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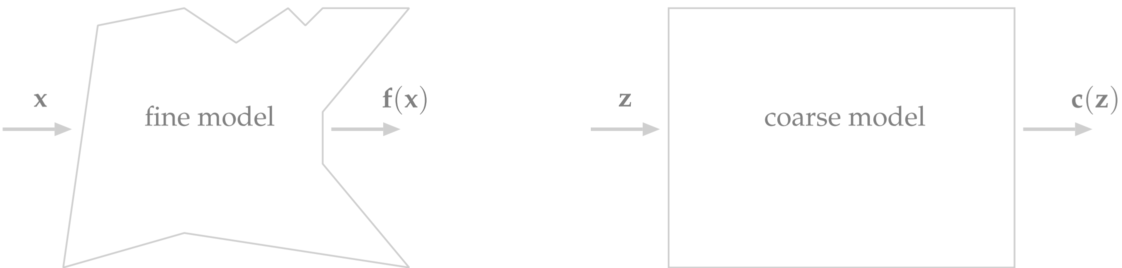
Surrogate-Based Optimization of Biogeochemical Models

A3: Algorithmic Optimal Control - C02 Uptake of the Ocean
(Prof. Dr. Thomas Slawig)

ICNAAM 2010



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Algorithmic Optimal Control - C02 Uptake of the Ocean

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General Research Aims

- CO_2 concentration has doubled since 1900
- To-date we assume $4 - 8°$C in the buisiness as usual case
- Agreement on the "2-degree-aim" until the year 2100
- This relates to a CO_2 emission reduction about 80% until 2050

$$\Downarrow$$

- Only sustainable energypolitics will not comply with this aim
- Think of carbon management/ sequestration approaches
- Increase our understanding of ocean change (past, present, future), the ocean's potential (marine ressources) and its risks

Algorithmic Optimal Control - C02 Uptake of the Ocean

- The ocean ↷ biggest CO_2 sink
- More than half of anthropogenic CO_2 stored for long time
  ↷ Crucial impact on climate
- Natural Sequestration based upon global CO_2 cycle
- "Physical + Biological CO_2 pump" are the operators
- Ocean Circulation + Biogeochemical Models indispensible

$$\Downarrow$$

- Optimization w.r.t. available measurement data (target)

↷ e.g. Improve determination of current/ future CO_2 sequestration potential

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The Biogeochemical Model

- Biogeochemical models = coupled PDE systems

  ↷ time-dependent advection-diffusion + nonlinear coupling terms

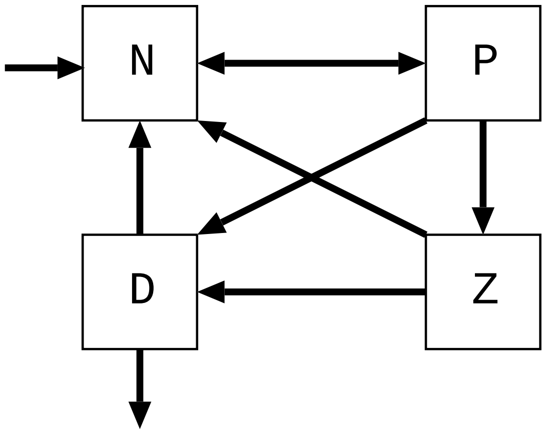
- Here: Ocean model data (velocity u_1) is used as a kind of forcing

  "offline mode" ↔ "online mode"

$$\frac{\partial \mathbf{y}^{(l)}}{\partial t} = \underbrace{-u_1 \frac{\partial \mathbf{y}^{(l)}}{\partial z}}_{\text{advection}} + \underbrace{\frac{\partial}{\partial z}\left(K_\rho \frac{\partial \mathbf{y}^{(l)}}{\partial z}\right)}_{\text{diffusion ("mixing")}} + \underbrace{Q^{(l)}(\mathbf{y}, t, u_2, \ldots, u_n)}_{\text{nonlinear coupling}}$$

$$\mathbf{y} = \left(\mathbf{y}^{(N)}, \mathbf{y}^{(P)}, \mathbf{y}^{(Z)}, \mathbf{y}^{(D)}\right)^T \quad , \quad \mathbf{y} \in [0,T] \times [0,H] \to \mathbb{R}^4.$$

