Solution of Optimization Problems with Adaptive and Reduced Order Models

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The problem of interest

$$\mathbf{q}_{\text{opt}} = \arg\min_{\mathbf{q}} \mathcal{J}(\mathbf{u}, \mathbf{q}) \qquad \text{subject to } \mathcal{F}(\mathbf{u}, \mathbf{q}) = 0$$

where

- $\mathbf{q}$ are the model parameters such as permeability field, material properties, initial and boundary conditions, or parameters defining topology;
- $\mathcal{F}(\mathbf{u}, \mathbf{q})$ is a constitutive/physical equation that provides model state $\mathbf{u}$ (e.g., displacements, stresses) given parameters $\mathbf{q}$ (e.g., topology) under certain conditions (e.g., loads);
- $\mathcal{J}(\mathbf{u})$ = performance metric that depends on model solution.

Model problem A

PDE (primal problem) "$\mathcal{F}(\mathbf{u},\mathbf{q}) = 0$":

$$\begin{aligned} -\nabla\cdot\left(\mathbf{q}(x)\,\nabla\mathbf{u}\right) &= \mathbf{f}(x)\,,\ x\in\Omega \\ \mathbf{u} &= \mathbf{g}(x)\,,\ x\in\Gamma=\partial\Omega\,, \end{aligned}$$

Find optimal parameter:

$$\mathbf{q}_{\rm opt}(x) = \arg\min_{\mathbf{q}}\ \mathcal{J}(\mathbf{u},\mathbf{q}) \quad \text{constrained by PDE: } \mathcal{F}(\mathbf{u},\mathbf{q}) = 0.$$

Cost functional:

$$\mathcal{J}(\mathbf{u},\mathbf{q}) = \underbrace{\frac{1}{2}\|\mathcal{H}(\mathbf{u})-\mathbf{o}\|^2_{\mathcal{L}^2(\Omega)}}_{\text{mismatch to observations}} + \underbrace{\frac{1}{2}\|\nabla(\mathbf{q}-\mathbf{q}_B)\|^2_{\mathcal{L}^2(\Omega)} + \frac{\beta}{2}\|\mathbf{q}-\mathbf{q}_B\|^2_{\mathcal{L}^2(\Omega)}}_{\text{regularization}}.$$

Model problem B: four-dimensional variational data assimilation (4D-Var)

$$
\begin{aligned}
\mathcal{J}(\mathbf{u}_0) &= \frac{1}{2}\left\|\mathbf{u}_0 - \mathbf{u}_0^b\right\|^2_{\mathbf{B}_0^{-1}} + \frac{1}{2}\sum_{i=1}^{N}\left\|\mathcal{H}(\mathbf{u}_i) - \mathbf{y}_i\right\|^2_{\mathbf{R}_i^{-1}} \\
\mathbf{q}_{\rm opt} = \mathbf{u}_0^a &= \arg\min \mathcal{J}(\mathbf{u}_0) \\
&\quad \text{subject to: } \mathbf{u}_i = \mathcal{M}_{t_0 \to t_i}(\mathbf{u}_0)\,, \quad i = 1, \cdots, N
\end{aligned}
$$

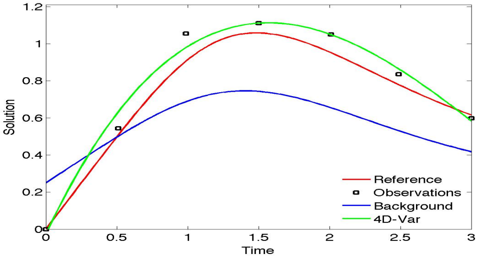


Figure : 4D-Var computes a MAP value of the initial condition of the dynamical system.

We need optimization methodologies that can use space/time adaptive models

- State-of-the-art forward model solvers are adaptive in space and time to maximize efficiency.
- Adaptive solvers can refine the mesh and the time step only where needed, to capture and track phenomena of interest, and to perform as few computations as possible.
- Previous research efforts have preferred the static approach due to the difficulties introduced by adaptive methods.
- However, there is a growing trend towards the use of space time adaptivity in the inverse problem community.

