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

FEM@LLNL Seminar

Kevin Chung

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Lawrence Livermore National Laboratory

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

R. K. SINGH, Y. FU, C. ZENG, D. T. NGUYEN, P. ROY, J. BAO, Z.XU, G.PANAGAKOS,
Chemical Engineering Journal 450 (2022) 138124.

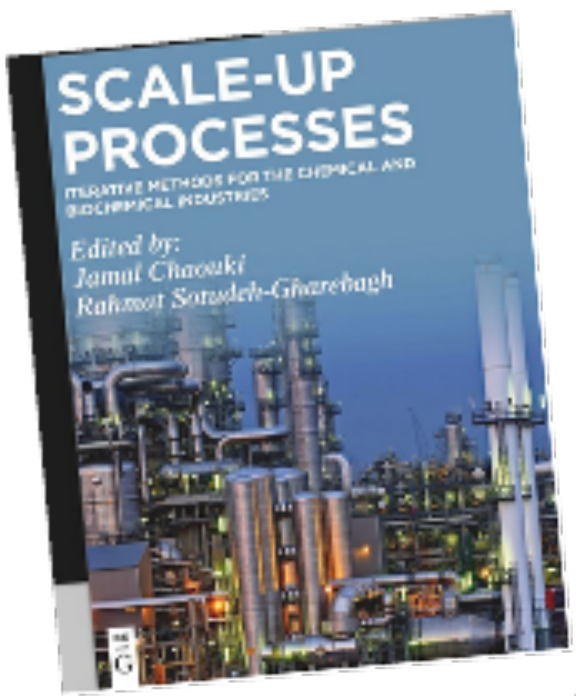
$\sim$35 years →

Industry scale
Conventional carbon-capture —

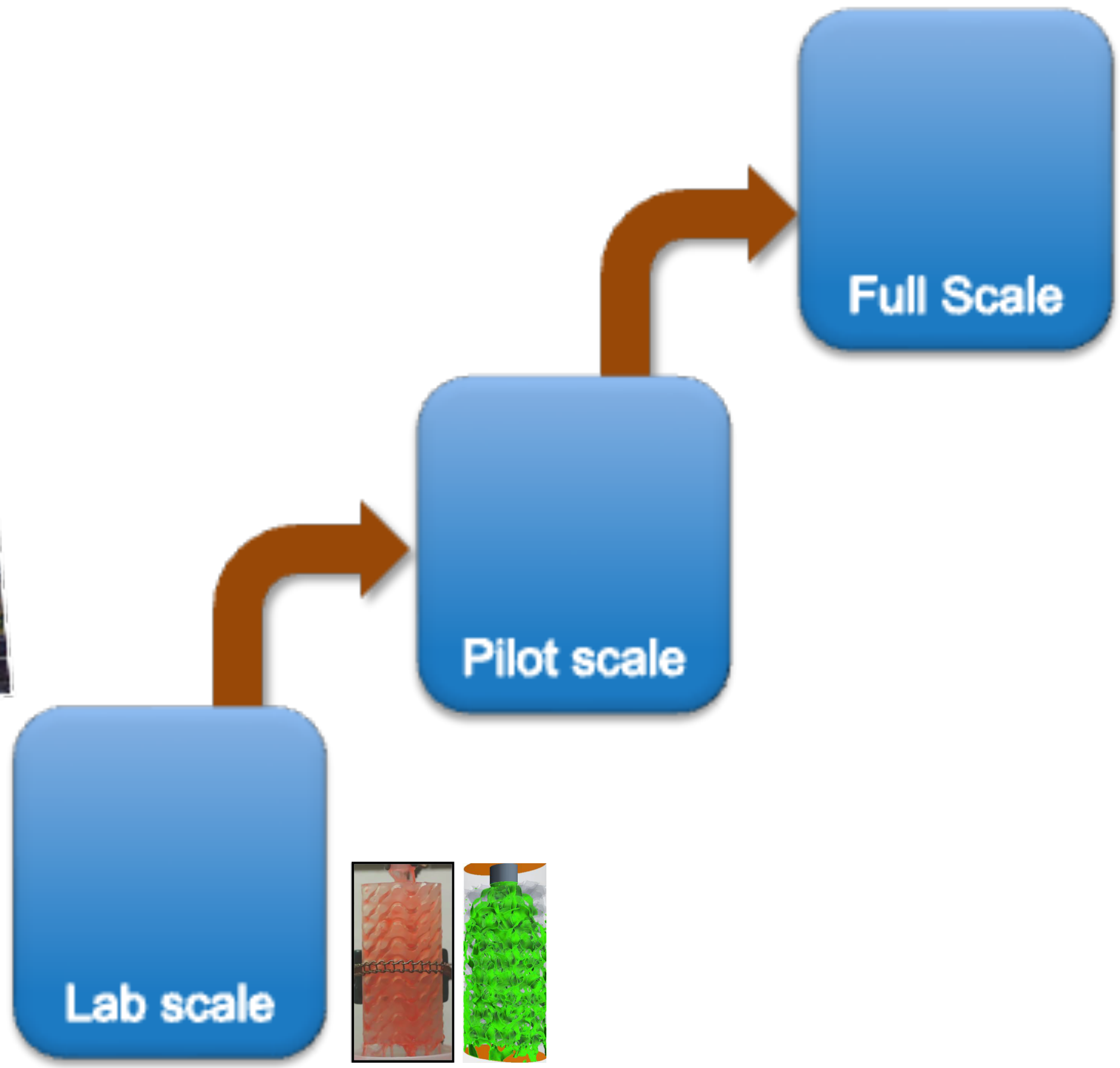
PETRA NOVA ABSORBER TOWER
Thompsons, TX

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

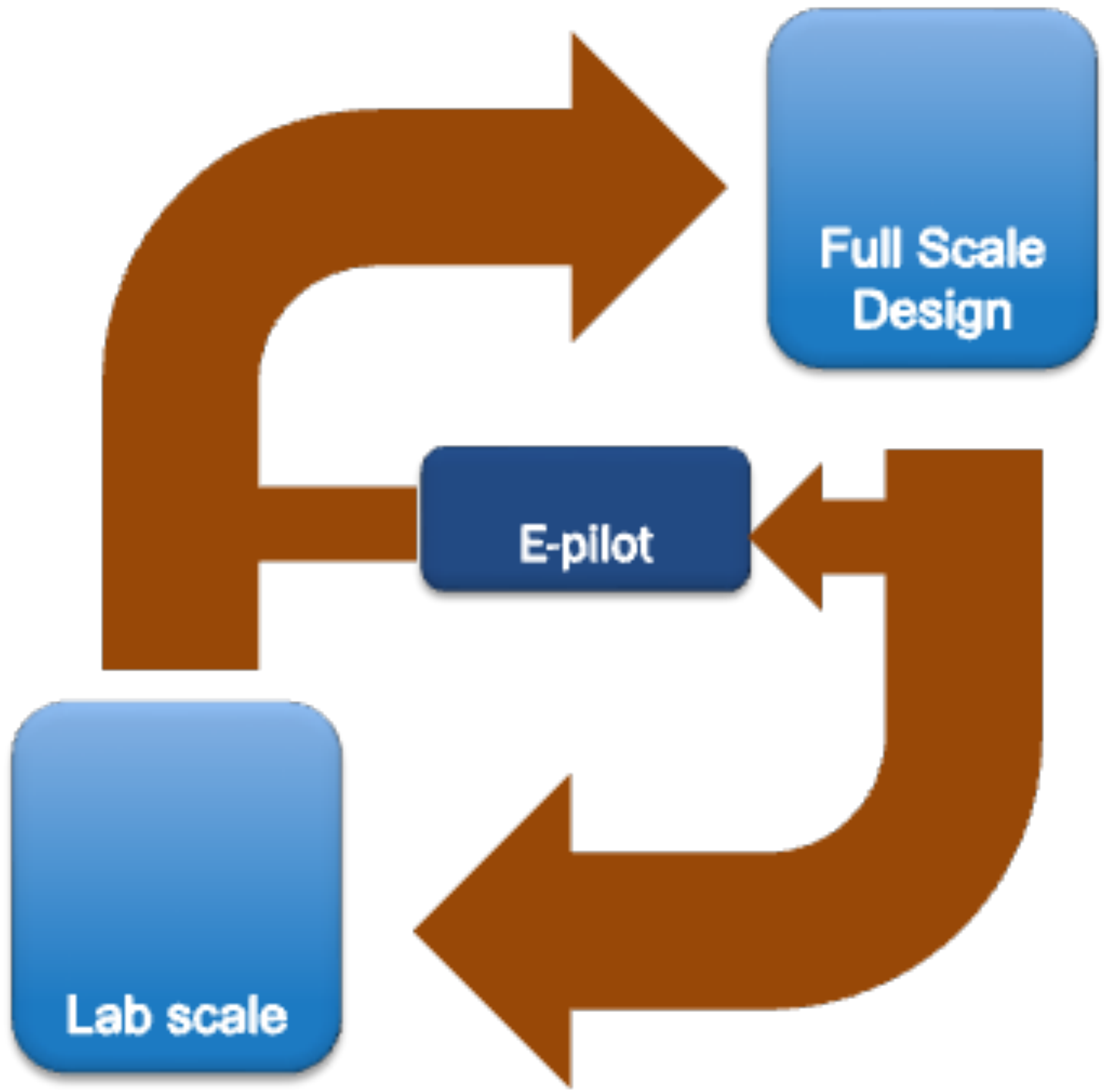


De Gruyter, 2021, Scale-Up Processes: Iterative Methods for the Chemical, Mineral and Biological Industries



E-pilot to accelerate industry deployment

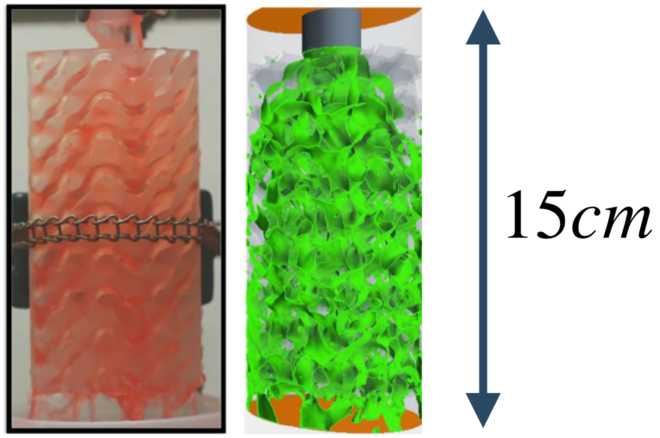
- Replace the physical pilot with computer simulations
- Feed back the design process beyond mere demonstration
  - Predict scaling behavior, failure modes, and emergent phenomena
  - Facilitate the design optimization



Conventional simulation is too expensive for E-pilot

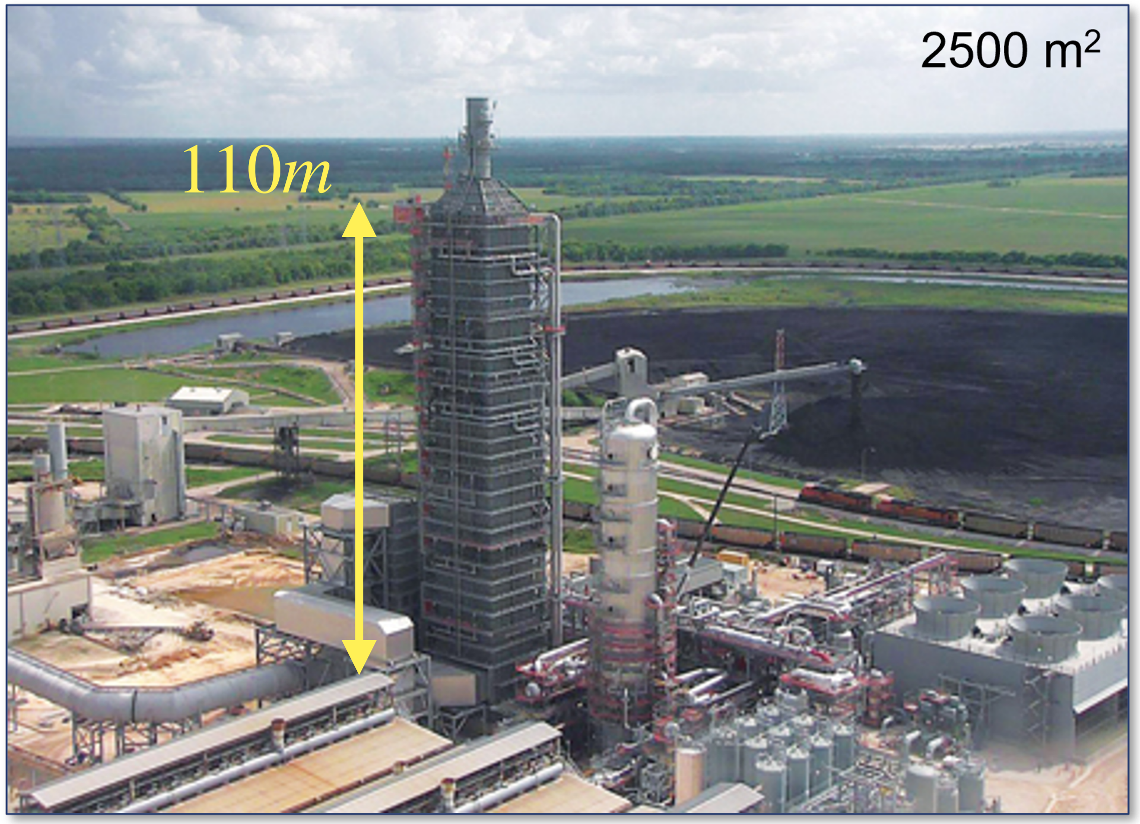
- Conventional simulation relies on high-fidelity discretization such as FEM, FVM, ...
- Even for lab scales, computationally expensive in both memory and time
- Approximation can be made for small scales (closure modeling, homogenization, ...), but often renders simulations to be inaccurate

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



R. K. SINGH, Y. FU, C. ZENG, D. T. NGUYEN, P. ROY, J. BAO, Z.XU, G.PANAGAKOS,
Chemical Engineering Journal 450 (2022) 138124.

$10^7 \times$ larger volume



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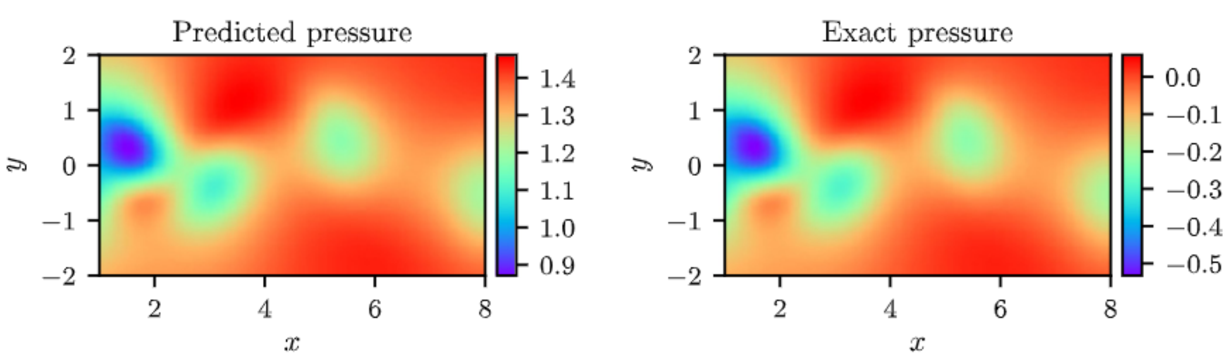
Machine learning is promising, but...