N : dissolved inorganic nitrogen
P : phytoplankton
Z : zooplankton
D : detritus



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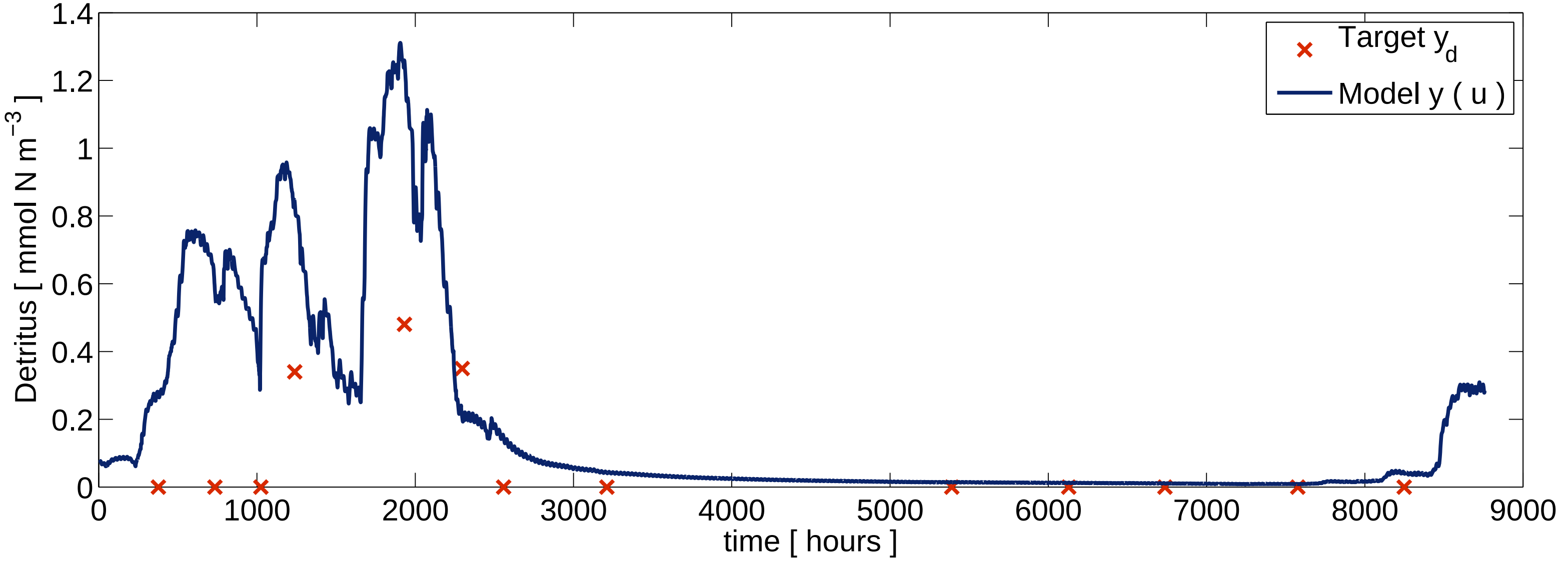
The Optimization (OPT) Problem

- Minimize distance between the model output $\mathbf{y}(\mathbf{u})$ and some target $\mathbf{y}_d$ (of least-squares type)

$$\min_{\mathbf{u}\in U} J(\mathbf{y}(\mathbf{u}),\mathbf{u}) := \left\| \mathbf{y}(\mathbf{u}) - \mathbf{y}_d \right\|_Y^2 + \alpha \cdot \| \mathbf{u} \|_U^2$$

$$U := \{ \mathbf{u} \in \mathbb{R}^n : \mathbf{b}_l \leq \mathbf{u} \leq \mathbf{b}_u \} \quad , \quad J : Y \times U \to \mathbb{R}$$

