What drives the glacial-interglacial cycle? A Bayesian approach to a long-standing model selection problem

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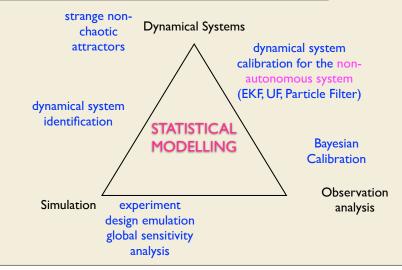
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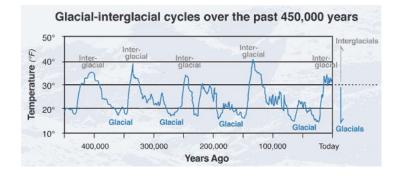
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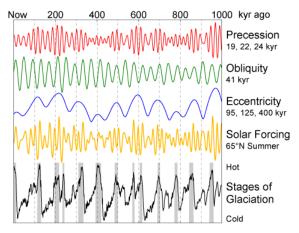
#### Glacial-Interglacial cycle



Cycle characterised by saw-toothed behaviour: slow accumulation and rapid terminations.

Approx 100 kyr period between cycles, but previously a 40 kyr period was observed.

## Milankovitch theory



Eccentricity: orbital departure from a circle, controls duration of the seasons Obliquity: axial tilt, controls amplitude of seasonal cycle Precession: variation in Earth's axis of rotation, affects difference between seasons

Insolation at  $65^{\circ}$  north: combination of these three terms, considered important.

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## 100kyr problem

Spectral analysis suggest the climate response has a period of  $\approx$  100kyr, but the orbital forcing at this period is small.

Eccentricity has 95 and 125kyr periods, but accounts for only 2% of the variation compared to the shifts caused by obliquity (41kyr period) and precession (21kyr period).

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Explanatory hypotheses

- Earth's climate may have a natural frequency of 100kyr caused by natural feedback processes
- 100kyr eccentricity cycle acts as a "pacemaker" to the system, amplifying the effect of precession and obliquity at key moments, triggering a termination.
- 21kyr precession cycles are solely responsible, with ice building up over several precession cycles, only melting after four or five such cycles.

## Current practice

Climate scientists want<sup>1</sup> to use palaeo-data to gather evidence for different hypotheses. They typically want to

- Compare models (and estimate parameters)
- Compare effects of different aspects of the solar forcing (all components have been argued for)
- Produce climate reconstructions (temperature chronologies)

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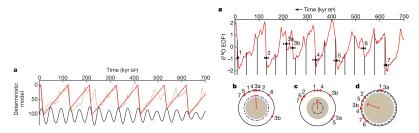
Current approaches tend to be statistically naive

- Models fit by eye,
- Model selection rarely tackled in a statistical manner, and when they do, questionable approaches are taken.

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## Example

Huybers and Wunsch 2005 argue that obliquity is the primary driver of glacial cycle



- Reduce the dataset to 7 termination times
- Look at the consistency of the phase of each components at terminations
- They propose a random walk model of ice volume with a 100kyr period

 $V_{t+1} = V_t + N(1,2)$  and if  $V_t > 90$ , terminate

and estimate the distribution of the test statistic under  $H_0$  (obliquity and termination are independent) by looking at obliquity phase during terminations in the model.

#### Our aim

Most simple models of the [...] glacial cycles have at least four degrees of freedom [parameters], and some have as many as twelve. Unsurprisingly [...this is] insufficient to distinguish between the skill of the various models (Roe and Allen 1999)

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Can we do any better?

- Aim to demonstrate the power of the Bayesian approach; demonstrate that a full analysis is feasible
- Use all the data, not just the termination times
- Estimate parameters rather than using hand tuned models

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• Deal with noisy records and age-model uncertainty

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Essentially a demonstration of recent Monte Carlo methodology (SMC<sup>2</sup>, PMCMC), and GPU computation.

Many aspects of the modelling could be improved, and be incorporated within this framework.

#### Models

A phenomenological approach is taken: idealised simple models based on a few hypothesised relationships that capture some aspect of the climate system.

Let  $X_t \in \mathbb{R}^p$  be the state of the climate at time *t*. Typically  $X_{1,t}$  = ice volume, and other components many represent CO<sub>2</sub>, ocean temp, etc, or be left undefined.