Challenge: seek optimal solution of continuous problem, but perform optimization with discrete model

Continuous inverse problem

$$
\begin{aligned}
\mathbf{q}_{\rm opt} &= \arg\min_{\mathbf{q}} \mathcal{J}(\mathbf{u}) \quad \text{subject to } \mathcal{F}(\mathbf{u},\mathbf{q}) = 0 \\
\text{(C-fwd)} \quad & \mathcal{F}(\mathbf{u}_{\rm opt},\mathbf{q}_{\rm opt}) = 0 \quad \Rightarrow \quad \mathbf{u}_{\rm opt} = \mathcal{M}(\mathbf{q}_{\rm opt}), \\
\text{(C-adj)} \quad & \mathcal{F}^*_{\mathbf{u}}(\mathbf{u}_{\rm opt},\mathbf{q}_{\rm opt}) \cdot \lambda_{\rm opt} = -\nabla_{\mathbf{u}} \mathcal{J}(\mathbf{u}_{\rm opt}), \\
\text{(C-opt)} \quad & \mathcal{F}^*_{\mathbf{q}}(\mathbf{u}_{\rm opt}) \cdot \lambda_{\rm opt} = 0 .
\end{aligned}
$$

In practice we solve a discrete inverse problem

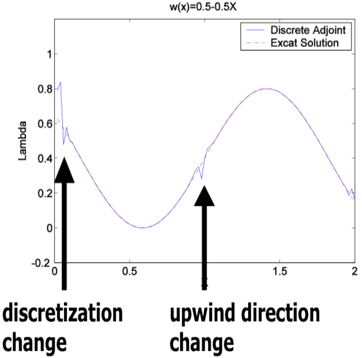
$$
\begin{aligned}
\mathbf{q}^h_{\rm opt} &= \arg\min_{\mathbf{q}} \mathcal{J}^h(\mathbf{u}) \quad \text{subject to } \mathcal{F}^h(\mathbf{u}^h,\mathbf{q}^h) = 0 \\
\text{(D-fwd)} \quad & \mathcal{F}^h(\mathbf{u}^h_{\rm opt},\mathbf{q}^h_{\rm opt}) = 0 \quad \Rightarrow \quad \mathbf{u}^h_{\rm opt} = \mathcal{M}^h(\mathbf{q}^h_{\rm opt}) \\
\text{(D-adj)} \quad & (\mathcal{F}^h_{\mathbf{u}^h})^*(\mathbf{u}^h_{\rm opt},\mathbf{q}^h_{\rm opt}) \cdot \lambda^h_{\rm opt} = -\nabla_{\mathbf{u}^h} \mathcal{J}^h(\mathbf{u}^h_{\rm opt}), \\
\text{(D-opt)} \quad & (\mathcal{F}^h_{\mathbf{q}^h})^*(\mathbf{u}^h_{\rm opt},\mathbf{q}^h_{\rm opt}) \cdot \lambda^h_{\rm opt} = 0 .
\end{aligned}
$$

Main point

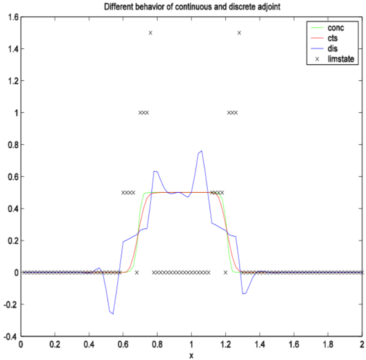
Proposition. [Sandu et al, 2006-2011]. To ensure that $\mathbf{q}^h_{\rm opt} \approx \mathbf{q}_{\rm opt}$ the scheme should posses:

$$\begin{aligned}
\text{Forward consistency} &: \quad \mathcal{F}^h \sim \mathcal{F} \\
\text{Adjoint consistency} &: \quad (\mathcal{F}^h_{\mathbf{u}})^* \cdot \lambda^h + \nabla_{\mathbf{u}^h} \mathcal{J}^h \sim (\mathcal{F}_{\mathbf{u}})^* \cdot \lambda + \nabla_{\mathbf{u}} \mathcal{J} \\
\text{Optimality consistency} &: \quad (\mathcal{F}^h_{\mathbf{q}})^* \cdot \lambda^h_{\rm opt} \sim \mathcal{F}^*_{\mathbf{q}} \cdot \lambda_{\rm opt}.
\end{aligned}$$

Challenge: consistency of the forward discretization is not automatically inherited by its discrete adjoint



(a) Third order upwind finite differences



(b) Finite volumes with minmod limiter

Figure : Discrete adjoints of numerical advection schemes can become inconsistent with the adjoint PDE. (a) Change of forward scheme computational pattern. (b) Active forward limiters act as pseudo-sources. [Liu and Sandu, 2005]

Challenge: consistency of the forward discretization is not automatically inherited by its discrete adjoint

