Model-order reduction for multiphysics reactor applications

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Department of Nuclear Engineering
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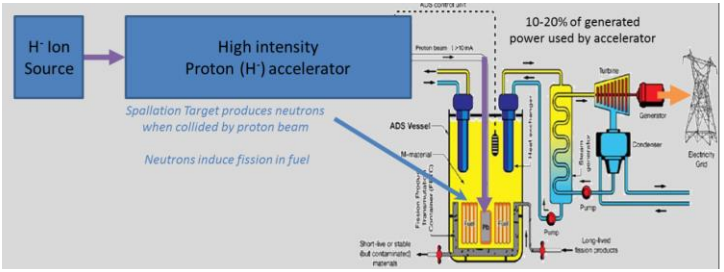
Joint ICTP-IAEA Advanced School/Workshop on Computational Nuclear Science and Engineering, May 26, 2022

← That's me (on GitHub)

← That's me (in real life)

- Accelerator-driven production of tritium (mid-90's)



$^{7}LiF - BeF_2 - {}^{233}UF_4$

- Near real-time PWR accident simulator for crisis management (early 2000's)

Reactor physics and Applied Math Department

cea

INP Grenoble

- 2004-present: Nuclear engineering, Texas A&M U.

Computational radiation transport, Multiphysics, and Predictive science https://multiphysics.engr.tamu.edu/

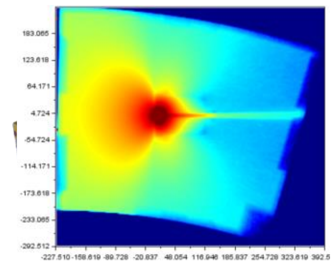
NUCLEAR ENGINEERING
TEXAS A&M UNIVERSITY

My research interests

- **Radiation transport**

  Predictive Science Academic Alliance Program (PSAAP)

  National Nuclear Security Administration

  CERT

  Center for Exascale Radiation Transport

  http://class.tamu.edu/cert

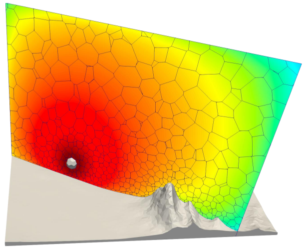
  Stockpile stewardship

  Lawrence Livermore National Laboratory

- **Multiphysics** software development (Griffin, Pronghorn, RELAP)

  MOOSE

  INL Idaho National Laboratory



- **Data sciences and machine-learning**

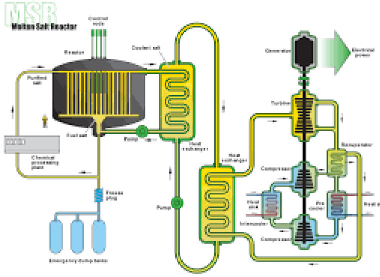
  Nuclear radiation effects

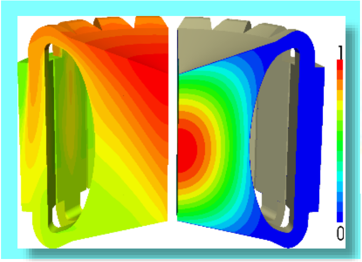
  DTRA DEFENSE THREAT REDUCTION AGENCY *Detect. Deter. Defeat.*

  Multiphysics model reduction

  NEUP Nuclear Energy University Program

  U.S. Department of Energy





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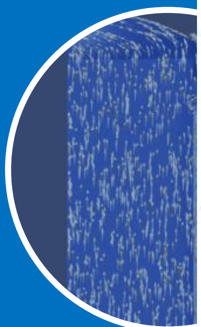

Modeling a... simulation...

- Developmen... / models for phenomena ... MSRs
- Application ... Science for r... design optim... and uncertai... quantificatio...
- System performance

...gies

- ...ent and ...tion of ...nd thermal
- ...totype built ...ring ...nd materials
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Education and training: development of human capital and expertise

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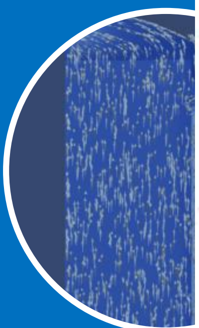