- Control variables $\mathbf{u}$ (scalar numbers) = 12 unknown physical/ biological parameters in the nonlinear coupling term $Q^{(l)}$



Surrogate-Based Optimization

- Aim : Reduce the overall number of high-fidelity model and gradient evaluations

- High-fidelity/ fine model $\mathbf{y}(\mathbf{u})$ $\curvearrowright$ replaced by computationally cheaper, less accurate surrogate with state $\mathbf{s}_k(\mathbf{u})$

$$\mathbf{u}_{k+1} = \min{}_{\mathbf{u}\in U} \; J\left(\mathbf{s}_k(\mathbf{u}), \mathbf{u}\right)$$

$$\mathbf{s}_k(\mathbf{u}_k) \approx \mathbf{y}(\mathbf{u}_k) \quad , \quad \left(\mathbf{s}_k'(\mathbf{u}_k) \approx \mathbf{y}'(\mathbf{u}_k) \right)$$

$$\hat{\mathbf{y}}(\mathbf{u}) \quad \xrightarrow{\text{alignment/ correction}} \quad \mathbf{s}_k(\mathbf{u})$$

- 0-oder and ideally also 1st-order similarity

- Groups of functional and physically-based surrogates

- Basis is a low-fidelity/ coarse model $\hat{\mathbf{y}}(\mathbf{u})$ which is then aligned/corrected through appropiate techniques to obtain the surrogate $\mathbf{s}_k(\mathbf{u})$

- Examples: coarser discretization , using analytical formulas if available, using simplified physics, . . .

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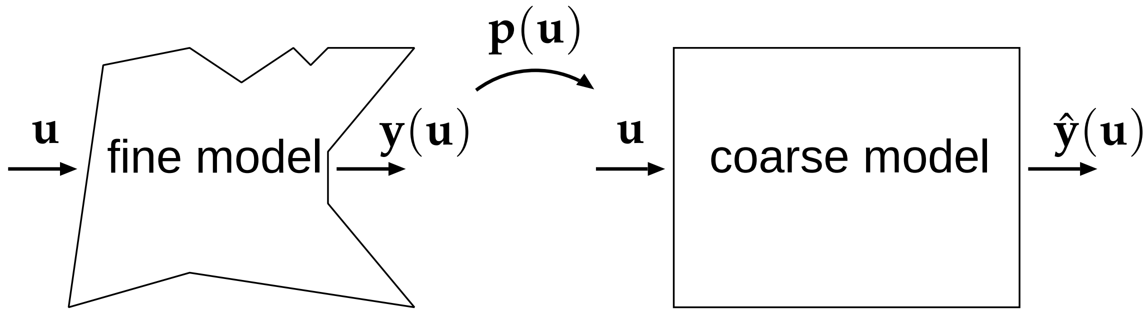
Space Mapping (SM) Optimization

Basic Concept



- SM uses a physically-based coarse model to create the surrogate
- Basic approach : Correction/ alignment through parameter mapping $\mathbf{p} : U \mapsto U$

$$\mathbf{u}_{k+1} = \min_{\mathbf{u}\in U} J\left(\mathbf{s}_k(\mathbf{u}), \mathbf{u}\right) \quad , \quad \mathbf{s}_k(\mathbf{u}) := \hat{\mathbf{y}}\left[\, \mathbf{p}_k(\mathbf{u}) \,\right]$$

$$\mathbf{p}_k(\mathbf{u}) = \mathbf{p}(\mathbf{u}_k) + \mathbf{p}'(\mathbf{u}_k)\,(\mathbf{u}_k - \mathbf{u})$$

