Supplementary Information for

Southern high-latitude terrestrial climate change during the Paleocene–Eocene derived from a marine pollen record (ODP Site 1172, East Tasman Plateau)

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State space models

State space models assume there is an underlying "true" system, and what we observe is corrupted by observational noise. In particular, we assume that the "true" DCA axis score and Sea Surface Temperature (SST) evolve according to a bivariate Wiener process (e.g. Varughese and Pienaar 2013), i.e. if $\mathbf{x}(t) = \{x_{\mathrm{DCA}}(t), x_{\mathrm{SST}}(t)\}$is a vector of the DCA axis score and SST,

$$\mathbf{x}(t + \mathrm{D}t) \sim \mathrm{MVN}(\mathbf{x}(t), \mathrm{D}t\ \mathrm{S}) \qquad \text{Eq. (1)}$$

where S is a covariance matrix:

$$\Sigma = \begin{Bmatrix} \sigma_{DCA}^2 & \sigma_{DCA}\sigma_{SST}\rho \\ \sigma_{DCA}\sigma_{SST}\rho & \sigma_{SST}^2 \end{Bmatrix} \qquad \text{Eq. (2)}$$

So, the "true" DCA axis score and SST both diffuse over time, and if they are correlated then the off-diagonal term in S will be non-zero, and can be read as a correlation between the true values.

We assume that the observed values of the DCA axis score and SST are corrupted by random noise, which we assume is independent and normally distributed:

$$SST_i \sim N\ (x_{\mathrm{SST}}(t(i))\ , t^2_{SST}) \qquad \text{Eq. (3)}$$

$$DCA_i \sim N\,(x_{\mathrm{DCA}}(d(i)),t^2_{DCA}) \qquad \text{Eq. (4)}$$

The correlation between observations decays with time, but we can estimate the correlation between SST and DCA based on:

$$\mathrm{corr(SST,DCA)} = \frac{\Delta t \rho \sigma_{DCA}\sigma_{SST}}{\sqrt{(\Delta dt+\tau^2_{DCA})(\Delta t\sigma^2_{SST}+\tau^2_{SST})}}. \qquad \text{Eq. (5)}$$

We compared 60 SST datapoints with our 40 values of the DCA Axis 1 scores. Because only six of the SST datapoints and DCA Axis 1 sample scores are from the exact same depths, we estimated the values of DCA Axis 1 sample scores and SST through multiple imputation (e.g. Nakagawa and Freckleton, 2008); the missing data are treated as extra variables that are estimated in the same model. We took a Bayesian approach to the model fitting, which requires setting prior distributinos on the parameters and missing data. The initial "true" values, $x_{\mathrm{DCA}}(t)$ and $x_{\mathrm{SST}}(t)$, were given independent normal priors with mean zero and standard deviation of 100. s_{DCA}, s_{SST}, t_{DCA} and s_{SST} were all given uniform priors between 0 and 100, and the prior for the correlation, r, was a uniform distribution between -1 and 1.

Two chains were run and after a burn-in of 10^6 iterations, a further 10^5 iterations were run, thinned to every 10th iteration to give a total of 20.000 draws from the posterior. The R script for the analysis is given below.

References

Nakagawa, S. and Freckleton, R.P.: Missing inaction: the dangers of ignoring missing data. Trends Ecol. Evol., 23, 592-596, doi: 10.1016/j.tree.2008.06.014.

Varughese, M. M. and Pienaar E. A. D.: Statistical inference for a multivariate diffusion model of an ecological time series. Ecosphere, 4, art104, doi: 10.1890/ES13-00092.1, 2013.

