An integrated and efficient framework for embedded Reduced Order Models for multifidelity Uncertainty Quantification

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Why multifidelity in Uncertainty Quantification?

Uncertainty Quantification
DoE and DoD deployment activities

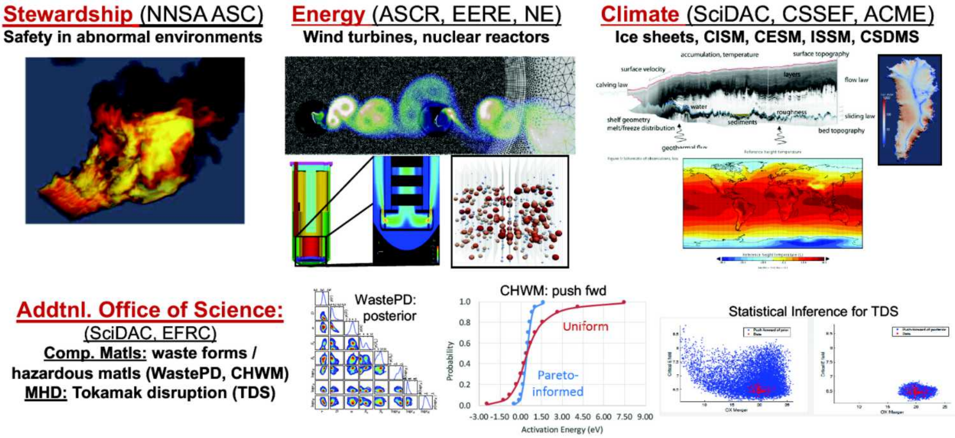


FIGURE: Courtesy of Mike Eldred

High-fidelity state-of-the-art modeling and simulations with HPC

- **Severe** simulations **budget constraints**
- **Significant dimensionality** driven by model complexity

Uncertainty Quantification for HF simulations
State-of-the-art

Two technologies are emerging as effective strategies to perform UQ for HF simulations:

- **Multifidelity** optimally fuses a handful of HF realizations with large sets of realizations from several lower fidelity models
- **Reduced Order Modeling (ROM)** creates a fast representation of the HF numerical model for a rapid *a posteriori* use

In principle ROM can be used (as it is) within a MF UQ framework as one model fidelity, however few questions need to be addressed:

- How accurate does ROM need to be to achieve a certain accuracy within the MF UQ?
- How is it possible to optimize the training step of ROM within a MF UQ workflow?

In this talk we try to explore how the coupling between ROM and MF UQ can be done efficiently

Multifidelity Sampling-based approaches

Uncertainty Quantification
Forward Propagation – Why Sampling Methods?

UQ context at a glance:

- High-dimensionality, non-linearity and possibly non-smooth responses
- Rich physics and several discretization levels/models available

Natural candidate:

- **Sampling**-based (MC-like) approaches because they are **non-intrusive**, **robust** and **flexible**...
- **Drawback:** Slow convergence $\mathcal{O}(N^{-1/2}) \rightarrow$ many realizations to build reliable statistics

Goal of the talk: **Reducing the computational cost** of obtaining MC reliable statistics

Pivotal idea:

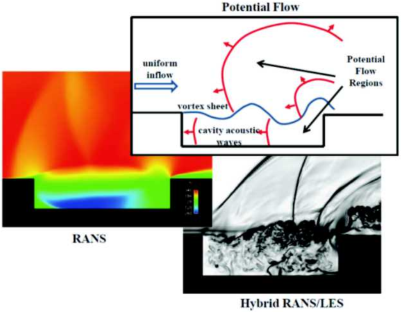
- Simplified (**low-fidelity**) models are **inaccurate** but **cheap**
  - **low-variance** estimates
- **High-fidelity** models are **costly**, but **accurate**
  - **low-bias** estimates

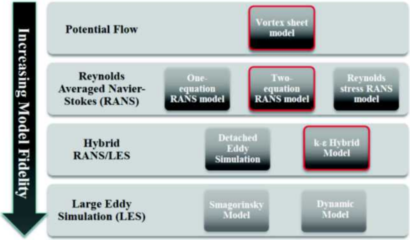
Uncertainty Quantification

Rich set of modeling choices – Discretization Vs Fidelity

Multi-fidelity: several accuracy levels available

- Physical models (Laminar/Turbulent, Reacting/non-reacting, viscous/inviscid...)
- Numerical methods (high/low order, Euler/RANS/LES, *etc*...)
- Numerical discretization (fine/coarse mesh...)
- Quality of statistics (long/short time history for turbulent flow...)





