Data-driven Discontinuous Galerkin FEM
Via Reduced Order Modeling and Domain Decomposition

FEM@LLNL Seminar

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Science of Scale-Up

- Among thousands of novel technologies, only a few are deployed to industry
- Average time from conception to commercialization: 35 years
- Can we bridge gaps to translate innovation to real-world impact?

Example: carbon-capture technology

Laboratory scale
two-phase direct air capture in triply periodic minimal surface geometry

Industry scale
Conventional carbon-capture — 2500 m²

PETRA NOVA ABSORBER TOWER
Thompsons, TX

R. K. SINGH, Y. FU, C. ZENG, D. T. NGUYEN, P. ROY, J. BAO, Z.XU, G.PANAGAKOS,
Chemical Engineering Journal 450 (2022) 138124.
Traditional pilot stage can be a major bottleneck

- New technology typically requires demonstration via a pilot plant
- Pilot-stage deployment itself can take years to design, construct and operate

*De Gruyter, 2021, Scale-Up Processes: Iterative Methods for the Chemical, Mineral and Biological Industries*
E-pilot to accelerate industry deployment

- Replace the physical pilot with computer simulations
- Feed back the design process beyond mere demonstration
  - Predict scaling behavior, failure modes, and emergent phenomena
  - Facilitate the design optimization
Conventional simulation is too expensive for E-pilot

- Conventional simulation relies on high-fidelity discretization such as FEM, FVM, ...
- Even for lab scales, computationally expensive in both memory and time
- Approximation can be made for small scales (closure modeling, homogenization, ...), but often renders simulations to be inaccurate

FVM on $\sim 10^6$ grid cells
3 days on 144 processes for simulating 30 seconds

Chemical Engineering Journal 450 (2022) 138124.

$10^7 \times$ larger volume
2500 m$^2$
110m
15cm

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Machine learning is promising, but…

- Neural networks are promising alternatives where there is no/little physics known, but lots of data available
- Challenge in scale-up: there is no data available at pilot/industry scale

How do we extrapolate in scale, only from small, lab-scale data?

### Physics-informed Neural Network

![Predicted pressure vs. Exact pressure](image)

Correct PDE

\[
\begin{align*}
\frac{\partial u}{\partial t} + (u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y}) &= -\frac{\partial p}{\partial x} + 0.01(u_{xx} + u_{yy}) \\
\frac{\partial v}{\partial t} + (u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y}) &= -\frac{\partial p}{\partial y} + 0.01(u_{xx} + u_{yy})
\end{align*}
\]

Identified PDE (clean data)

\[
\begin{align*}
\frac{\partial u}{\partial t} + 0.999(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y}) &= -\frac{\partial p}{\partial x} + 0.01047(u_{xx} + u_{yy}) \\
\frac{\partial v}{\partial t} + 0.999(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y}) &= -\frac{\partial p}{\partial y} + 0.01047(u_{xx} + u_{yy})
\end{align*}
\]

Identified PDE (1% noise)

\[
\begin{align*}
\frac{\partial u}{\partial t} + 0.998(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y}) &= -\frac{\partial p}{\partial x} + 0.01057(u_{xx} + u_{yy}) \\
\frac{\partial v}{\partial t} + 0.998(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y}) &= -\frac{\partial p}{\partial y} + 0.01057(u_{xx} + u_{yy})
\end{align*}
\]

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**M. Raissi, P. Perdikaris, G. E. Karniadakis,**

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**Neural Operator**

![Initial Vorticity vs. Prediction](image)

Figure 11: Zero-shot super-resolution

Vorticity field of the solution to the two-dimensional Navier-Stokes equation with viscosity \( \nu = 10^4 \) (Re\( \approx \) 200); Ground truth on top and prediction on bottom. The model is trained on data that is discretized on a uniform 64 \( \times \) 64 spatial grid and on a 20-point uniform temporal grid. The model is evaluated with a different initial condition that is discretized on a uniform 256 \( \times \) 256 spatial grid and a 80-point uniform temporal grid.

