Accelerating Physical Simulations with Reduced Order Models

Dylan Copeland, Siu Wun Cheung, Youngsoo Choi, Kevin Huynh

MLDL 2022

LLNL-PRES-833627

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

LLNL ROM Team

Dylan Copeland

Siu Wun (Tony) Cheung

Youngsoo Choi

Kevin Huynh

libROM
LIBRARY FOR REDUCED ORDER MODELS

Outline

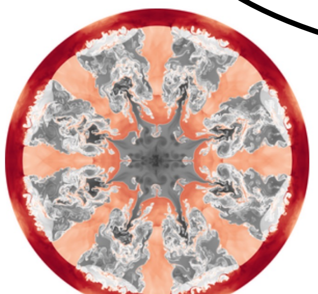
I. Linear subspace ROM
   - Nonlinear radiation diffusion

II. Time-windowing ROM
   - Lagrangian hydrodynamics

What is a reduced order model (ROM)?

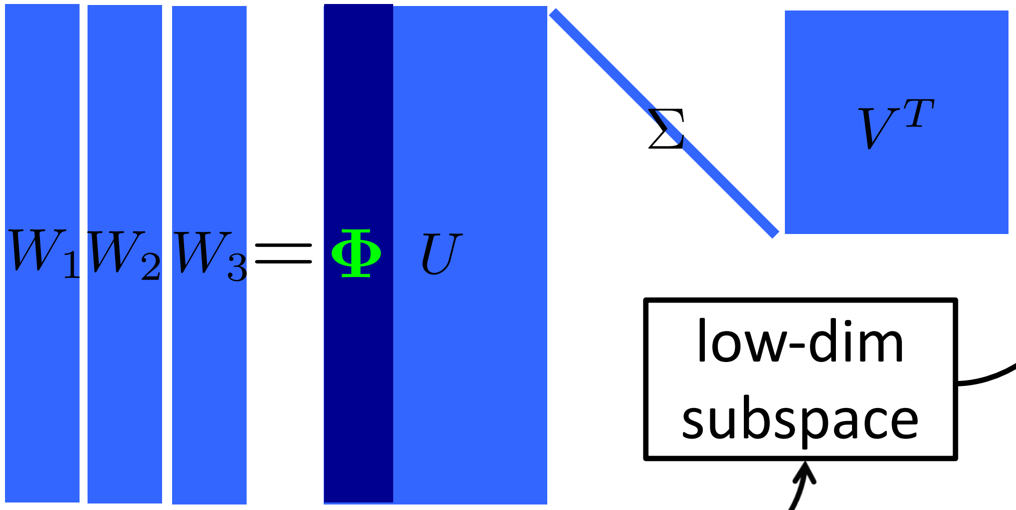
Goal: accelerate physics simulation without losing much accuracy by exploiting data and governing equations [**Data-driven and projection-based**].

high fidelity models / experiments



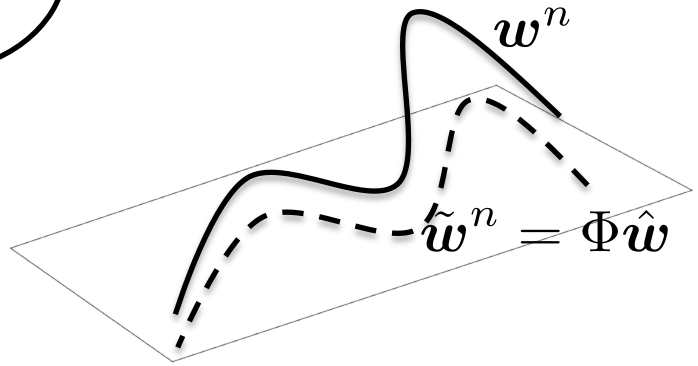
ICF-like Implosion (BLAST)

collect & compress data



low-dim subspace

project & propagate ***governing equation*** in time



approximate system solution

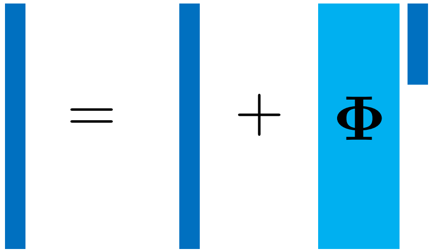
libROM
LIBRARY FOR REDUCED ORDER MODELS

Open source libROM (https://github.com/LLNL/libROM)

Reduced order model approach: projection-based (POD)

- Governing equation: $\dfrac{d\boldsymbol{w}}{dt} = \boldsymbol{f}(\boldsymbol{w}, t; \boldsymbol{\mu})$, $\quad \boldsymbol{w}, \boldsymbol{f} \in \mathbb{R}^{N_s}$
- Solution approximation:

$$\boldsymbol{w} \approx \tilde{\boldsymbol{w}} = \boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, \quad \boldsymbol{\Phi} \in \mathbb{R}^{N_s \times n_s}, \quad n_s \ll N_s$$



- Reduced system after Galerkin projection: $\dfrac{d\hat{\boldsymbol{w}}}{dt} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, t; \boldsymbol{\mu})$
- Euler time integrator: $\quad \hat{\boldsymbol{w}}_n = \hat{\boldsymbol{w}}_{n-1} + \Delta t \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, t; \boldsymbol{\mu})$

Scales with FOM size: $\mathbb{R}^{N_s}$ → Hyper-reduction (DEIM)

Radiation Diffusion

$$\eta_k \rho_k \frac{de_k}{dt} = c\eta_k \sigma_{p,k} (E - B(T(e_k))) + Q$$

$$\frac{dE}{dt} + \nabla \cdot F = -\sum_k c\eta_k \sigma_{p,k} (E - B(T(e_k))) - \frac{4}{3} EI : \nabla \mathbf{v} + S$$

$$\frac{1}{3}\nabla E = -\sum_k \eta_k \frac{\sigma_{r,k}}{c} F$$

$$c\mathcal{A}E - \mathcal{B}n \cdot F = \mathcal{C} \qquad \text{on boundary}$$

Nonlinear system solved on each implicit timestep:

$$\begin{cases} L_{\rho_k}\mathbf{k}_{\mathbf{e_k}} + H_k(\mathbf{k}_{\mathbf{e_k}}) - c\Delta t L_{\sigma_k}\mathbf{k}_{\mathbf{E}} & = S_{e_k} \\ \sum_k H_k(\mathbf{k}_{\mathbf{e_k}}) + L\mathbf{k}_{\mathbf{E}} + c\Delta t \sum_k L_{\sigma_k}\mathbf{k}_{\mathbf{E}} + D\mathbf{F} & = S_E \\ \frac{1}{c}R_\sigma \mathbf{F} + \frac{1}{3}R_n\mathbf{F} - \frac{1}{3}\Delta t D^T \mathbf{k}_{\mathbf{E}} & = S_F \end{cases}$$

$$\text{Backward Euler} \begin{cases} e_k^{n+1} = e_k^n + \Delta t \mathbf{k}_{\mathbf{e_k}}, \\ E^{n+1} = (L^{n+1})^{-1} L^n E^n + \Delta t \mathbf{k}_{\mathbf{E}} \end{cases}$$