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• Oscillators synchronised on the solar forcing (Saltzman and Maasch 1991),

$$dX_{1} = -(X_{1} + X_{2} + vX_{3} + F(\gamma_{P}, \gamma_{C}, \gamma_{E})) dt + \sigma_{1} dW_{1}$$
  

$$dX_{2} = (rX_{2} - pX_{3} - sX_{2}^{2} - X_{2}^{3}) dt + \sigma_{2} dW_{2}$$
  

$$dX_{3} = -q(X_{1} + X_{3}) dt + \sigma_{3} dW_{3}$$

• Models with switches in the ice volume (Tziperman 2006)

$$dX_1 = ((p_0 - KX_1)(1 - \alpha X_2) - (s + F(\gamma_P, \gamma_C, \gamma_E))) dt + \sigma_1 dW_1$$

 $X_2$  : switches from 0 to 1 when  $X_1$  exceeds some threshold  $X_u$ 

- $X_2$  : switches from 1 to 0 when  $X_1$  decreases below  $X_1$
- Models with switches dependent upon thresholds in the forcing (Parrenin and Paillard 2012)

#### Statistical model

These models are forced with some aspect of the solar forcing

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} = g(X_t, \theta) + F(t, \gamma)$$

where  $\gamma = (\gamma_P, \gamma_C, \gamma_E)$  controls the combination of precession, obliquity and eccentricity.

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Embed these models within a statistical state space model relating climate to observations

$$dX_t = g(X_t, \theta)dt + F(t, \gamma)dt + \Sigma dW$$
$$Y_t = d + sX_{1,t} + \epsilon_t$$

where we have 'noised-up' the models turning them into SDEs to account for model discrepancies.

Typically these models have 10-15 parameters that need to be estimated from the data.

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  - π(x|θ) = distribution of output x from your simulator when run using
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posterior 
$$= \pi(\theta|y) = \frac{\pi(y|\theta)\pi(\theta)}{\pi(y)} \propto \text{likelihood} \times \text{prior}$$

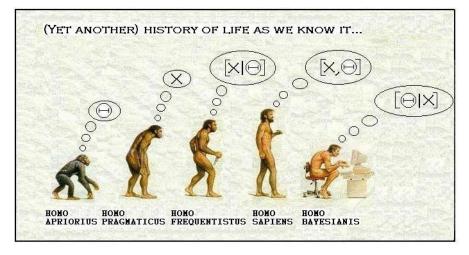
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Added difficulty:  $\pi(x|\theta)$  is usually unknown!



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Pros:

- Unified coherent approach to every problem.
- For hard problems, Bayesian approach usually more tractable.

Cons:

- Philosophical objections to subjectivism (priors!)
- No guarantee of frequentist coverage

The quantities we need to calculate are

• Climate reconstruction (filtering)

 $\pi(x_{1:T}|y_{1:T},\theta_m,\mathcal{M}_m) \propto \pi(x_{1:T-1}|y_{1:T-1},\theta)\pi(x_T|x_{T-1},\theta)\pi(y_T|x_T)$ 

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where  $x_{1:T} = (x_1, ..., x_T)$ 

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where  $x_{1:T} = (x_1, \dots, x_T)$ 

• Model calibration (marginal parameter posterior)

 $\pi(\theta_m|y_{1:T},\mathcal{M}_m)$ 

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• Model selection (model evidence/Bayes factors)

 $\pi(y_{1:T}|\mathcal{M}_m)$ 

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These are progressively more difficult to calculate, particularly as

$$\pi(X_{t+1}|X_t,\theta_m,\mathcal{M}_m)$$

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is unknown.

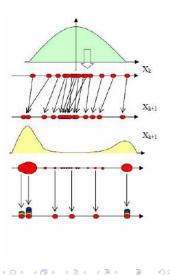
Filtering

Sequential Monte Carlo (SMC) methods are the natural approach for finding the filtering distributions  $\pi(x_{1:T}|y_{1:T},\theta)$ 

 Represent all distributions by collection of weighted particles {x<sup>(i)</sup>, w<sup>(i)</sup>}, e.g.,

$$p(x) \approx \sum w_0^{(i)} \delta_{x^{(i)}}(x)$$

• Sequentially build up approximation to  $\pi(x_{1:t}|y_{1:t},\theta)$ one step at a time.



