Interplay between Changing Climate and Species'

Ecology Drives Macroevolutionary Dynamics

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1 Ecological change provokes speciation and extinction, but our knowl-
2 edge of the interplay among the biotic and abiotic drivers of macroevo-
3 lution remains limited. Using the unparalleled fossil record of Ceno-
4 zoic macroperforate planktonic foraminifera, we demonstrate that
5 macroevolutionary dynamics depend upon the interaction between
6 species' ecology and the changing climate. This interplay drives
7 diversification, but differs between speciation probability and ex-
8 tinction risk: speciation was more strongly shaped by diversity-
9 dependence than by climate change, whereas the reverse was true for
10 extinction. Crucially, no single ecology was optimal in all environ-
11 ments and species with distinct ecologies had significantly different
12 probabilities of speciation and extinction. The ensuing macroevolu-
13 tionary dynamics depend fundamentally on the ecological structure
14 of species' assemblages.

15 The wide-ranging mechanisms that generate and maintain biodiversity have been grouped
16 in many different ways, but a fundamental distinction exists between biotic and abiotic
17 drivers (1–5). If interactions among species are the dominant drivers of evolution – as
18 in the “Red Queen” model (1, 4) – then diversification rates among groups of interact-
19 ing species are expected to show diversity-dependent dynamics with ongoing turnover at
20 equilibrium. A consequence of this mechanism is that diversification rates are expected

to decrease as a function of diversity. Conversely, if evolution is driven chiefly by changes in the physical environment – styled the “Court Jester” model (3) in contrast to the “Red Queen” – macroevolutionary dynamics should be dominated by clade-wide effects of abrupt abiotic perturbations. Although the interplay between these alternative drivers has long been recognized as fundamental for regulating diversity (6, 7), progress towards understanding their interaction has been slow (2). The fossil record’s incompleteness often necessitates temporally and taxonomically coarse paleontological analyses (7–10), while molecular phylogenies are restricted to extant species and therefore offer little insight into extinction (11, 12). To distinguish how interwoven biotic and abiotic processes regulate diversity, high-resolution data on multiple forcing mechanisms should be allied to paleontological, species-level phylogenies constructed on sufficiently complete fossil records over substantial periods of evolutionary history. This resolution is rare (2, 6), but Cenozoic macroperforate planktonic foraminifera provide a suitable record for testing these hypotheses (13).

Planktonic foraminifera are sexually-reproducing protists distributed throughout the world’s oceans. The calcium carbonate “shells” (tests) of dead individuals rain down on the ocean floor and can, under favorable conditions, generate continuous microfossil sequences that span millions of years. The group’s usefulness for stratigraphic correlation (14) and paleoclimatic reconstruction (15) has led to extensive documentation of their morphology (14) and depth habitats (15). The phylogenetic relationships within the macroperforate clade of the Cenozoic have recently been revised comprehensively (13)

applying Simpson’s evolutionary species concept (16). Under this concept, each species is intended to represent “a single line of descent” (16) that begins with a speciation (cladogenetic) event and ends in extinction. The completeness of this group’s fossil record is such that species have an 81% chance of being detected per million year interval (Fig. S2): this species-level fossil record is at least as good as the best-preserved genus-level records of macro-invertebrates (17).

The macroperforate clade has diversified from two species that survived the end-Cretaceous mass extinction into 32 morphologically distinct species today, though the rise in diversity has been far from smooth (Fig. 1). The sharpest fall in diversity was during the Eocene - Oligocene transition, when rapid global cooling led to the development of the Antarctic ice cap (15). This suggests that climate change has been important in macroevolution so we approximated the complex, multifaceted climate system using the mean and variability of oxygen isotopic composition of deep sea carbonates (15, 18). Clade growth ($\ln(\frac{N_{t+1}}{N_t})$, detrended, N_t is the number of species in each 1 million year bin t) was poorly predicted by climate (18, Fig. 2A, Table S1). Models based on diversity-dependence only used diversity at the start of each bin and assume a constant limit to niche availability (a taxonomic analogue to a demographic “carrying capacity”), but predictions were similarly poor (Fig. 2B, Table S1). The clade’s macroevolutionary dynamics are therefore not well-predicted by either a strictly abiotic (Fig. 2A) or a strictly biotic model (Fig. 2B).