Monte Carlo simulation
Introducing the spatial discretization

Problem statement: We are interested in the statistics of a functional (linear or non-linear) Q_M of the solution $\mathbf{u}_M$

$$Q_M = \mathcal{G}(\mathbf{u}_M) \quad \rightarrow \quad \mathbb{E}[Q_M]$$

- M is (related to) the number of **spatial** degrees of freedom
- $\mathbb{E}[Q_M] \xrightarrow{M \rightarrow \infty} \mathbb{E}[Q]$ for some RV $Q : \Omega \rightarrow \mathbb{R}$

$$\hat{Q}^{MC}_{M,N} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{i=1}^{N} Q^{(i)}_M ,$$

Looking at the **Mean Square Error (MSE)**:

$$\mathbb{E}\left[(\hat{Q}^{MC}_{M,N} - \mathbb{E}[Q])^2 \right] = \mathbb{V}\mathbf{ar}\left[\hat{\mathbf{Q}}^{\mathbf{MC}}_{\mathbf{M},\mathbf{N}} \right] + (\mathbb{E}[\mathbf{Q_M} - \mathbf{Q}])^{\mathbf{2}}$$

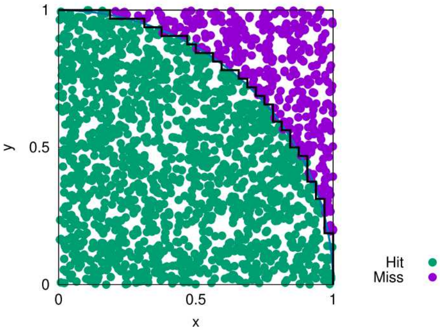
Accelerating Monte Carlo

Bringing multiple fidelity models into the picture

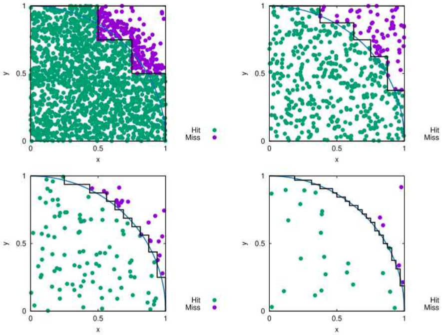
Pivotal idea:

- **High-fidelity** models are **costly**, but **accurate**
  - **low-bias** estimates
- Simplified (**low-fidelity**) models are **inaccurate** but **cheap**
  - **low-variance** estimates

Single Fidelity



Multi Fidelity

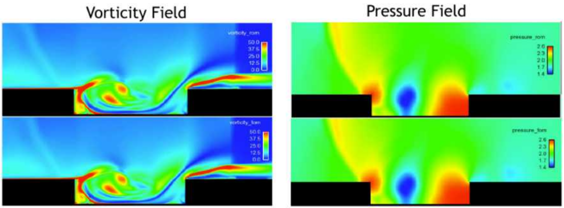


Reduced Order Modeling (ROM)

Reduced order Modeling
Generalities

LSPG ROM
- 32 min, 2 cores

High-fidelity
- 5 hours, 48 cores



ROM are used at Sandia for

- **Time critical decision:** Model predictive control and health monitoring
- **Many queries workflows:** Optimization and Uncertainty Quantification

Model Reduction Criteria

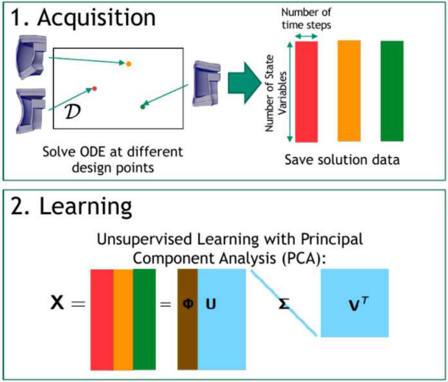
- **Accuracy:** achieve less than 1% error
- **Low cost:** achieve at least 100x computational saving
- **Property preservation:** preserves important physical properties
- **Generalization:** should work in every difficult cases
- **Certification:** accurately quantify the ROM error
- **Extensibility:** should work for many application codes

