.2.1 Basic assumptions ........................................... 15

2.3 Borehole climatology methods ....................................... 16

   2.3.1 Historical background ......................................... 16

   2.3.2 Functional space inversion .................................... 17

   2.3.3 Singular value decomposition method .......................... 19
2.3.4 Monte Carlo method ............................................ 22
2.3.5 Forward modelling methods ................................. 22

2.4 Complications and shortcomings of current methods .............. 23
2.4.1 Effects of seasonal snow cover and land use change .......... 24
2.4.2 Subsurface advection ........................................ 25
2.4.3 Smoothing constraints, model parameterisation and model uncertainty 26
2.4.4 Spatial signal and averaging of reconstructions ............... 28
2.4.5 Three-dimensional effects .................................. 28

2.5 Avenues for research ........................................... 29

3 Bayesian inference .................................................. 31
3.1 Bayes’ Law ....................................................... 31
3.2 Bayesian approach to inverse problems .......................... 32
3.2.1 Model choice and Ockham’s razor .......................... 33
3.3 Sampling algorithms: Markov chain Monte Carlo ................. 34
3.3.1 Posterior distributions and model averaging ............... 39
3.3.2 Other Bayesian methods .................................. 41
3.4 Bayesian methods in geophysics ................................ 43
3.5 Conclusions ...................................................... 45

4 Temperature reconstructions from single and multiple boreholes .... 46
4.1 Model setup ...................................................... 47
4.2 Bayesian formulation ......................................... 49
4.2.1 Prior ...................................................... 49
4.2.2 Likelihood .................................................. 51
4.2.3 Proposals .................................................. 52
4.3 Calculating the acceptance probability .......................... 55
4.3.1 Fixed dimension moves of time or temperature values ........ 55
4.3.2 Birth/death acceptance term ............................... 55
4.3.3 Derivation of the birth/death Jacobian term ............... 57
4.4 Synthetic Data ................................................ 58
4.4.1 Example I: Moberg et al. (2005) data .................... 58
4.4.2 Example II: Beck et al. (1992) data ................................. 63
4.5 Real Data ................................................................. 65
   4.5.1 Examples I: 5 profiles from the IHFC database located in the UK .. 65
   4.5.2 Joint inversion ...................................................... 69
   4.5.3 Examples II: 5 profiles from Sellafield, Cumbria. .................. 73
4.6 Discussion and Conclusions ............................................ 77

5 Spatial trends ............................................................ 80
   5.1 Introduction .......................................................... 80
   5.2 Background .......................................................... 81
   5.3 Methods .............................................................. 85
      5.3.1 Forward Model .................................................. 85
      5.3.2 Partition modelling and Voronoi tessellations ................... 86
      5.3.3 Bayesian Inference .............................................. 87
   5.4 Sampling algorithm .................................................. 88
      5.4.1 Prior information .............................................. 88
      5.4.2 Likelihood ...................................................... 90
      5.4.3 Proposal distributions ........................................ 91
      5.4.4 Proposal ratio terms ......................................... 94
      5.4.5 Calculating the acceptance term ............................ 96
   5.5 Synthetic case ....................................................... 99
   5.6 UK borehole dataset ................................................ 103
      5.6.1 Data sources .................................................... 103
      5.6.2 Sampling and posterior distributions ........................ 106
      5.6.3 Uniform prior on the number of partitions .................... 106
      5.6.4 Poisson prior constraining the number of partitions .......... 109
   5.7 Discussion and conclusions ....................................... 115

6 Transient three-dimensional heat transfer modelling .................. 120
   6.1 Finite element formulation ....................................... 122
   6.2 Steady state equations ............................................ 125
      6.2.1 Model validation ............................................... 128
6.3 Transient finite element solutions .............................................. 128
6.4 Computational issues ............................................................. 132
   6.4.1 Model validation ............................................................. 132
6.5 Boundary Conditions .............................................................. 133
6.6 Effects of isotropic and anisotropic thermal conductivity ............... 136
6.7 Summary ........................................................................... 138

7 Three-dimensional inversion using reversible jump MCMC ............ 139
   7.1 Introduction ................................................................. 139
   7.2 Model reduction using proper orthogonal decomposition ............. 141
      7.2.1 Reduced order model .................................................. 143
      7.2.2 Examples ................................................................. 145
   7.3 POD forward model with Bayesian Inference .............................. 148
   7.4 Synthetic cases ............................................................... 150
      7.4.1 Idealised examples 1D/3D ............................................. 151
      7.4.2 Basal heat flow example ............................................. 152
      7.4.3 Uncertainty in the thermal conductivity .......................... 153
      7.4.4 Thermal conductivity structure .................................... 155
   7.5 Discussion & Conclusions ................................................... 157

8 Three-dimensional inversion using the adjoint method ................. 161
   8.1 The adjoint method of gradient calculation ............................. 162
   8.2 The 1st order adjoint ....................................................... 163
      8.2.1 The 1st order gradient of the 3D FE heat conduction model ..... 165
      8.2.2 Verification of the 1st order gradient calculations .......... 167
   8.3 Optimisation Methods ....................................................... 167
      8.3.1 The functional ......................................................... 167
      8.3.2 Non-linear conjugate gradient method ........................... 169
   8.4 Synthetic Inversion Examples .............................................. 171
      8.4.1 Non-linear conjugate gradient .................................... 171
   8.5 Discussion and Conclusions ................................................ 172
9 Conclusions & Future work

9.1 Implications for further studies ........................................... 178
9.2 Future work ................................................................. 178

References ................................................................. 181

Appendices ................................................................. 196

A Bayesian methods .......................................................... 196
A.1 Bayes’ law ................................................................. 196
A.2 The reversible jump MCMC algorithm ................................. 197

B Gradient methods .......................................................... 198
B.1 Deriving an analytical gradient ........................................... 198
B.2 The method of conjugate gradients ..................................... 199

C Prior information choice .................................................. 201
C.1 Constraining the time points using a uniform prior distribution . 201

D Data sources ................................................................. 204
D.1 Proxy and instrumental data ............................................. 204
D.2 International Heatflow Commission database ....................... 205
D.3 Nirex Sellafield borehole data ......................................... 205

E Computer code and model output ....................................... 207
List of Figures

1.1 Millennial climate ......................................................... 4
1.2 Comparing NH surface temperatures ................................. 5

2.1 Thermal perturbations at depth due to varying surface temperatures 12
2.2 Underground effects of surface warming and cooling ............... 13
2.3 Underground temperature response .................................. 14
2.4 Borehole inversions: over-fitting .................................... 26
2.5 SVD examples ............................................................. 27
2.6 European GST reconstructions ........................................ 29

3.1 Illustrating the principle of Ockham’s razor: Bayesian evidence 34
3.2 Posterior expectation and credible limits ............................ 41

4.1 Model setup ............................................................... 49
4.2 Birth/death process for rj-MCMC ..................................... 54
4.3 Synthetic noise-free data inversion with rj-MCMC .................... 60
4.4 Synthetic noisy data inversion with rj-MCMC ......................... 60
4.5 Example models accepted by the rj-MCMC algorithm ............... 61
4.6 Comparing prior and posterior distributions ......................... 62
4.7 Likelihood and number of time-temperature points with iterations 62
4.8 Posterior on number of points in GST history ........................ 63
4.9 Posterior on the GST for the Beck et al. 1992 data example. ....... 64
4.10 Posterior GSTs for 5 UK boreholes ................................. 66
4.11 Mean data misfit ......................................................... 67
4.12 Mean data misfit ......................................................... 67
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.13</td>
<td>Conductivity values for Chalgrove and inferred GST histories</td>
<td>68</td>
</tr>
<tr>
<td>4.14</td>
<td>Posterior GST, simultaneous inversion 5 UK boreholes</td>
<td>70</td>
</tr>
<tr>
<td>4.15</td>
<td>Posterior GST, simultaneous inversion 2nd example</td>
<td>71</td>
</tr>
<tr>
<td>4.16</td>
<td>Proxies, instrumental data and the GST history</td>
<td>72</td>
</tr>
<tr>
<td>4.17</td>
<td>The locations of Briffa et al. (2001) proxy data sources</td>
<td>73</td>
</tr>
<tr>
<td>4.18</td>
<td>Sellafield boreholes map</td>
<td>74</td>
</tr>
<tr>
<td>4.19</td>
<td>Geology at Sellafield</td>
<td>74</td>
</tr>
<tr>
<td>4.20</td>
<td>Reduced profiles for the 5 borehole temperature profiles.</td>
<td>75</td>
</tr>
<tr>
<td>4.21</td>
<td>Inferred GST from Sellafield boreholes</td>
<td>75</td>
</tr>
<tr>
<td>4.22</td>
<td>Hydrogeology of the Sellafield area</td>
<td>76</td>
</tr>
<tr>
<td>5.1</td>
<td>Global surface air temperature trends</td>
<td>81</td>
</tr>
<tr>
<td>5.2</td>
<td>Spatial structure gridding in Pollack and Smerdon (2004)</td>
<td>82</td>
</tr>
<tr>
<td>5.3</td>
<td>An example of a Voronoi tessellation with 8 centres.</td>
<td>86</td>
</tr>
<tr>
<td>5.4</td>
<td>Voronoi setup for a birth move</td>
<td>92</td>
</tr>
<tr>
<td>5.5</td>
<td>BPM algorithm outline</td>
<td>94</td>
</tr>
<tr>
<td>5.6</td>
<td>Synthetic case: true model setup</td>
<td>99</td>
</tr>
<tr>
<td>5.7</td>
<td>Three N Hemisphere multi-proxy surface temperature reconstructions</td>
<td>99</td>
</tr>
<tr>
<td>5.8</td>
<td>Synthetic case: applied temperature histories</td>
<td>100</td>
</tr>
<tr>
<td>5.9</td>
<td>Posterior on the partition boundaries</td>
<td>101</td>
</tr>
<tr>
<td>5.10</td>
<td>Posterior value and the number of partitions</td>
<td>101</td>
</tr>
<tr>
<td>5.11</td>
<td>Posterior on the GST for synthetic case</td>
<td>102</td>
</tr>
<tr>
<td>5.12</td>
<td>UK GST reconstructions from Huang et al. (2000)</td>
<td>103</td>
</tr>
<tr>
<td>5.13</td>
<td>Huang et al. (2000) mean reconstruction from UK data</td>
<td>104</td>
</tr>
<tr>
<td>5.14</td>
<td>Conductivity data model</td>
<td>105</td>
</tr>
<tr>
<td>5.15</td>
<td>Posterior and number of partitions UK set</td>
<td>107</td>
</tr>
<tr>
<td>5.16</td>
<td>Posterior partition structure for the UK dataset</td>
<td>108</td>
</tr>
<tr>
<td>5.17</td>
<td>Posterior pdf of the GST histories in the 4 largest partitions</td>
<td>109</td>
</tr>
<tr>
<td>5.18</td>
<td>Comparison of 4 GSTs with instrumental data</td>
<td>109</td>
</tr>
<tr>
<td>5.19</td>
<td>Posterior mean GSTs for all 10 partitions</td>
<td>110</td>
</tr>
<tr>
<td>5.20</td>
<td>Historical instrumental stations</td>
<td>110</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>8.4</td>
<td>NLCG synthetic inversion example 2</td>
<td>173</td>
</tr>
<tr>
<td>C.1</td>
<td>Uniform time prior example</td>
<td>202</td>
</tr>
<tr>
<td>D.1</td>
<td>Moberg et al. (2005) reconstruction</td>
<td>204</td>
</tr>
<tr>
<td>D.2</td>
<td>Central England Temperatures</td>
<td>205</td>
</tr>
</tbody>
</table>
List of Tables

1.1 Proxy data source summary information ................................................. 4

2.1 Skin depths for sinusoidal temperature boundary conditions ................. 10

4.1 Beck et al. (1992) data ................................................................. 63

4.2 Borehole summary information for the 5 real data examples .................. 65

5.1 Borehole summary information for UK dataset ..................................... 105

D.1 Sellafield borehole summary information ............................................ 206

D.2 Depths of lithological units for the 5 Sellafield boreholes ...................... 206

D.3 Sellafield thermophysical data ............................................................ 206

E.1 Contents of data CD ............................................................................. 207
Chapter 1

Introduction

1.1 Palaeoclimate

The climate system is defined as the sum of the atmosphere, hydrosphere, biosphere, lithosphere and cryosphere and the interactions that occur between them. The climate is the long term average state of this complex system which can be quantified in different ways, be it the average surface air temperature, the average annual rainfall and so on. Over the last few decades the volatility of the past climate system has become more clearly understood as new evidence from ice cores and other sources has come to light, and as ever more realistic computer climate models make predictions of climatic changes caused by the anthropogenic altering of the atmospheric chemistry. For example, the longest temperature record derived indicated by oxygen isotope variations in the Antarctic EPICA ice cores shows that temperature has varied a great deal over the past 740,000 years, with numerous glacial and inter-glacial periods. The record culminates in a relatively short, stable inter-glacial, the Holocene which includes the time since the last de-glaciation up to the present day. However, even the Holocene has been the subject of climatic variations, such as the warm 'Holocene optimum’ at around 5000 years ago or the more recent 'Medieval Warm Period’ and 'Little Ice Age’. Understanding the causes of these and other past climatic variations is vital for making useful predictions about future changes in the climate. For this purpose, quantitative palaeo- reconstructions must be derived for climatic variables such as temperatures and for the forcings such as solar irradiance, volcanic activity and atmospheric chemistry.
In addition to the long records of temperatures derived from the polar ice cores (e.g. Dansgaard et al., 1993, EPICA, 2004), past temperatures can in general be derived from four sources of information. The first is the instrumental temperature record, which relates to most of the globe for the past 150 years (Jones et al., 1999), with longer records at certain locations in Europe. Although the accuracy of most of the records is high, their brevity makes their use for climate modelling and climate change detection limited. The second source of information is documentary evidence which comprise historical notes on the weather in the past, see for example Lamb (1982). Documentary evidence tends to focus on extreme events and so the data is often used more for comparisons with reconstructions from other methods, rather than for deriving reconstructions themselves. The third data source is proxy data and is so-called because it must be calibrated against instrumental temperatures in order to produce quantitative temperature reconstructions. Proxy data has the potential for much longer climate reconstructions, for example the temperature record from ice cores is a type of proxy reconstruction. However, the proxies can be subject to influences which cause a change in the temperature response over time. Sources of proxy data for temperature are tree ring widths and wood densities, coral growth layers, speleothems (e.g. stalagmites, stalactites) and sedimentary layers from lakes and the ocean bed.

The fourth type of temperature reconstruction is derived from data relating to systems which are sensitive to past temperatures but for which the level scientific understanding of the processes involved is higher. These types of systems can therefore be modelled numerically and thus there is no need to calibrate the measurements as is the case for the proxy data. These data types include glacier lengths, which have been measured for up to 300 years, providing reconstructions back 500 years (Oerlemans, 2005) and temperature depth measurements from boreholes (e.g. Pollack and Huang, 2000) which allow reconstructions of up to a few centuries depending on the depth range of measurements. In this second method, present day underground temperatures are related to heat transfer at the ground surface in the past through the law of heat conduction. Both this method and the glacier method are of particular relevance to climate modelling as the data and reconstruction methods involved are independent from those used in conventional proxy data reconstructions. The borehole method is the focus of this thesis and it is described
in detail in chapter 2. Since borehole reconstructions can only be derived for the past several centuries, a review of the current state of knowledge for this time period is given alongside an introduction to the other reconstruction methods employed.

1.2 Temperature reconstructions of the past millennium

The main temperature excursions of the past millennium are the so-called ’Medieval Warm period’, the ’Little Ice Age’ and more recently, global warming. The first of these is attributed to climatologist H.H. Lamb and is evident in his reconstruction back to AD900 of central England temperatures derived (for the time period prior to 1659) from documentary evidence (Lamb, 1965, 1982), see figure 1.1. More recently proxy and other data from across the globe have been used to derive reconstructions of past temperature variability. These include glacier lengths and borehole temperatures, whilst examples of the proxy indicators are tree rings, tree ring densities, coral layers, speleothems, varved sediments, ice core compositions and lake sediment cores. These latter data sources require calibration against relevant instrumental records. For example tree-ring widths are first detrended (for growth rates) and then calibrated against growth season temperatures from instrumental records (over a time period of overlap) to produce a palaeo-temperature series. For more detailed reviews of each data source see NRC (2006) and Jansen et al. (2007).

Different proxy methods are subject to various inherent obscuring factors. These include differing target seasons, meaning that a proxy data source is more sensitive to the climate at certain times in the year; coupling effects between different climatic factors e.g. between temperature and precipitation; differing spatial coverage; resolution differences and differences in calibration method. Table (1.1) indicates the properties of some commonly used proxy data sources compared with the borehole method. $C_{in}$ are correlations with the instrumental record for representative reconstructions as defined in Jones et al. (1998). Calibration is based on the assumption of a constant temporal response to changing climatic temperature with time. As an example, Briffa et al. (1998) among others note that tree-rings indices demonstrate a divergence from surface temperatures in the latter part of the 20th century, the cause of which is unknown although an anthropogenic
Chapter 1. Introduction

Figure 1.1: Surface temperatures over the past millennium from documentary evidence relating to central England (Lamb, 1965, 1982), two multi-proxy reconstructions relating to the full Northern hemisphere and the extra-tropical area of the northern hemisphere and instrumental data. The central England reconstruction shows much more variability than the proxy series, this could be due to the differing geographical coverage or differences in the reconstruction methodologies employed. Reproduced from Mann (2002).

Table 1.1: Proxy data source summary information

<table>
<thead>
<tr>
<th>Proxy</th>
<th>Target</th>
<th>Resolution</th>
<th>Obscuring factors</th>
<th>$C_m$ $^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tree rings and densities</td>
<td>growing season</td>
<td>annual</td>
<td>Removing growth trends problematic, can lead to reduced long-term climatic trends.</td>
<td>0.48-0.81</td>
</tr>
<tr>
<td>Corals (growth &amp; sediment)</td>
<td>seasonal/annual</td>
<td>annual</td>
<td>Affected by other factors e.g. sunlight, nutrient supply etc.</td>
<td>0.18 -0.41</td>
</tr>
<tr>
<td>Ice cores</td>
<td>annual</td>
<td>annual</td>
<td>Dependent on ice flow model and layer compaction.</td>
<td>0.26-0.30</td>
</tr>
<tr>
<td>Borehole temperatures</td>
<td>annual</td>
<td>poor</td>
<td>Air-ground temperature relationship complex, de-coupling can be induced by land use change, snow cover, topography and fluid flow.</td>
<td>0.42 $^b$</td>
</tr>
</tbody>
</table>

$^a$see Jones et al. (1998) for proxy details.

$^b$see Pollack and Smerdon (2004).

Influence is likely. Additionally, methods for removing the growth trend of a particular tree may also suppress low-frequency variations in tree-ring reconstructions (Briffa et al., 1998).

In order to minimise the influence of such effects on derived temperature reconstructions so-called multi-proxy reconstructions have been derived by combining data from
Figure 1.2: Reconstructions of North Hemisphere surface temperature trends over the last 1000 years. All reconstructions are derived from multi-proxy data, except Pollack and Smerdon (2004) which is calculated from global borehole temperatures and Huang (2004) which is based on a combination of proxy and borehole data. The proxy reconstructions have been smoothed with a 50-year filter (Mann, 2004). Data from Overpeck et al. (1997), Jones et al. (1998), Mann et al. (1999), Jones et al. (1999), Briffa (2000), Crowley and Lowery (2000), Briffa et al. (2001), Esper et al. (2002), Pollack and Smerdon (2004), Huang (2004) and Moberg et al. (2005).

many different sources (e.g. Mann et al., 1998, Jones et al., 1998, Mann et al., 1999, Esper et al., 2002, Mann and Jones, 2003, Moberg et al., 2005). This includes the well known ‘hockey stick’ reconstruction (Mann et al., 1999) which shows very little long-term variability until the 19th century and the onset of a strong warming to the present day. More recently different signals have been inferred from similar data using a variety of methods with more and more studies questioning the picture of relatively stable pre-19th century climate. A representative ensemble of such reconstructions is shown for comparison in figure 1.2 for which each reconstruction has been smoothed using a 50-year low-pass filter (Mann, 2004) for ease of comparison. The different reconstructions show many similar temperature variations, for example the slight warming to 1100 AD and subsequent cooling, but overall the magnitudes of the changes at longer timescales cover a wide range. The overall trend shows a medieval warm period centred on 1000-1100 AD followed by cooling to AD 1600 with subsequent warming to the present day. Although a number of the reconstructions are derived to before AD 1000, these are not shown due to the low
number of data sources used and the resultant uncertainties.

Reconstructions by Esper et al. (2002) and Moberg et al. (2005) shown in figure 1.2 both indicate much cooler conditions during the past few centuries, which are as low as 0.8°C below the 1961-1990 mean. These two reconstructions were both produced using methods explicitly designed to preserve the low frequency content of the proxy data in order to combat the problem of detrending in tree-ring data. These two reconstructions which are also consistent with the estimates of northern hemisphere temperatures derived from borehole temperatures (Huang et al., 2000, Pollack and Smerdon, 2004) which indicates 1.0°C warming over the last 500 years to AD 2000, see the dark grey line in figure 1.2. Hegerl et al. (2007) and Juckes et al. (2007) present new multi-proxy reconstructions which also show good agreement with borehole reconstructions for the last 500 years. Recently glacier length reconstructions have been derived which indicate warming (over the globe) of 0.6°C over the time period 1850 to 1990 Oerlemans (2005), consistent with both the borehole estimate and instrumental records. Finally the instrumental part of the central England series (back to 1659: the longest such record in the world) has been shown to be consistent with reconstructions from boreholes located in the UK and Ireland (Jones, 1999).

There exists a large range of temperature reconstructions from proxy data and other data sources for which the methods and data are entirely independent and which show good agreement with reconstructions from borehole temperatures. This provides a strong basis for further research into climate reconstruction from borehole data.

1.3 Motivation for studying borehole climatology

Given the apparent reconciliation of borehole temperature histories with proxy reconstructions at the hemispheric scale, as well as with instrumental and glacier reconstructions, it is necessary to invest more research in the borehole method to investigate ways of maximising the information content that can be extracted from the large worldwide borehole temperature data set. As well as the complex bio-physical processes that form the link between ground and air temperatures, there are a number of issues relating to how best to infer ground temperature histories from the available data. For example current methods
ignore issues of how models should be parametrized, use simple choices of prior information such as model smoothing and employ simple spatial data treatments. Additionally, there are no examples to date, of inverse schemes which can account for 3D thermal effects caused by the likes of topography and underground geological structure. In this thesis, new methods are presented to address some of these issues.

In chapter 2 the principles of borehole climatology are described. The current methods for extracting temperature histories and their spatial trends are discussed with a focus on the inherent drawbacks. Areas for potential improvement are outlined. This is followed by an introduction to Bayesian inference in chapter 3 and its use in geophysical inverse problems. Applications of newly developed methods in Bayesian statistics to other areas of geophysics are described and possible avenues for deployment in borehole climatology are discussed.

In chapter 4 a new method for inverting temperature-depth profiles, both individually and jointly, is given. This method relies on a Bayesian reversible jump Markov chain Monte Carlo (rj-MCMC) algorithm. Subsequently in chapter 5 the issues surrounding spatial variations of past temperatures and also how best to group or average multiple temperature reconstructions is approached from a Bayesian perspective. Here a Bayesian partition model is developed which automatically groups borehole data according to the jointly inferred temperature histories.

In chapters 6, 7 and 8 the assumption of purely vertical heatflow is relaxed and inversions are demonstrated with 3D forward models. Two methods are demonstrated, the first of which is an application of the rj-MCMC algorithm of chapter 4. In this case the forward model is too computationally expensive, and so the method of proper orthogonal decomposition is used to define a reduced order model. The second 3D inversion chapter details the application of a gradient based optimisation method which relies on the adjoint model for the gradient calculations. The thesis concludes with possibilities for further research using the methods presented here, as well as for future work in the field.
Chapter 1. Introduction

1.4 Publications resulting from the work in this thesis

Listed below are the refereed publications and conference presentations resulting from the work in this thesis.

Refereed publications:


Conference proceedings:


Chapter 2

Borehole climatology

2.1 Surface air and ground temperatures

Variations in surface temperatures at all time scales are propagated into the ground by heat conduction. Due to the low thermal conductivity of the rock the temperature variations are subjected to a low-pass filter so that high-frequency variations are rapidly damped out with depth below the surface. For example consider an oscillatory temperature boundary condition at the surface (e.g. diurnal or annual cycle) expressed as

\[ T_s = T_0 + \Delta T \cos(\omega t) \]  

(2.1)

where \(\omega\) is the circular frequency of the surface variation, \(\omega = \frac{2\pi}{\tau}\), where \(\tau\) is the time period and \(\Delta T\) is the amplitude of the variation. The subsurface temperature perturbation can then be shown to be an exponential function of depth and the wavelength of the boundary condition (Turcotte and Schubert, 2006):

\[ T(z,t) = T_0 + \Delta T \exp\left(-z\sqrt{\frac{\omega^2}{2\kappa}}\right) \cos\left(\omega t - z\sqrt{\frac{\omega^2}{2\kappa}}\right) \]  

(2.2)

where \(\kappa = \frac{k}{\rho c}\) the thermal diffusivity and \(k, \rho\) and \(c\) are the thermal conductivity, density and specific heat capacity respectively. The signal is attenuated according to frequency and depth, and a phase lag is introduced between the ground temperatures and the boundary
Table 2.1: Skin depths for oscillatory boundary conditions of different time periods assuming a uniform thermal diffusivity of $1 \times 10^{-6}$ m$^2$s$^{-1}$.

<table>
<thead>
<tr>
<th>Variation</th>
<th>time period rad s$^{-1}$</th>
<th>skin depth (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>daily</td>
<td>$7.27 \times 10^{-5}$</td>
<td>0.17</td>
</tr>
<tr>
<td>annual</td>
<td>$1.99 \times 10^{-7}$</td>
<td>3.17</td>
</tr>
<tr>
<td>decadal</td>
<td>$1.99 \times 10^{-8}$</td>
<td>10.03</td>
</tr>
<tr>
<td>centennial</td>
<td>$1.99 \times 10^{-9}$</td>
<td>31.7</td>
</tr>
</tbody>
</table>

condition which increases with depth below the surface. Therefore, only very low frequency variations will have significant influence on the temperatures at large depths. One way to quantify this is to consider the skin depth, which is the depth at which the perturbation has decayed to $1/e$ of its amplitude at the surface. In this case the skin depth is given by

$$d_\omega = \left(\frac{2\kappa}{\omega}\right)^{1/2}$$

(2.3)

Table 2.1 gives the skin depth for oscillatory variations of different time periods. The subsurface perturbations due to daily and annual variations in air temperatures have decayed to less than 0.01K at depths of 1.2m and 21.9m respectively, whilst the effect of more persistent long-term surface temperature changes can be found at larger depths. Variations from the last 500 years have influence at depths up to around 500m for example. Therefore accurate measurements of temperature over approximately this depth range can provide valuable information on past climatic changes.

2.2 Temperature and rock property measurements

To measure the rock temperatures a borehole is drilled, typically to a depth of a few hundred metres. A temperature sensitive probe is then lowered into the borehole in order to measure the groundwater temperature at a succession of depths below the surface. However, the process of drilling injects a large amount of energy into the rock and groundwater, and hence the temperatures in the borehole are measured a number of months or more after drilling is completed (Lachenbruch and Brewer, 1959). The groundrock and water is then expected to return to the temperatures of the surrounding rock over this time. The borehole must also have a small enough diameter to prevent significant verti-
cal, convective heat transfer in the ground water after drilling (Jessop, 1990). In certain cases cores are also retrieved from the borehole, these consist of sections of rock which, upon laboratory analysis, can yield measurements of thermal conductivity, density, heat capacity and porosity.

Generally thermistors or platinum resistance sensors are used in probes for measuring borehole temperatures. A thermistor can be connected to a Wheatstone bridge or used in an alternating current circuit. The former requires thicker wire to maintain accuracy and can require 2 minutes or more in order to equilibrate at each depth. The probe can be lowered more quickly when an AC current is used, in which case the signal frequency is proportional to the thermistor resistance. Accuracy can be better than 0.01K using the Wheatstone bridge. Depending on the logging speed, the AC current approach has an accuracy of around 0.05K with an absolute error of up to 0.5K (Beardsmore and Cull, 2001).

Typical geothermal gradients of 25-30Kkm$^{-1}$ can induce convective cells in boreholes with diameters greater than around 5cm (Diment, 1967, Gretener, 1967). Generally however the convective cell will be of the order of 1m in height and does not significantly affect the broader temperature trends measured in the borehole. The effect of convection within the water column of a borehole will be larger for boreholes with large diameters and where the geothermal gradient is higher.

Thermal conductivity values are generally obtained using a divided bar apparatus. This constitutes a warm and cool water container, which are in thermal contact with either side of a sample of rock. Brass plates are used to ensure good thermal contact and 4 temperature probes are used, 2 on ether side of the 2 copper plates. The water in the two containers is maintained at around 40°C and 25°C with the warmer at the top in order to minimise any convective heat transfer. The steady state temperatures are then used to determine the thermal conductivity of the rock. The results are usually accurate to around 5%.

For unconsolidated rock, a different setup is used whereby the mixture of (usually) sediment and water is packed into a cell so that heat sources can be applied. A primary source of error in these measurements relates to the how much water was present in the original subsurface environment, and how well the real rock-water combination can be
Figure 2.1: Temperature changes at the Earth’s surface, here $\Delta T$, cause a perturbation to the underground profile which is manifest as departures from the linear trend which is a function of the basal heat flow $q_0$ and the equilibrium surface temperature $T_{eq}$.

assumed to be homogeneous and isotropic.

Thermal conductivity can also be measured using a transient rather than steady-state experimental setup. One example is the needle probe which introduces a line heat source into the rock. Solutions for such a forcing are given by Carslaw and Jaeger (1959) and these can be used to calculate the thermal conductivity given temperature measurements in the vicinity of the probe. A disadvantage of this method is that the heat source can induce convection in especially porous rocks, leading to erroneous conductivity values. Beardsmore and Cull (2001) give details of more advanced transient measurement techniques using dual needle and sheet probes.

In order to identify the effect of long-term changes in the ground surface temperatures, the basal heat flow and long term equilibrium surface temperature must also be quantified. The basal heat flow comes from secular heat loss from the mantle as well as radiogenic heat production in both the crust and mantle. The value of the heat flow varies across the globe, but can be assumed to be constant over time periods of 1000s of years. The long term equilibrium temperature accounts for the average temperature at the surface. Thus if there have been no long-term variations in surface air temperatures, the temperatures $T(z)$ in a suitable borehole will increase with depth according to
Chapter 2. Borehole climatology

Figure 2.2: The effect of general warming or cooling on underground temperatures.

\[ T(z) = T_{eq} + q_0 R(z) \]  

(2.4)

where \( T_{eq} \) is the long-term equilibrium ground temperature, \( q_0 \) is the equilibrium basal heat flux and \( R(z) \) is the thermal resistance from the surface to depth \( z \) which is defined by

\[ R(z) = \int_0^z \frac{1}{k(z')} dz' \]  

(2.5)

where \( k \) is the thermal conductivity. This is illustrated in figure 2.1 by the dashed line, for the case of constant thermal conductivity and zero radiogenic heat production over the depth range plotted. In this case the temperature depth profile is then a linear function of depth.

We know however, that there have been significant variations of the surface tempera-
Figure 2.3: Underground reduced temperature response to a ground surface temperature history derived from Moberg et al. (2005) and Jones and Moberg (2003), see appendix D.1. The resultant temperatures are shown as deviations from the geothermal steady state. For comparison the same profile is shown degraded with Gaussian 0.1K noise.

Tectures over the past and these should be manifest to some degree in the subsurface temperature field \( T(z) \). For instance a long term warming signal will result in positive departures from the linear trend and a longer term cooling will result in negative departures. This is illustrated in figures 2.1 and 2.2. In reality the signal will be more complicated, involving for instance the Last Glacial maximum, the Medieval Warm Period (AD 900-1200), the Little Ice Age (AD 1500-1750) and warming since 1750 to the present. However, because the thermal signal is attenuated over time some of the perturbations from these changes will have decayed below the noise levels of the data, typically around \( 1 \times 10^{-2} \text{K} \) (Beltrami and Mareschal, 1992). The rate of attenuation means that it is unlikely that the distant past events are resolvable except for high quality borehole data and data from far northerly latitudes (where the signal would be expected to be stronger) and in boreholes drilled in ice (where the effects of noise are much smaller). However the older, but much larger amplitude temperature variations such as from the last glacial maximum to the Holocene climate are resolvable in borehole data of sufficient depth, usually of 2000m depth or more.
The effect of the signal attenuation is shown in figure 2.3 for typical rock properties. Here the underground response to surface forcing which constitutes a 2002 year palaeoclimate reconstruction is shown with depth and time. This is shown as the perturbations from the steady state, i.e. in reduced temperatures. The high frequency variations which result from the year to year variation are completely damped out for the depth range considered. The effects of the longer term centennial variations are clearly visible at depth, however, notice how the signal from the warm period at around AD 1000 is only just observed in the resultant $T(z)$ profile. For this reason studies of borehole temperatures therefore concentrate on reconstructions of the last deglaciation or the past 500 years only (e.g. Kukkonen and Jöeleht, 2003, Huang et al., 2000) and this depends on the depth range of the data under consideration.

2.2.1 Basic assumptions

Quantifying the heat conduction into the ground requires the diffusion equation which is derived from Fourier’s law and the conservation of energy:

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T)$$  \hspace{1cm} (2.6)

where $\rho c$ is the volumetric heat capacity, $k$ is the thermal conductivity, $t$ is time and $T$ is temperature field. For most studies of borehole temperatures, heat flow is assumed to be in the vertical direction only, and so this equation is simplified so that $T$ is dependent only on the depth $z$ and time $t$. In this purely conductive regime, the temperatures in the ground are a superposition of the equilibrium temperature value and that arising due to the time-varying upper-boundary temperature. The initial conditions are given by a linear trend as before (equation 2.4). The boundary conditions are the ground surface temperatures (GST) over time and the basal heat flux, which is treated as a constant over time-periods considered here.
\[
T(0, t) = T_{GST}(t) \tag{2.7}
\]
\[
k \frac{\partial T(z_b)}{\partial z} = -q_0 \tag{2.8}
\]

Subject to these boundary conditions the subsurface effects of the surface temperature variations in a purely conductive regime can be calculated. This is referred to as the forward problem. These solutions can be obtained either analytically (Carslaw and Jaeger, 1959, p. 63) or by using approximate methods such as finite differences or finite elements (e.g Lewis et al., 1996). In this work finite element methods are used so that both 1D and 3D solutions can be obtained. The finite element formulation used is described in chapter 6.

Given a forward problem for which the control parameters are unknown but of interest, an inverse problem must be solved. In this case the upper surface transient ground surface temperature (GST) values are the control parameters and these are inferred from the present day measured borehole temperatures by solving the inverse of the above forward problem. This is a non-linear problem which has mathematically an infinity of possible solutions (Menke, 1989) and so any inverse method must be designed to deal with this degeneracy by taking account of other a priori information. Dealing with the inverse problem is the main aim of this thesis and two methods are used, a Bayesian probabilistic approach (Mosegaard and Tarantola, 1995, Malinverno, 2000, Tarantola, 2005, Sambridge et al., 2006) and a gradient approach based on non-linear optimisation. In the next section a review of the current methods for solving this inverse problem is given. This is followed by a more general discussion of the real world obscuring factors which can have an impact on the derived reconstructions.

2.3 Borehole climatology methods

2.3.1 Historical background

Lane (1923) first noted that heat flow values need to be corrected for the effects of glacial temperatures and later Hotchkiss and Ingersoll (1934) and Birch (1948) made calculations
of the timing and magnitude of the last de-glaciation based on temperature measurements from mines. Beck and Judge (1969), Cermák (1971) and Anderssen and Saull (1973) demonstrated that borehole temperatures could be used to calculate ground surface temperature histories whilst Vasseur et al. (1983) introduced the idea of inverting a temperature-depth profile for past GST values. Lachenbruch and Marshall (1986) demonstrated the relevance of borehole temperatures to the global warming, after detecting strong 20th century warming in the Alaskan Arctic. Since then, there has been an upsurge of interest in using borehole temperature to measure past surface temperature changes across the globe. A variety of inverse methods have been developed, including a Bayesian least squares method (FSI: Shen and Beck (1991)), singular value decomposition (SVD: Mareschal and Beltrami (1992)), control theory (Kakuta, 1992), a Monte Carlo method (Dahl-Jensen et al., 1998), and an information criterion method (Woodbury and Ferguson, 2006). The FSI and SVD methods are the only methods with widespread use and these are described in detail below.

Data from across the globe have been analysed, with the majority in North America, Europe, South Africa and Australia. A global geothermal data-base of borehole profiles suitable for palaeoclimate inversion has been compiled from data from all the continents except Antarctica (Huang and Pollack, 1998). This database has been used to infer hemispheric and global GST trends over the past 500 years with consistent conclusions of 1°C warming over this period (Huang et al., 2000, Harris and Chapman, 2001, Beltrami and Bourlon, 2004, Pollack and Smerdon, 2004, Harris and Chapman, 2005). General reviews of the subject can be found in Pollack and Huang (2000), Majorowicz et al. (2004), Bodri and Cermak (2007) and González-Rouco et al. (2008), with the latter focusing on the interface with climate change modelling.