$$\mathbf{p}(\mathbf{u}_k) := \operatorname{argmin}_{\mathbf{u}\in U} \left\| \hat{\mathbf{y}}(\mathbf{u}) - \mathbf{y}(\mathbf{u}_k) \right\|^2$$

$$\hat{\mathbf{y}}_k(\mathbf{u}_k) \approx \mathbf{y}(\mathbf{u}_k)$$

Example: The Aggressive SM (ASM) Algorithm

- The ASM algorithm iteratively solves for a solution of the nonlinear system of equations

$$\mathbf{F}(\mathbf{u}) := \mathbf{p}_k(\mathbf{u}) - \hat{\mathbf{u}}^* = 0 \quad , \quad \hat{\mathbf{u}}^* := \min_{\mathbf{u}\in U} J\left(\hat{\mathbf{y}}(\mathbf{u}), \mathbf{u}\right)$$

$$\mathbf{p}_k(\mathbf{u}) = \mathbf{p}(\mathbf{u}_k) + \mathbf{p}'(\mathbf{u}_k)\,(\mathbf{u}_k - \mathbf{u})$$

- Using a globalized Quasi-Newton method with a Broyden rank-one update for the Jacobian $B_k \simeq \mathbf{p}'(\mathbf{u}_k)$

$$\mathbf{u}_{k+1} = \mathbf{u}_k + \sigma \cdot \mathbf{s}_k \quad , \quad B_k\,\mathbf{s}_k = -\mathbf{F}_k \quad , \quad \left\|\mathbf{F}(\mathbf{u}_{k+1})\right\|^2 \leq (1-\delta\cdot\sigma)\cdot\left\|\mathbf{F}(\mathbf{u}_k)\right\|^2$$

With $\mathbf{s}_k$ = descent direction for the merrit function $\|\mathbf{F}_k\|^2$

(assuming $B_k \simeq \mathbf{p}'(\mathbf{u}_k)$)

Example: Coarse Discretization

The Coarse Model

Discretized model equations with $\mathbf{y}_j \approx \big(\mathbf{y}(z_i, t_j)\big)_{i=1,\dots,K}$ and $A_j := A(t_j)$

$$\underbrace{\left[I - \tau \cdot A_j^{\text{diff}}\right]}_{:=B_j^{\text{diff}}} \mathbf{y}_{j+1} = \underbrace{\left[I + \tau \cdot A_j^{\text{adv}}\right]}_{:=B^{\text{adv}}} \circ B_j^Q \circ B_j^Q \circ B_j^Q \circ B_j^Q(\mathbf{y}_j)$$

$$B_j^Q(\mathbf{y}_j) := \left[I + \tau/4 \cdot Q_j(\mathbf{y}_j)\right] \quad , \quad j = 1, \dots, M$$

j	:	discrete time step
$A_j^{\text{diff}}, A^{\text{adv}}$	:	Spatial discretization of the sinking and diffusion term
Q_j	:	Nonlinear coupling in the four tracers
M, τ, K	:	Number, size of discrete time steps resp. vertical levels

High-fidelity model: $\tau = 1$ h

Low-fidelity model: $\hat{\tau} = \beta \cdot \tau$, e.g. $\beta = 2, 10, 20, 40, 80, \dots$

NOTE: Account for numerical instabilties due to $\hat{\tau} \not< C$

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The Future Ocean
The Model
The OPT Problem
Surrogate OPT
SM Optimization
Example
» The Coarse Model
» Numerical Stability
» Mapped Coarse Model
Conclusions