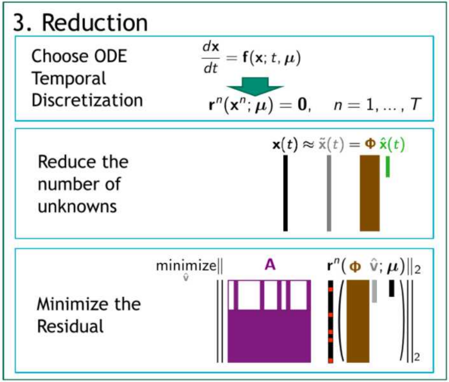
Reduced order Modeling

Least-squares Petrov-Galerkin (LSPG) – Workflow

High-Fidelity system of ODEs:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t; \boldsymbol{\mu}), \qquad \boldsymbol{x}(0; \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu})$$





- LSPG references: [Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]

Multifidelity UQ - ROM coupling

Multifidelity UQ and ROM coupling

Normalized cost with *a priori* ROM

- The variance reduction of the multifidelity scheme is

$$\mathbb{V}ar\left[\hat{Q}_N^{MF}\right] = \mathbb{V}ar\left[\hat{Q}\right]\left(1 - \frac{\mathbf{r-1}}{\mathbf{r}}\rho_1^2\right)$$

- Let's assume that ROM is the (only) LF model
- The optimal[1] number of HF and LF simulations can be obtained in closed form for an estimator variance ε^2

$$N = \frac{\mathbb{V}ar\left[Q\right]}{\varepsilon^2}\left(1 - \frac{r^\star - 1}{r^\star}\rho^2\right)$$

$$r^\star = \sqrt{\frac{\mathcal{C}_{FOM}}{\mathcal{C}_{ROM}}}$$

- The overall cost of the multifidelity estimator (normalized w.r.t. MC) is

$$\mathcal{C}_{MF}^{norm} = \left(1 - \frac{r^\star - 1}{r^\star}\rho^2\right)\left(1 + r^\star\frac{\mathcal{C}_{ROM}}{\mathcal{C}_{FOM}}\right).$$

NOTES:

- The cost $\mathcal{C}_{MF}^{norm}$ represents the efficiency of the MF UQ estimator
- Given a fixed value for both $\mathcal{C}_{FOM}$ and $\mathcal{C}_{ROM}$, then $\mathcal{C}_{MF}^{norm} = \mathcal{C}_{MF}^{norm}(\rho^2)$

[1] Minimum overall estimator cost for a target estimator variance

Multifidelity UQ and ROM coupling
Online ROM's cost integration

Can we be more efficient by designing the ROM to achieve an optimal correlation and cost trade-off within this framework?

We consider here (without lack of generality) two hyper-parameters for ROM:

- n_b number of basis terms for ROM
- k the multiplicative factor that controls the time step size (*i.e.* a time step $k\Delta t$ is used for ROM whereas Δt is used for FOM)

A complexity analysis can be conducted for both FOM and ROM

- Full order model
$$\mathcal{C}^{FOM} = n_t n_{nl} n_l \nu_{nnz} N.$$
- ROM based on QR decomposition
$$\mathcal{C}^{ROM,QR} = \frac{n_t}{k} n_{nl} \left(\alpha \nu_{nnz} N n_b + 2\alpha N n_b^2 + \alpha N n_b + n_b^2 \left(-\frac{2}{3} n_b^2 \right) \right)$$
- where
  - n_t is the number of time steps
  - n_{nl} is the number of iterations for the non-linear Newton-Raphson method
  - n_l is he number of iterations for the solution of the linear system
  - ν_{nnz} is the number of non-zero elements per row (*i.e.* spatial discretization stencil)
  - N is the number of spatial nodes
  - α is the hyper-reduction factor

Numerical results

Test case description
The Kuramoto-Sivashinsky equation

We consider the non-dimensionalized one-dimensional KS equation with homogeneous Dirichlet and Neumann boundary conditions,

$$\frac{\partial u}{\partial t} = -(u+c)\frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} - \nu \frac{\partial^4 u}{\partial x^4}$$
$$x \in [0, L], t \in [0, \infty),$$
$$u(0,t) = u(L,t) = 0,$$
$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0,$$
$$u(x,0) = u_0(x),$$

where L is the domain length ($L = 128$ in our tests), c is an advection parameter, and ν is the hyperviscosity parameter.