ROM Formulation of Radiation Diffusion

$$V_{e_k}^T L_{\rho_k} V_{e_k} \mathbf{u}_{\mathbf{e_k}} + V_{e_k}^T H_k(V_{e_k} \mathbf{u}_{\mathbf{e_k}}) - c\Delta t V_{e_k}^T L_{\sigma_k} V_E \mathbf{u}_\mathbf{E} = V_{e_k}^T S_{e_k}$$

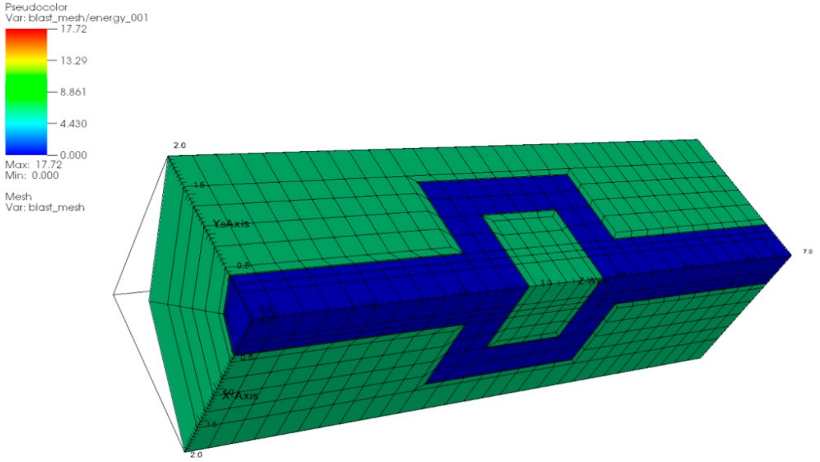
$$V_E^T \sum_k H_k(V_{e_k} \mathbf{u}_{\mathbf{e_k}}) + V_E^T L V_E \mathbf{u}_\mathbf{E} + c\Delta t \sum_k V_E^T L_{\sigma_k} V_E \mathbf{u}_\mathbf{E} + V_E^T D V_F \mathbf{u}_\mathbf{F} = V_E^T S_E$$

$$\frac{1}{c} V_F^T R_\sigma V_F \mathbf{u}_\mathbf{F} + \frac{1}{3} V_F^T R_n V_F \mathbf{u}_\mathbf{F} - \frac{1}{3} \Delta t V_F^T D^T V_E \mathbf{u}_\mathbf{E} = V_F^T S_F$$

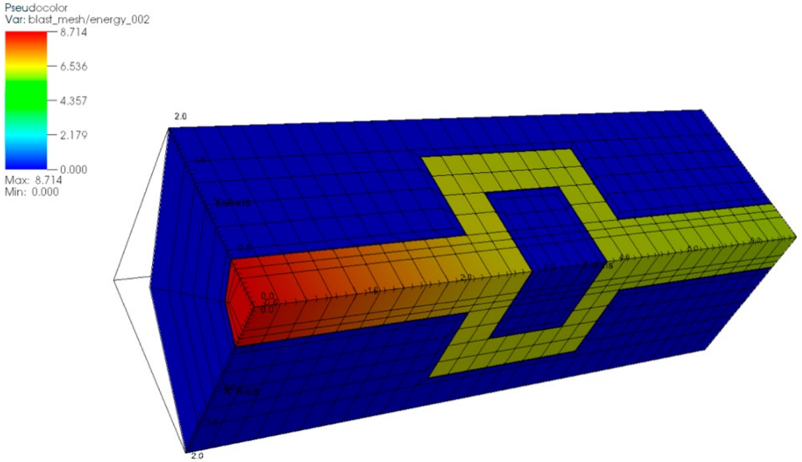
- Hyper-reduction (DEIM) is applied to the nonlinear terms and time-dependent terms (almost all terms).
- Newton’s method solves this small nonlinear system, with a direct solver for Jacobian.

3D Crooked Pipe Test in BLAST (t=600)

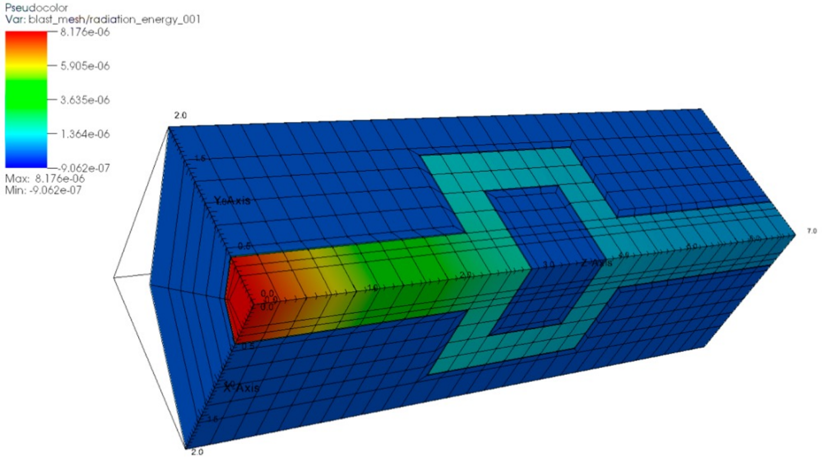
Material energy e_1



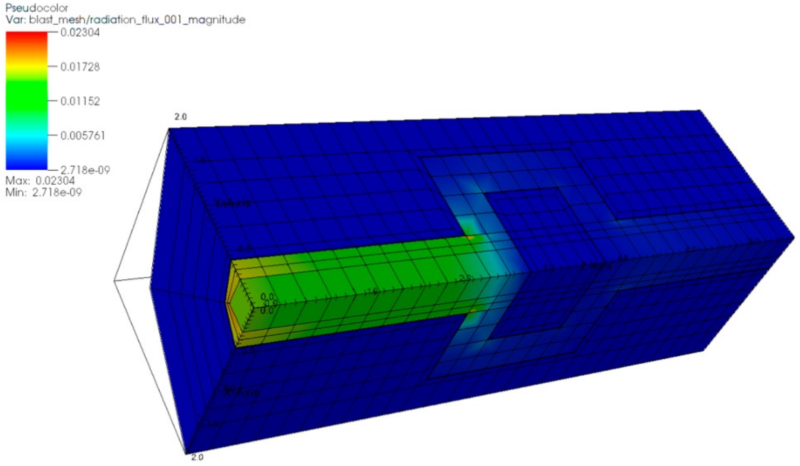
Material energy e_2



Radiation energy E



Radiation flux $|F|$



3D Crooked Pipe Test in BLAST (t=600)

DEIM	FEM order	e_1	e_2	E	F
No	1	4.3850e-04	0.0020195	0.019778	0.0061067
Yes	1	1.9267e-04	0.0014174	0.033249	0.0014944
No	2	2.24799e-04	0.00102656	0.0104595	0.00210421
Yes	2	3.76328e-04	6.51531e-04	0.0254946	0.00338081

Table 1: Relative $L^2(\Omega)$ errors.