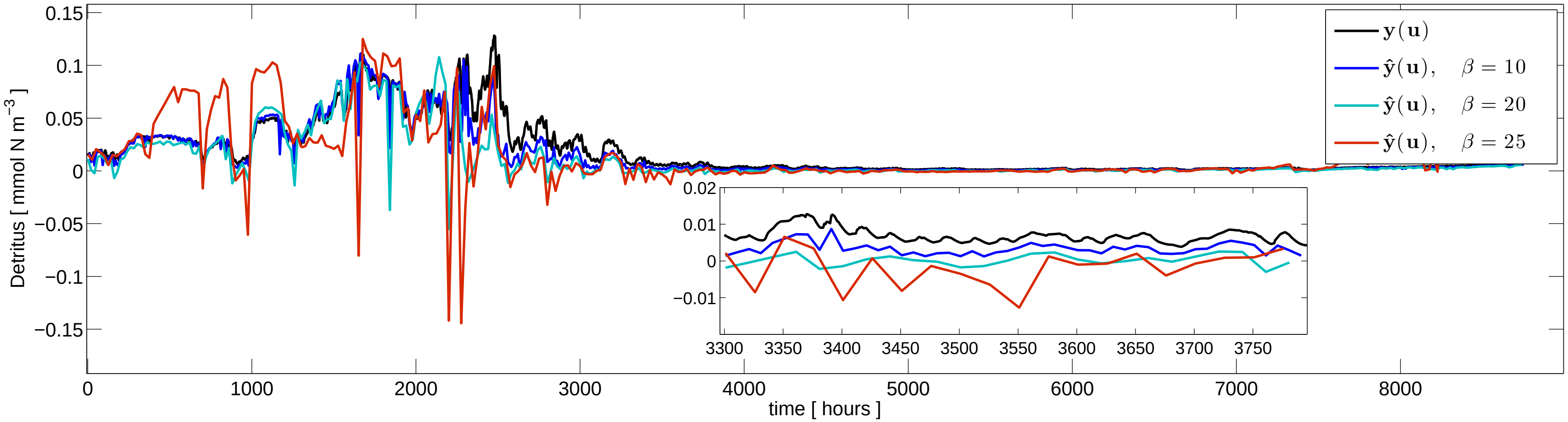
Numerical Stability

It can be shown that

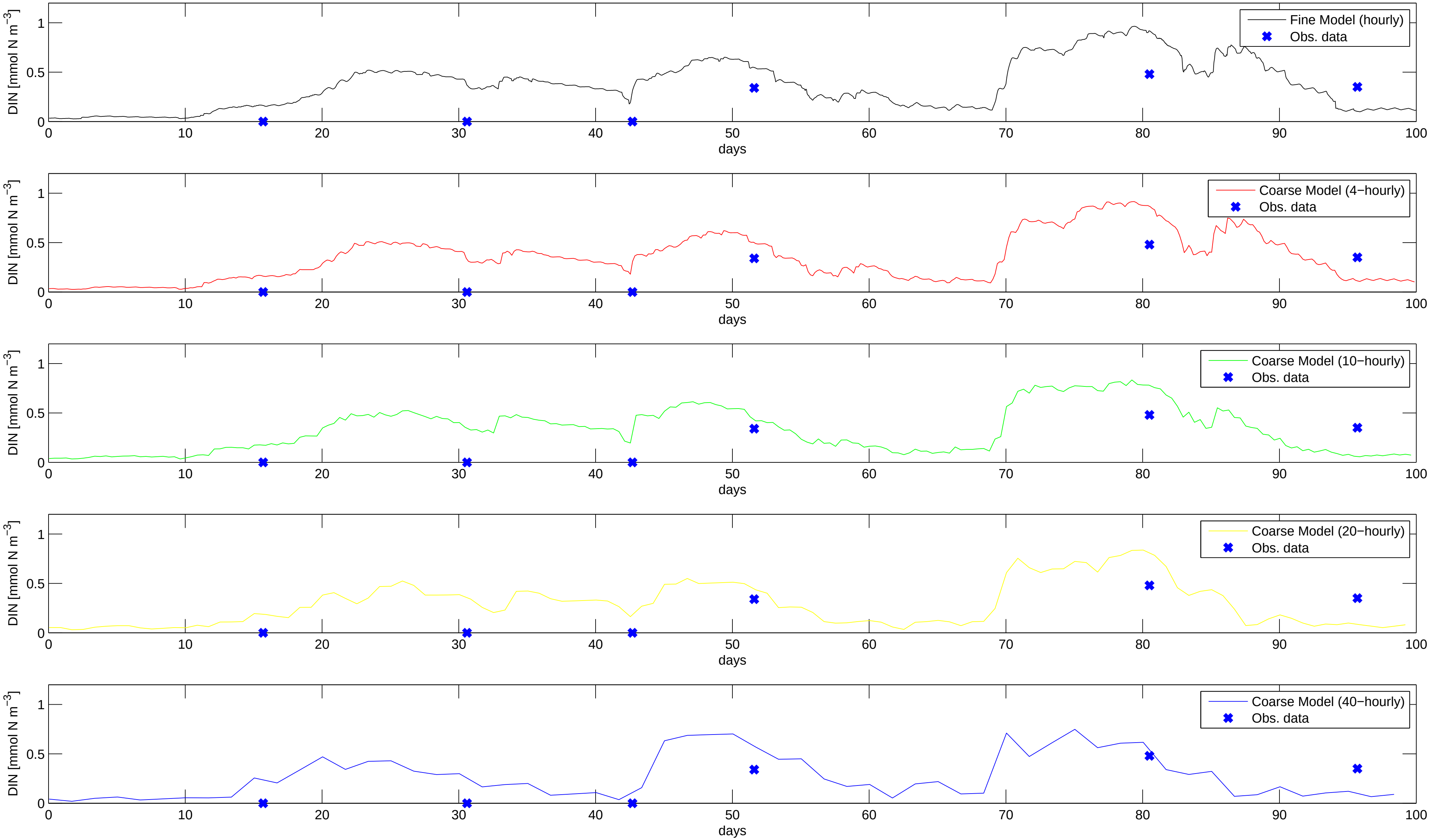
$$\left\|\mathbf{y}_j\right\| \leq \left(\prod_{m=0}^{j-1}\left\|B_m^{\text{diff}}\right\|\right)\cdot\left\|B^{\text{adv}}\right\|^j\cdot\prod_{m=0}^{j-1}\left\|L_m^Q\right\|^4 \quad , \quad L_m^Q := I+\tau/4\cdot Q_m'(0) \quad (1)$$

(since $Q_m(0) = 0$)
Hence a sufficient criterion for stability using this approximation of Q (!) is