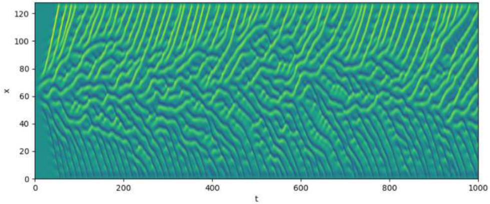


Figure: Space-time plot of the KS equation solution for $c = 0.0, L = 128.0, \nu = 1.0$.

Test case description

The Kuramoto-Sivashinsky equation – Quantities of Interest

In this study we considered four different quantities:

- Mean of a pointwise quantity

$$Q^1(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} u(x = 0.25L, t)\, dt,$$

- Mean of a squared pointwise quantity

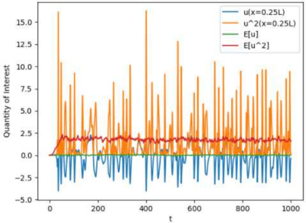
$$Q^2(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} u^2(x = 0.25L, t)\, dt,$$

- Mean of a spatially averaged quantity

$$Q^3(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \mathbb{E}[u]\; dt, \qquad \mathbb{E}[u] = \frac{1}{L}\int_0^L u(x,t)\, dx,$$

- Mean of a spatially averaged squared quantity

$$Q^4(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \mathbb{E}\left[u^2\right]\; dt, \qquad \mathbb{E}\left[u^2\right] = \frac{1}{L}\int_0^L u^2(x,t)\, dx,$$



MF UQ - ROM coupling

Exploring the existence of an optimal coupling region

On-line MF UQ – ROM coupling

- the hyper-parameters n_b (number of basis terms) and k (the time step factor) control the cost $\mathcal{C}_{ROM}^{norm}$
- the correlation between FOM and ROM is also a function of n_b and k
- the final MF UQ-ROM estimator's cost (normalized w.r.t. MC) is then function of n_b and k

$$\underset{n_b,k}{\operatorname{argmin}} \left(1 - \frac{r^\star(n_b,k) - 1}{r^\star(n_b,k)} \rho^2(n_b,k)\right) \left(1 + r^\star(n_b,k) \frac{\mathcal{C}_{LF}^{norm}(n_b,k)}{1}\right),$$

where

$$r^\star(n_b,k) = \sqrt{\frac{1}{\mathcal{C}_{LF}^{norm}} \frac{\rho^2(n_b,k)}{1-\rho^2(n_b,k)}},$$

Numerical tests procedure:

- The uncertainty parameters are randomly sampled and the inputs for N_{train} training data points are generated;
- FOM evaluations are generated for the training data;
- A POD basis $\mathbf{\Phi}$ is computed from the aggregation of the snapshots from the N_{train} FOM evaluations;
- For an assigned value of the parameters $\bar{n}_b$ and $\bar{k}$, ROM evaluations are generated for the training data;
- The correlation and the L2 error between the FOM and ROM QoI evaluations is computed.

NOTE: the normalized L2 error is defined as follows

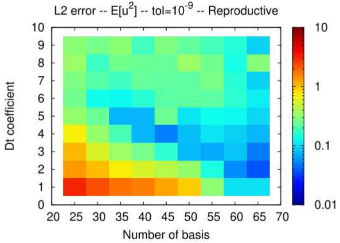
$$\|\mathbf{Q}_{FOM} - \mathbf{Q}_{ROM}\| = \frac{\sqrt{\sum_i \left(Q_{FOM}^{(i)} - Q_{ROM}^{(i)}\right)^2}}{\sqrt{\sum_i^{N_{train}} \left(Q_{FOM}^{(i)}\right)^2}},$$

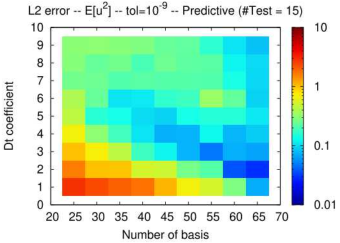
where the vector of realizations for the FOM and ROM are denoted as $\mathbf{Q}_{FOM}$ and $\mathbf{Q}_{ROM}$, respectively.