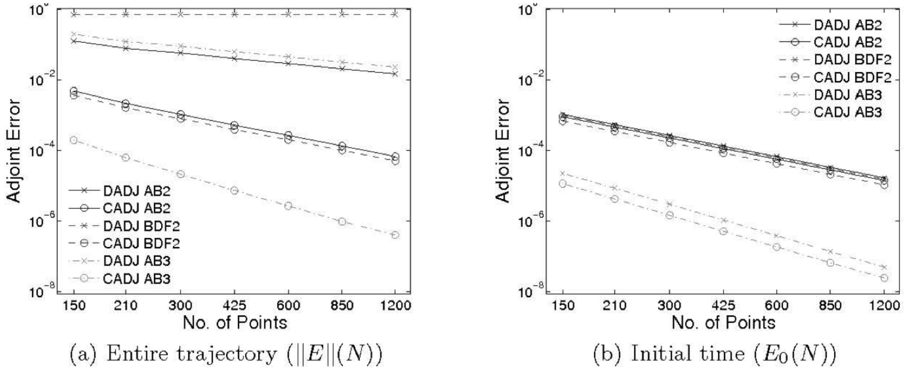


Figure : Adjoint orders of convergence for variable step size linear multistep methods [Sandu, 2007]

Challenge: duality framework for space-time inverse problems

Consider the following inverse problem:

$$
\begin{aligned}
\min_{\mathbf{u}^0,\mathbf{g},\mathbf{f}} \mathcal{J} &= \int_0^T \int_\Omega J_\Omega\left[C_\Omega\,\mathbf{u}\right] \mathrm{d}\mathbf{x}\,\mathrm{d}t + \int_0^T \int_\Gamma J_\Gamma\left[C_\Gamma\,\mathbf{u}\right] \mathrm{d}s\,\mathrm{d}t + \int_\Omega K_\Omega\left[E_\Omega\,\mathbf{u}\right] \\
\text{subject to} \quad \mathbf{u}_t &= N\left[\mathbf{u}\right] + \mathbf{f}\,,\ \mathbf{x}\in\Omega\,,\ t\in[0,T] \\
B[\mathbf{u}] &= \mathbf{g}\,,\ \mathbf{x}\in\Gamma\,,\ t\in[0,T] \\
\mathbf{u}(t=0,\mathbf{x}) &= \mathbf{u}^0\,,\ \mathbf{x}\in\Omega\,.
\end{aligned}
$$

Dual variable solves the adjoint problem:

$$
\begin{aligned}
-\boldsymbol{\lambda}_t &= L^*\,\boldsymbol{\lambda} + \mathbf{f}^{\mathrm{adj}}\,,\ \mathbf{x}\in\Omega\,,\ t\in[0,T] \\
B^{\mathrm{adj}}\,\lambda &= \mathbf{g}^{\mathrm{adj}}\,,\ \mathbf{x}\in\Gamma\,,\ t\in[0,T] \\
\boldsymbol{\lambda}(t=T,\mathbf{x}) &= E_\Omega^{\mathrm{adj}}\,k_\Omega\,,\ \mathbf{x}\in\Omega\,.
\end{aligned}
$$

Proposition (Alexe and Sandu, 2010)

The adjoint equation is well posed, if the differential operators that define the model and cost functional satisfy a set of three compatibility conditions on $\bar{\Omega}\times[0,T]$.

Adjoint sensitivity analysis for ODEs

Continuous forward equations

$$\mathbf{u}' = F(\mathbf{u}, t)\,, \quad t^0 \le t \le t^F\,; \quad \mathcal{J}(\mathbf{u}(t^F))\,.$$

Continuous adjoint equations

$$\lambda' = -F_{\mathbf{u}}^T(\mathbf{u}, t)\cdot\lambda\,, \quad \lambda^F = \left(\partial\mathcal{J}/\partial\mathbf{u}^F\right)^T\,, \quad t^F \ge t \ge t^0\,.$$

Discrete forward equations (Runge-Kutta method)

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h\sum_{i=1}^{s} b_i\, F\,(\,T_i,\, \mathbf{Y}_i\,)\,,$$

$$T_i = t_n + c_i\, h\,, \quad \mathbf{Y}_i = \mathbf{u}_n + h\sum_{j=1}^{s} a_{i,j}\, F\,(\,T_j,\, \mathbf{Y}_j\,)\,.$$