**N. Kovachki, Z. Li, B. Liu, K. Azizzadenesheli,**
**K. Bhattacharya, A. Stuart, A. Anandkumar,**
Our approach for extrapolation in scale

We already know the physics (equation) quite well. We just need to..

- **Solve it efficiently based on data**— Reduced Order Model (ROM)

- **Combine to a larger system**— Discontinuous Galerkin Domain Decomposition
Basis in Conventional FEM

Toy example: Poisson equation

\[-\nabla^2 q = f \equiv \sin 2\pi(k \cdot x + \theta)\]

\[q = 0 \quad x \in \partial \Omega\]

\[(\nabla q^\dagger, \nabla q)_\Omega = (q^\dagger, f)_\Omega + (q^\dagger, n \cdot \nabla q)_{\partial \Omega}\]

\[q, q^\dagger \in \mathbb{Q} = \left\{ q \in H^1(\Omega) \left| q|_\kappa \in V_s(\kappa) \quad \forall \kappa \in \mathcal{T}(\Omega) \right. \right\}\]

- Many mesh elements with simple geometry
  - \( \gtrsim 10^6 \) for typical 3D simulations
- Polynomial basis for each mesh element
- A large-size discretized equation

Can we use a basis that represents the solution more efficiently?
Basis identified from data

- Proper Orthogonal Decomposition (POD), Principal Component Analysis (PCA), ...
- Identifies major axes of snapshot scattering
- Reveals the low-dimensional manifold underlying physics

**Effective representation of solution with a low-dimensional basis inferred from data**

\[
\begin{align*}
Q & \approx \Phi \Sigma V^T \\
\end{align*}
\]

Example: from 2D to 1D

Example: flow past a cylinder

\[Q \approx \Phi \Sigma V^T\]

\[E \text{ffective representation of solution with a low-dimensional basis inferred from data}\]

\[k, \text{Taira, M. Hemati, S. Brunton, Y. Sun, K. Duraisamy, S. Bagheri, S. Dawson, C. Yeh, 2020, AIAA Journal, 58, 3, 998-1022}\]
Projection-based Reduced Order Model

- Galerkin projection of the physics equation onto POD basis space
  - In some sense, data-driven spectral method
- Much faster prediction with modest accuracy compared to full order model (FOM)
- Robust against extrapolation outside the training range

Full order model (FOM)

\[-\nabla^2 q = f \equiv \sin 2\pi (k \cdot x + \theta)\]

\[q = 0 \quad \text{for} \quad x \in \partial \Omega\]

\[(\nabla q^\dagger, \nabla q)_{\Omega} = (q^\dagger, f)_{\Omega} + (q^\dagger, n \cdot \nabla q)_{\partial \Omega}\]

\[q^{\dagger\top} L q = q^{\dagger\top} f \quad \forall q^\dagger\]

- Samples from random \(k\)

\[k = (k, k) \quad k \in U[0,1]\]

POD basis

\[\phi_1, \phi_2, \phi_3, \ldots\]

Reduced order model (ROM)

\[q \approx \Phi \hat{q}\]

\[q^{\dagger\top} L q \approx \hat{q}^{\dagger\top} \hat{L} \hat{q}\]

\[\hat{L} = \Phi^{\top} L \Phi\]

\[k = 1.65 \text{ prediction}\]

170 \times \text{speed-up with 2.7\% error}\]

This is good, but how do we predict for a large-scale system?
Using ROM as “element” with domain decomposition

- A large domain where we cannot obtain snapshot data, high-fidelity simulation
- Decompose the domain into smaller, repeatable subdomains
- Solve physics equation in each subdomain using ROM
- Enforce continuity/smoothness of the solution at interfaces

ROM can be used as element with appropriate interface handling

Physics equation at subdomain $m$

\[-\nabla^2 q_m = f_m\]

High-fidelity full-order model

\[L_m q_m = f_m\]

Reduced order model

\[\hat{L}_m \hat{q}_m = \hat{f}_m\]

