Reduced-Order Strategies for Efficient 4D-Var Data Assimilation

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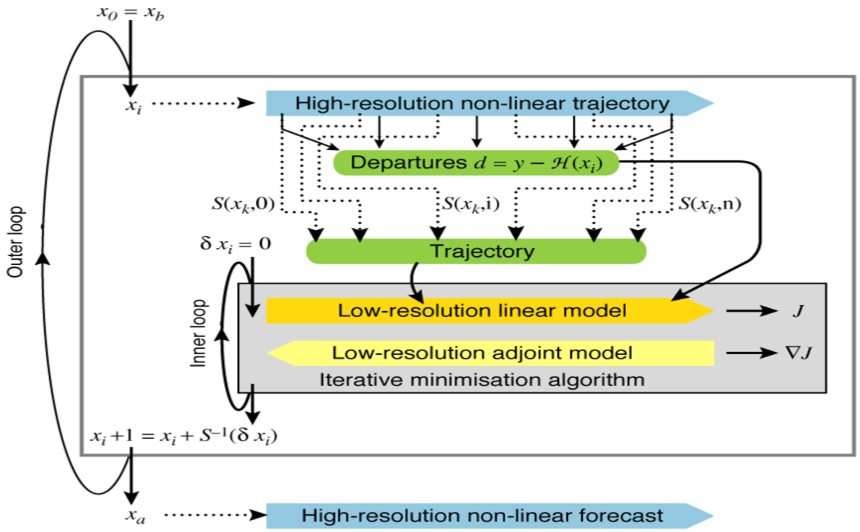
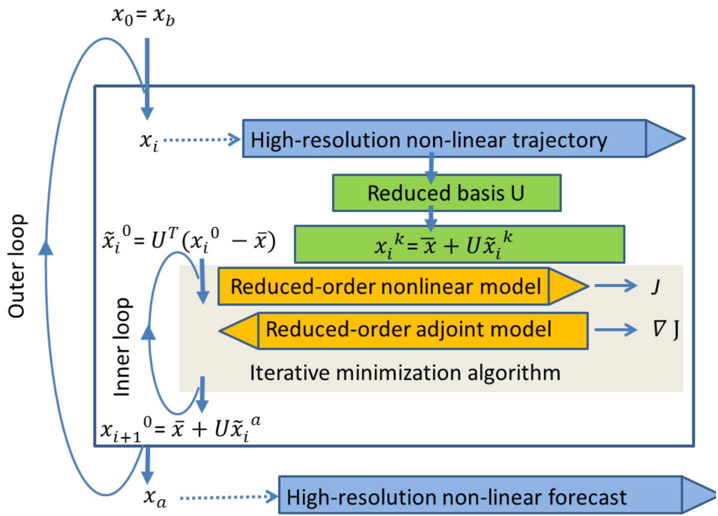
Outline

Incremental 4D-Var Data Assimilation Courtier et al. [9]



Reduced order data assimilation



Reduced order data assimilation

- Replace the current linearized cost function to be minimized in the inner loop.
- Surrogate models that accurately represent sub-grid-scale processes.- Benner et al. 2013.
- Highly non-linear observation operators fully derived in the reduced space.
- Experiments at increased space and time resolutions.
- Global convergence result for the solution of a trust region POD optimal control problem using time-dependent Navier-Stokes equations (NSE) for viscous incompressible fluids as constraint - Arian et al. 2000.

Proper Orthogonal Decomposition

- The desired simulation is well approximated in the input collection - Aubrey et al. 1988.
- Data analysis is conducted to extract basis functions, from experimental data or detailed simulations of high-dimensional systems
- Galerkin projections that yield low dimensional dynamical models.
- We assume a Petrov-Galerkin projection for constructing the reduced order models. U denotes the POD basis and the test functions are stored in W. $W^T U = I_k$, I_k being the identity matrix of order k. For simplicity we assume a POD expansion of $\mathbf{x} = U\tilde{\mathbf{x}}$.
- Standard POD models: Its nonlinear reduced terms still have to be evaluated on the original state space making the simulation of the reduced-order system too expensive.

Reduced Order Modelling

Standard POD

$$\tilde{N}(\tilde{\mathbf{x}}) = \underbrace{W^T}_{k\times n}\underbrace{U\tilde{\mathbf{x}}\odot U\tilde{\mathbf{x}}}_{n\times 1}, \tilde{N}(\tilde{\mathbf{x}}) \in \mathbb{R}^k \quad (1)$$

where $\odot$ is the componentwise multiplication Matlab operator and n is usually the number of spatial mesh points.