The discrete adjoint Runge-Kutta method

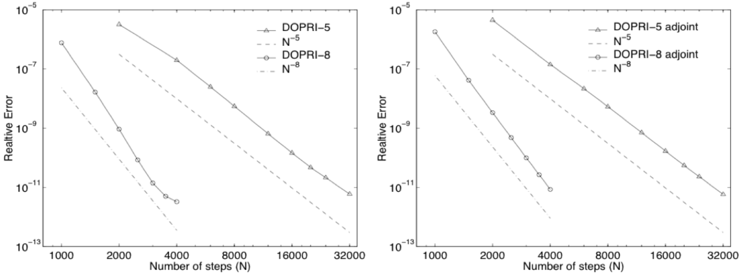
$$z_i = h\, F_{\mathbf{u}}^T\,(T_i, \mathbf{Y}_i)\cdot\left(b_i\,\lambda_{n+1} + \sum_{j=1}^{s} a_{j,i}\, z_j\right)\,, \quad i = s, \ldots, 1\,,$$

$$\lambda_n = \lambda_{n+1} + \sum_{j=1}^{s} z_j\,.$$

Results for discrete adjoint Runge Kutta methods

[Sandu, 2005]

- Nonstiff case: The discrete adjoint (of a RK method convergent with order p) converges with order p to the solution of the adjoint ODE.
- Stiff case: The discrete adjoint of a stiffly accurate RK method of order p with invertible A provides: an order p discretization of the adjoint of nonstiff variable; an order min(p,q+1,r+1) of the adjoint of stiff variable.



(a) Forward RK methods

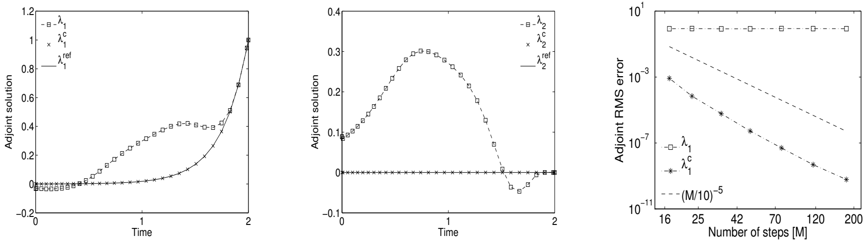
(b) Discrete adjoint RK methods

Figure : Orders of convergence for non-stiff problem `[Sandu, 2007]`

Discrete adjoints of adaptive time stepping algorithms

`[Alexe and Sandu, 2009b]` Discrete adjoints of adaptive time stepping algorithms are not *a priori* consistent. Post processing is required to restore the accuracy of the discrete adjoint trajectory.

`[Alexe and Sandu, 2009b]` Consistency re-established by zeroing out the spurious adjoint gradients or implementing a correction during post-processing.



(a) (b) (c)

Figure : DA solutions: inconsistent adjoint (a), consistent adjoint (b), and RMS errors (c) for the Prothero - Robinson IVP.

The adaptive mesh refinement process and grid transfers

- Solving the discrete primal problem with mesh refinement:

$$\mathbf{u}^{h,n+1} = \mathcal{I}_{n\to n+1}\left(\mathcal{S}_{n\to n+1}\left(\mathbf{u}^{h,n}\right)\right), \quad n = 0\ldots N-1 .$$

- The discrete adjoint procedure:

$$\boldsymbol{\lambda}^{h,n} = \mathcal{S}'^{\,*}_{n+1\to n}\left(\mathcal{I}^{T}_{n\to n+1}\,\boldsymbol{\lambda}^{h,n+1}\right), \quad N-1 \geq n \geq 0 ,$$

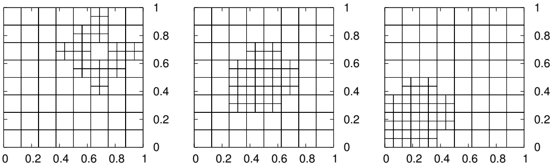
- Problem: Is the grid transfer operator dual consistent

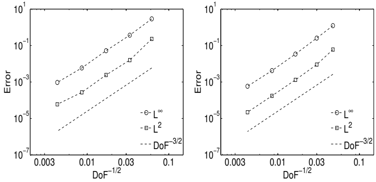
$$\mathcal{I}_{n+1\to n} = \mathcal{C}\cdot\left(\mathcal{I}_{n\to n+1}\right)^{T} \; ?$$

- Answer (FEM): `(Alexe and Sandu, 2010-11a)` Intergrid transfer operators for FEM h/p-adaptivity are dual consistent
- Answer (FVM): `(Alexe and Sandu, 2010,-11a)` Intergrid transfer operators based on high order polynomial interpolants become at most first order interpolants when transposed.

Dual consistency of space-time RK-DG discretizations on adaptive grids

`[Alexe and Sandu, 2010]` For space-time RK-DG discretizations the dual inherits the order of the primal discretization.





(a) Continuous adj. (b) Discrete adj.