## SMC

At time t - 1, suppose  $(X_{1:t-1}^n, W_{t-1}^n)_{n=1}^N$  is a collection of weighted particles approximating  $\pi(X_{1:t-1}|Y_{1:t-1}, \theta)$ 

- Sample ancestor particle index  $\mathcal{A}_{t-1}^n \sim \mathcal{F}(\mathcal{W}_{t-1}^n)$
- Propagate state particles  $X_t^n \sim q_t(\cdot|X_{t-1}^{\mathcal{A}_{t-1}^n}, heta, Y_t)$
- Weight state particles

$$w_t^n(X_{1:t}^n) = \frac{\pi(X_t^n | X_{t-1}^{\mathcal{A}_{t-1}^n}, \theta) \pi(Y_t | X_t^n)}{q_t(X_t^n | X_{t-1}^{\mathcal{A}_{t-1}^n}, \theta, Y_t)}, \qquad W_t^n = \frac{w_t^n(X_{1:t}^n)}{\sum_n w_t^n(X_{1:t}^n)}$$

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We need  $\pi(X_t|X_{t-1}, \theta)$  to cancel, but setting  $q = \pi$  can lead to extreme degeneracy, as too many proposals are in regions of low-posterior probability

We use the Golightly and Wilkinson (2006) approach to nudge the proposals towards the data.

#### Parameter estimation

SMC provides an unbiased estimate of the marginal likelihood

$$\pi(y_{1:T}|\theta) = \pi(y_1|\theta) \prod_{t=2}^T \pi(y_t|y_{1:t-1},\theta)$$

when we substitute the estimate

$$\tilde{\pi}(y_t|y_{1:t-1},\theta) = \frac{1}{M} \sum w_t^n$$

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for  $\pi(y_t | y_{1:t-1}, \theta)$ .

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for  $\pi(y_t | y_{1:t-1}, \theta)$ .

We can then use these estimates in a pseudo marginal scheme such as PMCMC (Andrieu *et al.* 2010) to estimate

$$\pi(\theta, x_{1:T}|y_{1:T})$$

and

$$\pi(\theta|y_{1:T})$$

# SMC<sup>2</sup>

We've found that  $SMC^2$  (Chopin *et al.* 2011) works well for our problem Basic idea:

- Introduce M parameter particles  $\theta_1, \ldots, \theta_M$
- For t = 1, ..., T
  - For each  $\theta_i$  run a particle filter targeting  $\pi(X_{1:t}|y_{1:t},\theta_i)$
  - Recalculate all the importance weights and resample if necessary

Note that to avoid particle degeneracy, it is still usually necessary to run a PMCMC sampler targeting  $\pi(\theta, X_{1:t}|y_{1:t})$  at each resampling step.

# SMC<sup>2</sup>

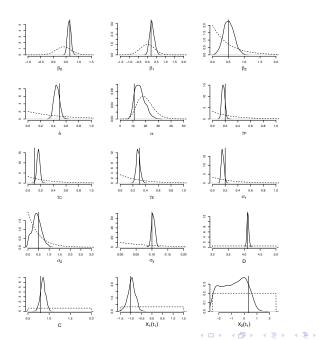
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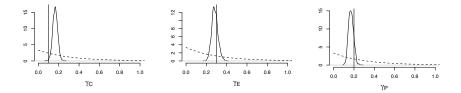
This takes 3-4 days on a standard server, or 4-6 hours on a GPU (2500 processors) with 1000  $\theta$  particles and 1000 X particles.

#### Results



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 $\gamma = (\gamma_P, \gamma_E, \gamma_C)$  controls the relative contribution of the three components of the orbital variations in the forcing.

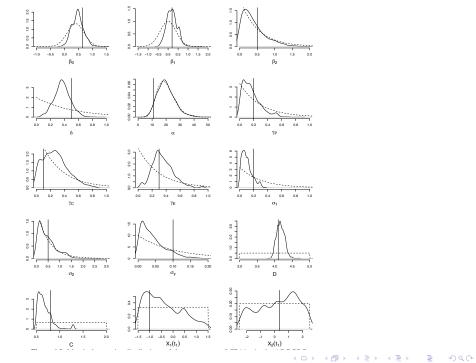


#### Alternative approaches

#### ABC

- Instead of approximating the likelihood (as in SMC<sup>2</sup>), we try to find  $\theta$  that give good match between observed and simulated data
- Allows us to calibrate on carefully chosen aspects of the system (period, volatility, etc), rather than just on the data.
- The loss of information from the ABC approximation is large, so the posteriors are usually much wider than with SMC<sup>2</sup>.

