Algorithmic Optimal Control - CO2 Uptake of the Ocean

Junior Research Group A3

Research Challenges and Recent Results

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Outline

- Some facts about „The Future Ocean“ ... general research aim ... our workgroup
- Oceanic CO2 uptake ... marine ecosystem models
- The underlying models ... the math behind
- One example
- Parameter optimization
- Current Research

Cluster of Excellence “The Future Ocean”

future ocean
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Computer Science, Mathematics

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Marine Science

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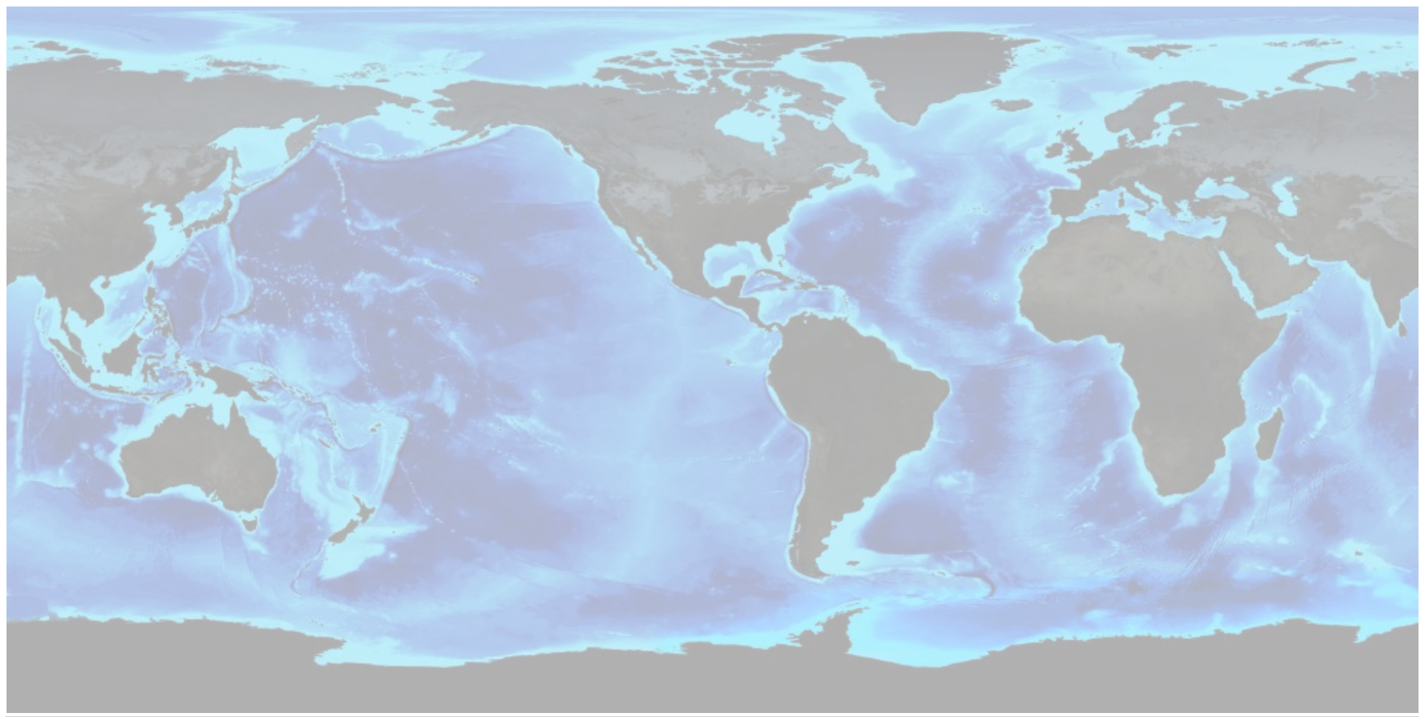


Economy

ifw

Art

muthesius
kunsthochschule

Furthermore ...

- medical scientists
- lawyers
- sociologists

General Research Aims

Some well known facts ...

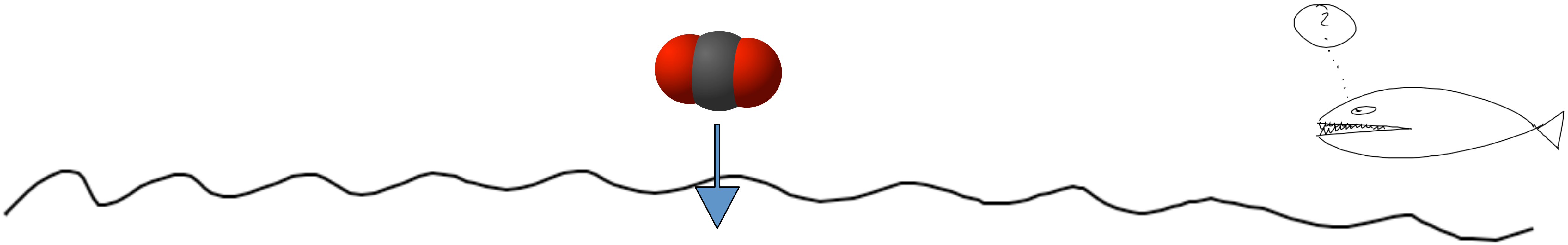
- CO_2 concentration has doubled since 1900
- To-date we assume $4-8^{\circ}C$ increase ... in the buisiness as usual case
- Agreement on the "2-degree-aim" until the year 2100
- This relates to a CO_2 emission reduction about 80% until 2050
- Only concentrating sustainable energypolitics will not comply with this aim
- Think of carbon management/sequestration approaches