2.3.2 Functional space inversion

The most common method used to infer GST reconstructions from borehole temperatures is called functional space inversion and it has been developed over a period of years (Shen and Beck, 1991, 1992, Shen et al., 1996, Huang et al., 1996, Șerban and Jacobsen, 2001). The method relies on the Bayesian least-squares theory of Tarantola and Valette (1982a,b) and progresses by minimising a functional which constitutes a data-fit and a
prior information term. The functional is given by:

\[
F = \frac{1}{2} (d - d_0)^T \cdot C_d^{-1} \cdot (d - d_0) + \frac{1}{2} (m - m_0)^T \cdot C_m^{-1} \cdot (m - m_0).
\] (2.9)

where \(d\) and \(d_0\) are the calculated and measured temperature data, \(m\) and \(m_0\) are the posterior and the a priori model parameters and \(C_d\) and \(C_m\) are the data and a priori model covariance matrices. \(C_d\) is used to quantify the noise in the data and \(C_m\) is used to add prior information to the inversion in order to constrain the solutions. The solution for \(F\) tending to zero is found using an iterative scheme thus:

\[
m_{k+1} = m_0 - C_m^{-1} \cdot G_k^T \cdot [G_k \cdot C_m \cdot G_k^T + C_d]^{-1} \\
\times [g(m_k) - d_0 - G_k \cdot (m_k - m_0)],
\] (2.10)

where \(m_k\) is the estimate of the GST history at the \(k^{th}\) iteration, \(m_0\) is the a priori model, \(g(m_k) - d_0\) is the data misfit vector and \(G_k\) is the gradient of the forward model with respect to the model parameters and is found by calculating the dual problem (also referred to as the adjoint method). This provides an analytical evaluation of the gradient vector. This method is explained in detail in chapter 8.

The a priori information is required to constrain the inverse solutions. Shen and Beck (1992) use a constraint that the GST history must be bounded and a smooth function of time. This is imposed by using a Gaussian prior covariance matrix (see also Şerban et al., 2001), which is calculated using

\[
C_{ij} = \sigma^2 \exp\left[ -\frac{1}{2} \frac{t(i) - t(j)}{L} \right]
\] (2.11)

where \(\sigma\) is the a priori standard deviation of the temperature history and \(L\) is the characteristic correlation time of the temperature history. Typical values for these two quantities are \(\sigma = 1.0\)K and \(L = 50\) years (e.g. Shen and Beck, 1992). More advanced formulations of the above covariance matrix can be found in Şerban and Jacobsen (2001) for which the
correlation time encompasses a range of values rather than a single value as above.

Shen and Beck (1992) show that values used in the a priori covariance matrix must be chosen carefully in order to infer GST signals from noisy data, and Shen et al. (1996) and Huang et al. (1996) demonstrate that spurious GST signals can be recovered when too much weight is given to noisy data. In order to deal with data from boreholes of differing depths, noise levels, sampling rates and data acquired by different research groups, Huang et al. (1996) developed a standardized procedure for inverting the data. This method has only 7 free parameters: 5 century temperature change rates, the basal heat flow and the equilibrium surface temperature. This leads to simplified estimates of past changes which are more generally comparable and so can be easily combined e.g. for hemispheric means.

It can be seen that for moderate noise in the borehole data, the FSI method can produce very inconsistent results (see figure 2.4 below), by reducing the number of free parameters to 7 a more generally applicable inverse algorithm has been produced. However, FSI remains sensitive to the specified errors on temperatures and sub-surface conductivities and it is also dependent on the parameterisation of the GST history.

Uncertainty in the GST reconstructions can be assessed by deriving the posterior model covariance matrix. This gives the standard deviation of each model parameter as well as the covariances between different model parameters.

### 2.3.3 Singular value decomposition method

The second most widely employed method for inverting borehole profiles uses singular value decomposition (Mareschal and Beltrami, 1992). This involves defining a forward model based on analytical solutions to the heat conduction equation. These solutions are for step increases in past temperature for a semi-infinite half space (Carslaw and Jaeger, 1959, p.63). The solutions can be assembled into a matrix $A$ which is calculated using the formula below for $j$ depths and $k$ time points:

$$A_{jk} = erf\left(\frac{z_j}{2\sqrt{\kappa t_{k-1}}}\right) - erf\left(\frac{z_j}{2\sqrt{\kappa t_k}}\right)$$

where $\kappa = \frac{k}{\rho c}$, the ratio of the thermal conductivity to the specific heat capacity, and
erfc is the complimentary error function. This matrix then forms an analytical forward relation when multiplied by a vector of the model parameters $\mathbf{m}$, which in this case are the equilibrium surface temperature, the basal heat flow and the step change GST values. Hence, $\mathbf{m} = [q_0, T_{eq}, T_1, T_2, \ldots, T_K]$ and the calculated temperature depth profile $\mathbf{\theta}$ is given by

$$A\mathbf{m} = \mathbf{\theta}$$

This is then the forward model used in the SVD method. The inverse solution is found by solving the singular value decomposition of the matrix $A$ giving

$$U\Delta V^T \mathbf{m} = \mathbf{\theta}$$

where $U$ is an $j \times j$ matrix spanning the data space, $V$ is a $k \times k$ matrix spanning the model space and $\Delta$ is a $j \times k$ diagonal matrix with entries equal to the $r(=\min(j,k))$ singular values $\lambda_r$. The temperature history $\mathbf{m}$ can then be found using the equation:

$$\mathbf{m} = V\Delta^{-1}U^T\mathbf{\theta}$$

The stability of the solution found in this way is adversely affected by very small singular values ($\lambda_r$). There are two ways to limit the influence of the small singular values on the results. In the first method, the singular vectors which correspond to singular value smaller than a choice cutoff (usually 0.05) are removed as these correspond with the majority of the noise in the system. However, by removing these vectors, the resolution is reduced, leading to smoother and more realistic GST solutions. There is then a trade off between GST model resolution and how well the data are fit by the model. This can be quantified by calculating the data and model resolution matrices (Menke, 1989, Beltrami et al., 1995). Results from the singular value cutoff method usually display prominent oscillations in the temperature history for recent times. These are difficult to remove from
the solutions and so an alternative method of damping the solution can be used. In this
the reciprocals of the singular values are damped according to:

\[
\frac{1}{\lambda_r} \rightarrow \frac{\lambda_r}{\lambda_r^2 + \epsilon^2},
\]

for which the value of \(\epsilon\) usually lies in the range 0.1 to 0.3.

SVD is attractive because of its simplicity, the availability of a tested code\(^1\) and its
widespread use (e.g. Beltrami and Mareschal, 1995, Beltrami et al., 1997, Beltrami and
Bourlon, 2004, González-Rouco et al., 2006). However, there is no physical link between
the data errors and the choice of SVD cutoff or damping factor \(\epsilon\), and it can be diffi-
cult to choose either value in an objective manner (Hartmann and Rath, 2005, Rath and
Mottaghy, 2007). The aforementioned code implements either an L-curve criterion or gen-
eralized cross-validation (Rath and Mottaghy, 2007) in order to deal with this. However, if
the SVD cutoff value is too high, the GST histories will be artificially smoothed and if it is
too low, the GST histories may include spurious variations which are not supported by the
data. For example Beltrami and Bourlon (2004) use SVD to derive a global temperature
history for the last 500 years. Their mean reconstruction includes a 1.0°C variation at
100 years b.p., but this is not supported either by instrumental data (Mann and Jones,
2003) or by other global borehole reconstructions (Huang et al., 2000). Features such as
this are undesirable and a more flexible method for dealing with data noise may help to
avoid such problems.

Comparisons of FSI with SVD methods (Shen et al., 1992, Beck et al., 1992, Shen et al.,
1996) show that given proper treatment of data noise both methods perform equally well.
However, because FSI is a Bayesian method, uncertainties in all model parameters can be
accounted for. A common example is the thermal conductivity, which is often not known
over the whole depth range of a borehole. FSI can take account of this uncertainty in
the inverse process leading to more realistic uncertainty estimates on the resultant GST
reconstructions.

\(^1\)http://www-users.rwth-aachen.de/volker.rath/downloads.html
2.3.4 Monte Carlo method

Dahl-Jensen et al. (1998) use a Markov Chain Monte Carlo -like method (e.g. Mosegaard and Tarantola, 1995) to invert two temperature depth profiles measured in ice in Greenland. The temperature histories are parametrized with a discrete number of points which are fixed in time. Using a Monte Carlo method (Keilis-Borok and Yanovskaya, 1967, Press, 1968), new GST history models $m'$ are randomly generated and then accepted with a probability $\alpha$, given by the ratio of the new data likelihood to the old:

$$\alpha = \min \left[ 1, \frac{L(m')}{L(m)} \right]$$

(2.17)

This is the classic Metropolis algorithm (Metropolis et al., 1953) and, as such, samples the posterior distribution of the temperatures histories according to Bayes’ Law (see next chapter 3), with the implicit assumption of uniform priors on the temperature values. However, before presenting the results, the sampled models $m_i$ are filtered according to a second misfit criterion, such that only models with a misfit less than the variance of the data are retained. Thus only the models which fit the data (according to the Metropolis algorithm) and satisfy this second criterion are used to build the histograms of the model parameters (heat flows and GST values).

Mareschal et al. (1999) and Kukkonen and Jöeleht (2003) use a similar Monte Carlo method to estimate past ground surface temperatures from geothermal heat flow data, but without this second data-fit criterion. In the latter the uncertainty ranges on the temperature values are large (up to $15^\circ$C at 100 years ago), this is most probably because of the lack of prior information used in the inverse model setup. In both cases GST model parameterisations must be chosen in advance, reflecting the depth range of the data and the expected resolution level with time before the present. This issue of model parameterisation choice is discussed below.

2.3.5 Forward modelling methods

A non-inverse approach to borehole data can be taken when boreholes are located close to meteorological stations. Surface air temperature series are used in a forward model to cal-
calculate simulated underground temperatures which are then compared with the measured borehole temperatures (Chapman et al., 1992, Gosnold et al., 1997, Harris and Chapman, 1998, Harris and Gosnold, 1999, Majorowicz et al., 2006). In order to optimize this data-fit, the surface air temperature series (usually of 100-150 years) is amalgamated with a step change (from pre-observation mean temperature value, POM) to form a POM-SAT time series. The step change is then optimised to fit the borehole data, so that the POM-SAT series gives an idea of the surface temperature changes prior to start of the meteorological record.

However, by using a step change in temperature, there is no way to discern between climatic effects and other factors influencing the thermal regime. Additionally the surface air temperature values used, may not correspond well with the actual ground temperatures which have forced the underground thermal regime, as there is often an offset between the two. There is also no objective way of deciding between one, two or more step changes of the POM value (except by trial and error) and little information on the resolution of the temperature history is produced.

Where much longer records can be used, such as those calculated from global climate model (GCM) runs, the comparisons between simulated and measured data can be more useful. For example Beltrami et al. (2006) demonstrate that the borehole temperatures in Canada are more consistent with anthropogenically forced (increasing CO$_2$ levels) GCM runs (1000 years) than those which are designed to replicate natural variability only.

### 2.4 Complications and shortcomings of current methods

Despite the main strengths of the borehole climate reconstruction methods, namely the absence of calibration stage, there are a number of other obscuring factors which must be taken into account. The physics of the ground surface energy exchange is extremely complicated and many of the key processes are still not understood very well. This calls into question the basic assumption of the borehole method: that ground and air temperatures track each other over time. Recently a number of studies have examined this aspect as well as the effects of other obscuring factors such as land use change, snow cover and sub-surface advection. In the following section, the results of these studies are described.
along with a discussion of limitations of current methods for obtaining reconstructions from borehole data.

2.4.1 Effects of seasonal snow cover and land use change

Snow cover has a large effect on ground temperatures which is a complex function of the snow thickness, its duration on the ground, latent heat effects and air temperatures (Zhang, 2005). For the winter months during which snow falls and settles, the snow cover effectively insulates the ground against colder air temperatures. When the snow melts, heat is drawn from the ground and the air. Additionally snow thickness varies with topography and from year to year (Zhang, 2005). Bartlett et al. (2005) demonstrate that the temperature offset between the ground surface (with snow) and the air will vary as a function of the average air temperature. Indicating a time-dependent coupling between air and ground surface temperatures which would make ground surface temperature histories less useful. However, over the period from 1970-2002, this variation is of the order 0.05K/decade, indicating a low sensitivity of the coupling to snow-cover changes, since the air temperature changes over this period are known to be large in the area under study.

Mann and Schmidt (2003) argue that GST and surface air temperatures are poorly coupled because of the insulating effects of snow-cover during winter time, leading to reconstructions which are biased towards larger amplitude trends. Mann et al. (2003) use optimal detection to find the climatic component contained in borehole temperature reconstructions, this is achieved by calculating the correlation to the 20th century instrumental temperature record. This method leads to reduced amplitude reconstructions for the last 500 years which are in better agreement with some other multi-proxy studies (e.g. Mann et al., 1999). However, Pollack and Smerdon (2004) demonstrate that errors in Mann et al. (2003) leave the ‘optimal’ GST trends closer to the unfiltered originals, see Rutherford and Mann (2004) for corrections. Additionally when at least 3 independent borehole reconstructions are averaged together the correlations with the 20th century instrumental temperatures can be greatly improved, an issue discussed further in this thesis in chapter 5.

In order to test the hypotheses that air and ground surface temperatures track each other over hundreds of years a 3-dimensional global climate model (GCM) must be used.
González-Rouco et al. (2003, 2006) use the shallow soil depth temperature series from such a GCM to force a series of synthetic temperature depth-profiles. These profiles are then inverted using the SVD method and the reconstructed GST histories are compared with the average surface air temperatures from the GCM run. The reconstructed GST histories correspond well with the surface air temperatures indicating that for this surrogate reality, air and ground temperatures are significantly correlated over long timescales (1000 years). Snow-cover, vegetation and soil hydrology (which are all incorporated into the GCM) therefore appear to have a second order effect only. These GCM models have a vegetation regime which is constant with time and this limitation has yet to be investigated further. It therefore appears that snow cover does not induce significant decoupling between long term ground and air temperature trends (González-Rouco et al., 2008).

Land use changes can have a large impact on the thermal conditions at the ground surface and the resultant subsurface temperature field (Lewis and Wang, 1992, Majorowicz and Skinner, 1997, Lewis and Wang, 1998, Lewis, 1998). For example deforestation leads to an increase in the amount of solar radiation reaching the ground surface and thus causes an increase in the average ground temperature of around 1-3 °C (Beltrami and Kellman, 2003, Nitoiu and Beltrami, 2005). Similarly constructions such as roads and buildings alter the amount of heat transferred into the ground from the atmosphere. The combined effects of land use changes are complex and therefore difficult to model. In addition the subsurface effects can penetrate laterally into the ground (Ferguson and Beltrami, 2006).

On the North American continent forest clearance and construction have occurred on a large scale in the past 150 years. Certain borehole profiles are therefore affected by this (Majorowicz and Skinner, 1997, Cermák and Bodri, 2001) causing large differences between the GST reconstructions and local instrumental temperature records. In general when boreholes are being selected for climate reconstructions, any indication of recent land surface change means that the borehole dataset is discarded (Huang and Pollack, 1998).

### 2.4.2 Subsurface advection

Subsurface advection of ground water can cause climate-like perturbations to the underground temperature profiles (Kukkonen et al., 1994, Reiter, 2005, Ferguson et al., 2006,
Majorowicz et al., 2006, Bense and Beltrami, 2007). In practice where there is evidence of advection, temperature profiles are generally discarded for use as palaeo indicators. However, downward propagation of water can be interpreted as GST warming in the past and therefore the effect can be difficult to isolate. In general the problem is worse for humid climates with ground rock that readily conducts water, such as highly fractured rocks and some basalts and sandstones, whereas boreholes in ice and in arid areas are likely to be free from advective disturbances (NRC, 2006). Comparison of 20th century instrumental records and borehole reconstructions shows no systematic offset related to precipitation levels (Pollack and Smerdon, 2004).

2.4.3 Smoothing constraints, model parameterisation and model uncertainty

Both of the inverse methods outlined in section 2.3.2 require the specification of a smoothing parameter (the autocorrelation function in FSI and the singular cutoff or damping parameter in SVD) so that the resultant inverse solutions take plausible values (e.g. Constable et al., 1987). Hartmann and Rath (2005) and Rath and Mottaghy (2007) show that it is difficult to objectively choose the magnitude of model smoothing that should be applied and they demonstrate with synthetic examples using noisy data that very smooth reconstructions are obtained which have difficulty capturing temperature variability before 200 years before present, see figure 2.5.

Another issue is the effect of model parameterisation on the inverse solution (e.g.
Figure 2.5: SVD inversion examples from Hartmann and Rath (2005), showing the true GST history alongside inversions of synthetic temperature profiles of depths 200-1000m, the synthetic data has been degraded with Gaussian noise of standard deviation 0.1K. Notice that little of true model variability before 200 years is captured by any of the inversions.

Malinverno, 2000, 2002). In figure 2.4a,b two different parameterisations have been used to invert the same 20 noisy realisations of a temperature-depth profile using the FSI method (Huang et al., 1996). In 2.4a FSI is applied with little success, only some of the 20 reconstructions recover the variability of the true model, whilst in 2.4b the model is simplified to 3 linear segments and there is improved agreement between the true model and the 20 reconstructions. Although the constraints applied in 2.4a could be optimised to produce more consistent results, the process involved is data-dependent and relies on user-specialisation. Determining which parameterisations are better suited to the data appears therefore to provide a method of producing more consistent and therefore robust GST histories.

In borehole climatology, little work has been aimed at expanding the role that model uncertainty plays in estimates of past climates, see for example Clow (1992), Beltrami and Mareschal (1995) and Dahl-Jensen et al. (1998). However, recent studies have shown the advantages of a probabilistic approach to inverse problems (Mosegaard and Tarantola, 1995, Malinverno and Torres-Verdín, 2000, Malinverno, 2002, Mosegaard and Sambridge, 2002) as it can lead to a fuller exploration of the model parameter space and more robust quantification of the model uncertainty. These methods are less likely to become entrapped in local minima, they are independent from the initial model and do not rely on the assumption of linearity. Estimates of uncertainty in GST reconstructions is important in
the context of the broader debate surrounding temperature changes of the past millennium, whilst the perceived uncertainty surrounding the borehole method will be lessened if more consistent reconstructions can be derived from similar data.

### 2.4.4 Spatial signal and averaging of reconstructions

It is only recently that the spatial component contained in geographically distributed profile locations has been examined (Majorowicz et al., 2002, Beltrami et al., 2003, Majorowicz et al., 2005, Pollack and Smerdon, 2004, Beltrami and Bourlon, 2004). Estimates of the spatial component have been derived by averaging individual reconstructions over a coarse spatial grid (e.g. $5^\circ \times 5^\circ$ or $1000\text{km} \times 1000\text{km}$). This is because the GST reconstructions are often found to show little correlation over relatively short geographical distances. Possible reasons for this include under-estimation of the data noise or local site-specific thermal perturbations. The aim of averaging the reconstructions is therefore to amplify coherent climate signal and reduce the combined noise signal. A drawback of this averaging process is that the individual reconstructions are not always optimally suited to the data being examined as each inversion is parametrized identically so that the resulting reconstructions are mathematically comparable. As borehole profiles are clustered sparsely across much of the globe, this averaging over the cells potentially leads to inconsistent weighting of the spatial signals and variable uncertainty, whilst larger scale averaging may remove any long-term spatial trends evident in the data. As an example, consider the inferred temperature trends in Europe from 123 profiles as calculated by Huang et al. (2000) and shown in figure (2.6). The diverging trends could be due to an underlying spatial signal, due to regional climatic variations, or they could be caused by a combination of local site specific noise sources. Averaging the reconstructions over a $5^\circ \times 5^\circ$ grid or over the whole area considered will not provide a very informative answer to this question, as possibly noisy and non-noisy data are averaged together.

### 2.4.5 Three-dimensional effects

Shen et al. (1995) showed that the effects of subsurface heterogeneity can have a large effect on the consistency of GST estimates from ensembles of boreholes. By taking into account the uncertainty associated with the physical structure of the underlying rock, ensembles
Figure 2.6: Inferred temperature histories for Europe from 123 borehole profiles (from Huang et al., 2000) with the borehole locations shown in the inset.

of synthetic and real boreholes yielded more consistent GST histories. Šafanda (1994), Kukkonen and Šafanda (1996), Kohl (1998), Šafanda (1999), Kohl (1999), Kohl et al. (2001), Serban et al. (2001), Gruber et al. (2004) and Noetzli et al. (2007) have investigated the effects of surface topography using 2D and 3D simulations and the results show that surface topography can cause significant departures from purely vertical heatflow, which is commonly assumed to be dominant. In these cases 1D inversions of temperature profiles would lead to misinterpretation of certain perturbations as climate signals. However, no GST reconstruction methods have so far taken account of these possible effects.

2.5 Avenues for research

It is clear that various factors must be considered at each profile location when borehole data are being selected for climate studies. In each case the evidence (if any) for subsurface advection, land use change, the presence of snow for significant periods during the year, equilibration after drilling and topography must be carefully examined. In fact geothermal
data is routinely screened for these effects. However, there are also other factors which are less easily identified which can also effect the reconstructions derived. The specific parameterisation of the inverse problem, the level of uncertainty ascribed to different parameters in the model, the prior information used to constrain the inversion, the way data are grouped for climate signal extraction and the effects of subsurface heterogeneity. The aim of this work is to develop new methods which can take account of some of these factors. Recent advances in Bayesian statistics (e.g. Denison et al., 2002) and adjoint methods (from meteorology) (e.g. Wang et al., 1992) form the basis of these new methods.
Chapter 3

Bayesian inference

In this chapter a brief introduction to Bayesian statistics is given in order to provide the theoretical underpinning for the methods employed in later chapters. After introducing Bayes’ law and its common interpretation, the probabilistic Bayesian approach to inverse problems is described along with the sampling algorithms commonly used. The advantages of model comparison (rather than parameter value comparison) are discussed and recent applications to geophysics problems are described. More complete descriptions of Bayesian statistics can be found in Bernardo and Smith (1994), MacKay (2003), Jaynes (2003), Tarantola (2005) and Sivia and Skilling (2006).

3.1 Bayes’ Law

Bayes’ law was originally derived by Thomas Bayes and published posthumously (Bayes, 1763). It was later independently discovered and applied in a variety of contexts by Laplace (1812). The law can be derived from elementary probability theory (see appendix A.1). The law states that for 3 quantities, a, b and c,

\[ p(a \mid b, c) = \frac{p(b \mid a, c) \ p(a \mid c)}{p(b \mid c)}. \]  

(3.1)

Here \( p() \) stands for probability and \( a \mid b \) implies conditional dependence of \( a \) given \( b \). The significance of this equation is that it allows transformation from one conditional
dependency to another. Thus if we have no information on a given $b$, we can quantify this by finding the dependence of $b$ given $a$. Re-writing the equation:

$$p(\text{theorem} \mid \text{data, prior}) = \frac{p(\text{data} \mid \text{theorem, prior}) p(\text{theorem} \mid \text{prior})}{p(\text{data} \mid \text{prior})}$$

the applicability of Bayes’ law becomes apparent, this interpretation of Bayes’ law is discussed in detail in Bernardo and Smith (1994). The left hand side gives the probability of a given theorem taking into account the given data and the prior information and is termed the posterior probability density function (pdf). Each of the other terms in this equation has a specific name, the first term in the numerator on the right hand side is called the likelihood and relates how successfully a particular theorem can predict the observed data, the second term is the prior probability accounting for the beliefs about the system and the denominator is termed the ‘evidence’ or marginal likelihood of the data. This term is given by the integral of the numerator of Bayes’ law over the model space.

$$p(\text{data} \mid \text{prior}) = \int p(\text{data} \mid \text{theorem, prior}) p(\text{theorem} \mid \text{prior}) \, dm$$

The evidence term accounts for the plausibility of one theorem or model parameterisation over another, thus models with different parameterisations can be compared using their respective evidence values. The posterior is the traditional target of Bayesian calculations and is often only calculated up to a constant of proportionality so that the evidence term is not calculated and only the relative values of the posterior are determined.

### 3.2 Bayesian approach to inverse problems

In the Bayesian formulation no distinction is made between model parameters and data values of a given system. All of these parameters are described by probability distributions, initially defined by the prior information. The inference process then proceeds by narrowing these prior distributions using the data (through the likelihood term) to pro-
duce the posterior distribution. Uncertainty associated with a particular parameter is then encompassed by the spread of the (marginalised) posterior distributions, i.e. the posterior pdf associated with a single model parameter.

Any Bayesian method therefore requires specification of a prior probability distribution which must reflect the a priori knowledge (or lack thereof) concerning the model (Scales and Tenorio, 2001, Curtis and Wood, 2004). So-called frequentists criticise this aspect of Bayesian methodology, arguing that it leads to subjective analysis which is contrary to basis scientific principles. However, there exists a range of compelling arguments for the use of prior information and also Bayesian methods in general (e.g. Bernardo and Smith, 1994). These are based on the mathematics of plausible and consistent reasoning which have been derived from logic theory by Richard Cox in the 1940s, see e.g. Jaynes (2003). More recently Jaynes (2003) and Sivia and Skilling (2006) argue that Bayesian inference is a mathematical encoding of logical scientific reasoning.

Another related issue is the notion of non-informative prior which is then thought to lead to a truly objective posterior. However, Denison et al. (2002) and others argue that a non-informative prior is a misnomer which can never by practically achieved and additionally can lead to biased estimates. For example, when parameters are subject to transformations, a presently vague prior distribution may become highly informative or biased (Scales and Tenorio, 2001).

In general the prior information can take the form of a most likely value and associated uncertainty, for example a Gaussian distribution with a specified mean and standard deviation. For situations with more uncertainty, a uniform distribution with upper and lower limits may be more appropriate.

3.2.1 Model choice and Ockham’s razor

One of the key advantages of the Bayesian approach is that it is naturally parsimonious (e.g. Jefferys and Berger, 1992, Denison et al., 2002, MacKay, 2003, Jaynes, 2003). This means that simple models which fit the data are preferred to more complex ones. For example, assuming that we have a complex and simple model that both fit the observed data, then, for non-diffuse priors, the support from the data (evidence) for a simpler model will be higher in the region of the observed data as it is spread over a smaller region in
data space. This is illustrated in figure (3.1) for single variables. Because all probability distributions are normalised, the model which can make a wider range of predictions (in data space) has a smaller probability value (evidence) compared to the simpler model. This is an example of what is often referred to as Ockham’s razor.

### 3.3 Sampling algorithms: Markov chain Monte Carlo

In general Bayesian inference involves possibly high dimension integrals which are rarely analytically tractable and for which numerical integration is of little use because of the high number of dimensions. Recent renewed interest in Bayesian inference is therefore due to the development of Markov chain Monte Carlo sampling strategies which allow sampling directly from the posterior distribution of Bayes’ law (e.g. Geman and Geman, 1984, Gilks et al., 1996). These algorithms are now routinely employed for Bayesian statistical calculations.

A Markov chain Monte Carlo algorithm is integration by Monte Carlo computed using a Markov chain. Monte Carlo is used for integrations which cannot be treated analytically or using other numerical methods. By generating n samples from the desired function and then averaging these, the integral can be found with the error on the estimate given as a function of 1/n. Therefore, increasing the number of samples n, then decreases the error on the integral estimate. Generating samples from the function may itself be difficult, but one way of overcoming this is to draw samples from a Markov chain whose stationary
distribution takes the form of the function of interest. A Markov chain is a sequence of random variables which are only dependent on the previous state and not on any produced before this, i.e.

\[ m_{t+1} = T(m_{t+1}, m_t). \quad (3.4) \]

\( m \) is then a Markov chain and \( T \) is the transition kernel of the chain. In order to sample from a distribution of interest the Markov chain must be stationary, i.e. the probability distribution which it is sampling, must not change over time. One way to achieve the stationarity of the Markov chain is to design the transition kernel \( T \), to satisfy detailed balance. This is defined by:

\[ T(m_a, m_b)\pi(m_b) = T(m_b, m_a)\pi(m_a) \quad (3.5) \]

where \( \pi(.) \) is the equilibrium probability for a particular state. This equation states that the probability of moving from a state \( m_a \) to another \( m_b \), is equal to moving from the state \( m_b \) to \( m_a \). A Markov chain which satisfies this equation is described as reversible. If we integrate both sides of equation 3.5 with respect to \( m_b \):

\[ \int T(m_a, m_b)\pi(m_b)dm_a = \pi(m_a). \quad (3.6) \]

The left hand side is the marginal likelihood of \( m_a \) assuming that \( m_b \) is from \( \pi(.) \). Since the right hand side is just \( \pi(m_a) \), this means that if \( m_a \) is from \( \pi(.) \) then if detailed balance is satisfied, \( m_b \) will also be from \( \pi(.) \).

Having shown that detailed balance is required in order that subsequent samples of a Markov chain are drawn from the same probability distribution we must now show how the transition of kernel of the Markov chain can be derived so that this probability distribution corresponds with the distribution of interest, In the Bayesian case this is the posterior distribution, (see Chib and Greenberg, 1995, for further details).
If we consider again the two points in model space $x$ and $y$, we may find that the probability of moving between them is not equal so that

$$\pi(x)T(x, y) > \pi(y)T(y, x)$$

(3.7)

In this case transitions to $y$ are more likely than transitions to $x$ and so the distribution that is sampled will not correspond with the true underlying one. A remedy is to correct the above relation with a factor $\alpha(x, y)$ which ensures that detailed balance is satisfied. Equation 3.7 now becomes

$$\pi(x)T(x, y)\alpha(x, y) = \pi(y)T(y, x)\alpha(y, x)$$

(3.8)

The probability of transitions from $x$ to $y$ needs to maximised and so we need to choose $\alpha(y, x)$ to be as large as possible. Setting this to 1 and rearranging leads to

$$\alpha(x, y) = \frac{\pi(y)T(y, x)}{\pi(x)T(x, y)},$$

(3.9)

whilst for the reverse case of equation 3.7, the opposite is true and

$$\alpha(y, x) = \frac{\pi(x)T(x, y)}{\pi(y)T(y, x)}.$$  

(3.10)

The probability of a move in model space must therefore be set to

$$\alpha(x, y) = \min[1, \frac{\pi(y)T(y, x)}{\pi(x)T(x, y)}],$$

(3.11)

since the probability cannot exceed 1. If a proposal distribution $q(y|x)$ is taken as the transition kernel, then equation is the Metropolis-Hastings algorithm (Metropolis et al., 1953, Hastings, 1970).
Metropolis’ original algorithm is formulated with two steps: a proposal and an acceptance or rejection of this proposal. A proposed model, \( m' \) is calculated from the current model, \( m \) using \( q(m' | m) \). If this model is accepted, \( m \) is discarded and replaced by \( m' \), if not, \( m' \) is discarded and the current model \( m \) is carried forward instead. For the Metropolis algorithm, the proposals are necessarily symmetric so that \( q(m' | m) = q(m | m') \) and hence the acceptance probability is given by:

\[
\alpha = \min \left[ 1, \frac{\pi(m')}{\pi(m)} \right].
\]

(3.12)

Thus from a starting model, \( m_0 \), a series of accepted models \( m_i, i=1, \ldots, M \), are produced and stored. The first \( n_b \) models are regarded as burn-in and are discarded. The remaining \((M-n_b)\) models then represent a good approximation to the target distribution \( \pi(.) \). Here \( M \) and \( n_b \) must be chosen empirically.

The M-H algorithm (Hastings, 1970) allows for non-symmetrical proposals such that \( q(m' | m) \neq q(m | m') \). These are taken into account in the acceptance term. The form of the algorithm is therefore identical but the M-H acceptance term is now

\[
\alpha = \min \left[ 1, \frac{\pi(m') q(m | m')}{\pi(m) q(m' | m)} \right].
\]

(3.13)

A further generalisation is taken by considering proposal functions, \( q(m' | m) \) in general state-space, such that \( m' = h(m, u) \) where \( u \) is a set of random numbers from some probability distribution, \( g(u) \). This distribution is required for the condition of detailed balance to hold. In this case since the two distributions are in different model or state spaces (for example of differing dimensionality) the change of variable needs to be accounted for and this can be achieved by using the change of variable formula. Thus the detailed balance condition of equation 3.8 now only holds when

\[
\pi(m)g(u)\alpha(m, m') = \pi(m')g'(u')\alpha(m', m)\left| \frac{\partial(m', u')}{\partial(m, u)} \right|
\]

(3.14)
where the last term accounts for the change of variable. As before taking the probabilities as large as possible leads to the acceptance probability which is now given by:

\[
\alpha = \min \left[ 1, \frac{\pi(m')}{\pi(m)} \frac{g'(u')}{g(u)} \left| \frac{\partial(m', u')}{\partial(m, u)} \right| \right] .
\] (3.15)

\(u'\) and \(u\) are generally sets of random numbers used to compute \(m'\) given \(m\). The last term in this acceptance probability is the determinant of the Jacobian which is defined as

\[
J = \left| \frac{\partial(m', u')}{\partial(m, u)} \right| .
\] (3.16)

As noted above, the introduction of this term to the acceptance probability allows proposals for models which are formulated on a different state-space. Significantly, the proposed model \(m'\) can be of a differing dimension to the current model \(m\). In this case the dimensions of the \(u'\) and \(u\) variables must balance, such that:

\[
d(m) + d(u) = d(m') + d(u')
\] (3.17)

where \(d(a)\) indicates the length of the vector \(a\). However this framework can also be used to construct more elaborate fixed dimension Metropolis-Hastings samplers (see e.g. Waagepetersen and Sorensen, 2001) and for many transdimensional implementations the Jacobian term still turns out to equal 1 (see chapter 5 for such an example). The reversible jump formulation above is just a further generalisation of the Metropolis-Hastings method and as such the M-H emerges as a special case in the above formulation. For more detailed accounts of the reversible jump methodology see Green (1995, 2001), Waagepetersen and Sorensen (2001), Green (2003).

In general \(\pi(.)\) can be split into the likelihood and prior terms as in Bayes’ law. This gives the usual form of the acceptance probability:
\[ \alpha = \min \left[ 1, \frac{p(m' | \psi)}{p(m | \psi)} \cdot \frac{p(d | m', \psi)}{p(d | m, \psi)} \cdot j(m') \cdot g_m(u') \cdot \left| \frac{\partial(m', u')}{\partial(m, u)} \right| \right] \] (3.18)

\[ \alpha = \min \left[ 1, \text{(prior ratio)} \cdot \text{(likelihood ratio)} \cdot \text{(proposal ratio)} \cdot |\text{Jacobian}| \right], \]

where jump probabilities \( j(m) \), have been inserted in order to account for \( m \) different proposal types now denoted \( g_m \). A further generalisation can be introduced so that the proposals are functions of the current model \( m \). This leads to the acceptance probability:

\[ \alpha = \min \left[ 1, \frac{p(m' | \psi)}{p(m | \psi)} \cdot \frac{p(d | m', \psi)}{p(d | m, \psi)} \cdot j(m') \cdot g_m(u) \cdot g_m(u') \cdot \left| \frac{\partial(m', u)}{\partial(m, u)} \right| \right] \] (3.19)

The significant advantage of rj-MCMC is that it allows jumps to models of differing dimensionality and hence the rj-MCMC algorithm can be applied to a range of problems for which M-H is not suited. In doing so models of differing dimensionality are sampled in proportion to their relative evidence values, although this value is not calculated in the algorithm. This property therefore ensures that the rj-MCMC algorithm satisfies Okham’s razor and thus preferentially samples simpler models which can adequately fit the data. This is to be expected since the rj-MCMC algorithm is sampling from the Bayesian posterior pdf which is a function of the evidence term (equation 3.3). The rj-MCMC algorithm is described in detail in appendix (A.2) and example applications can be found in Green (2001, 2003) and Denison et al. (2002). The rj-MCMC algorithm has proved useful in fields such as genomics and epidemiology and more recently geophysics (Malinverno, 2002, Andersen et al., 2003, Stephenson et al., 2006, Sambridge et al., 2006). Rj-MCMC is the sampling algorithm used in Bayesian parts of this thesis as it offers most flexibility in constructing and comparing different models.

### 3.3.1 Posterior distributions and model averaging

Once the samples from the posterior distribution have been collected, summaries of the resultant posterior pdf are often required. These usually take the form of means and
credible limits. In order to quantify the results robustly MCMC samples are used to evaluate the posterior expectation values of the model (e.g. Gilks et al., 1996). The expected value is given by the equation:

\[
E[f(m)] = \frac{\int f(m) \pi(m) dm}{\int \pi(m) dm}
\]  

(3.20)

where \( \pi(m) \) is the posterior distribution and \( f(m) \) is some function of interest. It is then possible to use the posterior samples generated by a Markov chain Monte Carlo algorithm to calculate this expectation value (Gilks et al., 1996), using the following equation:

\[
E[f(m)] = \frac{1}{n} \sum_{i=1}^{n} f(m).
\]  

(3.21)

In the case that \( f(m) \) is the model value, the expectation value is the posterior mean which is calculated by integrating across all models weighted by their posterior probability values (as models are sampled with frequency proportional to their posterior probability). This has the advantage that it gives a smoother result than any single sampled model but combines information from across the whole distribution.

One way of quantifying the posterior uncertainty for a particular parameter, say \( m \), is to calculate the 95% credible limits. These are the limits which enclose 95% of the posterior probability for a particular parameter, i.e. the limits must satisfy

\[
p(m_1 \leq m \leq m_2 | d, \varphi) = \int_{m_1}^{m_2} p(m | d, \varphi) dm = 0.95.
\]  

(3.22)

\( m_1 \) and \( m_2 \) are then the 95% credible limits for \( m \). The limits can be chosen in a number of ways, for example then could be symmetric about the posterior mean or median. Here the limits are found by removing the most extreme 2.5% of samples from the marginal posterior distribution of a parameter and taking the resulting minimum and maximum sample values. This corresponds with finding the narrowest interval which integrates to 95% probability (for a unimodal distribution). The posterior expectation value and the
95% credible limits are illustrated for an example probability distribution in figure 3.2. Notice that in this asymmetric case, the posterior mean value, which takes account of the full distribution does not coincide with the mode of the distribution.