Interface between subdomains $m$ and $n$

\[\llbracket q \rrbracket_{m,n} \equiv q_m - q_n = 0\]

\[\llbracket n \cdot \nabla q \rrbracket_{m,n} \equiv \frac{1}{2} (n_m \cdot \nabla q_m + n_n \cdot \nabla q_n) = 0\]

Corresponding reduced order model
With static condensation domain decomposition

- Component-wise reduced order model lattice-type structure design
  

  - Static-condensation reduced basis element method
    

- Split the solution into particular (interior) / homogeneous (interface) basis
- Limited to linear systems

**Physics equation**

\[ a(u, v) = f(v) \quad \forall v \in X_h(\Omega) \]

**Domain decomposition**

\[ u = \sum_m \left[ u_{m,p} + u_{m,h} \right] \quad u_{m,p}, u_{m,h} \in X_h(\Omega_m) \]

**Particular (interior) solution**

\[ a(u_{m,p}, v_m) = f(v_m) \quad \forall v_m \in X_0^h(\Omega_m) \]

\[ u_{m,p} = 0 \quad \text{on} \ x \in \partial \Omega_m \]

**Homogeneous (interface) solution**

\[ a(u_{m,h}, v_m) = 0 \quad \forall v_m \in X_0^h(\Omega_m) \]

\[ u_{m,h} = u_{n,h} \quad \text{on} \ x \in \partial \Omega_m \cap \partial \Omega_n \]
With least-square Petrov-Galerkin

- Domain decomposition least-square Petrov-Galerkin ROM
- Interface dofs are duplicated
- A least-square solution with interface constraint is sought
  - Sequential Quadratic Programming (SQP) method
    for associated Karush-Kuhn-Tucker system

Physics (discretized) equation
\[ r(x) = 0 \quad x \in \mathbb{R}^N \]

DD-LSPG solution
\[
\min_{(x_m^\Omega, x_m^\Gamma)} \frac{1}{2} \sum_m \left\| r_m(x_m^\Omega, x_m^\Gamma) \right\|^2
\]
such that
\[ P_m x_m^\Gamma - P_n x_n^\Gamma = 0 \quad \forall m, n \]

Two-domain schematic

A. N. Diaz, Y. Choi, M. Heinkenschloss
arXiv:2305.15163 (2023)
With least-square Petrov-Galerkin

- Domain decomposition least-square Petrov-Galerkin ROM
  
  

- Discretization-agnostic: FEM, FDM, ...

- Applicable for general nonlinear physics

- Difficulty in enforcing continuity
  
  - Strong enforcement can lead to a trivial interface solution
  
  - Stochastic weak enforcement does not respect the physics

\[
\begin{align*}
\min_{(x^\Omega_m, x^\Omega_m)} & \frac{1}{2} \sum_m \left\| r_m(x^\Omega_m, x^\Gamma_m) \right\|^2 \\
\text{such that} & \\
C_{m,n} (P_m x^\Gamma_m - P_n x^\Gamma_n) & = 0 \quad \forall m, n \\
C_{m,n} & \sim N[0,1^2]^{N_{mn}}
\end{align*}
\]

Burger’s equation

A. N. Diaz, Y. Choi, M. Heinkenschloss

arXiv:2305.15163 (2023)
Challenges in handling ROM interfaces

- POD (or other data-driven) basis does not guarantee the continuity/smoothness of the solution over interfaces
- Existing ROM+DD methods employ separate interface basis
  - Limited to linear system
  - Arbitrary weak enforcement of continuity

S. Mcbane, Y. Choi

A. N. Diaz, Y. Choi, M. Heinkenschloss
arXiv:2305.15163 (2023)
Discontinuous Galerkin domain decomposition

- DG basis does not have to match at element interface
- Discontinuity is allowed at interface, yet controlled under a desired numerical error
- Well-established: developed for various nonlinear physics
  - Poisson equation: P. Hansbo, GAMM-Mitteilungen 28.2 (2005)
  - ...
- Not limited to each finite element—same discretization can be used for general domain decomposition