Algorithmic Optimal Control - C02 Uptake of the Ocean

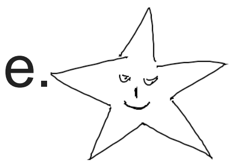
- Understanding the oceanic CO_2 uptake is of central importance for projections of climate change and oceanic ecosystems
- The ocean ➔ biggest CO_2 sink
- More than half of anthropogenic CO_2 stored for long time ➔ Crucial impact on climate
- Natural sequestration based upon global CO_2 cycle
- Furthermore additional C02 sequestration approaches are considered and analyzed

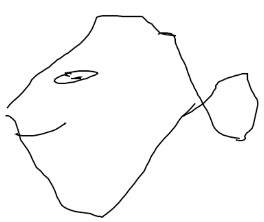
Marine Ecosystem Models - Oceanic CO2 Uptake ...

- ... is determined by the solution of CO2 in the water via the ocean surface

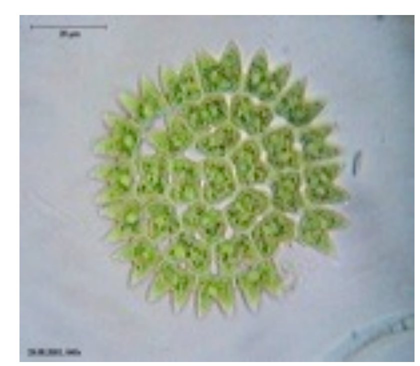


- ... and physical and biogeochemical processes in the water, i.e.





  - Ocean circulation
  - Photosynthesis (depends on nutrients), consumption by zooplankton, sinking of dead material, ...



Picture: Wagner GFDL

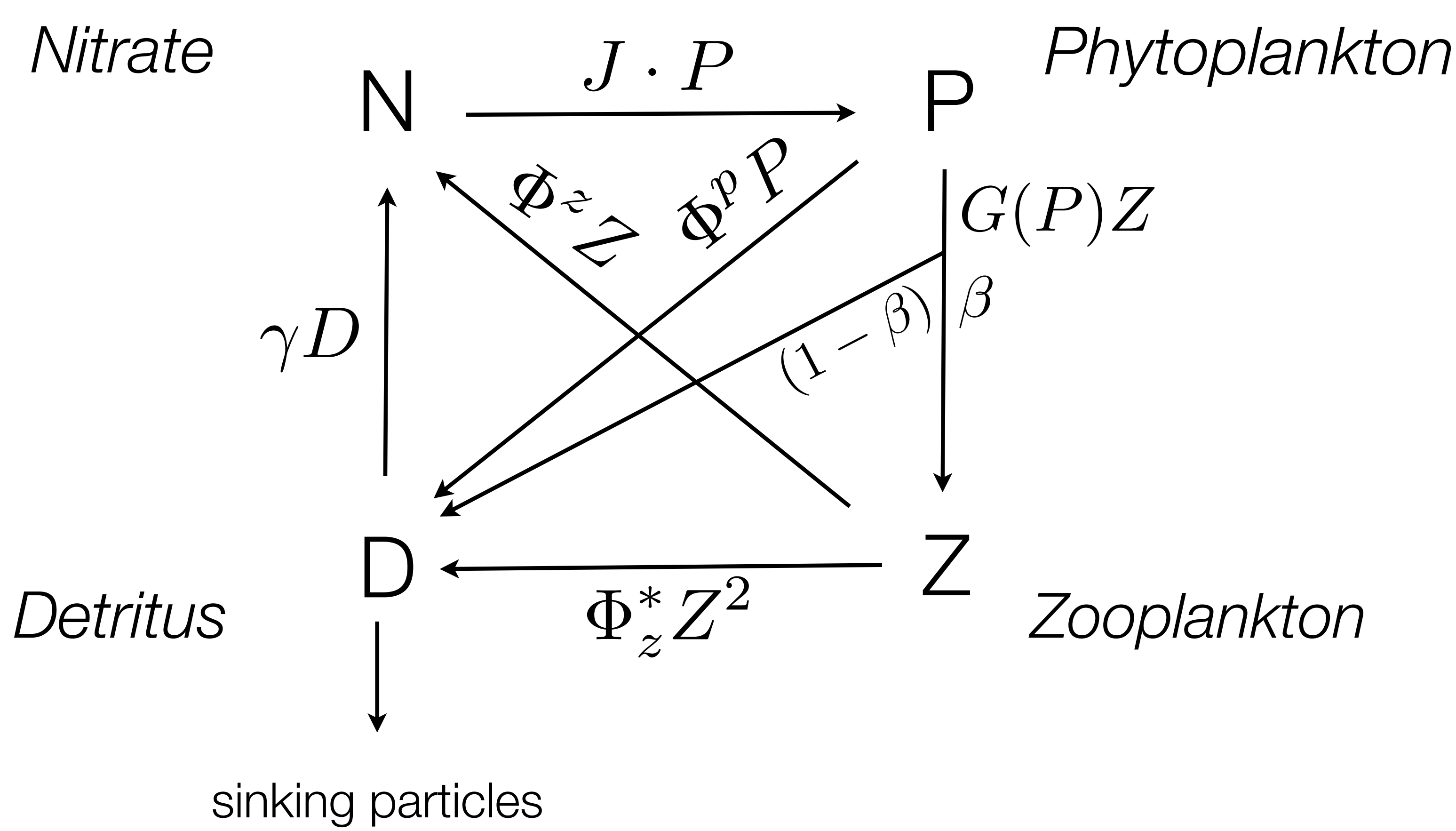
- Sinking dead organic material exports the carbon to the deeper ocean, below the upper mixed layer