Any clade will be comprised of species with distinct ecologies. If these ecologies have conferred a macroevolutionary advantage on certain species over others, models that incorporate ecology will provide a better description of observed changes in macroevolutionary dynamics than if all species are assumed equal. To test this hypothesis, we grouped species by their depth habitat and morphology, which taken together, we used as a proxy for species' ecology (18). Although it is impossible to obtain an experimental link between traits and fitness in fossils, certain traits are thought to indicate functional differences that reflect different ways of life. For example, the acquisition of spines occurred in the earliest Cenozoic, is hypothesized to indicate the transition to a carnivorous diet (19) and to have initiated the hosting of photosynthetic algal symbionts (20); while the evolution of a keel is thought in some instances to be associated with the invasion of new depth habitats (21). The assemblage in the warm Eocene oceans was dominated by species inhabiting the mixed layer, whereas most species in the stratified oceans of the Pliocene lived and reproduced near the thermocline where the temperature gradient is much steeper than elsewhere in the water column. The ecological composition of the clade has fluctuated (Fig. 1), with the relative dominance of each group apparently waxing and waning with the changing climate.

Ecology is more strongly predictive of clade growth than either climate or diversity, but model fit is at best moderate (Fig. 2C, Table S1). Models containing interactions among pairs of these variables are significantly and substantially better, but model support was strong only when species with distinct ecologies were permitted to respond differently

to changes in diversity and climate (evidence weight > 0.99 , Fig. 2F, Table S1). The importance of interactions among climate, diversity and ecology suggests that ecological variation enabled the clade’s standing diversity to respond rapidly to climatic fluctuations. This interpretation strengthens arguments that the “Red Queen” and “Court Jester” are not mutually exclusive hypotheses of evolutionary diversification (2).

Discrete-time analysis, such as that above, may introduce bias when diversification occurs in continuous time because there is no ideal bin length to maximize the accuracy of clade growth estimates (22). Here, we use the Euler-Lotka equation (22, 23) to provide an estimate of per-capita growth for an ecologically-structured clade with ongoing speciation and extinction. We used parametric survival analysis with censoring (24) to obtain parsimonious extinction and speciation functions (18, 25). This approach does not resort to discretizing a continuous process and allows direct testing of two cornerstone assumptions of macroevolutionary theory (26): a species’ age does not influence its chances of either going extinct (i.e., Van Valen’s law, 1) or of speciating.

Extinction risk increased with age when diversity dependence, climate change and species’ ecology were incorporated (Figs. 3, S3). This suggests rejection of Van Valen’s law (1, for similar patterns in morphospecies, see 27), though we note that the lower extinction risk of young species may reflect a veil line in the detection probability of short-lived species over the 65 million year Cenozoic era . We also found that the species most likely to speciate were young (Fig. S3). This result is consistent with the frequently-observed

103 “early-burst” pattern of diversification, in which rapid clade growth occurs over short
104 periods of geological time early in a clade’s history and thereafter slows due to diversity-
105 dependence (28). Speciation probability was affected more by biotic variables than by
106 abiotic ones, whereas the opposite was true for extinction risk (Fig. 3). Species’ ecol-
107 ogy meant that the impacts of diversity and climatic fluctuations were not felt uniformly
108 across the phylogeny: the extinction and speciation functions differed among species with
109 photosymbionts, keels and spines and between greenhouse and icehouse oceans (Fig. S3).
110 Identifying a fixed carrying capacity is non-trivial because the response of any assemblage
111 to climate change depends upon the species within it (Fig. S4) and differs between specia-
112 tion probability and extinction risk (Fig. 3). Not all species are one and the same: ignoring
113 ecological differences among them limits understanding of the clade’s macroevolutionary
114 dynamics.

115 The continuous-time model gives a deterministic measure of clade growth; we incor-
116 porated the impact of changing diversity and climate by parameterizing these variables
117 at speciation and thereby assume that conditions early in a species’ existence have long-
118 lasting evolutionary consequences. Taking an approach that spans the Cenozoic maxi-
119 mizes the number of bursts of diversification under investigation, but restricts our ability
120 to disentangle complex components of climate change and how they impact biodiversity.
121 Despite these limiting assumptions, the continuous-time model captured key features of
122 the macroevolutionary dynamics, such as highest clade growth in greenhouse and highly
123 stratified oceans (Fig. S4). The binned analysis is complementary to the continuous-time

one because it incorporates climate variability during a species' existence (though still assumes a single proxy for climate). The consistency of conclusions from the two approaches supports our interpretation that diversity-dependence, climate change and species' ecology interact to drive macroevolutionary dynamics. Approaches based only on extant diversity can identify some components of diversification (Table S4), but neglect competition among now-extinct species and therefore cannot reveal how biotic interactions among them affected diversity patterns in past environments (Fig. 4).

What biotic and abiotic factors should models of diversification consider? An often-invoked null hypothesis is constancy of birth and death rates, i.e. constant rates Markov (26). The ubiquitous significance of species level diversity-dependence in the models presented here violates this fundamental assumption. The less restrictive, equal-rates Markov model permits speciation and extinction probabilities to change through time, provided they do not vary among contemporaneous species (26). This assumption is opposed by our result that young species with similar ecologies are more likely to speciate under particular climatic conditions than older species with other ecologies (Figs. 3, S4). Finally, speciation probability was more strongly shaped by diversity-dependence than by climate change, whereas the reverse was true for extinction risk (Fig. 3): decomposing macroevolutionary dynamics into its constituent parts is a useful step towards a more complete understanding of how biodiversity is generated and destroyed (8).

