AMST Workshop 2016
Introduction to reduced order modelling
toward Pint+ROM4XDEM

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Outline

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Which are the challenges of reduced order modelling?

- Performing in real-time (on-fly) complex problem characterized by many parameters, solving low-dimensional problem;
- reducing significantly the computational complexity;
- evaluating multi-query tasks: uncertainty quantification analysis and data-driven model.

Active research lines:

- combination with domain decomposition algorithm in space
- combination with parallel-time integrator
- smart sampling of parameters in time and space
- adaptation with cheap cost on-fly for data-driven application
- combination with surrogate model

Parametrized partial differential equation

One of key feature of ROM is the possibility to exploit the affinely parametrization of the equations with respect to the parameters:

$$\frac{\partial(\rho c_p T)}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \lambda_{eff}\frac{\partial T}{\partial r}\right) + \sum_k \dot{\omega}_k H_k$$

$$-\lambda_{eff}\frac{\partial T}{\partial r}|_{r=0} = 0$$

$$-\lambda_{eff}\frac{\partial T}{\partial r}|_{r=R} = \alpha(T_R - T_\infty) + \dot{q}_{rad} + \dot{q}_{cond}$$

r is geometric parameter
c_p, λ_{eff} are the physical parameters.
The parameter of interest is:
$\mu = [r, c_p, \lambda_{eff}]$

$$\mu_2\frac{1}{\Delta t}M \cdot T^{k+1} + \frac{\mu_3}{\mu_1}AT^{k+1}(\mu) = \frac{1}{\Delta t}\mu_2 M \cdot T^k + f^k + \mu_3 g^k$$

Offline-online paradigm

Offline:

- Sampling the parameters in a physical predefinite range
- Define a manifold of snapshots $\mathcal{M} = \{T_i(\mu_i), \mu_i \in \mathcal{D}\} \subset \mathbb{R}^N$ with $\dim(\mathcal{M}) = m << \#dof$. Let $V := [T_1|\ldots|T_m]$.

Online:

- Select μ^{new}, express the solution

$$T(\mu^{new})^{k+1} = a_1^{k+1}(\mu^{new})T_1(\mu_1) + \ldots + a_m^{k+1}(\mu^{new}(t))T_m(\mu_m)$$

- The coefficients $\{a_1, \ldots, a_m\}$ are obtained solving :

$$\mu_2 \frac{1}{\Delta t} VMV^T \cdot \mathbf{a}^{k+1} + \frac{\mu_3}{\mu_1} VAV^T \mathbf{a}^{k+1} = \frac{1}{\Delta t}\mu_2 VMV^T \cdot \mathbf{a}^k + f^k + \mu_3 g^k$$

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Reduced Order Model recipes

Project-based methods:

- proper orthogonal decomposition (POD)
- reduced basis (be Greedy)
- Greedy-POD

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Project-based technique: proper orthogonal decomposition

How to reduce the information from the snapshots? How to quantify the information and the discard noise?

Algorithm 1: Proper orthogonal decomposition

Input : Preselected parameters $\mu_1, \ldots, \mu_m$ and snapshots $T_1, \ldots, T_m$, toll$= 0.1$

Output: Compressed POD basis $W_{POD} := [\phi_1 | \ldots | \phi_{POD}]$

1 Construct the covariance matrix C, whose entries $C_{i,j} = \langle T_i, T_j \rangle$;

2 Solve $C\psi = \lambda\psi$ with decreasing order $\lambda_m \geq \lambda_{m-1} \geq \ldots$;

3 Criteria $\frac{\|V - W_{POD} W_{POD}^T V\|_F}{\|W_{POD}\|_F} = \frac{\sum_{i=\mathrm{POD}}^m \lambda_i}{\sum_{i=1}^m \lambda_i} < \mathrm{toll}$;

4 Compute $\phi_i = \frac{1}{\sqrt{\lambda_i}} V\psi_i$ for $i = 1, \ldots, \mathrm{POD}$

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Project-based technique: reduced basis

Given m snapshots, which are the best snapshot parameter location ? Be greedy in selection!)

Algorithm 2: Greedy-Reduced Basis

Input : A set of parameters $\mathcal{D} = \{\mu_1, \ldots, \mu_m\}$, toll$= 1e - 6$

Output: Reduced basis $\mathbb{W}_{RB} := \mathrm{span}\,\{T_1, \ldots, T_{RB}\}$

1 Compute $T(\mu_n)$ for a random μ_n;

2 Add $T(\mu_n)$ to $\mathbb{W}_{RB}$ and perform the orthogonalization;

3 For each $\mu \in \mathrm{set}\,\{\mu_1, \ldots, \mu_m\} \setminus \mu_n$;

4 Solve the reduced system (compute the coefficient a) for μ;

5 Evaluate the (a-posteriori) error estimator $\eta(\mu)$;

6 Choose (the worst) $\mu_{n+1} = arg\,\max_{\mu \in \mathcal{D}} \eta(\mu)$;

7 If $\eta(\mu_{n+1}) > toll$, then set $n = n + 1$ and go to 2., otherwise terminate.

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Combine Greedy-POD for unsteady equations

