POD/DEIM Strategies for reduced data assimilation systems

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Outline

Motivation

Reduced Order Modelling

ROM 4D-Var DA systems - Choice of bases

4D-Var SWE DA reduced order systems

Numerical results
   Choice of POD bases
   Performances of ROM optimization framework

Conclusions and future research
Why do we need reduced order data assimilation?
Why do we need reduced order data assimilation?

- Replace the current linearized cost function to be minimized in the inner loop
- Low-rank surrogate models that accurately represent sub-grid-scale processes
- Highly non-linear observation operators
- Increased space and time resolutions
- Reduced computational complexity
The objective function $J$ to be optimized is defined based on model-data misfit penalty terms as:

$$J(x_0) = \frac{1}{2} (x^b - x_0)^T B_0^{-1} (x^b - x_0)$$

$$+ \frac{1}{2} \sum_{i=1}^{N} (y^i - H(x_i))^T R_i^{-1} (y^i - H(x_i)),$$

subject to

$$x_{i+1} = M_i x_i, \quad i = 0, \ldots, N - 1,$$
Strong Constraint 4D-Var Data Assimilation

The optimality conditions:

**Adjoint model:**\[ \lambda_i = M_i^T \lambda_{i+1} + H_i^T R_i^{-1} (y^i - H(x_i)), \quad i = N - 1, 1; \]
\[ \lambda_N = H_N^T R_N^{-1} (y^N - H(x_N)) \quad \text{and} \quad \lambda_0 = M_0^T \lambda_1. \]

(3)

**Cost function gradient:**\[ \nabla x_0 J = -B_0^{-1} (x^b - x_0) - \lambda_0 = 0; \]

(4)
Reduced Order Modelling

- dependent and independent of input

- For **linear models** we are able to produce input-independent highly accurate reduced models: balanced truncation, moment matching

- For general **nonlinear systems**, the transfer function approach is not yet applicable and input-specified semi-empirical methods are usually employed

- Data analysis is conducted to extract basis functions, from experimental data or detailed simulations of high-dimensional systems

- Standard POD Galerkin 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.

- EIM, DEIM, Gappy POD, MPIM, BPIM, TPOD
Proper Orthogonal Decomposition

\[ \frac{dx(t)}{dt} = F(x, t), \quad x(0) = x_0 \in \mathbb{R}^n. \] (5)

The corresponding time implicit (backward) Euler scheme is given by

\[ r^i(x_{t_i}) := x_{t_i} - x_{t_{i-1}} - \Delta t F(x_{t_i}) = 0, \quad \text{for } i = 1, \ldots, N_t, \quad N_t \in \mathbb{N}, \quad N_t > 0, \] (6)

where \( x_{t_i} \) denotes the state at time step \( t_i \) and \( r^i : \mathbb{R}^n \to \mathbb{R}^n \) denotes the residual operator at iteration \( t_i \).
Proper Orthogonal Decomposition

The method of POD consists in choosing a complete orthonormal basis $U = \{u_i\}$, $i = 1, \ldots, k$; $k > 0$; $u_i \in \mathbb{R}^n$; $U \in \mathbb{R}^{n \times k}$ such that the mean square error between $x(t)$ and POD expansion $x^{POD}(t) = \bar{x} + U\tilde{x}(t)$, $\tilde{x}(t) \in \mathbb{R}^k$ is minimized on average.

The POD dimension $k \ll n$ is chosen to capture the dynamics of the flow using an energy based analysis.

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

(7)

and the reduced operator $\tilde{r}^i : \mathbb{R}^k \to \mathbb{R}^k$ is defined as

$$
\tilde{r}^i : (\tilde{x}_{t_i}) \to \tilde{x}_{t_i} - \tilde{x}_{t_{i-1}} - \Delta t W^T F(\bar{x} + U\tilde{x}_{t_i}).
$$

(8)
<table>
<thead>
<tr>
<th>No. of spatial discretization points</th>
<th>CPU time (seconds)</th>
<th>SPOD</th>
<th>TPOD</th>
<th>POD/DEIM m=70</th>
<th>POD/DEIM m=180</th>
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<td>10^3</td>
<td>10</td>
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<td>TPOD</td>
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</tr>
</tbody>
</table>

**Table:** CPU time gains and the root mean square errors. $t_f = 3h$, $3h$ time integration window, 103, 776 spatial points. $k = 50$, DEIM points $m = 180, 70$.

![Graph](image1.png)  
(a) On-line stage  

![Graph](image2.png)  
(b) Off-line stage

**Figure:** Cpu time vs. the number of spatial discretization points for $t_f = 3h$;
ROM 4D-Var DA systems - Choice of bases

- 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 $U_f$

$$J^{POD}(\tilde{\mathbf{x}}_0) = \frac{1}{2}(\mathbf{x}^b - U_f \tilde{\mathbf{x}}_0)^T B_0^{-1} (\mathbf{x}^b - U_f \tilde{\mathbf{x}}_0)^T$$

$$+ \frac{1}{2} \sum_{i=1}^{N} (\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i))^T R_i^{-1} (\mathbf{y}^i - H(U_f \tilde{\mathbf{x}}_i))^T,$$  

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

(http://csl.cs.vt.edu)
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; It's not clear what information should be included in the reduced basis used for full space gradient equation projection.

- The “adjoint of reduced” (AR) model approach formulates the first order optimality conditions from the forward reduced order model.