FEM order	FOM energy	FOM flux	e_0	e_1	E	F	H_0	H_1
1	4928×3	16268	14	11	5	6	5	1
2	16632×3	53235	17	10	6	7	6	1

Table 2: Basis sizes.

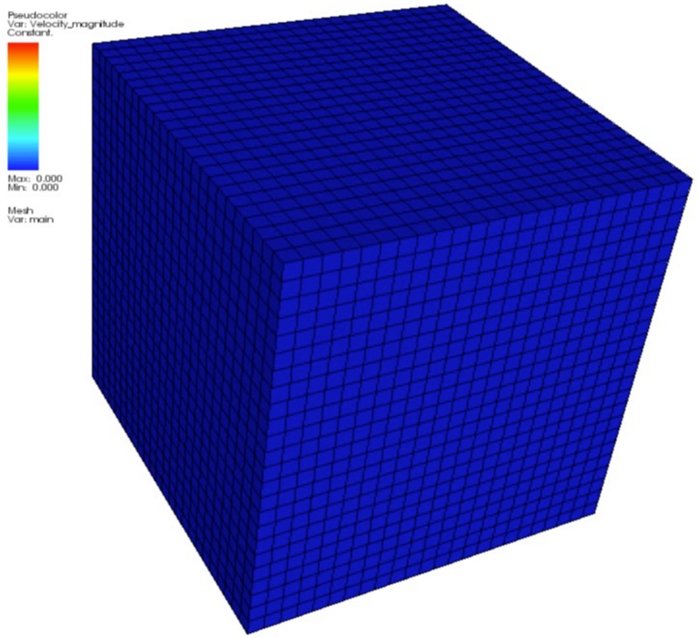
FEM order	FOM wall time	ROM speed-up	ROM-DEIM speed-up
1	55 s	4.6	**11.2**
2	586 s	7.5	**19.5**

Table 3: Run-time comparisons.

- FOM simulation used 8 MPI ranks, and ROM is serial, so speed-up could be multiplied by 8.

Challenges for linear subspace reduced order models

- This ROM formulation relies on a “*linear subspace*” solution representation
  - Cannot represent “*advection-dominated*” solution with a small basis
  - Sharp gradients, moving shocks, mesh deformation introduce extra challenges



- We need a more robust ROM approach!

Lagrangian hydrodynamics

- **Semi-discrete Lagrangian nonlinear conservation laws**

momentum conservation: $$\boldsymbol{M}_{\mathcal{V}} \frac{d\boldsymbol{v}}{dt} = -\boldsymbol{F} \cdot \mathbf{1}$$

energy conservation: $$\boldsymbol{M}_{\mathcal{E}} \frac{d\boldsymbol{e}}{dt} = -\boldsymbol{F}^T \cdot \boldsymbol{v}$$

equation of motion: $$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}$$

- **Explicit time integration with adaptive time-stepping: RK4, RK2-Average**
- **Mesh nodes move with the position variable $\boldsymbol{x}$**
- **Laghos[1] (high-order FEM Lagrangian hydrodynamics MFEM miniapp) is used for FOM simulation**
  - Kinematic space, $\mathcal{V} \subset \left[H^1(\tilde{\Omega})\right]^d$
  - Thermodynamics space, $\mathcal{E} \subset L_2(\tilde{\Omega})$

[1] Open source code; github page (https://github.com/CEED/Laghos)

ROM formulation for Lagrangian hydrodynamics

- **Substitute bases for each variable, then use Galerkin projection:**

momentum conservation: $\hat{\boldsymbol{M}}_{\mathcal{V}} \frac{d\hat{\boldsymbol{v}}}{dt} = -\boldsymbol{\Phi}_v^T \boldsymbol{F} \cdot \mathbf{1}$

energy conservation: $\hat{\boldsymbol{M}}_{\mathcal{E}} \frac{d\hat{\boldsymbol{e}}}{dt} = -\boldsymbol{\Phi}_e^T \boldsymbol{F}^T \cdot \boldsymbol{v}$

equation of motion: $\frac{d\hat{\boldsymbol{x}}}{dt} = \boldsymbol{\Phi}_x^T \boldsymbol{\Phi}_v \hat{\boldsymbol{v}}$

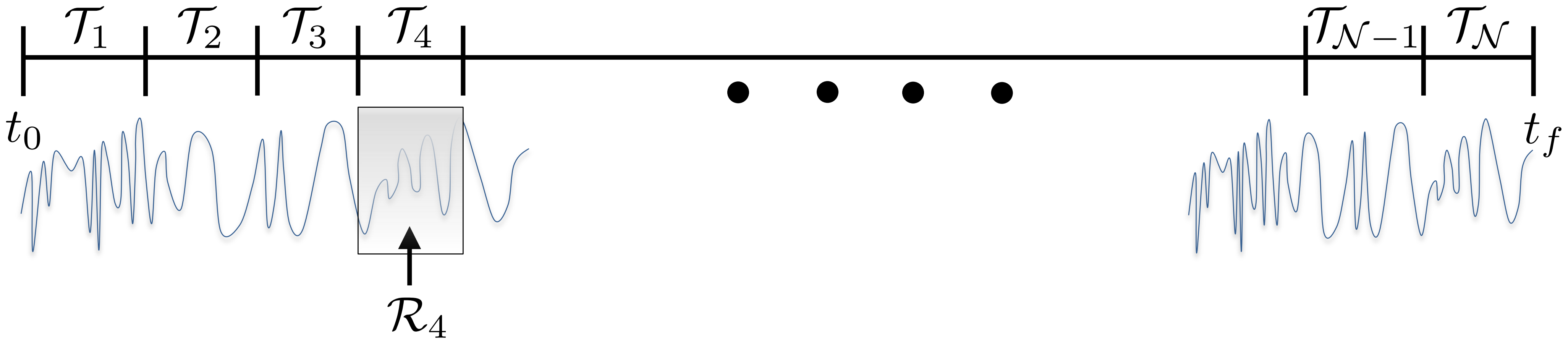
- **The reduced mass matrices:** $\hat{\boldsymbol{M}}_{\mathcal{V}} \equiv \boldsymbol{\Phi}_v^T \boldsymbol{M}_{\mathcal{V}} \boldsymbol{\Phi}_v, \quad \hat{\boldsymbol{M}}_{\mathcal{E}} \equiv \boldsymbol{\Phi}_e^T \boldsymbol{M}_{\mathcal{E}} \boldsymbol{\Phi}_e$
- **Formulating without FOM mass matrix inverses allows for much less DEIM sampling!**
- **Solution offsets are important for basis accuracy!**
- **Solution spaces (SNS) work well for the nonlinear terms (hyper-reduced by DEIM):** $\boldsymbol{f}_m = -\boldsymbol{F} \cdot \mathbf{1}, \qquad \boldsymbol{f}_e = -\boldsymbol{F}^T \cdot \boldsymbol{v}$

