POD/DEIM Strategies for reduced data assimilation systems

Răzvan Ștefănescu ¹  Adrian Sandu ¹  Ionel M. Navon ²

¹Computational Science Laboratory, Department of Computer Science, Virginia Polytechnic Institute and State University

²Department of Scientific Computing, The Florida State University
Outline

1. Data Assimilation
2. Reduced order data assimilation
3. Reduced Order Modelling
4. ROM 4D-Var DA systems - Choice of bases
5. 4D-Var SWE DA reduced order systems
6. Numerical results
7. Conclusions and future research
Data Assimilation

- Data assimilation - process of combining information from models, measurements, and priors - all with associated uncertainties - to obtain the best estimate of the state of a physical system.

- Two families of methods: variational and statistical methods.

- Variational methods - rooted in control theory and require developments of tangent linear and adjoint models.

- Statistical methods: Ensemble based sequential data assimilation and Bayesian inversion
4D-Var Data Assimilation

- 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

$$ x_{i+1} = M_i(x_i), \ i = 0, \ldots, N - 1, $$

- The optimality conditions:

  Adjoint model: $\lambda_i = M_i^T \lambda_{i+1} + H^T R_i^{-1} (y^i - H(x_i)), \ i = N - 1, 1;$

  $$\lambda_N = H^T R_N^{-1} (y^N - H(x_N))$$ and $\lambda_0 = M_0^T \lambda_1.$

  $\nabla_{x_0} \mathcal{L} = -B_0^{-1} (x^b - x_0) - \lambda_0 = 0;$
4D-Var Data Assimilation

Model state

Initial time $t_0$

Analysis time

4D-Var

Model trajectory from corrected initial $x_a$

Model trajectory from first guess $x_b$

3  6  9  12  15

Assimilation window

time
Incremental 4D-Var Data Assimilation Courtier et al. [8]
Reduced order data assimilation

\[ x_0 = x_b \]

Outer loop

High-resolution non-linear trajectory

Reduced basis \( U \)

\[ \tilde{x}_i^0 = U^T (x_i^0 - \bar{x}) \]

Reduced-order nonlinear model

Reduced-order adjoint model

Iterative minimization algorithm

Inner loop

\[ x_i^k = \bar{x} + U \tilde{x}_i^k \]

\[ x_{i+1}^0 = \bar{x} + U \bar{x}_i^a \]

High-resolution non-linear forecast

\[ J \]

\[ \nabla J \]
Why do we need 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 instead of linearized low-fidelity models.
- Suitable reduced order models can be derived successively and give global convergence results - Arian et al. [2] - This approach can be interpreted in the context of trust region methods using general nonlinear model functions with inexact gradient information.
- Highly non-linear and non-smooth observation operators.
- Increased space and time resolutions.
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

- Application of generalized transfer functions and generalized moment matching (Benner and Breiten [3]) for nonlinear model order reduction
Proper Orthogonal Decomposition

- The desired simulation is well approximated in the input collection.
- 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.
- 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.

- Tensorial POD - Stefanescu et al. [14] - "Comparison of POD reduced order strategies for the nonlinear 2D Shallow Water Equations"
- 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 $x = U \tilde{x}$. 

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POD/DEIM Strategies for reduced data assimilation systems
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 discrete optimality conditions; Reduced adjoint model approximates poorly its full counterpart and POD bases rely only on forward dynamics information.
To guide the POD bases snapshots selection process for Petrov-Galerkin based reduced data assimilation systems governed by non-linear models

Consistent reduced Karush Kuhn Tucker (KKT) optimality conditions and accurate reduced POD adjoint model solutions with respect to the full adjoint model outputs

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 $U_f$

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

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

subject to $\tilde{\mathbf{x}}_{i+1} = W_f^T M_i (U_f \tilde{\mathbf{x}}_i), \ i = 0, .., N - 1.$ (5)
ROM 4D-Var DA systems - Choice of bases

- Reduced adjoint model

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

\[
\tilde{\lambda}_N = U_f^T H^T R_N^{-1}(y^N - H(U_f \tilde{x}_N)) \quad \text{and} \quad \tilde{\lambda}_0 = U_f^T M_0^T W_f \tilde{\lambda}_1
\]

(7)

- Reduced Cost Function gradient

\[
\nabla_{\tilde{x}_0} \mathcal{L}^{POD} = -U_f^T B_0^{-1}(x^b - U_f \tilde{x}_0) - \tilde{\lambda}_0 = 0;
\]

(8)

Definition

A reduced KKT system is said to be consistent if it represents the first order optimality conditions of some reduced order optimization problem.
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, $\mathbf{x}_i \approx U_f \tilde{\mathbf{x}}_i$, $\lambda_i \approx U_a \tilde{\lambda}_i$, $i = 0, \ldots, N$.