- ... are governed by coupled systems of nonlinear parabolic partial differential equations for ocean circulation (ocean models) and transport of biogeochemical tracers (marine ecosystem models)

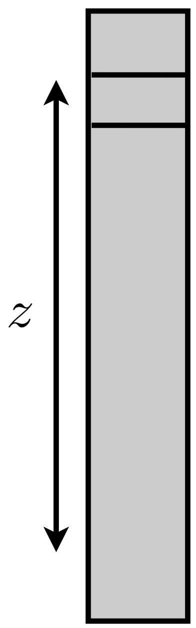
$$\frac{\partial y_i}{\partial t} = \underbrace{\operatorname{div}\left(\kappa \nabla y_i\right)}_{\text{diffusion}} + \underbrace{\operatorname{div}(\vec{v} y_i)}_{\text{advection}} + \underbrace{q_i(y_1, \ldots, y_n, T, S, u)}_{\text{tracer coupling}}$$

One Example ...

- Marine ecosystem model of NPZD type (Oschlies Garcon *Glob. Biogeochem. Cycles* 1999)
- Here: Ocean model data (velocity, diffusion coefficient, temperature) is precalculated by an ocean model (i.e. offline mode)



The Maths behind



$$\frac{\partial y_i}{\partial t} = \underbrace{\mathrm{div}\,(\kappa \nabla y_i)}_{\text{diffusion}} + \underbrace{\mathrm{div}(\vec{v} y_i)}_{\text{advection}} + \underbrace{q_i(y_1, \ldots, y_n, T, S, u)}_{\text{tracer coupling}}$$

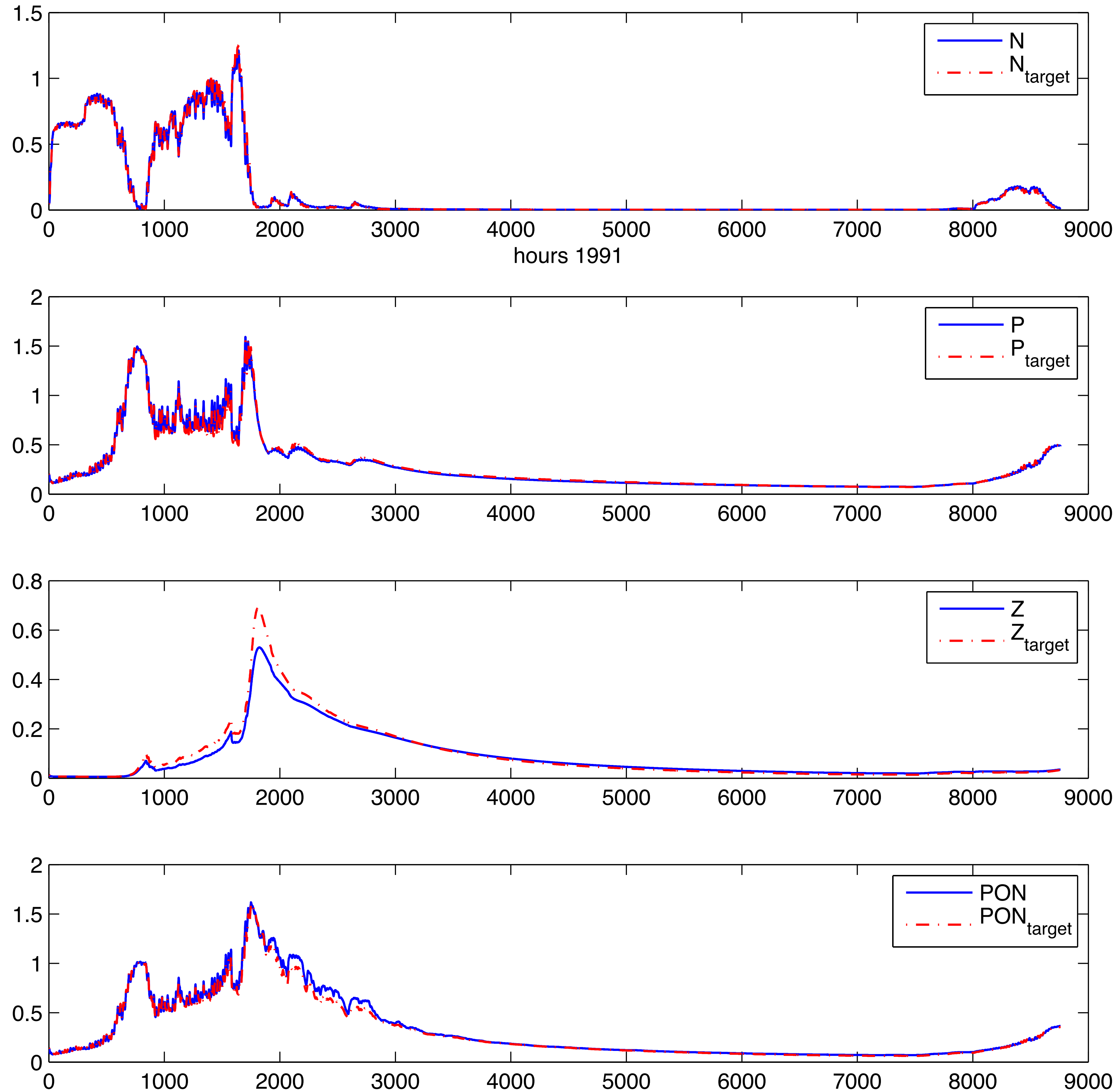
$$\begin{aligned}
q_1 &= -J(N,P)P + \gamma_m D + \Phi^z_m Z, \\
q_2 &= J(N,P)P - \Phi^p_m P - G(\epsilon, g)Z, \\
q_3 &= \beta G(\epsilon, g, P)Z - \Phi^z_m Z - \Phi^*_z Z^2, \\
q_4 &= (1-\beta)G(\epsilon, g, P)Z + \Phi^*_z Z^2 + \Phi^p_m P - \gamma_m D.
\end{aligned}$$