Tensorial POD

$$\tilde{N}(\tilde{\mathbf{x}}) = \left[\tilde{N}_i\right]_{i=1,..,k} \in \mathbb{R}^k;\ \tilde{N}_i = \sum_{j=1}^{k}\sum_{l=1}^{k} T_{i,j,l}\tilde{x}_j\tilde{x}_l. \quad (2)$$

$$\tilde{N}(\tilde{\mathbf{x}}) = \underbrace{\mathbf{T}}_{k\times k^2}\underbrace{\tilde{\mathbf{X}}}_{k^2\times 1}$$

$$T = \left(T_{i,j,l}\right)_{i,j,l=1,..,k} \in \mathbb{R}^{k\times k\times k},\ T_{i,j,l} = \sum_{r=1}^{n} W_{i,r}U_{j,r}U_{l,r}.$$

Reduced Order Modelling

Standard POD/DEIM

$$\tilde{N}(\tilde{\mathbf{x}}) \approx \underbrace{W^T V(P^T V)^{-1}}_{k \times m} \underbrace{\left((P^T U \tilde{x}) \odot (P^T U \tilde{x}) \right)}_{m \times 1} \tag{3}$$

where m is the number of interpolation points, $V \in \mathbb{R}^{n \times m}$ gathers the first m POD basis modes of the nonlinear term while $P \in \mathbb{R}^{n \times m}$ is the DEIM interpolation selection matrix (Chaturantabut [6], Chaturantabut and Sorensen [8, 7]).

Reduced Order Modelling

- We constructed reduced order Shallow Water Equations models - It shares characteristics with the real atmosphere.
- Alternating Direction Implicit scheme - accomodate for large CFL conditions.

	Full ADI SWE	Standard POD	Tensorial POD	POD/DEIM m=180	POD/DEIM m=70
CPU time	950.0314s	161.907	2.125	0.642	0.359
u	-	5.358e-5	5.358e-5	5.646e-5	7.453e-5
v	-	2.728e-5	2.728e-5	3.418e-5	4.233e-5
ϕ	-	8.505e-5e	8.505e-5	8.762e-5	9.212e-5

Table : CPU time gains and the root mean square errors for each of the model variables at $t_f = 3$h for a 3h time integration window. Number of POD modes was $k = 50$ and two tests with different number of DEIM points $m = 180, \; 70$ were simulated.$103,776$ spatial points.

ROM 4D-Var DA systems - Choice of bases

- The "adjoint of reduced" (AR) model approach formulates the first order optimality conditions from the forward reduced order model
- Consistent KKT discrete optimality conditions; Reduced adjoint model approximates poorly its full counterpart and POD bases rely only on forward dynamics information.
- The "reduced adjoint" (RA) approach projects the first order optimality equations of the full system onto the POD reduced spaces
- Accurate low-order surrogate models; Its not clear what information should be included in the reduced basis used for full space gradient equation projection

ROM 4D-Var DA systems - Choice of bases

- To guide the POD bases snapshots selection process for reduced data assimilation systems governed by non-linear models
- Consistent and accurate reduced Karush Kuhn Tucker (KKT) optimality conditions - accurate reduced POD adjoint model solutions and gradient with respect to their full counterparts
- Every type of reduced optimization involving adjoint models and projection based reduced order methods including reduced basis approach will benefit.

ROM 4D-Var DA systems - Choice of bases

- We derive the optimality conditions as in the AR approach
- Forward POD manifold U_f is computed using snapshots of the full forward model solution only $\mathbf{x} \approx U_f \tilde{\mathbf{x}}$
- Petrov-Galerkin (PG) projection; the test functions POD basis W_f is different than the trial functions POD manifold U_f

$$J^{POD}(\tilde{\mathbf{x}}_0) = \frac{1}{2}\left(\mathbf{x}^b - U_f\tilde{\mathbf{x}}_0\right)^T \mathbf{B}_0^{-1}\left(\mathbf{x}^b - U_f\tilde{\mathbf{x}}_0\right)^T + \frac{1}{2}\sum_{i=1}^{N}\left(\mathbf{y}^i - H(U_f\tilde{\mathbf{x}}_i)\right)^T R_i^{-1}\left(\mathbf{y}^i - H(U_f\tilde{\mathbf{x}}_i)\right)^T, \tag{4}$$

$$\text{subject to } \tilde{\mathbf{x}}_{i+1} = W_f^T M_i(U_f\tilde{\mathbf{x}}_i) = \tilde{M}_i(\tilde{\mathbf{x}}_i),\ \ i = 0, .., N-1. \tag{5}$$