- 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



Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999(uu_x + vu_y) = -p_x + 0.01047(u_{xx} + u_{yy})$ $v_t + 0.999(uv_x + vv_y) = -p_y + 0.01047(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998(uu_x + vu_y) = -p_x + 0.01057(u_{xx} + u_{yy})$ $v_t + 0.998(uv_x + vv_y) = -p_y + 0.01057(v_{xx} + v_{yy})$

M. Raissi, P. Perdikaris, G. E. Karniadakis,
2019, Journal of Computational physics, 378, 686-707

Neural Operator

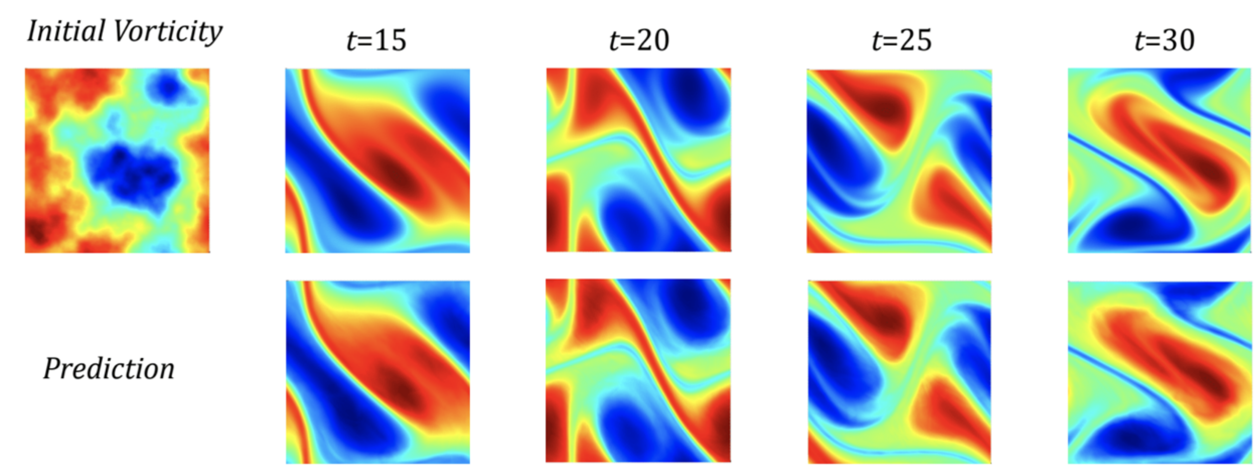


Figure 11: Zero-shot super-resolution
Vorticity field of the solution to the two-dimensional Navier-Stokes equation with viscosity $\nu = 10^4$ (Re$\approx$ 200); Ground truth on top and prediction on bottom. The model is trained on data that is discretized on a uniform 64×64 spatial grid and on a 20-point uniform temporal grid. The model is evaluated with a different initial condition that is discretized on a uniform 256×256 spatial grid and a 80-point uniform temporal grid.

N. Kovachki, Z. Li, B. Liu, K. Azizzadenesheli, K. Bhattacharya, A. Stuart, A. Anandkumar,
2023, Journal of Machine Learning Research, 24(89), 1-97.

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

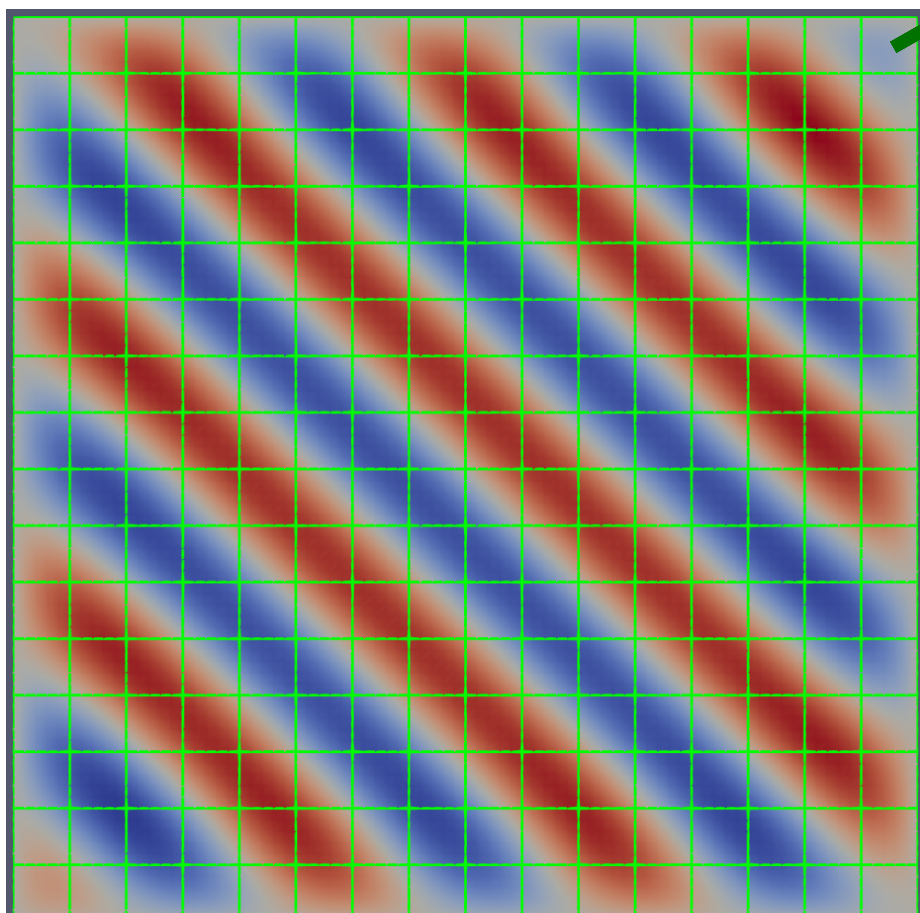
Toy example: Poisson equation

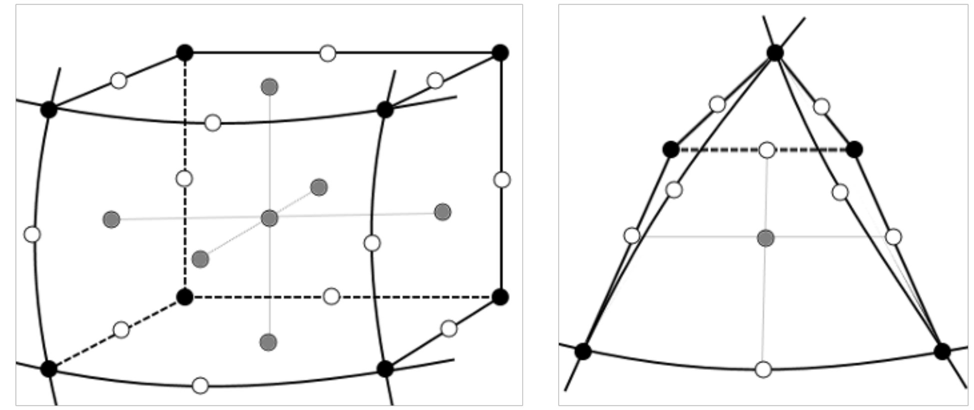
$$-\nabla^2 q = f \equiv \sin 2\pi(\mathbf{k}\cdot\mathbf{x}+\theta)$$

$$q = 0 \qquad \mathbf{x}\in\partial\Omega$$

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

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





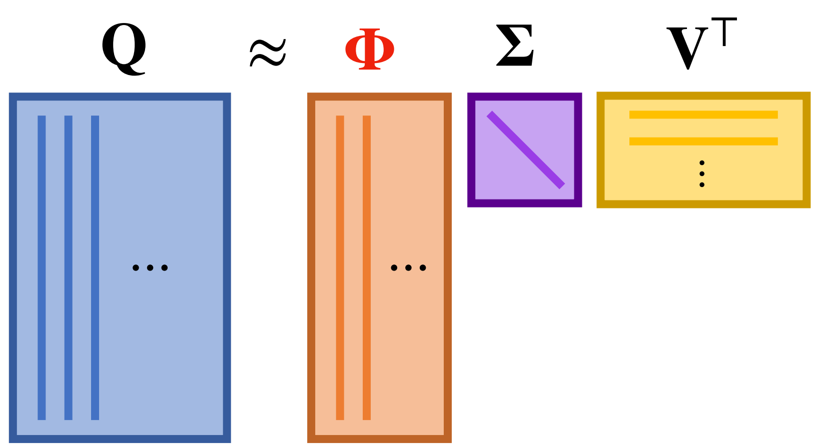
- Many mesh elements with simple geometry
  - $\gtrsim 10^6$ for typical 3D simulations
- Polynomial basis for each mesh element
- A large-size discretized equation

Can we use a basis that represents the solution more efficiently?

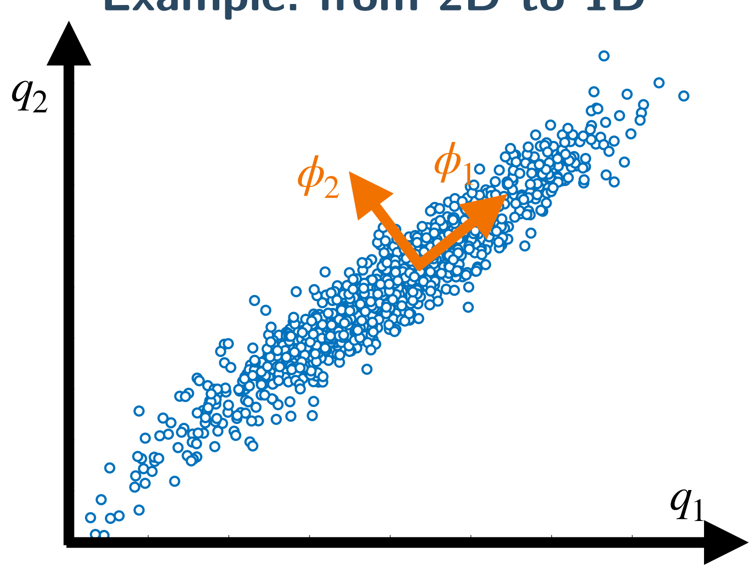
Basis identified from data

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

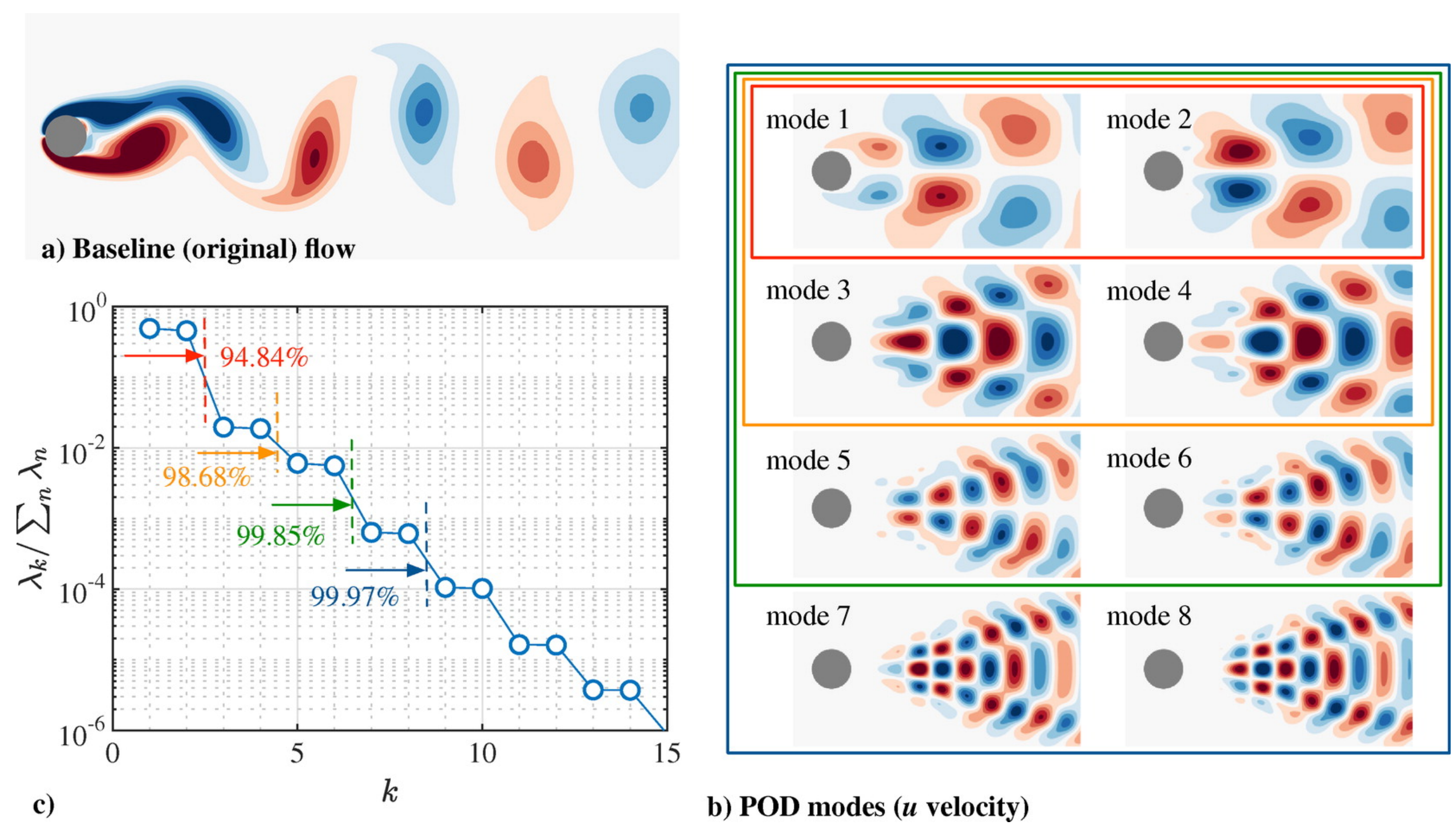
Effective representation of solution with a low-dimensional basis inferred from data



Example: from 2D to 1D



Example: flow past a cylinder



K. 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)

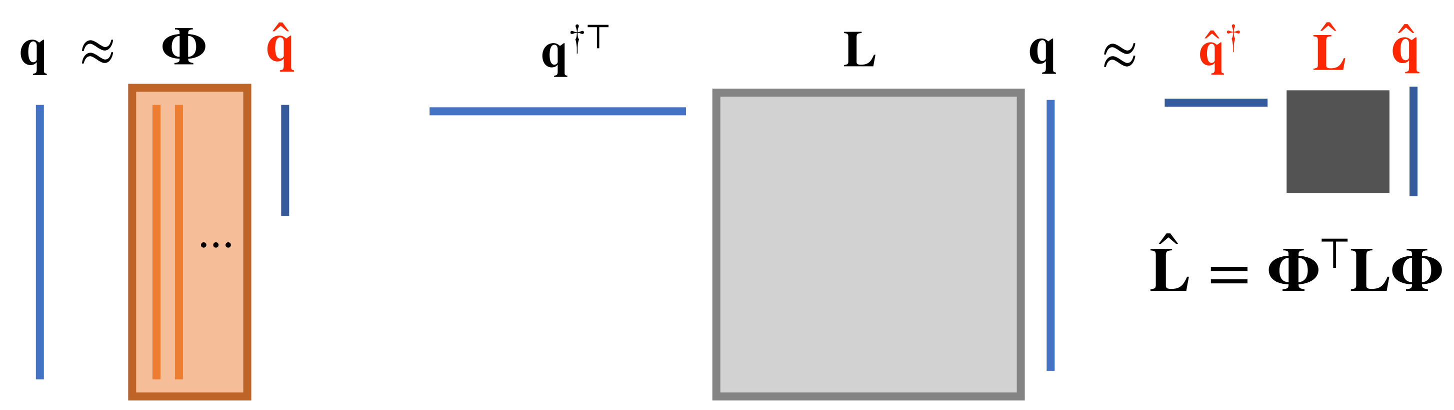
$$-\nabla^2 q = f \equiv \sin 2\pi(\mathbf{k}\cdot\mathbf{x}+\theta)$$

$$q = 0 \qquad \mathbf{x}\in\partial\Omega$$

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

$$\mathbf{q}^{\dagger\top}\mathbf{L}\mathbf{q} = \mathbf{q}^{\dagger\top}\mathbf{f} \qquad \forall \mathbf{q}^\dagger$$