$$J(N,P) = \min\{J_1(P), J_2(N)\}$$

$$G(\epsilon, g, P) = \frac{g\epsilon P^2}{g + \epsilon P^2}$$

A Typical Simulation Output

- Spring Bloom
- High-frequent oscillations
- Slight but global changes for different parameters



Improve models so they can be used e.g. for prediction of climate change ...

- Many parameters are used which ...
  ... are chosen such that the model output $\mathbf{y}(\mathbf{u})$ remains feasible (i.e. non-negative) and ...
  ... that given measurement data is matched $\mathbf{y}_d$

- For this purpose the aim is ...
  ... to minimize a least-squares type cost functional, measuring this misfit.

- Control vector $\mathbf{u}$ = unknown physical/ biological parameters in the nonlinear coupling terms q in the tracer transport equations

- Cost function may have lots of local minima + is high-dimensional

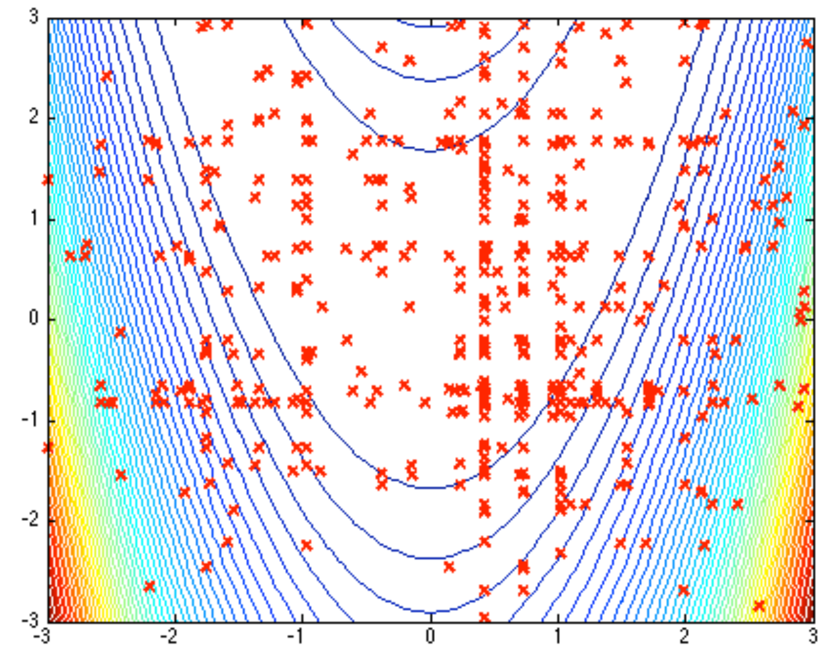
$$\min_{\mathbf{u}\in U} J(\mathbf{y}(\mathbf{u}),\mathbf{u}) := \left\|\mathbf{y}(\mathbf{u}) - \mathbf{y}_d\right\|_Y^2 + \alpha \cdot \|\mathbf{u}\|_U^2$$

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

What optimization methods can be used?

