# A Parareal Algorithm Applied on the Computation of Periodic States in Marine Ecosystems

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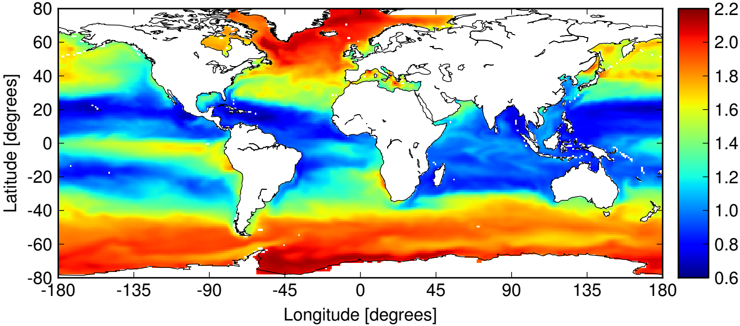
# Outline

# Motivation: Modeling the global carbon cycle

- **Ocean is a carbon sink**: $CO_2$ uptake via the sea surface
- **Transport and distribution** via ocean currents
- **Reactions** determined by ocean biogeochemical dynamics




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 calibration and assessment

**Fit model output to observed data**

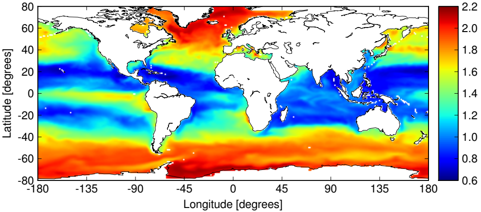
Optimize parameters $u$ in the underlying model

Formulation of the mathematical problem:

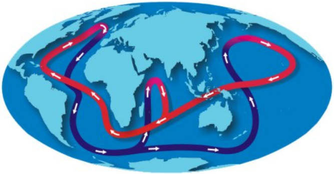
$y \in Y$ (either function space or, discretized, $\mathbb{R}^n$), $u \in \mathbb{R}^m$, $m \ll n$

$$\min J(y,u) = \frac{1}{2}\|y - y_{data}\|^2 + \frac{\alpha}{2}\|u - u_{est}\|^2$$

$$\text{s.t. model equations are fulfilled:} \quad e(y,u) = 0.$$

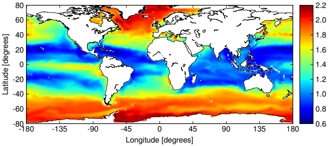


**Ocean circulation fields** **Tracer distribution**



online ⟷

⟶ offline




**Navier-Stokes equations** + **System of transport equations with nonlinear coupling**

Offline simulations:

- circulation fields pre-computed by ocean model
- used as forcing data for tracer transport model

# Offline state equation: Tracer transport model

- System of transport equations for biogeochemical tracers $y = (y_j)_j$:

$$\partial_t y_j = \underbrace{\mathrm{div}(\kappa \nabla y_j)}_{\text{diffusion}} - \underbrace{\mathrm{div}(\vec{v}\, y_j)}_{\text{advection}} + \underbrace{q_j(t, y, u)}_{\text{biogeochemistry}}, \qquad j = 1, \ldots, s$$

+ initial and boundary conditions.

- $u$: constant model parameters to be determined.
- Desired solution is a **steady annual cycle**:

$$y(t + T) = y(t), \quad t \in [0, T],$$

- for “climatological“ (annually periodic) forcing data and coupling terms

$$\begin{aligned} \kappa(t + T) &= \kappa(t), \\ \vec{v}(t + T) &= \vec{v}(t), \\ q_j(t + T, \cdot, \cdot) &= q_j(t, \cdot, \cdot), \qquad t \in [0, T]. \end{aligned}$$

# (Simplest) example: N-DOP model by Parekh et al.

- Transport equations:

$$\partial_t y_j = \mathrm{div}(\kappa \nabla y_j) + \mathrm{div}(v y_j) + q_j(t, y, u) \quad \text{in } \Omega \times (0, T), j = 1, 2.$$

- Coupling terms:

$$q_1 = \lambda y_2 + \begin{cases} -F(y_1), & \Omega_1 \text{ (upper layer)} \\ (1-\nu)E(y_1), & \Omega_2 \text{ (lower layer)} \end{cases}$$

$$q_2 = -\lambda y_2 + \begin{cases} \nu F(y_1), & \Omega_1, \\ 0, & \Omega_2 \end{cases} \qquad \nu \in (0, 1)$$

- Typical nonlinearity and non-local term:

$$F(y_1) = \alpha \frac{y_1}{y_1 + K},$$

$$E(y_1) = c \left[ \frac{z}{depth} \right]^m \int_{depth}^{0} (1-\nu) F(y_1) dz$$

- Nonlinear and nonlocal boundary condition (for mass conservation):

$$\partial_n y_j = b_j(y, u) \quad \text{on } \Gamma \times (0, T).$$

- Model: [Dutkiewicz et al., 2005], `mitgcm.org`.