DG domain decomposition provides simplicity/flexibility for data-driven FEM, without separate interface basis/handling

$$\mathbf{q}_m$$

$$\mathbf{q}_n$$

Physics equation

$$a(\mathbf{q}, \mathbf{q}^\dagger) = f(\mathbf{q}^\dagger) \quad \forall \mathbf{q}^\dagger \in X^h(\Omega)$$

DG domain decomposition

$$a(\mathbf{q}_m, \mathbf{q}_m^\dagger) + \sum_{\partial \Omega_m \cup \partial \Omega_n \neq \emptyset} \tilde{a}(\mathbf{q}_m, \mathbf{q}_n, \mathbf{q}_m^\dagger, \mathbf{q}_n^\dagger) = f(v_m) \quad \forall \mathbf{q}_m^\dagger, \mathbf{q}_n^\dagger \in X^h(\Omega)$$
Example: Poisson equation

\[-\nabla^2 q = f\]

- Interior Penalty Method
  
  *P. Hansbo*, GAMM-Mitteilungen 28.2 (2005)

\[\sum_{m} \left( \nabla q_{m}^\bot, \nabla q_{m} \right)_{\Omega_{m}} + \sum_{\Gamma_{m,n} \neq \emptyset} \left[ -\left( \left\{ n \cdot \nabla q_{m}^\bot \right\}, \left\{ q_{m} \right\} \right)_{\Gamma_{m,n}} - \left( \left\{ q_{m}^\bot \right\}, \left\{ n \cdot \nabla q \right\} \right)_{\Gamma_{m,n}} + \left( \gamma \Delta x^{-1} \left\{ q_{m}^\bot \right\}, \left\{ q_{m} \right\} \right)_{\Gamma_{m,n}} \right] = \sum_{m} \left( \nabla q_{m}^\bot, f \right)_{\Omega_{m}}\]

\[\sum_{m} q_{m}^\top L_{m} q_{m} + \sum_{\Gamma_{m,n} \neq \emptyset} \left( q_{m}^\top, q_{n}^\top \right) \left( \begin{array}{cc} L_{mm} & L_{mn} \\ L_{nm} & L_{nn} \end{array} \right) \left( \begin{array}{c} q_{m} \\ q_{n} \end{array} \right) = \sum_{m} q_{m}^\top f_{m} \quad \forall q_{m}^\bot \in \mathbb{R}^{N_{m}}\]

DG operators $L_{m}$, $L_{mm}$ can be seamlessly projected onto POD basis
Poisson equation—basis construction

- One unit component, 4225-dof FEM solution
- Sampling for POD basis construction \((M = 1)\)
  \[
  f = \sin 2\pi (k \cdot x + \theta) \quad k, k_b \sim U[-0.5, 0.5]^2
  \]
  \[
  q = \sin 2\pi (k_b \cdot x + \theta_b) \quad x \in \partial \Omega \quad \theta, \theta_b \sim U[0, 1]
  \]
- 4225 random samples on parameters
- Only 15 basis vectors can represent 99.77% of all samples

![POD mode Φ](image)

![Singular value spectrum](image)
ROM as a data-driven DG element

\[
\sum_{m} q_{m}^{\dagger} L_{m} q_{m} + \sum_{\Gamma_{m,n}=\emptyset} (q_{m}^{\dagger} L_{mn} q_{n}) = \sum_{m} q_{m}^{\dagger} f_{m} \quad \forall q_{m}^{\dagger} \in \mathbb{R}^{N_{m}}
\]

- Galerkin projection on POD basis space
  \[
  q_{m} \approx \Phi_{m} \hat{q}_{m} \quad q_{m}^{\dagger} \approx \Phi_{m} \hat{q}_{m}^{\dagger}
  \]

\[
\sum_{m} \hat{q}_{m}^{\dagger} L_{m} \hat{q}_{m} + \sum_{\Gamma_{m,n}=\emptyset} (\hat{q}_{m}^{\dagger} L_{mn} \hat{q}_{n}) = \sum_{m} \hat{q}_{m}^{\dagger} \Phi_{m}^{\dagger} f_{m} \quad \forall \hat{q}_{m}^{\dagger} \in \mathbb{R}^{\hat{N}_{m}}
\]