MF UQ - ROM coupling

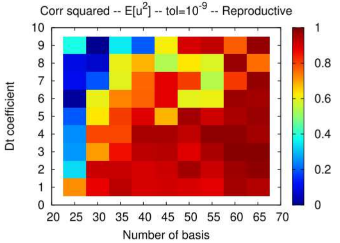
Reproductive Vs Predictive test scenarios ($c \sim \mathcal{U}(0.1, 0.5)$ and $\nu \sim \mathcal{U}(1, 2)$)

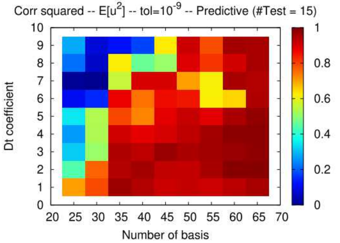
L2 error





Correlation squared

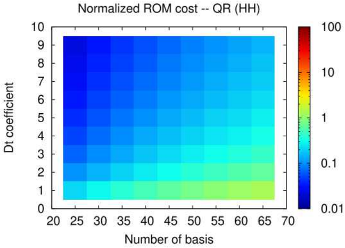


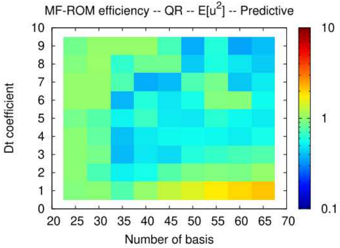


MF UQ - ROM coupling

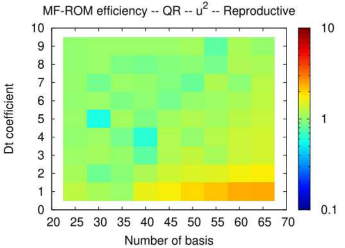
Estimator efficiency ($c \sim \mathcal{U}(0.1, 0.5)$ and $\nu \sim \mathcal{U}(1, 2)$)

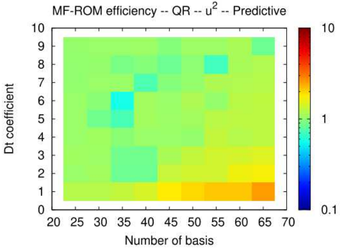
ROM (QR) – Cost and estimator efficiency for $\mathbb{E}\left[u^2\right]$





Reproductive Vs Predictive – A more challenging QoI u^2





Concluding remarks

Conclusions

Preliminary encouraging results, but more work is needed

Findings:

- A formal way of introducing ROMs within MF UQ has been developed
- In principle it is possible to tailor the ROM accuracy in order to maximize the estimator efficiency (compared to a plain MC)

Challenges:

- Kuramoto-Sivashinsky is a chaotic problem which poses great challenges for all ROMs algorithms
- Integral QoIs appear easier to represent. It is difficult to achieve a good overall estimator efficiency for pointwise QoIs.
- The non-linear relationships between the accuracy/cost for ROM as function of the hyper-parameters hampers the ability to obtain a closed form solution for both the optimal ROM and estimator parameters

Future directions (work in progress):

- Explore simpler problems to improve understanding of the interplay between the deterministic accuracy and the one obtained over the stochastic space by ROMs
- Explore the cost of a truly integrated approach based on a numerical optimization of the ROM hyper-parameters

THANKS!

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Supplemental Materials

Multifidelity

Focusing on the single low-fidelity case

- The goal of any multifidelity sampling strategy is to reduce the Monte Carlo variance
- In a control variate approach, this is done by introducing (correlated) low-fidelity models
- Each low-fidelity model introduces an unbiased term to be added to the original (HF only) MC estimator
- We need two different estimates of the low-fidelity mean ($\hat{Q}_1$ and $\hat{\mu}_1$)

$$\hat{Q}_N^{CV} = \hat{Q} + \beta \left(\hat{Q}_1 - \hat{\mu}_1 \right).$$

Multifidelity

Focusing on the single low-fidelity case

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$$\hat{Q}_N^{CV} = \hat{Q} + \beta \left(\hat{Q}_1 - \hat{\mu}_1 \right).$$

In practical situations

- the term $\hat{Q}_1$ is computed with the same set of samples available for the HF model
- the term $\hat{\mu}_1$ is unknown (low fidelity $\neq$ analytic function)
- we use an additional and independent set $\Delta^{\mathrm{LF}} = (\mathbf{r} - 1) N^{\mathrm{HF}}$

Finally the variance is

$$\mathbb{V}ar \left[\hat{Q}_N^{CV} \right] = \mathbb{V}ar \left[\hat{Q} \right] \left(1 - \frac{\mathbf{r} - \mathbf{1}}{\mathbf{r}} \rho_1^2 \right)$$

[1] Pasupathy, R., Taaffe, M., Schmeiser, B. W. & Wang, W., Control-variate estimation using estimated control means. *IIE Transactions*, **44**(5), 381–385, 2012

[2] Ng, L.W.T. & Willcox, K. Multifidelity Approaches for Optimization Under Uncertainty. *Int. J. Numer. Meth. Engng* 100, no. 10, pp. 746772, 2014.