R code Script for the state space model

wrote by Robert B. O'Hara

```
# Read in data, and merge into one data frame
DCA=read.xls("To bob.xlsx", sheet=2)
SST=read.xls("To bob.xlsx", sheet=3)
 names(SST)=c("Depth", "SST")

Data=merge(DCA,SST, by="Depth", all=T)
Data=Data[order(Data$Depth),]

# write.csv(Data, file="DCA_SST.csv")

# Write data for BUGS
DataToBUGS=list(NObs=nrow(Data), DCA=Data$DCA1, SST=Data$SST,
 Time=Data$Depth)
bugsData(DataToBUGS, "DCA_SSTbugs.txt")

# DataToBUGS=source("DCA_SSTbugs.txt")$value

# Plot the data
svg("Data.svg", width=8, height=6)
par(mfrow=c(2,1), mar=c(2,4,3,1), oma=c(2,0,0,0))
plot(DataToBUGS$Time, DataToBUGS$DCA, type="l", xlab="", ylab="DCA")
points(DataToBUGS$Time, DataToBUGS$DCA, pch=19,
 col=1+!is.na(DataToBUGS$SST), cex=0.5)
points(DataToBUGS$Time[!is.na(DataToBUGS$SST)],
 DataToBUGS$DCA[!is.na(DataToBUGS$SST)], pch=19, col=2, cex=0.5)
mtext("First DCA Coordinate", 3, line=0.5, adj=0.1)

plot(DataToBUGS$Time, DataToBUGS$SST, type="l", xlab="", ylab="Temperature")
points(DataToBUGS$Time, DataToBUGS$SST, pch=19,
 col=1+!is.na(DataToBUGS$DCA), cex=0.5)
points(DataToBUGS$Time[!is.na(DataToBUGS$DCA)],
 DataToBUGS$SST[!is.na(DataToBUGS$DCA)], pch=19, col=2, cex=0.5)
mtext("Sea Surface Temperature", 3, line=0.5, adj=0.1)
```

```
mtext("Depth", 1, line=2.53)
dev.off()

# Plot data with both SST and DCA
svg("Joint.svg", width=6, height=6)
par(mfrow=c(1,1), mar=c(4.1,4.1,1,1), oma=c(0,0,0,0))
plot(DataToBUGS$SST, DataToBUGS$DCA, xlab="Sea Surface Temperature",
 ylab="DCA score")
dev.off()

# Look at the correlation between values where we have both
cor(DataToBUGS$SST, DataToBUGS$DCA, use="c")

# The BUGS model: 2D diffusion + observation error
TheModel=function() {
 for(t in 1:NObs) {
	SST[t] ~ dnorm(X[t,1], tauSST)
	DCA[t] ~ dnorm(X[t,2], tauDCA)
 }
 for(p in 1:2) {
	X[1,p] ~ dnorm(0,0.0001)
 }
 for(t in 2:NObs) {
	for(p in 1:2) {
		for(pp in 1:2) {
			TauT[t,p,pp] <- Tau[p,pp]/max(sqrt(Time[t] - Time[t-1]),0.00001)
		}
	}
	X[t,1:2] ~ dmnorm(X[t-1,1:2], TauT[t,,])
 }
 for(p in 1:2) {
	SD.tau[p] ~ dunif(0,100)
	Sigma[p,p] <- SD.tau[p]*SD.tau[p]
	Sigma[p,3-p] <- rho*SD.tau[p]*SD.tau[3-p]
 }
 rho ~ dunif(-1,1)
 Tau[1:2,1:2] <- inverse(Sigma[,])

 Var[1,1] <- Sigma[1,1] + 1/tauSST
 Var[2,2] <- Sigma[2,2] + 1/tauDCA
 for(p in 1:2) {
	StdDev[p] <- sqrt(Var[p,p])
	Var[p,3-p] <- Sigma[p,3-p]
	for(pp in 1:2) {
		Corr[p,pp] <- Var[p,pp]/sqrt(Var[p,p]*Var[pp,pp])
	}
```

```
 }
 sdSST ~ dunif(0,100);tauSST <- pow(sdSST,-2)
 sdDCA ~ dunif(0,100);      tauDCA <- pow(sdDCA,-2)
}