# Model equations: Theory

Ecosystem model equation of *N-DOP* type in classical form:

$$
\begin{aligned}
\partial_t y_1 + \mathrm{div}(\vec{v}(t) y_1) - \mathrm{div}(\kappa \nabla y_1) - \lambda y_2 + d_1(y) &= 0 \quad \text{in } \Omega \times [0, T] \\
\partial_t y_2 + \mathrm{div}(\vec{v}(t) y_2) - \mathrm{div}(\kappa \nabla y_2) + \lambda y_2 + d_2(y) &= 0 \quad \text{in } \Omega \times [0, T] \\
\nabla y_j \cdot (\kappa \eta) + b_j(y) &= 0 \quad \text{on } \Gamma \times [0, T],\ j = 1, 2
\end{aligned}
$$

with

- $\Omega \subset \mathbb{R}^n$, $n \leq 3$, open, bounded, $\Gamma := \partial\Omega$
- $\vec{v} \in L^\infty(0, T; H^1(\Omega)^n)$ with $\mathrm{div}(\vec{v}(t)) = 0$ in $\Omega$ and $\vec{v}(t) \cdot \eta = 0$ on $\Gamma$
- $\kappa \in L^\infty(\Omega \times [0, T])$ with $\kappa_{\min} := \operatorname{ess\,inf}_{(x,t)} \kappa(x, t) > 0$
- $d$, $b$ reaction terms depending on space, time and an appropriate function space with $d(0) = 0 = b(0)$
- $\lambda > 0$

# Existence of nontrivial periodic solutions

**Theorem (Roschat 2014)**

*Let $C, \lambda > 0$. Under the assumptions*

- $d, b$ *are continuous*
- $\sum_{j=1}^{2}(\int_\Omega d_j(y,x,t)dx + \int_\Gamma b_j(y,s,t)ds) = 0$ *for almost all $t$ and all $y$*
- $\max\{|d_j(y,x,t)|, |b_j(y,x,t)|\} \leq M$ *for all $y$, $j = 1, 2$ and almost all $(x,t)$.*

*there is at least one periodic weak solution $y \in W(0,T;H^1(\Omega))^2$ of the ecosystem model equation with*

$$\text{mass}(y(t)) := \int_\Omega (y_1(t) + y_2(t))dx = C \quad \text{for all } t \in [0,T].$$

*In particular, the solution is not trivial.*

But: No result about uniqueness.

# Off-line simulation with transport matrices

- Instead of directly using the pre-computed forcing data ...

$$\frac{\partial y_j}{\partial t} = \text{div}(\kappa \nabla y_j) - \text{div}(\vec{v} y_j) + q_j(t, y, u), \quad j = 1, \ldots, s$$

- ... use discretized transport operators (matrices) in the *i*-th time step:

$$\mathbf{y}_{i+1} = \underbrace{A_{imp,i} \, (A_{exp,i}}_{\text{transport matrices}} \, \mathbf{y}_i + \Delta t \, q_i(\mathbf{y}_i, u)), \quad i = 1, \ldots$$

  $\mathbf{y}_i$: vector of all tracers at all grid points at time step *i*.
- Sparse implicit and explicit transport matrices:

$$A_{imp,i} = (I - \Delta t \, L_{imp,i})^{-1}$$
$$A_{exp,i} = (I + \Delta t \, L_{exp,i})$$

- Example resolution: 2.8125 deg ($128 \times 64$) surface grid, 15 vertical layers, 2880 time steps, matrix dimension per tracer $\approx 50'000$.
- Software METOS3D [Piwonski, Slawig 2015]: Marine Ecosystem Toolkit for Optimization and Simulation in 3-D, on github.

# Fixed-Point vs. Newton

- One time-step (e.g. 3 hours):

$$\mathbf{y}_{i+1} = \quad A_{imp,i}\left[A_{exp,i}\,\mathbf{y}_i + \Delta t\, q_i(\mathbf{y}_i, u)\right] \;=:\; g_i(\mathbf{y}_i, u), \quad i = 0, \ldots, n_{year} - 1.$$

- One year: ($\mathbf{y}^k$: all tracers at all grid points at one time step in year $k$.)

$$\mathbf{y}^{k+1} = \underbrace{g_{n_{year}-1} \circ \cdots \circ g_0}_{=:G \text{ (one model year)}}(\mathbf{y}^k, u)$$

- “Spin-up“ (pseudo time-stepping, fixed-point iteration):