Algorithm 3: Greedy-POD (Global trajectory)

Input : A parameter μ_1, set $n = 1$, N_1, N_2, $N_3 = 0$, $\mathcal{Z} = \emptyset$, toll$= 1e - 6$

Output: Reduced basis $\mathbb{W}_{POD} := \text{span}\left\{\tilde{\phi}_1, \ldots, \tilde{\phi}_{POD}\right\}$

1 Compute the trajectory $\left\{T^0(\mu_n), \ldots, T^K(\mu_n)\right\}$ for μ_n;

2 Compress $\langle \phi_1, \ldots, \phi_{POD} \rangle = POD(T^0(\mu_1), \ldots, T^K(\mu_1), N_1)$;

3 Enrich $\mathcal{Z} := \mathcal{Z} \cup \langle \phi_1, \ldots, \phi_{POD} \rangle$;

4 Set $N_3 = N_3 + N_2$;

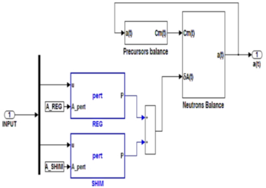
5 Compress $\langle \tilde{\phi}_1, \ldots, \tilde{\phi}_{N_3} \rangle = POD(Z, N_3)$;

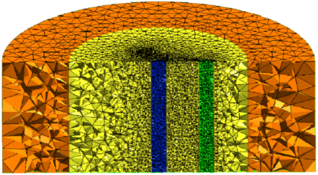
6 Set $W_{POD} = \text{span}\left\{\tilde{\phi}_1, \ldots, \tilde{\phi}_{N_3}\right\}$;

7 Choose (the worst) $\mu_{n+1} = arg\max_{\mu \in \mathcal{D}} \eta(t^K, \mu)$;

8 If $\eta(t^K, \mu_{n+1}) > toll$, then set $n = n + 1$ and go to 1., otherwise terminate.

Application of ROM recipes to multigroup neutronic diffusion





$$
\begin{cases}
\underline{\underline{V}}^{-1}\dfrac{\partial \underline{\Phi}}{\partial t} = \nabla\cdot\left(\underline{\underline{D}}\nabla\underline{\Phi}\right) - \underline{\underline{\Sigma}}_a\underline{\Phi} - \underline{\underline{\Sigma}}_s\underline{\Phi} + (1-\beta)\underline{\chi}_p\underline{F}^T\underline{\Phi} + \sum_m \lambda_m\underline{\chi}_d C_m + \underline{S} & (1) \\[2ex]
\dfrac{\partial C_m}{\partial t} = -\lambda_m C_m + \beta_m\underline{F}^T\underline{\Phi} \quad \text{for} \quad m = 1,\cdots,8 & (2)
\end{cases}
$$

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Evaluation of reactivity

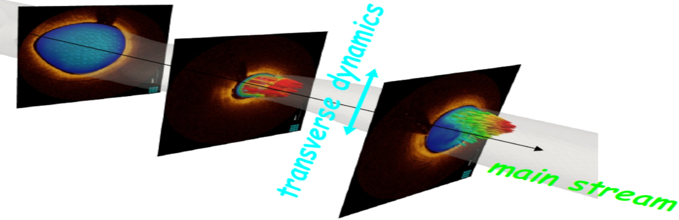
# of functions	Reactivity [pcm] Reference	POD	MM
1	3.4	-745.0	1.510
2	3.4	7.5	1.505
3	3.4	3.6	1.505
4	3.4	4.2	1.504
5	3.4	4.2	1.490
6	3.4	4.2	1.502
7	3.4	4.2	1.490
8	3.4	4.2	1.485
9	3.4	4.2	1.485
10	3.4	4.2	1.468
50	3.4	4.2	0.985
100	3.4	4.2	0.577

Limitations in ROM recipe

- computational cost in assembling the reduced system scales with the full dimension problem
- limitation in solving non-linear and parametric dependent problems
- adaptation requires to evaluate the full system

Surrogate model: HiMoD

Assuming a flow phenomena characterized by a main-stream dominant dynamics + transverse dynamics which are relevant only locally.



$$v_m^h(x,y) = \sum_{k=1}^{m} v_k^h(x)\phi_k(y) x \in \Omega_{1D} \; and \; y \in \Sigma_x$$

where ϕ_k are modal basis function that describe the transverse dynamics.