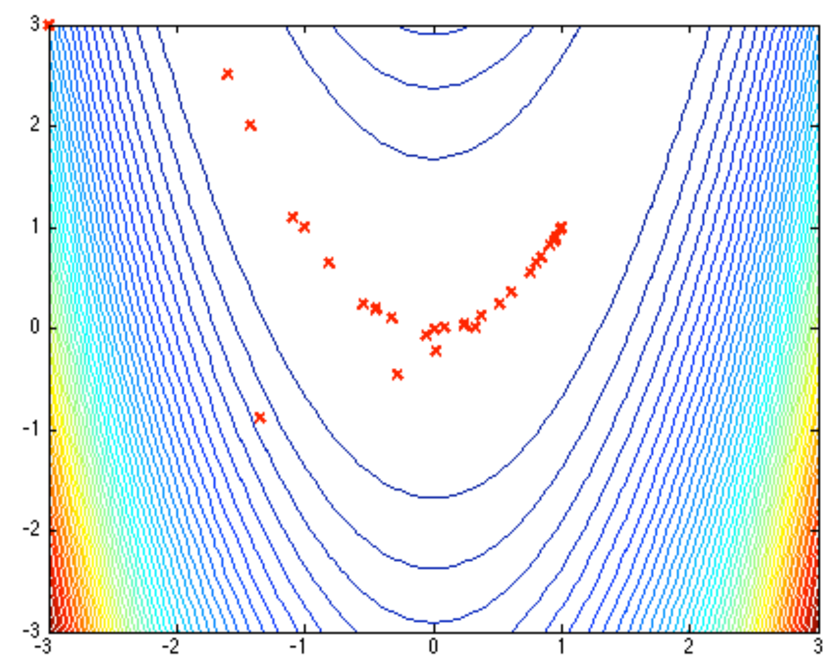
Using only function evaluations (evolutionary/genetic alg.):

- many evaluations necessary, hence need fast solver
- may find global optimum
- can easily treat box constraints



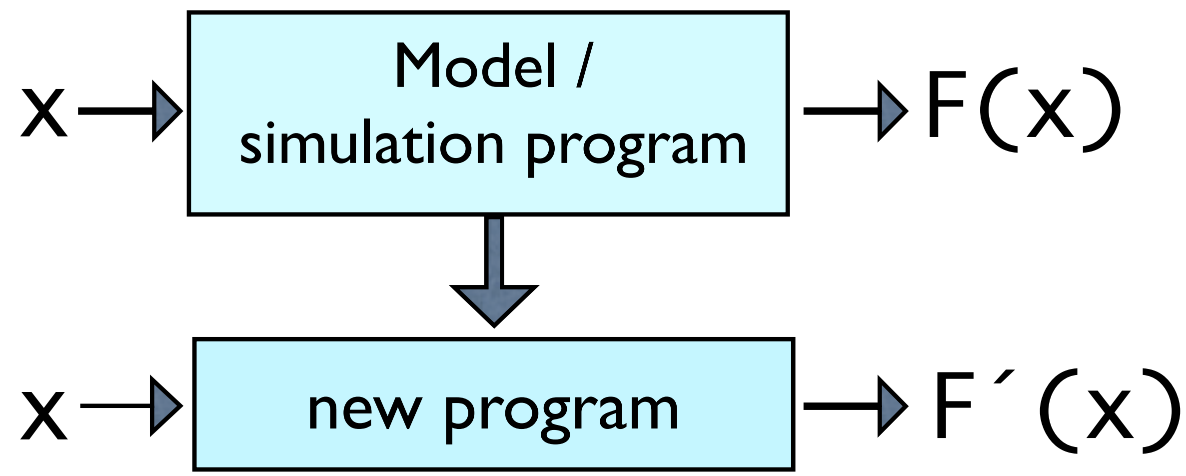
Using descent information (gradient, conjugate gradient, quasi-Newton/BFGS, SQP, active set, interior point methods ...)

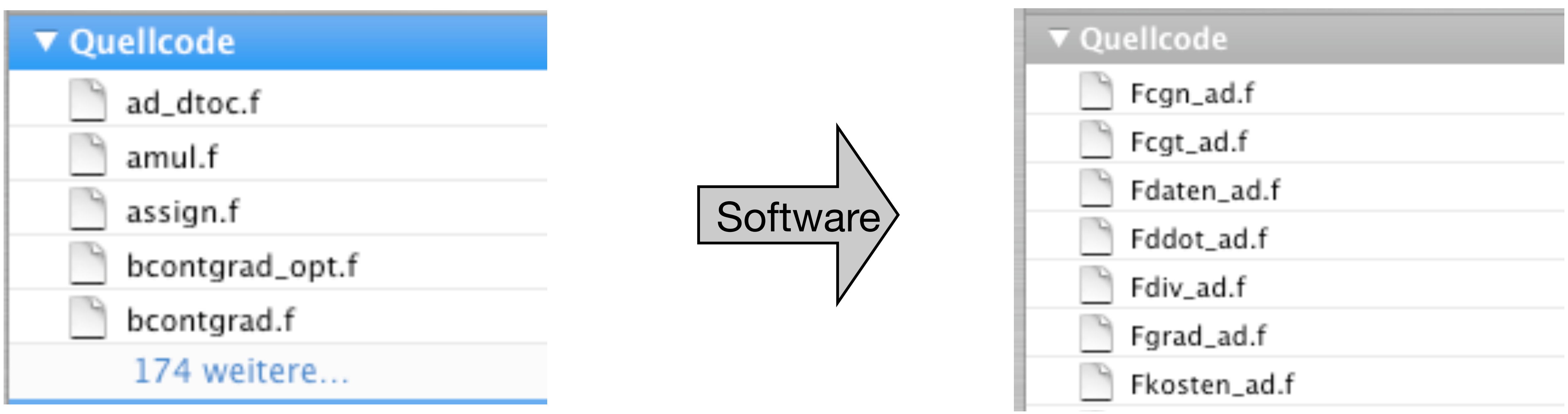
- need a formula for derivative/gradient (adjoint model)
- faster, migh become stuck in local optima
- need special treatment of constraints



An important technology we use ...