- Dimension reduction from \( N_{m} = 4225 \) to \( \hat{N}_{m} = 15 \)

\[
\hat{L}_{m} = \Phi_{m}^{\dagger} L_{m} \Phi_{m} \quad \hat{L}_{mn} = \Phi_{m}^{\dagger} L_{mn} \Phi_{n}
\]

- No particular basis/handling for interface

Simple extrapolation in scale only with component-scale data

Unit component ROM

32 \times 32\text{-component system}
Fast & Robust extrapolation in scale

- Over all scales, achieves $\sim 40 \times$ speed-up with $\sim 1\%$ relative error
- Can make a prediction for $\sim 10^4 \times$ larger system
  - FOM cannot be assemble over $\gtrsim 10^3 \times$ larger system at given memory limit
- Robust prediction against a qualitatively different problem out of training data

<table>
<thead>
<tr>
<th>Number of components</th>
<th>Solution time (s)</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>ROM: 1</td>
<td>FOM: 40</td>
</tr>
<tr>
<td>1000</td>
<td>ROM: 0.1</td>
<td>FOM: 400</td>
</tr>
<tr>
<td>10000</td>
<td>ROM: 0.01</td>
<td>FOM: 4000</td>
</tr>
<tr>
<td>100000</td>
<td>ROM: 0.001</td>
<td>FOM: 40000</td>
</tr>
<tr>
<td>1000000</td>
<td>ROM: 0.0001</td>
<td>FOM: 400000</td>
</tr>
</tbody>
</table>

Stokes flow DG formulation

\[-\nabla^2 \mathbf{u} + \nabla p = 0\]
\[\nabla \cdot \mathbf{u} = 0\]

\[\mathbf{q} = (\mathbf{u}, p) \quad \mathbf{q}^\dagger = (\mathbf{u}^\dagger, p^\dagger)\]


\[
\sum_m \left[ \langle \nabla \mathbf{u}^\dagger_m, \nabla \mathbf{u}_m \rangle_{\Omega_m} - \langle \nabla \cdot \mathbf{u}^\dagger_m, p_m \rangle_{\Omega_m} - \langle p^\dagger_m, \nabla \cdot \mathbf{u}_m \rangle_{\Omega_m} \right] \\
+ \sum_{\Gamma_{m,n} \neq \emptyset} \left[ -\langle \| \nabla \mathbf{u}^\dagger_m \|, \| \mathbf{u}_m \| \rangle_{\Gamma_{m,n}} - \langle \| \mathbf{u}^\dagger_m \|, \langle \nabla \cdot \mathbf{u}_m \rangle \rangle_{\Gamma_{m,n}} + \langle \gamma \Delta x^{-1} \| \mathbf{u}^\dagger_m \|, \| \mathbf{u}_m \| \rangle_{\Gamma_{m,n}} + \langle \| \mathbf{u}^\dagger_m \|, \langle p_m \rangle \rangle_{\Gamma_{m,n}} + \langle \langle p^\dagger_m \rangle, \langle p_m \mathbf{n} \cdot \mathbf{u}_m \rangle \rangle_{\Gamma_{m,n}} \right] = 0
\]

- Each DG operator has a saddle-point block matrix system

\[
\sum_m \mathbf{q}_m^\dagger \mathbf{L}_m \mathbf{q}_m + \sum_{\Gamma_{m,n} \neq \emptyset} \mathbf{q}_m^\dagger \mathbf{q}_n^\dagger \mathbf{L}_m \mathbf{L}_n^{-1} \mathbf{L}_n \mathbf{q}_n = \sum_m \mathbf{q}_m^\dagger \mathbf{f}_m \quad \forall \mathbf{q}_m \in \mathbb{R}^{N_m}
\]

\[
\mathbf{L}_m = \begin{pmatrix} \mathbf{K}_m & \mathbf{B}_m^\top \\ \mathbf{B}_m & \mathbf{0} \end{pmatrix} \\
\mathbf{L}_{m,n} = \begin{pmatrix} \mathbf{K}_{m,n} & \mathbf{B}_{m,n}^\top \\ \mathbf{B}_{m,n} & \mathbf{0} \end{pmatrix}
\]
Stokes flow with multiple ROM elements