Figure : Two-dimensional advection. Time-averaged L^2 and L^∞ errors with $p = 2$.

Model problem A revisited

Cost functional:

$$\mathcal{J}(\mathbf{u},\mathbf{q}) = \frac{1}{2}\|\nabla(\mathbf{q}-\mathbf{q}_B)\|^2_{\mathcal{L}^2(\Omega)} + \frac{\beta}{2}\|\mathbf{q}-\mathbf{q}_B\|^2_{\mathcal{L}^2(\Omega)} + \frac{1}{2}\|\mathcal{H}\mathbf{u}-\mathbf{o}\|^2_{\mathcal{L}^2(\Omega)} .$$

PDE constraint (primal problem):

$$\begin{aligned} -\nabla\cdot(\mathbf{q}(\mathbf{x})\,\nabla\mathbf{u}) &= \mathbf{f}(\mathbf{x})\,,\ \mathbf{x}\in\Omega \\ \mathbf{u} &= \mathbf{g}(\mathbf{x})\,,\ \mathbf{x}\in\Gamma=\partial\Omega\,, \end{aligned}$$

Adjoint problem:

$$\begin{aligned} -\nabla\cdot(\mathbf{q}\,\nabla\boldsymbol{\lambda}) &= \mathcal{H}^*(\mathcal{H}\mathbf{u}-\mathbf{o})\,,\ \mathbf{x}\in\Omega \\ \boldsymbol{\lambda} &= 0\,,\ \mathbf{x}\in\Gamma\,. \end{aligned}$$

Optimality condition:

$$\begin{aligned} -\Delta\,\mathbf{q}+\beta\,(\mathbf{q}-\mathbf{q}_B) &= -\Delta\mathbf{q}_B+\nabla\mathbf{u}\cdot\nabla\boldsymbol{\lambda}\,,\ \mathbf{x}\in\Omega\,, \\ \nabla\mathbf{q}\cdot\vec{\mathbf{n}} &= \nabla\mathbf{q}_B\cdot\vec{\mathbf{n}}\,,\ \mathbf{x}\in\Gamma\,. \end{aligned}$$

Primal symmetric interior penalty DG discretization

Primal problem: Find $\mathbf{u}^h \in \mathcal{U}_h^p$ s.t., $\forall\, \mathbf{w}^h \in \mathcal{U}_h^p$, we have:

$$
\begin{aligned}
\mathcal{N}^h(\mathbf{u}^h, \mathbf{w}^h) &= \int_\Omega \mathbf{f}^h\, \mathbf{w}^h\, \mathrm{d}\mathbf{x} + \mathcal{B}^h(\mathbf{g}^h, \mathbf{w}^h) \\
\mathcal{N}^h(\mathbf{u}^h, \mathbf{w}^h) &:= \int_\Omega \mathbf{q}^h\, \nabla \mathbf{u}^h \cdot \nabla \mathbf{w}^h\, \mathrm{d}\mathbf{x} + \int_{\Gamma_\mathcal{I} \cup \Gamma} \phi\, [\![\mathbf{u}^h]\!] \cdot [\![\mathbf{w}^h]\!]\, \mathrm{d}\mathbf{s} \\
&\quad - \int_{\Gamma_\mathcal{I} \cup \Gamma} \left([\![\mathbf{u}^h]\!] \cdot \{\mathbf{q}^h\, \nabla \mathbf{w}^h\} + \{\mathbf{q}^h\, \nabla \mathbf{u}^h\} \cdot [\![\mathbf{w}^h]\!] \right)\, \mathrm{d}\mathbf{s}\,, \\
\mathcal{B}^h(\mathbf{g}^h, \mathbf{w}^h) &:= -\int_\Gamma \mathbf{q}^h\, \mathbf{g}^h\, \nabla \mathbf{w}^h \cdot \vec{\mathbf{n}}\, \mathrm{d}\mathbf{s} + \int_\Gamma \phi\, \mathbf{g}^h\, \mathbf{w}^h\, \mathrm{d}\mathbf{s}\,.
\end{aligned}
$$

$$
\|\mathbf{v}\|_{\mathrm{DG}} := \left(\sum_{\kappa \in \mathcal{T}_h} \int_\kappa \mathbf{q}\, \nabla \mathbf{v} \cdot \nabla \mathbf{v}\, \mathrm{d}\mathbf{x} + \sum_{e \in \Gamma_\mathcal{I} \cup \Gamma} \hat{\phi}\, h^{-1} \int_e [\![\mathbf{v}]\!] \cdot [\![\mathbf{v}]\!]\, \mathrm{d}\mathbf{s} \right)^{1/2}, \ \forall\, \mathbf{v} \in \mathcal{U}\,.
$$