Relevant previous work

- Laghos (Lagrangian hydrodynamics high-order FEM solver) is based on:
  Dobrev, Kolev, Rieben, *High-order curvilinear finite element methods for Lagrangian hydrodynamics*, SIAM Journal on Scientific Computing, 34(5):B606–B641, 2012.
- Lagrangian POD for 1D convection-diffusion:
  Mojgani, Balajewicz, *Lagrangian basis method for dimensionality reduction of convection dominated nonlinear flows*, preprint arXiv:1701.04343, 2017.
- Dynamic mode decomposition (DMD) for 1D advection-diffusion:
  Lu, Tartakovsky, *Lagrangian dynamic mode decomposition for construction of reduced-order models of advection-dominated phenomena*, Journal of Computational Physics, 407:109229, 2020.
- In this work, time-windowing ROM is used for 2D and 3D Lagrangian advection-dominated problems.
- Copeland, Cheung, Huynh, Choi, *Reduced order models for Lagrangian Hydrodynamics*, Computer Methods in Applied Mechanics and Engineering, Volume 338, 114259, 2022.

Time-windowing ROM

- Decompose the whole-time domain into $\mathcal{N}$ small time windows

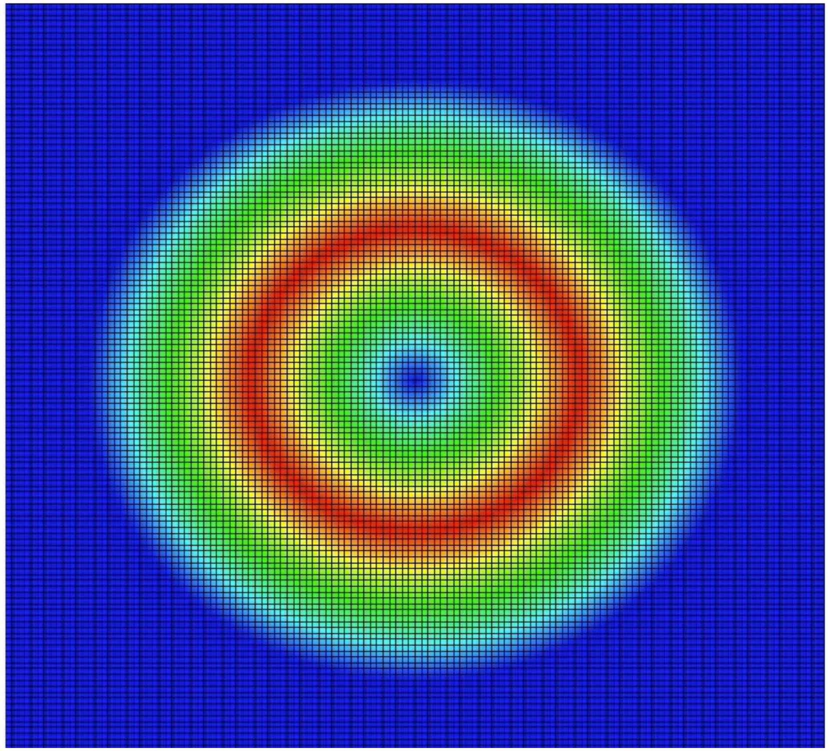


- Generate FOM solution data over the whole-time domain
- Extract each time window data and build a local ROM, $\mathcal{R}_k$, for k-th time window
- For parametric training, snapshots for all parameters are merged for each window
- Hyper-reduction is done with oversampled DEIM

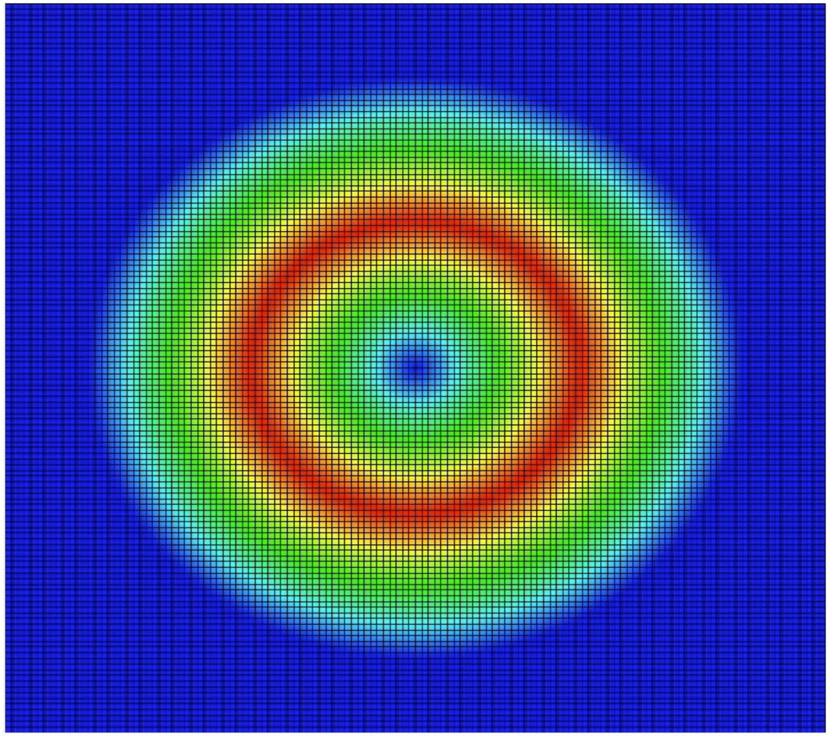
\+ Each local ROM must be accurate

\+ Local window basis size must be small to ensure speed

Gresho vortex (reproductive test, tf=0.62 sec)