- Flow problems for arrays of 5 unit objects

- 1400 samples on random $2 \times 2$ arrays with random in-flow conditions

$$
\mathbf{u} = \left( \begin{array}{c}
\mathbf{u}_0 + \Delta \mathbf{u} \sin 2\pi (\mathbf{k}_u \cdot \mathbf{x} + \theta_u) \\
\mathbf{v}_0 + \Delta \mathbf{v} \sin 2\pi (\mathbf{k}_v \cdot \mathbf{x} + \theta_v)
\end{array} \right) \quad \text{on} \quad \mathbf{x} \in \partial \Omega_{in}
$$

$$
\begin{align*}
\mathbf{u}_0, \mathbf{v}_0 & \sim U[-1,1] \\
\mathbf{k}_u, \mathbf{k}_v & \sim U[-0.5,0.5]^2 \\
\Delta \mathbf{u}, \Delta \mathbf{v} & \sim U[-0.1,0.1] \\
\theta_u, \theta_v & \sim U[0,1]
\end{align*}
$$

Sample 1 $|\mathbf{u}|$ 

Sample 2 $|\mathbf{u}|$

$\partial \Omega_{in}$ 

$\partial \Omega_{in}$

POD basis

$\Phi_1$ 

$\Phi_2$ 

$\Phi_3$
Unified POD basis

• POD is performed over the entire solution vector space

\[ Q \approx \Phi \Sigma V^T \]

\[ Q = \begin{pmatrix} u_1 & u_2 & \cdots \\ p_1 & p_2 & \cdots \end{pmatrix} \]

\[ \Phi = \begin{pmatrix} \Phi_u \\ \Phi_p \end{pmatrix} = \begin{pmatrix} \phi_{u1} & \phi_{u2} & \cdots \\ \phi_{p1} & \phi_{p2} & \cdots \end{pmatrix} \]

• POD basis is given as \((u, p)\) pairs
• \(u\) and \(p\) are constrained by linear correlation inferred from data
• FOM saddle-point operator becomes monolithic

FOM operator

\[ L = \begin{pmatrix} K & B^T \\ B & 0 \end{pmatrix} \]

ROM projection

\[ \hat{L} = \Phi^T L \Phi = \Phi_u^T K \Phi_u + \Phi_u^T B^T \Phi_p + \Phi_p^T B \Phi_u \]
Able to predict an emergent phenomenon

- Over all scales, achieves $\sim 15 \times$ speed-up with $\sim 1\%$ relative error
- Flow tends to accumulate over ‘empty’ components
  - $\sim 10 \times$ higher flow speed than training data
- Robust prediction with $\lesssim 3\%$ error for emergent phenomena

![Graphs and images showing computation time and accuracy for ROM and FOM, as well as a visual representation of a 32x32 array with a color scale for the vector field $\mathbf{u}$.]
Rapid convergence with basis dimension

- ROM is effective when physics underlies on a lower-dimensional subspace
- Rapid convergence can be achieved as the basis vectors span the underlying subspace

Poisson

Singular value spectrum

Stokes

Singular value spectrum
Steady Navier-Stokes— handling nonlinear advection

\[ \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p = 0 \quad \mathbf{q} = (\mathbf{u}, p) \quad \mathbf{q}^\dagger = (\mathbf{u}^\dagger, p^\dagger) \]