Reduced order model (ROM)

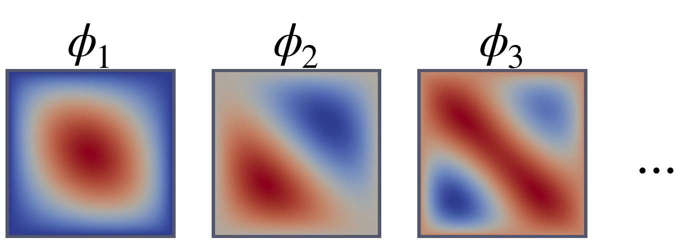


$$\hat{\mathbf{L}} = \mathbf{\Phi}^\top\mathbf{L}\mathbf{\Phi}$$

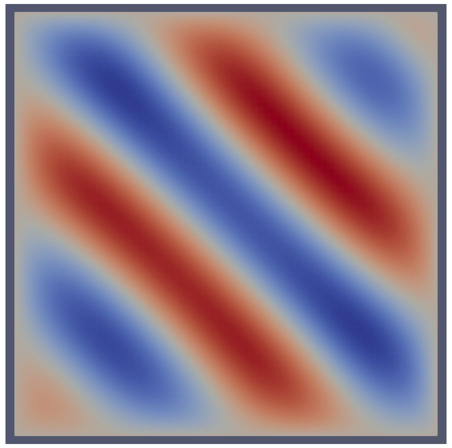
- Samples from random $\mathbf{k}$

  $\mathbf{k} = (k,k) \qquad k \in U[0,1]$

POD basis



$k = 1.65$ **prediction**



$170\times$ **speed-up with** $2.7\,\%$ **error**

```
spatial basis dimension is 4225 x 10
Project RHS on reduced basis.
Solve ROM.
ROM-solve time: 0.000235 seconds.
FOM-solve time: 0.040251 seconds.
Relative error: 2.68896E-02
```

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

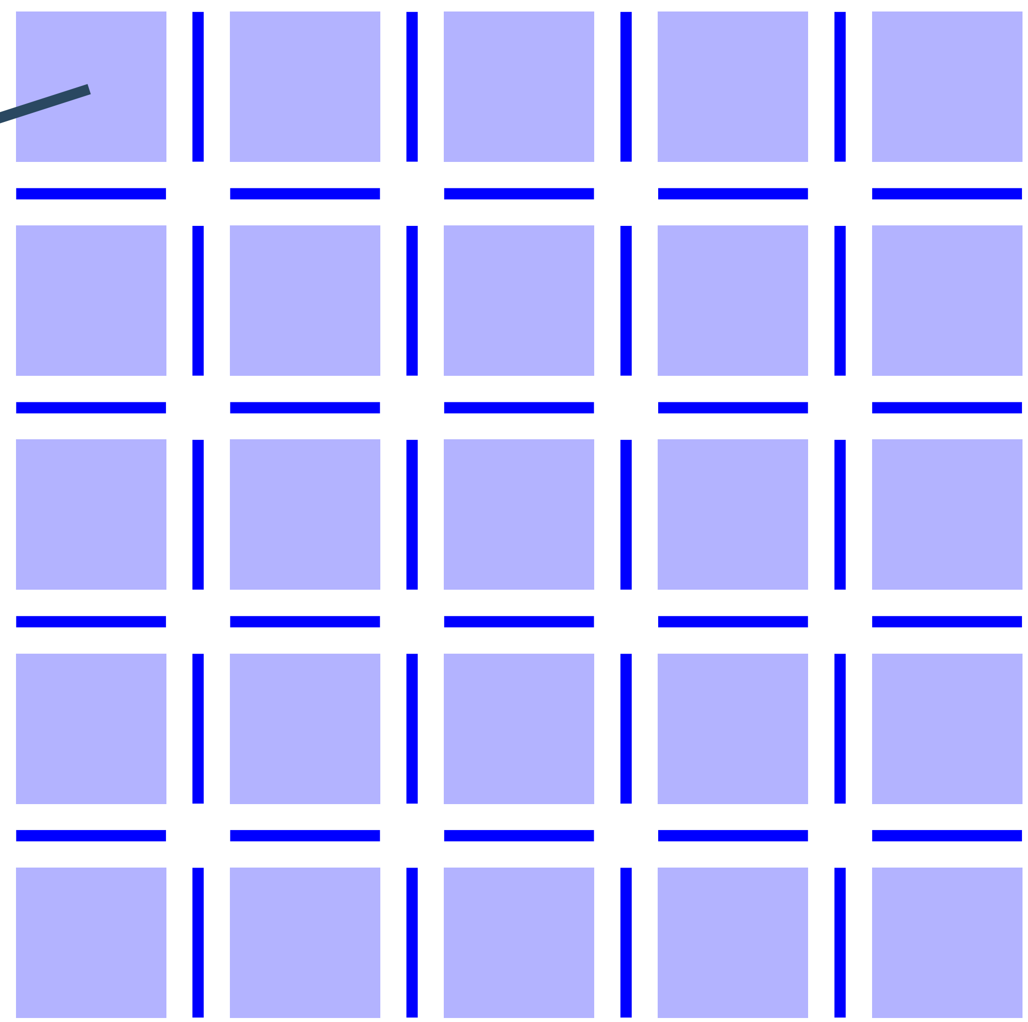
$$-\nabla^2 q_m = f_m$$

High-fidelity full-order model

$$\mathbf{L}_m \mathbf{q}_m = \mathbf{f}_m$$

Reduced order model

$$\hat{\mathbf{L}}_m \hat{\mathbf{q}}_m = \hat{\mathbf{f}}_m$$



Interface between subdomains m and n

$$[\![q]\!]_{m,n} \equiv q_m - q_n = 0$$

$$\{\!\{\mathbf{n} \cdot \nabla q\}\!\}_{m,n} \equiv \frac{1}{2}\left(\mathbf{n}_m \cdot \nabla q_m + \mathbf{n}_n \cdot \nabla q_n\right) = 0$$

Corresponding reduced order model

With static condensation domain decomposition

- Component-wise reduced order model lattice-type structure design
  S. Mcbane, Y. Choi, Computer Methods in Applied Mechanics and Engineering, 381 (2021)
  - Static-condensation reduced basis element method
    D. B. P. Huynh, D. J. Knezevic, A. T. Patera, Computer Methods in Applied Mechanics and Engineering, 259 (2013)
- Split the solution into particular (interior) / homogeneous (interface) basis
- Limited to linear systems

Physics equation

$$a(u, v) = f(v) \qquad \forall v \in X^h(\Omega)$$

Domain decomposition

$$u = \sum_m \left[u_{m,p} + u_{m,h} \right] \qquad u_{m,p}, u_{m,h} \in X^h(\Omega_m)$$

Particular (interior) solution

$$a(u_{m,p}, v_m) = f(v_m) \qquad \forall v_m \in X_0^h(\Omega_m)$$

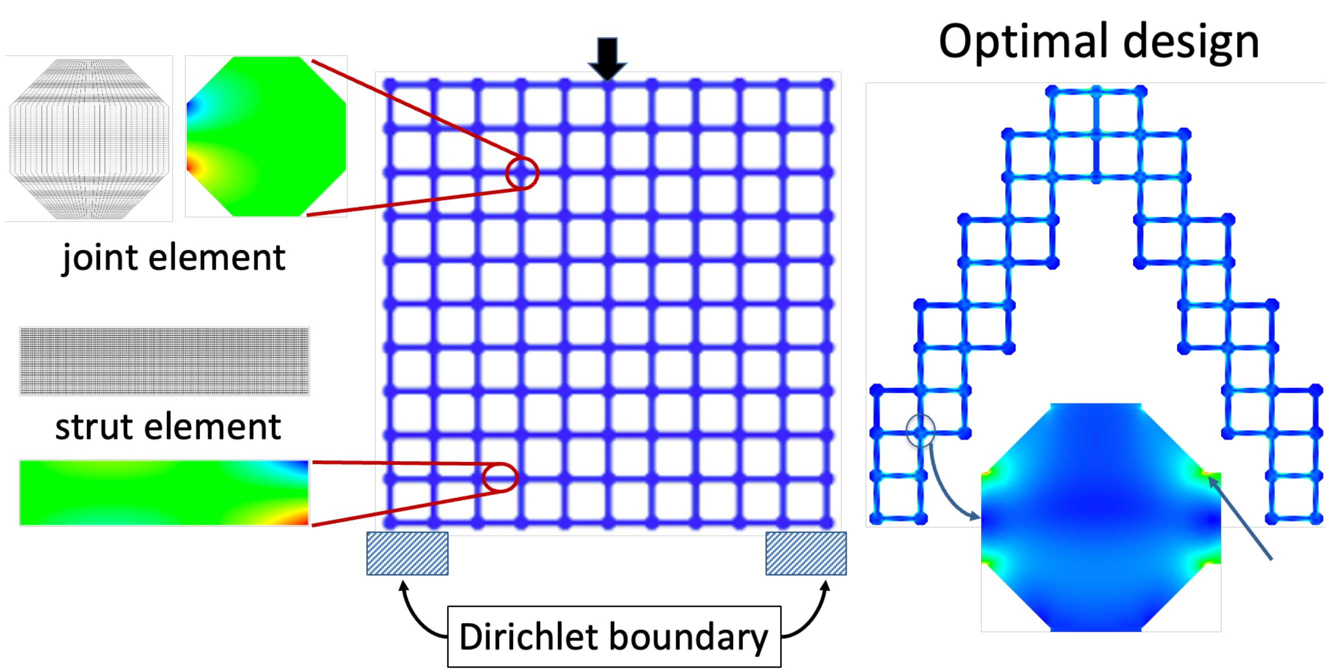
$$u_{m,p} = 0 \qquad \text{on } \mathbf{x} \in \partial\Omega_m$$

Homogeneous (interface) solution

$$a(u_{m,h}, v_m) = 0 \qquad \forall v_m \in X_0^h(\Omega_m)$$

$$u_{m,h} = u_{n,h} \qquad \text{on } \mathbf{x} \in \partial\Omega_m \cap \partial\Omega_n$$

Lattice-type structure design optimization



S. Mcbane, Y. Choi
Computer Methods in Applied Mechanics and Engineering, 381 (2021)

With least-square Petrov-Galerkin

- Domain decomposition least-square Petrov-Galerkin ROM
  C. Hoang, Y. Choi, K. Carlberg, Computer Methods in Applied Mechanics and Engineering, 384 (2021)
  A. N. Diaz, Y. Choi, M. Heinkenschloss, arXiv:2305.15163 (2023)
- 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

$$\mathbf{r}(\mathbf{x}) = \mathbf{0} \qquad \mathbf{x} \in \mathbb{R}^N$$

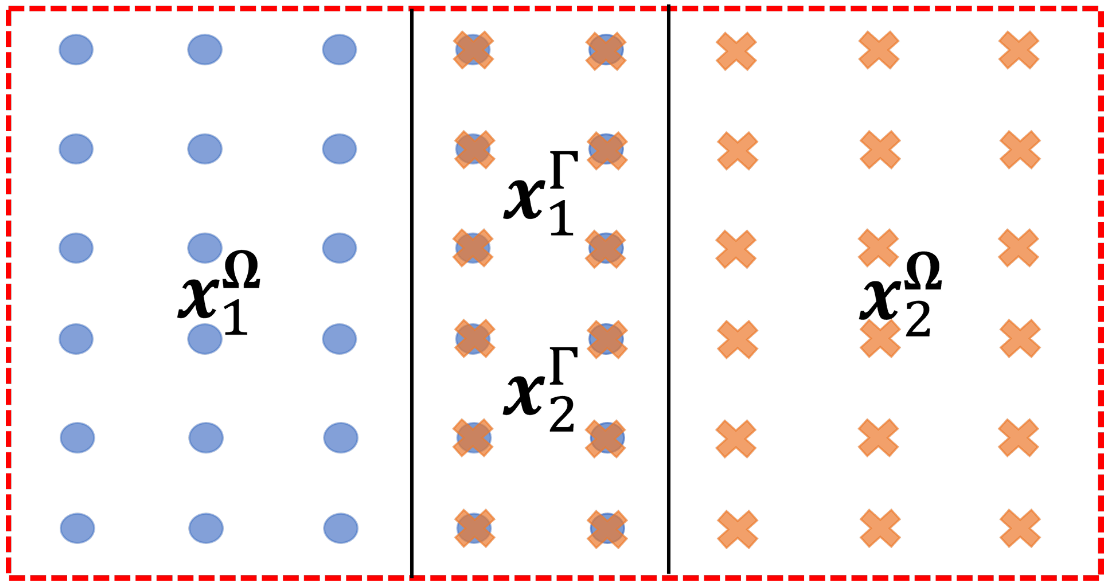
DD-LSPG solution

$$\min_{(\mathbf{x}_m^\Omega, \mathbf{x}_m^\Omega)} \frac{1}{2} \sum_m \left\| \mathbf{r}_m(\mathbf{x}_m^\Omega, \mathbf{x}_m^\Gamma) \right\|^2$$

such that

$$\mathbf{P}_m \mathbf{x}_m^\Gamma - \mathbf{P}_n \mathbf{x}_n^\Gamma = \mathbf{0} \quad \forall m, n$$

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
  C. Hoang, Y. Choi, K. Carlberg, Computer Methods in Applied Mechanics and Engineering, 384 (2021)
  A. N. Diaz, Y. Choi, M. Heinkenschloss, arXiv:2305.15163 (2023)
- 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