FOM



ROM

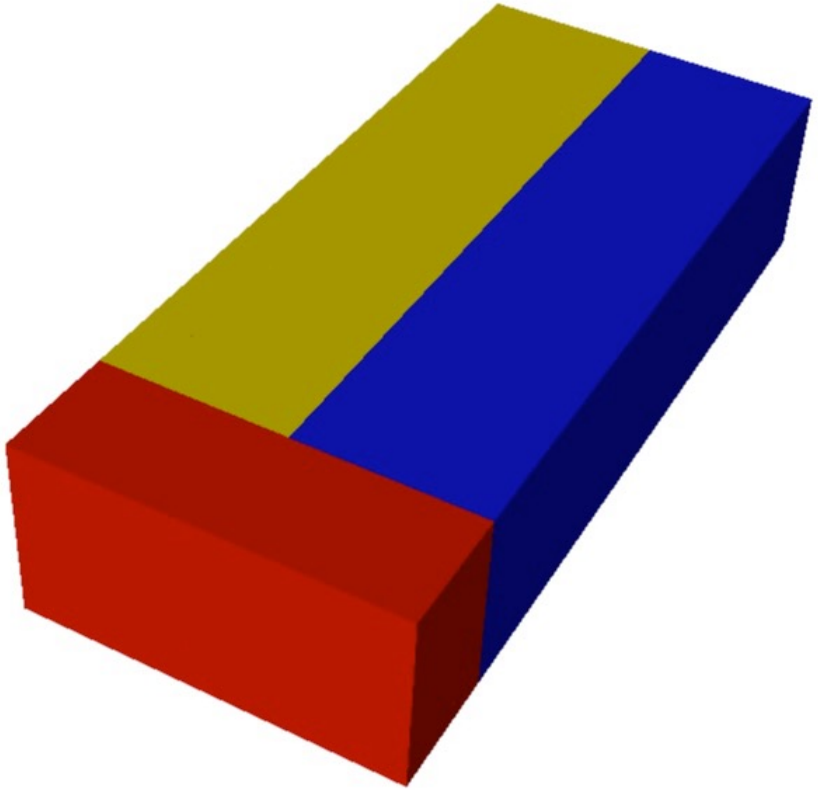
Kinematic dofs: 18,818, order 4
Energy dofs: 9,216, order 3
RK2-Average time integration
1672 FOM timesteps

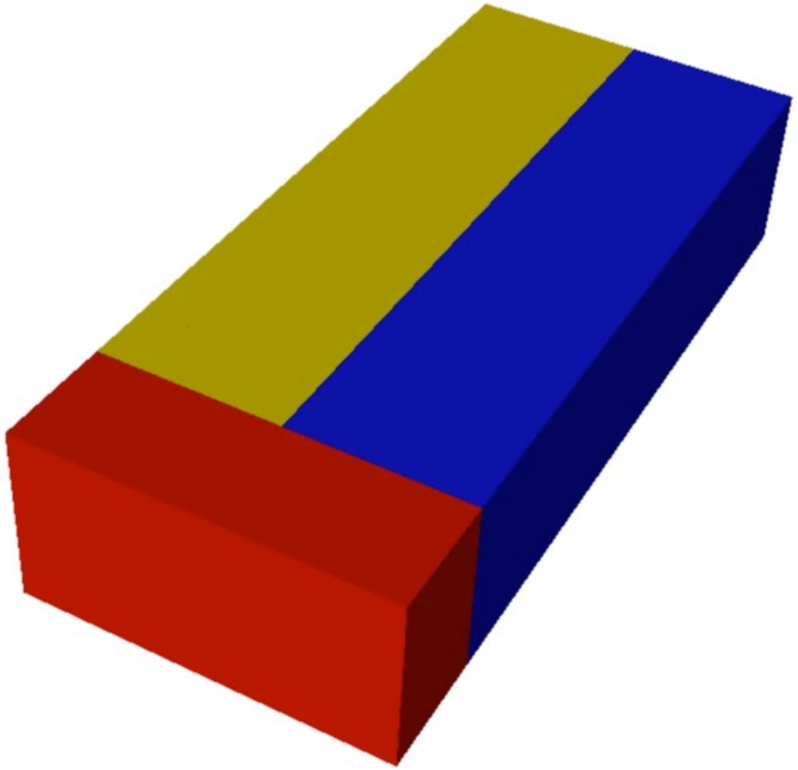
+ Speed-up: 25
- 335 windows
- Max basis size:
  position: 6
  velocity: 8
  energy: 10

Relative differences

Position: 4.3E-7
Velocity: 3.5E-6
Energy : 3.5E-7

Triple-point (reproductive test, tf=0.8 sec)





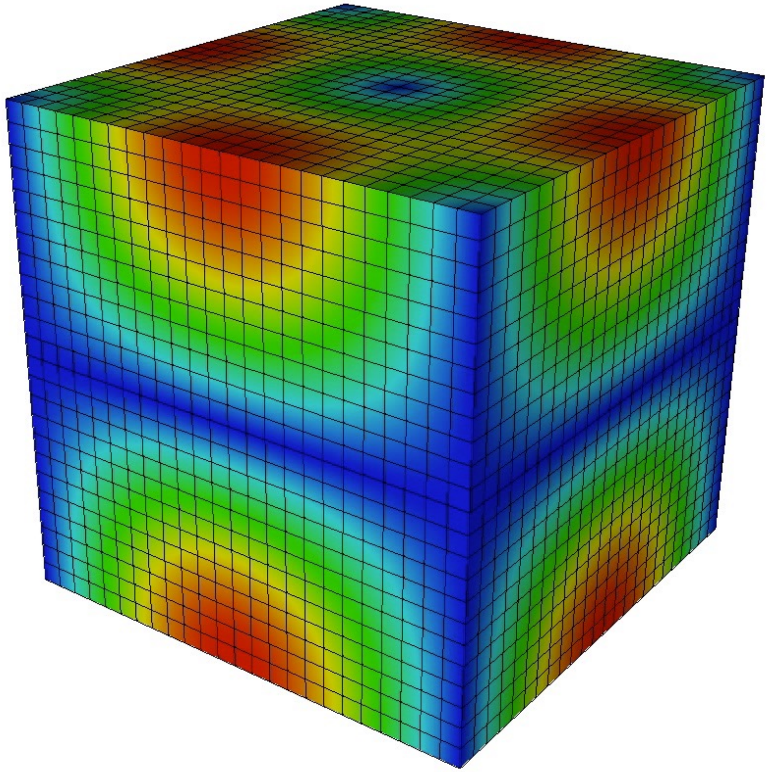
Kinematic dofs: 38,475, order 3
Energy dofs: 10,752, order 2
RK4 time integration, 193 FOM steps