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \sum_m \left[ \langle \mathbf{u}_m^\dagger, \mathbf{u}_m \cdot \nabla \mathbf{u}_m \rangle_{\Omega_m} + \langle \nu \nabla \mathbf{u}_m^\dagger, \nabla \mathbf{u}_m \rangle_{\Omega_m} - \langle \nabla \cdot \mathbf{u}_m^\dagger, p_m \rangle_{\Omega_m} - \langle p_m^\dagger, \nabla \cdot \mathbf{u}_m \rangle_{\Omega_m} \right] \]

+ \sum_{m,n \neq \emptyset} \left[ -\langle \nu \{ \{ \mathbf{n} \cdot \nabla \mathbf{u}_m^\dagger \}, \{ \mathbf{n} \mathbf{u}_m \} \} \rangle_{\Gamma_{m,n}} - \langle \nu \{ \{ \mathbf{u}_m^\dagger \}, \{ \mathbf{n} \cdot \nabla \mathbf{u}_m \} \} \rangle_{\Gamma_{m,n}} + \langle \Gamma_{m,n} \{ \{ \mathbf{n} \cdot \mathbf{u}_m^\dagger \}, \{ \mathbf{u}_m \} \} \rangle_{\Gamma_{m,n}} + \langle \{ \{ p_m^\dagger \}, \{ \mathbf{n} \cdot \mathbf{u}_m \} \} \rangle_{\Gamma_{m,n}} \right] = 0

- Naively, nonlinear weak-form is integrated over every element, every quadrature point
  - No benefit of dimension reduction
- Projection of a quadratic term is precomputed as a 3rd-order tensor operator
- While its complexity scales fast, a reasonable speed-up can be achieved with moderate basis dimension

FOM operator

\[ \mathbf{N}[\mathbf{q}] = \begin{pmatrix} \mathbf{K} + \mathbf{C}(\mathbf{u}) & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix} \]

ROM Tensor projection

\[ \mathbf{u}_m = \sum_i \phi_{u,i} \hat{u}_i \quad \mathbf{u}_m^\dagger = \sum_i \phi_{u,i} \hat{u}_i^\dagger \]

\[ \langle \mathbf{u}^\dagger, \mathbf{u} \cdot \nabla \mathbf{u} \rangle_{\Omega} = \sum_{i,j,k} \hat{u}_i^\dagger \left[ \phi_{u,i}^\dagger, \phi_{u,j} \cdot \nabla \phi_{u,k} \right]_{\Omega} \hat{u}_j \hat{u}_k = \sum_{i,j,k} \hat{u}_i^\dagger T_{ijk} \hat{u}_j \hat{u}_k \]

ROM projection

\[ \hat{\mathbf{N}} = \Phi_u^T \mathbf{K} \Phi_u + \mathbf{T}(\hat{\mathbf{u}}) + \Phi_u^T \mathbf{B}^T \Phi_p + \Phi_p^T \mathbf{B} \Phi_u \]
The choice of ROM basis must respect physics

- ROM with unified basis fails to converge in Newton iterations
- In unified basis vectors, \( \mathbf{u} \) and \( p \) are constrained by linear correlations from training data
  - Sufficient for linear Stokes flow system
- Linear correlations break down with nonlinear convection
- Separate basis for \( \mathbf{u} \) and \( p \) is necessary—leads to a similar saddle-point ROM operator

\[
\Phi = \begin{pmatrix} \Phi_u \\ \Phi_p \end{pmatrix} = \begin{pmatrix} \phi_{u1} & \phi_{u2} & \cdots \\ \phi_{p1} & \phi_{p2} & \cdots \end{pmatrix}
\]

Unified basis schematic

\[
\Phi = \begin{pmatrix} \Phi_u & 0 \\ 0 & \Phi_p \end{pmatrix}
\]

Separate basis schematic

\[
\hat{N}[q] = \begin{pmatrix} \Phi_u^T K \Phi_u + T(\mathbf{u}) & \Phi_u^T B^T \Phi_p \\ \Phi_p^T B \Phi_u & 0 \end{pmatrix}
\]