We conclude that neither the "Red Queen" nor the "Court Jester" is the dominant

macroevolutionary force; instead it is the interplay of biotic and abiotic variables that regulates diversity and drives speciation and extinction (Figs. 2, 3). Contrary to recent analyses of global marine diversity patterns (9), our results suggest that species' ecology plays a key role in determining overall diversity and gives clearer insights into macroevolutionary dynamics than is possible by treating clades as homogeneous wholes.

References

- [1] L. van Valen, A new evolutionary law. *Evol. Theor.* **1**, 1-30 (1973).
- [2] M. J. Benton, The red queen and the court jester: Species diversity and the role of biotic and abiotic factors through time. *Science* **323**, 728-732 (2009).
- [3] A. D. Barnosky, Distinguishing the effects of the red queen and court jester on miocene mammal evolution in the northern rocky mountains. *J. Vertrebr. Paleontol.* **21**, 172-185 (2001).
- [4] N. C. Stenseth, J. Maynard-Smith, Coevolution in ecosystems: red queen evolution or stasis? *Evolution* **38**, 870-880 (1984).
- [5] C. Venditti, A. Meade, M. Pagel, Phylogenies reveal new interpretation of speciation and the red queen. *Nature* **463**, 349-352 (2010).
- [6] J. W. Valentine, Determinants of diversity in higher taxonomic categories. *Paleobiology* **6**, 444-450 (1980).
- [7] D. Jablonski, Species selection: theory and data. *Ann. Rev. Ecol. Evol. Syst.* **39**,

501-524 (2008).

[8] J. Alroy, Dynamics of origination and extinction in the marine fossil record. *P. Natl. Acad. Sci. USA* **105**, 11536-11542 (2008).

[9] J. Alroy, The shifting balance of diversity among major marine animal groups. *Science* **329**, 1191-1194 (2010).

[10] M. Foote, Origination and extinction components of taxonomic diversity: Paleozoic and post-paleozoic dynamics. *Paleobiology* **26**, 578-605 (2000).

[11] A. Purvis, Phylogenetic approaches to the study of extinction. *Ann. Rev. Ecol. Evol. Syst.* **39**, 301-319 (2008).

[12] T. B. Quental, C. R. Marshall, Diversity dynamics: molecular phylogenies need the fossil record. *Trends in Ecol. & Evol.* **25**, 434-441 (2010).

[13] T. Aze, *et al.*, A phylogeny of cenozoic planktonic foraminifera from fossil data. *Biol. Rev.* **in press** (2011).

[14] W. A. Berggren, D. V. Kent, C. C. Swisher III, M.-P. Aubry, *A Revised Cenozoic Geochronology and Chronostratigraphy* (SEPM (Society for Sedimentary Geology), 1995).

[15] J. Zachos, M. Pagani, L. Sloan, E. Thomas, K. Billups, Trends, rhythms, and aberrations in global climate 65 ma to present. *Science* **292**, 686-693 (2001).

[16] G. G. Simpson, *Principles of Animal Taxonomy* (Columbia University Press, 1961).

[17] M. Foote, J. Sepkoski Jr., Absolute measures of the completeness of the fossil record. *Nature* **398**, 415-417 (1999).

- 184 [18] Materials and methods are available as supporting material on Science Online.
- 185 [19] C. Hemleben, D. Mühlen, R. K. Olsson, W. A. Berggren, Surface texture and the first
186 occurrence of spines in planktonic foraminifera from the early tertiary. *Geologische*
187 *Jahrbuch A* **128**, 117-146 (1991).
- 188 [20] R. D. Norris, Symbiosis as an evolutionary innovation in the radiation of paleocene
189 planktic foraminifera. *Paleobiology* **22**, 461-480 (1996).
- 190 [21] R. D. Norris, Extinction selectivity and ecology in planktonic foraminifera. *Palaeo-*
191 *geog., Palaeoclimatol., Palaeoecol.* **95**, 1-17 (1992).
- 192 [22] A. M. de Roos, Demographic analysis of continuous-time life-history models. *Ecol.*
193 *Lett.* **11**, 1-15 (2008).
- 194 [23] F. R. Sharpe, A. J. Lotka, A problem in age distribution. *Phil. Mag. Series 6* **21**,
195 435-438 (1911).
- 196 [24] J. Kalbfleisch, R. L. Prentice, *The Statistical Analysis of Failure Time Data* (New
197 York, John Wiley, 1980).
- 198 [25] K. P. Burnham, D. R. Anderson, *Model selection and multimodel inference. a practical*
199 *information-theoretical Approach*. (Springer-Verlag, New York., 2002).
- 200 [26] S. Nee, Birth-death models in macroevolution. *Ann. Rev. Ecol. Evol. Syst.* **37**, 1-17
201 (2006).
- 202 [27] N. A. Doran, A. J. Arnold, W. C. Parker, F. W. Huffer, Is extinction age dependent?
203 *Palaios* **21**, 571-579 (2006).
- 204 [28] A. B. Phillimore, T. D. Price, Density-dependent cladogenesis in birds. *PLoS Biol*

205 **6**, e71 (2008).