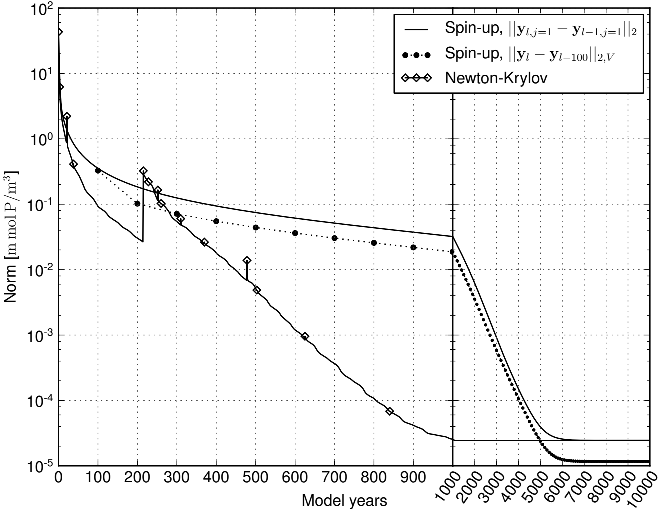
$$\mathbf{y}^{k+1} := G(\mathbf{y}^k, u), \qquad k = 1, 2, \ldots$$

- Newton-Krylov (matrix-free):

$$\text{solve} \quad \overbrace{G_y(\mathbf{y}^k, u)\Delta\mathbf{y}}^{\substack{\text{directional derivative} \\ \text{of one model year}}} = -G(\mathbf{y}^k, u)$$

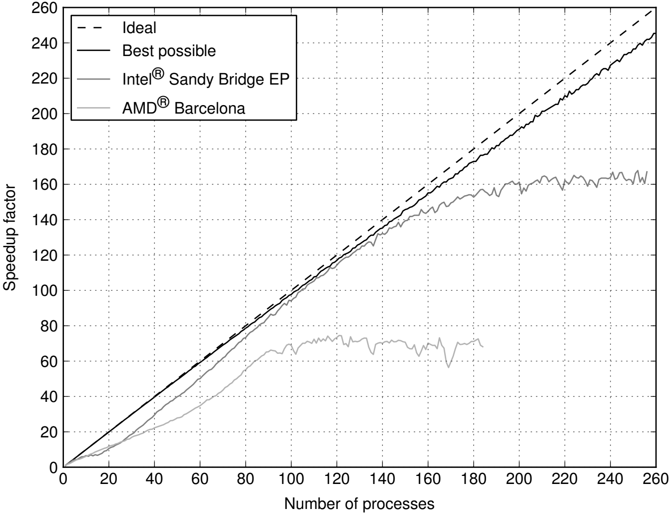
$$\mathbf{y}^{k+1} := \mathbf{y}^k + \Delta\mathbf{y}, \qquad k = 1, 2, \ldots$$

# Fixed-Point vs. Newton




Convergence towards a periodic solution.

# Spatial parallelization via domain decomposition




Theoretical and actual speedup of parallelized simulation runs.

# Numerical solution of the optimization problem

- Find $y \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, $m \ll n$

$$\min J(y,u) = \frac{1}{2}\|y - y_{data}\|^2 + \frac{\alpha}{2}\|u - u_{est}\|^2 \quad \text{s.t. } e(y,u) = 0.$$

- State $y$ is converged solution of a iteration (fixed-point or Newton):

$$y_{k+1} = G(y_k, u)$$

- Fixed-point: 3-10'000 years model time with 2880 times-steps each
- Newton: $\approx 1'000$ years model time.
- Spatial parallelization already exploited
- Ideally: even finer discretization
- Gradient based, iterative optimization: typically 100s of function evaluations
- $\Longrightarrow$ Acceleration techniques needed
- Motivation for additional parallelization in time

# First approach: *Parareal* with coarser time-steps

- Same spatial, but coarser temporal resolution:

$$\frac{\text{fine (original)}}{\text{coarse}} \text{ time-step} \hat{=} \frac{3}{192} \text{ hrs.} \hat{=} \frac{1}{64} \hat{=} \frac{2880}{45} \text{ steps/year}$$

- Result for 8 time intervals/processors (one year model time):

| Algorithm | Iteration | Accuracy Tracer 1 | Tracer 2 | mean time (s) |
|---|---|---|---|---|
| standard | | | | 221.000 |
| parareal | 1 | 7.69e-03 | 3.37e-03 | 56.126 |
| | 2 | 1.50e-03 | 7.28e-04 | 108.441 |
| | 3 | 7.73e-04 | 3.72e-04 | 160.303 |
| | 4 | 2.59e-04 | 1.17e-04 | 211.828 |
| | 5 | 5.65e-05 | 3.19e-05 | 262.946 |
| | 6 | 8.69e-06 | 4.64e-06 | 313.622 |
| | 7 | 5.55e-07 | 2.78e-07 | 363.646 |
| | 8 | 1.74e-13 | 8.89e-14 | 413.596 |

- Spin-up has ≈1e-04 accuracy, so (especially for the first steps) 1-3 parareal interations may be enough.

# Future work

Parameter ID in marine ecosystems:

- Repeat tests for complete spin-up.
- Micro-macro parareal:

  Generate matrices corresponding to coarser spatial mesh.

  Has to be done algebraically, since no coarser model available.
- Later: use current mesh (2.8 deg) as macro and an even finer one (1 deg) as micro.

Different project: Long-time paleo climate simulation

- Micro-macro setting for global climate models.