3.3.2 Other Bayesian methods

Although samples from a MCMC algorithm can be guaranteed to approximate the underlying posterior density, there is no guarantee of how effectively an MCMC algorithm will sample the model space as iterations progress. Firstly a sufficient number of ‘burn-in’ iterations must be discarded. This is because burn-in period of the chain will generally relate to samples from outside the posterior distribution. These burn-in iterations are necessary when the initial model used is a poor one, but the number of burn-in iterations will significantly decrease when the algorithm is initiated near to the high probability regions of the posterior distribution.

Secondly, poor proposal choices will lead to the model parameters remaining stationary for many iterations as these poor proposals are often rejected at the accept/reject stage. There are no formal rules for selecting the total number of iterations, the number of burn-in iterations or suitable proposal distributions. Often proposals are made using samples from the prior information, however, this may be prohibitive in cases where prior information is scant. Additionally the acceptance rate plays an important role in the efficiency of the algorithm. If the acceptance rate is too high or too low the MCMC algorithm is likely to spend too long in small regions of the model space leading to incomplete approximations.
of the true posterior distribution. In practice the chains of the model parameter values with iterations of the algorithm must be inspected to ensure that there is no overall trend which could indicate non-stationarity. A general and widely applied rule of thumb is to aim for acceptance rates of an MCMC algorithm of around 30% (Gilks et al., 1996).

In order to overcome problems of slow model parameter exploration several new algorithms have been designed. In the following these are briefly summarised along with some other methods often used in Bayesian inference. Gibbs sampling (Geman and Geman, 1984) allows calculation of the global posterior distribution by combining the conditional posteriors on each variable. In geophysics problems these conditional posteriors are not typically available and so Gibbs sampling cannot be used.

Bayesian information measures (e.g. Gallagher et al., 2005, Woodbury and Ferguson, 2006) are derived by approximating the posterior as a normal probability density function. These measures can be used to determine whether models are unnecessarily complicated and are thus over-fitting the data. However, rj-MCMC provides a more objective way of achieving this without resorting to any approximations, albeit at a higher computational cost.

Calculating the evidence term allows models of differing parameterisations to be objectively compared. For linear models whereby the prior, likelihood and also posterior all follow Gaussian distributions, the evidence can be calculated directly (Malinverno, 2000). In this case it is the product of the likelihood at the posterior mean and a so-called Ockham factor. However, in the more general non-linear problems the evidence must be calculated by an approximate method (much as the posterior must be approximated by MCMC). Methods for achieving this can be found in Newton and Raftery (1994), Gelfand and Dey (1994), Chib (1995), Chib and Jeliazkov (2001), Skilling (2004) and Chopin and Robert (2007). However, this is an area of ongoing research.

Simulated tempering (Marini and Parisi, 1992, Geyer and Thompson, 1995) involves introducing an extra parameter into the MCMC algorithm which is analogous to temperature in the optimisation method, simulated annealing. High values of the temperature effectively flatten out the posterior distribution allowing more rapid exploration of the model space by the MCMC algorithm. Example applications include Andersen et al. (2003). This method is particularly useful where there are found to be many interdepen-
dependencies between model parameters, which make MCMC exploration of the model space inefficient.

Jump Diffusion (e.g. Phillips and Smith, 1996) is an alternative method to the MCMC methods which can deal with variable dimensions. However, it has yet to be used as widely as the rj-MCMC method.

Delayed rejection (Green and Mira, 2001) is a method for improving acceptance rates in rj-MCMC by using information about rejected models to improve new proposals. Hence if a proposed model is rejected, instead of moving on to the next iteration of the algorithm, a second proposal is made which is additionally conditioned on the first unsuccessful one. The acceptance term in the rj-MCMC algorithm is then modified to take account of this process.

### 3.4 Bayesian methods in geophysics

Early uses of probabilistic methods in geophysics are due to Tarantola and Valette (1982a). In their method the data and model parameters are assumed to follow Gaussian distributions which are subsequently quantified by calculating the covariance matrices. Subsequently Mosegaard and Tarantola (1995), Mosegaard and Sambridge (2002) discuss applications of the Metropolis algorithm to inverse problems and real and synthetic data applications can be found in Schott et al. (1999), Grandis et al. (1999), Malinverno and Torres-Verdín (2000) and Ferrero and Gallagher (2002). It is often apparent that a smoothing function must be introduced into the a priori information in order to constrain the models. Malinverno (2002) argue against this constraint in the prior as it does not represent what is known a priori, rather it must be chosen to fit the model to the true values in the synthetic cases and thus can lead to reduced estimates of posterior uncertainty. A way around this problem is to take advantage of the parsimony of the Bayesian approach and employ a trans-dimensional sampler. Recently the reversible jump MCMC algorithm has been used for trans-dimensional Bayesian inference where the models are formulated with a variable number parameters and this number is then inferred from the data (and prior). Examples include inversion for underground electrical conductivity, seismic velocities and mixture modelling (Andersen et al., 2001, Malinverno, 2002, Andersen et al.,
Malinverno (2002) implements a rj-MCMC algorithm in which the Earth model is parametrized in terms of a variable number of layers. By taking advantage of the parsimony of a Bayesian formulation, it is shown how to solve non-linear inverse problems without resorting to subjective smoothing parameters. The algorithm design utilizes model proposals which are made independently of the current model state. This simplification means that the Jacobian in the acceptance term is always equal to 1. However, it is often easy to propose higher-likelihood models which are close to the current set and so this restriction may cause the algorithm to require many iterations which is problematic for computationally expensive forward models.

Sambridge et al. (2006) compare the Metropolis-Hastings and rj-MCMC algorithms mathematically with some simple examples and effectively perform 'within-model simulation' (Green, 2003). They show that the posterior distribution obtained in the trans-dimensional case is the sum of the fixed dimensional posteriors weighted by their respective evidence values, and highlight the importance of this the evidence term in model comparison. An automatic rj-MCMC algorithm (Green, 2003) is used, and this avoids the need for a complex computer code writing or debugging. However, this automatic method is only efficient when the number of model parameters is small, and so it is too restrictive for more complex applications.

More recently trans-dimensional sampling methods have been used to deal with data in 2D and 3D settings. In Stephenson et al. (2006) a partition model (Green, 1995, Denison et al., 2002) is employed to infer thermal histories from fission track data and to group these histories according to the spatial locations of the data. A rj-MCMC algorithm is used to infer the spatial component whilst secondary M-H algorithms are used in conjunction with optimization software to produce suitable model proposals in new spatial partitions. This method can be employed for inverse problems where spatial influences are important. The parsimonious nature of Bayes’ law ensures that the algorithm does not automatically divide the space into the maximum number of partitions (to maximise the data fit) but instead finds an objective balance between the data fit and the simplicity of the model.
3.5 Conclusions

Bayesian inference provides a well established method for combining prior information with data dependent information and for quantifying uncertainty in models. It also allows the formulation of the model to be investigated through model comparison using the Bayesian evidence term. Markov chain Monte Carlo methods currently provide the only method for Bayesian posterior sampling in complex real world problems, and reversible jump MCMC provides a method for comparing models with differing numbers of parameters. Previous applications in geophysics in general provide a basis for application to borehole temperature inversion. The development, testing and application to borehole climate reconstruction is then the subject of the next two chapters.
Chapter 4

Temperature reconstructions from single and multiple boreholes

In this chapter a novel Bayesian method for inverting temperature profiles is described. In this the inverse problem is cast in a probabilistic framework based on Bayes’ law. Model inference is made by quantifying the posterior probability density function (pdf) which is conditional on the borehole temperature data, through the likelihood function, and the prescribed prior information. In order to sample the posterior distribution a reversible jump Markov chain Monte Carlo sampling algorithm (rj-MCMC) (Green, 1995) is used. This enables a fully non-linear approach to the inverse problem in which full account can be taken of data uncertainty, a factor which may have biased previous ground surface temperature (GST) estimates (González-Rouco et al., 2008). The rj-MCMC provides a much more flexible framework for constructing and comparing models when compared to standard MCMC methods. For example in this context, past GST values at specified times in the past have been inferred from data (e.g. as in Dahl-Jensen et al., 1998, Kukkonen and Jöeleht, 2003, Mottaghy, 2007). However, the timing and number of the GST points can also be allowed to change according to the data. Taking advantage of the natural parsimony of the Bayesian method as described in chapter 3.2.1, it is then possible to infer the resolution of the GST history which is appropriate to the data. This is a feature which has not been dealt with in a specific manner before.

In this chapter the formulation and application of this algorithm to the GST inference
problem is described in detail in section 4.1 and 4.2, followed by examples using synthetic data (section 4.4) and real data from boreholes located in the UK (in section 4.5). The characterisation of the posterior probability pdf of the GST history leads to better understanding of the uncertainties compared with a single optimum model for which associated uncertainty is found by differentiating the likelihood with respect to the model parameters. Comparing the Bayesian rj-MCMC results with similar examples in the literature, shows that this new method is able to resolve temperature changes further back in time. This is because no explicit regularization is applied to the model values. Additionally, by comparing the prior and posterior probability distributions it is possible to identify which parts of the temperature reconstructions are supported strongly by the data and those aspects which are governed by the a priori information. This is not possible using current borehole climate reconstruction methods.

For realistic noisy synthetic data, it is shown that resolution decreases sharply into the past and that inference is only valid back to 500-750 years before the present for borehole data of 500m depth. Five borehole profiles from the UK indicate a warming trend over 500 years of between 0.6 and 1.8°C. However, only 2 of the reconstructions show good agreement with the nearest instrumental temperature record (Central England see appendix D.1). A joint inversion of the 5 datasets shows good agreement with this record and 2 local proxy tree-ring reconstructions. A joint inversion of data from Sellafield, Cumbria illustrates the method using noisier data.

### 4.1 Model setup

In order to find a solution to an inverse problem a forward model formulation is required. This provides the forward path from the system’s control parameters to the output of that system. In this case the forward problem involves solving the diffusion equation subject to specific boundary conditions. The diffusion equation in 1D is

\[
\rho C \frac{\partial T(z,t)}{\partial t} = \frac{\partial}{\partial z} \left( k(z) \frac{\partial T(z,t)}{\partial z} \right).
\]

where \( z \) is depth which is positive into the ground, \( t \) is time, \( T \) is the temperature and
k, \( \rho \) and \( C \) are the thermal conductivity, density and specific heat capacity respectively. Here the 1-D heat conduction equation is solved subject to two boundary conditions. The boundary conditions are an upper surface Robin boundary condition which is used to express the heat transfer from the air to the Earth through the surface heat transfer coefficient \( \beta \), and a lower surface Neumann boundary condition for basal heat flux:

\[
q(0, t) = \beta(T_{\text{air}}(t) - T(0, t)) \quad (4.2)
\]

\[
-k \frac{\partial T}{\partial z} |_{z_{\text{max}}} = q_0. \quad (4.3)
\]

where \( \beta \) is the heat transfer coefficient, \( T_{\text{air}} \) is the air temperature, \( T(z, t) \) are temperatures in the ground and \( q_0 \) is the basal heat flux, which is assumed to be constant with time.

In order to solve the forward problem efficiently a finite element approximation to equation (4.1) is used (e.g. Lewis et al., 1996). This allows the inclusion of radiogenic heat sources within the borehole depth range, the variability of the thermophysical properties with depth and also if required the thermal dependence of the rock thermophysical properties. Both the steady state and transient simulations are employed, the former used to calculate the equilibrium temperature depth profile subject to the equilibrium surface temperature \( T_{\text{eq}} \) and the basal heat flux. This steady state solution is then perturbed using a transient FE model. For 5 year time steps and a typical GST history (2000 years with a 1K step change at 1000 years), the maximum discretisation error is \( 6 \times 10^{-4} \text{K} \), well below typical data noise values. This error is insensitive to the spatial discretisation but scales with the length of the time-steps used.

The GST history is set up as a series of linear segments with the nodes of these segments being the \( k \) GST model parameters, i.e. \( \mathbf{m} = (T_i, t_i; i = 1, k) \), where \( T \) is temperature, and \( t \) is time. The model is allowed between \( k_{\text{min}} \) (=2) and \( k_{\text{max}} \) (=20) nodes with a maximum separation of \( L \) (= the duration of the reconstruction in years) and a minimum of the time-step used in the finite element approximation (=2-5 years), this is illustrated in figure 4.1. The rj-MCMC algorithm samples these \( k \) time and temperature parameters, the basal heat flux from below the borehole and the pre-reconstruction mean temperature \( T_{\text{eq}} \) and also the value of \( k \) itself.
Figure 4.1: (a) Example data plot showing the theoretical equilibrium profile (dashed line). (b) Model setup: the k circles denote the interpolation points for the GST history. These can move in time and new points can be added or deleted to vary the complexity of the GST history. The additional model parameters are $T_{eq}$, the long term pre-reconstruction mean GST and the heat flow, which is the lower boundary condition on the thermal model.

The parameter k represents an indication of the complexity of the model used. By allowing k to vary the question of model resolution is addressed more robustly than if k was arbitrarily fixed. However, k is not a physical quantity and cannot be directly measured and so it is only relevant for comparing the different models sampled by the rj-MCMC algorithm. This modelling scheme therefore corresponds to what statisticians call an open modelling perspective (Bernardo and Smith, 1994, Denison et al., 2002) whereby the range of models considered is not assumed to contain the ‘true’ model. However, this is also the case for any GST inversion model, as past temperature variations of various wavelength will have decayed in magnitude below the measurement error or the level of data noise. Thus real past temperature changes that occurred on scales from hourly to the decadal and even centennial are lost and cannot be represented in the model.

4.2 Bayesian formulation

4.2.1 Prior

In this work the prior information takes three forms. For the GST temperature values a most likely value is specified with the associated probability distribution designed to take
account of the full range of possible past variations. The second places a constraint on
the time points of the GST history, such that they are probabilistically biased towards
uniform spacing over the time domain. The basal heat flux, equilibrium temperature $T_{eq}$
and the number of GST points are constrained using uniform priors for which upper and
lower limits are specified.

The prior on the GST values is set to a multi-variate Gaussian distribution centred on
the present mean GST value (i.e. the value at zero years):

$$p(T_{GST} \mid \varphi) = \frac{1}{[(2\pi)^k \det C_{pr}]^{1/2}} \times \exp \left( -\frac{1}{2} (T_{GST} - T_{prior})^T C_{pr}^{-1} (T_{GST} - T_{prior}) \right)$$

In contrast to the FSI method (e.g. Shen and Beck, 1992), zero correlation is assumed
between the GST parameters so that $C_{pr}$ is a diagonal matrix with entries equal to 1.0 K²
(see Şerban and Jacobsen (2001) for a detailed discussion of correlated prior information
in this context). $T_{GST}$ is the current GST model, $T_{prior}$ is the prior mean value for the
GST model and $k$ is the number of GST interpolation nodes.

The time positions of the interpolation points are drawn using order statistics from a
uniform distribution over the time interval examined (Green, 1995, 2001). Thus the prior
distribution on the time locations is given by:

$$p(t \mid \varphi) = \frac{k! I[0 < t^1 < t^2 < \ldots < t^k < L]}{L^k}$$

where $t$ are the time points of the GST history, $L$ is the length of the time domain
($= t_{max} - t_{min}$) and $I$ is the order statistic uniform distribution. This form of prior helps
to ensure that very closely spaced interpolation points, which have negligible effect on
the likelihood and are inconsistent with the data (because of the spreading with time of
the thermal signal in the ground) do not emerge in the model. The effect of this prior
distribution choice is examined in Appendix C.
By setting a prior distribution on a non-physical quantity $k$, the meaning of models with different values of $k$ must be considered. In this context it is the expected resolution that is important because the original signal has been strongly filtered by thermal diffusion. Typical GST estimates derived from borehole temperature are of very low resolution, for example Huang et al. (1996) recommend century-long trends. Hence for reconstructions considered here, $k$ would be expected to take a value of around 5 (for equally spaced time points). By setting a uniform prior over the range $[2, 20]$ the resolution level of Huang et al. (1996) is included in the range of models considered. However, as the Bayesian approach is naturally parsimonious, unwarranted complexity is not introduced (i.e. more model parameters) if the data do not require it. For example if the true solution was a constant temperature over time, the algorithm would infer a posterior distribution with a maximum at $k=2$. Although more parameters could be used and still produce a constant temperature over time (with exactly the same data fit), the posterior probability would be lower than for the simpler model. This is because the more complex model is penalised through the increased number of terms in the prior.

The priors on basal heat flux and $T_{eq}$ values are uniform over the intervals $[0, 100]$ mWm$^{-2}$ and $[0, 15]$°C respectively.

4.2.2 Likelihood

The likelihood term is based on a least squares measure of the data misfit and takes the form of a multi-variate Gaussian pdf:

$$p(d_{obs} | m, \varphi, k) = \frac{1}{[(2\pi)^n \det C_d]^{1/2}} \times \exp \left( -\frac{1}{2} (d_{sim} - d_{obs})^T C_d^{-1} (d_{sim} - d_{obs}) \right)$$  \hspace{1cm} (4.6)

where there are $n$ data points, $d_{obs}$ are observed subsurface temperatures and $d_{sim}$ are the simulated underground temperatures which are calculated using the $T_{GST}$ vector (size $k$) according to the finite element method of section (4.1). $C_d$ is the data covariance matrix (here assumed to be diagonal). The errors on the data values are therefore assumed to be Gaussian and uncorrelated. The values used for $C_d$ are discussed with the descriptions of
synthetic and real data applications.

### 4.2.3 Proposals

In the generalized variable dimension case there are 5 types of changes to the model, each with an associated proposal function, which allow sampling of the model space. One of these change types is selected at random at each iteration of the rj-MCMC algorithm:

1. Perturb one temperature value, $T_i$.
2. Perturb one time value, $t_i$.
3. Create a new GST point (birth)
4. Delete one GST point (death)
5. Perturb the basal heat flux and $T_{eq}$ values for one borehole

The probability of selecting one of these change types is set to $1/5$ for all iterations, except for when the number of GST model points reaches $k_{min}$ or $k_{max}$. In the case that $k = k_{min}$, the death change and change v. (perturbing the heat flow and $T_{eq}$) have probability set to 0 and in the case that $k = k_{max}$, the birth step and change v. have probability set to zero. Option v. is not selected to improve efficiency and the birth and death steps are limited in this way to keep $k$ in the range $[k_{min}, k_{max}]$.

Although the choice of proposal distribution used in the rj-MCMC is essentially arbitrary, poor choices lead to very slow movement around the model space, such that convergence to the stationary distribution and exploration of the posterior distribution can take a very long time. It is therefore desirable to choose proposal distributions suitably such that the model space search is as efficient as possible.

The GST time points and GST values are updated individually, and are scaled so that proposals further back in time are larger. This is in order to improve the overall efficiency of the algorithm as the uncertainties are expected to expand with time before the present. If temperature value labelled i, ($i=1$ indicates the most recent times) is chosen for update and $k$ is the current number of GST model points, the new value $T'_i$ is given by:
Chapter 4. Temperature reconstructions from single and multiple boreholes

\[ T'_i = T_i + N(0, \sigma^m_T) \times \exp(i/k) \] (4.7)

where \( T \) and \( T' \) are the current and proposed GST values respectively and \( N(a,b) \) is a random Gaussian draw of mean \( a \) and standard deviation \( b \), and \( \sigma^m_T \) is a scaling factor for moving the temperature point (set to 0.1 for all cases here).

Similarly the time values are updated using:

\[ t'_i = t_i + [t_- - t_+] \times N(0, \sigma^m_t) \times \exp(i/k) \] (4.8)

where \( t \) and \( t' \) are the current and proposed GST time points respectively and \( \sigma^m_t \) is a scaling factor for moving the time point (set to 0.05 for all cases here). \( t_- \) and \( t_+ \) are the time values for the two adjacent GST model points. This proposal scales the time proposal to the width of the interval in which it is located and also exponentially with time in the past. These updates were found to give better mixing of the Markov chains, such that less iterations were required to quantify the posterior probability distributions. This move type is fully reversible (in that it satisfies detailed balance) as the time points are not allowed to cross each other.

The birth and death steps need to be designed so that one can exactly reverse the action of the other. Figure 4.2 illustrates the birth/death procedure employed. For a birth move, a time in the history is chosen at random and a GST interpolation point is added there. The current GST temperature at this time is then perturbed using a Gaussian distribution. The equations relating new and old points are

\[
\begin{align*}
t_* &= t_- + N(0, \sigma^b_t) \times (t_+ - t_-) \\
T_* &= \frac{(T_+ - T_-)}{(t_+ - t_-)} (t_+ - t_-) + N(0, \sigma^b_T) + T_- 
\end{align*}
\] (4.9) (4.10)

where \( t_* \) and \( T_* \) are the new time and temperature values, \( (t_-, T_-) \) and \( (t_+, T_+) \) are the co-ordinates of the two points either side, \( N(a,b) \) again is a random draw from a
Chapter 4. Temperature reconstructions from single and multiple boreholes

Figure 4.2: Upper panel: an example birth move, a random draw across the whole time domain determines the time position of the new point and a random draw from a Gaussian distribution determines the GST value at the new point. The distribution width has been exaggerated in order to improve clarity. Lower panel: an example death move.

normal distribution with a mean of \(a\) and a standard deviation of \(b\). \(\sigma_t\) is set to 1.0 and \(\sigma_T\) is the standard deviation of the proposal for the new temperature value. In this work \(\sigma_T = 10^{-6}\) has been used as it was found that this value led to good acceptance rates in the algorithm. For example, this stops the algorithm from having a near 100% acceptance rate for birth proposals and close to 0% for death proposals (or vice versa).

In the death step, an interpolation point is chosen at random and deleted, such that the GST curve is linearly interpolated from the two adjacent interpolation point temperatures. In both cases the GST history is returned to its current state if the proposal is not accepted (as defined by the acceptance criterion, equation 3.13).

The heat flow and \(T_{eq}\) temperatures are updated simultaneously using a bi-variate Gaussian proposal distribution. This is used because the heat flow and equilibrium temperature values for a particular borehole are negatively correlated. The required \(2 \times 2\) correlation matrix for each borehole is found by running an exploratory MCMC simulation before running the GST sampler in which these two parameters are updated singly.
4.3 Calculating the acceptance probability

For the heatflow and equilibrium temperature update the acceptance probability is given by

\[ \alpha = \min \left[ 1, \frac{p(d | m', \psi)}{p(d | m, \psi)} \right] \]

(4.11)

\[ = \min [1, \text{(likelihood ratio)}]. \]

4.3.1 Fixed dimension moves of time or temperature values

In the case that one temperature or time value is changed then the proposal is reversible and so the proposal ratio is equal to 1. The acceptance probability is then only dependent on the ratio of the likelihood terms and the prior ratio. For a temperature value perturbation the acceptance probability is given by:

\[ \alpha = \min \left[ 1, \frac{p(T' | \psi)}{p(T | \psi)} \cdot \frac{p(d | m', \psi)}{p(d | m, \psi)} \right] \]

(4.12)

\[ = \min [1, \text{(prior ratio) \cdot (likelihood ratio)}] \]

In the case that a time position is perturbed the prior ratio from equation (4.5) is introduced and so the acceptance term is given by:

\[ \alpha = \min \left[ 1, \frac{(t_+ - t_*)}{(t_* - t_-)} \cdot \frac{p(d | m', \psi)}{p(d | m, \psi)} \right] \]

(4.13)

\[ = \min [1, \text{(prior ratio) \cdot (likelihood ratio)}] \]

where \( t_- \) and \( t_+ \) are the GST model point times which are adjacent to the model point being perturbed \( t_* \).

4.3.2 Birth/death acceptance term

For the birth (and death) acceptance term, the prior and proposal ratio and also the Jacobian are required. The prior ratio takes account of the number of time steps and the
This last ratio is again calculated from equation (4.5). The prior ratio is then:

\[
\frac{p(m' \mid \varphi)}{p(m \mid \varphi)} = \frac{p(T' \mid \varphi) p(k + 1) k + 1 (t_+ - t_e)(t_e - t_-)}{p(T \mid \varphi) p(k) \frac{L}{(t_+ - t_-)}}
\]  

(4.14)

The proposal ratio reflects the probability of choosing a point for birth or death move, and is given by

\[
\frac{q(m \mid m')}{q(m' \mid m)} = \frac{L \; d_{k+1}}{(k + 1) \; b_k}
\]  

(4.15)

where \( k \) is the current model size, \( d_{k+1} \) is the death move probability and \( b_k \) is the birth probability. The ratio \( L/(k+1) \) accounts for the probability of choosing a point for a birth or death step. For a birth, the location of the time point is chosen with probability = \( 1/L \), i.e. uniform over the duration of the GST history. For the reverse death an existing point is selected with a probability = \( 1/(k+1) \) (since this is reversing a birth step from \( (k+1) \) to \( k \)). The ratio of the two values, \( b_k \) and \( d_{k+1} \) is \( \frac{1}{5} \) as there are 5 proposal types to choose from in each case. However, when \( k \) has reached the value \( k_{min} \) or \( k_{max} \) the proposal ratio for a birth or death change is different because there are less proposals types to choose from. Option v is not allowed (heat flow and \( T_{eq} \)) when the minimum or maximum dimension limit has been reached. Hence, for \( k = k_{min} \) only two options remain: birth or perturb a temperature, \( T_i \). For \( k = k_{max} \) only three options remain: death, perturb a temperature, \( T_i \) or perturb a time point \( t_i \). This leads to the proposal ratios for birth (at \( k = k_{min} \)) and death (at \( k = k_{max} \)) as follows:

\[
\begin{align*}
\frac{q(m \mid m')}{q(m' \mid m)}_b & = \frac{L}{(k_{min} + 1)} \; \frac{b_{k_{min}}}{b_k} = \frac{2L}{5 (k_{min} + 1)} \\
\frac{q(m \mid m')}{q(m' \mid m)}_d & = \frac{(k_{max} - 1) \; b_{k_{max} - 1}}{L \; d_{(k_{max})}} = \frac{3(k_{max} - 1)}{5L}
\end{align*}
\]  

(4.16)
4.3.3 Derivation of the birth/death Jacobian term

The equations relating the new temperature and time points to the current points are given again for clarity (equations 4.9 and 4.10):

\[
t_+ = t_- + \sigma_t \times u_2(0,1) \times (t_+ - t_-) \tag{4.17}
\]
\[
T_+ = \frac{(T_+ - T_-)}{(t_+ - t_-)} (t_+ - t_-) + u_1(0,1) \times \sigma_T + T_- \tag{4.18}
\]

where \(t_+\) and \(T_+\) are the new time and temperature values, \((t_-, T_-)\) and \((t_+, T_+)\) are the co-ordinates of the two points either side. Now substituting \(t_+\) into equation (4.18) gives:

\[
T_+ = (T_+ - T_-)\sigma_t \times u_2(0,1) + u_1(0,1) \times \sigma_T + T_- \tag{4.19}
\]

Equations (4.17) and (4.19) are required for calculating the Jacobian term. This is achieved by omitting the parameters which are unchanged by the birth or death move. This leads to a 2×2 determinant:

\[
|J| = \begin{vmatrix}
\frac{\partial(T_+, t_+)}{\partial(u_1, u_2)} \\
\frac{\partial(T_+, t_+)}{\partial(u_1, u_2)}
\end{vmatrix}
= \begin{vmatrix}
(T_+ - T_-) & \sigma_t \\
\sigma_T(t_+ - t_-) & 0
\end{vmatrix}
= -\sigma_t \sigma_T(t_+ - t_-) \tag{4.20}
\]

where the 4 terms have been derived by differentiating equations (4.17) and (4.19). Notice that the determinant of this Jacobian results in a negative quantity. Since the Jacobian term represents a mapping of the relative dimensions of the two subspaces this negative is not relevant in the acceptance probability, and if the terms are defined in a different order in equation 4.20 then the determinant become positive:

\[
|J| = \begin{vmatrix}
\frac{\partial(t_+, T_+)}{\partial(u_1, u_2)} \\
\frac{\partial(t_+, T_+)}{\partial(u_1, u_2)}
\end{vmatrix}
= \begin{vmatrix}
\sigma_T(t_+ - t_-) & 0 \\
(t_+ - t_-) & \sigma_t
\end{vmatrix}
= \sigma_t \sigma_T(t_+ - t_-) \tag{4.21}
\]
The acceptance term for a birth move is then:

\[
\alpha = \min \left[ 1, \frac{p(k+1)}{p(k)} \left( \frac{k}{L} \right) \frac{(t_s - t_\ast)(t_\ast - t_\ast)}{(t_+ - t_-)} \times \frac{p(T' | \varphi, k+1)}{p(T | \varphi, k)} \times \frac{p(d | m', \varphi, (k+1))}{p(d | m, \varphi, k)} \times \frac{L d_{k+1}}{b_k(k+1)} \times \frac{1}{(\sigma_T \sigma_l)(t_+ - t_-)} \right].
\]

(4.22)

where the first ratio term always takes the value 1. The corresponding acceptance term for a death step, has the same form but with appropriate re-labelling such that the current model is dimension k, moving via death to a model of dimension (k-1). The ratio terms also need to be inverted (Green, 1995):

\[
\alpha = \min \left[ 1, \frac{p(k-1)}{p(k)} \left( \frac{k}{L} \right) \frac{(t_+ - t_-)}{(t_+ - t_\ast)(t_\ast - t_-)} \times \frac{p(T' | \varphi, k-1)}{p(T | \varphi, k)} \times \frac{p(d | m', \varphi, (k-1))}{p(d | m, \varphi, k)} \times \frac{kb_{k-1}}{d_kL} \times \frac{1}{(\sigma_T \sigma_l)(t_+ - t_-)} \right].
\]

(4.23)

4.4 Synthetic Data

In order to evaluate the effectiveness of this Bayesian rj-MCMC method, it is first tested on synthetic data which have been designed to be similar to real data. The uncertainties which may be associated with the various model parameters can then be assessed.

4.4.1 Example I: Moberg et al. (2005) data

For the first synthetic example a temperature-depth profile is calculated using a surface air temperature (SAT) series as the ground surface temperature history. In this first case a well known SAT reconstruction (Moberg et al., 2005) and an instrumental SAT series (Jones and Moberg, 2003) have been amalgamated to produce a 2002 year SAT history (see appendix D.1). This is then used as a GST forcing for calculating the subsurface temperature values in a synthetic profile of depth 500m with values at 5m intervals. The thermal diffusivity was set to \(4 \times 10^{-7} \text{m}^2\text{s}^{-1}\) and the heat flow and \(T_{eq}\) to 60 mWm\(^{-2}\) and 9.6°C respectively. The temperature-depth values were then degraded with normally distributed 0.1K(=standard deviation) noise. The algorithm was tested on both the noise...
free and 0.1 K noise cases. The rj-MCMC algorithm was run for 500,000 iterations with
the last 400,000 used to generate the posterior distributions of GST, heat flow and $T_{eq}$.
This amalgamated SAT history is the same as the temperature series used for synthetic
experiments in Woodbury and Ferguson (2006), where the authors use empirical Bayes
methods to recover the GST histories. Comparisons between those results and the new
ones obtained here are made below.

Figures 4.3 and 4.4 show the posterior distributions for the noise free and 0.1 K noise
cases. The P scale is the posterior probability of the GST value at a given time. The
posterior distributions of heat flow and $T_{eq}$ values can be reasonably well fitted with
a Gaussian curve. For this synthetic case the posterior means and standard deviations
for the heat flow and $T_{eq}$ values were $(60.8 \pm 0.8)$ mWm$^{-2}$ and $(9.4 \pm 0.3)$ °C respectively.
These values are slightly biased from the true values, possibly by the action of the prior
information which does not correspond well with the first 1000 years of the GST history
in the true model.

In figure 4.5 examples of temperature histories accepted by the algorithm are shown
alongside the true model over the last 1300 years of the reconstruction. Over the period
shown it is possible to see that the number of points corresponds well with the long term
trends in the true model.

The expectation model defined in the previous chapter as the posterior mean, has the
advantage that it gives a smoother result than any single sampled model (which would
all consist of linear segments). However, it combines information from all of the sampled
models and therefore takes fuller account of the uncertainty. To illustrate this both the
posterior mean model and the maximum likelihood model are shown in figure 4.4. The
maximum likelihood model does not fit within the 95% credible intervals and appears to
over fit the data. The mean however, corresponds well with the true model and is much
smoother than the maximum likelihood model.

The Bayesian 95% credible interval is calculated by removing 2.5% of the smallest and
largest GST values at each time point to give a range of GST values which have a 95%
posterior probability of enclosing the true model. This range can be affected by the choice
of prior information, but for sensible prior choices, it gives a good idea of the changing
resolution with time.
Chapter 4. Temperature reconstructions from single and multiple boreholes

Figure 4.3: rj-MCMC inversion: synthetic data with no noise added. The synthetic data are calculated using surface air temperature reconstruction (Moberg et al., 2005) and instrumental data (Jones and Moberg, 2003) shown as the true model. The posterior mean is the expected value integrated across all models, the posterior distribution is shown in the 'P' colour-scale and the 95% credible intervals are shown as the dashed lines.

Figure 4.4: rj-MCMC inversion: synthetic data with Gaussian random noise added (mean 0.0K and standard deviation 0.1K). The true model has been 50 year smoothed. The maximum likelihood GST history is shown for comparison with the posterior mean. The mean shows much better agreement with the true model as it combines information from all the models sampled whereas the maximum likelihood model is just the single model which provides a best fit to the data. The posterior distribution is shown in the colour-scale and the 95% credible intervals are shown to illustrate the increasing uncertainty with time.
Figure 4.5: Examples of GST models accepted by the algorithm and how they compare with the true model. A smoothed version of the true model is shown for ease of comparison. Notice how the algorithm converges on a number of points (k) which appears well suited to the number of low-frequency change-points in the true temperature history. For the time period shown there are 3 points.

In the noise free case the GST has been well recovered across most of the time domain. However, in the more realistic noisy example, this is not the case and the reconstruction has slightly underestimated the warmth at 1000 years and the cool period around 400 years. The 95% credible interval becomes wider and more asymmetric than in the noise free example.

In figure 4.6 the posterior for the noisy data simulation is plotted at 4 times in the past and compared with the prior distribution and the true values (over a range of ±5 years). For the recent past the algorithm samples with high probability close to the true model values, as would be expected in this form of problem in which the resolution is expected to deteriorate back in time. Further back in time the posterior distribution becomes progressively more influenced by the prior. For example the posterior at 2000 years is effectively the same as the prior, indicating that no information has come from the data about the GST at this time. This type of observation can be used with real data examples to ascertain which parts of the GST reconstruction are actually supported by the data. In figure 4.7 the log likelihood and number of GST points are shown for the noisy case. The likelihood is stable above the expectation value (-188.4) and shows that
Figure 4.6: Posterior probability distributions at 4 times before present (2000, 1000, 500 and 200 years).

Figure 4.7: The log-likelihood and the number of time-temperature points in the GST history. The dashed line indicates the expected likelihood value when the data are fitted to exactly the expected noise value. The log likelihood value when the true model is used is -189.72, which is in the middle of the values sampled by the algorithm. The algorithm has explored models from size 3-7 with 4 showing most support from the data (see figure 4.8).

The algorithm is stable around this value. The data support between 3 and 7 points in the GST history. 52% of sampled models consisted of 4 GST points (see figure 4.8).

The results here show better resolution than the identical synthetic example (with 0.1K normally distributed noise) of Woodbury and Ferguson (2006) where no pre-20th century variation is captured. Another similar synthetic example with 0.1K noise is described by Hartmann and Rath (2005) using the SVD method, for which little variation prior to 1800
Chapter 4. Temperature reconstructions from single and multiple boreholes

Figure 4.8: Posterior probability density function of the number of GST points for the noisy synthetic case as sampled by the reversible jump MCMC algorithm. The data clearly favour a GST history with only 4 or 5 points.

Table 4.1: Beck et al. (1992) data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>True Value</th>
<th>$\sigma_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>temperature (K)</td>
<td>see fig. 4.9</td>
<td>$\pm$ 20 mK</td>
</tr>
<tr>
<td>thermal conductivity (W m$^{-1}$ K$^{-1}$)</td>
<td>2.5</td>
<td>$\pm$ 0.25</td>
</tr>
<tr>
<td>specific heat capacity (J m$^{-3}$ K$^{-1}$)</td>
<td>$2.5 \times 10^6$</td>
<td>$\pm 0.25 \times 10^6$</td>
</tr>
<tr>
<td>rate of heat production (W m$^{-3}$)</td>
<td>$1.0 \times 10^{-6}$</td>
<td>$\pm 0.5 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

is resolved and the average pre-1800 GST signal is somewhat biased compared to the true model. Here some of the variation of the past millennium for a 500m synthetic profile is recovered. Additionally inference about resolution changes over time are possible and it can be ascertained which parts of the reconstruction relate to the data or to the inverse methodology (in this case prior information, in other methods model smoothing).

4.4.2 Example II: Beck et al. (1992) data

In this case a synthetic data set published in Beck et al. (1992) is used in order aid comparison with the 5 inverse methods used in that paper. The data consist of temperature-depth values at 10m intervals to 600m depth calculated using a known GST history and a set of thermophysical property values and radiogenic heat values. All of these values are then degraded with Gaussian noise before inversion to mimic the effect of measurement errors. The true value and the Gaussian standard deviation for each parameter are shown in table 4.1. In the original paper 5 different inversion methods were tested on this data set. Four of the methods rely on the total least squares (Tarantola and Valette, 1982a, Shen and
Beck, 1991) whilst the other is singular value decomposition (Mareschal and Beltrami, 1992). For the noisy data set DS2 (examined here) all 5 methods either underestimate the cool period at 350 years before present or overestimate more recent variations.