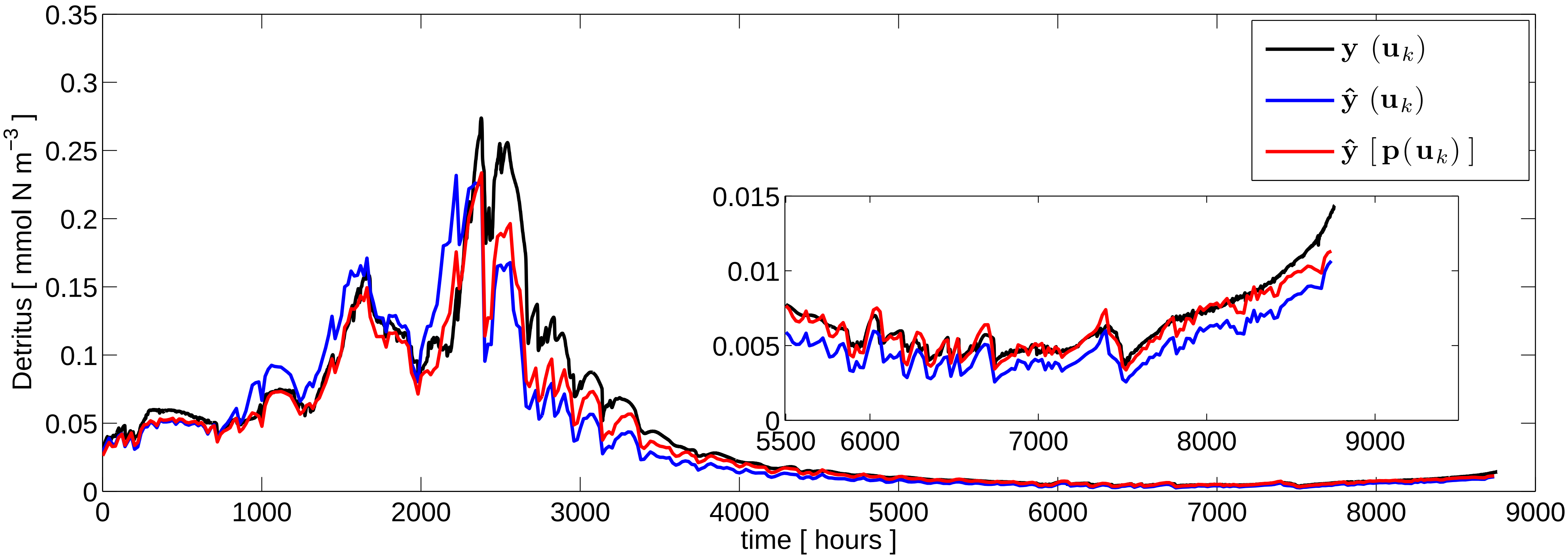
$$\left\|B_m^{\text{diff}}\right\| \leq 1 \quad , \quad \left\|B^{\text{adv}}\right\| \leq 1 \quad , \quad \left\|L_m^Q\right\| \leq 1 \quad . \qquad (2)$$