- Algorithmic or Automatic Differentiation (AD)
- Generation of new computer code that compute derivatives, e.g. for optimization or sensitivities





subroutine f (x, y, ...)

subroutine g_f (x, g_x, y, g_y, ...)

Ongoing Research ...

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Model Validation

(J. Rückelt, joru@informatik.uni-kiel.de)

Questions arise ...

- Can the model reproduce real data? Is the model output injective? Is the model output independent of initial values? How is the dependency on data errors/uncertainties?

- Method: SQP solver, repeated starts from randomly chosen parameters, AD generated gradients = useful tool for parameter optimization

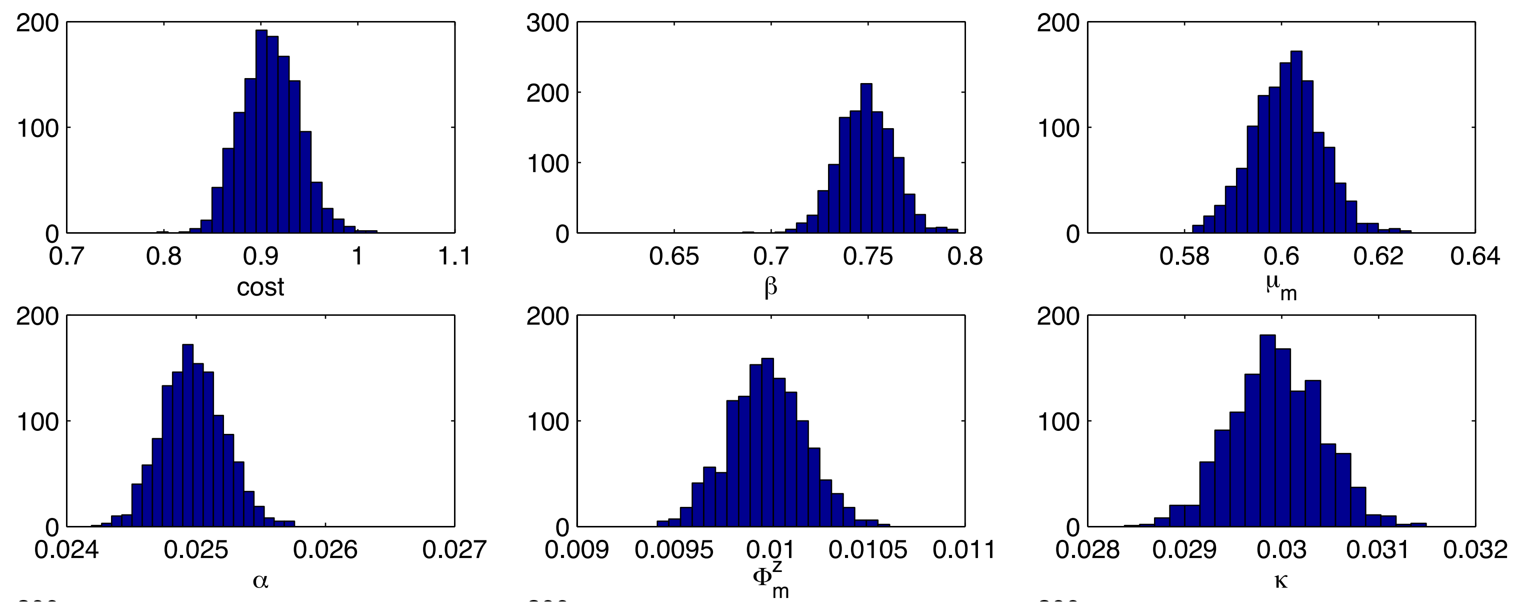
- Test: Reconstruction of random parameters up to arbitrary precision (albeit only with additional restriction on P)