ROM 4D-Var DA systems - Choice of bases

- *Reduced adjoint model*

$$\tilde{\lambda}_i = U_f^T \mathbf{M}_i^T W_f \tilde{\lambda}_{i+1} + U_f^T \mathbf{H}^T R_i^{-1} \big(\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i)\big), \; i = \overline{N-1, 1};$$
$$\tilde{\lambda}_N = U_f^T \mathbf{H}^T R_N^{-1} \big(\mathbf{y}^N - H(U_f \tilde{\mathbf{x}}_N)\big) \text{ and } \tilde{\lambda}_0 = U_f^T \mathbf{M}_0^T W_f \tilde{\lambda}_1 \tag{6}$$

- *Reduced Cost Function gradient*

$$\nabla_{\tilde{\mathbf{x}}_0} J^{POD} = -U_f^T \mathbf{B}_0^{-1} \big(\mathbf{x}^b - U_f \tilde{\mathbf{x}}_0\big) - \tilde{\lambda}_0 = 0; \tag{7}$$

ROM 4D-Var DA systems - Choice of bases

- RA approach: the full forward and adjoint models and the gradient are projected onto separate reduced manifolds
- U_f, U_a and U_g are the trial POD reduced subspaces and W_f, W_a and W_g are the test functions POD manifolds, $\mathbf{x}_i \approx U_f \tilde{\mathbf{x}}_i$, $\lambda_i \approx U_a \tilde{\lambda}_i$, $i = 0, .., N$.
- *Reduced forward model:*

$$\tilde{\mathbf{x}}_{i+1} = \tilde{M}_i(\tilde{\mathbf{x}}_i), \ i = 0, .., N-1. \tag{8}$$

- *Reduced adjoint model:*

$$\begin{aligned} \tilde{\lambda}_i &= W_a^T \mathbf{M}_i^T U_a \tilde{\lambda}_{\mathbf{i+1}} + W_a^T \mathbf{H}^T R_i^{-1} \big(\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i\big), \ i = \overline{N-1, 1} \\ \tilde{\lambda}_N &= W_a^T \mathbf{H}^T R_N^{-1} \big(\mathbf{y}^N - H(U_f \tilde{\mathbf{x}}_N)\big) \text{ and } \tilde{\lambda}_0 = \ W_a^T \mathbf{M}_0^T U_a \tilde{\lambda}_1, \end{aligned} \tag{9}$$

- *Reduced Cost Function gradient*

$$\nabla_{\tilde{\mathbf{x}}_0} J^{POD} = -W_g^T \mathbf{B}_0^{-1} \big(\mathbf{x}^b - U_f \tilde{\mathbf{x}}_0\big) - W_g^T U_a \tilde{\lambda}_0 = 0; \tag{10}$$

ROM 4D-Var DA systems - Choice of bases

- *AR adjoint model:*

$$\tilde{\lambda}_i = U_f^T \mathbf{M}_i^T W_f \tilde{\lambda}_{i+1} + U_f^T \mathbf{H}^T R_i^{-1}\left(\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i)\right),\ i = \overline{N-1, 1};$$
$$\tilde{\lambda}_N = U_f^T \mathbf{H}^T R_N^{-1}\left(\mathbf{y}^N - H(U_f \tilde{\mathbf{x}}_N)\right) \text{ and } \tilde{\lambda}_0 = U_f^T \mathbf{M}_0^T W_f \tilde{\lambda}_1 \tag{11}$$

- *RA adjoint model:*

$$\tilde{\lambda}_i = W_a^T \mathbf{M}_i^T U_a \tilde{\lambda}_{\mathbf{i+1}} + W_a^T \mathbf{H}^T R_i^{-1}\left(\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i)\right),\ i = \overline{N-1, 1}$$
$$\tilde{\lambda}_N = W_a^T \mathbf{H}^T R_N^{-1}\left(\mathbf{y}^N - H(U_f \tilde{\mathbf{x}}_N)\right) \text{ and } \tilde{\lambda}_0 = W_a^T \mathbf{M}_0^T U_a \tilde{\lambda}_1, \tag{12}$$

- For Petrov Galerkin and Galerking projections:

$$W_f = U_a = U_g,\ \text{and } W_a = U_f = W_g,\ \text{and } U_f = U_a = U_g. \tag{13}$$