Here results from the RJ-MCMC algorithm indicate that the cool period at 300-500 years before present cannot be fully resolved, and that the expected value for this cool period is approximately -0.5°C. This magnitude is much smaller than that in the true model and this is most likely to be due to the the short duration of this temperature excursion in relation to its age (200 years at 300-500 years ago) and the effect of the noise on all of the model parameters. The underestimation of the GST signal in this case demonstrates a useful feature relating to the parsimony of the Bayesian approach. If the support from the data is inconclusive, then the Bayesian method will tend towards the prior distribution, in this case therefore the prior indicates no change in GST over time. The 95% credible limits are very asymmetric at the cool time period in the true model, and indicate that a cooling to -1.0°C at around 400 years should not be ruled out by the data. This again shows that the overall posterior distribution contains useful information which cannot be conveyed by a single (e.g. best data-fit) model.

Although the noise factors for all of the model parameters are realistic, in practice this synthetic example is perhaps overly artificial because the large amplitude and rapidity of temperature changes are unlikely to have occurred in recent climatic record (large, very
Table 4.2: Borehole summary information for the 5 real data examples.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>Depth(m)</th>
<th>No. values</th>
<th>Lat.</th>
<th>Long.</th>
<th>Log date</th>
<th>Heat flow(mWm$^{-2}$)</th>
<th>$T_{eq}(^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wythcomber (A)</td>
<td>292</td>
<td>80</td>
<td>50.65</td>
<td>-3.37</td>
<td>1983.5</td>
<td>39.0 ± 2.0</td>
<td>12.5 ±0.34</td>
</tr>
<tr>
<td>Venn (B)</td>
<td>299</td>
<td>92</td>
<td>50.71</td>
<td>-3.32</td>
<td>1983.5</td>
<td>47.6 ± 1.1</td>
<td>11.4 ±0.19</td>
</tr>
<tr>
<td>Seabarn (C)</td>
<td>320</td>
<td>16</td>
<td>50.62</td>
<td>-2.53</td>
<td>1978.5</td>
<td>60.0 ±0.9</td>
<td>9.2 ±0.19</td>
</tr>
<tr>
<td>Chalgrove (D)</td>
<td>323</td>
<td>100</td>
<td>51.66</td>
<td>-1.05</td>
<td>1983.5</td>
<td>44.8 ±0.6</td>
<td>11.6 ±0.15</td>
</tr>
<tr>
<td>Worcester (E)</td>
<td>298</td>
<td>92</td>
<td>52.22</td>
<td>-2.2</td>
<td>1983.5</td>
<td>44.6 ±1.3</td>
<td>9.5 ±0.23</td>
</tr>
</tbody>
</table>

The values quoted for the heat flow and $T_{eq}$ are the posterior pdf means and standard deviations as sampled by the rj-MCMC algorithm. These posterior distributions are well approximated by a Gaussian distribution.

rapid temperature jumps have only been found to occur during glacial times and are called Dansgaard-Oeschger events). This example however, does demonstrate the increasing lack of resolution of the borehole reconstruction method for events successively further back in time.

4.5 Real Data

4.5.1 Examples I: 5 profiles from the IHFC database located in the UK

The real data used in this section were selected from the International Heat Flow Commission borehole climatology database (Huang and Pollack, 1998). Summary information for the boreholes examined is given in table 4.2. These data have been judged to be of good enough quality for palaeoclimate studies and specifically there is no evidence of vertical thermal convection. The 5 selected borehole data comprise temperature-depth profiles and thermal conductivity measurements with a minimum and maximum depths of 262m and 323m respectively. Values used for the volumetric heat capacity are $3.75 \times 10^5 Jm^{-3}K^{-1}$ for all the boreholes and measured data were used for the thermal conductivity. The noise term (standard deviation) used in the likelihood term was found by examining how well the data could be fit using an initial exploratory rj-MCMC run. This initially led to a standard deviation of 0.05K chosen for all of the data.

The profiles have been inverted both individually and jointly using simultaneous inversion (Beltrami and Mareschal, 1992, Beltrami et al., 1992, Pollack et al., 1996, Beltrami et al., 1997). In the latter case a joint likelihood is used in which it is assumed that the errors on the temperature data measured in each borehole are statistically independent from those in the other boreholes. This leads to the following likelihood formulation:
Figure 4.10: Posterior probability distributions for the individually inverted boreholes. The locations of these are shown in the inset map, and the details are given in table (4.2).

\[
p(d_{i=1,n_b} | m, \varphi, k) = p(d_1 | m, \varphi, k) \times \ldots \times p(d_{n_b} | m, \varphi, k) = \prod_{i=1}^{n_b} p(d_i | m, \varphi, k)
\]  

(4.24)

where as before \( m \) refers to the model (GST and heat flow parameters), \( \varphi \) refers to prior information, \( k \) is the model dimensionality, \( d_i \) is the data from borehole number \( i \) and there are \( n_b \) boreholes.

By using a posterior probability rather than average functional misfits, this formulation means boreholes for which the GST history signal is more uncertain, will have a smaller influence on the overall result as their posterior probability values will always be lower than those with a more robust signal. The priors used in the real cases are similar to those used for the synthetic, but with the prior mean set to the equilibrium temperature for each borehole.

The inferred heat flow and \( T_{eq} \) values for the 5 boreholes are given in table 4.2. Since
the posterior distributions for heat flow and $T_{eq}$ are close to Gaussian, the mean and standard deviations as sampled by the rj-MCMC algorithm are quoted. In figure 4.10 the individual posterior distributions of GST for the 5 boreholes are shown. Again, the P scale indicates posterior probability value showing the resolution of the GST signal with time. Comparing the posterior width of the GST signals for each reconstruction (as in figure 4.6) shows that borehole D has the smallest uncertainties associated with the GST reconstruction, whereas C has the largest. Borehole B has the smallest misfit with the data and for comparison the mean misfits for boreholes B and D are shown in figure 4.11 and 4.12. In all 5 cases the data misfit is acceptable given the expected noise in the data.

The differences in magnitudes of surface warming between the 5 boreholes are relatively large. The southern boreholes (A, B and C) show an average of 1.5K warming over 500 years whereas the central set (D and E) showing an average of 0.5K. Over the time period from 1659-1987 the Central England temperature (CET) record shows up to 1.5 K warming whilst synthetic examples with the CET record show that 0.5-0.6K of the warming signal (to AD 1983) is resolved by borehole inversion (although this is dependent on the assumption used for the synthetic test, that the GST does not change prior to the CET record commencing). In order to ascertain which warming signal is closer to the truth, the remaining 17 UK boreholes must be analysed. This is done in the next chapter 5 using a more advanced method.
Figure 4.13: Conductivity data for Chalgrove. Posterior GST history for conductivity model (1). Posterior GST history for conductivity model (2).

Effects of thermal conductivity value choice

Considering the data from borehole located at Chalgrove, the conductivity values from cores using the divided bar and needle probe method are available for depths 91m-322m. In the previous inversion, the values at shallower depths have been taken as $k = 1.5\, \text{Wm}^{-1}\text{K}^{-1}$, which is close to the average value for the shallower measurements. However, if we take this value to equal the nearest measured data, the value will be $1.87\, \text{Wm}^{-1}\text{K}^{-1}$. These values lead to ratios of thermal diffusivity to conductivity of $4.0\times10^{-6} \, \text{m}^2\text{s}^{-1}$ and $4.99\times10^{-6} \, \text{m}^2\text{s}^{-1}$ when a volumetric heat capacity of $3.75\times10^5 \, \text{Jm}^{-3}\text{K}^{-1}$ is used. These ratio values are both within 20% of $4.4\times10^{-6} \, \text{m}^2\text{s}^{-1}$, which is a generally accepted range for thermal diffusivity of a variety of rock types (e.g. Mottaghy, 2007). However, this small change in thermal conductivity leads to contrasting inferred GST histories as shown in figure 4.13, alongside the equivalent reconstruction from Huang et al. (2000). The inferred GST history for $k = 1.5\, \text{Wm}^{-1}\text{K}^{-1}$ is more consistent with climate knowledge of warming over the past several centuries and so it can be inferred that this conductivity value is closer to the true value.

The large effect caused by this change in thermal conductivity value underlines the
importance of choosing values carefully where core data are not available. Typically this should be based on standard values for the rock formations. A plausible alternative is to assign the unmeasured values a probability distribution which would take into account the a priori uncertainty. However, unless this pdf is fairly well constrained, the resulting GST reconstructions have been found to contain almost no inferred temperature variations as the variety of acceptable a priori conductivity values leads to a posterior with large credible bounds on the GST history. Many multi-borehole studies have assumed a uniform thermal diffusivity for all profiles of $1 \times 10^{-6} \text{ m}^2\text{s}^{-1}$, but it is not clear to what extent the actual departures from this uniform value may have caused some of the variations in the individual inferred GST histories evident in the global data set (Huang et al., 2000, Beltrami and Bourlon, 2004).

4.5.2 Joint inversion

In order to combat the influence of obscuring factors which may have corrupted the climate signal previous studies have relied on joint inversion. This is implemented here using the rj-MCMC algorithm. For the joint inversion, the GST applied to each borehole is defined as deviations from the individual $T_{eq}$ at each borehole (each of which is sampled by the rj-MCMC algorithm also). This allows for differences in the mean conditions at each site (e.g. due to latitude or altitude) whilst allowing a common long-term climatic signal to be inferred. The joint posterior probability distribution for the 5 boreholes is shown in figure 4.14 indicating a warming of approximately 1.0K over the 350 years to 1983. This has been calculated with a noise parameter $\sigma_d=0.05\text{K}$ and with the prior standard deviation of $\sigma_p =1.0\text{K}$.

The 95% credible intervals for the joint inversion, are wider and show increased asymmetry compared to the 5 individual inversions shown in figure 4.10. This increased uncertainty appears to be caused by the incompatibility of the 5 profiles, such that it is difficult to find a GST trend which can fit all 5 data sets. In this case, the choice of grouping of the 5 boreholes appears not to be supported by the data.
Chapter 4. Temperature reconstructions from single and multiple boreholes

Figure 4.14: Posterior probability distribution for the simultaneous inversion of the 5 boreholes shown as deviations from the steady state. The prior is centred on zero change with a standard deviation of 1.0K and the expected noise level of the data has a standard deviation of 0.05K.

Effect of the prior distribution choice and noise level

In a number of similar joint inversion experiments with synthetic data it was found that the mechanics of the MCMC algorithm mean that if poor choices of the heat flow or equilibrium surface temperature are proposed and accepted, the joint climate signal (from reduced temperatures) can become contaminated and this leads to spurious GST reconstructions. Chouinard and Mareschal (2007) also found that joint inversions (using the singular value decomposition method described in chapter 2.3.3) are prone to a parameter trade-off between the equilibrium parameters and the GST values. Their solution is to reduce all the profiles before inversion, i.e. subtracting the calculated equilibrium profile from the data. This makes sense for the SVD method as the two controlling model parameters are assumed to take single values. In the Bayesian context used here, the profiles cannot be reduced in the same way, as the two parameters are taken as probability distributions with loose a priori distributions. Additionally if the parameters were taken as single values, then this would artificially remove some of the inherent uncertainty in the overall model.

In synthetic cases a solution was to decrease the width of the prior pdf near to the start time of the reconstruction. This helped bias the GSTs from compensating for poor choices of the heat flow and equilibrium temperature parameters. This also makes sense.
Figure 4.15: Posterior probability distribution for the simultaneous inversion of the 5 boreholes shown as deviations from the steady state. In this example $\sigma_p$ varies linearly from 0.1K at the beginning of the reconstruction, to 1.0K at the present and the expected data noise level $\sigma_d = 0.1K$.

because the models here all assume that the GST histories are constant before the time period of the reconstruction.

In this real data example, it was demonstrated that modifying the prior in this way had little effect on the resultant posterior GST reconstruction. As a result in addition to tightening the prior on the GST values, the estimated noise parameter for each borehole data set was loosened to a value of $\sigma_d = 0.1K$. This then allows the algorithm more freedom as to which models are acceptable in light of the data. Employing this here, the jointly inferred GST history for the 5 selected UK boreholes becomes simpler in terms of less variations with time and is in better agreement with proxy and instrumental data reconstructions (e.g. Briffa et al., 2001); showing a minimum in the 17th Century and approximately 0.8K warming to the present day. The joint posterior pdf of the GST history is shown in figure 4.15 and in figure 4.16 two proxy reconstructions, the Central England temperature series (Manley, 1974, Parker et al., 1992) and the joint posterior mean borehole reconstruction are compared. The series show good agreement over long time scales with all 4 series showing approximately 0.8K warming since 1600. However, the two proxy reconstructions diverge from the continued warming trend of the instrumental record after AD 1950, this
Figure 4.16: Comparison over time periods 1500-1987 of two composite European tree-ring reconstructions (Briffa et al., 2001), the Central England temperature series and the posterior mean GST history reconstructed from the 5 boreholes described in the previous section. The borehole reconstruction has been shifted along the temperature axis.

is attributed to the divergence problem (see chapter 1.2). At higher frequencies the instrumental series and proxy reconstructions are also divergent. For comparison the locations of the European proxy data sources are shown in figure 4.17. The area covered by these 2 proxies sets includes much of southern Europe as well as Scandinavia and parts of Russia, but the data are relatively sparse around the British Isles. This may explain some of the shorter-term divergences between the instrumental and proxy records over the period 1659-1983.

Differences between proxy reconstructions and borehole reconstructed GSTs are commonly ascribed to a combination of factors: (i) the differing locations of the boreholes and proxy sites, (ii) the divergence problem affecting earlier sections of the tree ring reconstructions, (iii) the summer temperature bias of the tree ring proxy, (iv) the tendency for tree-ring reconstruction methods to underestimate low-frequency variations as the signal is partially removed together with the tree’s growth trend, (v) the effect of the assumption of no pre-reconstruction variations in the borehole GST model or (vi) the effects of snow cover on GST estimates. The results here, the proxy reconstructions of (Briffa et al., 2001) and the instrumental record for central England together indicate that these factors may be of less importance in the British Isles than for other regions of the globe.
4.5.3 Examples II: 5 profiles from Sellafield, Cumbria.

In this section the simultaneous rj-MCMC algorithm is applied to a suite of borehole temperature data from Sellafield in Cumbria, north west England acquired by Nirex and now held by the British Geological Survey (BGS). This consists of 5 temperature depth logs and the associated lithologies with thermophysical measurements for the majority of all 5 boreholes. The data are summarised in appendix D.3 and a map of the area is shown in figure 4.18. The geological setting of 2 of the wells is illustrated in figure 4.19 which shows a cross section from WSW to ENE through borehole numbers 2 and 3. Overall a number of sedimentary layers overlay a thicker layer of Borrowdale Volcanic rocks, with the lithologies dipping towards the coast. The temperature and geological data for the 5 boreholes are provided by the BGS and are summarised in Nirex (1997). The overall Sellafield database includes 30 temperature-depth profiles. However, the majority of these were found to be unsuitable for ground surface temperature history reconstructions. The reduced profiles for the 5 selected profiles are shown in figure 4.20. These are as sampled by the rj-MCMC algorithm used in this chapter and show that the ground surface at Sellafield has experienced recent warming. At greater depths, evidence of a variety of thermal processes are evident including local influences of faulting especially in borehole 3 and
fluid flow. Significant thermal disturbances of up to 1.5°C from the expected equilibrium values are present in the temperature log for borehole 3 below 1000m (not shown), and so data from below 950m are not included in the inversion.

Due to the likely thermal disturbances from fluid flow and land use changes in the area, the 5 borehole data sets have been inverted simultaneously only. As in the previous section, the model consists of 1 GST history of length L and in this case 5 $T_{eq}$ temperature values and 5 heat flow values. These then account for the equilibrium thermal conditions
at each site and thus account for differences due to localized affects. The prior information and proposal functions are identical to that used in the first IHFC data joint inversion of the previous section.

The five boreholes are much deeper than those from the IHFC database and so the length of the reconstruction has been changed from 500 years to 10,000 years. The errors on the temperature data are again assumed to be Gaussian and uncorrelated with a standard deviation $\sigma_T = 0.1K$, as used in the second joint inversion of the IHFC data.

Figure 4.21 depicts the posterior probability distribution of the ground surface temperature history over the last 1000 years. No significant variations were evident before
this time period and the onset of warming at 700 before present. This warming is almost certainly due to ground water flow in the vicinity of the boreholes (e.g Kukkonen et al., 1994). The posterior GST is not correlated with instrumental records for central England or with proxy studies (Briffa et al., 2001). Additionally the amplitudes of the variations (2.5°C between 1800 and 1991) are too large to be realistically related to long-term climatic changes. The Sellafield geology includes a layer of sandstones and shales which lie over a bed of the Borrowdale volcanic rock. Studies have shown that ground water percolates from the nearby hills in the Lake District towards the coast through the shallow layers of rock (Chaplow, 1996, McKeown et al., 1999), with the near surface flow most significant further inland. One explanation for the posterior GST history shown in figure 4.21 is then that the downward velocity of the ground water leads to cooler temperatures at depth and this can be interpreted as the large warming over the period from 200 years b.p to the 1991. The reduced temperature profiles in figure 4.20 indicate a positive temperature anomalies at depths of 200-500m and this could be related to upward ground water flow.
in the underlying formations. This most probably caused the 'warm' period in the GST history at 400 years b.p. Both of the groundwater flows are illustrated along with the basic geology in figure 4.22.

In conclusion, although the Sellafield dataset represents an extremely comprehensive set of geological and geophysical information, the influence of groundwater flow across the whole area is too large to allow inference of past ground surface temperatures using simple 1D heat conduction forward models. Incorporation of heat advection by groundwater flow into a suitable 2/3D forward model may allow this effect to be accounted for, so that the effects of past GST variations and fluid flow can be separated. However, the accuracy of the advection calculations would need to be smaller than the perturbations due to climate change and so of the order of 0.01K. This would only be feasible if the geological formations and the groundwater flows are very well characterised. For 1D heat conduction methods, it has been shown that joint inversion fails to constructively infer past GST variations and this lends support to careful selection of borehole profiles used for inversion (Huang and Pollack, 1998, Chouinard and Mareschal, 2007).

4.6 Discussion and Conclusions

In this chapter the use of Bayesian inference for inferring past climate from borehole temperatures is demonstrated. In order to achieve this, reversible jump Markov chain Monte Carlo sampling is used and this allows efficient exploration of model space by sampling models of varying dimension. The advantages of this approach mean that the inverse problem can be treated in a fully non-linear manner and that explicit regularization of the model parameters is not required, thus avoiding the need to find an optimal regularization value (Hartmann and Rath, 2005) and also reducing the possibility of artificially smoothing the reconstruction. Instead the posterior probability distribution of the GST is conditioned on the measured data and the prior information. The expected model, determined from the posterior, provides an integration over all models and therefore better captures the variability in the range of possible solutions than any other single (e.g. best) model. This posterior distribution incorporates the uncertainty due to the information loss from diffusion of the thermal signal and noise on the data and allows identification
of any non-uniqueness or poor resolution of GST or thermal equilibrium parameters. By comparing the posterior distribution with the prior it is possible to infer which parts of the distribution are supported by the data. Using the trans-dimensional form of MCMC, the complexity of the GST reconstruction is addressed in terms of the support from the data for models of differing dimensionalities.

In this chapter the results have been presented in terms of posterior means and 95% credible limits and these are useful quantities for summarising the results of Bayesian sampling. However, the aim of the whole approach is to quantify the posterior distribution and so the key result is actually the family of sampled GST histories for each case. The sampled GST models would be of most use in further studies as they could be used for example in further Bayesian sampling schemes for combining the borehole data analysed here with other borehole or even proxy data.

In any Bayesian formulation, the outcome is to some extent influenced by the choice of prior information. However, it is impossible to define totally non-informative priors and so sensible choices relating realistic a priori uncertainties must be made (e.g. Scales and Tenorio, 2001, Curtis and Wood, 2004). The priors used in this work are constant with time so that a priori no GST change is assumed. However, the prior distribution (i.e. its width) is designed to account for likely past variations. This is a good test of the methodology in the first case. However, the prior distribution is a flexible tool and could be used to incorporate information from instrumental data or other palaeoclimate reconstructions as well as the associated uncertainties. A different prior on the time locations of the nodes of the temperature history, which biases the model towards more nodes in the recent past, may help to improve the resolution of the recent part of the reconstruction. In appendix C an example is calculated with uniform prior on the time point locations.

A further issue surrounding the choice of prior constraints is whether the priors imposed translate well under different transformations in the multi-dimensional model space. This is an issue where uniform prior distributions are used as there is a large amount of injected information surrounding the prior bounds. In this work, uniform constraints are used as prior information for both the heat flow and equilibrium temperatures ($q_0$ and $T_{eq}$) and also the number of time temperature points. In theory the specified bounds for these parameters could lead to very biased sampling as the integrated prior distribution will have
most of the density concentrated around the extreme values. However, in our sampling these parameters do not approach any of the applied uniform probability limits except for the lower limit (=2) on the number of time-temperature points. This prior bias seems therefore to have had a small effect on the sampling results described.

Examples from the International HeatFlow commission database indicate a compelling warming trend in the British Isles over the last 500 years. The results show between 0.5 and 1.5 °C of warming as inferred from individual boreholes and around 0.8°C of warming when inverted jointly. This latter result is in good agreement with hemispheric borehole estimates from Huang et al. (2000) and Beltrami and Bourlon (2004) and the trend is concordant with multi-proxy studies such as Moberg et al. (2005) and Hegerl et al. (2007). However, there are a number of assumptions which should be tested before the results are accepted. The choice of conductivity values where no measurements are available appears to be important, and is something that has not been dealt with in previous studies. More significantly is the choice of which boreholes to invert jointly. If many borehole profiles are included which are corrupted partially with site specific noise, the overall signal will be subject to increased uncertainty and may lead to both under or over-estimates of past GST variability. This has been demonstrated by simultaneous inversion of 5 profiles from Sellafield. In the next chapter the issue of how boreholes are grouped for inversion is explored using a Bayesian partition model which allows the objective selection of borehole groupings which is entirely dependent on the data and uniform spatial prior information.
Chapter 5

Spatial trends

5.1 Introduction

Records of surface temperatures indicate that the average global surface air temperature has risen by 0.6°C over the course of the 20th Century. Examination of the spatial component of the numerous instrumental series indicates a high degree of heterogeneity across the globe. For example, observed surface air temperatures from 1880 to the present day (figure 5.1) show larger amplitude warming in continental Canada and Greenland, whereas some other parts of the globe have seen a moderate cooling over the same time period. Some of these spatial variations back in time have also been inferred by geothermal studies, especially using data from Canada (Pollack and Huang, 2000, Majorowicz et al., 2002, Beltrami et al., 2006, Stevens et al., 2008). However, the geothermal methods for inferring spatial variability are relatively simple and rely on a priori division of the space into smaller regions, so that the contained ground temperature history (GST) reconstructions can be averaged together. A related issue in borehole climatology is that in order to derive robust estimates of GST histories from real data, the profiles must be treated jointly in some fashion (Pollack et al., 1996, Beltrami et al., 1997, Pollack and Smerdon, 2004). However, it is not always obvious how borehole data can be grouped to produce the most robust reconstructions. The employed inverse algorithm and the method of dealing with data noise are important factors.

Linking these two issues, a Bayesian approach is used which relies on Partition Modelling of Denison et al. (2002). This allows a robust approach to the problem, whereby
the relative support for differing model parameterisations is quantified, so that instead of resorting a priori to a certain model setup, a variety of configurations is examined and tested against the data. This then allows both the spatial component and the uncertainty in the data to be explicitly taken into account by the probabilistic modelling formulation.

5.2 Background

Recently multiple borehole profiles have been examined jointly in order to infer spatial variations of past surface temperatures resolvable in borehole data (Majorowicz et al., 2002, Beltrami et al., 2003, Majorowicz et al., 2005, Pollack and Smerdon, 2004, Beltrami and Bourlon, 2004). These estimates of the spatial component are derived by averaging the individual reconstructions over pre-defined areas (e.g. $5^\circ \times 5^\circ$ or geographical regions) to give the best estimate of the reconstructed GST history in each cell or region. For example, estimated GST trends in Canada, where the largest number of studies have been
Chapter 5. Spatial trends

Figure 5.2: 124 European borehole locations from Huang and Pollack (1998) (red crosses). Shaded boxes indicate 5° × 5° cells containing 3 or more borehole profiles. If grid cells with less than 3 boreholes are ignored (as in Pollack and Smerdon, 2004) then 18 borehole profiles would be omitted from this dataset.

made, broadly show delayed onset of warming from the east to west of the continent over the last few hundred years (e.g. Majorowicz et al., 2002).

However, even over relatively short geographical distances, reconstructed GST trends are often poorly correlated with each other. Despite careful screening of the data, the influences of site-specific thermal perturbations such as those caused by underground fluid flow, land use change or topographic variations are impossible to completely exclude. Additionally, under-estimation of the data noise during the inversion process can result in spurious GST reconstructions, the severity of which is dependent on the sophistication of the employed inverse method. The aim of averaging or jointly inferring GST histories is therefore to amplify the coherent climate signal and reduce the combined noise from the non-climatic factors and the measurement errors (Beltrami and Mareschal, 1992, Pollack et al., 1996, Huang et al., 2000).

A drawback of averaging reconstructions using existing inverse methods is that for each individual reconstruction, the estimated noise level cannot be tailored to the profile in question. This is because each inversion must be parameterised consistently so that the resulting reconstructions are mathematically comparable (Beltrami et al., 1997, Huang
et al., 2000, Beltrami et al., 2003). A second issue arises because a choice must be made as to how the borehole profiles are grouped together for joint inversion or averaging of reconstructions. Averaging over a pre-defined grid, with a minimum number of profiles per cell (Pollack and Smerdon, 2004), is undesirable because a number of borehole profiles are ignored (as they lie in grid cells with too few boreholes) and many grid cells will have much larger numbers of boreholes compared to neighbouring ones, leading to uneven uncertainty on the GST reconstructions across a spatial domain. This is illustrated in figure 5.2 for 124 European borehole locations. In this example a $5^\circ \times 5^\circ$ grid means that 18 profiles are discarded as the grid occupancy varies from 1 to 22. Averaging across larger areas would appear to be a more robust approach, but this may mask any actual spatial climatic trends. The only way to decide on a more suitable set of averaging regions would be to carefully examine the reduced temperature profiles in advance (e.g. Majorowicz et al., 2002) or to resort to information on current state of expected climatic trends e.g. from climate modelling experiments or other palaeoclimate data sources.

Here the use of a Bayesian Partition Model (Green, 1995, Denison et al., 2002, Stephen-son et al., 2006) is considered as a possible method for dealing with both of the issues described. The GST histories can be inferred jointly from multiple temperature-depth profiles of possibly varying noise levels. Crucially, the areas over which these joint inversions are performed can be determined directly from the borehole data themselves. This is achieved by resorting to a fully Bayesian (probabilistic) formulation in which models of differing parameterisations are constructed and then objectively compared using a MCMC algorithm. The partition model is setup so that the spatial domain under consideration is divided into a set of smaller partitions, each of which is assumed to pertain to an independent GST history. The aim of the approach is to infer both the partition structure and the GST in each partition directly from the observed temperature-depth profile at each borehole location. In this work this posterior probability density function (pdf) of the partitions and the partition GST histories is approximated by sampling with a reversible jump Markov chain Monte Carlo (rj-MCMC) algorithm (Green, 1995). This algorithm allows for models of varying dimensionality, which means that models with different numbers of partitions (and therefore different numbers of GST histories) can be compared. In doing this the standard birth/death type proposals (Green, 1995, Denison et al., 2002)
are used whereby extra partitions are added or removed one at a time in the algorithm. However, in order to deal with the inverse problem of estimating an appropriate GST history for each partition, a second rj-MCMC algorithm is additionally used to sample from the conditional posterior pdf of the GST conditioned on the boreholes enclosed by that particular partition. The overall methodology, which therefore relies on two separate rj-MCMC samplers, is then capable of sampling for an appropriate number of independent GST histories in the total spatial domain, as well as appropriate temporal resolution levels of the different temperature histories in each partition.

Using Bayesian Partition modelling in this way it should then be possible to infer the number of independent GST histories which are supported by the data from a collection of borehole profiles, conditioned on the estimated level of data noise for each profile and the relative location of each borehole. This method will then have implications where profiles have either been inappropriately averaged together, or in datasets for which spatial trends in the past surface temperatures are important. A first case study which is explored in this chapter, is a set of 23 borehole data of which 22 have been previously examined (Huang et al., 2000) (these reconstructions are shown in figure 5.12 and will be discussed further later). These GST reconstructions are extremely variable and this appears to undermine the utility of the borehole climate reconstruction method. The aim of this work is then to investigate whether the large range in estimated GST trends is due to site specific noise (fluid flow, land use change, topography), mis-appreciation of the noise levels of the data or an underlying spatial trend in past temperatures.

The 1D forward model setup used here is described in section 5.3.1. In sections 5.3.2 and 5.3.3 a brief introduction to Partition Modelling and Bayesian inference is given. The implementation of the rj-MCMC algorithm is described in detail in section 5.4. This is followed in section 5.5 by a test example illustrated using synthetic data for which the algorithm is shown to quickly converge on the true spatial setup. In section 5.6 the methodology is applied to 23 real borehole temperature profiles from the UK, 22 from the database of Huang and Pollack (1998). Preliminary results show that the data favour 8 or 9 separate partitions. The inferred GST histories for the larger partitions show a large range of inferred temperature histories, implying that the data cannot provide a good constraint on past climate. Furthermore, although the trend for 2 of the partitions shows
good agreement, the possibility of systematic errors (which are present in the other large partitions) makes direct interpretation of the reconstructed temperature history difficult. This UK dataset should therefore not be used for climate reconstruction purposes without at least (i) acquiring more detailed site information for each borehole and (ii) using a more advance forward model which includes more of the important heat transfer processes such as surface topography or subsurface advection.

5.3 Methods

5.3.1 Forward Model

The employed forward model was described in chapter 4. The heat flow is assumed to be only in the vertical direction with no advective component. Thus thermal perturbations in the subsurface from the long term equilibrium are the result of time-varying ground surface temperature only. The relevant form of the heat conduction equation in 1D is:

\[
\rho C \frac{\partial T(z, t)}{\partial t} = \frac{\partial}{\partial z} \left( k(z) \frac{\partial T(z, t)}{\partial z} \right),
\]

where \( z \) is depth, \( t \) is time, \( \rho \) is the rock density, \( c \) is the rock specific heat capacity and \( k \) is the rock thermal diffusivity. The present day temperature-depth profile can then be expressed in terms of the equilibrium thermal conditions, the past surface temperature variations and random measurement error:

\[
T(t_{\text{present}}, z) = T_{eq} + q_0 \int_0^{z_{\text{max}}} \frac{1}{k(z)} dz' + T_s(z) + \epsilon_d
\]

where \( T_{eq} \) is the long-term equilibrium surface temperature, \( q_0 \) is the basal heat flow, \( T_s(z) \) is the subsurface perturbation at depth \( z \) due to past surface temperature variations and \( \epsilon_d \) is the measurement error.

As in the preceding chapter, the conduction equation is solved numerically by the method of finite elements. In order to account for background geothermal heat flow, a steady state solution is first derived and this is then perturbed using a transient FE model.
to give the final temperature-depth values. These are then compared with the measured data through the likelihood function to give the likelihood value.

5.3.2 Partition modelling and Voronoi tessellations

To divide up the space over which the boreholes are located, Voronoi tessellations are used (e.g. Green, 1995, Denison et al., 2002, Blackwell and Møller, 2003). This allows divisions of a specified space into regions defined by tessellation centres $C_i$. Each Voronoi tessellation region is formed by including in a tessellation, say $R_1$ associated with centre $C_1$, all the points in space which are closer to $C_1$ than to any other centre, $C_i$. This distance can be measured in a variety of manners (Denison et al., 2002), but in this work the standard Euclidean distance metric is used:

$$D(x_a, x_b) = \sum_i (x_{ai} - x_{bi})^2$$ (5.3)

Figure 5.3 depicts an example Voronoi tessellation which has 8 centres.

Applications of Voronoi tessellations and partition modelling can be found in a range

In this work each partition pertains to an independent GST history. Thus the number of partitions, \( n_c \), can vary over the range \( 1, n_b \) where \( n_b \) is the number of boreholes. When the number of partitions is 1, all of the borehole profiles fall within the same Voronoi region and so are fitted with a common GST history. For \( n_c = n_b \), each borehole is located in a separate Voronoi cell and so a different GST history is fitted to each profile. The latter setup will therefore provide the best fit to the data, however, the aim of Bayesian partition modelling is to find an appropriate and objective balance between the number of partitions (in a sense, a measure of the model complexity), and the quality of the fit to the observed data. The prior information plays a key role in achieving this balance (see section 5.4.1).

### 5.3.3 Bayesian Inference

The parameters of interest are \( C \), the locations of the Voronoi centres, \( \theta \) the GST histories in each partition and \( q_0 \) and \( T_{eq} \) the geothermal heat flux and surface equilibrium temperature at each borehole respectively. These model parameters are encapsulated by

\[
m = (C, \theta, q_0, T_{eq}).
\]

(5.4)

where \( C_i \in \mathbb{R}^2 \) and \( \theta_i \in \mathbb{R}^{k_i} \) (\( k_i \) is the number of time and temperature points, \( t_j, T_j, j = 1, k_i, \) in GST history \( \theta_i \)) are defined for each partition and \( q_0^j \) and \( T_{eq}^j \) are defined for each borehole.

In theory all of the parameters of the simulation could be incorporated into this set \( m \); including for example, the thermal conductivity values and even the temperature data themselves (e.g. Gallagher, 1990). In this work \( m \) is limited to the Voronoi centres and those parameters that have been of most interest in similar work, namely the GST
histories and the background equilibrium thermal conditions (Huang et al., 2000, Beltrami et al., 2003). Casting the problem in a probabilistic framework using Bayesian inference (e.g. Mosegaard and Tarantola, 1995, Tarantola, 2005) allows for uncertainty in all model parameters. The probability distribution of the four model parameter vectors conditioned on the data and prior information is then given by Bayes’ law (e.g. Bernardo and Smith, 1994), see chapter (3.3) and appendix (A.2).

At first sight, it might be anticipated that the rj-MCMC algorithm will tend to a solution with \( n_b \) partitions such that each borehole profile is individually fitted and the lowest possible misfit to all the data is achieved. However, Bayesian inference is naturally parsimonious and avoids overly complex models (Jefferys and Berger, 1992). In this work the evidence is not calculated, instead the rj-MCMC algorithm samples models of different dimensionality in proportion to their evidence (Green, 2003, Sambridge et al., 2006). Thus the method will tend to favour the simplest model which can adequately fit the data. In the synthetic examples presented it is demonstrated that the Bayesian method preferentially samples simpler models. This is achieved without needing to specify a restrictive prior on the number of partitions.

### 5.4 Sampling algorithm

#### 5.4.1 Prior information

In any Bayesian formulation prior information for all model parameters must be specified. In inverse problems the prior information acts to ensure that the solutions have acceptable or physically reasonable values (Scales and Tenorio, 2001, Curtis and Wood, 2004). In this work the prior information is chosen to correspond with what is usually known in a typical data situation.

Treating the prior probability hierarchically, the terms in \( \theta \) can be separated from those in \( C \):

\[
p(C, \theta \mid \varphi) = p(\theta \mid C, \varphi)p(C \mid \varphi)
\]  

(5.5)
Here a continuous uniform prior is employed for the positions of the Voronoi centres and a
discrete uniform prior is used for the number of the Voronoi centres (Denison et al., 2002):

\[ p(C) = \frac{n_c!}{(\Delta x \Delta y)^{n_c}} \times p(n_c) \]  \hspace{1cm} (5.6)

where \( \Delta x = x_{\text{max}} - x_{\text{min}} \) and \( \Delta y = y_{\text{max}} - y_{\text{min}} \) are the dimensions of the spatial domain
(rectangular) and are both equal to 1.0 in all the examples presented. A uniform proba-
bility distribution over the range \((1,n_b)\) is used as the prior on the number of partitions
i.e. \( p(n_c) = 1/n_B \). A more conservative choice would be a Poisson distribution with an
expected value. However, in order to demonstrate the efficacy of the partition modelling
method, the more general prior term is used initially.

The prior information on the GST model parameters \( \theta_i \) is the same as used in chapter
4. The prior distribution on the past temperature values is given by:

\[ p(T_i \mid \psi) = \frac{1}{[(2\pi)^{k_i} \det \mathbf{C}_\psi]^{1/2}} \exp \left[ -\frac{1}{2} (T_i^{\text{GST}} - T^{\psi})^T \mathbf{C}_\psi^{-1} \right. \]
\[ \left. \times (T_i^{\text{GST}} - T^{\psi}) \right] \]  \hspace{1cm} (5.7)

where \( T_i^{\psi} \in \mathbb{R}^{k_i} \) gives the most likely values at each of the \( k_i \) time-points. In this work \( T^{\psi} \)
takes the same value at all time-points so that the prior is biased towards temperatures
histories with no change (Huang et al., 2000). The values used for \( T^{\psi} \) and \( \mathbf{C}_\psi \) are given
alongside the specific examples described in sections 5.5 and 5.6. When combining the prior
for multiple partitions, the GST histories in each partition are assumed to be independent
such that the prior term for GST for the \( n_c \) partitions is given by the product of the
individual prior terms:

\[ p(T \mid \psi) = \prod_{i=1}^{n_c} p(T_i \mid \psi), \]  \hspace{1cm} (5.8)

where there are \( n_c \) partitions or independent GST histories.

The prior distribution for the positions of the nodes, used to parameterise the GST
histories, is a uniform order statistic distribution (e.g. Green, 1995). The prior on the

\[ p(t_i \mid \varphi) = \frac{k_i! \times t_1^i \times (t_2^i - t_1^i) \times \ldots \times (L - t_{k_i}^i)}{L^{k_i}}. \]  

(5.9)

Again the terms for each partition are independent and so can be combined as a product:

\[ p(t \mid \varphi) = \prod_{i=1}^{n_c} p(t_i \mid \varphi). \]  

(5.10)

The prior on the number of points in the GST history is uniform over the range [1-20),

hence the prior probability of a GST model of dimension \(k\) is \(p(k) = 1/19\), the combined

prior for \(n_c\) partitions is \(p(\mathcal{P}) = \prod_{i=1}^{n_c} p(k_i)\).