The Coarse Model



Mapped Coarse Model

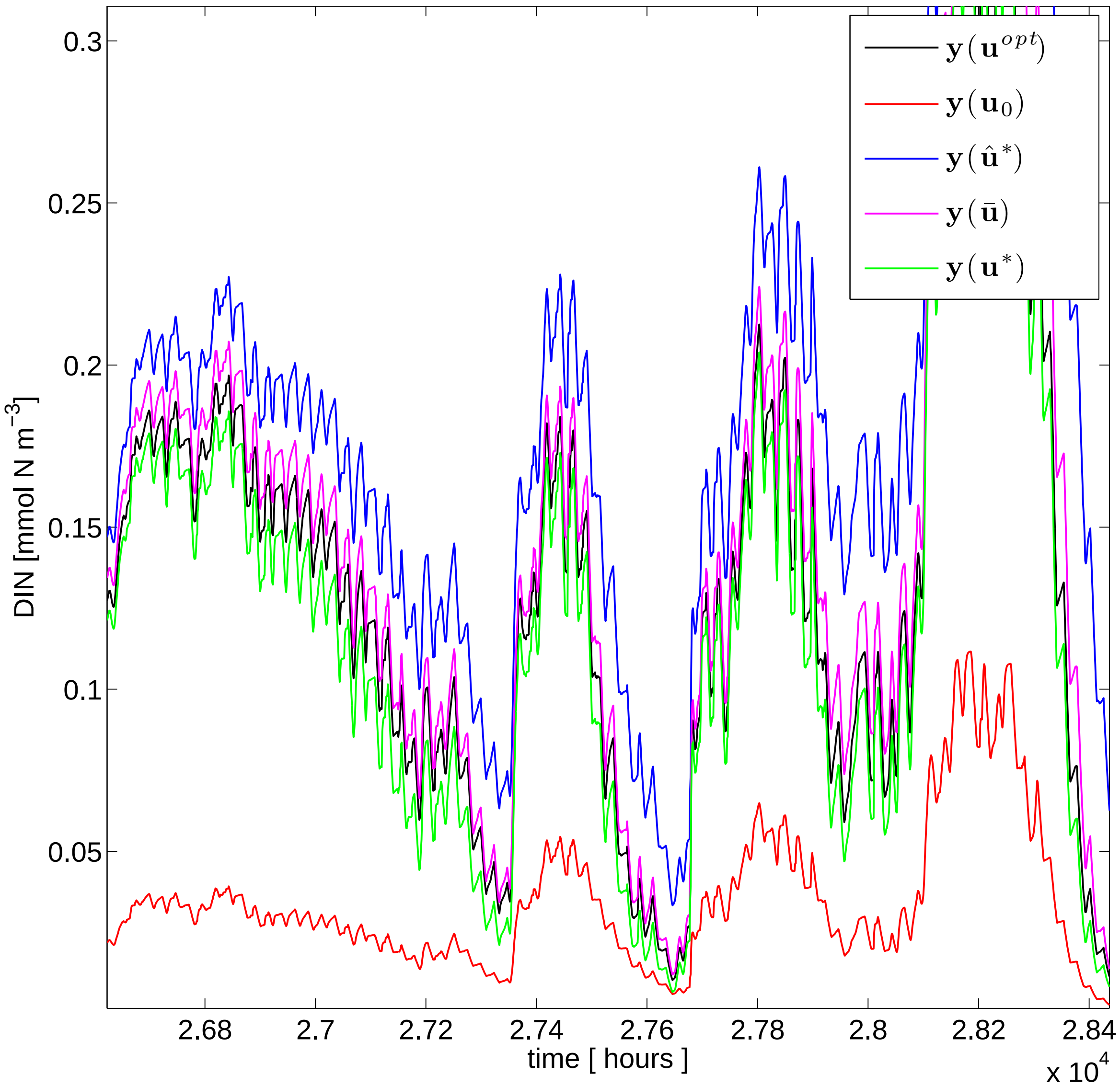


Obviously surrogate's 1st order information corresponds

$$\hat{\mathbf{y}}_k(\mathbf{u}_k) \quad = \quad \hat{\mathbf{y}}[\,\mathbf{p}(\mathbf{u}_k)\,] \quad \simeq \quad \mathbf{y}(\mathbf{u}_k)$$

ASM vs Direct Optimization

iterate $\mathbf{u}_k$		min J	min $\hat{J}$
$\mathbf{u}_0$	J_0	$4.31e-02$	$4.31e-02$
	$\delta\mathbf{u}_k$	$1.92e+00$	$1.92e+00$
$\hat{\mathbf{u}}^*$	J	-	$1.56e-03$
	J/J_0	-	$3.61e-02$
	$\delta\mathbf{u}_k$	-	$8.17e-01$
			ASM
$\mathbf{u}^*, \bar{\mathbf{u}}$	J	$3.29e-05$	$3.73e-04$
	J/J_0	$7.63e-04$	$8.65e-03$
	$\delta\mathbf{u}_k$	$4.75e-01$	$5.42e-01$
	time	4215 s	1851.4 s
	# iter.	27	38 (33 + 5)



$$\delta\mathbf{u}_k := \left\| \mathbf{u}_k - \mathbf{u}^{\text{opt}} \right\|_{\text{rel}} \; , \; J =: J(\mathbf{y}(\mathbf{u}), \mathbf{u}) \; , \; \hat{J} =: J(\hat{\mathbf{y}}(\mathbf{u}), \mathbf{u})$$

Conclusions

- E.g. improve prediction of the CO_2 uptake of the ocean

  ↷ Optimization of transport + ocean models

- Surrogate approach: Seek for a reduction in total # of high-fidelity model evaluations and derivatives in particular for more time-consuming 3-D models

- A coarser discretized model can be used as a basis to create a surrogate (mostly easy to implement)

- Numerical Stability issues might place significant limitations

  ↷ Preanalysis indispensible !

- ASM : This basic approach of SM Optimization already yields a reasonable solution and reduction in total optimization cost

Thank you for your attention

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