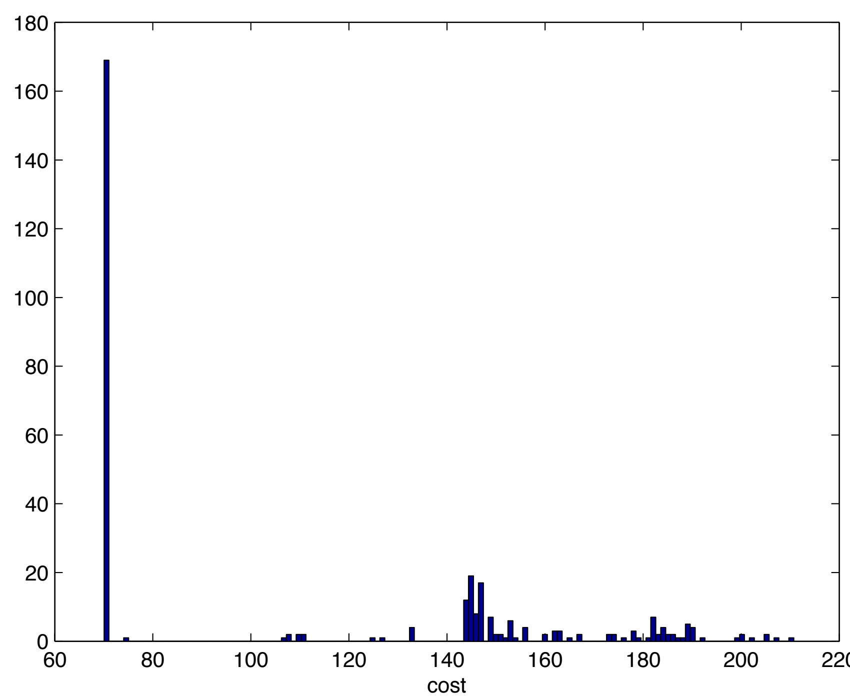
- Actual optimization: 320 starts, 180 'identical' minima with less than 1% spread in parameters

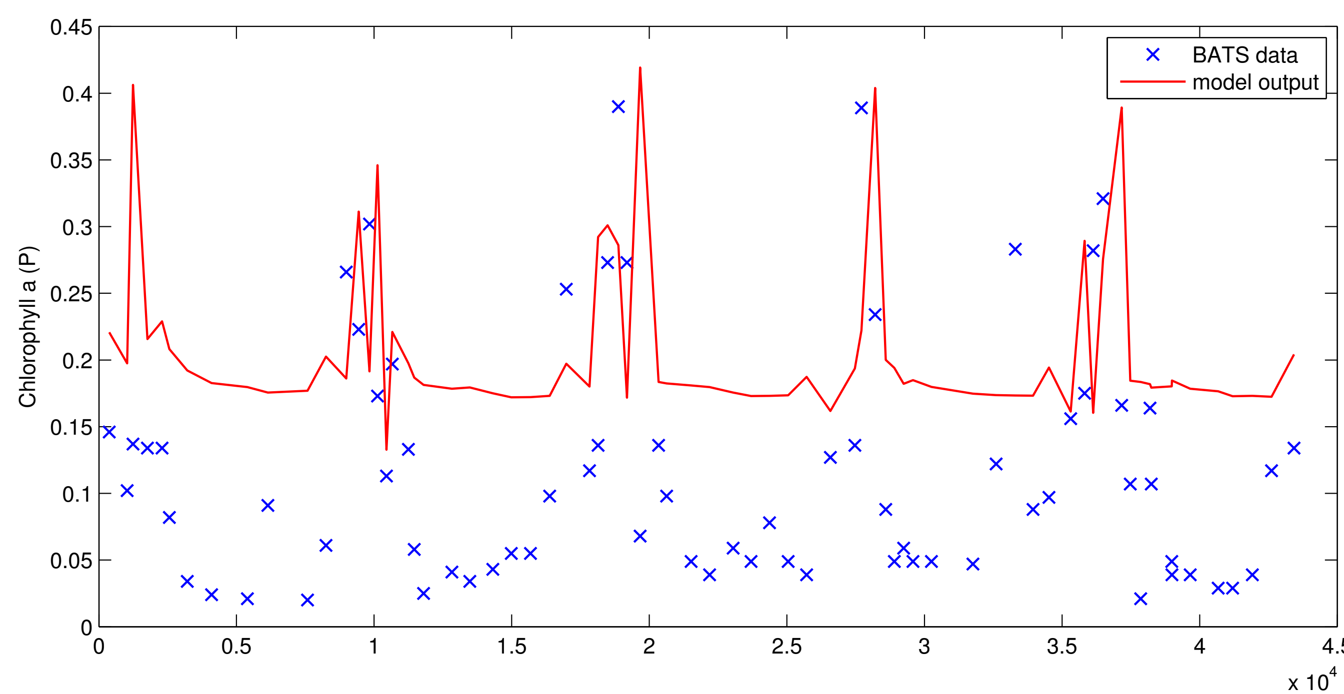
Model Validation

(J. Rückelt, joru@informatik.uni-kiel.de)

- Calculate the uncertainties (if the model is not too big & our optimizer ist fast)
- Shown are optimal parameters values when introducing gaussian data errors/uncertainties
- For this model the results above remain valid for real data, even though the model fit is not optimal







Linear Quadratic Optimal Control

(M. El Jarbi, mej@informatik.uni-kiel.de)

- Application of Linear Quadratic Optimal Control (LQOC) approach
- The aim is ...
  ... to minimize the cost/misfit subject to the following linear dynamics:

$$\begin{aligned} \dot{x}(t) &= A(t)x(t) + B(t)u(t), \quad t > t_0 \\ x(t_0) &= x_0, \end{aligned}$$