POD+HiMoD = HiPOD

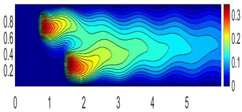


Figure: HiMoD simulation

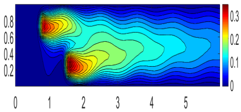


Figure: 6 POD basis

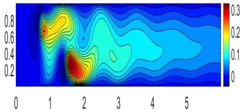


Figure: Two POD basis

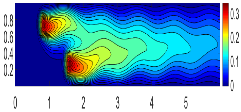


Figure: 19 POD basis

Advanced model reduction: Gappy POD

Algorithm 4: POD evolution basis

Input : A set of parameter $\mu_1, \dots, \mu_m$, *toll*

Output: POD basis $W(POD, \beta_j)$ for the $j-$th time step

1 Fix the $j - th$ time, collect all snapshots at this time:
$Y^j = [T(\mu_1, t^j), \dots, T(\mu_m, t^j)]$;

2 Compute the POD basis,
$W(POD, \beta_j) = [\phi_1^j | \dots | \phi_{\beta_j}^j] = POD(Y^j, \beta_j)$;

How to determine online the coefficient z_k^j of the expansion $T^{j(0)}(t^j, \mu_{new}) = \sum_{k=1}^{\beta_j} z_k^j \phi_k^j$ for the “optimal“ guest of the Newton-like method at the $j-$th time step?

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Algorithm 5: Forecasting method

Input : Evolution POD basis, $\alpha_{max} \geq max_j \beta_j$

Output: Forecasting guest $T(t^{n+1} + c_1 \Delta t^n)$ for new parameter

1 For each time step $n = 1, \dots, K$;

2 If the forecast $T(t^{n+1} + c_1 \Delta t^n)$ is available then set the initial guess $T^{n(0)}$, otherwise from previous time step. ;

3 Solve Newton-method and compute $T(t^n)$ with the given initial guest.;

4 Let K_n the number of Newton iteration at time n.;

5 If $K_n \geq toll$ and $(n-1) \geq \max_j \beta_j$ then ;

6 Set the memory $\alpha = min(n-1, \alpha_{max})$ and compute z^j coefficient using the previous α time information, solving:;

7 $z_j = arg\min_{z \in \mathbb{R}^{\beta_j}} \|Z(n,\alpha)W(POD,\beta_j)z - Z(n,\alpha)[T(t^0 + c_1 \Delta T), \dots, T(t^{K-1} + c_1 \Delta T)]^T\|$;

8 where $Z(n,\alpha) = [\mathbf{e}_{n-\alpha-1}, \dots, \mathbf{e}_{n-1}]^T$.;

Definition of SDC sweep

Given an ODE (or a unsteady PDEs reduced to an ODE) of the form

$$y'(t) = f(t, y(t)) \quad \text{with } y(t_0) = y_0$$

Let $[t^n, t^{n+1}]$ be the interval where we apply the time-integration; and $t^n \leq t_0 \leq \ldots \leq t_{M-1} \leq t^{n+1}$. A sweep of deferred correction algorithm (SDC) based on backward-Euler is defined by solving iteratively

$$y^{k+1}(t_{m+1}) = y^{k+1} + \Delta t_m(f(t_{m+1}, y^{k+1}(t_{m+1})) - f(t_{m+1}, y^k(t_{m+1})))$$

where $Q_m^{m+1} = \delta t \sum_{i=0}^{M}(q_{m+1,i} - q_{m,i}) f(t_i, y_i^k)$ and $q_{m,j}$ are obtain the quadrature point of high-order collocation integration. The convergence is monitored by the residual.

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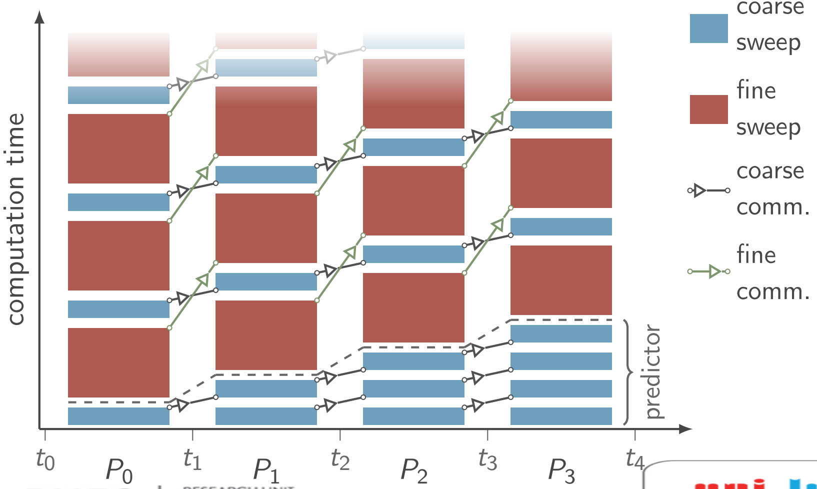
Parallelism-in-Time: PFASST

How to extend this concept in exascale multilevel space-time parallelism?



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How to combine PinT with model reduction?

- Construct for each time step a evolving ROM basis
- Construct a coarse sweep online based on Gappy-POD

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Research questions

- How to quantify the goodness of on-fly model from engineering point of view ?
- How much can benefit XDEM from model reduction ?
- How much can increase its scalability from PinT+ROM?
- How the reduction model in different modules can interact?