Relative differences

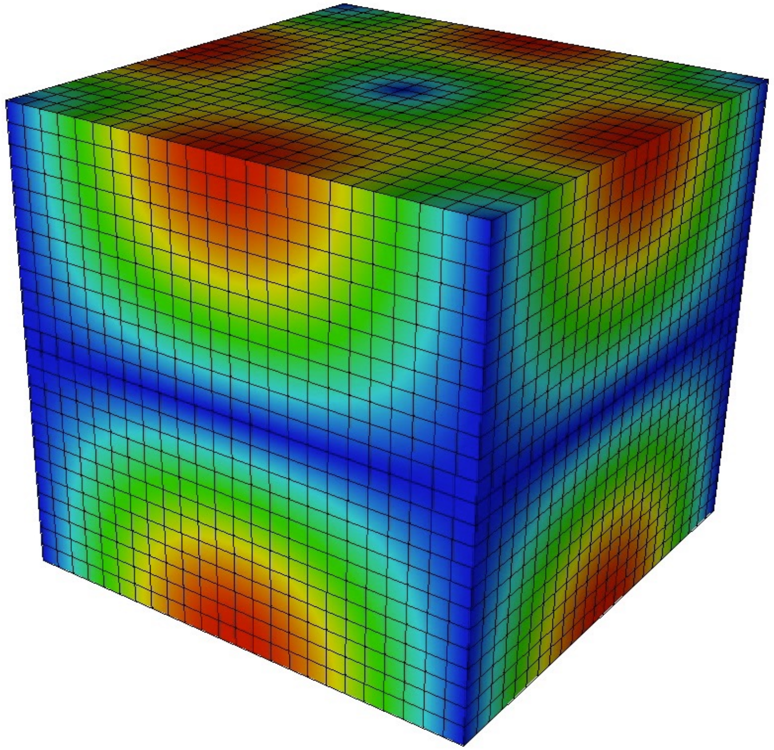
Position: 3.8e-5
Velocity: 9.3e-4
Energy : 7.0e-4

+ Speed-up: 75
- 39 windows
- Max basis size:
  position: 5
  velocity: 7
  energy: 8

Taylor–Green (reproductive test, tf=0.25 sec)



FOM



ROM

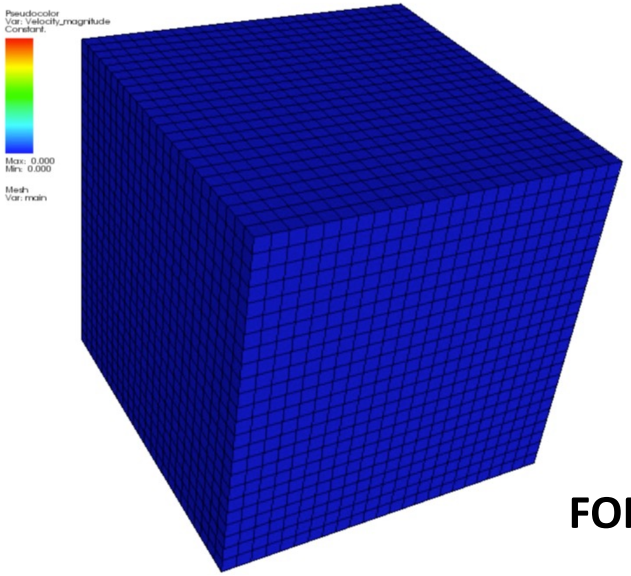
Kinematic dofs: 14,739, order 3
Energy dofs: 4,096, order 2
RK4 time integration, 897 FOM steps

Relative differences

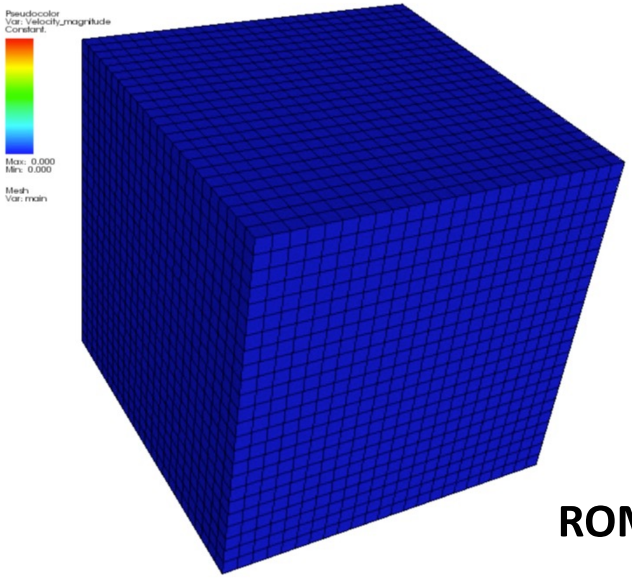
Position: 7.0e-9
Velocity: 1.2e-6
Energy : 5.4e-8

+ Speed-up: 23
- 180 windows
- Max basis size:
  position: 2
  velocity: 3
  energy: 5

Sedov blast (reproductive test, tf=0.8 sec)



FOM



ROM

Kinematic dofs: 14,739, order 3
Energy dofs: 4,096, order 2
RK4 time integration, 719 FOM steps
Delta function energy source at origin

No time–windowing

Relative differences

Position: 0.0001
Velocity: 0.0097
Energy : 0.0002

- + Speed-up: 1.7
- Basis size:
  - position: 29
  - velocity: 169
  - energy: 26

