Parameter Estimation for Marine Ecosystem Models in 3-D

J. Piwonski, T. Slawig

CAU - Christian-Albrechts-Universität zu Kiel

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future ocean
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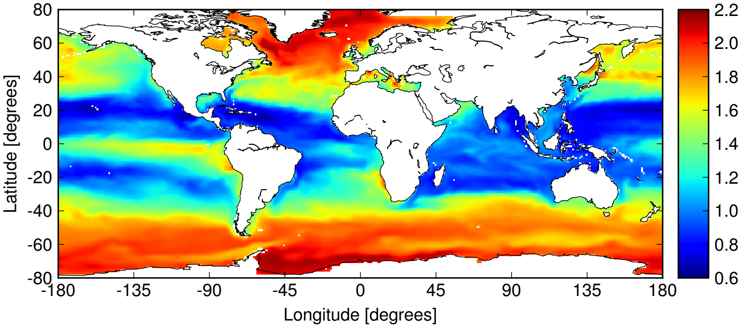
Outline

- Motivation
- Model evaluation
  - Transport matrices
  - Biogeochemical model interface
  - Solver software
- Optimization
  - Twin experiment
  - World Ocean Atlas 2005 data

Motivation

- **Global carbon cycle**, CO_2 uptake of the world's oceans
- **Ocean Biogeochemical Dynamics** [Sarmiento and Gruber, 2006]



Simulated concentration of nutrients (phosphate, PO_4^{3-}) at the surface layer in $m\,mol\;P/m^3$. The longitudinal and latitudinal resolution is at $1.0°$.

Model evaluation

- **System of transport equations** for biogeochemical tracers:

$$\frac{\partial y_i}{\partial t} = \underbrace{\nabla \cdot (\kappa \nabla y_i)}_{\text{diffusion}} - \underbrace{\nabla \cdot (v\, y_i)}_{\text{advection}} + \underbrace{q_i(y, \mathbf{u}, b, d)}_{\text{bgc model}}, \quad i = 1, \ldots$$

- **Climatological** (annual periodic) forcing

$$\begin{aligned} \kappa(t+1) &= \kappa(t), & b(t+1) &= b(t), & t \in [0, 1[\\ v(t+1) &= v(t), & d(t+1) &= d(t) \end{aligned}$$

- Solution is a **steady annual cycle** (equilibrium)

$$y(t+1) = y(t)$$

Off-line simulation

- **Transport Matrix Method** [Khatiwala et al., 2005]

$$\mathbf{y}_{j+1} = \underbrace{\mathbf{A}_{imp,j}\,(\mathbf{A}_{exp,j}}_{\text{transport matrices}}\,\mathbf{y}_j + \Delta t\, q_j(\mathbf{y}_j, \mathbf{u}, \mathbf{b}_j, \mathbf{d}_j)), \quad j = 1, \ldots$$

- **Sparse** implicit and explicit transport matrices

$$\begin{aligned} \mathbf{A}_{imp,j} &= (\mathbf{I} - \Delta t\, \mathbf{L}_{imp,j})^{-1} \\ \mathbf{A}_{exp,j} &= (\mathbf{I} + \Delta t\, \mathbf{L}_{exp,j}) \end{aligned}$$

Biogeochemical model interface

- **Water column** model (1-D)
- **Any number** of
  - tracers, n
  - layers, n_y
  - parameters, m
  - boundary data, n_b
  - domain data, n_d
- Realization in **Fortran:**

```
subroutine bgc(n, ny, m, nb, nd, dt, q, t, y, u, b, d)
  integer :: n, ny, m, nb, nd
  real*8  :: dt, q(ny, n), t, y(ny, n), u(m), b(nb), d(ny, nd)
end subroutine
```

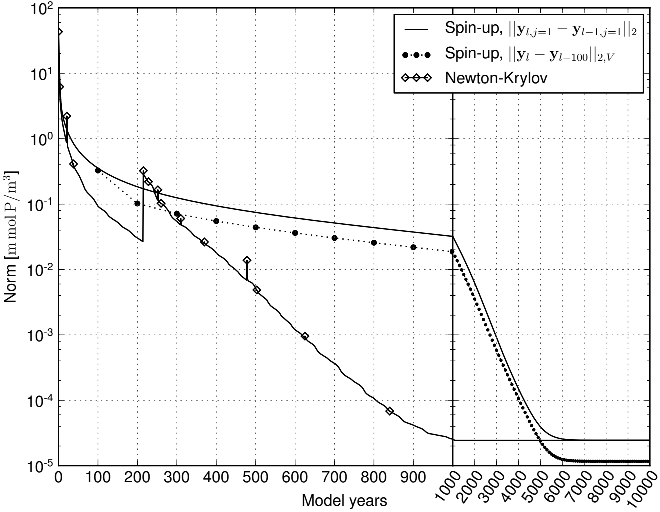
Solver software

- **Metos3D** [Piwonski and Slawig, 2014]
  - **Fixed point iteration**
  - **Newton-krylov solver**
- `github.com/metos3d`
- **PETSc** based implementation in **C** [Balay et al., 1997]