- Reduced forward model:
  \[ \tilde{\mathbf{x}}_{i+1} = W_f^T M_i(U_f \tilde{\mathbf{x}}_i), \quad i = 0, \ldots, N - 1. \]  

- Reduced adjoint model:
  \[
  \tilde{\lambda}_i = W_a^T M_i^T U_a \tilde{\lambda}_{i+1} + W_a^T H^T R_i^{-1}(\mathbf{y}_i - H(U_f \tilde{\mathbf{x}}_i)), \quad i = N - 1, 1
  \]
  \[
  \tilde{\lambda}_N = W_a^T H^T R_N^{-1}(\mathbf{y}_N - H(U_f \tilde{\mathbf{x}}_N)) \quad \text{and} \quad \tilde{\lambda}_0 = W_a^T M_0^T U_a \tilde{\lambda}_1,
  \]
ROM 4D-Var DA systems - Choice of bases

- **AR adjoint model:**

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

(11)

- **RA adjoint model:**

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

(12)

- For Petrov Galerkin and Galerkin projections - ARRA technique

\[
W_f = U_a \quad \text{and} \quad W_a = U_f, \quad \text{and} \quad U_f = U_a.
\]

(13)
Theorem

Assume that the model operators $\mathcal{M}_{i,i+1} : \mathbb{R}^{N_{\text{state}}} \to \mathbb{R}^{N_{\text{state}}}$, $i = 0, \ldots, N - 1$ and observation operators $\mathcal{H}_i : \mathbb{R}^{N_{\text{state}}} \to \mathbb{R}^{N_{\text{obs}}}$, $i = 0, \ldots, N$ belong to $C^2[\mathbb{R}^{N_{\text{state}}}]$ and the high-fidelity and AR optimization problems admit unique optimal pairs $(x^a, \lambda^a) \in \mathbb{R}^{N_{\text{state}} \times N} \times \mathbb{R}^{N_{\text{state}} \times N}$ and $(\tilde{x}^a, \tilde{\lambda}^a) \in \mathbb{R}^{k \times N} \times \mathbb{R}^{k \times N}$, with projection $(\hat{x}^a, \hat{\lambda}^a) = (U_f \tilde{x}^a, W_f \tilde{\lambda}^a)$ laying in the neighbourhood of $(x^a, \lambda^a)$.

Then there exist “impact factors” $\xi, \nu_i$ and $\mu_i \in \mathbb{R}^{N_{\text{state}}}$, $i = 0, \ldots, N$ 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

$$\varepsilon(\hat{x}_0) - \varepsilon(x^a_0) \approx \Delta_{\text{fwd}} + \Delta_{\text{adj}} + \Delta_{\text{opt}}. \quad (14)$$
Forward model contribution:

\[ \Delta_{\text{fwd}} = - \sum_{i=0}^{N-1} v_{i+1}^T \left( U_f W_f^T - I \right) M_{i,i+1}(x_i^a) \]  

(15a)

Adjoint model contribution

\[ \Delta_{\text{adj}} = -\mu_N^T \left( W_f U_f^T - I \right) H_N^T R_N^{-1} (y_N - \mathcal{H}_N(x_N^a)) \]

\[- \sum_{i=0}^{N-1} \mu_i^T \left( W_f U_f^T - I \right) \left[ M_{i,i+1}^T \lambda_{i+1}^a + H_i^T R_i^{-1} (y_i - \mathcal{H}_i(x_i^a)) \right], \]

(15b)

Optimality equation contribution:

\[ \Delta_{\text{opt}} = -\xi^T \left( W_f U_f^T - I \right) B_0^{-1} (x_0^b - x_0^a). \]

(15c)
ROM 4D-Var DA systems - Choice of bases

Definition

The triplet \((x, \lambda, \nabla x_0 \mathcal{L}) \in \mathbb{R}^{N_{\text{state}} \times N} \times \mathbb{R}^{N_{\text{state}} \times N} \times \mathbb{R}^{N_{\text{state}}}\) is said to be KKT-feasible if \(x\) is the solution of the forward model (2) initiated with a given \(x_0 \in \mathbb{R}^{N_{\text{state}}}\), \(\lambda\) is the solution of the adjoint model (3) linearized across the trajectory \(x\), and \(\nabla x_0 \mathcal{L}\) is the gradient of the Lagrangian function computed from (4).
Definition