Combining the prior terms for the temperatures \(T_i\), the time points \(t_i\) and the number

of \((t,T)\) points in each partition \(k\), gives us the prior used in the acceptance term \(\alpha\). This

then takes the form:

\[ \pi(\theta \mid \varphi) = \prod_{i=1}^{n_c} p(T_i \mid \varphi) \cdot p(t_i \mid \varphi) \cdot p(k_i) \]  

(5.11)

The prior distributions for the heat flow and equilibrium surface temperatures \((q_0, T_{eq})\) are set to uniform over the range [5,150]mW and [-5,15]°C. The prior terms relating
to these two quantities will always cancel in the acceptance term \(\alpha\) (provided no values

outside of the specified ranges are accepted) and so these terms are omitted in the following
equations.

5.4.2 Likelihood

The likelihood term for a particular borehole is assumed to be a multi-variate Gaussian
distribution with uncorrelated parameters and is a function of the calculated temperature
profile (using finite elements) and the measured temperature profile:
\[ p(d \mid m, k, \varphi) = \frac{1}{\{(2\pi)^n \det C_d\}^{1/2}} \exp \left[ -\frac{1}{2} (d_{sim} - d_{obs})^T C_d^{-1} \times (d_{sim} - d_{obs}) \right] \]  
\[ (5.12) \]

where there are \( n \) data points, \( d_{sim} \) and \( d_{obs} \) are the simulated and observed subsurface temperatures respectively and \( C_d \) is the data covariance matrix (here assumed to be diagonal). The errors on the data are therefore assumed to be Gaussian and uncorrelated. The values used for \( C_d \) are discussed later with the descriptions of synthetic and real data applications. By assuming the errors on the measured data in each borehole are statistically independent from other boreholes, the joint likelihood for an ensemble of borehole profiles can be simplified thus:

\[
p(d_{j=1,n_b} \mid m, k, \varphi) = p(d_1 \mid m, k, \varphi) \times p(d_2 \mid m, k, \varphi) \times \cdots \times p(d_{n_b} \mid m, k, \varphi),
\]

\[ = \prod_{j=1}^{n_b} p(d_j \mid m_{v(j)}, k_{v(j)}, \varphi). \]  
\[ (5.13) \]

where \( d_j \) is the data for borehole \( j \), \( m \) is the current model and \( m_{v(j)} \) is the relevant set of model parameters for borehole \( j \), where \( v(j) \) gives the Voronoi partition in which borehole \( j \) is located.

### 5.4.3 Proposal distributions

In order to sample the posterior distribution 1 of 6 proposal types is chosen. These are designed for efficiency in moving around the model space, and focus mainly on the partition structure. These are summarised as:

i. Birth: add a new Voronoi centre with the position found by drawing from the prior distribution on \( C \),

ii. Death: delete one Voronoi centre chosen randomly from the current set,

iii. Move an existing Voronoi centre to a position drawn from the prior on \( C \)
iv. Perturb one Voronoi centre by drawing from a normal distribution centred on its current position.

v. Update the heat flux ($q_0$) and equilibrium surface temperature ($T_{eq}$) for 1 borehole site.

vi. Propose a new GST history ($\theta_i'$) for partition $i$.

Each possible proposal is selected with equal probability ($=1/6$), except when the number of partitions is 1 or at the maximum, in which case we do not allow death or birth, respectively. When the Voronoi centres are changed in the first 4 ways, the overall structure is recalculated. Often the majority of the tessellation boundaries will remain unchanged relative to the borehole locations. However, each time a new data configuration is arrived at (i.e. a different grouping of the boreholes in 1 or more Voronoi polygons) a proposal for a new GST history must be made. In figure (5.4) this is illustrated for the case of a birth from 2 partitions to 3: there is no obvious choice for the GST histories $\theta_i'$ of the new partitions. Moreover, the proposal probability for the reverse proposal (i.e. the corresponding reduction in the number of partitions) is also required in order to satisfy detailed balance of the Markov chain. When a proposal for $\theta_i$ is required in this way or because option (v) is selected, a secondary rj-MCMC algorithm is run (e.g. Stephenson et al., 2006) unless the proposed partition has been previously sampled. This secondary algorithm gives an approximation to the conditional posterior of the GST history in a
partition, conditional on the set of borehole profiles enclosed by that partition. One of the GST histories sampled by the secondary rj-MCMC, $\theta_s$ is then randomly selected and set as the proposal $\theta'_i$. This means that the proposal function for $\theta'_i$ has no dependence on the current state of $\theta_i$ and thus the proposal term is greatly simplified. These proposal distributions are stored for cases in which the algorithm proposes to move back to a previously sampled state, in which case a new model is randomly drawn from the stored distribution.

The secondary rj-MCMC algorithm is as described in chapter 4 and so does not need to be described in detail here. However, many of the details of the secondary rj-MCMC algorithm are similar to those used in the main algorithm. The priors on the GST histories and the likelihood formulation are both as described above for the main rj-MCMC. The only difference is that in order to constrain the model space when inverting a number of borehole profiles simultaneously, the prior on the GST temperatures is modified so that the standard deviation varies linearly from 0.1K to 1.0K over the reconstruction time length. This prior structure prevents large changes in the GST values compensating for poor proposals of the basal heat flux or equilibrium surface temperature. The narrower prior range in the past also makes sense, because the model setup assumes no changes in GST prior to onset of the reconstruction, an assumption common to most GST reconstruction methods. This problem in joint inversion has also been identified by Chouinard and Mareschal (2007) using a singular value decomposition inversion method. The authors resorted to inverting reduced temperature profiles only (i.e. subtracting a calculated equilibrium temperature-depth profile from the measured data).

In both the main and secondary algorithms, the heat flow and equilibrium surface temperature are updated using a bi-variate Gaussian proposal distribution with an assumed correlation between the two parameters for each borehole of 75%. The standard deviations for each parameter are $4 \times 10^{-5}$Wm$^{-2}$ and $4 \times 10^{-2}$K respectively. The values sampled by the secondary algorithm for these two parameters are not ‘returned’ to the main algorithm except at initialisation before the first iteration of the main rj-MCMC algorithm.

The overall algorithm is summarised graphically in figure 5.5.

Bayesian Partition Model Method Outline

\[ m \in \{ C, \Theta, q^0, T_{eq} \} \]

Initialise \( m \)

Draw \( u = U(0, 6) \)

- If \( u < 1 \), Birth
- If \( 1 \leq u < 2 \), Death
- If \( 2 \leq u < 3 \), Move
- If \( 3 \leq u < 4 \), Perturb
- If \( 4 \leq u < 5 \), GST
- If \( 5 \leq u < 6 \), HtF & Teq

\( m' \)

Draw GST from 2nd RJ-MCMC

- If \( C_i' \neq C_i \) or (GST = true)

Store \( m \)

Draw \( U(0,1) \); if \( \alpha(m', m) > U \)

- If \( \text{HtF & Teq} = \text{true} \)

Store \( m' \)

\[ \text{Figure 5.5: A flowchart showing the stages of each iteration of the BPM algorithm} \]

5.4.4 Proposal ratio terms

The proposal ratio used in the main rj-MCMC algorithm can be simplified by separating out the 4 model parameters:
\[
\frac{q(m | m')}{q(m' | m)} = \frac{q(C, \theta, q_0, T_{eq} | C', \theta', q'_0, T'_{eq})}{q(C', \theta', q'_0, T'_{eq} | C, \theta, q_0, T_{eq})} = \frac{q(C | C')}{q(C' | C)} \cdot \frac{q(\theta | \theta', C')}{q(\theta' | \theta, C)} \cdot \frac{q(q_0, T_{eq} | q'_0, T'_{eq})}{q(q'_0, T'_{eq} | q_0, T_{eq})}
\]

(5.14)

The proposal ratio for centres given a perturb, move or GST update is equal to unity. For a birth step it is given by:

\[
\frac{q(C | C')}{q(C' | C)}_b = \frac{1/(n_c + 1)}{(1/(\Delta x \Delta y))}
\]

(5.15)

This accounts for choosing a \(C_i\) point at random (on a spatial domain size \((1/\Delta x) \times (1/\Delta y)\)). The \(1/n_c + 1\) term accounts for choosing that point for death (following the birth, so that the proposal is reversible).

In the proposal ratio the choices of model parameters for a particular partition must also be taken into account. This means that the proposal distributions used to generate the model parameters in each partition must be drawn from a normalised probability distribution. In the proposal 1 GST history \(\theta'_i\) is randomly selected from those sampled. The probability distribution is calculated for each model parameter \((k_i, t^k_i, T^k_i)\) in \(\theta'_i\), using 24 year and 0.1K increments for time and temperature respectively. This is conditional on the remaining model parameters taking their sampled values in \(\theta'_i\) and leading to a proposal probability \(p(\theta'_i)\) which is the product of these individual probabilities. The probability for a particular proposal is then of the form

\[
\frac{q(\theta'_i | \theta_i, C')}{q(\theta'_i | \theta_i, C)} = \frac{p(\theta_i)}{p(\theta'_i)}
\]

(5.16)

where

\[
p(\theta_i) = p(k_i) \cdot p(t_i | k_i) \cdot p(T_i | t_i, k_i)
\]

(5.17)

The third term of equation (5.14) is given by
and is equal to 1 as the proposal distribution is a bi-variate Gaussian centred on the current values with a fixed covariance matrix (it does not change between iterations). This term can therefore be discarded in subsequent equations.

The overall proposal ratio (equation 5.14) is then given by the products of the proposal probabilities in each partition before and after a proposal is made multiplied by the proposal ratio for \( \mathbf{C} \) the Voronoi centres and the proposal ratio for the proposal type (birth, death, move, perturb etc.) Thus for a birth move, the proposal ratio is given by:

\[
\frac{q(m | m')} {q(m' | m)} = \frac{\Delta x \Delta y} {n_c + 1} \times \frac{d_{n_{c+1}}}{b_{n_c}} \times \frac{\prod_{i=0}^{n_c} p(\theta_i)} {\prod_{i=0}^{n_{c+1}} p(\theta'_i)},
\]

(5.19)

where there are \( n_c \) partitions originally and \( n_{c+1} \) partitions in the proposed model and \( b_{n_c} \) and \( d_{n_{c+1}} \) both take the value 1/6 unless the number of partitions reaches the maximum value (or minimum in the case of a death move). In order to keep the number of partitions in the model in the range \((1,n_B)\) birth (death) moves are not allowed when the number of partitions reaches the maximum (minimum) of this range. The proposal ratio for the move type will therefore be different from 1. In the case that \( n_C = 1 \), the move type proposal ratio for a birth is given by \( d_2 / b_1 = 1/6 \) and in the case that \( n_C = n_B \), the move type proposal ratio for a death is given by \( b_{n_B-1} / d_{n_B} = 1/6 \).

### 5.4.5 Calculating the acceptance term

When the number of centres changes through a birth or death move, the Jacobian needs to be calculated. However, for the choices of birth and death used here the Jacobian turns out to equal 1. For the birth step:
\( c'_s = (x_{\min} + u(0, \sigma_x), y_{\min} + v(0, \sigma_y)) \) \hspace{1cm} (5.20)

\[
|J|_b = \frac{\partial c'_s}{\partial (u,v)} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 1, \hspace{1cm} (5.21)
\]

where \( u(a,b) \) and \( v(c,d) \) are random draws from a uniform distribution over the range \( a \) to \( b \) or \( c \) to \( d \) respectively. \((\Delta x, \Delta y)\) is the domain under consideration. The Jacobian is found by considering only the model parameters which are affected by the proposal. In this case the other centres are all unchanged and so only \( c'_s \), the new centre is considered.

The GST values, \( \theta \) do come into this calculation because they are proposed independently of the current state (see equation 5.14). Since the Jacobian for a death move is \( |J|_d = |J|_b^{-1} \), this quantity takes the value 1 for a death step also.

The prior ratios for the Voronoi centres \( C \) will cancel except in the cases of a birth or death. For a birth proposal type the prior ratio on the Voronoi centres is given by:

\[
\frac{p(C')}{p(C)} = \frac{n_c + 1}{\Delta x \Delta y} \hspace{1cm} (5.22)
\]

This term will then cancel with the first term of the proposal ratio given by equation 5.19. The same terms appear inverted in the death move equations and will therefore cancel out in a similar manner.

Combining the prior, proposal and likelihood ratios, the acceptance term for a birth step is:

\[
\alpha = \min \left[ 1 - \prod_{i=1}^{n_c+1} p(T'_i | \psi) \cdot p(t'_i | \varphi) \cdot p(k'_i) \cdot \prod_{j=1}^{n_b} \frac{p(d_j | m'_u(j), k'_v(j), \psi)}{p(d_j | m_u(j), k_v(j), \varphi)} \cdot \frac{d_{n_{C+1}}}{b_{n_C}} \right] ,
\]

\[
\times \left[ \prod_{i=1}^{n_c} p(\theta_i) \right] \cdot \prod_{i=1}^{n_c+1} p(\theta'_i) \hspace{1cm} (5.23)
\]

The acceptance term for a death move is similar to that for a birth. In general each ratio term in the birth move acceptance term is inverted. The proposal probabilities for
Chapter 5. Spatial trends

98

a death move are different if the algorithm reaches the maximum number of points. For
the death step in which one of the Voronoi centres is deleted (with all the other remaining
centres constant) the proposal ratio is given by the inverse of that for the birth move:

\[
\frac{q(C | C')}{q(C' | C)} = \frac{b_{nC-1}}{d_{nC}} \times \frac{1/(\Delta x \Delta y)}{1/(nc)}. \tag{5.24}
\]

In general the ratio \(b_{nC-1}/d_{nC}\) is equal to one but takes the value \(1/6 \cdot 1/5\) when the number
of centres reaches the maximum. This proposal ratio is needed to satisfy detailed balance
as it takes account of not being able to choose a birth move at this stage. The general
death move acceptance probability is given by

\[
\alpha = \min \left[ 1, \prod_{i=1}^{n_i} \frac{p(T'_i | \varphi) \cdot p(t'_i | \varphi) \cdot p(k'_i)}{p(T_i | \varphi) \cdot p(t_i | \varphi) \cdot p(k_i)} \cdot \prod_{j=1}^{n_j} \frac{p(d_j | m'_{v(j)}, k'_{v(j)}, \varphi)}{p(d_j | m_{v(j)}, k_{v(j)}, \varphi)} \cdot \frac{b_{nC-1}}{d_{nC}} \right]. \tag{5.25}
\]

For a move or perturb, or a GST history update the proposal probability ratio of
equation (5.24) is always equal to one and so can be omitted. The acceptance term is then
calculated according to:

\[
\alpha = \min \left[ 1, \prod_{i=1}^{n_i} \frac{p(T'_i | \varphi) \cdot p(t'_i | \varphi) \cdot p(k'_i) \cdot p(\theta_i)}{p(T_i | \varphi) \cdot p(t_i | \varphi) \cdot p(k_i)} \cdot \prod_{j=1}^{n_j} \frac{p(d_j | m'_{v(j)}, k'_{v(j)}, \varphi)}{p(d_j | m_{v(j)}, k_{v(j)}, \varphi)} \cdot \frac{b_{nC-1}}{d_{nC}} \right]. \tag{5.26}
\]

and for a heat flux and \(T_{eq}\) update the prior and proposal terms dependent on \(\theta, T, t\)
and \(k\) can be omitted so that the acceptance term in this case is the ratio of the likelihood
values:

\[
\alpha = \min \left[ 1, \prod_{j=1}^{n_j} \frac{p(d_j | m'_{v(j)}, k'_{v(j)}, \varphi)}{p(d_j | m_{v(j)}, k_{v(j)}, \varphi)} \right]. \tag{5.27}
\]
Chapter 5. Spatial trends

5.5 Synthetic case

In this first example an arbitrary partition structure is set up on a square of dimensions 1×1, by selecting 3 points as the centres. 10 points in the square were selected as the locations of the synthetic borehole profiles (figure 5.6). The GST histories in each partition were based on 3 well known surface air temperature reconstructions (Mann et al., 1999, Crowley and Lowery, 2000, Moberg et al., 2005). 600 annual temperature values to 1980 (1979 for Moberg et al., 2005) were first smoothed with a low pass filter for clarity, see

Figure 5.6: True model set-up for the synthetic test case. Borehole locations are given by crosses, the partition boundaries show how the profiles are grouped according to the applied surface GST history.

Figure 5.7: Surface temperature reconstructions for the NH by Crowley and Lowery (2000), Mann et al. (1999), Moberg et al. (2005).
Figure 5.8: Temperature histories modified from figure 5.7 to give the 3 GST histories used as the true forward model for the synthetic data case.

The resultant temperature histories have then been modified to give markedly different trends over the 600 year time period and are shown in figure 5.8. The temperature profiles were calculated at 2.5m depth intervals to a maximum depth of 500m with 600 1 year timesteps using the finite element model of section 5.3.1. Each profile was degraded with normally distributed random noise with a standard deviation of 0.1K. The model set up (figure 5.6) shows how the 3 different GST histories have been applied to the 10 synthetic profiles. For simplicity all of the profiles were initialised with a heat flux of 60mWm$^{-2}$ and an equilibrium surface temperature of 9.0°C.

The Bayesian Partition Modelling (BPM) algorithm was run for 80,000 iterations with 3500 iterations in each run of the secondary rj-MCMC algorithm, the first 500 of which were discarded each time as burn-in. The model was initialised with 1 partition and the secondary algorithm was used to generate an initial GST history for this partition, with the $q_0$ and $T_{eq}$ values initialised to the secondary rj-MCMC sample means. The algorithm then progresses as described in the previous section.

The resulting samples of all of the model parameters are used to generate posterior probability distributions. The algorithm was found to converge on the true partition
In figure (5.9) the 2D posterior distribution of the inferred partition boundaries is shown. It is clear that this distribution is concentrated around the boundaries of the true partition model (figure 5.6). In figure (5.10) the evolution of the number of partitions with
rj-MCMC iterations together with the likelihood × prior value (proportional to the posterior probability value) is shown. Although the algorithm has sampled 4 partitions, the preferred model has 3 partitions (with a high probability). This is because the introduction of extra partitions results in lower values for the posterior. This is the natural parsimony feature of Bayesian inference as described in section 5.3.3, such that the improved data fit (greater likelihood) is counteracted by the reduction in the value of the prior term, as the number of parameters increases. Figure 5.11 shows the conditional posterior distributions for the 3 temperature histories derived from the mode partition structure, which is equal to the
true model setup. The true GST histories are shown for comparison in dashed lines. For each partition the posterior mean GST as inferred by the algorithm matches well with the true GST history.

Having demonstrated the Bayesian partition method on synthetic data the BPM algorithm is now applied to the 23 UK borehole data sets described earlier.

5.6 UK borehole dataset

5.6.1 Data sources

![Figure 5.12: Locations of the 23 boreholes used in this study. The maximum temperature measurement depth at each borehole is indicated proportionally by the diameter of the circle marker. The deepest is J (Morley) at 823m and the shallowest is U (Mount) at 261m. Reconstructions (Huang et al., 2000) from these boreholes (excluding borehole O).]

In the real data case 22 boreholes have been taken from the Huang and Pollack (1998) database and 1 other has been provided by the British Geological Survey (Rollin, 1987). Previous GST reconstructions from the 22 boreholes have been derived by Huang et al. (2000) and are used in hemispheric and global estimates of surface temperature changes. The 22 borehole locations and the individually derived reconstructions are shown in figure 5.12 (left and right panel respectively). The authors emphasise that these individual reconstructions are not necessarily optimal as the methods they used have been designed for consistency in analysing 837 worldwide borehole profiles rather than for deriving optimal individual reconstructions. For comparison figure 5.13 shows the mean of these 22 reconstructions with the Central England instrumental temperature series (CET) and Lamb’s
Figure 5.13: Huang et al. (2000) mean reconstruction from UK data compared with Central England temperatures and estimated pre-1659 temperatures of Lamb (1965, 1982).

documentary temperature reconstruction for earlier periods. The Huang et al. (2000) average appears to underestimate variations from before around 1750. This may be due to the averaging process, or due to noise in the reconstructions. It was noted in chapter 1.2 that Jones (1999) found good agreement between Huang’s reconstruction average and the CET. However, in that analysis Jones (1999) additionally included 4 borehole reconstructions from Ireland, all of which show much larger cooling into the past (up to 3.5°C over 500 years). The effect of these 4 reconstructions is then to reduce the pre-1750 average reconstructed temperatures. The pitfalls of averaging reconstructions have been described earlier in this chapter, but this example provides further evidence that this process can yield undesirable, or at least variable results.

Table 5.1 summarises the 23 data sets used, giving the maximum depth of temperature measurements, the range of depths of conductivity measurements, the borehole longitude and latitude and the date of logging. The heat flux and equilibrium surface temperatures given in the table, are the starting values used in the algorithm. The spatial domain is chosen to be a square with south west and north east vertices at (longitude, latitude) (-9°,48°) and (3°,60°) respectively. This domain is purposefully larger than the area enclosed by the boreholes so that the spatial component of the overall model is not prone to edge effects (Blackwell and Møller, 2003).

As shown in table 5.1 there is a reasonable amount of thermal conductivity data from
Table 5.1: Borehole summary information for UK dataset.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>Depth (m)</th>
<th>Cond. z-range Long.</th>
<th>Lat.</th>
<th>Log date</th>
<th>q0 (mWm(^{-2}))</th>
<th>T(_{eq}) ((^{\circ})C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Withycombe</td>
<td>262</td>
<td>16-262</td>
<td>-3.37</td>
<td>50.65</td>
<td>1983</td>
<td>52.9</td>
</tr>
<tr>
<td>B Venn</td>
<td>307</td>
<td>18-305</td>
<td>-3.32</td>
<td>50.71</td>
<td>1984</td>
<td>57.1</td>
</tr>
<tr>
<td>C Chard</td>
<td>289</td>
<td>37-289</td>
<td>-2.93</td>
<td>50.85</td>
<td>1984</td>
<td>50.4</td>
</tr>
<tr>
<td>D Seabarn</td>
<td>420</td>
<td>18-415</td>
<td>-2.53</td>
<td>50.62</td>
<td>1979</td>
<td>61.2</td>
</tr>
<tr>
<td>E Worcester</td>
<td>298</td>
<td>33-298</td>
<td>-2.2</td>
<td>52.22</td>
<td>1984</td>
<td>43.4</td>
</tr>
<tr>
<td>F Chalgrove</td>
<td>323</td>
<td>91-322</td>
<td>-1.05</td>
<td>51.66</td>
<td>1984</td>
<td>51.7</td>
</tr>
<tr>
<td>G Tydd</td>
<td>294</td>
<td>51-295</td>
<td>0.12</td>
<td>52.74</td>
<td>1984</td>
<td>56.6</td>
</tr>
<tr>
<td>H Stowlangtoft</td>
<td>277</td>
<td>13-276</td>
<td>0.85</td>
<td>52.28</td>
<td>1984</td>
<td>35.9</td>
</tr>
<tr>
<td>I Crewe</td>
<td>296</td>
<td>53-296</td>
<td>-2.47</td>
<td>53.09</td>
<td>1984</td>
<td>58.6</td>
</tr>
<tr>
<td>J Morley</td>
<td>823</td>
<td>10-830</td>
<td>-1.29</td>
<td>52.76</td>
<td>1987</td>
<td>56.6</td>
</tr>
<tr>
<td>K Cleethorpes</td>
<td>290</td>
<td>80-290</td>
<td>-0.03</td>
<td>53.54</td>
<td>1985</td>
<td>72.2</td>
</tr>
<tr>
<td>L Shipston</td>
<td>549</td>
<td>9-547</td>
<td>-1.17</td>
<td>54.02</td>
<td>1987</td>
<td>59.9</td>
</tr>
<tr>
<td>M Thornton</td>
<td>287</td>
<td>42-288</td>
<td>-3.02</td>
<td>53.89</td>
<td>1984</td>
<td>52.2</td>
</tr>
<tr>
<td>N Clitheroe</td>
<td>341</td>
<td>81-301</td>
<td>-2.37</td>
<td>53.86</td>
<td>1985</td>
<td>45.1</td>
</tr>
<tr>
<td>O * Wray</td>
<td>303</td>
<td>100-301</td>
<td>-2.56</td>
<td>54.09</td>
<td>1986</td>
<td>40.2</td>
</tr>
<tr>
<td>P Shap</td>
<td>301</td>
<td>10-300</td>
<td>-2.68</td>
<td>54.47</td>
<td>1983</td>
<td>73.5</td>
</tr>
<tr>
<td>Q Skiddaw</td>
<td>265</td>
<td>10-281</td>
<td>-3.06</td>
<td>54.67</td>
<td>1983</td>
<td>125.4</td>
</tr>
<tr>
<td>R Silloth</td>
<td>340</td>
<td>48-340</td>
<td>-3.37</td>
<td>54.88</td>
<td>1982</td>
<td>53.1</td>
</tr>
<tr>
<td>S Cairngorn</td>
<td>282</td>
<td>10-296</td>
<td>-3.67</td>
<td>57.14</td>
<td>1983</td>
<td>75.9</td>
</tr>
<tr>
<td>T Ballater</td>
<td>290</td>
<td>10-298</td>
<td>-2.99</td>
<td>57.07</td>
<td>1983</td>
<td>75.6</td>
</tr>
<tr>
<td>U Mount</td>
<td>261</td>
<td>10-260</td>
<td>-2.75</td>
<td>57.0</td>
<td>1983</td>
<td>69.9</td>
</tr>
<tr>
<td>V Bennachie</td>
<td>282</td>
<td>10-294</td>
<td>-2.55</td>
<td>57.28</td>
<td>1983</td>
<td>81.5</td>
</tr>
<tr>
<td>W Ballymacilroy</td>
<td>493</td>
<td>61-500</td>
<td>-6.33</td>
<td>54.79</td>
<td>1980</td>
<td>59.5</td>
</tr>
</tbody>
</table>

* Not previously selected by Huang and Pollack (1998).

Figure 5.14: Given temperature data spaced at 5m depth intervals and arbitrarily spaced conductivity data a conductivity model is calculated at 1m intervals and then linearly interpolated to the 5m spacing.

For depth ranges where no conductivity measurements are available the nearest measured value is used. This is illustrated for an example borehole in figure 5.14.

Since the range of dates at which the 23 boreholes have been logged is small (1979-1987), this is not taken into account in this model. Thus all boreholes are assumed to be
logged at 1987. Because of the low resolution of the GST reconstructions this assumption should have a small overall effect on the reconstructed temperatures.

5.6.2 Sampling and posterior distributions

The reconstruction length is set to 756 years using $63 \times 12$ year timesteps in each 1D finite element model. This length of the reconstruction period is chosen to reflect the time over which GST reconstructions can be made for boreholes of 500m depth (as in the synthetic examples in chapter 4.4.1). Many of the boreholes in this dataset are considerably shorter with maximum depth ranges of 250m-350m. In these cases the prior can be expected to become dominant so that the inferred posterior GST history will show zero change where the data do not support otherwise.

The BPM algorithm is initialised with one partition and by using the secondary rj-MCMC algorithm to find a suitable GST history for this initial partition. The $q_0$ and $T_{eq}$ values are also initialised to the secondary rj-MCMC sample means derived for this single partition. The algorithm was run for 120,000 iterations. The covariance matrices used in equation (5.12) are assumed to be diagonal, with the standard deviation of the data error taken to be the same for each borehole. A value of 0.1K is used a so-called 'loose inversion', in order to account for large errors in the data. A more conservative estimate may otherwise lead to spurious variations in the reconstructed temperatures. This choice is also supported by the joint inversion examples using real data from the previous chapter, for which the noise standard deviation value of 0.1K led to much more consistent and realistic GST histories.

5.6.3 Uniform prior on the number of partitions

Figure 5.15 depicts the progress of the algorithm in the first case for which a uniform prior on the number of Voronoi centres is used. The method shows a clear preference for 9 partitions of the borehole datasets. There is a very small probability of sampling 10 partitions as evidenced by the excursion at just before 60,000 iterations. The partition structure settled on the mode configuration after 4700 iterations and here burn-in is assumed to last 15,000 iterations.

In figure 5.16 the posterior pdf of the partition boundaries is shown. This has been
calculated for every 50th sample from the posterior over the 120,000 iterations, not including the first 15,000 iterations. The posterior here shows how the boreholes are grouped in the 9 partitions on which the rj-MCMC algorithm has converged. The partitions are labelled by Roman numerals so that the inferred GST reconstructions can be identified. The two largest partitions, numbers II and VII, are inferred to contain 7 and 5 boreholes respectively, whilst the remaining partitions contain either 1 or 2 boreholes only. Due to the larger number of boreholes in partitions II and VII, the inferred GST histories for these two partitions are expected to represent more robustly the past climate, and so these are shown in figure 5.17. The 95% Bayesian credible limits are indicated by the grey shaded regions and give an indication of the level of uncertainty surrounding the mean inferred trends. In both case these trends show a warming from the time period of around AD 1600 or before, to the present day with indication of a cooling from the start of the reconstruction period in partition II. For partition II the warming from 1650 to 1987 is around 1.0°C whereas for partition VII the warming is much less at 0.4°C. The flatter part of the GST reconstruction for this partition may be attributable to the shallower depths of the boreholes. In figure 5.18 the posterior means for these two partitions as well as partition V are compared with the CET record, these are shown as deviations from the 1951-1979 mean. Partition V is included because an almost identical GST trend is inferred as for

Figure 5.15: Posterior value and the number of partitions as a function of the rj-MCMC iterations. The burn-in is assumed to end at 15,000 iterations.
partition II. In this figure the inferred GST histories for partitions II and V show reasonable agreement with the CET record, although it is impossible to estimate a trend from the CET prior to 1750. The temperature minimum at around 1650 is in agreement with trends from a variety of Northern Hemisphere multi-proxy reconstructions (e.g. Moberg et al., 2005, Hegerl et al., 2007). However, the magnitude of warming varies between 0.4°C and 1.0°C over the reconstruction length, which indicates that even this subset of the data provides a poor constraint on the magnitude of temperature change over this time period.

In figure 5.19 the mean GST reconstructions for all 9 partitions are shown together. This ensemble of GST histories shows marginally less variability than the equivalent reconstructions of Huang et al. (2000) shown in figure 5.12. The GST histories with larger numbers of the partitions, shown in thick black lines, show more realistic amplitudes of past variations, compared with many of the GST histories which are inferred from singly occupied partitions. This indicates that the borehole data which have been inferred to lie singly in separate partitions are likely to be influenced by non-climatic factors. Furthermore, factors causing the large differences between II and VII (the larger partitions)
Figure 5.17: Posterior mean GST histories for the two partitions with the largest numbers of boreholes. The posterior 95% credible intervals are indicated by the grey shaded regions.

Figure 5.18: Comparisons of the two largest partitions (II and VII), partition V and the Central England temperature record.

must be systematic because of the larger number of boreholes which are inferred for these partitions.

5.6.4 Poisson prior constraining the number of partitions

In order to explore the influence of the prior pdf in this problem, a Poisson prior on the number of partitions was also used. In this, the expected number of partitions was set to 1, as the area covered by the boreholes is small enough to be considered a single climatic zone. This assertion is supported by the instrumental temperature records for the UK
Figure 5.19: The posterior mean GST histories for all 10 partitions. The reconstructions are labelled corresponding to figure (5.23) and the two partitions with more than 2 boreholes are shown by the darker lines.

Figure 5.20: Locations of MetOffice historical instrumental data stations.

which show similar trends over the past 150 years, shown in figures 5.20 and 5.21. A truncated Poisson pdf is used as the maximum number of partitions is set to equal the number of the boreholes. The truncated Poisson pdf is given by
Figure 5.21: The 5 longest instrumental records from the Met. Office data set (UKMO, 2006) and the Central England temperature series (Parker et al., 1992, Manley, 1974) as deviations from the 1971-2000 annual mean and decadally smoothed, unless otherwise noted.

Figure 5.22: Posterior value and the number of partitions as a function of the rj-MCMC iterations. The burn-in is assumed to end at 40,000 iterations.

\[ p(n_c) = \frac{1}{\sum_{i=1}^{n_B} \frac{\lambda^i}{i!}} \frac{\lambda^{n_c} e^{-\lambda}}{n_c!} \]  
\hspace{1cm} (5.28)

where \( \lambda \) is the expected value, \( n_c \) is the number of partitions and \( n_b \) is the number of boreholes. The first term can be ignored as it is independent of \( n_c \) and so will always cancel in the acceptance probability. The second term will cancel except in a birth or death proposal, in which case taking \( \lambda=1 \), the ratio of the terms will be \( 1/(n_c+1) \) for a birth and \( n_c \) for a death move.

For this Poisson prior case, the evolution of the posterior value and the number of
partitions is shown in figure (5.22), and the posterior distribution of the partition boundaries is shown in figure (5.23). The data show a very clear preference for 8 partitions with no excursions to higher or lower dimensions after burn-in. Four of the partitions shown in figure (5.23), labelled I, II, V and VI, contain 6, 6, 5 and 2 boreholes respectively. The temperature histories inferred in these 4 partitions can be taken as the most robust because of the inferred agreement between more than one borehole profile in each of these partitions (the remaining partitions contain only 1 borehole each). Therefore in figure (5.24) the posterior mean GST history and the 95% credible interval for each of these partitions is shown. All 4 of the posterior pdfs of the reconstructed GSTs show warming although there is again, large variability in both the magnitude and timing. Partitions II and V show very strong agreement, with both depicting evidence for a cool period centred on AD 1600-1650 and 0.7-0.9°C warming to the 1987. The cool period appears to have occurred somewhat later in partition II which is located further south. The data in both of these partitions indicate that a warmer period preceded the temperature minimum of AD
Figure 5.24: Posterior mean GST histories for the four partitions with the largest numbers of boreholes. The posterior 95% credible intervals are indicated by the grey shaded regions. The trends have been shifted along the temperature axis for clarity: I -1.0°C, V +0.5°C, VI +1.0°C

1600-1650. The posterior GST history for partition I shows a very different trend, with only 0.2°C warming, almost all of which is inferred to have occurred before AD 1400. The trend for partition VI shows around 0.6°C warming only since 1900 with the preceding temperature variations most likely dominated by the prior (centred on zero change) as the 2 boreholes in this partition are both less than 300m deep.

In figure (5.25) the posterior mean reconstructed GST histories for these 4 partitions are compared with a 50-year smoothed version of the CET record (Manley, 1974, Parker
et al., 1992). The 5 temperature histories are plotted with respect to deviations from the 1950-1979 mean. The reconstructed temperature trends for partitions II and V show good agreement with the CET record although there may be slight overestimation of the warming. The histories for partitions II and V are also commensurate with a Medieval
Warm Period (e.g. Lamb, 1982). However, partition I shows a different overall trend to all 3 of the other large partitions and the CET record. Partition I is also the largest inferred in the model and so this again indicates that some systematic error is biasing the 6 boreholes in this partition. Partition VI shows warming only during the 20th century and this is in conflict with the CET record.

The similarity of the reconstructed temperature trends across these two larger partitions (II and V) which are spread across a large part of the examined area, indicates that the inferred variations may be robust. However, since systematic errors appear to be important in partitions I and VII there may also be some systematic error affecting the GST histories partitions II and V. This possibility will be difficult to ignore without resorting to a more detailed study of the present and past conditions at each borehole. These effects could include historical vegetation clearance for example, or even similar topographic or hydrological conditions (e.g. the boreholes could all be located on slopes of similarly sized hills, leading to topographically induced groundwater flow near to the surface.)

The partition scheme has grouped the data according to similar GST trends and so boreholes inferred to lie singly in separate partitions are likely to be heavily influenced by local noise factors. This is the case here for boreholes D, F, R and W (partitions III, IV, VII and VIII). For comparison the posterior mean GST histories for all 8 partitions are shown in figure (5.26). The inferred GST histories for these separated partitions display larger amplitude changes than those inferred from the larger partitions and it is clear that non-climatic influences are significant for the data from many boreholes. The inferred GST reconstructions for the four larger partitions show 3 distinct GST trends only one of which is consistent with the CET record. It is therefore again concluded that these 23 datasets provide a poor constraint on past climate in the region.

5.7 Discussion and conclusions

In this chapter a novel method for inferring both spatial and temporal trends in ground surface temperatures jointly inferred from collections of borehole temperature profiles has been demonstrated. The efficacy of this Bayesian Partition modelling method has been
Chapter 5. Spatial trends

tested with realistic synthetic data, for which the algorithm is able to correctly group borehole profiles according to the applied GST history. This method therefore allows the data to determine the optimum grouping for joint inversion which takes account of the relative locations of the profiles.

In the synthetic case presented, the Bayesian Partition algorithm demonstrates the natural parsimony which allows the rj-MCMC algorithm to preferentially sample simple models which in this case correspond with the true model used. In other synthetic experiments the algorithm has converged on partition structures for which partitions defined in the true model are merged in the posterior distribution. This happens where the data can be fit to an adequate degree with the same GST history. The tendency towards simpler models is a crucial feature, as it allows more useful models of the underlying trends in past GSTs. This is as opposed to simply optimising the fit separately at each borehole, which can lead to a more confused and possibly misleading set of GST reconstructions.