DD-LSPG solution

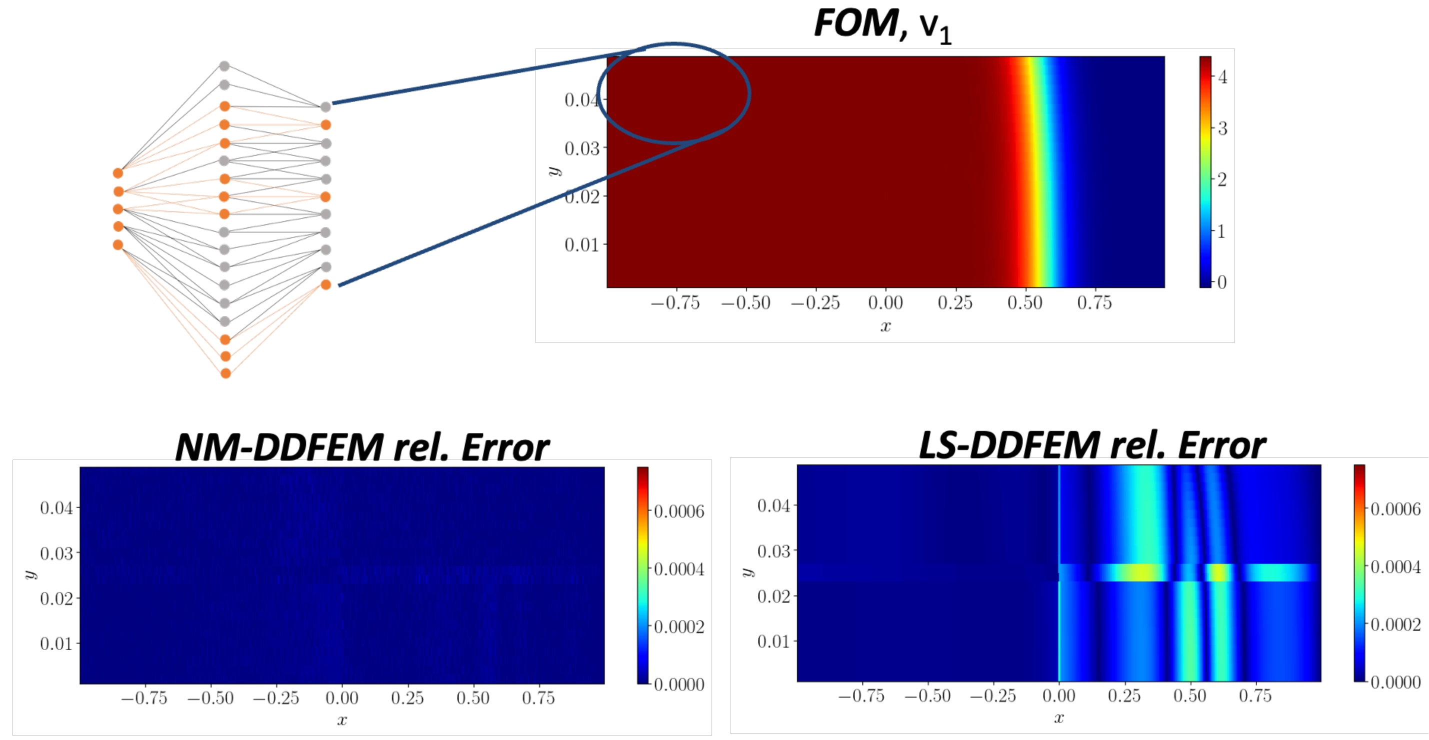
$$\min_{(\mathbf{x}_m^\Omega, \mathbf{x}_m^\Omega)} \frac{1}{2} \sum_m \left\| \mathbf{r}_m(\mathbf{x}_m^\Omega, \mathbf{x}_m^\Gamma) \right\|^2$$

such that

$$\mathbf{C}_{m,n}\left(\mathbf{P}_m\mathbf{x}_m^\Gamma - \mathbf{P}_n\mathbf{x}_n^\Gamma\right) = \mathbf{0} \quad \forall m, n$$

$$\mathbf{C}_{m,n} \sim N[0,1^2]^{N_{mn}}$$

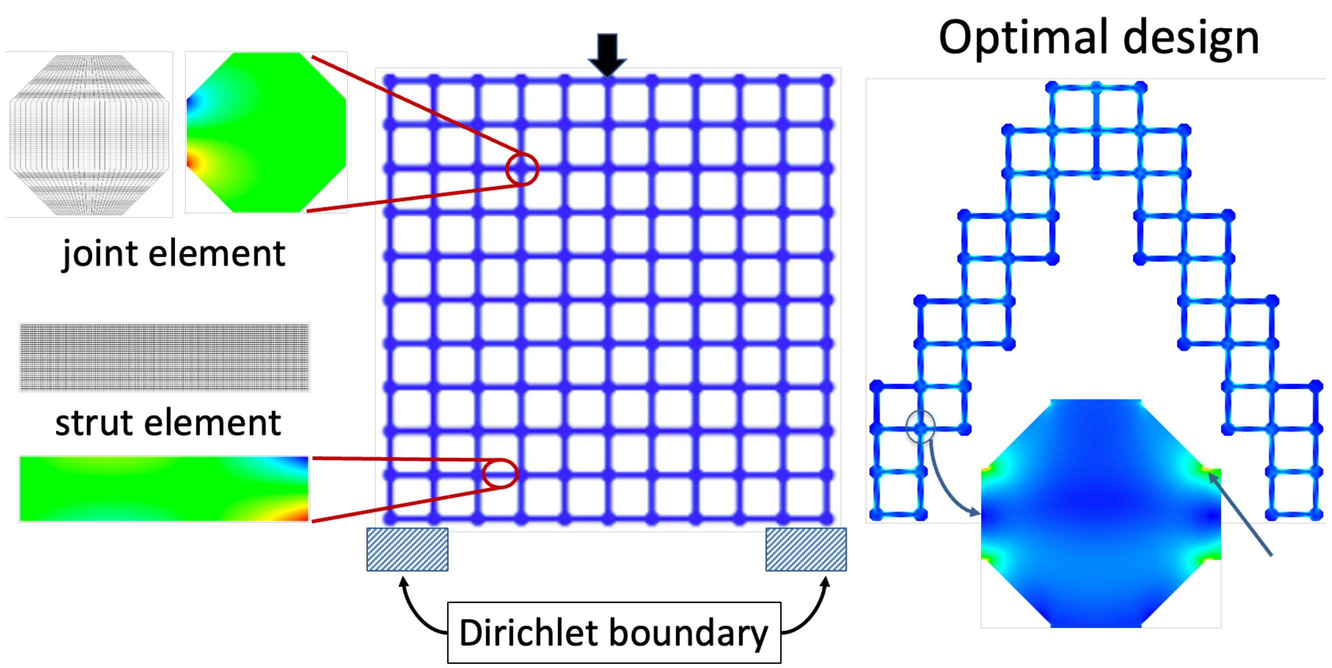
Burger's equation



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



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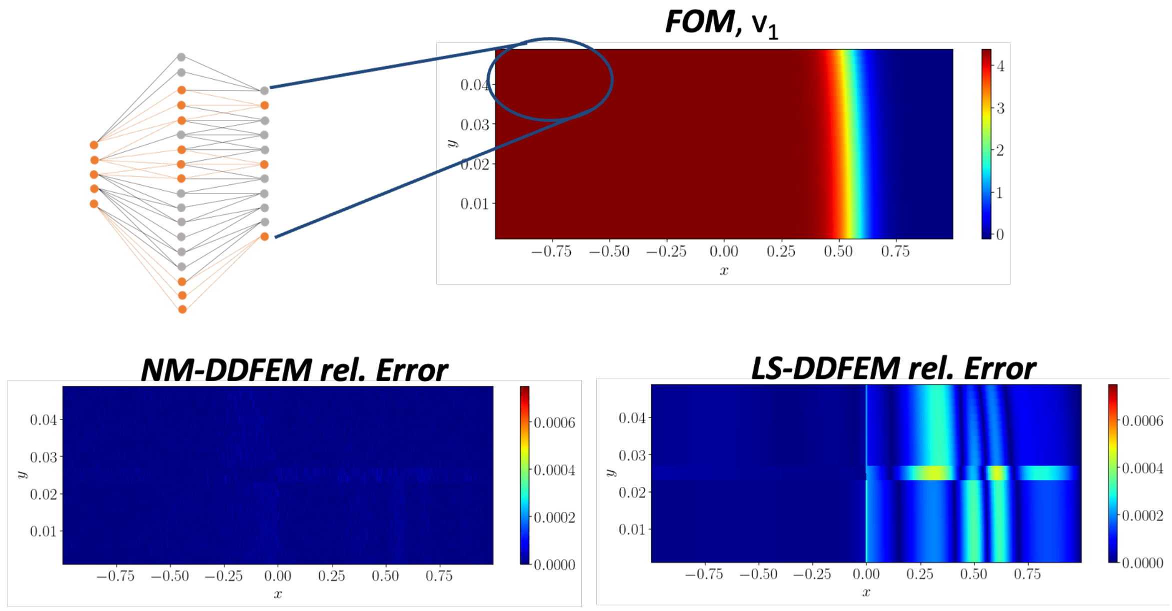
Computer Methods in Applied Mechanics and Engineering, 381 (2021)

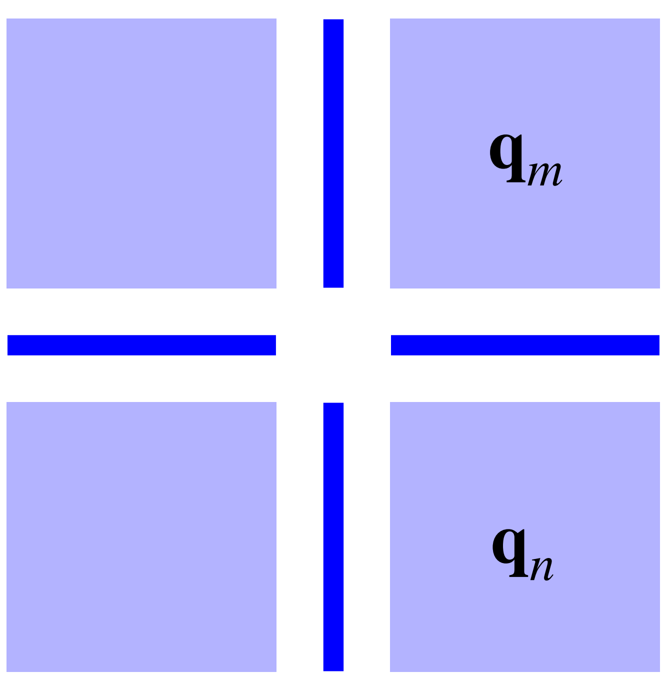


A. N. Diaz, Y. Choi, M. Heinkenschloss
arXiv:2305.15163 (2023)

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)
  - Steady Stokes flow: ***A. Toselli,*** Mathematical Models and Methods in Applied Sciences 12.11 (2002)
  - Incompressible/compressible Navier-Stokes flow: ***B. Cockburn, G. E. Karniadakis, C.-W. Shu,*** Springer Berlin Heidelberg, (2000)
  - ...
- 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



$[\![\mathbf{q}]\!]_{m,n}$

$\{\!\{\mathbf{n}\cdot\nabla\mathbf{q}\}\!\}_{m,n}$

Physics equation

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

DG domain decomposition

$$a(\mathbf{q}_m,\mathbf{q}_m^\dagger) + \sum_{\partial\Omega_m\cup\partial\Omega_n\neq\varnothing} \tilde{a}(\mathbf{q}_m,\mathbf{q}_n,\mathbf{q}_m^\dagger,\mathbf{q}_n^\dagger) = f(v_m) \qquad \forall \mathbf{q}_m^\dagger,\mathbf{q}_n^\dagger \in X^h(\Omega)$$

Example: Poisson equation

$$\boxed{-\nabla^2 q = f}$$

- Interior Penalty Method

  P. Hansbo, GAMM-Mitteilungen 28.2 (2005)

$$\sum_m^M \left\langle \nabla q_m^\dagger, \nabla q_m \right\rangle_{\Omega_m} + \sum_{\Gamma_{m,n}\neq\varnothing} \left[-\left\langle \{\!\{\mathbf{n}\cdot\nabla q^\dagger\}\!\}, [\![q]\!] \right\rangle_{\Gamma_{m,n}} - \left\langle [\![q^\dagger]\!], \{\!\{\mathbf{n}\cdot\nabla q\}\!\} \right\rangle_{\Gamma_{m,n}} + \left\langle \gamma \Delta\mathbf{x}^{-1} [\![q^\dagger]\!], [\![q]\!] \right\rangle_{\Gamma_{m,n}} \right] = \sum_m^M \left\langle \nabla q_m^\dagger, f \right\rangle_{\Omega_m}$$

$$\sum_m^M \mathbf{q}_m^{\dagger\top} \mathbf{L}_m \mathbf{q}_m + \sum_{\Gamma_{m,n}\neq\varnothing} \begin{pmatrix} \mathbf{q}_m^{\dagger\top} & \mathbf{q}_n^{\dagger\top} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{mm} & \mathbf{L}_{mn} \\ \mathbf{L}_{nm} & \mathbf{L}_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{q}_m \\ \mathbf{q}_n \end{pmatrix} = \sum_m^M \mathbf{q}_m^{\dagger\top} \mathbf{f}_m \qquad \forall \mathbf{q}_m^\dagger \in \mathbb{R}^{N_m}$$

DG operators $\mathbf{L}_m$, $\mathbf{L}_{mn}$ can be seamlessly projected onto POD basis

Poisson equation— basis construction

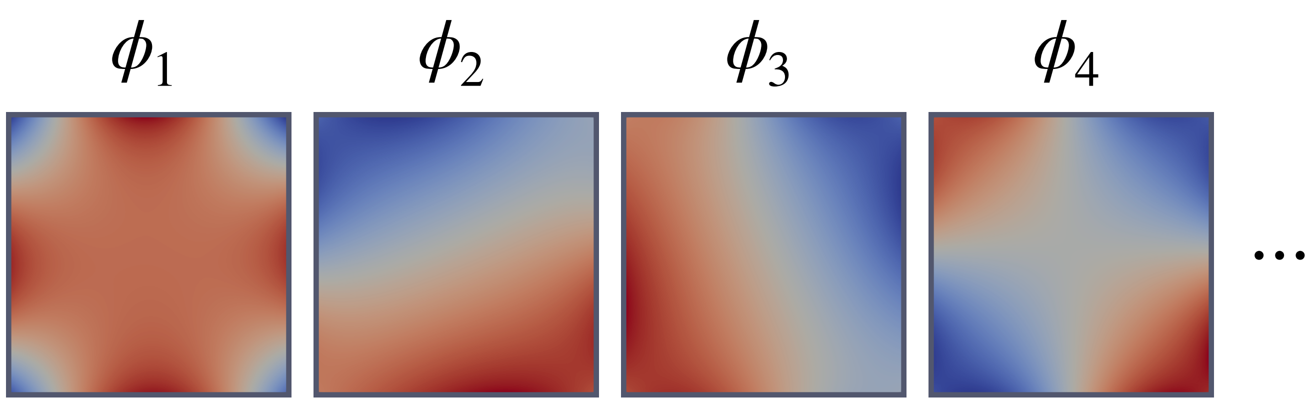
- One unit component, 4225-dof FEM solution
- Sampling for POD basis construction ($M = 1$)

$$f = \sin 2\pi(\mathbf{k} \cdot \mathbf{x} + \theta) \qquad \mathbf{k}, \mathbf{k}_b \sim U[-0.5, 0.5]^2$$

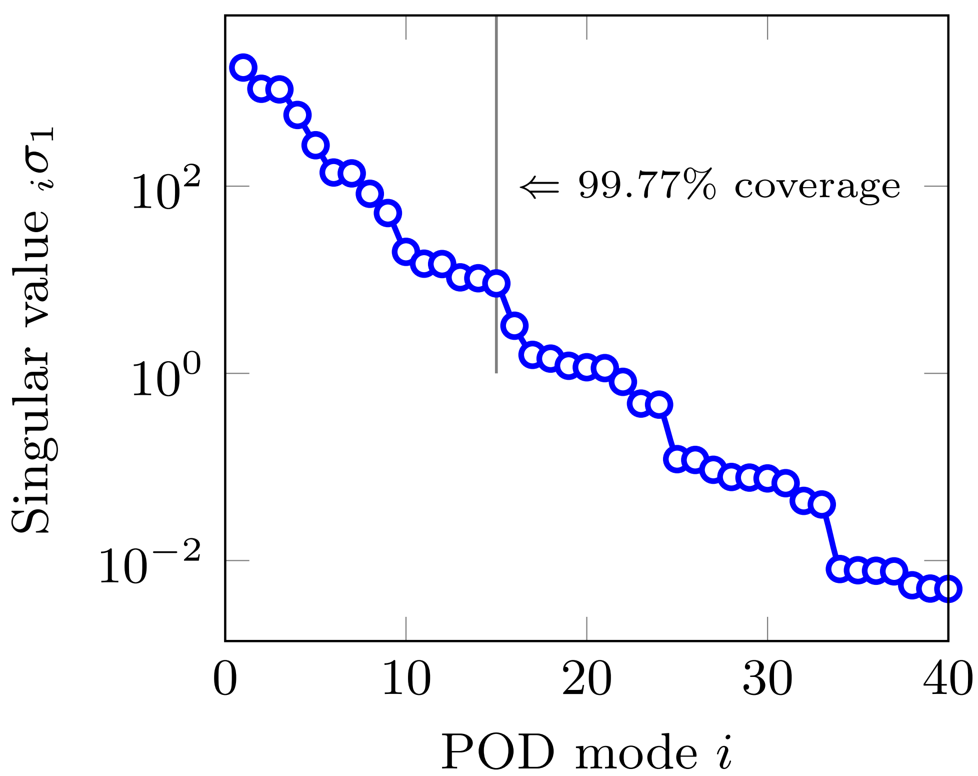
$$q = \sin 2\pi(\mathbf{k}_b \cdot \mathbf{x} + \theta_b) \quad \mathbf{x} \in \partial\Omega \qquad \theta, \theta_b \sim U[0, 1]$$