writeModel(TheModel, "BUGSmodel.bug")

# Function to simulate initial values for the MCMC
SimInits=function(dat) {
#dat=DataToBUGS
  Use=!is.na(dat$SST) & !is.na(dat$DCA)
  DCA.lm=lm(dat$DCA[Use]~dat$SST[Use])
  DCA.newdata=data.frame(SST=dat$SST[is.na(dat$DCA)])
  DCApred=rnorm(sum(is.na(dat$DCA)), predict(DCA.lm,
 newdata=DCA.newdata),sd(resid(DCA.lm))/sqrt(2))
  DCAinit=ifelse(!is.na(dat$DCA), dat$DCA, DCApred)

  SST.lm=lm(dat$SST[Use]~dat$DCA[Use])
  SST.newdata=data.frame(DCAT=dat$DCA[is.na(dat$DCA)])
  SSTpred=rnorm(sum(is.na(dat$SST)), predict(SST.lm,
 newdata=SST.newdata),sd(resid(SST.lm))/sqrt(2))
  SSTinit=ifelse(!is.na(dat$SST), dat$SST, SSTpred)

  list(
    DCA=ifelse(!is.na(dat$DCA), NA, DCApred),
    SST=ifelse(!is.na(dat$SST), NA, SSTpred),
    X=cbind(
      rnorm(length(dat$DCA), DCAinit, sd(DCAinit)/sqrt(2)),
      rnorm(length(dat$SST), SSTinit, sd(SSTinit)/sqrt(2)) ),
      sdDCA=sd(dat$DCA, na.rm=T)/4, sdSST=sd(dat$SST, na.rm=T)/4,
    SD.tau=rgamma(2,10,100), rho=rbeta(1,48,2)
  )
}
# SimInits(DataToBUGS)

# Run BUGS
NChains=2  # 2 chains (mixes well, but takes time to converge)
bugsInits(replicate(NChains, SimInits(DataToBUGS), simplify=F), NChains,
        paste("DCA_SSTinits", 1:NChains,".txt",sep=""))

modelCheck("BUGSmodel.bug")
modelData("DCA_SSTbugs.txt")
modelCompile(NChains)
modelInits(paste("DCA_SSTinits", 1:NChains,".txt",sep=""))

# Burn in for 10^6 iterations
# Could do in 1 line, but sometimes BUGS traps, and this lets it continue
```

```
modelUpdate(1e4, thin=10) # 10k
modelUpdate(1e4, thin=10) # 20k
modelUpdate(1e4, thin=10) # 30k
modelUpdate(1e4, thin=10) # 40k
modelUpdate(1e4, thin=10) # 50k
modelUpdate(1e4, thin=10) # 60k
modelUpdate(1e4, thin=10) # 70k
modelUpdate(1e4, thin=10) # 80k
modelUpdate(1e4, thin=10) # 90k
modelUpdate(1e4, thin=10) # 100k

modelSaveState("DCA_SST1mInits")
# Record interesting variables
samplesSet("StdDev")
samplesSet("sdDCA")
samplesSet("sdSST")
samplesSet("rho")

# Run for another 10^5 iterations, thin to every 10
modelUpdate(1e3, thin=10) # 1k
modelUpdate(1e3, thin=10) # 2k
modelUpdate(1e3, thin=10) # 3k
modelUpdate(1e3, thin=10) # 4k
modelUpdate(1e3, thin=10) # 5k
modelUpdate(1e3, thin=10) # 6k
modelUpdate(1e3, thin=10) # 7k
modelUpdate(1e3, thin=10) # 8k
modelUpdate(1e3, thin=10) # 9k
modelUpdate(1e3, thin=10) # 10k

# Check convergence by eye
samplesHistory("rho")

# Save posteriors
samplesStats("*")
samplesCoda("*", "BasicModel")

rho=samplesSample("rho")

library(MCMCglmm) # only for posterior.mode

posterior.mode(rho)
HPDInterval(rho)
```