ROM 4D-Var DA systems - Choice of bases

Theorem

Assume that in an open subset there exist unique solutions for the high-fidelity $\mathbf{x}_0^a$ and AR reduced order $\tilde{\mathbf{x}}_0^a$ optimization problems . Assume that the model and observation operators $\mathcal{M}$ and $\mathcal{H}_i, \ i = 0, .., N$ are twice continuously differentiable and the Hessian of the cost function $\mathcal{J}$ evaluated at the minimizer of high-fidelity problem is positive definite. Then there exist "impact factors" ξ, ν_i and $\mu_i \in \mathbb{R}^M, \ i = 0, .., N$ such that the error in a component of the high-fidelity optimizer computed using the minimizer of reduced order problem is approximated to first order by formula

$$\varepsilon(\hat{\mathbf{x}}_0) - \varepsilon(\mathbf{x}_0^a) \approx \Delta_{fwd} + \Delta_{adj} + \Delta_{opt}, \tag{14}$$

where $\hat{\mathbf{x}}_0 = U_f \tilde{\mathbf{x}}_0^a$.

- Becker and Vexler 2005.

ROM 4D-Var DA systems - Choice of bases

Forward model contribution:

$$\Delta_{\mathrm{fwd}} = -\sum_{i=0}^{N-1} \nu_{i+1}^T \Big(U_f W_f^T - I \Big) \mathcal{M}_{i,i+1}(\mathbf{x}_i) \tag{15a}$$

Adjoint model contribution

$$\Delta_{\mathrm{adj}} = -\mu_N^T \Big(W_f U_f^T - I \Big) \mathbf{H}_N^T \mathbf{R}_N^{-1} (\mathbf{y}_N - \mathcal{H}_N(\mathbf{x}_N)) - \sum_{i=0}^{N-1} \mu_i^T \Big(W_f U_f^T - I \Big) \Big[\mathbf{M}_{i,i+1}^T \lambda_{i+1} + \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)) \Big], \tag{15b}$$

Optimality equation contribution:

$$\Delta_{\mathrm{opt}} = -\xi^T \Big(W_f U_f^T - I \Big) \mathbf{B}_0^{-1} (\mathbf{x}_0^{\mathrm{b}} - \mathbf{x}_0). \tag{15c}$$

4D-Var SWE DA reduced order systems

Algorithm 1 Standard and Tensorial POD SWE DA systems

Off-line stage

1: Generate initial conditions **u**, **v** and ϕ.
2: Solve full forward ADI SWE model to generate state variables snapshots.
3: Solve full adjoint ADI SWE model to generate adjoint variables snapshots.
4: Compute one 4D-Var iteration
5: Compute a POD basis using snapshots describing dynamics of the forward and adjoint trajectories and $\mathbf{B}_0^{-1}\left(\mathbf{x}^b - U_f\tilde{\mathbf{x}}_0\right)$.
6: Compute reduced order model coefficients.

4D-Var SWE DA reduced order systems

Algorithm 1 Standard and Tensorial POD SWE DA systems

On-line stage - Minimize reduced cost functional J^{POD} (4)

1: Solve forward reduced order model (5)
2: Solve adjoint reduced order model (6)
3: Compute reduced gradient (10)

Decisional stage

4: Project the suboptimal reduced initial condition generated by the on-line stage and perform steps 1 and 2 of off-line stage. Using full forward information evaluate the high-fidelity J. If $\|J\| > \varepsilon_3$ or $|\nabla J| > \varepsilon_4$ then continue the off-line stage from step 3, otherwise STOP.

4D-Var SWE DA reduced order systems

- The on-line stage - minimization of the cost function J^{POD} performed on a reduced POD manifold
- The stoping criteria are

$$\|\nabla J^{POD}\| \leq \varepsilon_1,\ \|J^{POD}_{(i+1)} - J^{POD}_{(i)}\| \leq \varepsilon_2,\ \mathrm{MXFUN} \leq iter_{Max} \qquad (16)$$

- The off-line stage - outer iteration - general stopping criterion

$$\|J\| \leq \varepsilon_3 \text{ or } |\nabla J| \leq \varepsilon_4.$$

Numerical Results

- ADI SWE model
- 3% Gaussian perturbations added to the initial conditions of Grammeltvedt [10] and generate twin-experiment observations at every grid space point location and every time step
- Background state is computed adding a 5% Gaussian perturbations to Grammeltvedt initial conditions.
- Background and Observation error covariance matrices are diagonal.
- The length of the assimilation window: $3h$.
- BFGS optimization method (CONMIN)
- We use $\varepsilon_1 = 10^{-14}$ and $\varepsilon_2 = 10^{-5}$.
- We select 31×23 mesh points 91 time steps and use 50 POD basis functions. MXFUN is set to 25 and $\varepsilon_3 = 10^{-16}$ and $\varepsilon_4 = 10^{-12}$.