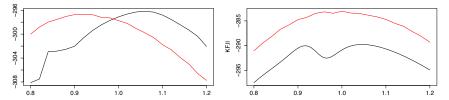
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#### Alternative approaches

Instead of using the particle filter (SMC) to do the filtering, we would like to use the unscented Kalman filter (UKF) or EnKF.

- Assumes π(x<sub>t</sub>|y<sub>1:t</sub>) is Gaussian and uses Sigma-point particles to estimate mean and variance.
- Much cheaper than *SMC* or *MCMC* approaches.
- We found the UKF works well for filtering (location), less well for parameter estimation, and terribly for model selection.



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## Bayes factors

Consider comparing two models,  $\mathcal{M}_1$  and  $\mathcal{M}_2$ .

Bayes factors (BF) are the Bayesian approach to model selection.

$$\frac{\mathbb{P}(\mathcal{M}_1|\mathcal{D})}{\mathbb{P}(\mathcal{M}_2|\mathcal{D})} = \frac{\pi(\mathcal{M}_1)}{\pi(\mathcal{M}_2)} \frac{\mathbb{P}(\mathcal{D}|\mathcal{M}_1)}{\mathbb{P}(\mathcal{D}|\mathcal{M}_2)}$$
  
posterior odds = prior odds × Bayes factor

where

$$B_{12} = \frac{\mathbb{P}(\mathcal{D}|\mathcal{M}_1)}{\mathbb{P}(\mathcal{D}|\mathcal{M}_2)} = \frac{\int \pi(\theta_1|\mathcal{M}_1)\mathbb{P}(\mathcal{D}|\theta_1,\mathcal{M}_1)d\theta_1}{\int \pi(\theta_2|\mathcal{M}_2)\mathbb{P}(\mathcal{D}|\theta_2,\mathcal{M}_2)d\theta_2}$$

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$B_{12}$ range	$\mathbb{P}(\mathcal{M}_1 D)$ range	Interpretation
1–3	0.5-0.75	Barely worth mentioning
3–10	0.75 - 0.91	Substantial
10-30	0.91-0.97	Strong
30–100	0.97- 0.99	Very strong
> 100	0.99-1	Decisive

# Bayes factors

Advantages:

- Provide evidence in favour of a model
- Provides an automatic form of Occam's razor.
- Do not require models to be nested
- Asymptotic consistency

Disadvantages

- Hard to calculate
- Sensitive to choice of prior
- Integrated likelihood may not be desirable treatment
  - predictive evaluation via scoring rules? (not p-values)

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#### Model selection

To compare models  $\mathcal{M}_1$  and  $\mathcal{M}_2,$  we want to find the Bayes factor

$$B_{12} = \frac{\pi(y_{1:T}|\mathcal{M}_1)}{\pi(y_{1:T}|\mathcal{M}_2)}$$

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Values of  $B_{12} > 100$  indicate 'decisive' evidence in favour of  $\mathcal{M}_1$ .

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Values of  $B_{12} > 100$  indicate 'decisive' evidence in favour of  $M_1$ . SMC<sup>2</sup> can be used to provide an unbiased estimate of

$$\pi(y_{1:T}|\mathcal{M})$$

for any model.

However, the variance of our estimates are typically an order of magnitude, so don't consider  $B_{12}$  to be large until we see values > 1000.

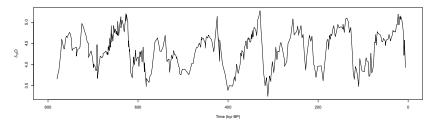
## Results

We generate simulated data from SM91, using both the astronomically forced and unforced version of the model

Model		Evidence $\pi(y_{1:N} \mathcal{M}_m)$		
		SM91-unforced	SM91-forced	
SM91	Forced	$5.6 imes10^{28}$	$1.4 imes10^{41}$	
	Unforced	$1.1 imes10^{30}$	$2.4 imes10^{18}$	
T06	Forced	$3.6 imes10^{20}$	$2.6 imes10^{30}$	
	Unforced	$1.1 imes10^{22}$	$2.9 imes10^{14}$	
PP12	Forced	$2.8 imes10^8$	$2.1 imes10^{18}$	

- Strongest evidence for the true model found each time
- Unforced model is special case of forced model with 3 parameters set to zero, so we expect it to be harder to select the unforced model.
- For the data generated from the forced model, the forced version of the wrong model is preferred.