Plate I.

All specimens are from the Paleocene and Eocene of ODP Site 1172. Scale bars equal 10 μm.

1. *Gleicheniidites senonicus* Ross, 1949; Sample 17R-4, 40–42 cm (629.87–629.89 rmbsf), Slide 4, England-Finder coordinates L9.
2. *Evansispora senonica* Raine, 2008; Sample 17R-7, 20–22 cm (634.17–634.19 rmbsf), Slide 1, E35.
3. *Cyathidites australis* Couper, 1953; Sample 15R-5, 134–136 cm (612.85–612.87 rmbsf), Slide 1, C24/3.

4.-5. *Ceratosporites* spp. complex; Sample 15R-5, 134–136 cm (612.85–612.87 rmbsf), Slide 2, P38; Sample 15R5, 124–126 cm (612.75–612.77 rmbsf), Slide 1, M26/4.

6. *Podocarpidites exiguus* Harris, 1965; Sample 20R-5, 40–43 cm (660.18–660.21 rmbsf), Slide 1, Q28/3.
7. *Phyllocladidites mawsonii* Cookson, 1947 *ex* Couper, 1953; Sample 20R-5, 40–43 cm (660.18–660.21 rmbsf), Slide 1, M20.
8. *Araucariacites australis* Cookson, 1947; Sample 17R-6, 40-42 cm (631.37–631.39 rmbsf), Slide 1, O22.
9. *Dilwynites granulatus* Harris, 1965; Sample 19R-1, 40–42 cm (644.58–644.6 rmbsf), Slide 2, Q22.
10. *Spinizonocolpites prominatus* (McIntyre) Stover and Evans, 1973; Sample 15R-4, 135–137 cm (611.36–611.38 rmbsf), Slide 1, E28/1.
11. *Cycadopites follicularis* Wilson & Webster, 1946; Sample 15R-3, 40–42 cm (608.9–608.92 mbsf), Slide 2, M33/1.
12. *Arecipites* sp.; Sample 14R-3, 40–42 cm (599.74–599.76 rmbsf), Slide 4, N20/4.

Plate II.

All specimens are from the Paleocene and Eocene of ODP Site 1172. Scale bars equal 10 μm.

1. *Banksieaeidites arcuatus* Stover in Stover and Partridge 1973, Sample 15R-7, 40–42 cm (614.91–614.93 rmbsf), Slide 2, G15/4.
2. *Propylipollis latrobensis* (Harris) Martin and Harris, 1974; Sample 15R-6, 50–52 cm (613.51–613.53 rmbsf), Slide 1, X19/1.
3. *Proteacidites teuiexinus* Stover in Stover and Partridge, 1973; Sample 15R-5, 114–115 cm (612.65–612.66 rmbsf), Slide 1, E16/2.
4. *Proteacidites adenanthoides* Cookson, 1950; Sample 15R-5, 5–7 cm (611.56–611.58 rmbsf), Slide 1, U32.
5. *Myricipites harrisii* (Couper) Dutta and Sah, 1970; Sample 15R-5, 44–45 cm (611.95–611.96 rmbsf), Slide 1, Q20.

6. *Gambierina edwardsii* (Cookson and Pike) Harris, 1972; Sample 20R-5, 40–43 cm (660.18–660.21 rmbsf), Slide 2, V22/1.
7. *Malvacipollis subtilis* Stover in Stover and Partridge, 1973; Sample 15R-5, 19–21 cm (611.7–611.72 rmbsf), Slide 1, X29.
8. *Nothofagidites* cf. *endurus* (Cookson) Harris, 1965; Sample 20R-1, 40–42 cm (654.18–654.20 rmbsf), Slide 2, N24.
9. *Nothofagidites brachyspinulosus* (Cookson) Harris, 1965; Sample 15R-3, 40–42 cm (608.9–608.92 rmbsf), Slide 2, Y49.
10. *Alisporites* sp.; Sample 18R-6, 40–42 cm (641.97–641.99 rmbsf), Slide 1, R26/4 [reworked].
11. *Cannanoropollis* sp.; Sample 20R-4, 40–42 cm (658.67–658.69 rmbsf), Slide 2, Q29/2 [reworked].
12. *Protohaploxypinus* sp.; Sample 20R-5, 40–43 cm (660.18–660.21 rmbsf), Slide 1, C28/3 [reworked].