Time–windowing

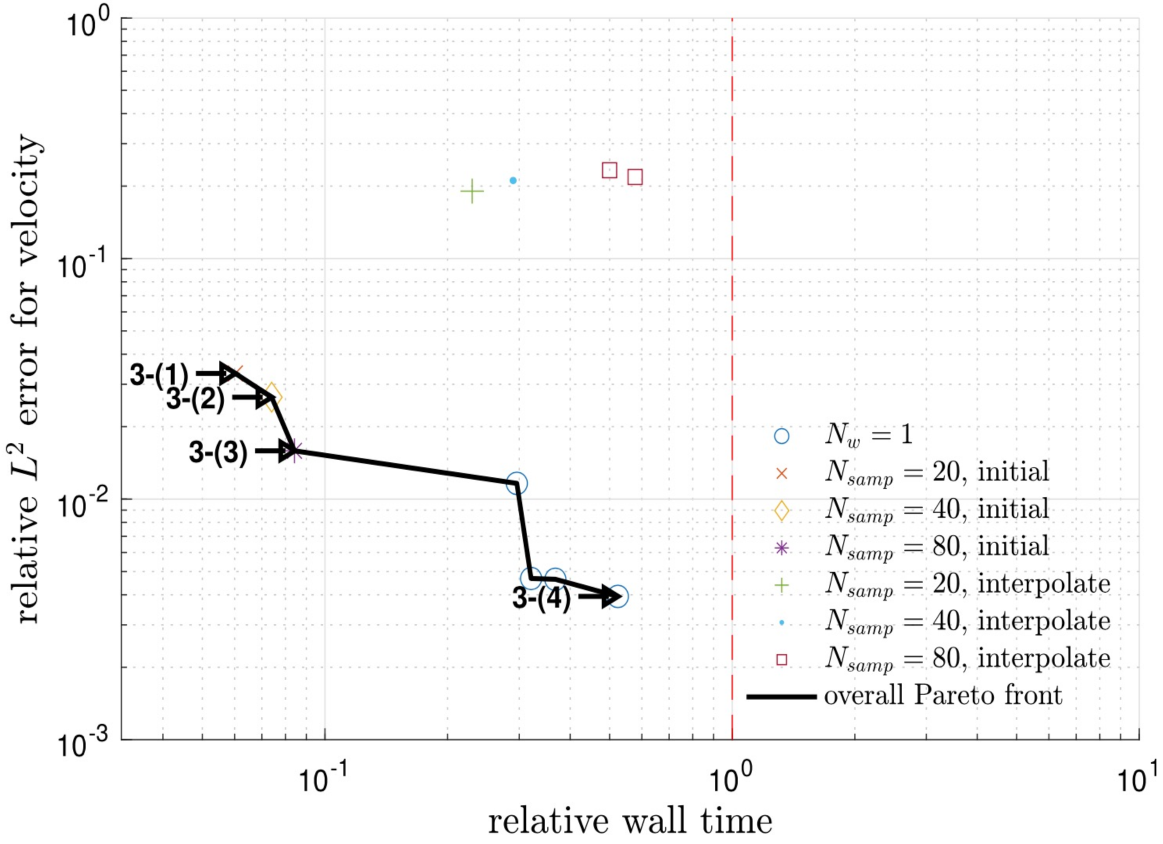
Relative differences

Position: 3.9e-5
Velocity: 4.6e-4
Energy : 3.0E-5

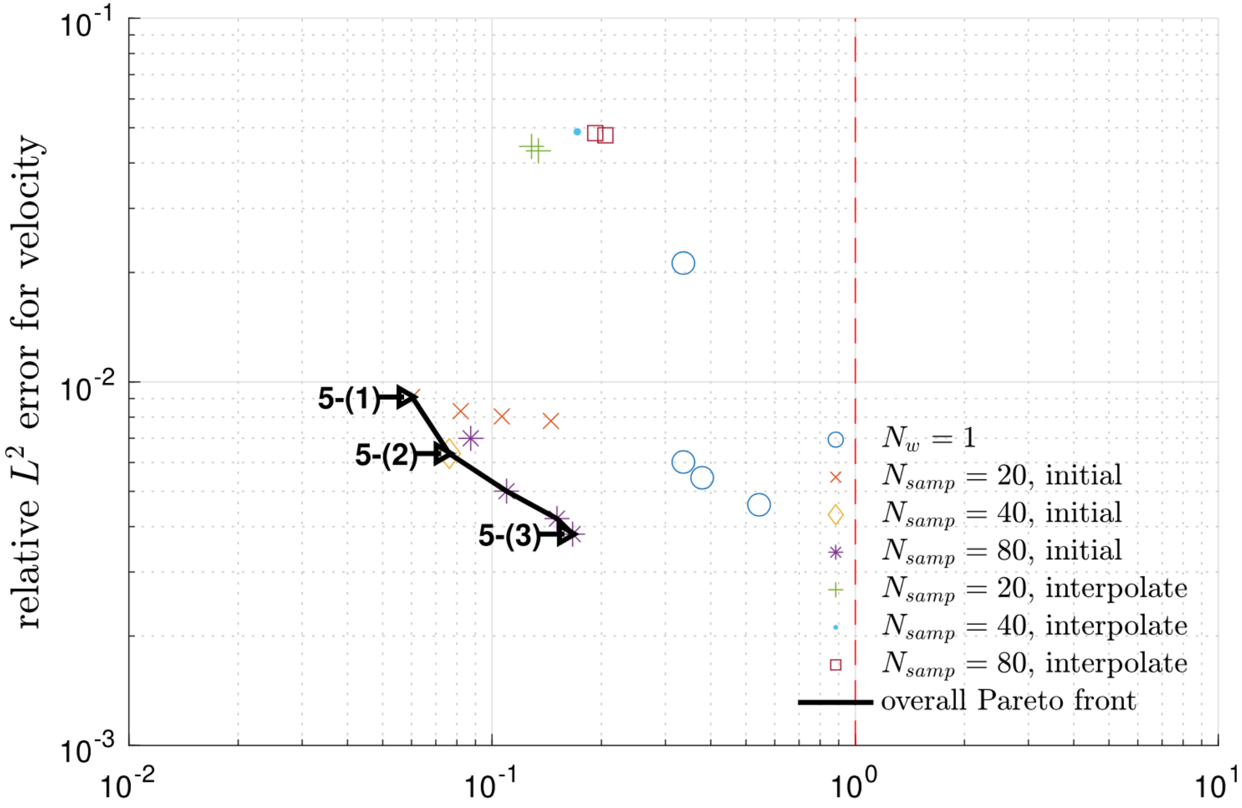
- + Speed-up: 26
- 144 windows
- Max basis size:
  - position: 7
  - velocity: 10
  - energy: 7