A first case study has been made using a dataset of 23 boreholes located in the United Kingdom. Using this dataset a previously large range of GST histories has been slightly reduced, by examining the support from the data for independent temperature histories. The preliminary results indicate that for this dataset, the data favour a partition structure with 8 or 9 independent GST trends. However, examination of instrumental data covering the period 1850-present from the Meteorological Office Historical Instrumental Station dataset (figures 5.20 and 5.21) indicates that the long term changes in surface temperature are very similar across the whole of the country. The posterior mean GSTs for the larger partitions show good agreement with each other and thus support the idea of a single GST history for the UK, with an inferred warming of between 0.7°C and 1.0°C. However, in both the examples presented, large partitions are inferred which show clearly contrasting GST histories and which are mostly inconsistent with the CET record. The results therefore strongly indicate that, in a 1D conduction dominated regime, these data do not provide a robust signal of past ground surface temperatures. Therefore these 23 datasets should not be used for future climate reconstruction purposes without further site analyses and more advanced forward modelling.

However, this algorithm is fairly sensitive to the starting values used for the basal heat flux and equilibrium temperature at each site. In this work suitable values have been found
by running a preliminary MCMC run for which only these two quantities are updated. In general it would be desirable for the algorithm to be able to explore the model space sufficiently that the initial values are less important. Introducing more informative prior information is method of reducing size of the model space and thus allowing the algorithm to explore reasonable models more efficiently. This prior information could take the form of an expected temperature trend (GST history) over time based on instrumental or proxy data. Additionally more informative prior constraints could be applied to each heat flux and equilibrium temperature value. A more general method for increasing the efficiency of the model space search is simulated tempering (Marini and Parisi, 1992, Geyer and Thompson, 1995) which samples from a series of modified posterior pdfs which are parameterised in terms of a temperature value, where higher temperatures allow much more efficient mixing of the MCMC algorithm by effectively flattening out the pdf. A simpler method for increasing the efficiency of the model space search is to set the algorithm to resample a certain partition (i.e. re-run the secondary rj-MCMC algorithm) with a certain probability (rather than drawing from previously calculated samples). This probability can be set to 1% and leads to improved mixing of the main rj-MCMC chain. This is because the values of the heat flow and equilibrium temperature \(q_0\) and \(T_{eq}\) which may have changed between proposals for a particular partition are taken account of when the secondary rj-MCMC algorithm is re-run.

A different method for dividing up the space may allow the partitions with similar GST histories (e.g. II and V in the Poisson case), to be parameterised with 1 GST history rather than 2. To achieve this the set of partitions could be parameterised in terms of the coloured polygons rather than Voronoi generating centres, as used here. In this way partitions which are physically separated by data points identified as outliers, could be allowed to have the same colour (or GST history). Andersen et al. (2003) describe in detail a rj-MCMC algorithm for sampling in this manner in the context of a non-linear inverse problem.

Disagreement between the GST signals from the region indicates that most of these data for the UK are likely to be affected by other factors such as land use and topography. A feature of the methodology developed here is that these boreholes can be identified automatically and their influence on the inferred climatic histories can be excluded. In
the future work aimed at finding spatial trends in real data, it would be preferable to use the BPM algorithm to analyse datasets which have been subject to more rigorous quality control. For example Chouinard and Mareschal (2007) analysed 194 borehole temperature-depth profiles from Canada and selected only 28 of these for climate reconstruction purposes.

For simplicity in analysing the results, the inferred GST histories in this chapter have been presented in terms of the posterior mean models and the posterior 95% credible intervals. However, the actual posterior samples are the real results and these would be of most use in future work, since they could be used in future sampling schemes. Since the results from real data here indicate that the data are less useful for climate reconstructions, the posterior distributions of the GST histories are not so useful for such purposes. However, in similar future work it would be beneficial to make both the means and credible intervals as well as the complete family of sampled models available to others.

One possible future development for this field is the use of more sophisticated error analysis. For example, it is likely that underground fluid flow contributes to the temperature-depth data errors, even if only on a small scale (such as the 1m convective cells in the groundwater described in chapter 2.2). The assumptions that the errors are Gaussian and uncorrelated have been assumed in this work and almost all previous borehole-climate studies. However, errors caused by fluid flow will never satisfy these assumptions, since advection will be correlated across certain geological structures (or across the convective cells) and because the errors are systematic. A method for including this information in the error covariance matrix may help with identifying whether a borehole is suitable for climate reconstruction purposes.

The Bayesian Partitioning algorithm is fairly computationally burdensome as it relies on two different rj-MCMC samplers. For example, the real data cases took over 45 hours of computation on a Pentium 4 3.2GHz Linux PC. In order to apply this method to a larger dataset, this algorithm would therefore benefit from parallelisation. Running multiple algorithms would not necessarily improve the efficiency of the model space exploration. However, where proposal choices lead to more than 1 partition being updated in a single iteration, the calculations for each partition could be sent to separate processors.

Finally, the methods presented here could be developed in order to incorporate proxy
data together with the borehole temperatures. Implementing a Bayesian calibration method for the proxy data, the borehole data could serve as a prior (through the heat conduction forward model) on low-frequency variations of the reconstructions from proxy data.
Chapter 6

Transient three-dimensional heat transfer modelling

The majority of methods used for inferring past ground surface temperatures (GST) from borehole data suffer from the restrictive assumption that heatflow is only in the vertical direction. This means that accounting for the effects of the setting or terrain of a particular borehole in the reconstruction of past climate is difficult, and so many borehole temperature profiles cannot be used. Terrain can have a significant impact on the ground thermal regime (Lewis and Wang, 1992, 1998), as the surface energy balance is modified. For example many different factors have an influence on underground temperatures including, vegetation changes, the presence of water bodies, total incident solar radiation, the release of latent heat or from lateral heat flow variations in the ground caused by the variation of the thermophysical values. Many of these processes are complex and as such difficult to simulate numerically without a large amount of site-specific or meteorological data (e.g. Noetzli et al., 2007). Two factors which could be incorporated into a modelling and inversion scheme for general purpose use (i.e. for which meteorological data are not required) are surface topography and subsurface thermophysical variations, in particular of thermal conductivity.

Surface topographic variations cause departures from purely vertical heat flow. The slope of the ground surface and the temperature distribution on this surface can lead to curved isotherms and in extreme cases, nearly horizontal heat flow. The variation of
air temperature with altitude leads to lateral heat flow across hills and around valleys and differences in solar insolation across mountains and hills cause further asymmetries in underground temperature profiles (Blackwell et al., 1980). Kohl (1999) compares a variety of methods for evaluating the subsurface effects of topography in 3D and finds that finite element methods are best suited. Kohl (1999) also demonstrates that 1D inversions for past GSTs of synthetic temperature-depth profiles calculated using a 3D method, show pronounced cooling and reduced warming when the temperature-depth profiles are located at topographic peaks, and the opposite effects for profiles located in topographic troughs. For a sinusoidal topography of amplitude 100m and wavelength of 20km, the topographically induced effect leads to an error in the GST reconstruction (compared with a flat surface) of 1K at 200 years before present (abp) for a step change GST model of +1K at 200 abp and -1K at 100 abp. This effect is clearly of importance when inferring GST histories for the last few hundred years in a range of typical settings.

Variations of thermal conductivity with depth and also laterally are often neglected in inversion of borehole data for past climate. The effects, however, of neglecting to account for these variations can be strong (Shen et al., 1995, Kukkonen and Šafanda, 1996, Clauser et al., 1997). In many real data cases, palaeo-temperatures, topography and sub-surface conductivity have been identified as the dominant influences on subsurface temperatures (e.g. Kukkonen and Šafanda, 1996, Kohl, 1999, Șerban et al., 2001). For example analysis of two sets of 107 borehole profiles in 2 parts of Canada show topography to be the dominant influence in 28 of these (Chouinard and Mareschal, 2007). However, to date only one study has focused on incorporating these effects into an inverse scheme for reconstructing past GSTs (Kohl and Gruber, 2003). In other examples, Kukkonen and Šafanda (1996) resort to a trial and error 2D forward modelling approach and Kohl (1999) performs data corrections so that 1D inversions can be used. All other GST reconstruction methods rely on the assumption of purely conductive 1D vertical heat flow. As a result much borehole data must be excluded from palaeoclimate work, and for some data the assumption of 1D heat flow may not be valid, leading to spurious GST reconstructions.

In this chapter a 3D transient finite element (FE) heat transfer model is derived and tested so that it may be used in conjunction with an inverse method to infer GST histories. This 3D formulation is a natural extension of the 1D FE forward model used in chapters
Chapter 6. Transient three-dimensional heat transfer modelling

4 and 5. A 3D model has the advantage that heat flow can be considered both vertically and laterally and as such a variety of effects due to the setting of a particular borehole can be accounted for. These include the thermal perturbations due to hills and valleys and also where appropriate other surface effects such as water cover or constructions and buildings. The underground structure can also be considered so that lateral variations and anisotropy of thermal conductivity can be accounted for.

This chapter builds on previous studies with an aim to incorporate the experience gained from the various forward modelling surveys into the process of solving the inverse problem in 3D. This is described using two methods in two subsequent chapters. In the first the Bayesian reversible jump MCMC method of chapter 4 is applied in chapter 7 and in chapter 8 a gradient based optimisation method is demonstrated which relies on the adjoint of the FE forward model. In this chapter, the next two sections, 6.2 and 6.3, contain detailed descriptions of the finite element discretisation for Fourier’s law and the diffusion equation. This is followed by a discussion of the applied boundary conditions, with examples of the effects of this can have on the resultant temperature distributions. In section 6.6 examples are given of transient calculations to estimate for a typical case, the effects of typical subsurface thermal conductivity anisotropy.

6.1 Finite element formulation

The method of finite elements is a numerical technique for efficiently solving partial differential equations or integral equations. The finite element method is a generalisation of both finite difference and finite volume methods and involves discretisation of the continuous equations using basis functions which interpolate between the nodes or discretisation points. The method provides appropriate approximating functions for solving the Galerkin discretisation of a continuous equation. It can be shown for the Galerkin representation and hence for finite element method that as the number of discretisation points or nodes tends to infinity, the approximate solution will converge to the exact solution.

In this work linear basis functions are used in both the time and space domains and a theta time stepping method is formulated which is a combination of implicit and explicit differencing schemes. The combination is controlled by the value of theta, if theta is equal
to 1/2, the method is the familiar Crank-Nicholson. The boundary conditions are applied at the upper and lower surfaces, with zero gradients at the sides boundaries. For the upper surface a Robin boundary condition is applied and this accounts for heat transfer between the air and the ground. The coupling between the two is controlled by the factor $\beta$. In all simulations presented, $\beta$ is kept constant and takes the value of 5.0. See Stieglitz and Smerdon (2007) for time-variant $\beta$ in 1D forward modelling examples.

The finite element grid upon which the equations are solved is generated using GEM, a mesh generation package used for the Imperial College Ocean Model. An example of a mesh generated by this programme is shown in figure 6.1. In the examples presented, the nodal spacing is similar magnitude over the whole space with more horizontal divisions close to the borehole at the centre. For larger simulations the refinement could be varied in order to keep computation times reasonable or to resolve boundaries between known geological formations.

The temperature field in the volume is approximated by the nodal temperature values:
Figure 6.2: (a) 1D linear basis functions for element $\xi$, $N_1(\xi) = (1-\xi)/2$ and $N_2(\xi) = (1+\xi)/2$. (b) The combination of the two basis functions to give the finite element function $\bar{T}$.

\[ T(x,t^n) = \sum_{j=1}^{N} N_j(x)T^n_j \]  

(6.1)

where $N_j$ are a set of piece-wise linear basis functions. These functions take a tri-linear form and so that for a vertex placed at $(\xi_1, \xi_2, \xi_3)$, the basis function takes the form $\frac{1}{8}(1 - \xi_1)(1 - \xi_2)(1 - \xi_3)$. These are illustrated for the 1D case in figure 6.2. For 3D example the shape functions take the form:

\[ N_1 = (1 - \xi_1)(1 - \xi_2)(1 - \xi_3)/8 \]  

(6.2)

\[ N_2 = (1 + \xi_1)(1 - \xi_2)(1 - \xi_3)/8 \]  

(6.3)

\[ N_3 = (1 + \xi_1)(1 + \xi_2)(1 - \xi_3)/8 \]  

(6.4)

\[ N_4 = (1 + \xi_1)(1 + \xi_2)(1 + \xi_3)/8 \]  

(6.5)

\[ N_5 = (1 - \xi_1)(1 + \xi_2)(1 - \xi_3)/8 \]  

(6.6)

\[ N_6 = (1 - \xi_1)(1 + \xi_2)(1 + \xi_3)/8 \]  

(6.7)

\[ N_7 = (1 - \xi_1)(1 - \xi_2)(1 + \xi_3)/8 \]  

(6.8)

\[ N_8 = (1 + \xi_1)(1 - \xi_2)(1 + \xi_3)/8 \]  

(6.9)

where $\xi_1, \xi_2, \xi_3$ are the local co-ordinates on the hexahedral element, so that each varies from -1 to 1 over the length of the edges of that element (Piggot, 2005).
Figure 6.3: (a) The model setup used in the 3D simulations, where $T_{air}$ indicates the air temperatures. In the transient simulation it represents the past climate in which we are interested and in the steady state simulation this quantity is denoted by $T_{eq}$. $k$, $c$ and $\Gamma$ are the thermal conductivity, heat capacity and density respectively and these may vary over the volume. The additional parameter is the basal heat flux, $q_0$ applied to the base of the model. (b) The surface topography profile used in the synthetic examples with non-flat upper boundary.

6.2 Steady state equations

For the initial steady state calculation the equation to be solved is Fourier’s law:

$$\nabla \cdot (k \cdot \nabla T) = -q$$

(6.10)

where $k$ is the thermal conductivity and $q$ is heat flow. The boundary conditions are then defined by two constants: the surface equilibrium temperature $T_{eq}$ and the basal heat flux $q_0$:

$$q = \beta(T - T_{eq}) |_{\Gamma_{\infty}}$$

(6.11)

$$-k \cdot \nabla T = q_0 |_{\Gamma_{b}}$$

(6.12)

where $\Gamma_{b}$ denotes the lower surface and $\Gamma_{\infty}$ denotes the upper surface in contact with the air. This model setup is shown schematically in figure 6.3.

In order to solve this equation by finite elements it is first necessary to consider the
variational formulation of the problem. This requires the introduction of a set of trial functions, \( \tau \), and weighting functions, \( \omega \). The strong variational formulation is to find \( T \) such that:

\[
\int_{\Omega} \left[ \nabla \cdot (k \cdot \nabla T) + Q \right] W \, d\Omega = 0 \quad (6.13)
\]

where \( T \) and \( W \) are from the sets \( \tau \) and \( \omega \) respectively. If we do not assume that all the trial functions satisfy the boundary conditions then we can re-write this equation to include the boundary conditions:

\[
\int_{\Omega} \left[ \nabla \cdot (k \nabla T) + Q \right] W \, d\Omega + \Psi \int_{\Gamma_1} [T - f] W \, d\Gamma + \phi \int_{\Gamma_2} [k \frac{\partial T}{\partial n} + \chi] W \, d\Gamma = 0 \quad (6.14)
\]

where \( \Psi \) and \( \phi \) are arbitrary constants. By manipulating equation 6.14 a weak formulation can be derived. Assuming the functions involved are sufficiently smooth. Using the relation:

\[
[\nabla \cdot (k \cdot \nabla T)]W = \nabla \cdot [W k \cdot \nabla T] - k \cdot \nabla T \cdot \nabla W \quad (6.15)
\]

and the divergence theorem gives:

\[
\int_{\Omega} k \cdot \nabla T \cdot \nabla W \, d\Omega = \int_{\Omega} Q W \, d\Omega + \int_{\Gamma_1} W k \frac{\partial T}{\partial n} \, d\Gamma - \int_{\Gamma_2} W \omega \, d\Gamma + \psi \int_{\Gamma_1} [T - f] W \, d\Gamma \quad (6.16)
\]

when \( \phi \) is taken as \(-1\). If we require the trial set \( \tau \) (of \( T \)) to satisfy the boundary condition, the \( T-f \) term can become zero and if we require the trial set \( \omega \) (of \( W \)) to satisfy boundary condition then this can be re-written:

\[
\int_{\Omega} k \cdot \nabla T \cdot \nabla W \, d\Omega = \int_{\Omega} Q W \, d\Omega - \int_{\Gamma_2} W \omega \, d\Gamma \quad (6.17)
\]
Chapter 6. Transient three-dimensional heat transfer modelling

This is then the weak formulation from which the finite-element solution can be derived.

The trial sets of $T$ and $W$ are now assumed to satisfy the boundary conditions. The temperature and weighting functions are now written in terms of shape or basis functions, $N_i$:

$$
\tau^{(M+1)} = (T = \sum_{j=1}^{(M+1)} T_j N_j) \quad (6.18)
$$

$$
\omega^{(M+1)} = (W = \sum_{j=1}^{(M+1)} b_j N_j)
$$

with the basis functions as in equations 6.2-6.9. Substituting equations 6.18 into equation 6.17, results in a matrix relationship (e.g. Lewis et al., 1996):

$$
K T = Q - q \quad (6.19)
$$

here $T$ are the temperatures at the nodes and $q$ are the heat flow values at the nodes and $Q$ accounts for heat production within the volume (here set to zero). The matrix $K$ and vectors $Q$ and $q$ have elements:

$$
K_{ij} = \int_{\Omega} k \cdot \nabla N_j \cdot \nabla N_i \; d\Omega \quad (6.20)
$$

$$
Q_i = \int_{\Omega} \hat{Q} N_i \; d\Omega + \psi \int_{\Gamma_1} [\hat{T} - \hat{f}] N_i \; d\Gamma \quad (6.21)
$$

$$
q_i = \int_{\Gamma} \hat{q} N_i d\Gamma \quad (6.22)
$$

where $\hat{\cdot}$ denotes nodal values and for which $\hat{T} = \hat{f}$ so that the second term in $Q_i$ disappears. In this work the steady state solution, $T_{st}$ is then used as the initial condition for the transient finite-element simulation.
Chapter 6. Transient three-dimensional heat transfer modelling

6.2.1 Model validation

The steady state finite element model can be tested by calculating the geothermal profile for a cuboid volume with constant thermal conductivity over the volume for a given basal heat flux and surface temperature. Since both the finite element basis functions and the true (analytical) solutions are linear functions of depth, the solutions from the two methods should correspond exactly. In figure 6.4 the FE solution is shown for boundary conditions of basal heat flux of 60\,mWm\(^{-2}\) and upper surface temperature 0°C. In this case, the differences between the finite element solution and values calculated using Fourier’s Law are negligible and of the order \(1\times10^{-14}\,\text{K}\).

6.3 Transient finite element solutions

By following a similar procedure as in section (6.2) but starting instead with the time dependent heat conduction equation, a transient finite element formulation can be derived. The diffusion equation is
Chapter 6. Transient three-dimensional heat transfer modelling

\[ \nabla \cdot (k \cdot \nabla T) + Q = \rho c \frac{\partial T}{\partial t} \quad (6.23) \]

subject to the two boundary conditions:

\[ q = \beta (T - T_\infty) |_{\Gamma_\infty} \quad (6.24) \]
\[ -k \nabla T = q_0 |_{\Gamma_b} \quad (6.25) \]

and the initial conditions \( T = T_{st} \), where \( T_\infty \) is the surface air temperature (varying over time), and \( q_0 \) is the basal heat flow. The Galerkin representation (after integration by parts) becomes

\[ - \int \left[ \nabla \cdot k \cdot \nabla T_i N_i + N_i Q + N_i \rho c \frac{\partial T}{\partial t} \right] dV - \int N_i q d\Gamma_q - \int N_i \beta (T - T_\infty) d\Gamma_\infty = 0 \quad (6.26) \]

Now using the approximation \( \hat{T} \) for the temperature values, this equation becomes:

\[ - \int \left[ \nabla \cdot k \cdot \hat{T} N_i \right] dV + \int N_i Q dV - \int N_i \rho c N_j dV \frac{\partial \hat{T}}{\partial t} - \int N_i q d\Gamma_q - \int N_i \beta N_j \hat{T} d\Gamma_\infty + \int N_i 2T_\infty d\Gamma_\infty = 0 \quad (6.27) \]

where there are \( n \) spatial elements. By substituting the shape functions and discretised temperatures this equation can be written in terms of \( T \) and its time derivative:

\[ M \frac{dT}{dt} + KT = f \quad (6.28) \]

In which \( M \) is given by:

\[ M_{ij} = \int_{\Omega} p_{ij} c_{ij} N_j N_i dV \quad (6.29) \]
The upper surface boundary condition is given in $f$:

$$f_\infty = \int_{\Gamma_\infty} \beta (T_\infty - T_{z=0}) N_i \, d\Gamma_\infty$$  \hspace{1cm} (6.30)$$

where $\Gamma_\infty$ denotes the surface exchanging heat with the air. The $\beta T_{z=0}$ term is then transferred to the other side of the equation so that the matrices $K$ and $f$ (including possible radiogenic heating $Q$) become:

$$K = \int [k \nabla \cdot N_j T_i \cdot] \, dV + \beta \int_{\Gamma_\infty} N_i N_j \, d\Gamma_\infty$$  \hspace{1cm} (6.31)$$

$$f_i = \int N_i Q \, dV - \int q N_i \, d\Gamma_q + \beta \int_{\Gamma_\infty} N_i T_\infty \, d\Gamma_\infty$$  \hspace{1cm} (6.32)$$

where $T_\infty$ are the air temperatures used for the Robin boundary condition and $Q$ is heat production within the volume (here set to zero).

The resulting differential equation is then discretised in time by finite difference method, which relates the temperature distribution at time step $m+1$ to the previous step $m$. By defining a parameter $\theta$ for which $0 \leq \theta \leq 1$ explicit and implicit finite differencing schemes (forward and backward) can be combined (e.g. Zienkiewicz and Morgan, 1983, Lewis et al., 1996). In general this scheme takes the form:

$$\frac{u_j^{m+1} - u_j^m}{\Delta t} = \frac{1}{(\Delta z)^2} \left[ \theta \delta^2 \times u + j^{m+1} + (1 - \theta) \delta^2 \times u + j^m \right]$$  \hspace{1cm} (6.33)$$

Applying this to equation 6.28 the theta-method for time-stepping the finite element model is derived:
\[
\frac{M}{\Delta t}\left[\theta(T^{m+1} - T^m) + (1 - \theta)(T^{m+1} - T^m)\right] + \\
K(1 - \theta)T^m + K\theta T^{m+1} = (1 - \theta)f^m + \theta f^{m+1}
\]

(6.34)

and the forcing vector \( f \) is given by:

\[
f_\infty = \int_{\Gamma_\infty} \beta(T_\infty - T_{z=0})N_i N_j d\Gamma_\infty + \int_{\Gamma_b} N_j N_i q_0 d\Gamma_b
\]

(6.35)

where \( \infty \) represents the upper surface, and \( b \) indicates the basal surface of the model. The time-stepping equation can be re-arranged to give:

\[
\left(\frac{M}{\Delta t} + \theta K\right)T^{m+1} + \left(-\frac{M}{\Delta t} + (1 - \theta)K\right)T^m = (1 - \theta)f^m + \theta f^{m+1}
\]

(6.36)

and re-writing in terms of new matrices \( A \) and \( B \):

\[
AT^{m+1} + BT^m = (1 - \theta)f^m + \theta f^{m+1}
\]

(6.37)

where \( A \) and \( B \) are given by:

\[
A = \left(\frac{M}{\Delta t} + \Phi K\right)
\]

(6.38)

\[
B = \left(-\frac{M}{\Delta t} + (1 - \Phi)K\right)
\]

(6.39)

Equation 6.37 then constitutes the transient component of the 3D FE model.
6.4 Computational issues

In the following the finite element mesh is generated over a spatial domain of 1000m × 1000m and with vertical extent which depends on the topography used. For the typical scenario the model depth ranges from 500m to 600m with 80 divisions in the vertical direction and 24 each in the x and y directions. The total number of finite element nodes produced by the mesh generation software is then around 20,000. The time-steps are 1.0 years and in the synthetic examples there are 700 steps, giving a reconstruction length of 700 years. This value is chosen as it is at the limit of how far into the past the method can resolve realistic temperature variations, as demonstrated in chapter 4. Taking a finite difference approach this leads to the ratio

$$\frac{\Delta z^2 / \kappa}{\Delta t} = \frac{6.25^2 / 6.67 \times 10^{-7}}{3.16 \times 10^7} = 1.9$$

which is greater than 1 as generally required, this also holds for the horizontal spacing of 50m. The matrix equations in the full finite element model are solved by the method of conjugate gradients, whilst in the reduced model a partial pivoting Gaussian elimination scheme is used as the matrices are no longer positive definite or symmetric.

6.4.1 Model validation

Solutions from the transient 3D FE model can be compared with those obtained analytically. Assuming a model with a flat surface and with a $\Delta T$ step increase in surface temperature at t before present, the analytical solution (Carslaw and Jaeger, 1959) for a semi-infinite half-space is given by

$$T_t(z) = \Delta T \text{erfc} \left[ \frac{z}{2\sqrt{\kappa t}} \right]$$

where $z$ is depth, $t$ is time since the step change, $\kappa = \frac{k}{\rho c}$ and erfc is the complimentary error function which is given by
Chapter 6. Transient three-dimensional heat transfer modelling

Figure 6.5: The difference between the 3D FE solution and the analytical solution over the simulated volume (500×500×500 m) given a 1°C step increase in surface temperature at 150 years before present. The maximum absolute difference is $5.5 \times 10^{-3}$ °C.

\[
\text{erfc}(\theta) = 1 - \frac{2}{\sqrt{\pi}} \int_0^\theta e^{-x^2} \, dx
\] (6.42)

In this example $\Delta T = 1.0$°C and $t = 150$ years, for FE timesteps of 6 years and with a spatial discretisation of 50m in the x-y plane and 10m in the z (vertical direction) the maximum absolute difference between the FE and analytical solutions is found to be $5.5 \times 10^{-3}$°C. Figure 6.5 shows the variation of error introduced by the FE approximation over a 500m×500m×500m volume. For 1 year timesteps (as used in the synthetic examples below) the maximum error is found to be $3.7 \times 10^{-3}$°C.

6.5 Boundary Conditions

The atmospheric lapse rate varies from 3 to 10K km$^{-1}$ depending on the air moisture content and temperature. The average surface value can be taken as 6.5K km$^{-1}$. This means that for a 100m rise in altitude, the temperature of the air will on average be reduced by 0.65K. This is significant in terms of climatological investigations because it is comparable to the strength of atmospheric warming over the twentieth century for example. The effect of a lapse rate is illustrated in figures (6.6) and (6.7) whereby the same
Chapter 6. Transient three-dimensional heat transfer modelling

Figure 6.6: The underground temperature response to GST forcing using surface air temperature reconstruction of Moberg et al. (2005) with the equilibrium temperature set to 9.0°C and the heat flux set to zero for clarity.

Figure 6.7: The underground reduced temperature response to GST forcing as in figure 6.6 but with the boundary condition modified to take account of an atmospheric lapse rate of 6°Ckm\(^{-1}\).
Chapter 6. Transient three-dimensional heat transfer modelling

3D volume is subject to a ground temperature history based on Moberg et al. (2005). In this synthetic model, the surface topography varies by from 525m to 600m over a distance of 1000m with a central 200m wide plateau at a height of 550m. In the first case the lapse rate effect is ignored and the resultant isotherms lie close to parallel to the ground surface. In the more realistic example whereby the surface temperature boundary condition is modified by a lapse rate of 5Kkm$^{-1}$, the subsurface isotherms are considerably different and demonstrate induced lateral heatflow. These perturbations due to the topography are of a similar magnitude and at similar depths to the perturbations due to varying climate. Therefore a 3D model is required to interpret underground temperatures located in moderately hilly terrains.

In reality the orientation of the ground surface will also have an effect on underground temperatures (Blackwell et al., 1980). Any surface which is predominantly sun-facing will, on average, absorb a larger amount of solar energy, causing the ground to be warmer than on surfaces which are exposed to less solar radiation. The difference between surface ground temperatures on North and South facing slopes can be up to 3°C, causing heat flow which can be almost horizontal in extreme topography. In Blackwell et al. (1980) and Šafanda (1999) the relationship between total solar irradiation and ground surface temperatures is found to be approximately linear, giving a gradient of $4 \times 10^{-3} \, ^\circ C/(kWhm^{-2}yr^{-1})$ whereas Šafanda (1994) and Gruber et al. (2004) assume a constant offset in surface temperature between north and south slopes for extreme gradients. However, more realistic methods have also been utilized for predicting ground temperatures from meteorological data or regional climate model simulations which utilize energy balance models. For example, Noetzli et al. (2007) use output from a regional climate model to drive an energy balance model coupled with a 3D FE model in order to simulate underground temperatures below extreme topographies.

In practice, the quantities required by an energy balance model, such as total insolation, diffuse sky and land radiation and sensible and latent heat fluxes may not be available and so it is likely that a simpler method will find wider applicability. In this work the approach of Kohl (1999) is used and the effects of irradiation differences are ignored. Therefore the ground surface temperatures are modified as a function of altitude only. This is a reasonable assumption for sites where topographic variations are relatively small.
i.e. not corresponding to mountainous terrains. A surface temperature lapse rate of 5 K km\(^{-1}\) (Kohl, 1999) is used which is similar to estimates calculated by extrapolating temperatures from boreholes at various altitudes to the ground surface. Values of 4.7 and 4.0 K km\(^{-1}\) have been found by Kubík (1990) and Šafanda (1999) respectively.

### 6.6 Effects of isotropic and anisotropic thermal conductivity

In the majority of borehole climate inversion methods, the subsurface thermal conductivity is assumed to be laterally homogeneous, and in many studies is assumed to be constant with depth. In many real data cases these assumptions have proven too restrictive and more realistic models should be used. One issue in geothermics is the possible influence of conductivity anisotropy whereby the thermal conductivity varies as a function of the direction. This has been encountered in real data cases (e.g. Clauser and Huenges, 1995, Kukkonen and Šafanda, 1996, Clauser et al., 1997) and presents an obscuring factor which would hinder the recovery of past climate changes from borehole data. Anisotropy of rock properties can exist on scales from microscopic to the scale of geological formations, and can be caused by the orientations of the crystalline structures or by folding and orogeny of the rock formations (Clauser and Huenges, 1995). Here the 3D FE model is used to assess the magnitude of the effect for typical conductivity values.

Consider a dipping geological section (figure 6.8) with anisotropic conductivity so that the thermal conductivity parallel to the formation, \(k_\parallel\) is not equal to the conductivity perpendicular to the formation \(k_\perp\). A typical ratio for these two parameters is 1.5 with the parallel conductivity usually taking the higher value (Kukkonen and Šafanda, 1996). The conductivities for the cartesian co-ordinates can be calculated using

\[
k_x = \sqrt{k_\perp^2 \sin^2 \phi + k_\parallel^2 \cos^2 \phi} \quad (6.43)
\]
\[
k_y = k_\parallel \quad (6.44)
\]
\[
k_z = \sqrt{k_\perp^2 \cos^2 \phi + k_\parallel^2 \sin^2 \phi} \quad (6.45)
\]

In order to test the thermal effect of this type of anisotropy, a 3D transient FE model
was setup as shown in figure 6.8. In the first case $k_\parallel$ was set to $2.25 \text{W}(\text{mK})^{-1}$ and $k_\perp$ to $1.5 \text{W}(\text{mK})^{-1}$, i.e. an anisotropy factor $(\frac{k_\parallel}{k_\perp})$ of 1.5. The dip angle was set to $\varphi=30^\circ$. In the second case, the conductivity was made isotropic so that $k_x=k_y=k_z$ with $k_z$ equal to the vertical conductivity in the anisotropic case. The difference between the two temperature
fields is shown in figure 6.9, the absolute maximum difference between the two simulations is $6.9 \times 10^{-2}$ °C. If the anisotropy factor is reduced to 1.1, the maximum difference between the isotropic and anisotropic temperature fields becomes $2.9 \times 10^{-2}$ °C. These differences are comparable with the typical error values of borehole temperature measurements. The effect of anisotropic conductivity can therefore be significant for palaeoclimate inversion and accounting for such effects in real case 3D studies could be important. In such a real data study Kukkonen and Šafanda (1996) find a similar magnitude of the anisotropic conductivity effects (-0.11 to 0.08 K), however, in that case regions of extremely high conductivity of up to $7$W(mK)$^{-1}$ at depths of 600-1200m meant that anisotropic effects were of second order importance compared to those of heat flow refraction by these high conductivity regions.

6.7 Summary

A 3 dimensional finite element method provides an ideal method for evaluating the subsurface thermal effects from a variety of sources. The finite element method provides a flexible tool for simulating ground temperatures, as the mesh on which the heat conduction equations are solved can be optimised to the particular problem at hand. Thus variations in surface topography and thermal conductivity can be much more flexibly incorporated compared to analytical methods (e.g Birch, 1950, Lachenbruch, 1957, 1969, Turcotte and Schubert, 2006). In this chapter the influence of the variation of ground surface temperatures with altitude and the effects of conductivity anisotropy have been briefly examined. In both cases the thermal effects could have strong influence on inferred ground surface temperature histories when data are inverted in 1D. In the next chapters two methods of inversion using this 3D model are demonstrated using a variety of synthetic data designed for similarity to real data cases to which 1D methods have been previously applied.
Chapter 7

Three-dimensional inversion using reversible jump MCMC

7.1 Introduction

As described in chapter 2 the majority of ground surface temperature (GST) reconstruction methods are formulated with the assumption that heatflow is purely vertical (e.g. Shen and Beck, 1992, Mareschal and Beltrami, 1992). However, the importance of accounting for 3-dimensional effects has been highlighted in a number of geothermal studies (Šafanda, 1994, Shen et al., 1995, Kukkonen and Šafanda, 1996, Kohl, 1999, Kohl et al., 2001). Two factors that should be considered for a variety of settings are the effects of subsurface thermal conductivity variations and the subsurface thermal signatures of varying surface topography (Lachenbruch, 1969, Blackwell et al., 1980, Shen et al., 1995, Kukkonen and Šafanda, 1996, Šafanda, 1999). Using a 1D forward model, these factors may lead to spurious GST reconstructions.

In this chapter the first of two methods is presented for dealing with these issues by forming an inverse scheme which utilizes a reduced-order version of the transient 3D finite element heat transfer forward model described in the preceding chapter. This 3D forward model has been linked to the Bayesian trans-dimensional inverse approach for inferring GST histories, introduced in chapter 4. This method utilises reversible jump Markov chain Monte Carlo (rj-MCMC) sampling (Green, 1995), so that the number of variables in the model can be varied. As before the number of points used to parameterise the GST
history is allowed to change so that the resolution of the GST history over time can be inferred. This relies on the natural parsimony of the Bayesian approach, whereby simpler models which can adequately fit the data are preferred over more complex models. The Bayesian framework allows for uncertainty in all model parameters and so for example, the conductivity over the volume can be treated as unknown in all or part of the volume (e.g. measurements are more likely to be available at the borehole from cores). This has the advantage that the specified range of plausible conductivity values will be taken into account in the reconstruction of past GSTs rather than relying on a single set of values.

In order to make the inverse calculations in a reasonable time, a reduced-order model is used instead of the full finite element simulation. This is found by using the method of proper orthogonal decomposition (also known as principal components or Karhunen-Loève) whereby the output from an initial forward run of the full-scale FE model is subject to an eigenvalue decomposition. The leading eigenvectors are then used to construct a reduced model (Sirovich and Kirby, 1987, Sirovich, 1987a,b, Holmes, 1996) which preserves the dominant behaviour of the original output. Because the dominant modes are generally contained in just a few of the eigenvectors, the reduced-order model is of much lower-dimension compared to the original simulation. The degree to which the first few eigenvalues dominates the complete set of eigenvalues determines the accuracy of the reduced-order model and the errors introduced by reducing the forward model can therefore be kept small (a comparison of full and reduced-order model output is given in section 7.2.2).

Bayesian inference and the rj-MCMC algorithm used have been described in detail in chapters 3 and 4 and so this is not repeated here. Instead, first a description of model reduction using proper orthogonal decomposition is given. This is followed by the derivation of the reduced forward model in section 7.2. Subsequently examples of reduced models are shown alongside comparisons between the reduced-order and full model counterparts. In section 7.4 synthetic examples are shown to demonstrate how the inverse method performs on realistic data in 3D settings. Comparisons between GST reconstructions obtained when using a 1D forward model are shown. The effects of uncertain thermal conductivity and also of incorrectly assuming lateral geological homogeneity are also assessed. The chapter concludes with ideas for future research.
7.2 Model reduction using proper orthogonal decomposition

Proper orthogonal decomposition (POD), also known as Karhunen-Loève or principal component analysis was independently discovered by Kosambi (1943), Loève (1945) and Karhunen (1946). It provides a method for describing large data sets using a small number of dominant vectors or principal components. The method is used extensively as a descriptor for large datasets. The method has the advantage that it is completely data dependent. Recently the POD method has been used in conjunction with so-called snapshot data (Sirovich and Kirby, 1987, Sirovich, 1987a,b, Holmes, 1996) in order to derive reduced order numerical models. Output data from a particular computer model are used to derive a reduced description of that simulation. The solutions obtained in this way can be shown to be optimal representations in a least-squares sense and the accuracy can be controlled by calculating the energy percentage contained in the reduced representation.

An introduction to model reduction can be found in Astrid (2004) whilst a mathematical analysis of POD in general is found in Rathinam and Petzold (2003). Examples of model reduction applications can be found in Cao et al. (2006), Luo et al. (2007) and Fang et al. (2008).