- 4225 random samples on parameters
- Only 15 basis vectors can represent 99.77% of all samples

POD mode $\mathbf{\Phi}$



Singular value spectrum



ROM as a data-driven DG element

$$\sum_m^M \mathbf{q}_m^{\dagger\top}\mathbf{L}_m\mathbf{q}_m + \sum_{\Gamma_{m,n}\neq\emptyset} \begin{pmatrix}\mathbf{q}_m^{\dagger\top} & \mathbf{q}_n^{\dagger\top}\end{pmatrix}\begin{pmatrix}\mathbf{L}_{mm} & \mathbf{L}_{mn}\\ \mathbf{L}_{nm} & \mathbf{L}_{nn}\end{pmatrix}\begin{pmatrix}\mathbf{q}_m\\ \mathbf{q}_n\end{pmatrix} = \sum_m^M \mathbf{q}_m^{\dagger\top}\mathbf{f}_m \qquad \forall \mathbf{q}_m^\dagger \in \mathbb{R}^{N_m}$$

- Galerkin projection on POD basis space

$$\mathbf{q}_m \approx \mathbf{\Phi}_m\hat{\mathbf{q}}_m \qquad \mathbf{q}_m^\dagger \approx \mathbf{\Phi}_m\hat{\mathbf{q}}_m^\dagger$$

$$\sum_m^M \hat{\mathbf{q}}_m^{\dagger\top}\hat{\mathbf{L}}_m\hat{\mathbf{q}}_m + \sum_{\Gamma_{m,n}\neq\emptyset} \begin{pmatrix}\hat{\mathbf{q}}_m^{\dagger\top} & \hat{\mathbf{q}}_n^{\dagger\top}\end{pmatrix}\begin{pmatrix}\hat{\mathbf{L}}_{mm} & \hat{\mathbf{L}}_{mn}\\ \hat{\mathbf{L}}_{nm} & \hat{\mathbf{L}}_{nn}\end{pmatrix}\begin{pmatrix}\hat{\mathbf{q}}_m\\ \hat{\mathbf{q}}_n\end{pmatrix} = \sum_m^M \hat{\mathbf{q}}_m^{\dagger\top}\mathbf{\Phi}_m^\top\mathbf{f}_m \qquad \forall \hat{\mathbf{q}}_m^\dagger \in \mathbb{R}^{\hat{N}_m}$$

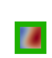
- Dimension reduction from $N_m = 4225$ to $\hat{N}_m = 15$

$$\hat{\mathbf{L}}_m = \mathbf{\Phi}_m^\top\mathbf{L}_m\mathbf{\Phi}_m \qquad \hat{\mathbf{L}}_{mn} = \mathbf{\Phi}_m^\top\mathbf{L}_{mn}\mathbf{\Phi}_n$$

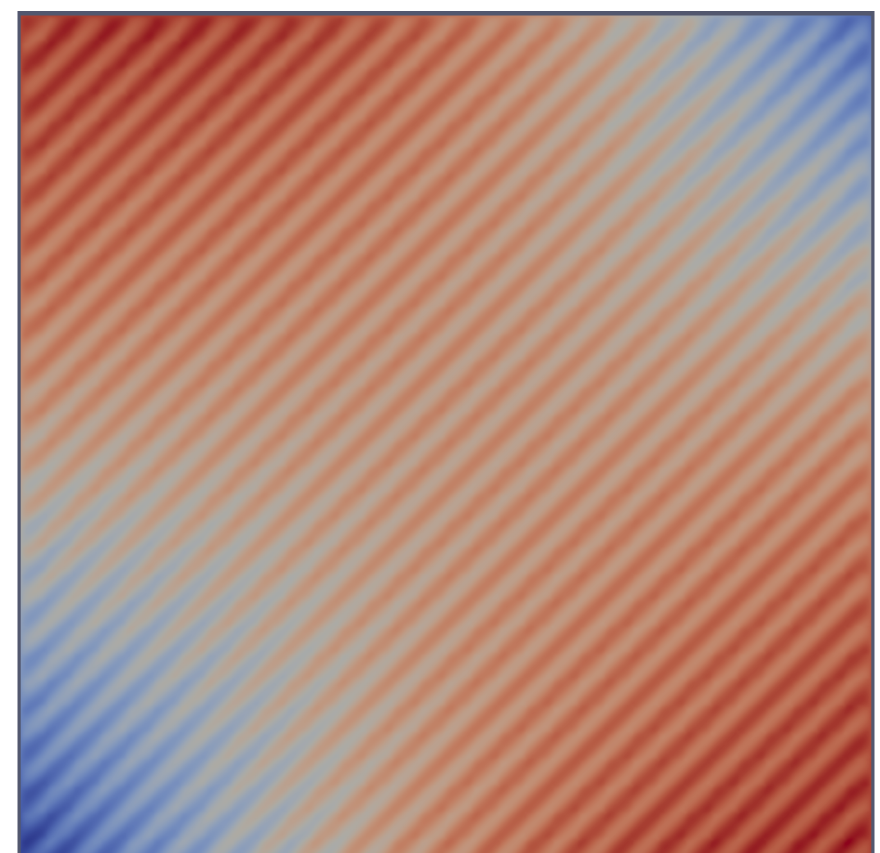
- No particular basis/handling for interface

Simple extrapolation in scale
only with component-scale data

Unit component ROM



32×32-component system

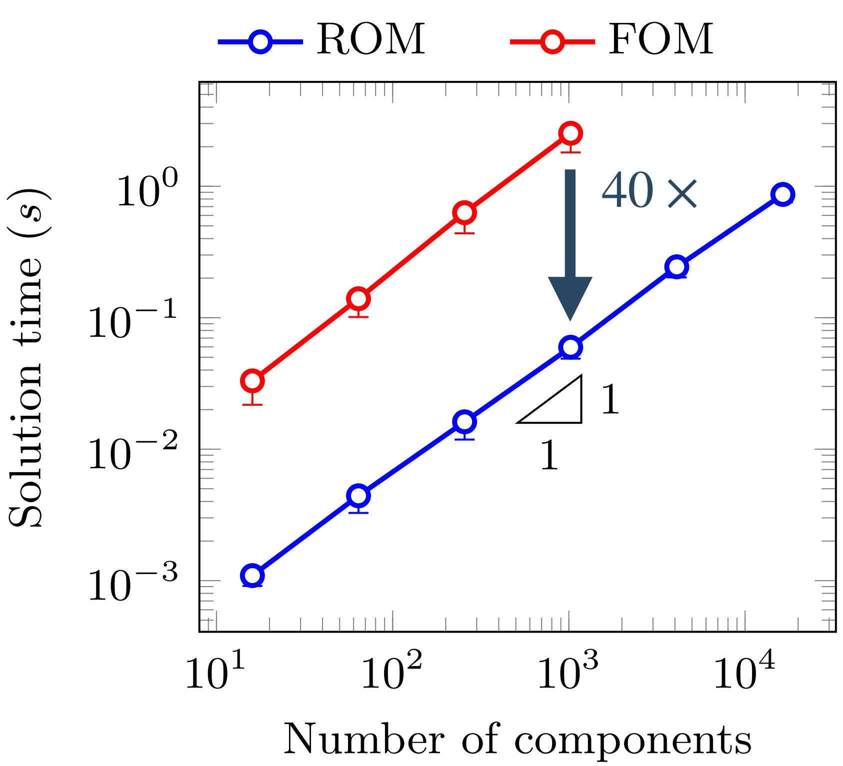


Fast & Robust extrapolation in scale

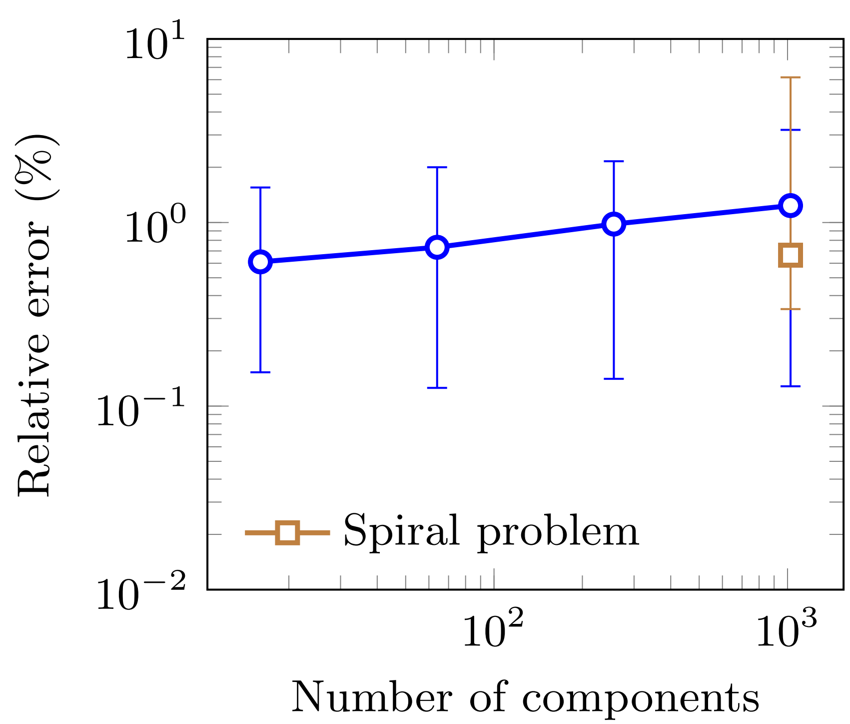
S. Chung, Y. Choi, P. Roy, T. Moore, T. Roy, T. Y. Lin, D. Y. Nguyen, C. Hahn, E. B. Duoss, S. E. Baker,
"Train Small, Model Big: Scalable Physics Simulators via Reduced Order Modeling and Domain Decomposition",
arXiv:2401.10245 (2024) (submitted to Computer Methods in Applied Mechanics and Engineering)

- 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

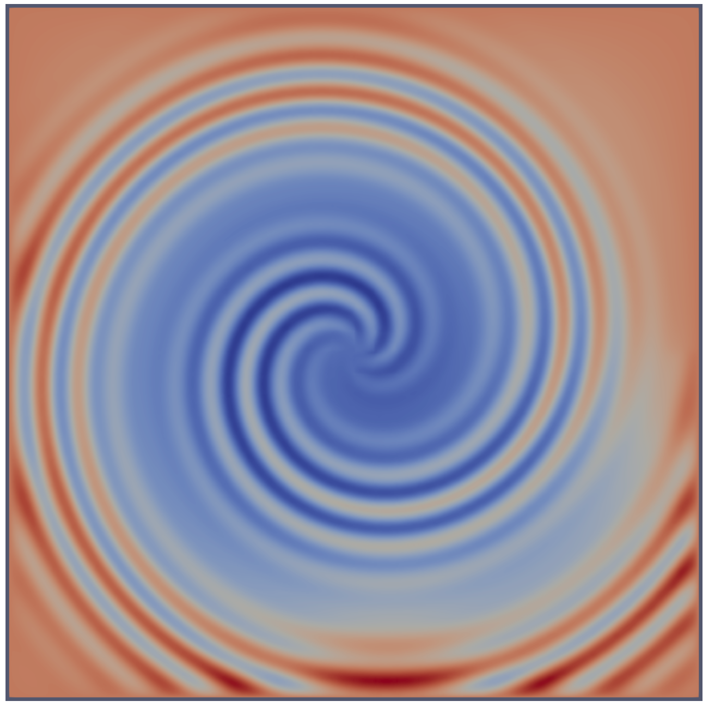
Computation time



Accuracy



32×32 **Spiral problem**



Stokes flow DG formulation

$$\begin{aligned} -\nabla^2 \mathbf{u} + \nabla p &= 0 \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \qquad \mathbf{q} = (\mathbf{u}, p) \qquad \mathbf{q}^\dagger = (\mathbf{u}^\dagger, p^\dagger)$$

- ***A. Toselli,*** Mathematical Models and Methods in Applied Sciences 12.11 (2002)

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

$$+ \sum_{\Gamma_{m,n} \neq \varnothing} \left[-\left\langle \{\!\{ \mathbf{n} \cdot \nabla \mathbf{u}_m^\dagger \}\!\}, [\![\mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} - \left\langle [\![\mathbf{u}_m^\dagger]\!], \{\!\{ \mathbf{n} \cdot \nabla \mathbf{u}_m \}\!\} \right\rangle_{\Gamma_{m,n}} + \left\langle \gamma \Delta \mathbf{x}^{-1} [\![\mathbf{u}_m^\dagger]\!], [\![\mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} + \left\langle [\![\mathbf{n} \cdot \mathbf{u}_m^\dagger]\!], \{\!\{ p_m \}\!\} \right\rangle_{\Gamma_{m,n}} + \left\langle \{\!\{ p_m^\dagger \}\!\}, [\![\mathbf{n} \cdot \mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} \right] = 0$$

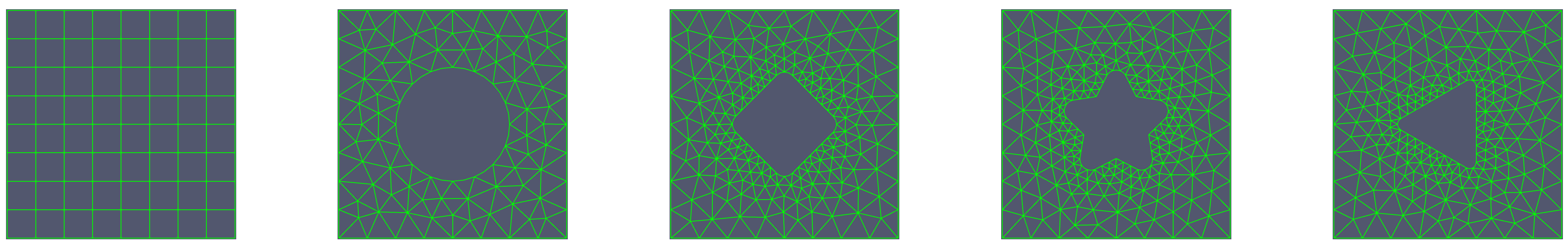
- Each DG operator has a saddle-point block matrix system

$$\sum_m^M \mathbf{q}_m^{\dagger\top} \mathbf{L}_m \mathbf{q}_m + \sum_{\Gamma_{m,n} \neq \varnothing} \begin{pmatrix} \mathbf{q}_m^{\dagger\top} & \mathbf{q}_n^{\dagger\top} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{mm} & \mathbf{L}_{mn} \\ \mathbf{L}_{nm} & \mathbf{L}_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{q}_m \\ \mathbf{q}_n \end{pmatrix} = \sum_m^M \mathbf{q}_m^{\dagger\top} \mathbf{f}_m \qquad \forall \mathbf{q}_m^\dagger \in \mathbb{R}^{N_m}$$

$$\mathbf{L}_m = \begin{pmatrix} \mathbf{K}_m & \mathbf{B}_m^\top \\ \mathbf{B}_m & \mathbf{0} \end{pmatrix} \qquad \mathbf{L}_{m,n} = \begin{pmatrix} \mathbf{K}_{m,n} & \mathbf{B}_{m,n}^\top \\ \mathbf{B}_{m,n} & \mathbf{0} \end{pmatrix}$$