[3] Peherstorfer, B., Willcox, K. & Gunzburger, M., Optimal Model Management for Multifidelity Monte Carlo Estimation. *SIAM J. Sci. Comput.* 38(5), A3163A3194, 2016.

Reduced order Modeling

Generalities

- The HF model is considered the Full Order Model from the ROM perspective
- After the semi-discretization in space a parametrized set of ODEs is obtained

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t; \boldsymbol{\mu}), \qquad \boldsymbol{x}(0; \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu}),$$

  where $\boldsymbol{x}^0(\boldsymbol{\mu})$ denotes the parameterized initial condition.
- A time-discretization method is required for the numerical solution, *e.g.* a linear k-steps method

$$\boldsymbol{r}^n(\boldsymbol{x}^n; \boldsymbol{\mu}) = \boldsymbol{0}, \quad n = 1, \dots, N_t,$$

  where the time-discrete residual $\boldsymbol{r}^n : \mathbb{R}^N \times \mathcal{D} \to \mathbb{R}^N$ is defined as

$$\boldsymbol{r}^n : (\boldsymbol{\xi}; \boldsymbol{\nu}) \mapsto \alpha_0 \boldsymbol{\xi} - \Delta t \beta_0 \boldsymbol{f}(\boldsymbol{\xi}, t^n; \boldsymbol{\nu}) + \sum_{j=1}^{k} \alpha_j \boldsymbol{x}^{n-j} - \Delta t \sum_{j=1}^{k} \beta_j \boldsymbol{f}(\boldsymbol{x}^{n-j}, t^{n-j}; \boldsymbol{\nu}).$$

  Here, $\Delta t \in \mathbb{R}_+$ denotes the time step, $\boldsymbol{x}^k$ denotes the numerical approximation to $\boldsymbol{x}(k\Delta t; \boldsymbol{\mu})$, and the coefficients α_j and $\beta_j, j = 0, \dots, k$ with $\sum_{j=0}^{k} \alpha_j = 0$ define a particular linear multistep scheme.

In this talk we focus on Least-Square Petrov-Galerkin

Reduced order Modeling
Least-squares Petrov-Galerkin (LSPG)

- Projection-based ROM compute an approximation $\tilde{\boldsymbol{x}} \approx \boldsymbol{x}$ that lies in a low-dimensional affine trial subspace $\tilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) \in \boldsymbol{x}^0(\boldsymbol{\mu}) + \text{Ran}(\boldsymbol{\Phi})$, i.e.,

$$\tilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu}) + \boldsymbol{\Phi}\hat{\boldsymbol{x}}(t;\boldsymbol{\mu}),$$

  where $\boldsymbol{\Phi} \in \mathbb{R}^{N\times p}$ is the reduced-basis matrix of dimension $p \leq N$ ($\boldsymbol{\Phi}^T\boldsymbol{\Phi} = \boldsymbol{I}$)
- $\hat{\boldsymbol{x}} : [0,T] \times \mathcal{D} \to \mathbb{R}^p$ denotes the generalized coordinates
- Ran$(\boldsymbol{A})$ denotes the range of a matrix $\boldsymbol{A}$
- LSPG substitute the approximation $\boldsymbol{x} \leftarrow \tilde{\boldsymbol{x}}$ into the FOM ODE, and subsequently minimizes the ODE residual in a weighted ℓ^2-norm, i.e.,

$$\hat{\boldsymbol{x}}^n = \underset{\hat{\boldsymbol{z}}\in\mathbb{R}^p}{\arg\min} \|\boldsymbol{A}\boldsymbol{r}^n(\boldsymbol{x}^0(\boldsymbol{\mu}) + \boldsymbol{\Phi}\hat{\boldsymbol{z}};\boldsymbol{\mu})\|_2.$$

- To ensure an N-independent operation count a sparse weighting matrix should be selected

$$\boldsymbol{A} = (\boldsymbol{P}_r\boldsymbol{\Phi}_r)^+\boldsymbol{P}_r \quad \text{and}$$
$$\boldsymbol{A} = \boldsymbol{P}_r$$

  in the case of gappy POD and collocation, respectively.