In general the snapshot data \( S_i, i=1,\ldots,m \), is an \( n \) dimensional vector which has been sampled \( m \) times. The mean vector is found from this dataset:

\[
\bar{S}_j = \frac{1}{m} \sum_{i=1}^{m} S_{i,j}, j = 1,\ldots,n. \tag{7.1}
\]

and \( S \) is then modified to give a zero-mean set of numbers. Thus a new ensemble is formed by subtracting this mean from the values in each vector:

\[
\Psi_{ij} = S_{ij} - \bar{S}_j, j = 1,\ldots,n. \tag{7.2}
\]

An optimal (in a least squares sense) representation \( \Phi_{ij} \), of this data set can be found using the following relation:
\[ \Phi_j = \sum_{i=1}^{m} a_{ij} \Psi_{ij}, j = 1, \ldots, n. \]  
(7.3)

where \( a \) are the reduced order variables, in the reduced order FE model \( a \) will correspond with temperatures in the full FE model. The basis functions, \( \Phi_j \) must maximise

\[ \frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{n} (\Psi_{ij} \Phi_j)^2, \]  
(7.4)

subject to

\[ \sum_{j=1}^{n} (\Phi_j)^2 = 1. \]  
(7.5)

Singular value decomposition is used to find the optimal basis functions \( \Phi_j \). This is done by decomposing the matrix \( \Psi_{ij} \),

\[ \Psi_{ij} = U \Delta V^T, \]  
(7.6)

where \( U \) are the singular vectors and the diagonal entries of \( \Delta, \lambda_i \) are the singular values. Singular value decomposition is equivalent to the eigenvalue decomposition for a square matrix. The POD basis functions are then given by the singular vectors corresponding to the \( k_r \) largest singular values of the decomposition:

\[ \Phi_i = \Psi_{ij} U_i / \sqrt{\lambda_i}, \quad i = 1, \ldots, k_r. \]  
(7.7)

Here \( k_r \) must be large enough that the majority of the information in the original set is captured in the reduction. The ratio of the sums of the first \( k_r \) singular vectors to the sum of all of the singular values must be kept close to 1. For example
where the value of $\gamma$ is usually chosen to be 0.99 or larger.

### 7.2.1 Reduced order model

The steady state finite element model is given by

$$ K \mathbf{T} = \mathbf{Q} \quad (7.9) $$

This equation can be reduced using a set of basis function, in this case $\Phi_s$ which are derived using the method of the previous section from a set of snapshot data $S_s$. This snapshot data is found by evaluating the full-scale steady state FE model at a number of different values of the basal heat flux and the equilibrium surface temperature, $q_0$ and $T_{eq}$. The basis functions $\Phi_s$ are then calculated from this steady state snapshot data according to the method in the previous section. The reduced order steady state model is then given by:

$$ \hat{K} \mathbf{a}_{eq} = \hat{\mathbf{Q}} \quad (7.10) $$

where

$$ \hat{K} = \Phi_s^T K \Phi_s \quad (7.11) $$

$$ \hat{\mathbf{Q}} = \Phi_s^T \mathbf{Q} \quad (7.12) $$

$$ T_{eq} = \Phi_s a_{eq} \quad (7.13) $$

In a similar manner the transient reduced order model can be derived from the FE implementation. The FE model is given by:
where $T_m$ are the nodal temperature values at time-step $m$. This model can be reduced using the POD basis function $\Phi_t$ which are derived from the SVD applied to snapshot data $S_t$ which are the collected output from a single full transient FE simulation. The transient reduced order model is then given by

$$\hat{A}a^{m+1} + \hat{B}a^m = (1 - \theta)\hat{f}^m + \theta\hat{f}^{m+1}$$  \hspace{1cm} (7.15)$$

where

$$\hat{A} = \Phi_t^T A \Phi$$ \hspace{1cm} (7.16)$$

$$\hat{B} = \Phi_t^T B \Phi$$ \hspace{1cm} (7.17)$$

$$\hat{f}^m = \Phi_t^T f^m$$ \hspace{1cm} (7.18)$$

and $a$ are the POD coefficients (e.g Astrid, 2004). Applying this to the 3D FE heat transfer model, $\hat{A}, \hat{B} \in \mathbb{R}^{k_r \times k_r}$ and $a \in \mathbb{R}^{k_r}$. The solution of the reduced order model after the final time-step, $a$ can then be converted back to physical temperatures using the relation

$$T = \Phi_t a.$$  \hspace{1cm} (7.19)$$

Since $k_r \ll n$ (=number of nodes in the FE mesh), the POD model has a much smaller dimension than the FE model. Both equations (7.14) and (7.15) are of the same form so that the number of time-steps in the reduced transient model is the same as in the full simulation. In the following section examples of model reduction are given for 1D and 3D FE simulations where $k_r$ is of the order 8 and the number of nodes in the original model $n$, is of the order 100 to 20,000.
Chapter 7. Three-dimensional inversion using reversible jump MCMC

7.2.2 Examples

In this first example the POD basis functions \( \Phi_i \) for a transient 1D FE model are found by eigenvalue decomposition using the Matlab \texttt{eig} function. In figure 7.1 solutions from a reduced order transient finite element model are compared with those from a transient 1D FE model. The original model used to generate the snapshot data consists of 100 spatial nodes and the reduced model has 5 eigenvectors. The maximum absolute difference between two results is less than \( 3 \times 10^{-3} \text{K} \), which is below typical estimates of data noise (0.05 K).

In the second example the reduced order and FE steady state and transient models are compared for 3D implementations. In both cases, the full scale 3D FE model is reduced using POD with the basis vectors found using the method of singular value decomposition (Lehoucq et al., 1998). The domain is 1000\times 1000 \text{m} with a laterally symmetric surface topography, which ranges from 600m to 525m, with a central 200m wide plateau at 550m. The full model has 18,949 nodes and the transient model is run for 330 time-steps of 6 years, the reduced model has the same number of time-steps, but is constructed using just
Figure 7.2: The temperature difference between the steady state FE and POD models for basal heat flux of 60mWm$^{-2}$ and equilibrium surface temperature of 9.0°C.

8 of the leading singular vectors. The applied boundary condition is a linear increase in surface temperature of 1K over the 1980 years.

For the steady state formulation, a series of full steady state FE models are evaluated over a range of the two controlling model parameters, basal heat flux and equilibrium surface temperature, from 55 to 65 mWm$^{-2}$ in 35 increments and 8.5 to 9.5 °C in 10 increments, respectively. For the steady state simulation the snapshot data are therefore generated by 350 steady state FE model forward evaluations. The 350 resulting temperature-depth profiles were then used as the snapshot data for the steady state POD model. The transient snapshot data were collected at every timestep of a single evaluation of the transient FE model, with an applied sinusoidal surface temperature boundary condition.

The difference in °C between the full and reduced model outputs for the steady state calculations are shown in figures 7.2 and 7.3. In the first figure the $q_0$ and $T_{eq}$ take values in the middle of the range (60mWm$^{-2}$ and 9.0°C respectively) used to generate the snapshot data, whereas for the second figure the values are chosen to lie outside of this range (50mWm$^{-2}$ and 10.0°C respectively). The mean and maximum absolute errors for these two experiments are then $4.19\times10^{-11}$K and $9.14\times10^{-11}$K, and $9.90\times10^{-10}$K and $9.02\times10^{-9}$K respectively. In the latter case, the discrepancies with the FE model are more than 20 times larger and the pattern over the volume is more randomized. However, at
Figure 7.3: The temperature difference between the steady state FE and POD models for basal heat flux of $50\text{mWm}^{-2}$ and equilibrium surface temperature of 10.0°C. The values fall outside the range used to generate the steady state snapshot data and the resultant errors are larger and more asymmetric than in figure 7.2.

$10^{-8}\text{K}$, these errors are still insignificant for geothermal forward modelling.

The POD-FE discrepancy for the transient component is shown in 7.4. In the transient case the maximum absolute error is found to be $2.05\times10^{-3}\text{K}$ whilst the average absolute error is $9.40\times10^{-4}\text{K}$. If the number of singular vectors in the transient POD model is reduced from $k_r=8$ to $k_r=4$, the mean absolute error increases to $2.82\times10^{-3}\text{K}$. For the transient POD model the full eigenvalues series is approximated by the first $n = 15$ values only. The energy content of these model reductions, given by equation (7.8), is 99.13% for the $k_r=4$ eigenvector reduction and 99.98% for the $k_r=8$ eigenvector reduction respectively. These values are unchanged if 5 more eigenvalues are included (i.e. $n = 20$), indicating that these and the subsequent singular values are small enough to be ignored.

The accuracy of the POD model can only be guaranteed when the reduced model boundary conditions correspond closely with the boundary conditions used to generate the snapshot data. However, for nearly linear problems such as the heat conduction system considered here, this condition is less important and the results here demonstrate that when the boundary condition used to generate the snapshot data is different from that used in the reduced order model, the accuracy of the reduced order model is still sufficient. This then implies that for repeated reduced model evaluations each requiring a different BC (e.g. as required for rj-MCMC inversions) only one full scale FE simulation
Figure 7.4: The deviation between a full 3D FE model and the associated POD reduced model both forced with surface temperature increasing linearly by 1°C over 1980 years. In the full model there are 18,949 spatial nodes whereas the reduced model is constructed using the 8 leading eigenvectors. Both models have 330×6yr timesteps. The maximum deviation between the two model outputs is $2.05 \times 10^{-3}$°C.

would be needed to generate suitable snapshot data.

7.3 POD forward model with Bayesian Inference

By reducing the heat transfer model using POD the forward problem can be evaluated at a rate of 10.5 per minute which is much faster than the full forward model. This enables the forward model to be used in a MCMC algorithm for inversion such as in chapter 4, despite the large number of forward evaluations required. This is not the first attempt to perform GST inversion using a higher-dimensional model: Kohl and Gruber (2003) use a 2D model linked with a least-squares inversion code, however, the employed inverse method was unable to resolve suitable inverse solutions because of the large number of free parameters.

The model parameters under consideration here are the ground temperature history, the equilibrium thermal conditions and the subsurface geological structure (thermal conductivity, specific heat capacity). Here initially, the geological structure and underground temperatures (at the borehole) are treated as known quantities. The objective is then to
quantify posterior pdf of the remaining four model parameter vectors and scalars. This is a similar setup as in chapter 4 except there, heatflow is assumed to be in vertical direction only. The model parameters of interest for the Bayesian inference algorithm are then encompassed by \( m \):

\[
m = \{ t, T, q_0, T_{eq} \}
\]  

(7.20)

where \( t_i, T_i, i=1, \ldots, s \) (time, temperature) are used to parameterise the ground surface temperature history with linear interpolation, and \( q_0 \) and \( T_{eq} \) are the equilibrium heat flux density and long term equilibrium surface temperature respectively. The latter two are required to separate the climatic components of the underground temperature perturbations from the steady state geothermal profile. A schematic of this model setup was shown in the previous chapter in figure 6.3.

Here the prior information and proposal choices are the same as those used in chapter 4, and hence the acceptance probabilities used in the rj-MCMC algorithm are all as given before (equations 4.11, 4.12, 4.13, 4.22 & 4.23).

The prior on the temperature values is taken to be a multi-variate Gaussian with a mean of zero and a diagonal covariance matrix. In these examples the diagonal values correspond to a standard deviation on the GST values of 0.5°C. This is a smaller value than used in previous chapters because the amplitude of the true model used in these experiments is also smaller. As before the second prior constraint places a probabilistic limit on the spacing of the time nodes \( t_i \) so that there is a probabilistic bias towards uniform spacing over the time domain. This takes the form of a uniform order statistics distribution (e.g. Green, 1995). The number of points \( k \), in the GST history is subject to a uniform prior distribution over the range \((k_{min}, k_{max})\) where \( k=k_{min} \) indicates a linear trend over time. Similarly the basal heat flux and equilibrium surface temperature values are subject to a uniform prior distribution with limits at \((5, 100)\) mWm\(^{-2}\) and \((5,15)\)°C respectively.

Assuming the measurement errors on the borehole temperature data are normally distributed and independent between different depths, the likelihood function can be taken
as a multi-variate Gaussian. The covariance function is then a diagonal matrix with the values given by the square of standard deviation of the Gaussian error at each data point, as in previous chapters this value is $\sigma_d = 0.1K$. 

### 7.4 Synthetic cases

In this first example a 3D geometry is used which is designed to be representative of typical moderate topography as in Kohl (1999). The model has a horizontal extent of 1000×1000m and varies from 700m to 500m in the vertical direction. In the vertical direction the nodal spacing is 6.25m and in the horizontal direction the nodal spacing is 50m in the central 200m and 100m outside of this region. The model has 1 borehole which is located at 100,100 m. A forward model is run with 700×1 year timesteps with a surface boundary condition based on the last 700 years of the well known surface temperature reconstruction by Moberg et al. (2005). The resultant temperature field (minus the background equilibrium) is shown in figure 7.5.
Chapter 7. Three-dimensional inversion using reversible jump MCMC

7.4.1 Idealised examples 1D/3D

The data produced by the forward calculation at the borehole site are degraded with 0.1K normally distributed noise as in synthetic examples in chapters 4 and 5. The rj-MCMC algorithm is then run for 20,000 iterations with the first 2500 iterations discarded as burn in. The resultant posterior samples are shown for a simplified case in figure 7.6 for which...
the heat flow and equilibrium surface temperature are treated as known. Apart from the noise on the data this represents a realistic ideal inversion case against which to make further comparisons. The posterior mean in this examples shows excellent agreement with the true model with the posterior mean GST correctly identifying a cool period centred on 400 years b.p. For comparison, the same temperature data were inverted using a 1D forward model and the same rj-MCMC inference scheme. The resultant posterior on the past GSTs is depicted in figure 7.7. Here the effects of topography on the recovery of past surface temperatures is obvious as the posterior on the GST diverges during most of the reconstruction period from the true values, with no inferred cool period centred on 400 years b.p. This example clearly demonstrates the strong effect that even moderate topographic variations can have on inferred GST histories.

7.4.2 Basal heat flow example

In this more realistic example, a similar example is calculated with a surface topography varying from 525m to 600m and with the borehole located at 500m, 500m. The resultant temperature data were then inverted with the 3D forward model using rj-MCMC. However, the basal heat flux and equilibrium surface temperature are treated as unknown and the initial temperature of the GST history is also treated as unknown. This results in a larger model space and so more MCMC iterations are required to properly sample the posterior pdf. In addition the data have been truncated above 20m depth to mimic real data acquisition. The rj-MCMC algorithm was run for 50,000 iterations. Figure 7.8 shows the posterior pdf for the GST and the number of time-temperature points k. The data favour a model with 3 time-temperature points. In this case the uncertainty of the GST model increases much more into the past and reflects this more realistic model setup. The posterior mean shows good agreement with the true model with a minimum in temperature occurring at around 350 years. The higher-frequency variations in the true model are not resolved by the posterior, and this reflects the low resolution of the system as expected because of the diffusion of the temperature signal over time and because of the noise which has been added to the synthetic data. The slight underestimation of the true amplitude of the cooling (0.15°C versus 0.3°C in the true model) is also an artefact of the information loss due to diffusion as comparisons of the noise free and noisy cases in
7.4.3 Uncertainty in the thermal conductivity

In the third synthetic example it is assumed that the thermal conductivity values over the volume have not been measured and only estimates are available. This corresponds to chapter 4 demonstrate (figures 4.3 and 4.4). The posterior distribution shown to illustrate the range of models sampled by the algorithm. The preference here is for 3 segments in the temperature history.

Figure 7.8: Posterior probability density function on the past GST values as sampled by the rj-MCMC algorithm (50,000 iterations) for noisy synthetic data with 3D forward model allowing also for the uncertainty on the basal heat flux and equilibrium surface temperature.

Figure 7.9: Posterior probability density function of the past GSTs as sampled by the rj-MCMC algorithm (50,000 iterations) for noisy synthetic case in figure 7.8 but with thermal conductivity values sampled from a normal distribution $N(2.0,0.25)$ to mimic real data cases where measurements of the thermal conductivity are scarce.
a real situation whereby the effects of surface topography on temperatures in a borehole may be strong, but for which no cores are available from the borehole. In order to take account of this, the thermal conductivity distribution is assigned a prior pdf from which the model samples values for each forward calculation. The conductivity is assumed to be isotropic. The prior pdf is taken as a normal distribution of mean \(2.0 \text{ W(mK)}^{-1}\) and standard deviation \(0.25\text{W(mK)}^{-1}\). The conductivity values for each mesh point in the 3D model are then sampled from this prior pdf at each evaluation of the forward model with a random draw.

The resultant effect on the GST reconstructions can be seen by comparing figures 7.8 and 7.9, where the latter shows the posterior pdf for the reconstructed GSTs conditioned on the same data as in the previous example, but with the thermal conductivity prior as described above. In the latter case the inferred GST is somewhat muted compared to previous examples and shows a small bias towards models with less time-temperature points. The overall width of the 95\% credible limits on the GST history remain similar in both cases. The overall effect of the uncertainty on the thermal conductivity is then to slightly flatten the inferred GST history. This is caused by the wider range of GST histories which can now fit the data equivalently and so the prior on the GST history (which is biased towards a flat model) is more dominant. In this case however, the posterior GST is still gives reasonable agreement with the true model. The agreement between the models will then deteriorate as the prior on the thermal conductivity becomes increasingly vague. Comparing the posterior of the number of time-temperature points with that in figure 7.8 shows a slight decrease in the number of 2 segment models sampled and an increase in the number of 3 segment models sampled. It is expected that for this case where the data places a looser constraint on the model the preference would be for simpler models. The fact that there is no clear trend between figures 7.8 and 7.8 indicates either that the uncertainty range on the conductivity may be too small to have a significant effect, or that the acceptance rates are altered by drawing from a prior on the thermal conductivity and thus making direct comparison difficult. Finally, the model reduction is based on snapshot data calculated with one set of thermal conductivity values. Further forward modelling tests with the reduced model are required to determine how accurately the reduced model performs with different thermal conductivity values than those used to
produce the snapshot data.

7.4.4 Thermal conductivity structure

A common assumption in 1D GST inversions is that the underlying geological structure is laterally homogeneous. However, the validity of this assumption can rarely be tested as 3D heat transfer models as used here, are infrequently employed. Here this assumption is tested using a realistic synthetic example whereby the true geological structure is used in the forward model to calculate synthetic data, but then ignored in the inversion. The forward model is setup with three sloping geological layers of differing thermal conductivities. In the inversion, the conductivity layers are assumed to be horizontal and take thermal conductivity values which occur at the borehole position (500m,500m) in the forward model.

The synthetic data have been recalculated to account for the three parallel layers assumed to have a dip angle of 8.53° corresponding to a vertical rise of 150m over 1000m horizontally. The layers from surface downwards have isotropic thermal conductivity values of 1.5, 2.0 and 3.0 W(mK)$^{-1}$ respectively. This thermal conductivity setup is depicted in figure 7.10. For comparison, the forward model is forced with the same surface temperature reconstruction as in previous examples and is setup with a basal heat flux of 60mWm$^{-2}$ and an equilibrium surface temperature of 9.0°C. Again the surface temper-
Figure 7.11: Posterior probability density function of the past GSTs as sampled by the rj-MCMC algorithm (50,000 iterations) for the noisy synthetic case corresponding to the conductivity structure of figure 7.10 but with assumed lateral homogeneity so that the values at the borehole are assumed for the whole volume.

The surface temperature is modified according to the ground surface lapse rate of 5K km\(^{-1}\). The surface topography is also identical to previous examples.

In figure 7.11 the posterior pdf of the GST history is depicted after rj-MCMC sampling of 50,000 iterations. It can be seen that the posterior mean GST somewhat underestimates the past temperature variations shown in the true model. Although a general cool period is inferred, the amplitude and timing is more modest (around -0.1K rather than -0.3K). The use of the incorrect thermal conductivity profile appears to have biased the temperature history somewhat, with the temperature minimum shifted forwards from around 400 years in the true model to 200 years in the posterior mean. The probability distribution of the number of time-temperature points shows more preference for complex models as compared with the example in figure 7.8. This is most likely due to the added complexity introduced by varying the thermal conductivity over the volume. In this case the effect of the (incorrect) assumption of lateral thermal conductivity homogeneity is relatively small, other geometries and thermal conductivity values may lead to larger errors in the inferred GST histories. This example though contains relatively large thermal conductivity variations, and so in many real data cases where surface topography is not significant, the assumption of lateral geological homogeneity should not lead to significantly affected GST reconstructions.

The comparisons of the number of time-temperature points (k) sampled have only
been possible here as the same data have been inverted each time with identical prior constraints. In the more general case the comparisons of the posterior samples of $k$ for different data will have much less significance.

### 7.5 Discussion & Conclusions

In this chapter a method for performing simulations and inversions using a 3D numerical forward model has been demonstrated. One problem is that full 3D models are too expensive or slow and the aim here has been to develop a forward model strategy that is efficient enough that an MCMC inversion method could be applied. This necessarily implies the use of a further approximation to the finite element method. However, the errors introduced in this problem have been shown to be small enough for accurate inversions to be considered. In order to achieve this, the method of proper orthogonal decomposition has been applied to a conventional 3D finite element heat transfer model such that a reduced order model is produced. This reduced order model is then taken as the forward model and is linked with a Bayesian approach to the inverse problem introduced in chapter 4.

This approach therefore allows inclusion of a range of processes in the forward model which could not previously be accounted for when inverting borehole data for past surface temperatures. In particular the effects of variable surface topography and heterogeneous subsurface conductivity values can be taken into account and this will allow the setting of a particular borehole dataset to be included in the inversion. This should allow more data to be used for climate reconstruction purposes and additionally datasets which have been previously treated with 1D models may now yield more consistent GST reconstructions. The trans-dimensional sampling method allows for models of differing dimensionality such that the resolution of the GST history with time is inferred from the data and this means that as in chapter 4, no smoothing of the GST history is required.

Previously Kohl (1999) showed that the effects of topography could be eliminated from temperature-depth profiles by performing a correction, which relies on 3D forward calculations and subtracting the resulting equilibrium temperature profile from the measured profile. This has the disadvantage that the basal heat flow and equilibrium surface temperature as well as the underground conductivities must be calculated separately from the
inversion for the GST histories. In our approach these quantities are inferred jointly from the data along with the GSTs which is a more robust approach, as the inferred GST signal depends strongly on the values chosen for each of these other quantities.

In this chapter the overall method has been demonstrated using synthetic data, which have been degraded with noise in order to replicate realistic data sources. The resultant GST histories show similar resolution to those obtained in 1D settings. For comparison, the same data have been treated with the an identical inverse method but utilizing instead a 1D forward model. In examples of moderate topography (200m over 1km) the resultant GST histories are shown to be significantly affected and the 1D inversion results do not recover the true GST trends. This is potentially significant for many previous borehole climate reconstruction studies. Although many boreholes are located in areas of relatively uniform topography (such as the Great Plains of the USA and parts of the Canadian Cordillera), great care should be taken in choosing borehole profiles for climatic studies where topography deviates from these types of conditions, as all methods used to date rely on 1D models. In practice the effects of topography may be expected to cancel upon averaging of multiple reconstructions, since boreholes could be located on as well as below hills. However this is difficult to justify without further testing and the 3D simulation and inversion methods presented here would be good tools for this purpose.

The complete family of sampled models are useful for future work and are more useful than the posterior means and credible intervals which summarise the results. However, all of the data analysed in this chapter is synthetically generated and these posterior samples are only likely to be used in real data cases. In these 3D cases the sampled models are even more useful because of the high computational cost of the inversion compared to 1D examples. Therefore it would be useful in 3D inversion examples to make the complete ensemble of sample GST models available over the internet.

The effect on the posterior inferred GST histories of uncertainty of thermal conductivity is assessed and this leads to smoother GST histories with wider 95% credible intervals, reflecting the decreasing resolving ability of the method as the knowledge of the thermal conductivity becomes less certain. The impact of assuming lateral homogeneity of the geological structure (but using the correct topography) has also been assessed for a synthetic case with moderate variations in thermal conductivity. This shows that for large
differences between the true and assumed thermal conductivity models, the inferred GSTs are still relatively close to the true model, although, in this case this assumption leads to slight underestimation of the timing of the GST trends. The assumption is therefore likely to be valid in a range of settings, where large variations of the thermal conductivity (> 2.0W(mK)$^{-1}$) do not occur.

In the more complex cases it has been found by numerical experiments, that the data spacing plays a role in how well the true GST model is recovered. For data spacing vertically down the borehole of 10m or more, the model can underestimate the true variations whereas for the spacing of 6.25m used here the amplitude and timing of the GST changes is relatively well recovered. Modern day borehole data acquisition frequently relies on continuous temperature logging so this data-spacing issue may only be relevant to older data.

A chief limitation for the methods introduced here is the paucity of appropriate geological data for which they can be employed. Much of the borehole data currently available for palaeoclimate reconstruction does not have appropriate subsurface geological data. However, topographic data at reasonable horizontal resolution of 90m is available for the globe, with higher 30m resolution data available for the U.S. High resolution DEM data for the UK is available from the British Geological Survey and this would allow topographic influences in the UK IHFC datasets to be included.

Regional averages of GST histories are particularly important in real data settings in order that robust climate histories can be derived. The method used here could be employed at locations where it is warranted, whilst the 1D equivalent could be employed for other sites. Regional averages could then be found by averaging the posterior mean GST deviations over time or by joint sampling from the inferred posterior distributions. For closely spaced boreholes a single 3D forward model could be used to model all of the sites together. In that case it may be found that the simple parameterisation of the equilibrium surface temperature as a function of altitude (using a lapse rate) is inadequate. In this case the Bayesian methodology used here could be extended to estimate spatial variations of this parameter using for example Bayesian partition modelling (Denison et al., 2002). This may then allow the influence of historical land cover differences from one borehole to another to become apparent.
In future work, the forward model could be modified to simulate underground advection of ground water. This advection-diffusion model could then also be reduced using the POD method and linked with a suitable inversion scheme. Because of the trade-off between the influence of groundwater flow and palaeoclimate on underground temperatures, some method for assessing a priori the fluid velocities would be required. This could be obtained from detailed geological investigations of the site under consideration or by the use of a hydrogeological fluid flow model.
Chapter 8

Three-dimensional inversion using the adjoint method

Having introduced the first method for inversion in three dimensions using reversible jump Markov chain Monte Carlo sampling, this chapter details the development and application of the second method for which a non-linear conjugate gradient method is employed (e.g. Pain et al., 2002). For rectangular matrices the linear conjugate gradient method is equivalent to Lanczos’ algorithm (e.g. Golub and Van Loan, 1996, chapter 10.2.5), a method used to calculate the singular value decomposition (SVD) of a matrix. Therefore, the NLCG method applied here is a non-linear analogue of the SVD method widely used for borehole data inversion as in Mareschal and Beltrami (1992) and described previously in chapter 2.3.3. Comparisons between the NLCG method and the rj-MCMC methods developed in this thesis are therefore useful for illustrating the differing features of the two approaches.

Optimisation based inverse procedures require some sort of regularisation term in order to constrain the solutions to physically realistic values (Constable et al., 1987). This is analogous to the prior information term used in Bayesian methods. In this work the regularisation term penalises the absolute derivative of the temperature history with time so that the inverse solution is constrained to be flat or constant with time unless the data demand otherwise. Generally the method is designed so that initial model updates are to smooth models, whilst subsequent iterations can introduce more detailed variations as
Chapter 8. Three-dimensional inversion using the adjoint method

this regularisation penalty is somewhat relaxed.

The gradient calculations are achieved efficiently by using the adjoint method (e.g. Wang et al., 1992). This means that these calculations are exact for the finite element (FE) discretisation used here. After introducing the adjoint method in general, the specific application to the FE model of chapter 6 is detailed. This is followed by a description of the functional and regularisation constraints. The employed optimisation method is described in section 8.3 and this is followed by a series of synthetic examples in section 8.4. A discussion of the results and comparisons with results from the previous chapter are given in section 8.5

8.1 The adjoint method of gradient calculation

The adjoint formulation provides a method for analytically evaluating the gradient of a system by algebraic manipulation of the governing equations. Typically the adjoint is used in optimization and sensitivity analysis of large systems governed by partial differential equations. The adjoint calculation is similar in computational expense to the forward evaluation, and so in fields such as fluid dynamics and geology it provides a much more efficient alternative to numerical methods such as finite differences.

The use of adjoint methods has been widespread in the field of meteorology since the 1970s where it is used for 3 or 4 dimensional variational data assimilation (e.g. Wang et al., 1992). More recently the adjoint method has been used in other fields including, inverse tomography (Tarantola, 1984), borehole temperature inversion (Shen and Beck, 1991), 3D resistivity inversion (Pain et al., 2002), ocean modelling (Fang et al., 2006), and hydrogeology (Hier-Majumder et al., 2006). In this work the adjoint method is applied in a similar manner to Shen and Beck (1991) where the 1st order gradient is used in a least-squares Bayesian inversion scheme (see chapter 2.3.2). However, here the forward model is formulated in 3D and an optimisation method is used rather than Bayesian least-squares.

An alternative to the adjoint method is automatic differentiation (e.g. Bischof et al., 2003, Rath et al., 2006, Sambridge et al., 2007), whereby the differential of a model with respect to certain variables can be found by differentiating the computer code itself. This is automatic as the original code is run line for line to calculate the differential by coupling
with a suitable automatic differentiation compiler. Since the forward model applied in this work is relatively simple, automatic differentiation is not explored and instead the adjoint model is derived algebraically.

8.2 The 1st order adjoint

The 1st order adjoint method can be used to derive the exact gradient of the cost functional with respect to the model parameters. This can be applied in one of two ways, either by applying the adjoint method to the governing differential equation(s) and then applying the finite element discretisation to the resulting equations, or by applying the adjoint method to the discretised equations, which is the method used here.

In this first section the adjoint formulation is illustrated using a generic discretised partial differential equation. This is represented by the matrix equation:

\[ A\phi = s. \]  
(8.1)

Here \( \phi \) is the vector of variables which we wish to find and is a general function of the model vector \( m \). Now defining the functional as \( F \), and taking the partial derivative w.r.t. the model parameters, the gradient can be written as:

\[ \frac{\partial F}{\partial m} = \left( \frac{\partial \phi}{\partial m} \right)^T \frac{\partial F}{\partial \phi}. \]  
(8.2)

Taking the gradient of equation (8.1) w.r.t. the model vector:

\[ \frac{\partial A}{\partial m} \phi + A \frac{\partial \phi}{\partial m} = \frac{\partial s}{\partial m}. \]  
(8.3)

This can be re-arranged for \( \frac{\partial \phi}{\partial m} \):
\[
\frac{\partial \phi}{\partial m} = -A^{-1}\left( \phi \frac{\partial A}{\partial m} - \left( \frac{\partial s}{\partial m} \right) \right) \tag{8.4}
\]

In this work \( \frac{\partial A}{\partial m} \) is equal to zero (because \( A \) depends solely on the discretisation). Equation (8.4) can then be substituted into equation (8.2) to give:

\[
\frac{\partial F}{\partial m} = \left( \frac{\partial s}{\partial m} \right)^T \cdot \left( A^{-T} \frac{\partial F}{\partial \phi} \right) \tag{8.5}
\]

The bracketed term on the RHS can be found by introducing the adjoint variables, \( \phi^* \),

\[
\phi^* = A^{-T} \cdot \frac{\partial F}{\partial \phi} \tag{8.6}
\]

re-arranged to give

\[
A^T \phi^* = \frac{\partial F}{\partial \phi} \tag{8.7}
\]

This is the first order adjoint model, so named because the matrix \( A \) is transposed. The solution of this equation given by \( \phi^* \) is then substituted back into equation 8.5 to give the gradient:

\[
\frac{\partial F}{\partial m} = \left( \frac{\partial s}{\partial m} \right)^T \phi^*. \tag{8.8}
\]

Since equation (8.7) is of similar scale to the forward problem (equation 8.1), the gradient can be found in approximately the same amount of time as two runs of the forward model. This is a marked improvement on the \( m \) (=number of time-steps) runs required by finite differences. Additionally the gradient calculated above is the exact gradient of
the particular discretisation used. In the next section the application of this method to
the transient component of the 3D finite element heat transfer model described in chapter
6 is demonstrated.

8.2.1 The 1st order gradient of the 3D FE heat conduction model

Derivation of $\frac{\partial s}{\partial m}$

The vector $s$ contains the model source terms relating to the boundary conditions. In the
3D discretisation these take the form of Robin boundary condition applied to the upper
surface elements:

$$s^i_j = \beta \Delta t T^{i}_{\text{air}} \int N_k ds, j = 1, \ldots, S_n \quad (8.9)$$

where superscripts (i) refer to timestep and subscripts (j) to the FE node, there are
$S_n$ surface nodes (in contact with the air) and the integration is over the surface basis
functions. The constant $\beta$ is the air to ground heat transfer coefficient introduced in

This is then differentiated w.r.t. the model vector $m$:

$$m = \begin{pmatrix}
T^1_{\text{air}} \\
T^2_{\text{air}} \\
\vdots \\
T^{m-1}_{\text{air}} \\
T^m_{\text{air}}
\end{pmatrix} \quad (8.10)$$

given m time-steps in the model.
The differential is then
\[
\frac{\partial s}{\partial m} = \beta \Delta t \int N_k ds \times
\begin{pmatrix}
1 & 1 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{pmatrix}
\begin{pmatrix}
0 & 0 & \cdots & 0 \\
1 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{pmatrix}
\begin{pmatrix}
0 & 0 & \cdots & 0 \\
1 & 1 & \cdots & 0
\end{pmatrix}
\tag{8.11}
\]

\[
\begin{pmatrix}
0 & \cdots & \cdots & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\end{pmatrix}
\tag{8.12}
\]

where the 1s correspond to surface nodes and 0s (in the same row) denote the remaining FE nodes. Each row corresponds to one time step, so that each block matrix is \( m \times n \) and the whole matrix is \( m \times (m \times n) \).

**Adjoint model** \( A^T \phi^* = \frac{\partial F}{\partial \phi} \)

The adjoint system of the forward model is given by:

\[
\begin{pmatrix}
A_l & B_l & 0 & \cdots & 0 \\
0 & A_l & B_l & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\vdots & \vdots & \ddots & B_l & \vdots \\
0 & \cdots & 0 & A_l & \vdots
\end{pmatrix}
\begin{pmatrix}
\phi^{1s} \\
\phi^{2s} \\
\vdots \\
\phi^{ns}
\end{pmatrix}
= \begin{pmatrix}
0 \\
\vdots \\
\vdots \\
2(T^{obs} - T^m)
\end{pmatrix}
\tag{8.13}
\]

This must be solved from bottom to top leading to a reverse-time version of the original forward model. The solution forms a block matrix \( \phi^* \).

**The gradient**

The multiplication of terms (8.11) and the solutions \( \phi^* \) of (8.13) gives:
Chapter 8. Three-dimensional inversion using the adjoint method

\[ \frac{\partial F}{\partial m} = \left( \frac{\partial s^1}{\partial m} \quad \frac{\partial s^2}{\partial m} \quad \cdots \quad \frac{\partial s^{m-1}}{\partial m} \quad \frac{\partial s^m}{\partial m} \right) \begin{bmatrix} \phi^{*1} \\ \phi^{*2} \\ \vdots \\ \phi^{*m-1} \\ \phi^{*m} \end{bmatrix} \]  \hspace{1cm} (8.14)

The gradient at timestep \( i \) is then calculated by

\[ \left. \frac{\partial F}{\partial m} \right|_i = \beta \Delta t \sum_{i=1}^{S_n} \phi^{*i} \int N_k ds, \]  \hspace{1cm} (8.15)

where the summation is over the \( S_n \) surface nodes and the integration is of the FE basis functions over the surface of the mesh.

### 8.2.2 Verification of the 1st order gradient calculations

The first order gradient can be compared to that derived using either a finite difference calculation or by deriving the gradient for an analytical solution (see appendix B.1). In both cases the gradient derived from the adjoint agrees well. Examples of the gradient calculated using adjoint, finite differences and analytical methods is shown in figures 8.1 and 8.2. The two solutions diverge at the final time-steps which can be attributed to the oscillatory behaviour of the finite element method at the initial timestep of the adjoint model, corresponding to the final time-step of the gradient. This effect can be reduced by using variable sized time-steps with smaller steps towards the end of the simulation.

### 8.3 Optimisation Methods

#### 8.3.1 The functional

The functional quantifies the progress of the inversion method by measuring the fit between the measured and simulated data. This quantity must be reduced in magnitude to the expectation value (calculated using the data-noise level). In geophysical inverse problems the functional will usually include terms which constrain the solutions in some way, usually
by penalizing departures from smooth models (Constable et al., 1987). In this work the functional includes a regularisation term which penalizes deviations in the temperature history model from the smoothest (i.e. no change) model. This is formed by the square of the differential of the temperature history with time, for which the continuous and discretised equations are given by:

$$F_r = \frac{1}{2} \lambda \int \nabla^T m k_{sm} \nabla m \, d\Omega$$

$$F_r = \frac{1}{2} \lambda m^T K_r m$$

where $k_{sm}$ is a regularisation matrix, $K_{ri,j} = \int \nabla^T N_i \nabla N_j \, d\Omega$, where $N_i$ are the temporal basis functions. The data-fit contribution to the functional is given by:
Chapter 8. Three-dimensional inversion using the adjoint method

\[ F_d = \frac{1}{2} (d - d_{\text{obs}})^T C_d^{-1} (d - d_{\text{obs}}) \]  

(8.18)

where \( C_d \) is the data covariance matrix. The overall functional \( F \), is given by a combination of the data-fit and regularisation terms:

\[ F = F_d + F_r \]

\[ = \frac{1}{2} (d - d_{\text{obs}})^T C_d^{-1} (d - d_{\text{obs}}) + \frac{1}{2} \lambda m^T K m, \]  

(8.19)

where the value of \( \lambda \) controls the relative influence of the regularisation term versus to the data-fit term.

8.3.2 Non-linear conjugate gradient method

The linear conjugate gradient method is described in appendix B.2. The non-linear conjugate gradient is similar to the linear method and can be applied to any continuous differentiable function. However, unlike for the linear method, the choice of the update length \( \alpha \) has no straightforward interpretation and for this reason, a line-search method is required. A bracketing method, which is described below, has been used.