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210 13.

211 **Supporting Online Material**

212 Full Methods, including additional References

213 Figs. S1 - S4

214 Tables S1 - S4

Figure Legends

Fig. 1. The relative frequencies of morphologies (**A**) and depth habitats (**B**) of macroperforate planktonic foraminifer species across the Cenozoic (13) has fluctuated substantially. Time (million years before present) is based on the marine geological time scale (14); “Pl” and “Pt” refer to Pliocene and Pleistocene, respectively.

Fig. 2. Discrete time models incorporating interactions among diversity, climate and species’ ecology outperformed all others. The dashed grey line is $y=x$; a model that predicted observed clade growth perfectly would have points only on this line. For all summary statistics and models, see Table S1.

Fig. 3. Speciation probability and extinction risk varied significantly with species’ age (**A**), diversity (**D**), climate (**C**), species’ ecology (**E**) and their interactions (letter combinations). The dashed lines denote a difference in corrected Akaike Information Criterion ($\Delta AICc$) of 2; interactions that did not reach this threshold for “substantial” support and inclusion in the model (25) are not shown (18).

Fig. 4. The impact of extinction on macroevolutionary dynamics of macroperforate planktonic foraminifera is clear when fossil species are used (blue), but not when analysis is based solely on extant lineages (red). Time (million years before present) is based on the marine geological time scale (14); “Pl” and “Pt” refer to Pliocene and Pleistocene, respectively.

Predicted Clade Growth

Observed Clade Growth, $\ln(N_{t+1}/N_t)$

log lineages

**Interplay between Changing Climate and Species' Ecology
Drives Macroevolutionary Dynamics:**

Supporting Online Material

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1 Full Methods

2 1.1 Cenozoic macroperforate planktonic foraminifera

3 The complete phylogeny of Cenozoic macroperforate planktonic foraminifer species was
4 developed from paleontological work that details the evolutionary relationships and tem-
5 poral distributions of species identified morphologically and without molecular evidence
6 (13). Under favorable conditions, the tests (shells) of dead individuals sink and accumulate
7 continuously on the seabed forming an unparalleled resource for stratigraphic correlation
8 (14), paleoclimatic reconstruction (15) and macroevolutionary research. Substantial tem-
9 poral intergradation of morphospecies meant that we chose to perform all analyses on the
10 phylogeny of evolutionary species' lineages (16) (hereafter, species) to minimize inflation
11 of speciation and extinction rates caused by “pseudospeciation” and “pseudoextinction”
12 (29). In $\sim 85\%$ of cases, persistent ancestry at the time of speciation (cladogenesis) could
13 be assigned on the basis of morphological similarity (13). Each morphospecies was as-
14 signed to one of 19 groups delimited on test morphology and one of 6 delimited on inferred
15 depth habitat (13).

16 1.2 Mathematical & Statistical Models

17 The support for particular statistical models was assessed using an information theoretic
18 approach (25), selecting the model with most support among various combinations of di-
19 versity, climate, species' ecology as main effects and their two-way interactions (30).

1.2.1 Explanatory Variables

Models were constructed using data on all species that originated during the Cenozoic; two species (*Hedbergella holmdelensis* and *H. monmouthensis*) persisted through the end-Cretaceous mass extinction around 65 million years ago and were excluded from all analysis (31).

Because the planktonic foraminifera are distributed throughout the oceans, it is appropriate to compare their evolutionary patterns with the global climatic history of the Cenozoic era. Although climate change is complex and multifaceted, the oxygen isotopic composition ($\delta^{18}\text{O}$) of deep sea carbonates provides a single time series recording direct, independent evidence for “trends, rhythms and aberrations” of Cenozoic climate history (15, 32). Isotopic signature shows substantial site-specificity (15), which we removed using a generalised additive model (GAM, 33) for use in our models. The $\delta^{18}\text{O}$ record (32) was regressed against age and the mean-centred, fitted values from the model were our paleoclimatic proxy. We set the upper limit on the number of knots, i.e. the “wiggleness” (33) of the curve, at 900 because the default settings (~ 9) capture the trends but not the aberrations and there were substantial improvements in fit (assessed by minimizing the general cross validation scores, 33) between intermediate (~ 90) and higher orders of magnitude, but not thereafter (Fig. S1). The climate at identical times was modeled as identical across all oceans on Earth; replicated time horizons were therefore removed to leave 14,572 values.