Stokes flow with multiple ROM elements

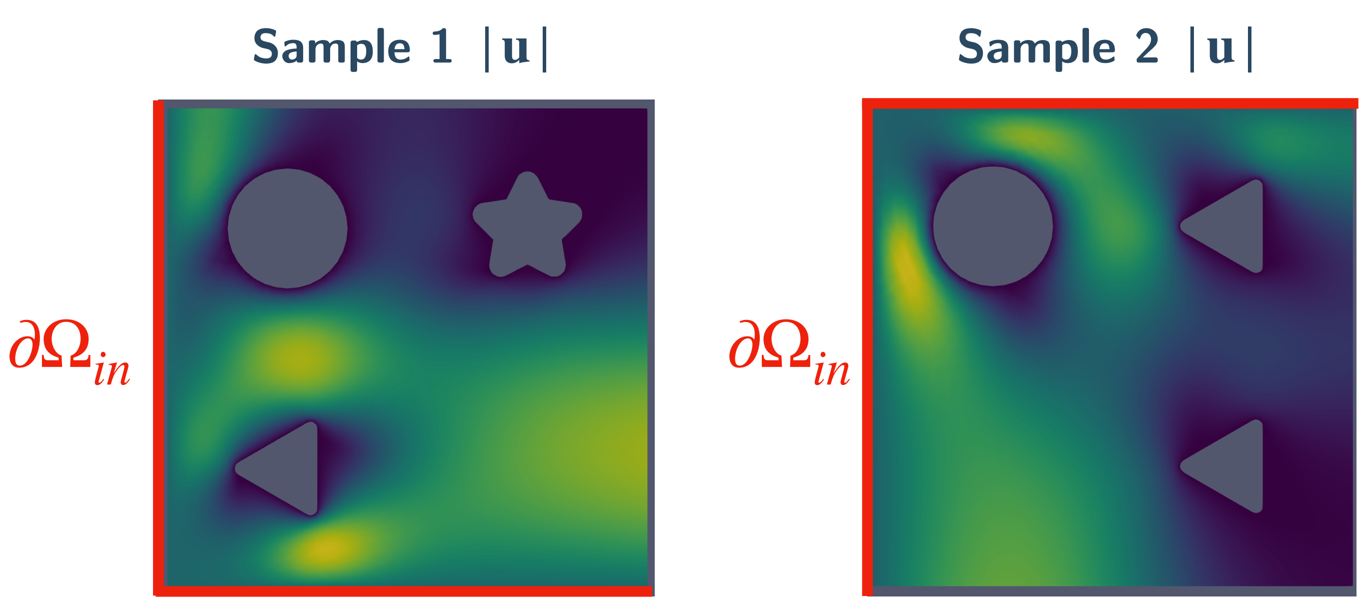
- Flow problems for arrays of 5 unit objects

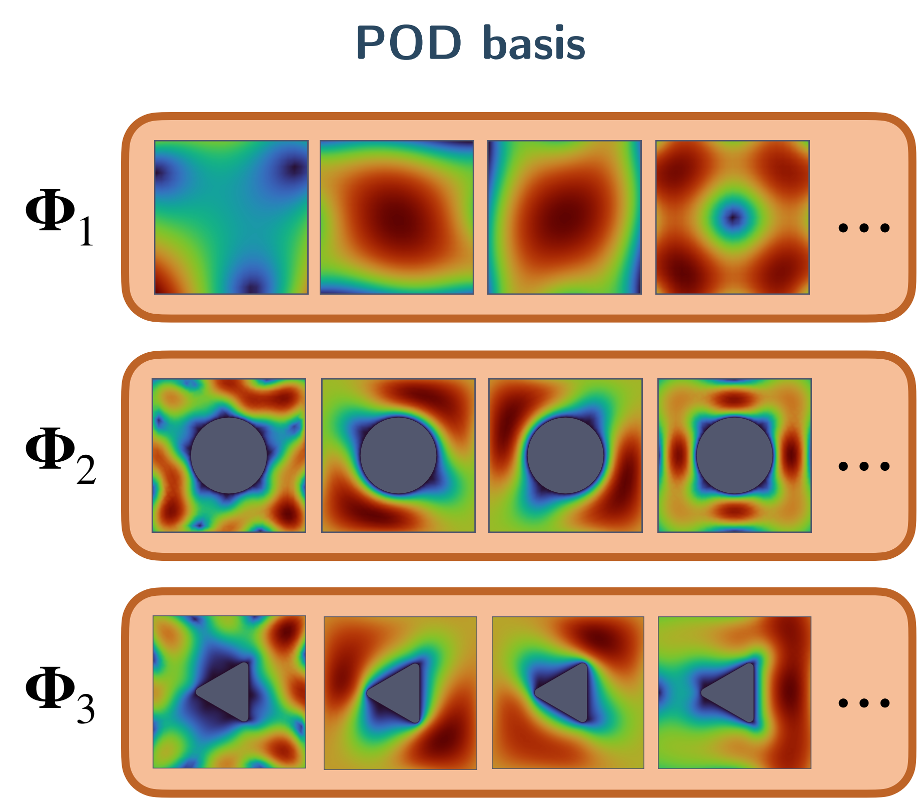


- 1400 samples on random 2×2 arrays with random in-flow conditions

$$\mathbf{u} = \begin{pmatrix} u_0 + \Delta u \sin 2\pi(\mathbf{k}_u \cdot \mathbf{x} + \theta_u) \\ v_0 + \Delta v \sin 2\pi(\mathbf{k}_v \cdot \mathbf{x} + \theta_v) \end{pmatrix} \quad \text{on } \mathbf{x} \in \partial\Omega_{in}$$

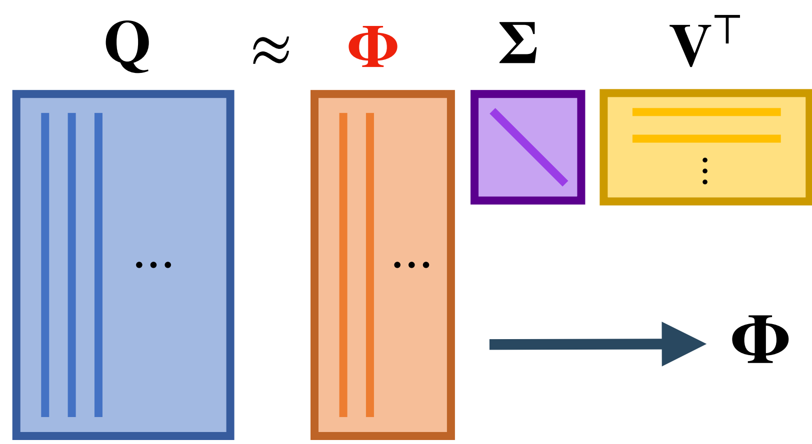
$$u_0, v_0 \sim U[-1,1] \qquad \mathbf{k}_u, \mathbf{k}_v \sim U[-0.5,0.5]^2$$
$$\Delta u, \Delta v \sim U[-0.1,0.1] \qquad \theta_u, \theta_v \sim U[0,1]$$





Unified POD basis

- POD is performed over the entire solution vector space



$$\mathbf{Q} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots \\ p_1 & p_2 & \cdots \end{pmatrix} \qquad \boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\Phi}_u \\ \boldsymbol{\Phi}_p \end{pmatrix} = \begin{pmatrix} \phi_{u1} & \phi_{u2} & \cdots \\ \phi_{p1} & \phi_{p2} & \cdots \end{pmatrix}$$

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

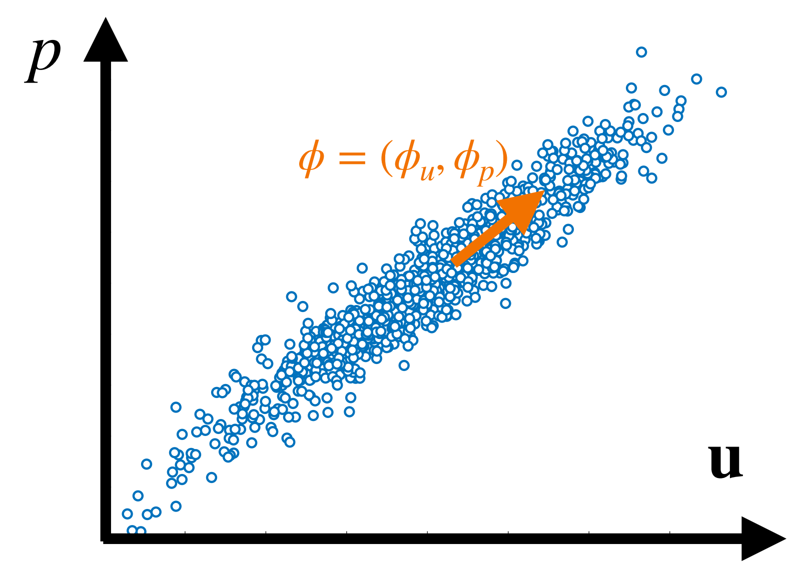
FOM operator

$$\mathbf{L} = \begin{pmatrix} \mathbf{K} & \mathbf{B}^\top \\ \mathbf{B} & \mathbf{0} \end{pmatrix}$$

ROM projection

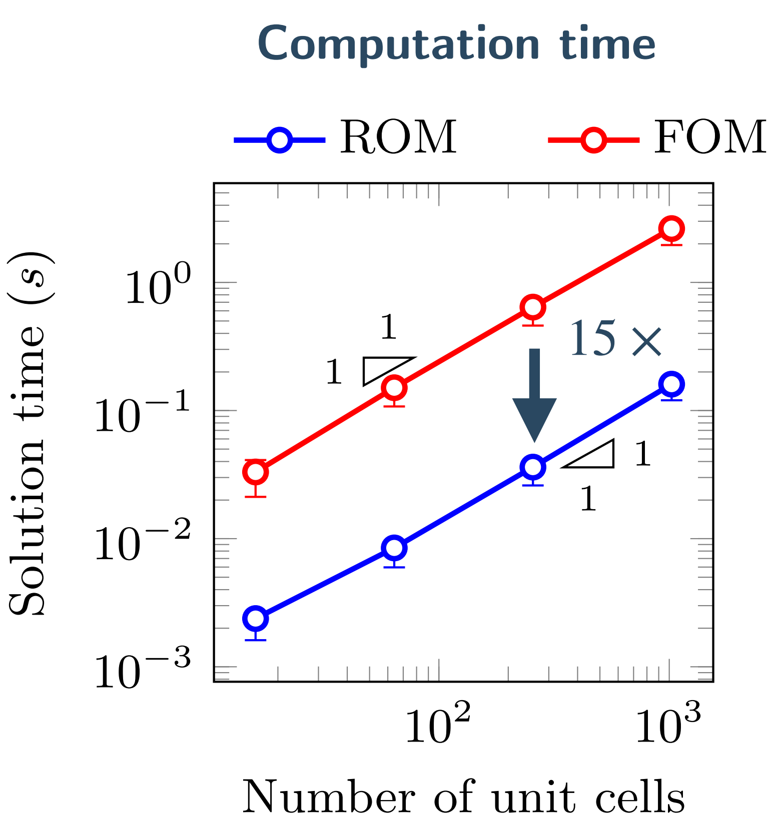
$$\begin{aligned} \hat{\mathbf{L}} &= \boldsymbol{\Phi}^\top \mathbf{L} \boldsymbol{\Phi} \\ &= \boldsymbol{\Phi}_u^\top \mathbf{K} \boldsymbol{\Phi}_u + \boldsymbol{\Phi}_u^\top \mathbf{B}^\top \boldsymbol{\Phi}_p + \boldsymbol{\Phi}_p^\top \mathbf{B} \boldsymbol{\Phi}_u \end{aligned}$$