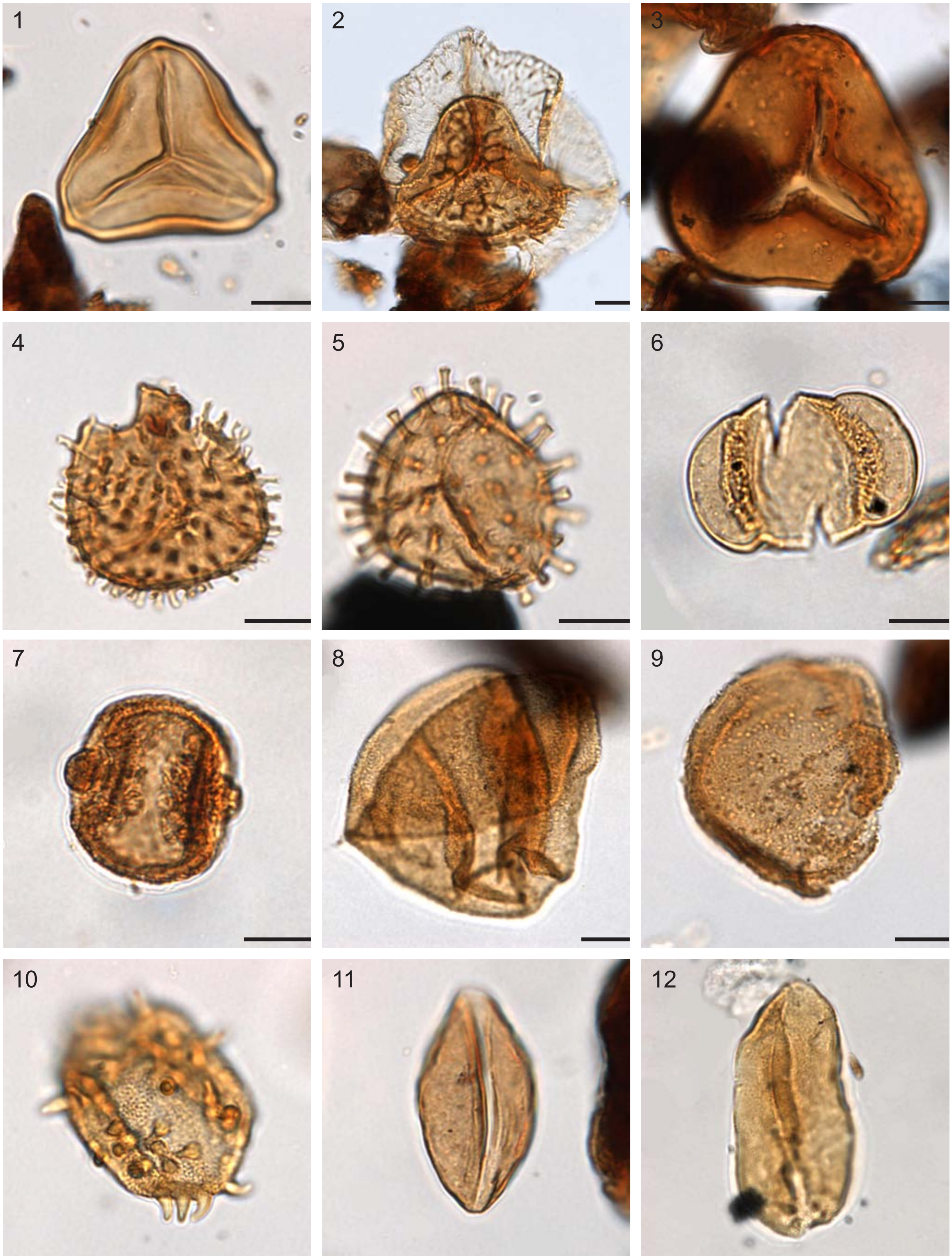

Plate I.