# Results: ODP677



We use the ODP677 stack (a composite record from multiple cores), which has been dated by two authors:

- Lisiecki and Raymo (2005) used orbital tuning
- Huybers 2007 used a depth-derived age model (no orbital tuning)

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# Results: ODP677

Model		Evidence		
		ODP677: H07(unforced)	ODP677: LR04(forced)	
SM91	Forced	$4.0  imes 10^{24}$	$1.1  imes 10^{28}$	
	Unforced	$3.5 imes10^{26}$	$1.6 imes10^{18}$	
T06	Forced	$3.3 imes10^{25}$	$4.5 imes10^{29}$	
	Unforced	$1.7 imes10^{28}$	$3.3 imes10^{21}$	
PP12	Forced	$1.5 imes10^{22}$	$1.8 imes10^{34}$	

The dating method applied changes the answer

- Using Huybers' non-orbitally tuned data, we find evidence in favour of the unforced T06 model.
- Using Lisiecki's orbitally tuned data, we find strong evidence for PP12 a tuned model (PP12)

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Moreover, orbitally tuned data leads us to strongly prefer the orbitally tuned version of each model (and vice versa)

# Results: ODP677

Model		Evidence		
		ODP677: H07(unforced)	ODP677: LR04(forced)	
SM91	Forced	$4.0  imes 10^{24}$	$1.1  imes 10^{28}$	
	Unforced	$3.5 imes10^{26}$	$1.6 imes10^{18}$	
T06	Forced	$3.3 imes10^{25}$	$4.5 imes10^{29}$	
	Unforced	$1.7 imes10^{28}$	$3.3 imes10^{21}$	
PP12	Forced	$1.5 imes10^{22}$	$1.8 imes10^{34}$	

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Moreover, orbitally tuned data leads us to strongly prefer the orbitally tuned version of each model (and vice versa)

The age model used to date the stack (often taken as a given) has a strong effect on model selection conclusions

## Age model

Can we also quantify chronological uncertainty?

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Target

$$\pi(\theta, T_{1:N}, X_{1:N}|y_{1:N})$$

where  $T_{1:N}$  are the times of the observation  $Y_{1:N}$ , which were previously taken as given.

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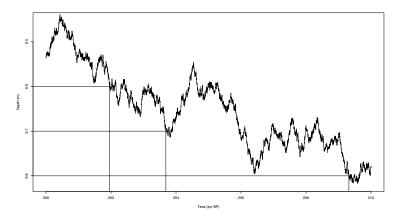
where  $T_{1:N}$  are the times of the observation  $Y_{1:N}$ , which were previously taken as given.

Propose a simple age model for sediment accumulation: Let H be the depth in the core, with  $H_N = 0$  at  $T_N = 0$ 

$$\mathrm{d}H = -\mu_{s}\mathrm{d}T + \sigma\mathrm{d}W$$

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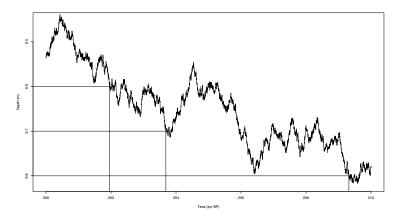
Slices are then taken through the core at specific depths  $H_1, \ldots, H_N$ .



There may have been multiple times when a certain depth was reached: the most recent time is the age of that slice, i.e., it is a first passage problem. Given  $(T_m, H_m)$ , then  $T_{m-1}$  is the first passage time of  $H_{m-1}$  with

$$T_{m-1}|T_m \sim IG\left(T_m - \frac{H_{m-1} - H_m}{\mu_s}, \frac{(H_{m-1} - H_m)^2}{\sigma_s^2}\right)$$

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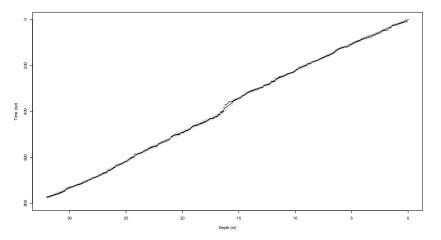
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We then add a model to account for compaction in the core, and apply Bayes theorem to find  $\pi(T_m|T_{m-1})$  so that we can run the model forward in time

### Simulation study results (n = 321) - age vs depth

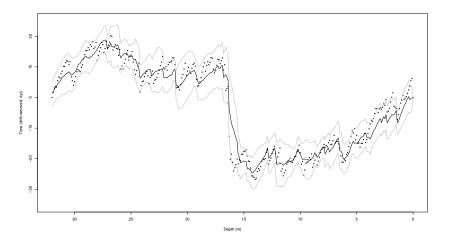
Dots = truth, black line = estimate, grey = 95% Cl

We use simulated data from the CR12 model, with parameter values, and initial conditions comparable to real data. We consider the period 780 kyr to the present.