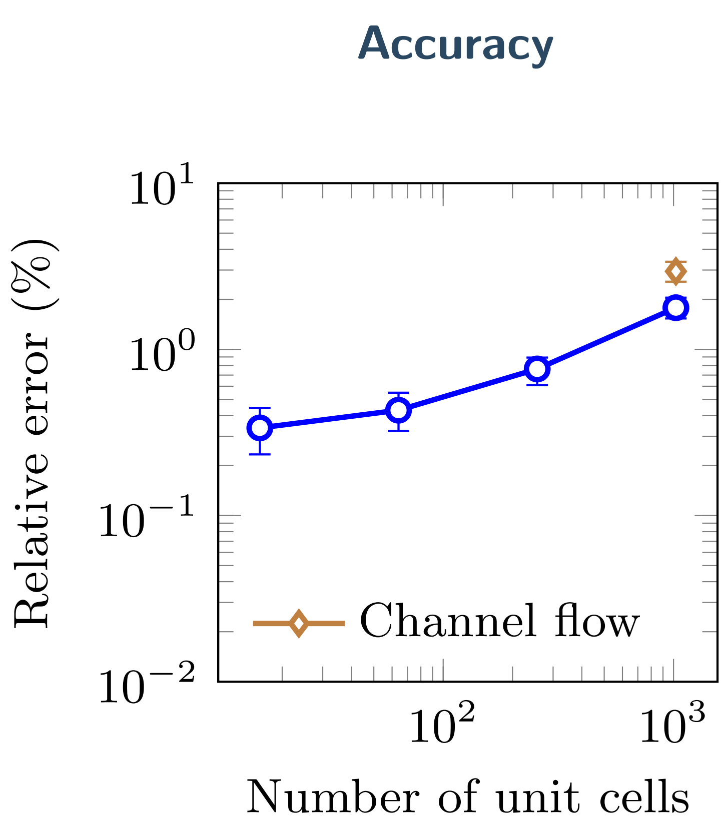
Unified basis schematic

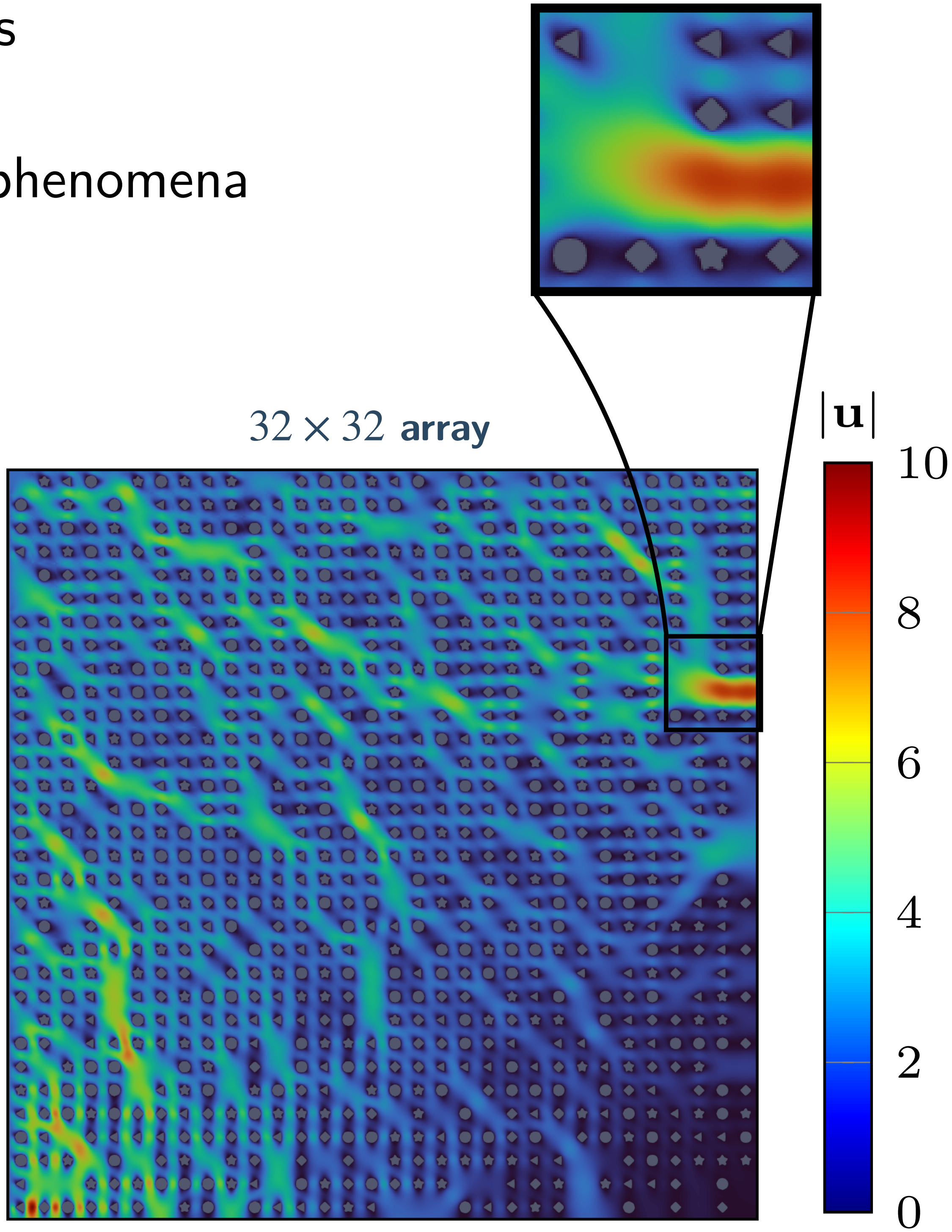


Able to predict an emergent phenomenon

- 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

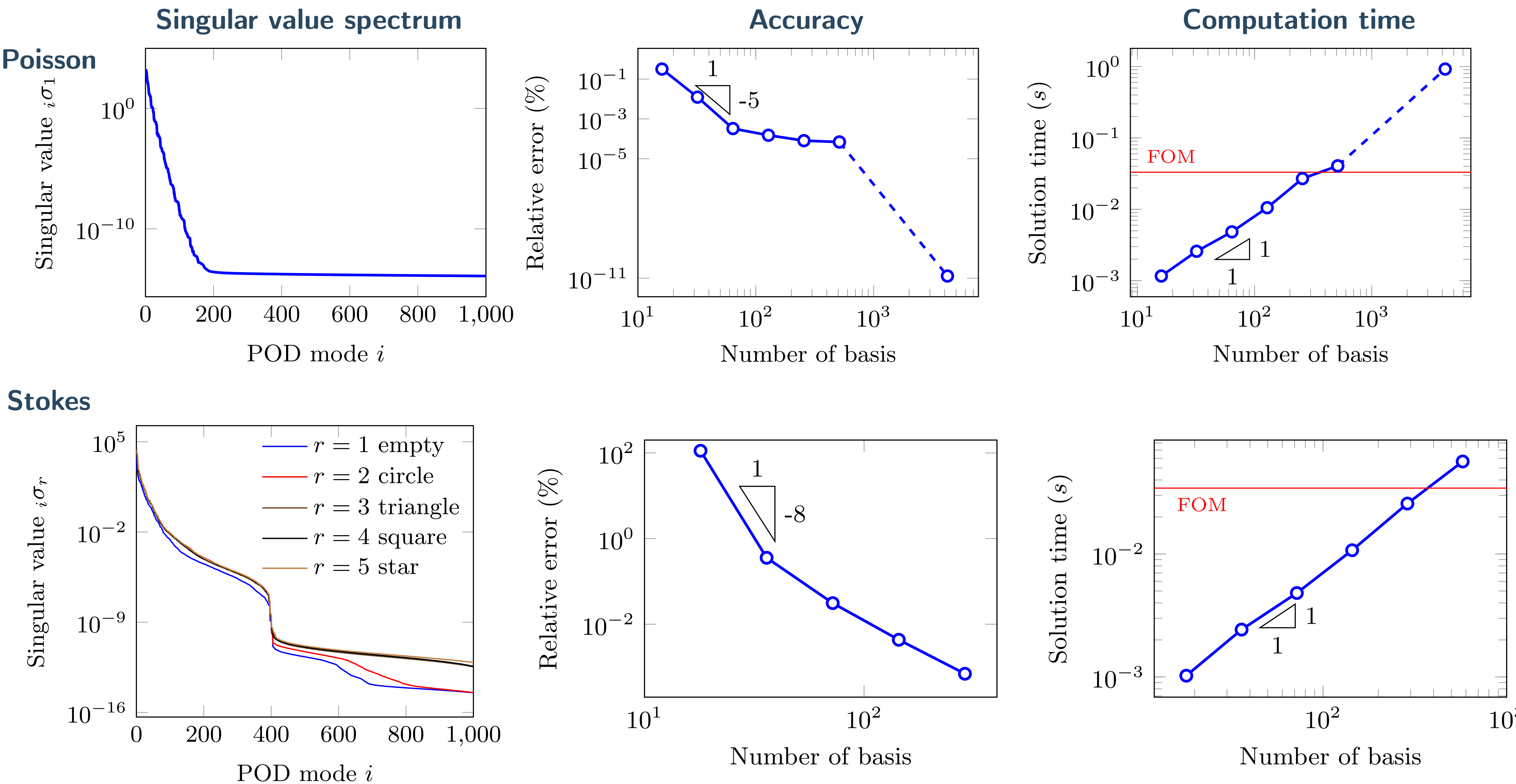






Rapid convergence with basis dimension

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



Steady Navier-Stokes— handling nonlinear advection

$$\begin{aligned} \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u} + \nabla p &= 0 \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned} \qquad \mathbf{q} = (\mathbf{u}, p) \qquad \mathbf{q}^\dagger = (\mathbf{u}^\dagger, p^\dagger)$$

FOM operator

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

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

$$+ \sum_{\Gamma_{m,n}\neq\emptyset} \left[-\left\langle \nu\{\!\{\mathbf{n}\cdot\nabla\mathbf{u}_m^\dagger\}\!\}, [\![\mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} - \left\langle \nu[\![\mathbf{u}_m^\dagger]\!], \{\!\{\mathbf{n}\cdot\nabla\mathbf{u}_m\}\!\} \right\rangle_{\Gamma_{m,n}} + \left\langle \gamma\Delta\mathbf{x}^{-1}[\![\mathbf{u}_m^\dagger]\!], [\![\mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} + \left\langle [\![\mathbf{n}\cdot\mathbf{u}_m^\dagger]\!], \{\!\{p_m\}\!\} \right\rangle_{\Gamma_{m,n}} + \left\langle \{\!\{p_m^\dagger\}\!\}, [\![\mathbf{n}\cdot\mathbf{u}_m]\!] \right\rangle_{\Gamma_{m,n}} \right] = 0$$

- 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

ROM Tensor projection

$$\mathbf{u}_m = \sum_i \phi_{u,i}\hat{u}_i \qquad \mathbf{u}_m^\dagger = \sum_i \phi_{u,i}\hat{u}_i^\dagger$$

ROM projection

$$\hat{\mathbf{N}} = \mathbf{\Phi}_u^\top\mathbf{K}\mathbf{\Phi}_u + \mathbf{T}(\hat{\mathbf{u}}) + \mathbf{\Phi}_u^\top\mathbf{B}^\top\mathbf{\Phi}_p + \mathbf{\Phi}_p^\top\mathbf{B}\mathbf{\Phi}_u$$

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

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

$$\boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\Phi}_u \\ \boldsymbol{\Phi}_p \end{pmatrix} = \begin{pmatrix} \phi_{u1} & \phi_{u2} & \cdots \\ \phi_{p1} & \phi_{p2} & \cdots \end{pmatrix}$$

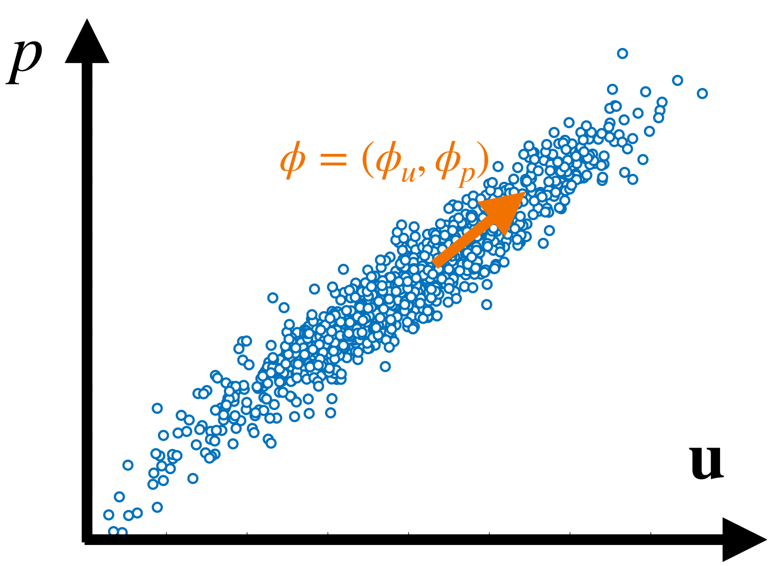
Unified basis schematic

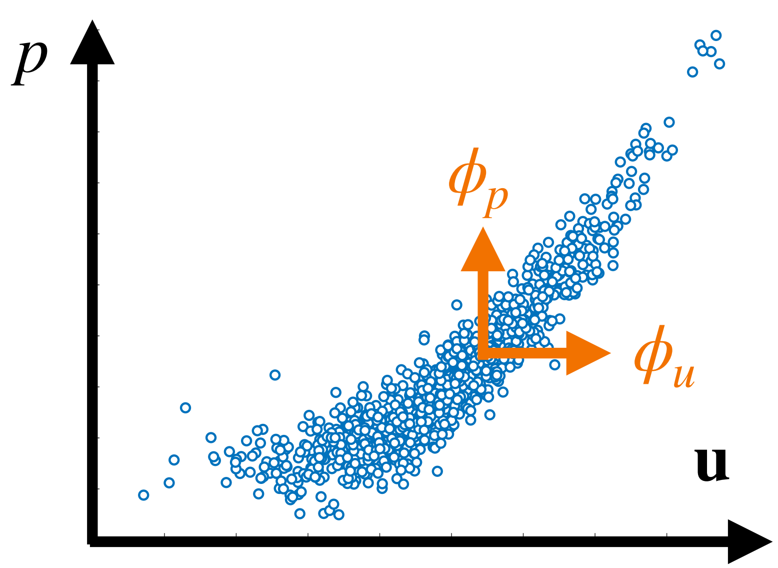
$$\boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\Phi}_u & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Phi}_p \end{pmatrix}$$

Separate basis schematic

New ROM projection

$$\hat{\mathbf{N}}[\mathbf{q}] = \begin{pmatrix} \boldsymbol{\Phi}_u^\top \mathbf{K} \boldsymbol{\Phi}_u + \mathbf{T}(\mathbf{u}) & \boldsymbol{\Phi}_u^\top \mathbf{B}^\top \boldsymbol{\Phi}_p \\ \boldsymbol{\Phi}_p^\top \mathbf{B} \boldsymbol{\Phi}_u & \mathbf{0} \end{pmatrix}$$





Newton iterations for 8×8 array at $\mathrm{Re} = 1$

```
||r|| = 54.6169
||r|| = 0.0938665, ||r||/||r_0|| = 0.00171863
||r|| = 0.166563, ||r||/||r_0|| = 0.00304966
||r|| = 16.5694, ||r||/||r_0|| = 0.303374
||r|| = 3204.19, ||r||/||r_0|| = 58.6667
||r|| = 106117, ||r||/||r_0|| = 1942.93
||r|| = 1.74169e+08, ||r||/||r_0|| = 3.18891e+06
||r|| = 1.87222e+12, ||r||/||r_0|| = 3.42791e+10
||r|| = 1.46324e+14, ||r||/||r_0|| = 2.6791e+12
```

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**
  O. Ladyzhenskaya, (1963) *I. Babushka,* (1971) *F. Brezzi,* (1974)
- 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 $\mathbf{u}$ components, p is underdetermined

Incompressible, divergence-free condition

$$\nabla \cdot \mathbf{u} = 0$$

Divergence-free ROM basis

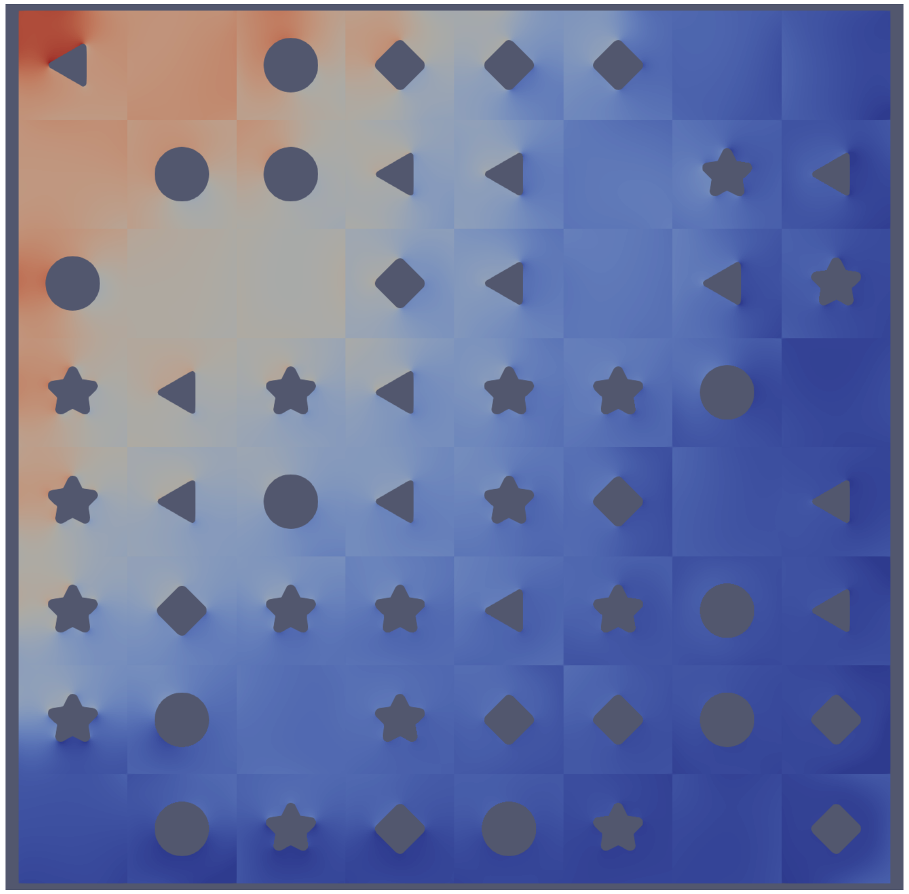
$$\nabla \cdot \phi_{u,i} \approx 0 \qquad \forall i$$

$$\text{Or, } \mathbf{B}\boldsymbol{\Phi}_u \approx \mathbf{0}$$

ROM projection

$$\hat{\mathbf{N}}[\mathbf{q}] = \begin{pmatrix} \boldsymbol{\Phi}_u^\top \mathbf{K} \boldsymbol{\Phi}_u + \mathbf{T}(\mathbf{u}) & \boldsymbol{\Phi}_u^\top \mathbf{B}^\top \boldsymbol{\Phi}_p \\ \boldsymbol{\Phi}_p^\top \mathbf{B} \boldsymbol{\Phi}_u & \mathbf{0} \end{pmatrix}$$

Pressure at $\mathrm{Re} = 1$, $4.2\,\%$ error



Augment velocity basis to stabilize pressure

- Supremizer enrichment for stabilizing pressure
  F. Ballarin, A. Manzoni, A. Quarteroni, G. Rozza, International Journal for Numerical Methods in Engineering 102.5 (2015) 1136-1161
- Demonstrated the speed-up/accuracy at Re=10
- Ongoing demonstration for higher Reynolds numbers