Predictive ROM in Laghos: Sedov blast with parameter variation

Energy source relative magnitude parameter training values: μ in {0.8, 1, 1.2}



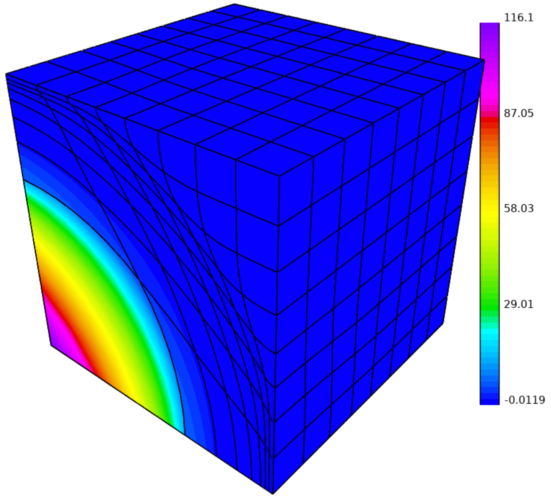
μ = 0.7 predictive, extrapolating

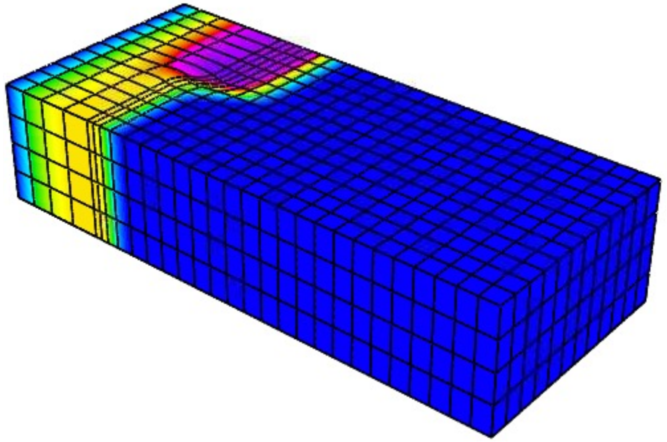


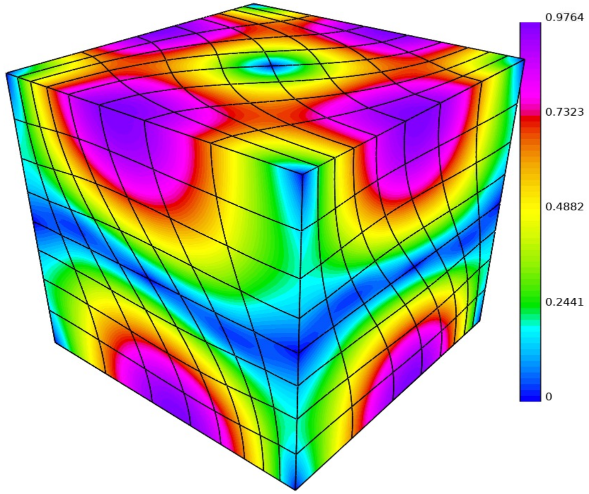
μ = 0.9 predictive, interpolating

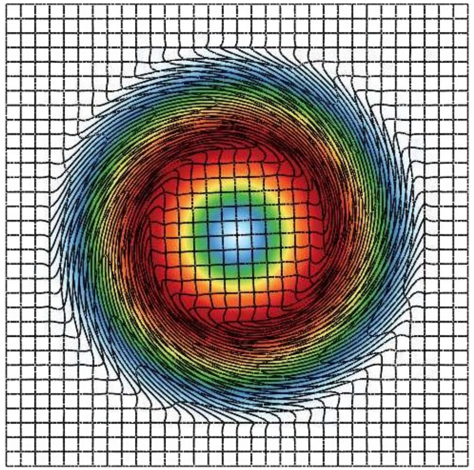
Summary and future work

+ Linear subspace ROM works well for nonlinear diffusion problems
+ Time-windowing ROM achieved good accuracy and speed-up for hydrodynamics
+ Speed-up should be greater for larger problems (higher order, larger mesh)
+ Parametric cases were solved accurately and robustly
+ libROM is efficient, scalable, and parallel



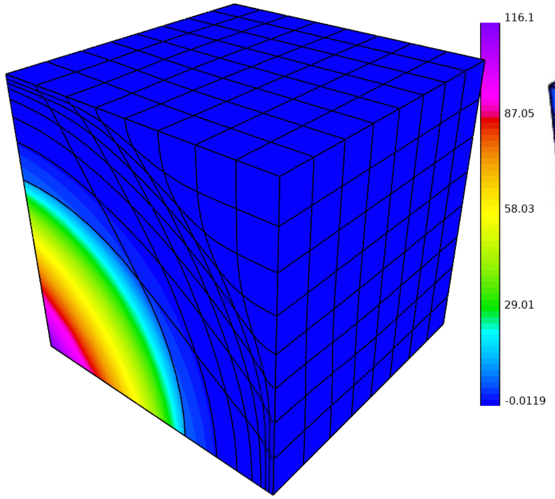


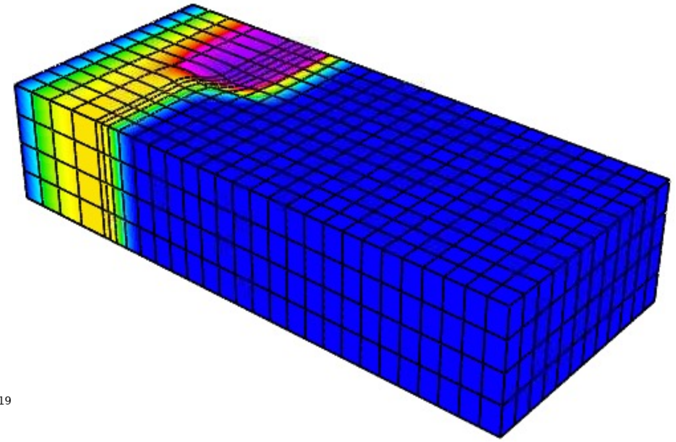


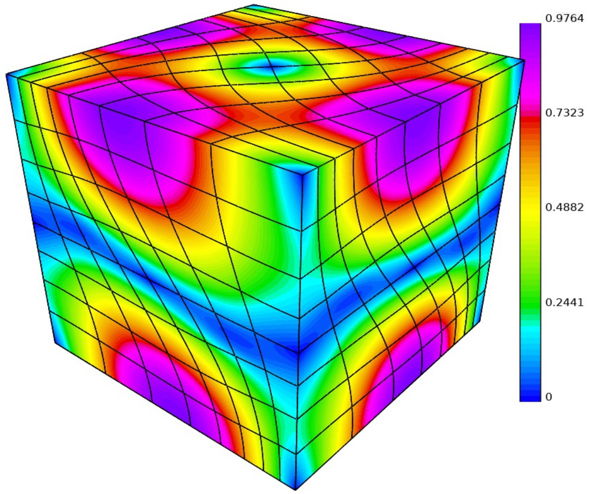


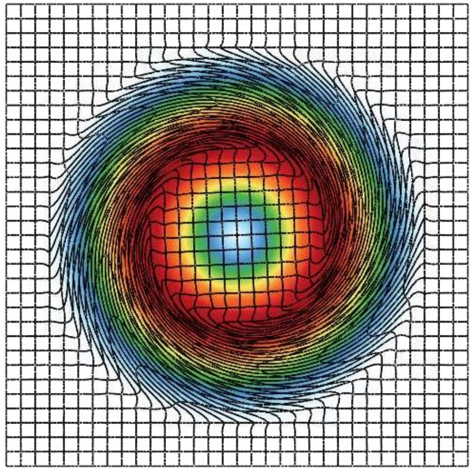
Summary and future work

- **Future work**
  - Develop space-time ROM or nonlinear manifold ROM for these applications.
  - Apply ROM to more challenging applications, such as ALE hydrodynamics.









Thank you for your attention!

copeland11@llnl.gov

Lawrence Livermore National Laboratory