- Consistent KKT reduced optimality conditions; Reduced adjoint model approximates poorly its full counterpart and POD bases rely only on forward dynamics information.
ROM 4D-Var DA systems - Choice of bases

- RA approach: the full forward and adjoint models are projected onto separate reduced manifolds

- $U_f$ and $U_a$ are the trial POD reduced subspaces and $W_f$ and $W_a$ are the test functions POD manifolds, $x_i \approx U_f \tilde{x}_i$, $\lambda_i \approx U_a \tilde{\lambda}_i$, $i = 0, \ldots, N$.

- **Reduced forward model:**

  \[
  \tilde{x}_{i+1} = \tilde{M}_i \tilde{x}_i, \quad \tilde{M}_i = W_f^T M_i U_f, \quad i = 0, \ldots, N - 1. \tag{11}
  \]

- **Reduced adjoint model:**

  \[
  \tilde{\lambda}_i = W_a^T M_i^T U_a \tilde{\lambda}_{i+1} + W_a^T H^T R_i^{-1} (y^i - H(U_f \tilde{x}_i)), \quad i = N - 1, 1
  \]

  \[
  \tilde{\lambda}_N = W_a^T H^T R_N^{-1} (y^N - H(U_f \tilde{x}_N)) \quad \text{and} \quad \tilde{\lambda}_0 = W_a^T M_0^T U_a \tilde{\lambda}_1, \tag{12}
  \]
ROM 4D-Var DA systems - Choice of bases

▶ AR adjoint model:

\[
\tilde{\lambda}_i = U_f^T M_i^T W_f \tilde{\lambda}_{i+1} + U_f^T H^T R_i^{-1} (y^i - H(U_f \tilde{x}_i)), \quad i = N-1, 1; \\
\tilde{\lambda}_N = U_f^T H^T R_N^{-1} (y^N - H(U_f \tilde{x}_N)) \quad \text{and} \quad \tilde{\lambda}_0 = U_f^T M_0^T W_f \tilde{\lambda}_1
\] (13)

▶ RA adjoint model:

\[
\tilde{\lambda}_i = W_a^T M_i^T U_a \tilde{\lambda}_{i+1} + W_a^T H^T R_i^{-1} (y^i - H(U_f \tilde{x}_i)), \quad i = N-1, 1 \\
\tilde{\lambda}_N = W_a^T H^T R_N^{-1} (y^N - H(U_f \tilde{x}_N)) \quad \text{and} \quad \tilde{\lambda}_0 = W_a^T M_0^T U_a \tilde{\lambda}_1,
\] (14)

▶ For Petrov Galerkin and Galerking projections:

\[
W_f = U_a \quad \text{and} \quad W_a = U_f, \quad \text{and} \quad U_f = U_a.
\] (15)
4D-Var SWE DA reduced order systems

**Algorithm 4.1** Standard and Tensorial POD SWE DA systems

**Off-line stage**

1. Generate background state $u$, $v$ and $\phi$.
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. For each state variable compute a POD basis using snapshots describing dynamics of the forward and its corresponding adjoint trajectories.
5. Compute tensors as $T$ required for reduced Jacobian calculations. Calculate other POD coefficients corresponding to linear terms.
4D-Var SWE DA reduced order systems

Algorithm 4.1 Standard and Tensorial POD SWE DA systems

On-line stage - Minimize reduced cost functional $J^{POD}$ (9)

1: Solve forward reduced order model
2: Solve adjoint reduced order model
3: Compute reduced gradient

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 $J$ in (1). If $\|J\| > \varepsilon_3$ 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 stopping criteria are

  \[ \| \nabla J^{POD} \| \leq \varepsilon_1, \quad \| J^{POD}_{(i+1)} - J^{POD}_{(i)} \| \leq \varepsilon_2, \quad \text{MXFUN} \leq \text{iter}_{Max} \]  

(16)

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

  \[ \| J \| \leq \varepsilon_3 \]
Numerical Results

- ADI SWE model
- 10% uniform perturbations on the initial conditions of Grammeltvedt and generate twin-experiment observations at every grid space point location and every time step
- Background state is computed using a 5% perturbations of the initial conditions
- The length of the assimilation window: 3h.
- BFGS optimization method (CONMIN)
- We use $\varepsilon_1 = 10^{-14}$ and $\varepsilon_2 = 10^{-5}$. 

Numerical results [18/22] (http://csl.cs.vt.edu)
AR - no need for implementing the full adjoint SWE model since the POD basis relies only on forward trajectories snapshots.

We select $31 \times 23$ mesh points 91 time steps and use 50 POD basis functions. MXFUN is set to 25 and $\varepsilon_3 = 10^{-16}$

**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 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 $\varepsilon_3 = 10^{-1}$.

![Iteration performance](image1)

![Time performance](image2)

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

Conclusions and future research

- Consistent reduced KKT optimality conditions + accurate reduced POD adjoint model solutions with respect to the full adjoint model.

- Petrov-Galerkin projection - test functions POD bases of the forward and adjoint models have to match the trial functions POD bases of the adjoint and forward models.

- Galerkin projection - one single POD basis is required.

- Applicable for all type of reduced optimization involving adjoint models and projected based reduced order methods.

- For meshes of $151 \times 111$ points or higher the hybrid POD/DEIM reduced data assimilation system is approximately 10 times faster than the full space data assimilation system.

- A-posteriori error estimation apparatus - hybrid POD/DEIM SWE 4D-Var system - POD basis construction and selection of DEIM.

(http://csl.cs.vt.edu)


R. Stefanescu, I.M. Navon, Max Marchand, Henry Fuelberg 1D+4D-VAR data assimilation of lightning with WRFDA system using nonlinear observation operators, Submitted to MWR, 2013.