The non-linear conjugate gradient method is given by:

\[ m_{i+1} = m_i + \alpha d_i \]  

(8.20)

with the initial search direction given by \( d_1 = -g_1 \), where \( g_1 \) is the gradient for the initial model. For subsequent iterations the conjugate directions are calculated using the Polak-Ribière formula:

\[ d_{(i+1)} = -g_i + \beta d_i \]  

(8.21)

\[ \beta = \frac{(g_{(i+1)})^T (g_{(i+1)} - g_i)}{(g_i)^T g_i} \]

A line search is used to find a suitable value of \( \alpha \) at each iteration. This is achieved by progressive bracketing of the minimum by fitting a parabola to the misfit function.
evaluated at three points along the current search direction. The first 3 points along the current search direction are found by

\begin{align}
    n_1 &= 0.0 \\
    n_2 &= 0.5 \times I_s \left/ \max(g) \right. \\
    n_3 &= I_s \left/ \max(g) \right.
\end{align}

(8.22)  
(8.23)  
(8.24)

where \( \max(g) \) is the largest absolute value of the elements of the gradient and \( I_s \) is a tunable parameter which controls the step-length of the line search. In examples presented here, this takes an empirical value of 5.0. These three positions lead to 3 forward model evaluations and resulting functional values \( F_1, F_2 \) and \( F_3 \). Subsequent values are chosen by quadratic interpolation of the 3 functional values, placing the new value, \( n_i \) at the minimum point of this quadratic function. The forward model is then re-evaluated to give \( F_i \) and \( n_i \) then replaces one of the existing points if \( F_i \) is smaller than at least one of \( F_{1,2,3} \), so that the further point from the new one is replaced. If the new point functional \( F_i \) is larger than the current 3 then the new point is replaced by a point halfway between the two current points nearest two \( n_i \).

This process is repeated for a defined number of iterations or until the update in the functional falls below a defined tolerance level. Once a suitable minimum has been located in one direction the control variables are updated and a new gradient is found. The line search is then employed in the same manner along the next search direction calculated using equation (8.21).

The total number of iterations used depends on how the convergence of the overall algorithm is defined. In Constable et al. (1987) the algorithm is terminated once the data misfit part of the functional has fallen below the expected value. This expected value is equal to \( N/2 \) for the functional in equation 8.18 where \( N \) is the number of data points. An alternative explored here is to terminate the algorithm once the mean update at the data-points is less than a certain tolerance.
Chapter 8. Three-dimensional inversion using the adjoint method

Figure 8.3: The inverse GST models with iterations and on the right the value of the functional with iterations. The termination criterion here stops the algorithm after 5 iterations.

8.4 Synthetic Inversion Examples

8.4.1 Non-linear conjugate gradient

In this example the model is setup with surface topography as in the synthetic examples of the previous chapter. The thermal conductivity was setup in both the forward and inverse models as in figure 7.10. The data have been degraded with 0.1K standard deviation Gaussian random noise. The NLCG algorithm was run for a maximum of 35 iterations each with 6 line search iterations. At each iteration the smoothness constraint, $F_r$, is reduced by 10%. The initial model is uniform GST values of 10.0°C, which is a reasonable starting model, forcing the algorithm only to introduce deviations when supported by the data.

In order to ensure that the model does not overfit the data, a termination criterion is required. Here the NLCG algorithm is stopped once the functional update corresponds an average update at each data point of less than 0.01K, i.e. when the functional changes by less than 0.4. The regularisation term is initially set to equal $1 \times 10^7$ and is reduced by 10% at each iteration. The step-length parameter $I_s$ is set to equal 5.0.

In figure 8.3 this procedure is illustrated, and here the inversion is stopped after 5 iterations. The solution shows fair agreement with the true model, depicting a general cool period in the past, with subsequent warming. However, the model appears to be more sensitive to recent events and so the minimum of the cool period is inferred to have occurred
at around 200 years rather than at 400 years as in the true model. A direct comparison with similar results from the Bayesian rj-MCMC method in the previous chapter can be made between this figure and figure 7.6 for which the Bayesian posterior mean correctly indicates a temperature minimum at 400 abp. Further comparisons between the two methods are discussed below.

Notice, in figure 8.3 also a set of rapid variations between 20 years and the present. These variations appear to be an artefact of the gradient calculation and the lack of constraint for the very recent as the data are taken from depths greater than 20m. These variations are therefore only penalised in the functional through the regularisation term and are therefore difficult to remove with increased regularisation without obscuring part of the true trend at earlier times (e.g. Chouinard and Mareschal, 2007). A plausible solution is to cut off the inverse model at 10-20 apb, or to average the GST values over this period, here the former option used.

Since gradient optimisation methods cannot guarantee convergence to a particular functional minimum, it is necessary to use multiple trials which are started from different positions in the model space. Therefore for comparison the inversion of the data used in figure 8.3 inverted again with the model initiated as $T = 8.0^\circ$C. The resultant inverse solutions are shown in figure 8.4. In this example the algorithm is again terminated after 5 iterations and the final model has almost the same functional value. However, here the inverse solution GST history does not show the same variation over time, instead showing a general warming over the whole reconstruction length. It therefore appears that in this example the algorithm has converged to a different functional minimum leading to a modestly different inverse GST history.

8.5 Discussion and Conclusions

The gradient optimisation methods present a different approach to Bayesian inference used in the majority of this thesis. Optimisation method seek to minimise some of form of functional which is specifically designed so that the algorithm can converge on physically realistic solutions. This means that optimisation methods typically involve a number of empirical parameters that require tuning to the problem at hand and which have a direct
Figure 8.4: The inverse GST models with iterations and on the right the value of the functional with iterations as in figure 8.3 but with a starting model of $T=8.0^\circ$C.

influence on the final solution. Additionally, since gradient methods have no mechanism for dealing automatically with local minima in the functional surface, multiple runs from differing starting positions are typically required.

Realistic synthetic examples indicate that the inverse solutions which are dependent on the gradient of the functional w.r.t. model parameters are more sensitive to the recent times. This means that it is difficult for the method to recover the correct timing of past temperature changes. Evidence from repeated inversions with differing starting models shows that approximately equal data fits can be obtained for solutions with quite different GST histories. This is due to the degeneracy of the inverse solutions caused by the noise in the data, and is a feature with is dealt with robustly in a Bayesian formulation, but apparently not by this optimisation method.

In contrast the Bayesian inference methods lead to the derivation or approximation of a posterior probability which rigorously combines all the information both from the data and prior information. The number of tunable parameters is less, although care must be taken in the design of the method for sampling from the posterior. Since the Bayesian inference method relies solely on information from the forward model (and prior) it appears to produce more robust estimates of past changes (c.f. figures 7.6 and 8.3).

However, the rj-MCMC method used is expensive, typically requiring 10,000s of forward model evaluations. In contrast the optimisation method require only around 40 equivalent forward model evaluations (taking 5 iterations each with 6 line search itera-
tions and 1 gradient evaluation, this totals $5 \times 6 + 5 \times 2 = 40$, since the gradient evaluation requires the equivalent of 2 forward model evaluations). In summary, the purpose of the study at hand may help to determine the method used. For extremely large data sets or 3D models, it may only be feasible to use an optimisation type method unless the forward model is parallelised efficiently, but this is then prone to converging on poor solutions. Some sort of hybrid scheme involving both gradient and an rj-MCMC methods could therefore be useful. For example, the faster gradient inversions could be used to approximate the prior pdf of the temperature histories by collecting the results from multiple starting points, this could then serve to reduce the plausible model space (and hence computation time) of a final 3D forward model rj-MCMC run using the methods described in the previous chapter.

In future work the 2nd order adjoint gradient of the FE model could be derived and used in a Newton type inverse procedure (Pain et al., 2002). This may then provide better sensitivity to past climatic events, just as Pain et al. (2002) shows that the 2nd order gradient inversions for electrical resistivity provide higher sensitivity at locations further from the electrical receivers.
Chapter 9

Conclusions & Future work

In this thesis I have focussed on developing new methods for inverting borehole temperature data in order to reconstruct past surface temperature variations. In chapter 4 a new method for inverting borehole profiles singly and jointly was presented. For this a trans-dimensional Bayesian approach was used which relies on reversible jump Markov chain Monte Carlo (MCMC) sampling. The models of the past variations are parameterised simply in terms of a variable number of time-temperature points. The natural parsimony of the Bayesian approach then allows objective inference of the optimal number of these nodes conditioned on the data and prior. This method represents a departure from previous work as there is no explicit regularisation of the temperature history and this allows better resolution of the temperature variations back in time. Sampling the full posterior distribution of the model parameters leads to more rigorous quantification of the model uncertainty which, along with the prior, is useful in determining how far into the past the reconstruction is determined by the data. Results from UK data suggest a warming of 0.8°C from approximately 1600-1650 to the year 1987, in agreement with regional instrumental and proxy data.

In chapter 5 the issues of how to optimally group multiple borehole data before joint inversion and how to infer spatial variations in past temperature variations from these multiple boreholes are addressed using a Bayesian partition model. In this method the space in which the boreholes are located is divided into a set of partitions each of which is assumed to relate to an independent temperature history. The number and positions of these partitions can then be inferred again using a reversible jump MCMC algorithm,
Chapter 9. Conclusions & Future work

whilst the joint GST history in each partition is inferred using the method described in the preceding paragraph. As the Bayesian formulation naturally penalises unwarranted complexity, the partition model is shown to find a balance between data fit achieved with more partitions and the prior terms which penalise these extra partitions. This means that boreholes are grouped according to the inferred joint history where the data can be reasonably fit according to the estimated data uncertainty. Application to 23 borehole data sets from the UK indicates that the majority of the boreholes are corrupted by non-climatic influences, including some groups with systematic errors. These results therefore show that the 23 datasets should not be used for climate reconstruction purposes without further site analyses and more advanced forward modelling schemes.

In chapters 6, 7 and 8 the forward model is reformulated in three dimensions so that the setting of the particular borehole can be better taken into account. In this a 3D transient finite element heat transfer (FE) model has been used and combined with two inverse methods. The first is an implementation of the reversible-jump MCMC method of chapter 4 and the second is the method non-linear conjugate gradients. Since the number of the forward model evaluations required by MCMC methods is very large, some way of reducing the computation time of the FE model was required and here model reduction was achieved using proper orthogonal decomposition. This allows a much faster forward model which can then be used in rj-MCMC algorithm.

Synthetic data calculated with topographical variations using the FE model were then inverted using this 3D rj-MCMC method and the 1D method of chapter 4. Comparisons of the resulting posterior distributions demonstrate the effect of the topography on the resultant GST reconstructions. The discrepancy introduced when using a 1D forward model is relatively large and this suggests that a 3D model should be used for real data cases located in areas of even moderate topographical variations. A 3D inversion was also used to test the common assumption of lateral conductivity homogeneity in a realistic synthetic inversion example. The results show that the effects on the resultant GST history are small, implying that this assumption will be valid in many real data cases.

Results from inversions using the non-linear conjugate gradient algorithm show that the method can converge on unrealistic solutions if regularisation of the temperature history over time is not carefully applied. Examples with different starting values also illustrate
Chapter 9. Conclusions & Future work

that the method is prone to converge on different solutions. The NLCG method is more practical where either a larger FE model is required or where the reconstruction length is too long for reasonable computation times with a MCMC simulation. Using the NLCG method to approximate a prior distribution of the GST history may be a useful way of combining this method with the more computationally expensive rj-MCMC method, so that the reduced model space (defined by this prior) implies less MCMC iterations will be required.

The specific contributions of this thesis to the field of borehole palaeo-climatolgy are:

A new method for inferring past surface temperatures from single and multiple borehole profiles. Using the reversible jump Markov chain Monte Carlo Bayesian sampling it is possible to infer the model complexity that is appropriate to the data. This then avoids the need to specify a model smoothing over time and thus leads to more realistic temperature reconstructions for which the uncertainty is fully accounted for in the posterior probability density function.

The first method specifically designed to infer spatial trends in ensembles of borehole profiles. A Bayesian partition model is used to group multiple borehole temperature profiles according to the inferred temperature history. This leads to better estimates of spatial signals so that data which are corrupted by noise can be identified by the size of the groups in which they are inferred to lie. Analysis of real data from the UK shows that some of the borehole data is in near agreement with long instrumental temperature record, but the majority of the borehole datasets are dominated by non-climatic influences, which are mostly localised but with some systematic non-climatic errors which are common to many boreholes.

The first 3D simulation inversion method for inferring past surface temperature changes in complex settings. Using a 3D finite element model and a reduced model a method has been designed and tested which allows borehole data to be inverted in a 3D setting using Bayesian rj-MCMC sampling or a non-linear conjugate gradient method. It has been shown that for moderate topographic variations the thermal effects
on underground temperatures can be significant, thus leading to biased GST reconstructions when a 1D method is used.

9.1 Implications for further studies

The aim of this thesis has been to develop new methods for borehole inversion in the palaeoclimate context, and as such this work has necessarily focussed on synthetic data examples. The results in this thesis indicate that applying these new methods to existing data could help to provide new insights into long term past surface temperature changes at the Earth’s surface. A key issue for climate reconstruction of the past millennium has been the debate over the magnitude of surface temperature variations (e.g. Mann et al., 1999, Huang et al., 2000, Briffa and Osborn, 2002, Esper et al., 2002, Moberg et al., 2005, Hegerl et al., 2007, Juckes et al., 2007). Results in this work indicate that the methods presented are superior to established GST inversion techniques and they highlight that for previous methodologies data uncertainty, model regularisation (smoothing in time) and averaging of borehole reconstructions can have an effect on the inferred GST changes, an issue touched upon by (González-Rouco et al., 2008). Future work aimed at analysing a larger portion of the IHFC data and other newer data with these new methods is unlikely to drastically alter the global estimate of GST change over the past 500 years although the timing of the inferred GST changes may change. New analyses may provide interesting evidence of spatial variations which are not evident in the UK data analysed in this thesis. The amount of acceptable data used for GST reconstructions is now theoretically widened as the 3D structural effects can now be included in the inverse models. Where suitably applied, this may help to reduce some of the spread in inferred GST trends of large borehole datasets (e.g Huang et al., 2000).

9.2 Future work

In many of the preceding chapters, ideas for developing the methods presented have been described. These include more informative prior information choices and different parameterisations of the partition model using parameterised polygons instead of Voronoi tessellations. However, in this section I focus on possible methods of combining borehole
and proxy data which are based on some of the work in this thesis.

To date there have been a limited number of studies involving both proxy and borehole data. In Beltrami et al. (1995) and Beltrami and Taylor (1995) proxy data (tree rings or ice borehole oxygen isotope values) are calibrated to surface temperatures using borehole data. This is achieved by transforming the proxy data using the resolution matrix of borehole data inversion (Menke, 1989, Beltrami and Mareschal, 1995) so that the proxy index is directly comparable with the borehole reconstruction. A linear fit between the two is derived and then applied to the original proxy data to derive a high-resolution temperature reconstruction. Huang (2004) uses proxy temperature reconstructions as prior information for inverting global borehole temperatures. The resultant reconstructions preserve the high-frequency content of the proxy data but at low-frequency, the trends are dictated by the borehole reconstructions.

In a Bayesian context, conditioning the new overall reconstruction on the individual reconstructions (as in Huang, 2004) involves specifying a distribution or uncertainty level for each reconstruction- a potentially subjective step in the methodology. A more flexible basis for combining both types of data source would be to condition the reconstruction on both data sources rather than on the reconstructions. For the borehole, this is the temperature-depth data, whilst for the proxies, the data would constitute appropriate instrumental temperature series. Hence, features of the borehole or proxy data which are possibly non-climatic are not forced into the reconstruction since the reconstructions are derived simultaneously from all of the available data. In this way a prior distribution is specified for the temperature changes over time (e.g. as specified for the GST models in this work) and appropriate uncertainty factors for the borehole and instrumental data are used.

A Bayesian calibration process would also allow incorporation of the uncertainty in other factors in the proxy methods, for example the removal of the growth trend from tree ring data. Unfortunately to date there have been no implementations of Bayesian methods in dendro-climatology or multi-proxy reconstructions of the last millennium. However, Robertson et al. (1999) demonstrate a Bayesian Kernel based method for proxy climate reconstruction and Haslett et al. (2006) provide an overview of more recent literature in a variety of related topics, additionally Buck et al. (2006) use a non-parametric Bayesian
methods to produce a radio-carbon dating calibration curve and this method may also be suited to proxy data.
References


181
References


EPICA Community Members.


References


References


References


References


Robertson, I., D. Lucy, L. Baxter, A. Pollard, R. Aykroyd, A. Barker, A. Carter, V. Swit-


Wang, Z., I. Navon, F. Ledimet, and X. Zou (1992). The 2nd-Order Adjoint Analysis -


Appendix A

Bayesian methods

A.1 Bayes’ law

Bayes’ law can be derived from elementary probability theory by considering the definition of a conditional probability:

\[
p(A | B) = \frac{p(A \cap B)}{p(B)}, \quad (A.1)
\]

\[
p(B | A) = \frac{p(B \cap A)}{p(A)},
\]

where \(p(A | B)\) means the probability of \(A\) given that \(B\) has occurred and \(p(A \cap B)\) means the probability of \(A\) and \(B\) occurring. These two equations can be combined using the relation \(p(A \cap B) = p(B \cap A)\) so that:

\[
p(A | B)p(B) = p(A \cap B) = p(B \cap A) \quad (A.2)
\]

\[
= p(B | A)p(A)
\]

\[
p(A | B) = \frac{p(B | A)p(A)}{p(B)}. \quad (A.3)
\]

Equation A.3 is then Bayes’ law.
A.2 The reversible jump MCMC algorithm

The reversible jump algorithm proceeds in the same manner as Metropolis-Hastings, but using instead the more generalised form of the proposal acceptance term $\alpha$. This modification then accounts for proposals to differing state spaces including to models of differing dimensionality if required (Green, 1995, 2001, 2003). Algorithm A.2 summarises the actual calculations made in RJ-MCMC and equation A.4 gives the more general form of the acceptance probability.

**Algorithm 1** Reversible Jump MCMC algorithm

```
Initialize with $m_0$

for $i = 1$ to $N$
    Sample $q(m' | m)$
    Sample a uniform random number $U(0,1)$
    if $U \leq \alpha(m', m)$ then
        $m \leftarrow m'$
    else
        discard $m'$, store $m$
    end if
end for
```

$$
\alpha = \min \left[ 1, \frac{p(m' | \varphi)}{p(m | \varphi)} \cdot \frac{p(d | m', \varphi)}{p(d | m, \varphi)} \cdot \frac{q(m | m')}{q(m' | m)} \cdot |J| \right] \tag{A.4}
$$

$$
= \min \left[ 1, \text{(prior ratio)} \cdot \text{(likelihood ratio)} \cdot \text{(proposal ratio)} \cdot |\text{Jacobian}| \right]
$$

where the Jacobian, $J$, is calculated by differentiation:

$$
J = \frac{\partial(m', u')}{\partial(m, u)} \tag{A.5}
$$

and $u'$ and $u$ are functions used to probabilistically calculate $m'$ dependent $m$. 
Appendix B

Gradient methods

B.1 Deriving an analytical gradient

In order to derive an analytical gradient with which to compare the adjoint gradient calculation, an analytical solution to the heat conduction equation is required. This is discussed in chapter 2.3.3 and is given again for a series of step increases in the surface temperature:

\[ T_i(z) = \sum_{i} \Delta T_i \text{erfc} \left[ \frac{z}{2\sqrt{\kappa t_i}} \right] \]  

(B.1)

where

\[ \text{erfc}(\theta) = 1 - \frac{2}{\sqrt{\pi}} \int_{0}^{\theta} e^{-x^2} \, dx \]  

(B.2)

This can be represented by a matrix equation:

\[ T_j = A_{jl} m_l \]  

(B.3)

where \( A \) is a matrix of analytical solutions of the heat conduction equation (Carslaw and Jaeger, 1959, Mareschal and Beltrami, 1992):
Appendix B. Gradient methods

\[
A_{jl} = \text{erfc}\left(\frac{z_j}{2\sqrt{\kappa t_{k-1}}}ight) - \text{erfc}\left(\frac{z_j}{2\sqrt{\kappa t_k}}\right) \tag{B.4}
\]

In equation B.3 \(T_j\) are the temperature values measured at \(J\) depths \(z_j\). \(\mathbf{m}_t\) are the model parameters, the surface temperatures over time. Equation B.4 can then be differentiated with respect to the surface temperatures \(\mathbf{m}_t\) leading to:

\[
\frac{\partial T_j}{\partial \mathbf{m}_t} = A \tag{B.5}
\]

The gradient, which is the differential of the functional with respect to the model parameters (surface air temperatures) can now be calculated from

\[
G = \frac{\partial F}{\partial \mathbf{m}_t} = \frac{\partial \left[ (\mathbf{T}(z) - \mathbf{d})C_d^{-1}(\mathbf{T}(z) - \mathbf{d}) \right]}{\partial \mathbf{m}_t} \\
= 2\frac{\partial \mathbf{T}(z)}{\partial \mathbf{m}_t}C_d^{-1}(\mathbf{T}(z) - \mathbf{d}) \\
= 2AC_d^{-1}(\mathbf{T}(z) - \mathbf{d}) \tag{B.6}
\]

B.2 The method of conjugate gradients

Given a linear forward problem, for which the misfit functional \(f(\mathbf{m})\) is the discrepancy between the true and the current solutions. The steepest descent method is given by the update vector \(\mathbf{r}\):

\[
\mathbf{Am} = \mathbf{b} \tag{B.7}
\]
\[
f(\mathbf{m}) = (\mathbf{b} - \mathbf{Am}) \cdot (\mathbf{b} - \mathbf{Am}) \tag{B.8}
\]
\[
\mathbf{r}_i = \frac{\partial f}{\partial \mathbf{m}}(\mathbf{m}) \tag{B.9}
\]
\[
\mathbf{m}_{i+1} = \mathbf{m}_i - \mathbf{r}_i \tag{B.10}
\]
For linear problems, a large number of iterations can guarantee convergence. This method is refined by using a line-search to find a suitable model distance to move in any given direction:

\[
m_{i+1} = m_i - \alpha r_i \tag{B.11}
\]

\[
\alpha = \frac{r_i^T r_i}{r_i^T A r_i} \tag{B.12}
\]

Steepest descent which can often take many steps along the same direction, often with subsequent steps undoing steps made in previous iterations. A modification of the steepest-descent above is the conjugate gradient method which avoids this pitfall by making a series of steps along a set of \( A \)-orthogonal directions. This means that subsequent iterations do not back-track in the same way as is possible with steepest descent.

Two vectors, say \( x \) and \( y \), are \( A \)-orthogonal if they satisfy

\[
x^T A y = 0 \tag{B.13}
\]

which leads to a line search optimum for \( A \)-orthogonal directions:

\[
\alpha = \frac{r_i^T r_i}{d_i^T A d_i} \tag{B.14}
\]

where \( d_0 \) are the search directions and \( r_0 \) are the data residuals. This leads to the standard method of conjugate gradients described by algorithm 2.

**Algorithm 2** Conjugate gradient algorithm

```
Initialize with \( d_1 = r_1 = b - A m_1 \)
for \( i = 1 \) to \( n \) do
  \( \alpha_i = \frac{r_i^T r_i}{d_i^T A d_i} \)
  \( r_{i+1} = r_i - \alpha_i A d_i \)
  \( m_{i+1} = m_i + \alpha_i d_i \)
  \( \beta_{i+1} = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i} \)
  \( d_{i+1} = r_{i+1} + \beta_{i+1} d_i \)
end for
```
Appendix C

Prior information choice

C.1 Constraining the time points using a uniform prior distribution

In chapters 4, 5 and 7 the time points of the ground surface temperature histories have been constrained using a uniform order statistics prior (see equation 4.5). This prior acts to bias the times points to being uniformly spaced out over the time domain. Here a uniform prior which places no constraint on the spacing is explored for completeness. A uniform probability distribution on a set of k points takes the form (e.g. Denison et al., 2002):

\[ p(t) = \frac{k!}{(t_{max} - t_{min})^k K - 1} \]  \hspace{1cm} (C.1)

where the range of the possible times is \((t_{max}, t_{min})\) and \(K\) is the maximum allowed number of points and 2 is the minimum number allowed in the model setup. This places a uniform prior constraint on the number of points and on the time position of each of the points. The \(k!\) term then accounts for exchangeability of each of the \(k\) points. In a birth step of the reversible jump MCMC algorithm the prior ratio for the birth proposal will be

\[ \frac{p(t')}{p(t)} \bigg|_b = \frac{k + 1}{(t_{max} - t_{min})} \]  \hspace{1cm} (C.2)
and for a death proposal this ratio is

\[
p(t')^d \cdot p(t)\]

\[
\frac{p(t')}{p(t)} = \frac{(t_{\text{max}} - t_{\text{min}})}{d - 1}
\]

Multiplying each term respectively by the proposal term for the move type leads to

\[
\frac{q(m | m')}{q(m' | m)} \cdot \frac{p(t')} {p(t')} = \frac{d_{k+1}} {b_k}
\]

for the birth proposal and for the death proposal

\[
\frac{q(m | m')}{q(m' | m)} \cdot \frac{p(t')} {p(t')} = \frac{b_{k-1}} {d_k}
\]

as the terms in \(k\) and \(L\) (=\(t_{\text{max}} - t_{\text{min}}\)) cancel in both cases. The overall birth acceptance probability is then given by
\[ 
\alpha = \min \left[ 1, \frac{p(k+1)}{p(k)} \times \frac{p(T' \mid \varphi, k+1)}{p(T \mid \varphi, k)}, \right. \\
\left. \quad \times \frac{p(d \mid m', \varphi, (k+1))}{p(d \mid m, \varphi, k)} \times \frac{d_{k+1}}{b_k} \times \frac{1}{(\sigma_T \sigma_I)(t_+ - t_-)} \right], 
\] (C.6)

whilst for the death proposal it is given by

\[ 
\alpha = \min \left[ 1, \frac{p(k-1)}{p(k)} \times \frac{p(T' \mid \varphi, k-1)}{p(T \mid \varphi, k)}, \right. \\
\left. \quad \times \frac{p(d \mid m', \varphi, (k-1))}{p(d \mid m, \varphi, k)} \times \frac{b_{k-1}}{d_k} \right], 
\] (C.7)

The acceptance probability for the temperature perturb is given earlier by equation 4.12. For this uniform prior this acceptance probability is also used for the time perturb proposal. For a heat flux and \( T_{eq} \) update the acceptance probability is given by equation 4.11.

A synthetic example was calculated using the modified acceptance probabilities described above. For this example the Beck et al. (1992) data set example of chapter 4.4.2 was used. The modified RJ-MCMC algorithm was run for 100,000 iterations with the first 20,000 removed as burn in. The resultant posterior pdf of the temperature history is shown in figure C.1. Comparison of the two posterior distributions of the GST history (figures 4.9 and C.1) shows little difference with both results showing a preference for cooling to around 0.5°C at 300 years before present and neither method able to resolve the very brief cool excursion at 200 years. The asymmetry of the credible limits in both cases show that the data and prior do not rule out cooler temperatures at 300 years.

This examples demonstrates that the uniform order statistics prior distribution used in this thesis does not impart a strong bias on the posterior distributions obtained. In future work a prior distribution which biases the model towards placing more time points in the recent past may prove effective and help to provide better resolution of the inferred temperature history over the last one or two centuries.
Appendix D

Data sources

D.1 Proxy and instrumental data

The instrumental and proxy data used for the synthetic inversions are available at the World Data Center for Paleoclimatology http://www.ncdc.noaa.gov/paleo/recons.html. Figure D.1 shows the temperature data used in synthetic examples. This is a compilation of reconstructed northern hemisphere temperatures (Moberg et al., 2005) and instrumental data (Jones and Moberg, 2003).

Figure (D.2) shows the Central England temperature record (Manley, 1974, Parker et al., 1992) which is the longest accurate instrumental temperature series from anywhere

![Deviation from 1960-1991 mean](image)

**Figure D.1:** Surface temperature data used in synthetic inversion cases: proxy reconstruction (Moberg et al., 2005) and instrumental measurements (Jones and Moberg, 2003).
in the world. For the earliest part of the record from 1659 to October 1722 the monthly values are given to the nearest whole degree, but with a period from 1699 to 1706 given to the nearest 0.1°C. The varying precision of the record accounts for the changing quality level of data at different times in the past. Uncertainty on the more recent part of the record has been investigated by Parker and Horton (2005) and a discussion of the record as a whole is given by Jones (1999).

D.2 International Heatflow Commission database

The UK borehole data is included in the World Data Center Borehole Paleoclimate data set which is available at http://www.ncdc.noaa.gov/paleo/borehole/ borehole.html. This set includes individually derived GST reconstructions (Huang et al., 2000). However, the data for the UK must be obtained separately from the British Geological Survey (BGS) (Rollin, 1987).

D.3 Nirex Sellafield borehole data

Tables D.1, D.2 and D.3 give the basic information from the Nirex Sellafield data set. For the 5 boreholes examined there are temperature-depth data, thermophysical values from cores and the depths of the main lithological units in each borehole.
## Table D.1: Sellafield borehole summary information for BH2,3,4,5 and 7a.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>Depth range(m)</th>
<th>No. values</th>
<th>$q_0$($\text{mWm}^{-2}$)</th>
<th>$T_{eq}$($^\circ\text{C}$)</th>
<th>Log date</th>
</tr>
</thead>
<tbody>
<tr>
<td>BH2</td>
<td>14.6, 1602.34</td>
<td>10,444</td>
<td>62.1</td>
<td>8.13</td>
<td>16.01.1992</td>
</tr>
<tr>
<td>BH4</td>
<td>8.45, 1258.32</td>
<td>8,213</td>
<td>59.2</td>
<td>8.37</td>
<td>20.12.1991</td>
</tr>
<tr>
<td>BH5</td>
<td>0.18, 1249.85</td>
<td>8,203</td>
<td>58.2</td>
<td>8.42</td>
<td>20.7.1992</td>
</tr>
<tr>
<td>BH7a</td>
<td>0.00, 1004.72</td>
<td>6,601</td>
<td>61.1</td>
<td>8.76</td>
<td>29.9.1992</td>
</tr>
</tbody>
</table>

## Table D.2: Depths of lithological units for the 5 Sellafield boreholes

<table>
<thead>
<tr>
<th>Borehole</th>
<th>formation</th>
<th>upper depth(m)</th>
<th>lower depth(m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BH2</td>
<td>Quaternary</td>
<td>5.02</td>
<td>33.05</td>
</tr>
<tr>
<td></td>
<td>Calder Sandstone</td>
<td>33.05</td>
<td>62</td>
</tr>
<tr>
<td></td>
<td>St Bees Sandstone</td>
<td>62</td>
<td>400.72</td>
</tr>
<tr>
<td></td>
<td>Brockram</td>
<td>400.72</td>
<td>467.55</td>
</tr>
<tr>
<td></td>
<td>Borrowdale Volcanic Group</td>
<td>467.55</td>
<td>1610</td>
</tr>
<tr>
<td>BH3</td>
<td>Ormskirk Sandstone</td>
<td>6.56</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td>Calder Sandstone</td>
<td>50</td>
<td>579.5</td>
</tr>
<tr>
<td></td>
<td>St Bees Sandstone</td>
<td>579.5</td>
<td>1133.98</td>
</tr>
<tr>
<td></td>
<td>St Bees Shale</td>
<td>1133.98</td>
<td>1269.24</td>
</tr>
<tr>
<td></td>
<td>St Bees Evaporites</td>
<td>1269.24</td>
<td>1315.22</td>
</tr>
<tr>
<td></td>
<td>Brockram</td>
<td>1315.22</td>
<td>1473.82</td>
</tr>
<tr>
<td></td>
<td>Carboniferous Limestone</td>
<td>1473.82</td>
<td>1622.82</td>
</tr>
<tr>
<td></td>
<td>Borrowdale Volcanic Group</td>
<td>1622.82</td>
<td>1952.32</td>
</tr>
<tr>
<td>BH4</td>
<td>Quaternary</td>
<td>5.02</td>
<td>27.31</td>
</tr>
<tr>
<td></td>
<td>Calder Sandstone</td>
<td>27.31</td>
<td>29</td>
</tr>
<tr>
<td></td>
<td>St Bees Sandstone</td>
<td>29</td>
<td>366</td>
</tr>
<tr>
<td></td>
<td>Brockram</td>
<td>366</td>
<td>411.75</td>
</tr>
<tr>
<td></td>
<td>Borrowdale Volcanic Group</td>
<td>411.75</td>
<td>1260</td>
</tr>
<tr>
<td>BH5</td>
<td>Quaternary</td>
<td>5.02</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>Calder Sandstone</td>
<td>9</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>St Bees Sandstone</td>
<td>69</td>
<td>406.11</td>
</tr>
<tr>
<td></td>
<td>Brockram</td>
<td>406.11</td>
<td>489.83</td>
</tr>
<tr>
<td></td>
<td>Borrowdale Volcanic Group</td>
<td>489.83</td>
<td>1260</td>
</tr>
<tr>
<td>BH7a</td>
<td>Quaternary</td>
<td>6.15</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>Calder Sandstone</td>
<td>30</td>
<td>57.5</td>
</tr>
<tr>
<td></td>
<td>St Bees Sandstone</td>
<td>57.5</td>
<td>405.3</td>
</tr>
<tr>
<td></td>
<td>St Bees Shale</td>
<td>405.3</td>
<td>482.7</td>
</tr>
<tr>
<td></td>
<td>Brockram</td>
<td>482.7</td>
<td>523.3</td>
</tr>
<tr>
<td></td>
<td>Carboniferous Limestone</td>
<td>523.3</td>
<td>577.83</td>
</tr>
<tr>
<td></td>
<td>Borrowdale Volcanic Group</td>
<td>577.83</td>
<td>1010</td>
</tr>
</tbody>
</table>

## Table D.3: Thermophysical properties for Sellafield area formation rocks.

<table>
<thead>
<tr>
<th></th>
<th>Quat.</th>
<th>Calder</th>
<th>St Bees SS</th>
<th>Shale</th>
<th>Brockham</th>
<th>Carb</th>
<th>BVG</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$(Wm$^{-1}$ K$^{-1}$)</td>
<td>3.1</td>
<td>3.3</td>
<td>3.1</td>
<td>3.1</td>
<td>2.5</td>
<td>2.7</td>
<td>2.5</td>
</tr>
<tr>
<td>$C$(Jkg$^{-1}$ K$^{-1}$)</td>
<td>845</td>
<td>845</td>
<td>845</td>
<td>845</td>
<td>1133</td>
<td>1133</td>
<td>843</td>
</tr>
<tr>
<td>$A$(Wm$^{-3}$)</td>
<td>1.0×10$^{-6}$</td>
<td>1.0×10$^{-6}$</td>
<td>1.0×10$^{-6}$</td>
<td>1.0×10$^{-6}$</td>
<td>1.7×10$^{-6}$</td>
<td>1.0E-6</td>
<td>2.0×10$^{-6}$</td>
</tr>
<tr>
<td>$\rho$(gcm$^{-3}$)</td>
<td>2.094</td>
<td>2.904</td>
<td>2.326</td>
<td>2.761</td>
<td>2.634</td>
<td>2.717</td>
<td>2.712</td>
</tr>
</tbody>
</table>
Appendix E

Computer code and model output

The attached CD contains all of the computer code used in this work as well as all the processed output files. A table of contents of the CD is given below in table E.1.

<table>
<thead>
<tr>
<th>Relevant chapters</th>
<th>CD directory</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>RJ-MCMC</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/RJ_MCMC_code</td>
<td>Source code</td>
</tr>
<tr>
<td></td>
<td>/BeckSynthetic</td>
<td>Beck et al. example</td>
</tr>
<tr>
<td></td>
<td>/MobergSyntheticCases</td>
<td>Moberg et al. Synthetic cases</td>
</tr>
<tr>
<td></td>
<td>/boreholes</td>
<td>5 UK real data examples</td>
</tr>
<tr>
<td>5</td>
<td>BPM</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/Code</td>
<td>Source code</td>
</tr>
<tr>
<td></td>
<td>/Synthetic</td>
<td>Synthetic BPM output</td>
</tr>
<tr>
<td></td>
<td>/UK_Uniform</td>
<td>UK BPM output for uniform prior case</td>
</tr>
<tr>
<td></td>
<td>/UK_Poisson</td>
<td>UK BPM output for Poisson prior case</td>
</tr>
<tr>
<td></td>
<td>/UKboreholedata</td>
<td>Complete UK dataset</td>
</tr>
<tr>
<td>6-8</td>
<td>3DCodes</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/gem</td>
<td>Mesh generation software</td>
</tr>
<tr>
<td></td>
<td>/potinv</td>
<td>3D simulation and inversion routines</td>
</tr>
<tr>
<td></td>
<td>/temsuf.f</td>
<td>Surface boundary condition routine</td>
</tr>
<tr>
<td>7</td>
<td>3DRJ-MCMCinversion</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/1Dinvversionsof3Ddata</td>
<td>Example from figure 7.7</td>
</tr>
<tr>
<td></td>
<td>/3DLapseRateEx</td>
<td>Example from figure 7.6</td>
</tr>
<tr>
<td></td>
<td>/BasalHtFinEx</td>
<td>Example from figure 7.8</td>
</tr>
<tr>
<td></td>
<td>/UncertainConductivityExample</td>
<td>Example from figure 7.9</td>
</tr>
<tr>
<td></td>
<td>/Homogeneity</td>
<td>Example from figure 7.11</td>
</tr>
<tr>
<td>8</td>
<td>NLCG</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/1</td>
<td>Example from figure 8.3</td>
</tr>
<tr>
<td></td>
<td>/2</td>
<td>Example from figure 8.4</td>
</tr>
<tr>
<td>5</td>
<td>Matlab</td>
<td></td>
</tr>
<tr>
<td></td>
<td>/VoronoiMat.m</td>
<td>Function to plot Voronoi tessellation</td>
</tr>
<tr>
<td></td>
<td>/VoronoiScript.m</td>
<td>Script to plot pdf of Voronoi partitions</td>
</tr>
</tbody>
</table>