Theorem

For sufficiently large penalty $\hat{\phi} > 0$, there exists C independent of h such that

$$
\left\|\mathbf{u} - \mathbf{u}^h\right\|_{\mathrm{DG}} \le C\, h^{\min(p+1,s)-1}\, \|\mathbf{u}\|_{\mathcal{H}^s(\mathcal{T}_h)}\,.
$$

A priori error analysis for the optimal solution

Proposition (Alexe and Sandu, 2011b)

The following a priori bound holds for the optimal solution error (SIPG DG):

$$\left\|\mathbf{q}_*^h - \mathbf{q}_*\right\|_{\mathcal{H}^s(\mathcal{T}_h^q)} \quad \leq \quad C(r,p)\, h^{\min(p+1,s)-3/2} \left(\|\mathbf{u}\|_{\mathcal{H}^s(\mathcal{T}_h)} + \|\boldsymbol{\lambda}\|_{\mathcal{H}^s(\mathcal{T}_h)}\right) \ .$$

Proof. The equation for the discrete optimal solution error is a perturbed SIPG discretization. Bound these perturbations and asses their impact on the solution via Lax Milgram theorem.

Comment. Stronger bounds can be obtained for optimization with continuous Galerkin approach.

Numerical Results: Convergence

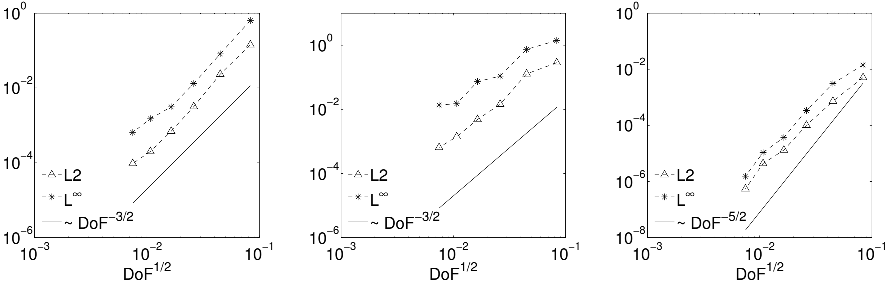


Figure : Convergence of the discrete optimal (left), primal (center), and dual (right) solutions for test B. The errors correspond to the converged solutions on each mesh level, and are plotted versus $h \sim \mathrm{DoF}^{-1/2}$.

A posteriori estimation allows to use adaptivity to control errors in optimal solution

[Alexe and Sandu, 2011b] Consider error functional defined as:

$$E[\mathbf{q}] : \mathcal{Q} \rightarrow \mathbb{R}$$

1. Solve the Hessian equation for $\boldsymbol{\sigma}_{\mathbf{q}}$ using quasi-Newton approximation.

$$j_{\mathbf{q},\mathbf{q}}[\mathbf{q}_*]\,(\phi, \boldsymbol{\sigma}_{\mathbf{q}}) = E_{\mathbf{q}}[\mathbf{q}_*]\,(\phi)\;, \quad \forall \phi \in \mathcal{Q}$$

2. Given $\boldsymbol{\sigma}_{\mathbf{q}}$, solve the tangent linear model to obtain $\boldsymbol{\sigma}_{\mathbf{u}}$.

$$0 = \mathcal{A}_{\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{u}}) + \mathcal{A}_{\mathbf{q}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{q}}) \quad \Leftrightarrow \quad \boldsymbol{\sigma}_{\mathbf{u}} = U'[\mathbf{q}_*]\,\boldsymbol{\sigma}_{\mathbf{q}}$$

3. Given $\boldsymbol{\sigma}_{\mathbf{q}}$ and $\boldsymbol{\sigma}_{\mathbf{u}}$, solve the second order adjoint model to obtain $\boldsymbol{\sigma}_{\boldsymbol{\lambda}}$.

$$\begin{aligned} 0 \;=\;& \mathcal{J}_{\mathbf{u},\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{u}}) + \mathcal{J}_{\mathbf{q},\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{q}}) \\ & -\mathcal{A}_{\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\boldsymbol{\lambda}}) - \mathcal{A}_{\mathbf{u},\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{u}}) - \mathcal{A}_{\mathbf{q},\mathbf{u}}\,[\boldsymbol{\xi}_*]\,(\boldsymbol{\sigma}_{\mathbf{q}}) \end{aligned}$$