New ROM projection

Newton iterations for \( 8 \times 8 \) array at \( \text{Re} = 1 \)

\[
\begin{align*}
||r|| &= 54.6169 \\
||r|| &= 0.0938665, \quad ||r||/||r\ 0|| = 0.00171863 \\
||r|| &= 0.166563, \quad ||r||/||r\ 0|| = 0.00304966 \\
||r|| &= 16.5694, \quad ||r||/||r\ 0|| = 0.383374 \\
||r|| &= 3204.19, \quad ||r||/||r\ 0|| = 58.6667 \\
||r|| &= 106117, \quad ||r||/||r\ 0|| = 1942.93 \\
||r|| &= 1.74169e+08, \quad ||r||/||r\ 0|| = 3.18891e+06 \\
||r|| &= 1.87222e+12, \quad ||r||/||r\ 0|| = 3.42791e+10 \\
||r|| &= 1.46324e+14, \quad ||r||/||r\ 0|| = 2.6791e+12
\end{align*}
\]
ROM also must satisfy necessary physics conditions

- Naive separation of velocity/pressure leads to spurious pressure modes
- Solution space for saddle-point systems must satisfy the **inf-sup condition**
  
  
- Just as for standard FEM, ROM basis is also subject to the same inf-sup condition
- ROM basis, inferred from incompressible flow data, is also divergence-free
- Without compressible \( u \) components, \( p \) is underdetermined

Incompressible, divergence-free condition

\[ \nabla \cdot \mathbf{u} = 0 \]

Divergence-free ROM basis

\[ \nabla \cdot \phi_{u,i} \approx 0 \quad \forall i \]

Or, \( B\Phi_u \approx 0 \)

ROM projection

\[
\hat{\mathbf{N}}[\mathbf{q}] = \begin{pmatrix}
\Phi_u^T \mathbf{K} \Phi_u + \mathbf{T}(\mathbf{u}) & \Phi_u^T B^T \Phi_p \\
\Phi_p^T B \Phi_u & 0
\end{pmatrix}
\]
Augment velocity basis to stabilize pressure

- Supremizer enrichment for stabilizing pressure
  

- Demonstrated the speed-up/accuracy at Re=10

- Ongoing demonstration for higher Reynolds numbers

\[
\phi_{s,i} = \nabla \phi_{p,i}
\]

Or
\[
\Phi_s = B \Phi_p
\]

Orthonormalization
\[
\Phi_s = GS[\Phi_s]
\]

Augment velocity basis
\[
\tilde{\Phi}_u = (\Phi_u \ Ph_s)
\]
Toward general nonlinear physics

- **Standard FEM**
  - Analytical, polynomial basis
  - Weak-form evaluation at prescribed quadrature points/weights
- **Data-driven FEM**
  - Data-inferred POD basis
  - Data-inferred, **empirical** quadrature points (EQP)

**EQP non-negative least-square problem**

Find minimum $N_k > 0$ and $\{w_k\}, \{x_k\}$ such that

$$\max_{s, i} \left| \left\langle \phi_i, N[q_s] \right\rangle_{\Omega} - \sum_{k}^{N_k} w_k \phi_i(x_k) N[q_s(x_k)] \right| < \epsilon$$

**Performance comparison**

<table>
<thead>
<tr>
<th></th>
<th>Tensor</th>
<th>EQP</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Vel error</strong></td>
<td>0.17%</td>
<td>0.36%</td>
</tr>
<tr>
<td><strong>Pres error</strong></td>
<td>0.35%</td>
<td>0.32%</td>
</tr>
<tr>
<td><strong>Speed-up</strong></td>
<td>10.47x</td>
<td>10.25x</td>
</tr>
</tbody>
</table>
Moving forward—

- **scaleupROM**: [https://github.com/LLNL/scaleupROM.git](https://github.com/LLNL/scaleupROM.git)
- Active development toward more complex physics
  - Unsteady N-S flow, nonlinear elasticity, ...
- Preconditioning for ROM-FEM

Preconditioner for iterative ROM-FEM solver

Data center heat exchanger

Direct air capture column
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Thank you for your attention. Any questions?