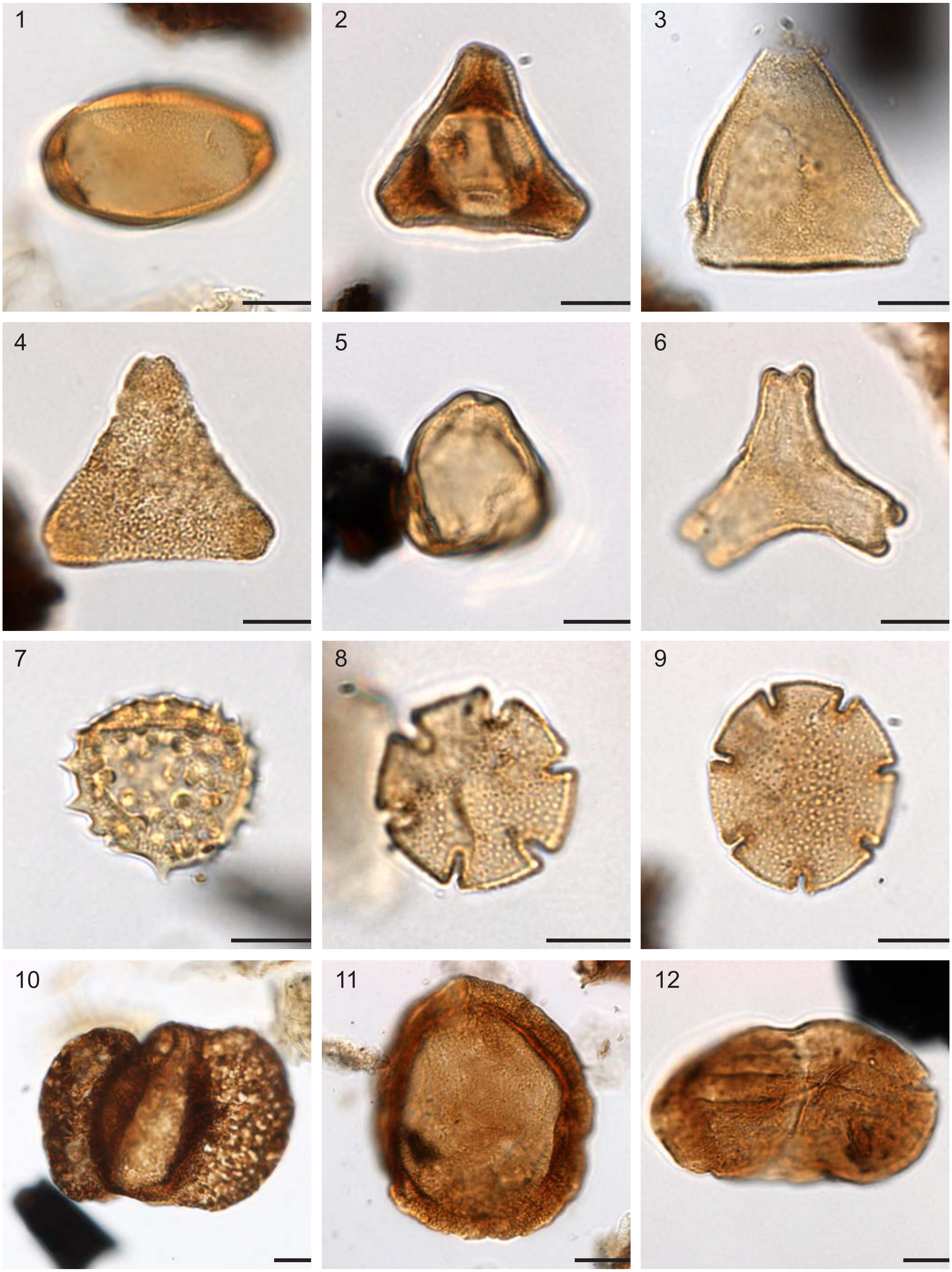

Plate II.