4. Estimate the element-wise error using the dual weighted residual formula

$$\begin{aligned} E[\boldsymbol{\xi}_*^h] - E[\boldsymbol{\xi}_*] \;=\;& \mathcal{A}[\mathbf{u}^h, \mathbf{q}^h](\Delta\boldsymbol{\sigma}_{\mathbf{u}}) \\ & + \mathcal{J}_{\mathbf{u}}[\mathbf{u}^h, \mathbf{q}^h](\Delta\boldsymbol{\sigma}_{\boldsymbol{\lambda}}) - \mathcal{A}_{\mathbf{u}}[\mathbf{u}^h, \mathbf{q}^h](\Delta\boldsymbol{\sigma}_{\boldsymbol{\lambda}}, \boldsymbol{\lambda}^h) \\ & + \mathcal{J}_{\mathbf{q}}[\mathbf{u}^h, \mathbf{q}^h](\Delta\boldsymbol{\sigma}_{\mathbf{q}}) - \mathcal{A}_{\mathbf{q}}[\mathbf{u}^h, \mathbf{q}^h](\Delta\boldsymbol{\sigma}_{\mathbf{q}}, \boldsymbol{\lambda}^h) + h.o.t. \end{aligned}$$

Meshes generated by the aposteriori error control

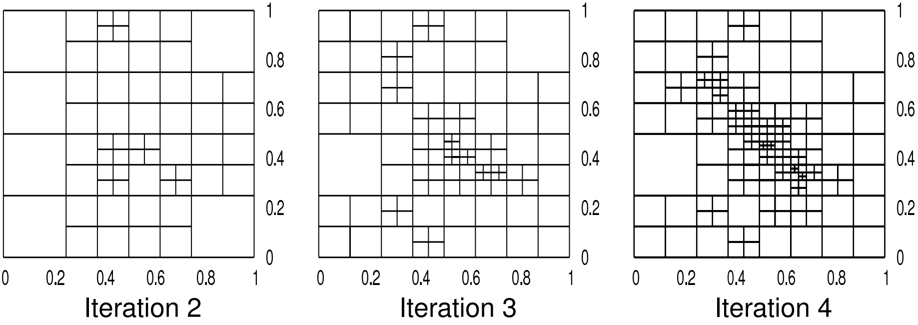
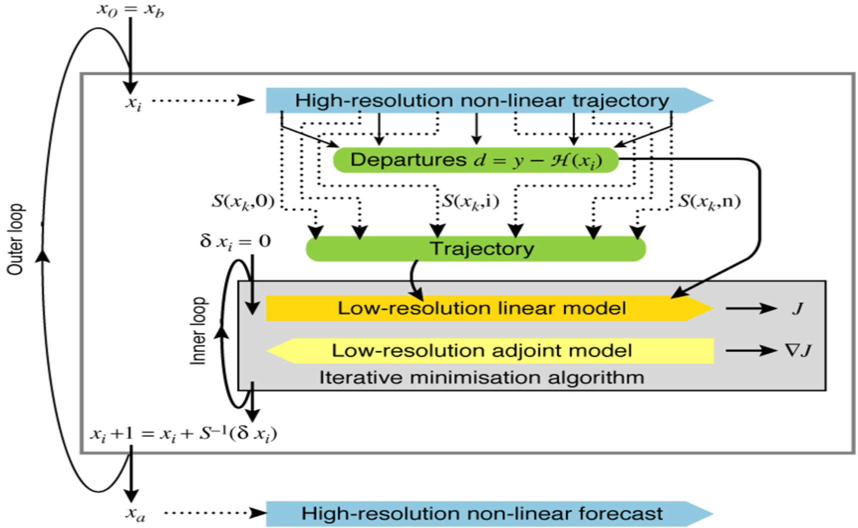


Figure : Optimization meshes generated by aposteriori error estimation algorithm for numerical test B.

Using reduced order models as surrogates to speed up optimization problems



Example of ROM: Proper Orthogonal Decomposition

- Full continuous model:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{F}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{x}_0 \in \mathbb{R}^n.$$

- POD chooses orthonormal basis $U \in \mathbb{R}^{n \times k}$, $k \ll n$, such that the mean square error between $\mathbf{x}(t)$ and POD expansion is minimized:

$$\mathbf{x}^{POD}(t) = \bar{x} + U\widetilde{\mathbf{x}}(t), \ \widetilde{\mathbf{x}}(t) \in \mathbb{R}^k.$$

- Reduced order continuous model:

$$(W^T U) \frac{d\widetilde{\mathbf{x}}(t)}{dt} = W^T \mathbf{F}\Big(\bar{x} + U\widetilde{\mathbf{x}}(t), t\Big), \quad \widetilde{\mathbf{x}}(0) = W^T \Big(\mathbf{x}(0) - \bar{x}\Big).$$