Let \((x, \lambda, \nabla x_0 L) \in \mathbb{R}^{N_{\text{state}} \times N} \times \mathbb{R}^{N_{\text{state}} \times N} \times \mathbb{R}^{N_{\text{state}}}\) be a KKT-feasible triplet of the full order optimization problem (1). If for any positive \(\varepsilon_f, \varepsilon_a\) and \(\varepsilon_g\) there exists \(k \leq N_{\text{state}}\) and three bases \(\bar{U}, \bar{V}\) and \(\bar{W} \in \mathbb{R}^{N_{\text{state}} \times k}\) such that the reduced KKT-feasible triplet \((\tilde{x}, \tilde{\lambda}, \nabla \tilde{x}_0 L^{\text{POD}}) \in \mathbb{R}^{k \times N} \times \mathbb{R}^{k \times N} \times \mathbb{R}^{k}\) of the reduced optimization problem (5) satisfies:

\[
\|x_i - \bar{U}\tilde{x}_i\|_2 \leq \varepsilon_f, \quad i = 0, \ldots, N, \quad (16a)
\]
\[
\|\lambda_i - \bar{V}\tilde{\lambda}_i\|_2 \leq \varepsilon_a, \quad i = 0, \ldots, N, \quad (16b)
\]
\[
\|\nabla x_0 L - \bar{W}\nabla \tilde{x}_0 L^{\text{POD}}\|_2 \leq \varepsilon_g, \quad (16c)
\]

then the reduced order AR KKT system built using \(U_f = \bar{U}, \ W_f = [\bar{V}, \bar{W}]\) that generated \((\tilde{x}, \tilde{\lambda}, \nabla L^{\text{POD}}_{\tilde{x}_0})\) is said to be accurate with respect to the full order KKT system.
Algorithm 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.
Algorithm 1 Standard and Tensorial POD SWE DA systems

On-line stage - Minimize reduced cost functional $J^{POD}$ (5)

1: Solve forward reduced order model (6)
2: Solve adjoint reduced order model (7)
3: Compute reduced gradient (8)

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.
The on-line stage - minimization of the cost function $J^{POD}$ performed on a reduced POD manifold

The stopping criteria are

$$\| \nabla J^{POD} \| \leq \varepsilon_1, \quad \| J_{(i+1)}^{POD} - J_{(i)}^{POD} \| \leq \varepsilon_2, \quad \text{MXFUN} \leq \text{iter}_{\text{Max}} \quad (17)$$

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

$$\| J \| \leq \varepsilon_3$$
Three POD based reduced order models will be considered for deriving reduced order SWE data assimilation systems: standard Proper Orthogonal Decomposition (SPOD), tensorial POD (TPOD) and standard POD/Discrete Empirical Interpolation Method (POD/DEIM)

The reduced Jacobians are obtained using tensorial calculus for all three ROMs and their computational complexity depends only on $k$ the dimension of POD basis - Stefănescu and Sandu [15]

The methods differ in the way the nonlinear terms are treated - polynomial quadratic nonlinearity $u^2$. 
4D-Var SWE DA reduced order systems

**Standard POD**

\[
\tilde{N}(\tilde{u}) = \underbrace{W^T}_{k \times \text{state}} \underbrace{\tilde{U} \odot \tilde{U}}_{\text{state} \times 1}, \tilde{N}(\tilde{u}) \in \mathbb{R}^k \tag{18}
\]

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

**Tensorial POD**

\[
\tilde{N}(\tilde{u}) = \left[ \tilde{N}_i \right]_{i=1,\ldots,k} \in \mathbb{R}^k; \quad \tilde{N}_i = \sum_{j=1}^{k} \sum_{l=1}^{k} T_{i,j,l} \tilde{u}_j \tilde{u}_l. \tag{19}
\]

\[
\tilde{N}(\tilde{u}) = \underbrace{T}_{k \times k^2} \underbrace{\tilde{U}}_{k^2 \times 1}
\]

\[
T = \left( T_{i,j,l} \right)_{i,j,l=1,\ldots,k} \in \mathbb{R}^{k \times k \times k}, \quad T_{i,j,l} = \sum_{r=1}^{n} W_{i,r} U_{j,r} U_{l,r}.
\]
4D-Var SWE DA reduced order systems

Standard POD/DEIM

\[ \tilde{N}(\tilde{u}) \approx W^T V (P^T V)^{-1} \left( (P^T U\tilde{u}) \odot (P^T U\tilde{u}) \right) \]

(20)

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 [5], Chaturantabut and Sorensen [7, 6], Stefanescu and Navon [13]).
4D-Var SWE DA reduced order systems

\[ F_{11}(u, \phi) = u \odot A_x u + \frac{1}{2} \phi \odot A_x \phi, \quad F_{12}(u, v) = v \odot A_y u \]

\[ F_{21}(u, v) = u \odot A_x v, \quad F_{22}(v, \phi) = v \odot A_y v + \frac{1}{2} \phi \odot A_y \phi, \]

\[ F_{31}(u, \phi) = \frac{1}{2} \phi \odot A_x u + u \odot A_x \phi, \quad F_{32}(v, \phi) = \frac{1}{2} \phi \odot A_y v + v \odot A_y \phi. \]