Set up

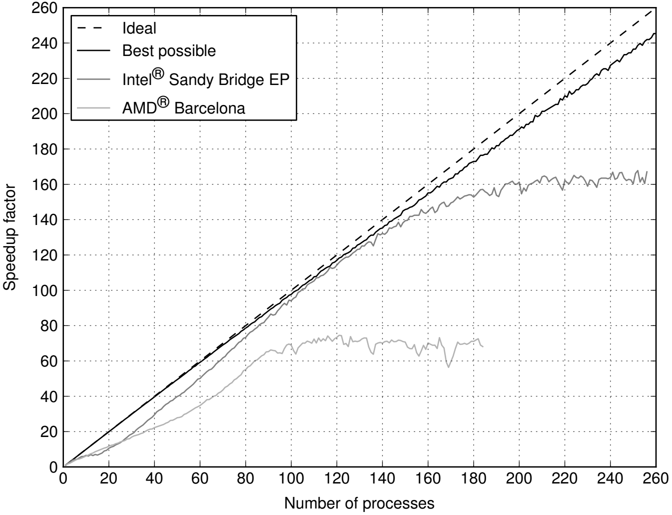
- **Transport matrices:**
  - Longitudinal and latitudinal: $\mathbf{2.8125}^\circ$ (128×64 surface grid)
  - Vertical: **15 layers**
  - Temporal: **2880 time steps**, $\Delta t = 1/2880$
- **Biogeochemical model:**
  - **N-DOP**, [Dutkiewicz et al., 2005], **`mitgcm.org`**
  - Boundary data (isolation): **latitude, ice cover**
  - Domain data: **depths, heights**

Solution



Convergence towards a periodic solution.

Solution cont'd



Theoretical and actual speedup of parallelized simulation runs.

Optimization

- **Problem:**

$$\min_{\mathbf{u}\in U} J(\mathbf{u})$$

- **Cost function:**

$$J(\mathbf{u}) = \frac{1}{2}||\mathbf{y}(\mathbf{u}) - \mathbf{y}_d||^2_{2(,V)}$$

- **Admissible set:**

$$U = \{\mathbf{u} \in \mathbb{R}^m : \mathbf{b}_l \leq \mathbf{u} \leq \mathbf{b}_u\}$$

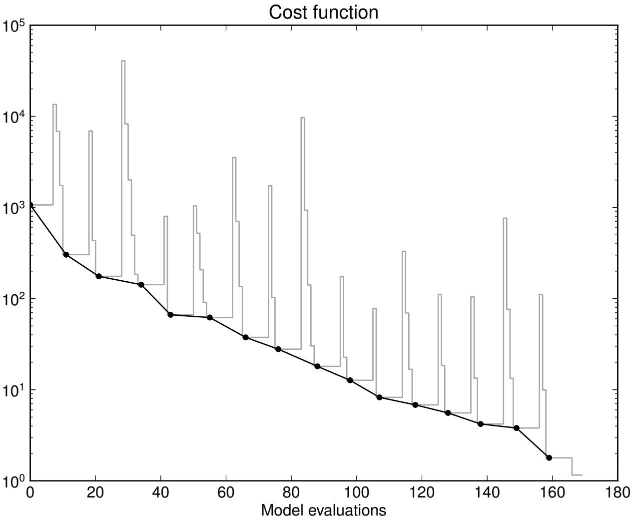
Set up

- **Optimizer:**
  - `fmincon`, Matlab[1]
- **Parameters:**

$\mathbf{u}$	Description	$\mathbf{u}_d$	$\mathbf{b}_l$	$\mathbf{b}_u$
u_1	DOP remineralization rate	0.5	0.25	0.75
u_2	maximum community production	2.0	1.5	200.0
u_3	fraction of DOP	0.67	0.05	0.95
u_4	PO4 half saturation	0.5	0.25	1.5
u_5	light half saturation	30.0	10.0	50.0
u_6	light attenuation	0.02	0.01	0.05
u_7	power law remineralization coefficient	0.858	0.7	1.5

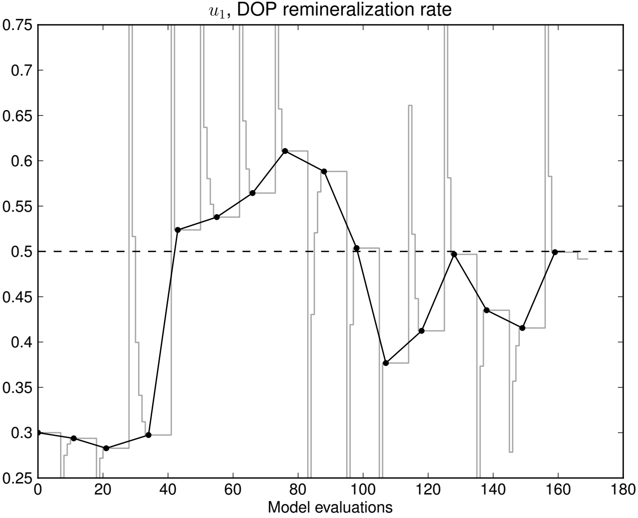
[1] Matlab is a registered trademark of The Mathworks Inc.