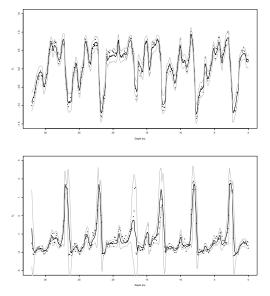


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#### Simulation study results - age vs depth (trend removed) Dots = truth, black line = estimate, grey = 95% CI

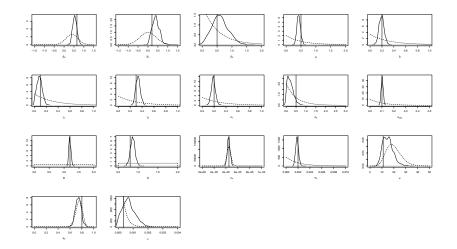


#### Simulation study results - climate reconstruction Dots = truth, black line = estimate, grey = 95% CI



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### Simulation study results - parameter estimation



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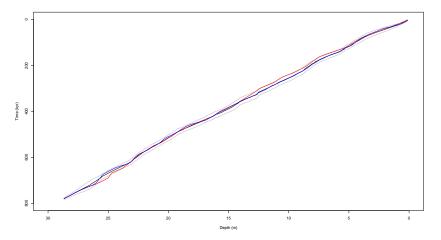
### Results for ODP846 core

- ODP846 contains a marker for the Brunhes-Matuyama magnetic reversal at 780kyr, allowing us to give a strong prior for T<sub>1</sub> (±2kyr).
- Has again been dated by two groups
  - Lisiekci and Raymo (LR04): graphical correlation of 57 cores. The stack is then orbitally tuned
  - Huybers and Wunsch 2004 (HW04) use a depth-derived age model. They decompact each core, fit a linear age model, then average over many several realisations and to get a distribution for 17 age control points(ACPS), such as terminations. Average ages for the the ACP events are then found, and a linear age model is fitted between consecutive ACPs

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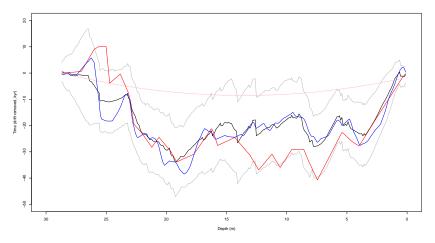
#### Results for ODP846 - age vs depth

Black = posterior mean, grey = 95%Cl, red = H07, blue = LR04



Our results come with uncertainty bounds (HW04 estimate accuracy of  $\pm$ 9kyr for all ages). Moreover, the full joint distribution for all quantities is available if required.

Results for ODP846 - age vs depth (trend removed) Black = posterior mean, grey = 95%CI, red = H07, blue = LR04

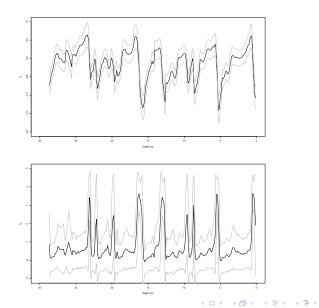


Note that these age estimates now depend explicitly on the model CR12.

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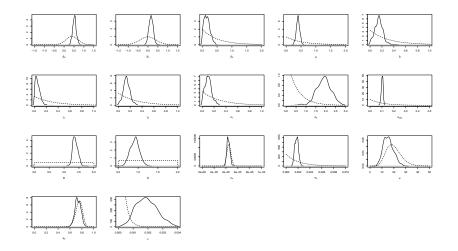
#### Results for ODP846 - climate reconstruction

We can now give climate reconstructions that account for age uncertainty.



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### Results for ODP846 - parameter estimates



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# Conclusions

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- However, the results are very sensitive to the age model applied to the data.
- Monte Carlo methodology and computer power are now sufficiently advanced that we can tackle the joint reconstruction, age model, and model selection problems in a fully Bayesian manner
  - $\blacktriangleright$  but it remains computationally expensive. The age model results take  $\sim$  1 week to compute per model.

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Still to do/issues:

- Model selection with inferred age models
- Multiple cores/stacks
- More sophisticated models
- Large variance in the BF estimates
- Prior distribution selection

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Thank you for listening!

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