<table>
<thead>
<tr>
<th></th>
<th>Full ADI SWE</th>
<th>Standard POD</th>
<th>Tensorial POD</th>
<th>POD/DEIM m=180</th>
<th>POD/DEIM m=70</th>
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<tr>
<td>CPU time</td>
<td>950.0314s</td>
<td>161.907</td>
<td>2.125</td>
<td>0.642</td>
<td>0.359</td>
</tr>
<tr>
<td>(u)</td>
<td>-</td>
<td>5.358e-5</td>
<td>5.358e-5</td>
<td>5.646e-5</td>
<td>7.453e-5</td>
</tr>
<tr>
<td>(v)</td>
<td>-</td>
<td>2.728e-5</td>
<td>2.728e-5</td>
<td>3.418e-5</td>
<td>4.233e-5</td>
</tr>
<tr>
<td>(\phi)</td>
<td>-</td>
<td>8.505e-5e</td>
<td>8.505e-5</td>
<td>8.762e-5</td>
<td>9.212e-5</td>
</tr>
</tbody>
</table>

**Table:** CPU time gains and the root mean square errors for each of the model variables at \(t_f = 3h\) 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.
4D-Var SWE DA reduced order systems

Figure: Cpu time vs. the number of spatial discretization points for $t_f = 3h$; number of POD modes = 50; two different numbers of DEIM points 70 and 180 have been employed.
Numerical Results

- ADI SWE model
- 10% uniform perturbations on the initial conditions of Grammeltvedt [9] 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 $\varepsilon_2 = 10^{-5}$.
- We select $31 \times 23$ mesh points 91 time steps and use 50 POD basis functions. MXFUN is set to 25 and $\varepsilon_3 = 10^{-16}$
Numerical Results - Choice of POD basis

(a) Forward model snapshots only     (b) Forward and adjoint models snapshots

Figure: The decay around the singular values of the snapshots solutions for $u$, $v$, $\phi$ for $\Delta t = 960s$ and integration time window of $3h$. 
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 has to be incorporated into POD basis.
POD/DEIM SWE 4D-Var DA system

- Mesh of $31 \times 23$ and $17 \times 13$ points, a POD basis dimension of $k = 50$, and various number of DEIM interpolation points are used. MXFUN is set to 100 and $\varepsilon_3 = 10^{-16}$

![Graph showing evolution of cost function and gradient norm as a function of the number of minimization iterations for different number of mesh points and various number of DEIM points.](image)

(a) Number of mesh points $31 \times 23$  
(b) Number of mesh points $17 \times 13$

Figure: Standard POD/DEIM ADI SWE 4D-Var system – Evolution of cost function and gradient norm as a function of the number of minimization iterations for different number of mesh points and various number of DEIM points.
Hybrid POD/DEIM SWE 4D-Var DA system

(a) Tangent Linear and Adjoint test

(b) Cost function and gradient decays

Figure: Tangent linear and adjoint test for standard POD/DEIM SWE 4D-Var system. Optimization performances of Standard POD/DEIM and Hybrid POD/DEIM 4DVAR ADI 2D shallow water equations for 50 DEIM points and \( n = 17 \times 13 \) space points.
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

- New 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 feasible reduced POD KKT conditions.

- 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 and the correlation matrix must contain snapshots from both forward and adjoint full models. Include also the optimality condition information.
Conclusions and future research

- Every type of reduced optimization involving adjoint models and projected based reduced order methods including reduced basis approach benefit from the new strategies.

- The POD/DEIM approximations of four nonlinear terms involving height field out of ten partially lost their accuracy during the optimization where input data are different than the ones used to generate the interpolation points - Hybrid tensorial POD/DEIM 4D-Var SWE.

- 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.
Conclusions and future research

- This rate increases directly proportional with the mesh size

- Stabilization strategies proposed by Amsallem and Farhat [1], Bui-Thanh et al. [4] 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. [10], Rapún and Vega [12]);

- Exploit the structure of the weak constraints variational approach (Trémolet [17]), consistent reduced KKT conditions (Stefănescu et al. [16]) and formulate a piecewise-in-space-time approximation strategy that uses different ROMs on different subintervals, and constructs them concurrently;

- Develop reduced order parallel 4D-Var framework using Augmented Lagrangian (Rao and Sandu [11]).
Manuscripts related to the present research effort


Manuscripts related to the present research effort

POD/DEIM Strategies for reduced data assimilation systems

Thank You