Many of the 19 morphogroups recognised in (13) consisted of very few species; we therefore pooled them into operational groups based on morphological innovations associated with exploitation of distinct ecological niches (presence/absence of keels, spines and

photo-symbionts; see main text). Of the 8 possible combinations of these binary morphological traits, six were observed across the 210-species phylogeny (group size ranged from 11 to 63). Depth habitat was similarly re-cast as a three-way categorical variable (mixed layer in tropical/subtropical oceans, thermocline and sub-thermocline; see main text) by assimilating the 10 species that inhabit upwelling zones or high latitudes into the mixed layer and sub-thermocline groups, respectively. The thermocline is the point in the water column where the temperature gradient is steepest.

1.2.2 Discrete-time models

The usual approach to circumvent the coarse temporal resolution of much of the fossil record is to amalgamate events in supposedly homogeneous periods of time and analyse diversification, origination and extinction rates within these discrete bins (8, 9). We used bin lengths of 1 myr for our discrete analysis to trade-off temporal replication against data completeness (Fig. S2): at a bin length of 1 million years, species have an 81% chance of being detected in the Neptune database (34, 35).

Clade growth ($\ln(\frac{N_{t+1}}{N_t})$ where N_t denotes the number of species at time t) was detrended by taking first differences and then regressed against diversity at time t (ln-transformed), species ecology (proportions of species in the operational groups defined in §1.1.1 at time t), climate (mean [to investigate the direction of change] and range [to investigate the impact of climate variability within the bin] from time t to time $t + 1$ of the fitted values from the GAM) and two-way interactions in a linear least-squares model. For model selection procedure, see §1.2.4. Interactions among species' ecology groups were not incorporated because bins early in the sequence (when there are very

few species in low numbers of operational groups) have significantly high influence on all model fits, suggesting over-parameterization (36). We present results with the first bin omitted because the number of species rose from 2 to 7 during this bin, which artificially increased variance explained in the models and produced unsatisfactory diagnostic plots (36). The ranking of most important models was unchanged between models using all data and those presented with this one outlier removed.

1.2.3 Continuous-time models

Functions for extinction and speciation were obtained independently, and then united in the continuous-time diversification model developed by Lotka (23) and extended by de Roos (22) to incorporate multiple types of individuals or, as here, species. Species' duration was regressed against ecology (as the binary groups defined in §1.1.1), overall diversity, climate and all two-way interactions using parametric survival regression models (24) to obtain parsimonious functions for speciation and extinction as detailed in §1.2.4. To control for the effect of diversity dependence and climate on clade growth, we assume that conditions early in a species' existence have long-lasting evolutionary consequences and remain constant as at the time of speciation; therefore climate variability was not incorporated in this analysis. In addition, we tested for a non-linear response by fitting our climate proxy additionally as a quadratic term. Minimum adequate models for speciation and extinction were obtained independently (Tables S2, S3) and then united in the continuous-time model. We used censoring when the last appearance date of a species was not an extinction or speciation date, as appropriate. For extinction functions, this meant censoring extant species and in the ~15% of cases where neither descendant could

87 be identified unequivocally as the continuation of the ancestor; for speciation functions,
88 it meant censoring extant species and extinct species that did not speciate.

We modeled time to speciation or extinction as Weibull random variables. A Weibull random variable a consists of two parameters – scale (λ) and shape (k) – and has probability density function:

$$f(a; k, \lambda) = \begin{cases} \frac{k}{\lambda} \left(\frac{a}{\lambda}\right)^{k-1} e^{-\left(\frac{a}{\lambda}\right)^k} & \text{if } a \geq 0 \\ 0 & \text{if } a < 0 \end{cases}$$

where λ is the scale parameter and k the shape parameter; both λ and k are strictly positive. If $k \neq 1$ then the hazard function, i.e. instantaneous risk of failure (24), changes with age (a). A biological interpretation of $k < 1$ is elevated extinction of young species (hazard decreases with age); if $k > 1$ then the converse is true and species are more likely to go extinct as they get older. A value of $k = 1$ indicates constant hazard; under this scenario the Weibull distribution simplifies to the exponential distribution. For our purposes, this case indicates that species have a constant probability of extinction throughout their existence, i.e. follow Van Valen’s Law (1). Here, “hazard” represents the instantaneous probability of speciation or extinction of a species of age a . The Weibull hazard takes the form:

$$h(a; k, \lambda) = \frac{k}{\lambda} \left(\frac{a}{\lambda}\right)^{k-1}$$

According to the model (22, 23), the deterministic estimate of clade growth r is obtained by solving the following integral:

$$1 = \int_0^\infty e^{-r\alpha} b(\alpha) F(\alpha) d\alpha$$

$F(\alpha)$ in the Euler-Lotka equation is survival up to age α , which can be solved using hazard rates in the system of ordinary differential equations (ODEs) below. Following de Roos (22), let $L(a, r) = \int_0^a e^{-r\alpha} b(\alpha) F(\alpha) d\alpha$ and then solve the following system of ODEs under initial conditions of $S(0) = 1$ and $L(0, r) = 0$:

$$\frac{dS}{da} = -(m(a) + r)S(a) \quad \frac{dL}{da} = b(a)S(a)$$

where $m(a)$ is the extinction hazard and $b(a)$ the speciation hazard modeled as Weibull random variables. $b(a)$ and $m(a)$ contained statistically significant effects of photo-symbionts, keels and spines (Fig. S3, Table S3). Let $\mathbf{L}(A_m, r)$ be the matrix that relates the proportion of speciations in group i from an ancestral species in group j at a given age m :

$$\mathbf{L}(A_m, r) = \begin{bmatrix} L_{11}(A_m, r) & \cdots & L_{61}(A_m, r) \\ \vdots & \ddots & \vdots \\ L_{16}(A_m, r) & \cdots & L_{66}(A_m, r) \end{bmatrix}$$

The matrix is of rank 6 because that is the number of statistically-distinct groups observed; the main diagonal indicates species with the same morphology as their immediate ancestor while the off-diagonal elements relate species of a one type to ancestors of another type. Each element of $\mathbf{L}(A_m, r)$ is $L(a, r)$ as in the single-type case above for a particular combination of spines, keels and symbionts, scaled by the probability of having an ancestor of a particular group (we assumed this probability was constant and estimated it using observed mean transition rates). The system of ODEs outlined above is thus replaced by a multivariate version and, in this “multiple ecologies” case, r is the largest root (eigenvalue) of the multi-state dynamical system (22):

$$\det(\mathbf{L}(A_m, r) - \mathbf{I}) = 0$$

where *det* indicates determinant and $\mathbf{I}$ the identity matrix. r was obtained numerically (37), using Newton-Raphson iteration procedures.

1.2.4 Model Selection

The statistical models with most support were obtained by fitting multiple combinations of explanatory variables (diversity, climate and ecology) as main effects and two-way interactions. We selected the most parsimonious model based on the corrected Akaike Information Criterion (AICc, 25). AICc provides a compromise between explanatory power and parameters used scaled by a correction factor for small sample size (as sample size increases, AICc converges on the “uncorrected” Akaike Information Criterion); if multiple models differed by < 2 values ($\Delta AICc < 2$) then all have “substantial” support and we prefer that with the fewest parameters as the most parsimonious (25). We also report model weights, which sum to 1 and can be interpreted as evidence weights, i.e. the probability that a particular model provides the optimal description of the data among the set of candidate models (25).

The improvement of fit in discrete models (Fig. 2) and the contributions to extinction and speciation hazards (Fig. 3) were calculated following a procedure for obtaining phenomenological time series models (30). The approach entails fitting combinations of explanatory variables and then comparing among them using some metric of explanatory power (r^2 , AICc, ...). We calculated the difference in model fit between two candidate models using differences in AICc values because of the multi-parameter nature of the ecological groups. The difference between model fit of the minimum adequate (i.e., best) model and all other possibilities was calculated by removing each focal variable (including

interactions) in turn and comparing this new model with the minimum adequate model. The height of each bar in Fig. 3 is therefore the difference in AICc when each term is removed from the minimum adequate model, i.e., a measure of variance explained by that term only (30) and corrected for the degrees of freedom used by it (25).

The validation of the continuous-time model (Fig. S4) set the initial estimate of r for low diversities ($N=10$) at 0.3, and then iterated through increasing diversities using the preceding estimate of r for the initial estimate at subsequent diversity levels while holding the climate constant. Once r had been estimated for all diversity values in each climate state, climate was incremented (across the inter-quartile range) and the above procedure repeated until the lattices were filled.

1.2.5 Implementation and Software

All graphics were produced and analyses performed in the R environment for graphical and statistical computing (38) using the deSolve (37), mgcv (33), LASER (39), paleoPhylo (40) and survreg packages.

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2 Supplementary Figures

Figure S1. At a bin length of 1 million years, Cenozoic macroperforate planktonic foraminifer species have a per-bin probability of 81% of being detected in the Neptune database (34, 35), suggesting that this species-level fossil record is at least as good as the best genus-level records among macro-invertebrate groups (17). Data was downloaded from Neptune on 11-11-2010.