- The NPZD model is nonlinear,
  ➔ essential for applying a (LQOC) design is the linearization of the nonlinear differential equation

$$A(t) = \frac{\partial f}{\partial y}(y_d(t), u_d),$$

$$B(t) = \frac{\partial f}{\partial u}(y_d(t), u_d)$$

J. Piwonski, jpi@informatik.uni-kiel.de)

Marine **E**cosystem **O**ptimization and **S**imulation **T**oolbox in **3D**

- Framework towards ...
  ... parameter optimization of global marine ecosystem models (i.e. ocean circulation models coupled to 3D marine ecosystem models)
- Transport Matrix approach [Khatiwala et al., 2004]
- Flexible enough for different resolutions
- The software is ...
  - based on the spin-up framework by [Khatiwala, 2007]
  - written using the PETSc library only, http://www.mcs.anl.gov/petsc
- It admitts ...
  - Scalable Nonlinear Equation Solvers (globalized Newton-Krylov, Trust region)
  - Flexible FORTRAN/C interface for general marine ecosystem models

Surrogate-Based Optimization

(M. Priess, mpr@informatik.uni-kiel.de)

- Actual optimization process involves ...

  ... evaluations of the high-fidelity model
  + its sensitivitiy

- High computational cost and maybe ...
- ... sensitivities even not available

- High-fidelity model repaced by cheaper surrogate

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

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

Key points ...

- Fine model evaluated once or a few times only per iteration
- Number of iterations needed to yield satisfactory solution is small
- Accurate (at least locally) and cheap surrogate model
- smooth, easy to optimize

Types of Surrogates

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Functional:

Constructed without any particular knowledge of the system, based on sampled data and algebraic expressions, cheap to evaluate

Popular techniques:

Low-order polynomials, Radial basis functions, Kriging

Physically based:

Based on knowledge about the physical system in question, constructed from low-fidelity model, exist independently of the physical system, inherits more caharacteristics of the system, typically more expensive

Popular techniques:

Response correction, Space Mapping

The Low-Fidelity Model

- Low-fidelity model implementation from discretized model equations:

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

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

- For the low-fidelity model use: state $\hat{\mathbf{y}}$ with coarsening factor $\hat{\tau} = \beta \cdot \tau$

Numerical Issues ...

- When chosing a coarse discretization one has to take into account ...
  - numerical instabilities
  - noisy model output due to low resolution of the model (huge peaks, maybe negative)

- The stability condition is determined mainly by the term: h/v

  (where h denotes the size of the discrete spatial step and v the ocean circulation)

- Aggressive Space Mapping approach (firstly developed by John W. Bandler et., 1994)

$$\mathbf{s}_k(\mathbf{u}) := \hat{\mathbf{y}}\left[\mathbf{p}_k(\mathbf{u})\right] \quad , \quad \mathbf{p}_k(\mathbf{u}) = \mathbf{p}(\mathbf{u}_k) + \mathbf{p}'(\mathbf{u}_k)\,(\mathbf{u} - \mathbf{u}_k)$$

$$\hat{\mathbf{u}}_k = \mathbf{p}(\mathbf{u}_k) := \mathrm{argmin}_{\mathbf{u}\in U} \;||\,\hat{\mathbf{y}}(\mathbf{u}) - \mathbf{y}(\mathbf{u}_k)\,||_Y^2$$

- Solving a (conditionally equivalent) nonlinear system of equations ...

$$\mathbf{F}(\bar{\mathbf{u}}) := \mathbf{p}(\bar{\mathbf{u}}) - \hat{\mathbf{u}}^* = 0 \quad , \quad \hat{\mathbf{u}}^* := \mathrm{argmin}_{\,\mathbf{u}\in U}\, J\,(\,\hat{\mathbf{y}}(\mathbf{u}), \mathbf{u}\,)$$

- ... using a Quasi-Newton iteration with a Broyden rank-one approximation of the Jacobian of the mapping + 1st order Taylor approximation as above

$$\mathbf{u}_{k+1} = \mathbf{p}_k^{-1}(\hat{\mathbf{u}}^*) = \mathbf{u}_k + \mathbf{d}_k \quad , \quad B_k\,\mathbf{d}_k = -\mathbf{F}(\mathbf{u}_k) = -\,(\mathbf{p}(\mathbf{u}_k) - \hat{\mathbf{u}}^*)$$

$$B_{k+1} = B_k + \frac{(\mathbf{y}_k - B_k\,\mathbf{d}_k)\;\mathbf{d}_k^T}{\mathbf{d}_k^T\,\mathbf{d}_k} \quad .$$

Correction Approaches ...

- Elemental response correction Ai,j

$$s_k(\mathbf{u}, z_i, t_j) := A_{i,j} \cdot \tilde{\tilde{y}}(\mathbf{u}, z_i, t_j) \quad , \quad A_j := \tilde{y}(\mathbf{u}, z_i, t_j) / \tilde{\tilde{y}}(\mathbf{u}, z_i, t_j)$$

- Exact 0-order consistency in the point u and also good agreement in neighbourhood u + ε

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

- i.e. the surrogate provides a very reasonable approximation of the fine model (even without including sensitivity information !)

- Now replacing the high-fidelity model in the optimization in iteration k

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

Thank you for

your attention !

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