Numerical Results - Choice of POD basis

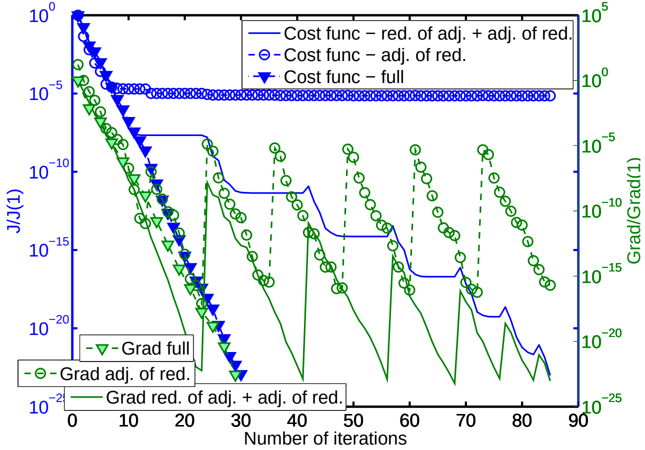
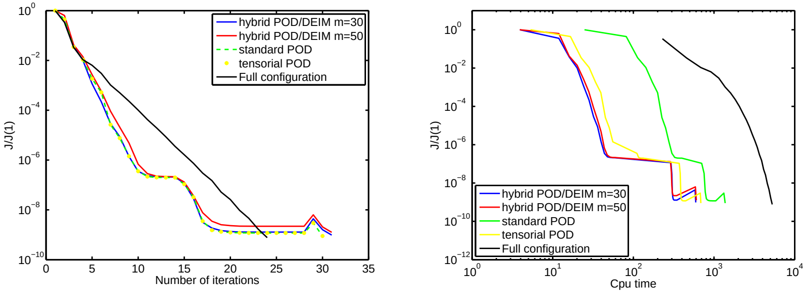


Figure : Tensorial POD/4DVAR ADI 2D Shallow water equations – Evolution of cost function and gradient norm as a function of the number of minimization iterations. The information from the adjoint equations and gradient has to be incorporated into POD basis.

POD based SWE 4D-Var DA systems

- $n = 151 \times 111$ space points, number of POD basis modes $k = 50$, $\text{MXFUN} = 15$ and $\varepsilon_3 = \varepsilon_4 = 10^{-3}$,.



(a) Iteration performance (b) Time performance

Figure : Number of iterations and CPU time comparisons for the reduced Order SWE DA systems vs. full SWE DA system.

Conclusions and future research

- New efficient POD bases selection strategies for POD based reduced 4DVar data assimilation systems governed by nonlinear state models using both Petrov-Galerkin and Galerkin projections.
- Consistent reduced Karush Kuhn Tucker (KKT) optimality conditions + accurate reduced POD adjoint model solutions and gradient with respect to their full counterparts.
- Galerkin projection - one single POD basis is required and the correlation matrix must contain snapshots from both forward and adjoint full models. Include also the optimality condition information.

Conclusions and future research

- The speed up gain increases directly proportional with the the mesh size
- Stabilization strategies proposed by Amsallem and Farhat [1], Bui-Thanh et al. [5] must be pursued in order to obtain feasible Petrov-Galerkin reduced order data assimilation systems
- Multifidelity techniques: Local in time adaptive ROMs. (Peherstorfer et al. [13], Rapún and Vega [16]);
- Exploit the structure of the weak constraints variational approach (Trémolet [20]), consistent and accurate reduced KKT conditions (Stefănescu et al. [19]) and formulate a piecewise-in-space-time approximation strategy that uses different ROMs on different subintervals, and constructs them concurrently;
- Expand the research for WRF.

Manuscripts related to the present research effort

- R. Stefanescu, A. Sandu, I.M. Navon POD/DEIM Strategies for reduced data assimilation systems, Journal of Computational Physics,2015.
- R. Stefanescu, A. Sandu, I.M. Navon Comparison of POD reduced order strategies for the nonlinear 2D Shallow Water Equations, International Journal for Numerical Methods in Fluids, 2014.
- R. Stefanescu, I.M. Navon, POD/DEIM Nonlinear model order reduction of an ADI implicit shallow water equations model, Journal of Computational Physics, Vol 237 , pp 95–114, 2013.

POD/DEIM Strategies for reduced data assimilation systems

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