Model problem B revisited

- Full 4D-Var optimization:

$$\min \quad J(\mathbf{x}_0) = \frac{1}{2}\left(\mathbf{x}^b - \mathbf{x}_0\right)^T \mathbf{B}_0^{-1}\left(\mathbf{x}^b - \mathbf{x}_0\right) + \frac{1}{2}\sum_{i=1}^{N}\left(\mathbf{y}^i - H(\mathbf{x}_i)\right)^T R_i^{-1}\left(\mathbf{y}^i - H(\mathbf{x}_i)\right),$$

$$\text{subject to } \mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i),\ i = 0, .., N-1,$$

- Reduced-order 4D-Var:

$$\min \quad J^{POD}(\widetilde{\mathbf{x}}_0) = \frac{1}{2}\left(\mathbf{x}^b - U_f\widetilde{\mathbf{x}}_0\right)^T \mathbf{B}_0^{-1}\left(\mathbf{x}^b - U_f\tilde{\mathbf{x}}_0\right)^T + \frac{1}{2}\sum_{i=1}^{N}\left(\mathbf{y}^i - H(U_f\widetilde{\mathbf{x}}_i)\right)^T R_i^{-1}\left(\mathbf{y}^i - H(U_f\widetilde{\mathbf{x}}_i)\right)^T,$$

$$\text{subject to } \widetilde{\mathbf{x}}_{i+1} = \tilde{M}_i(\widetilde{\mathbf{x}}_i),\ \tilde{M}_i = W_f^T M_i U_f,\ i = 0, .., N-1.$$

Numerical Results with 2D Shallow Water Model

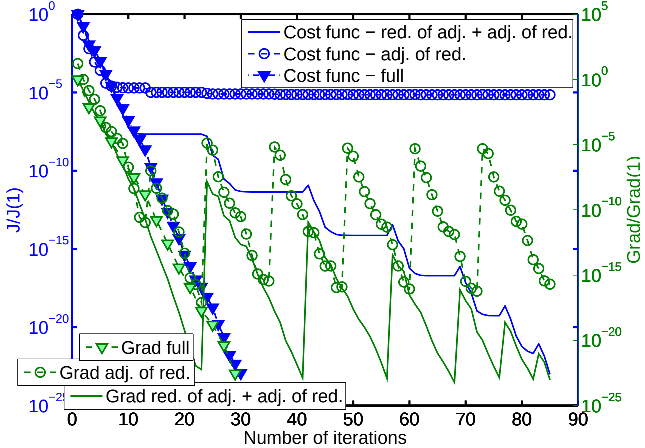


Figure : Tensorial POD/4DVAR 2D Shallow water equations. Evolution of cost function and gradient norm as a function of the number of minimization iterations. The information from the adjoint equations has to be incorporated into POD basis.

POD based SWE 4D-Var DA systems

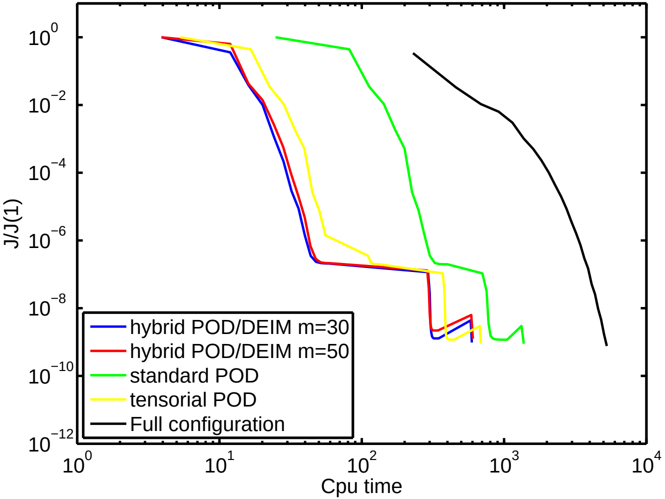


Figure : CPU time comparison for the reduced vs. full order SWE DA systems.

Conclusions

- Correct optimal solutions can be computed if forward, dual, and optimal consistency; this constraints the forward discretization (e.g., RK DG)
- Special issues posed by adaptive algorithms:
  - Space and time mesh refinements,
  - Solution limiters,
  - Grid transfer operators,
  - Both *a priori* and *a posteriori* error analysis and estimation.
- The discrete duality framework enables the solution of optimization problems to benefit from all the adaptive features listed above.
- These principles applied to optimization with reduced order models lead to considerable improvements in CPU time.