Figure S2. **Generalised additive models (33) were used to remove site specificity from the record of oxygen isotopic composition of deep sea (benthic) carbonates of the Cenozoic era (15, 32).** We increased the number of knots k because the default settings (top, $k < 9$) captured the trends in climate but not the aberrations (note the Paleocene-Eocene Thermal Maximum around ~ 55 million years ago, for example); the general cross validation scores for the curves were similar at intermediate $k < 90$ and high $k < 900$ levels, but inspection of diagnostic plots (residuals vs fitted values) were satisfactory only for the high level (note the Paleocene-Eocene Thermal Maximum around ~ 55 million years ago, for example).

Figure S3. **Extinction and speciation hazards for statistically distinct ecological groups changed in rank between Greenhouse and Icehouse oceans.** Hazard functions give the instantaneous probability of the modeled event. Color codes are: blue - spinose; green - keeled; red - symbionts; purple - spinose and symbionts; and black all others. Curves are drawn (up to the maximum recorded duration for the focal group) at the 1st and 3rd climate quartiles to represent the greenhouse and icehouse oceans at overall mean diversity.

Figure S4. **The continuous-time model captured key features of the clade’s macroevolutionary dynamics, including increased clade growth r at low and high values of our climate proxy and how different assemblages produce very different estimates of r even when all other parameters remain constant.** High $\delta^{18}\text{O}$ values reflect “greenhouse” oceans, whereas low $\delta^{18}\text{O}$ values are found in the more stratified oceans of today. The top panel is model estimates of r prior to the Eocene-Oligocene (E-O) transition; the middle panel is for the whole Cenozoic as reported in the main text; and the bottom panel for the post E-O assemblage.

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3 Supplementary Tables

Model	r^2	Parameters	AICc	Δ AICc	Model Weight	Panel
MAM of D*C*E	0.6618	13	-247.2	0.0	0.9999	2f
D*E	0.4628	10	-227.3	19.9	0.0000	
D*C+E	0.4618	11	-224.2	23.0	0.0000	
D+E	0.3025	6	-221.5	25.7	0.0000	
D+C*E	0.5872	17	-220.5	26.7	0.0000	
Full	0.7255	23	-219.5	27.7	0.0000	
C*E	0.5450	16	-218.1	29.1	0.0000	2e
D+C+E	0.3090	8	-217.0	30.2	0.0000	
E	0.2060	5	-215.8	31.4	0.0000	2c
D*C	0.2598	7	-215.3	31.9	0.0000	2d
D	0.0459	2	-211.1	36.1	0.0000	2b
C+E	0.2093	7	-211.1	36.1	0.0000	
C	0.0533	4	-207.1	40.1	0.0000	2a
D+C	0.0468	4	-206.7	40.5	0.0000	

Table S1. **The best discrete-time models (ranked according to the corrected Akaike Information Criterion, AICc) featured interactions among diversity (D), climate (C) and species' ecology (E).** Letter combinations indicate multiple driver models with * indicating multiplicative effects (up to second-order only) and + additive effects. Model weights can be interpreted as the probability that the model is the best of those fitted; r^2 is the adjusted value from a standard least-squares model (36) with sample size = (number of bins) - 1. "MAM" abbreviates "minimum adequate model" (see §1.2.4).

Group	Extinction	Speciation
Symbionts	$\zeta + \kappa D + \eta O$	$\zeta + \epsilon^{sy} + \kappa D + \eta O$
Spinose	$\zeta + \epsilon^{sp} + \kappa D + \eta O$	$\zeta + \epsilon^{sp} + \kappa D + (\eta + \eta^{sp})O$
Spinose & Symbionts	$\zeta + \epsilon^{sp} + \kappa D + \eta O$	$\zeta + \epsilon^{sp} + \epsilon^{sy} + \kappa D + (\eta + \eta^{sp})O$
Keeled	$\zeta + \epsilon^{kl} + \kappa D + \eta O$	$\zeta + \kappa D + \eta O$
Keeled & Symbionts	$\zeta + \epsilon^{kl} + \kappa D + \eta O$	$\zeta + \epsilon^{sy} + \kappa D + \eta O$
Other (Intercept)	$\zeta + \kappa D + \eta O$	$\zeta + \kappa D + \eta O$

Table S2. **Variables included to obtain the scale parameters in the Weibull hazard functions for the six statistically-distinct ecological groups observed.** Capital letters refer to non-constant variables (D and O are overall diversity and oxygen isotope ratios, respectively); greek letters are parameters estimated from parametric survival regression (24). ζ indicates intercept; κ diversity-dependence; ϵ intercept adjustments for keeled (kl), spinose (sp) and symbiont (sy) groups; η deep-sea (benthic) oxygen isotope ratios as the climate proxy; η^{sp} is the interaction between climate and spinose species.