Supremizer from pressure basis

$$\overline{\phi}_{s,i} = \nabla \phi_{p,i}$$

Or $\overline{\mathbf{\Phi}}_s = \mathbf{B}\mathbf{\Phi}_p$

Orthonormalization

$$\mathbf{\Phi}_s = \mathrm{GS}\left[\overline{\mathbf{\Phi}}_s\right]$$

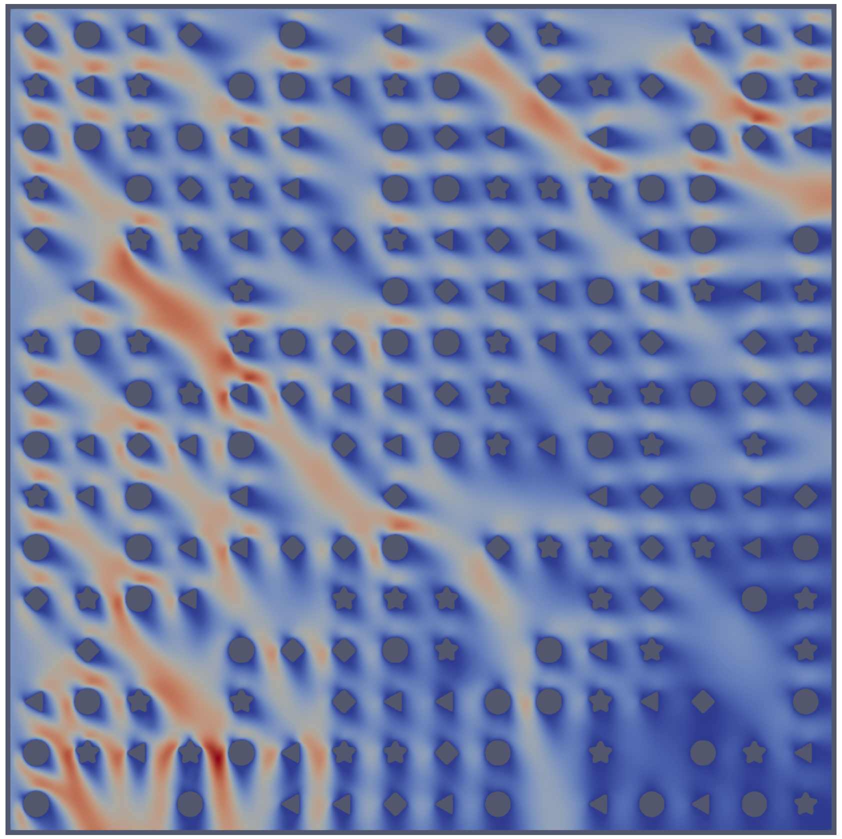
Augment velocity basis

$$\tilde{\mathbf{\Phi}}_u = \left(\mathbf{\Phi}_u \quad \mathbf{\Phi}_s\right)$$

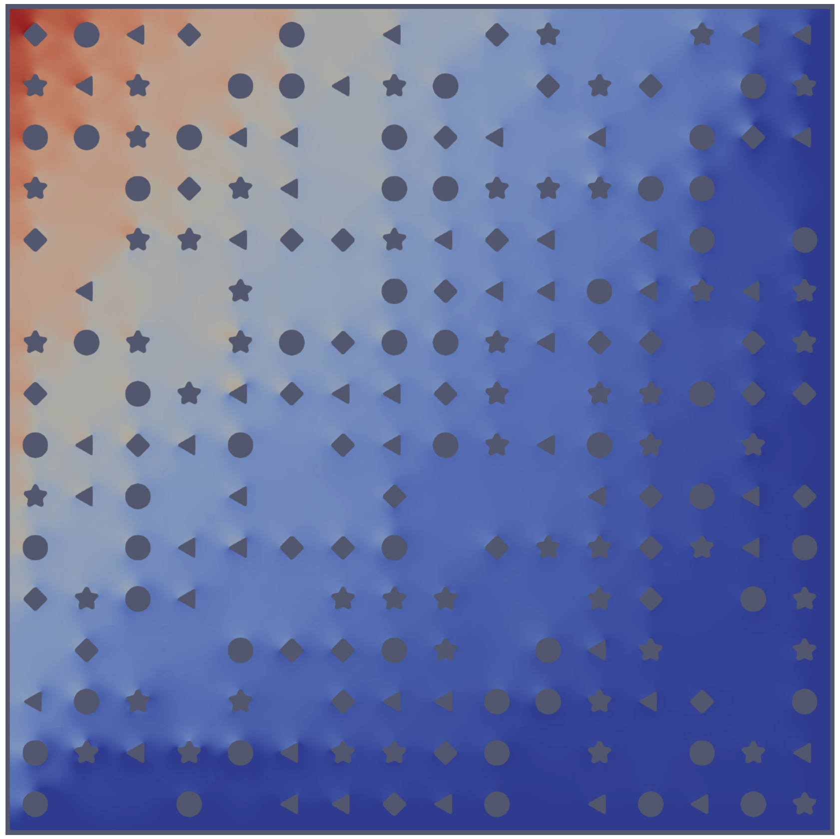
Prediction for 16×16 array, $\mathrm{Re} = 10$

$(n_u, n_s, n_p) = (40{,}40{,}40)$ **basis,** $18.7\times$ **speed-up**

Flow speed, $1.3\,\%$ **error**



Pressure, $0.9\,\%$ **error**



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)

T. Chapman, P. Avery, P. Collins, C. Farhat,
International Journal for Numerical Methods in Engineering 109.12 (2017) 1623-1654

EQP non-negative least-square problem

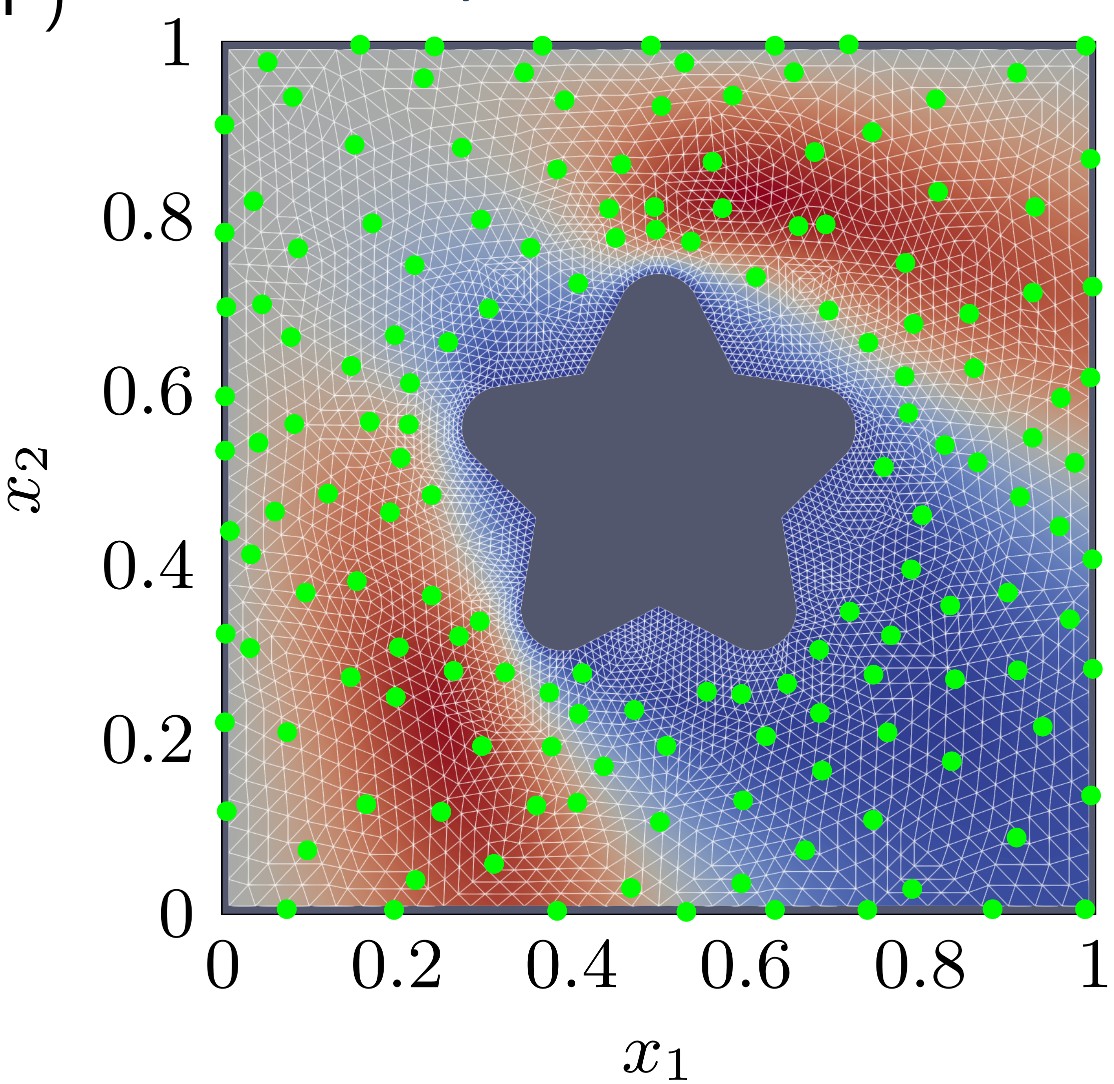
Find minimum $N_k > 0$ and $\{w_k\}$, $\{\mathbf{x}_k\}$ such that

$$\max_{s,i} \left\| \left\langle \phi_i, \mathcal{N}[\mathbf{q}_s] \right\rangle_\Omega - \sum_k^{N_k} w_k \phi_i(\mathbf{x}_k) \mathcal{N}[\mathbf{q}_s(\mathbf{x}_k)] \right\| < \epsilon$$

Performance comparison

	Tensor	EQP
Vel error	0.17%	0.36%
Pres error	0.35%	0.32%
Speed-up	10.47x	10.25x

ROM prediction with 155 EQP



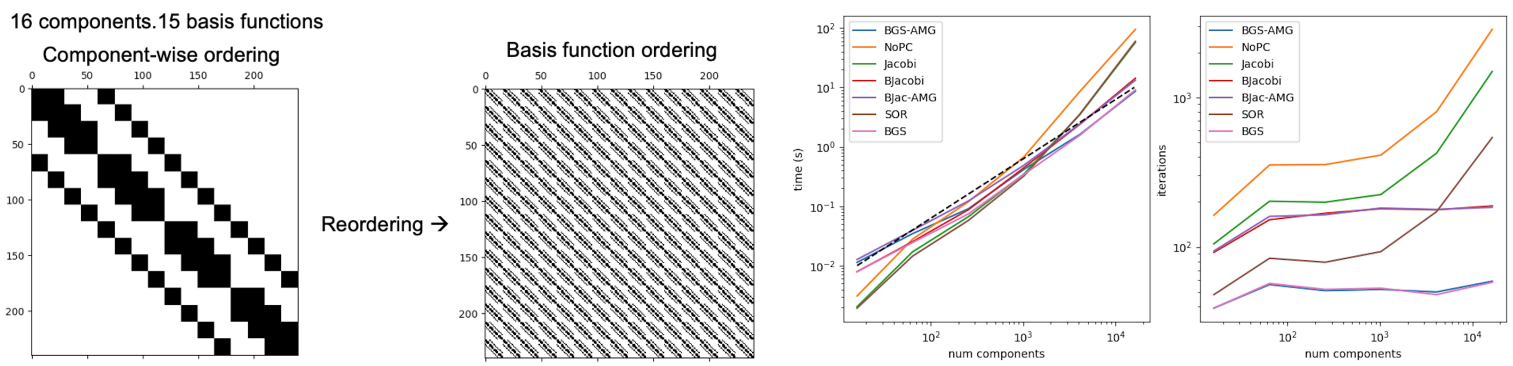
Moving forward—

S. Chung, Y. Choi, P. Roy, T. Moore, T. Roy, T. Y. Lin, D. Y. Nguyen, C. Hahn, E. B. Duoss, S. E. Baker,
"Train Small, Model Big: Scalable Physics Simulators via Reduced Order Modeling and Domain Decomposition",
arXiv:2401.10245 (2024) (submitted to Computer Methods in Applied Mechanics and Engineering)

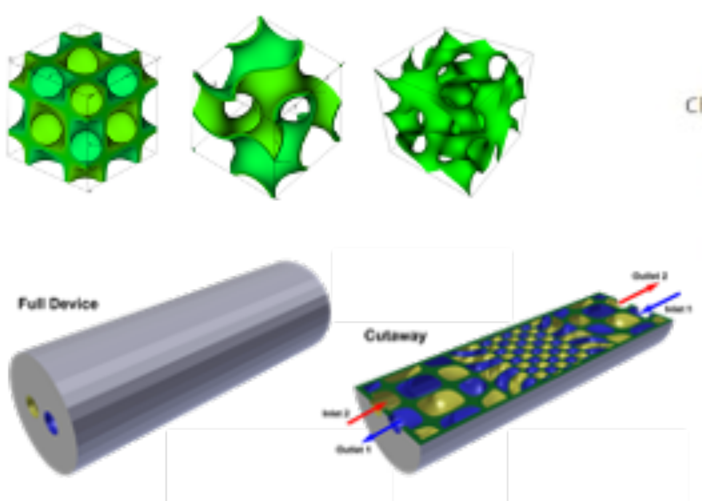
- scaleupROM: https://github.com/LLNL/scaleupROM.git
- Active development toward more complex physics
  - Unsteady N-S flow, nonlinear elasticity, ...
- Preconditioning for ROM-FEM

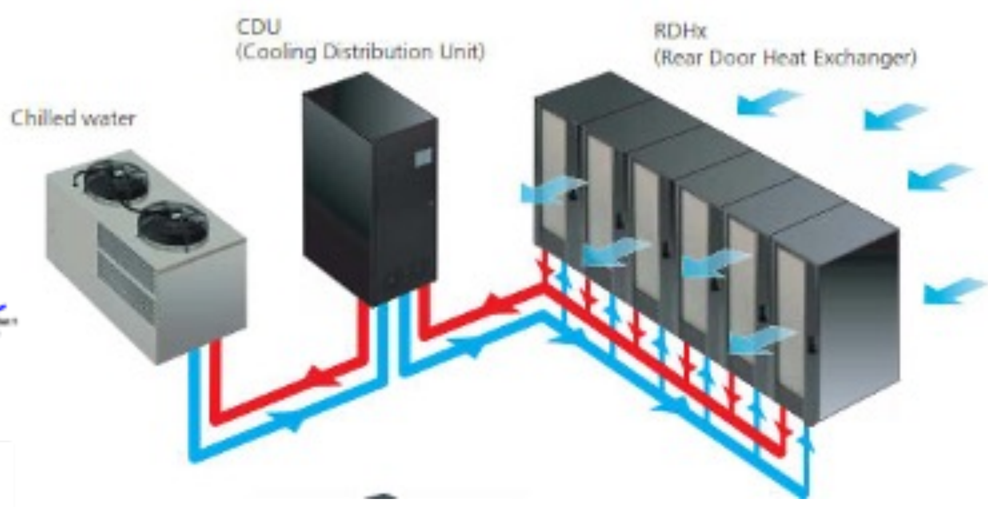
Direct air capture column

Preconditioner for iterative ROM-FEM solver



Data center heat exchanger





Acknowledgement

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Science of ScaleUp Reduced Order Modeling Team


Youngsoo Choi


Pratanu Roy


Thomas Roy


Tiras Lin


Du Nguyen


Thomas Moore
(Currently at QUT)


Chris Hahn


Eric Duoss


Sarah Baker

libROM
LIBRARY FOR REDUCED ORDER MODELS

LLNL libROM group

Siu Wun Cheong
Dylan Copeland
Eric Chin
Coleman Kendrick
William Anderson
Paul Tranquilli

Thank you for your attention. Any questions?

Lawrence Livermore National Laboratory