Twin experiment



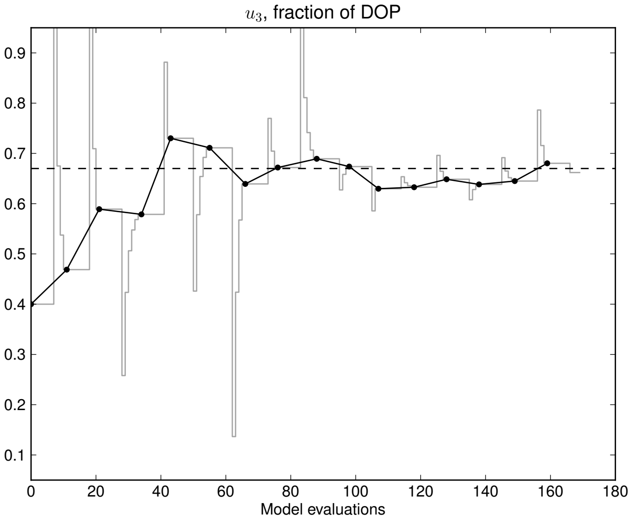
Decay of the unweighted cost function.

Twin experiment cont'd



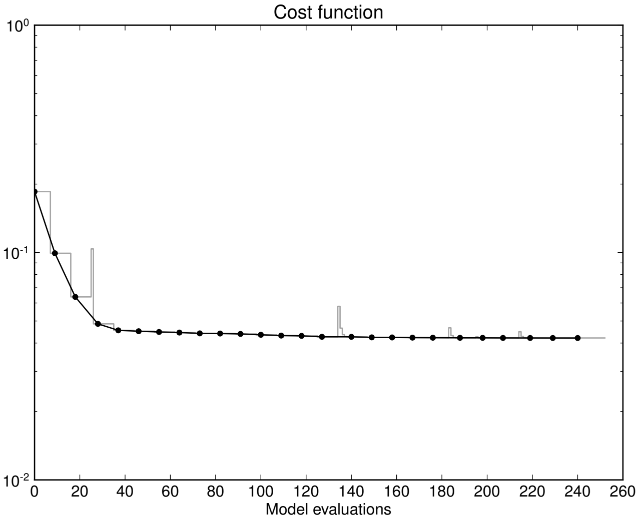
Convergence towards the reference parameter $u_{d,1}$.

Twin experiment cont'd



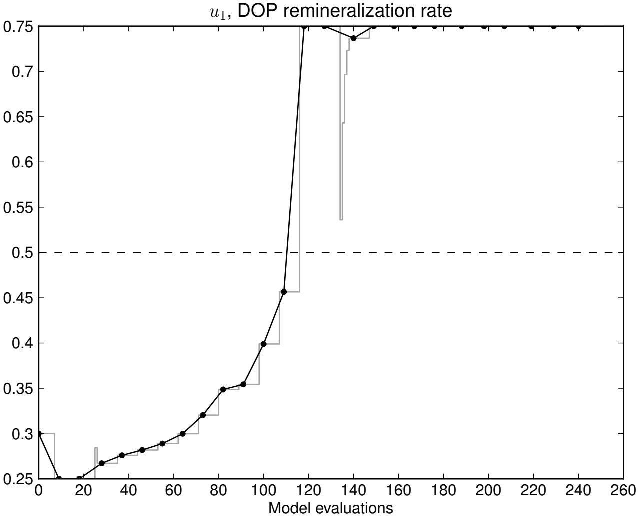
Convergence towards the reference parameter $u_{d,3}$.

World Ocean Atlas 2005



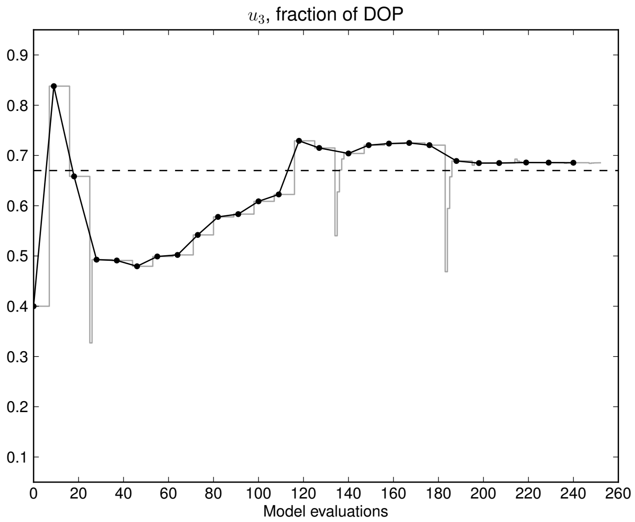
Decay of the weighted cost function. Weights are relative volumes.

World Ocean Atlas 2005 cont'd



Behavior of the parameter u_1.

World Ocean Atlas 2005 cont'd



Behavior of the parameter u_3.

Thanks

Thanks for your attention!