Parameter	Extinction				Speciation			
	Coef.	S.E.	z	p	Coef.	S.E.	z	p
ζ	2.325	0.103	22.7	***	2.445	0.154	15.8	***
κ	-0.737	0.255	-2.88	**	0.785	0.180	4.37	***
η	0.155	0.082	1.90		-0.209	0.154	-1.36	
ϵ^{sp}	0.405	0.142	2.86	**	0.397	0.184	2.16	*
ϵ^{kl}	-0.393	0.241	-1.63					
ϵ^{sy}					-0.712	0.234	-3.036	**
η^{sp}					0.843	0.249	3.385	***
κ^{sp}	0.838	0.324	2.59	**				
η^{kl}	0.634	0.232	2.73	**				
$\ln(k)$	-0.194	0.063	-3.08	**	0.164	0.059	2.77	**

Table S3. **Coefficients (Coef., with standard errors [S.E.], z-values and p-value codes) used in the extinction and speciation functions, obtained independently using parametric survival analysis with censoring (24).** The parameter codes are: ζ intercept; κ diversity-dependence; ϵ intercept adjustments for keeled (kl), spinose (sp) and symbiont (sy) groups, respectively; η deep-sea (benthic) oxygen isotope ratios as the climate proxy; η^{sp} is the interaction between climate and spinose species; k is the shape parameter. The p-value codes are: *** $p < 0.001$; ** $p < 0.01$; * $p < 0.05$; $p > 0.05$; blank lines indicate that these terms were only significant for the other hazard. For model selection procedure, see §1.2.4. The corrected Akaike Information Criterion (AICc) scores were 1042.1 and 1153.4 for extinction and speciation, respectively.

Model	Parameters	AICc	Δ AICc	Model Weight
Birth-Death	2	85.61	0.00	0.288
Pure Birth	1	86.00	0.10	0.274
Exponential diversity-dependent speciation	2	86.91	1.30	0.151
Logistic diversity-dependent speciation	2	88.00	2.39	0.087
Exponentially declining speciation	3	87.58	2.43	0.086
Exponentially increasing extinction	3	87.62	2.46	0.084
Variable extinction and speciation	4	88.94	4.43	0.031

Table S4. **The best-supported, most-parsimonious model based on extant species only was a pure-birth model, highlighting the difficulty in inferring patterns of extinction based on extant species only.** Gamma (41) was -1.496 ($p > 0.05$ on a one-tailed test assuming complete taxon sampling), indicating a failure to reject the null hypothesis that speciation rates have decreased over time. Models were fitted using the LASER package (39); for model selection procedure, see §1.2.4.

4 References

29. S. Stanley, S. *Macroevolution: pattern and process* (W.H. Freeman and Co., San Francisco, 1979).
30. T. Coulson, et al., Estimating the functional form for the diversity dependence from life-history data. *Ecology* **89**, 1661-1674 (2008)
31. R. K. Olsson, C. Hemleben, W. A. Berggren & B. T. Huber, *Atlas of Paleocene Planktonic Foraminifera*. No. 85 in Smithsonian Contributions to Paleobiology (Smithsonian Institution Press, 1999)
32. J. C. Zachos, G. R. Dickens & R. E. Zeebe An early Cenozoic perspective on greenhouse warming and carbon-cycle dynamics. *Nature* **451**, 279-283 (2008).
33. S. N. Wood, *Generalized Additive Models: An Introduction with R*, Texts in Statistical Science (Chapman and Hall, Boca Raton, FL, 2006)
34. Lazarus, D. B. Neptune: a marine micropaleontology database. *Math. Geol.*, **26**, 817-832 (1994).
35. Spencer-Cervato, C. The Cenozoic deep sea microfossil record: explorations of the DSDP/ODP sample set using the Neptune database. *Paleont. Elect.*, **2**, (1999).
36. Fox, J. A. *An R and S-PLUS Companion to Applied Regression* (Sage Publications, Thousand Oaks, California, 2002).
37. Soetaert, K., Petzoldt, T. & Setzer, R. W. Solving Differential Equations in R: Package deSolve. *J. Stat. Soft.* **33**, 1-25 (2010).
38. R Development Core Team, *R: a language and environment for statistical computing* (Vienna, 2010)

- 149 39. Rabosky, D. L. LASER: A Maximum Likelihood Toolkit for Detecting Temporal
150 Shifts in Diversification Rates From Molecular Phylogenies. *Evolutionary Bioinfor-*
151 *matics Online* **2**, 257-260 (2006)
- 152 40. Ezard, T.H.G. & Purvis, A. paleoPhylo: free software to draw paleobiological phy-
153 logenies. *Paleobiology* **35**, 460-464 (2009).
- 154 41. Pybus, O. G. & Harvey, P. H. Testing macro-evolutionary models using incomplete
155 molecular phylogenies. *Proc. Roy. Soc. Lond. B* **267**, 2267-2272 (2000).