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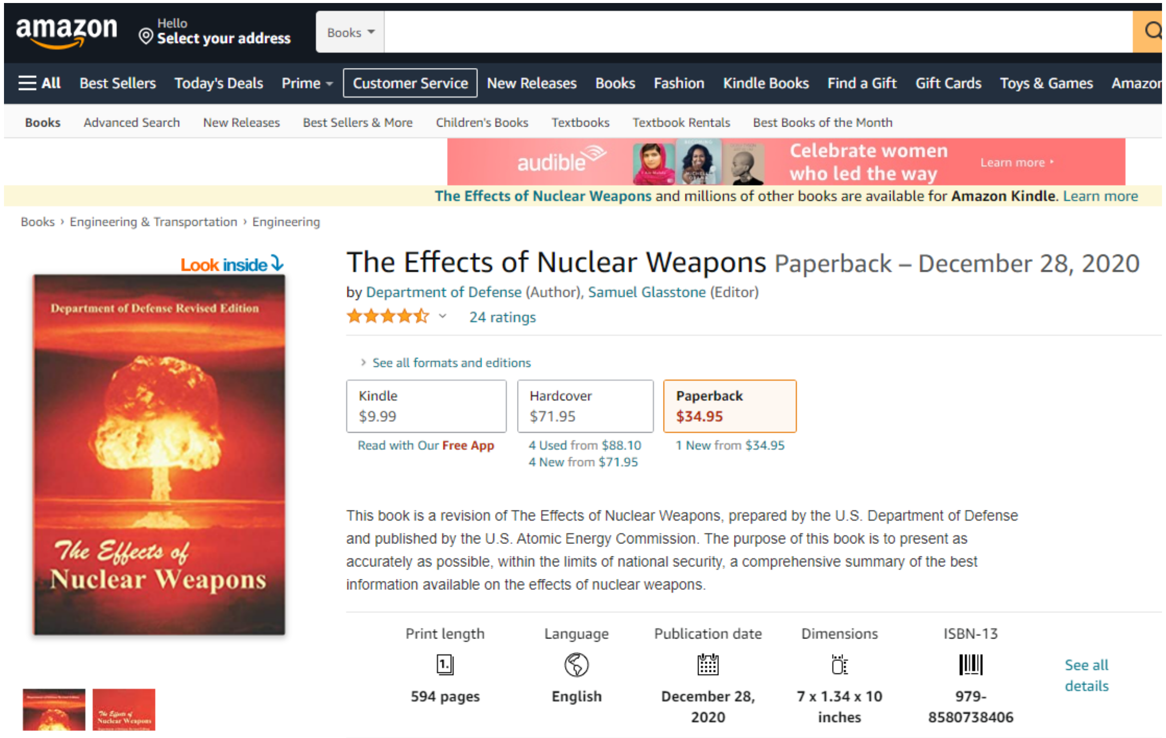
  - ***DOD/DTRA (2017-2021)***
  - ***Highlights:***
    - **Development of reduced-order models for radiation transport**



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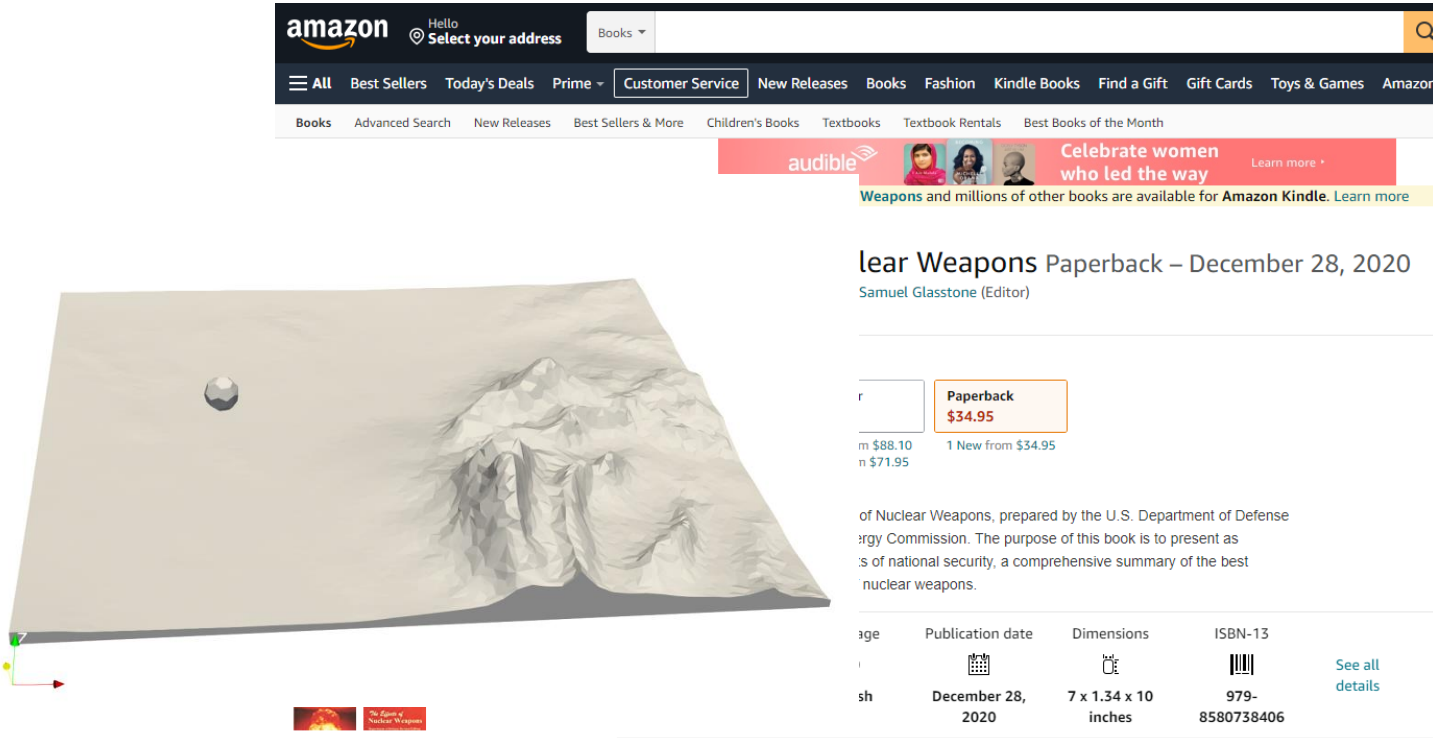

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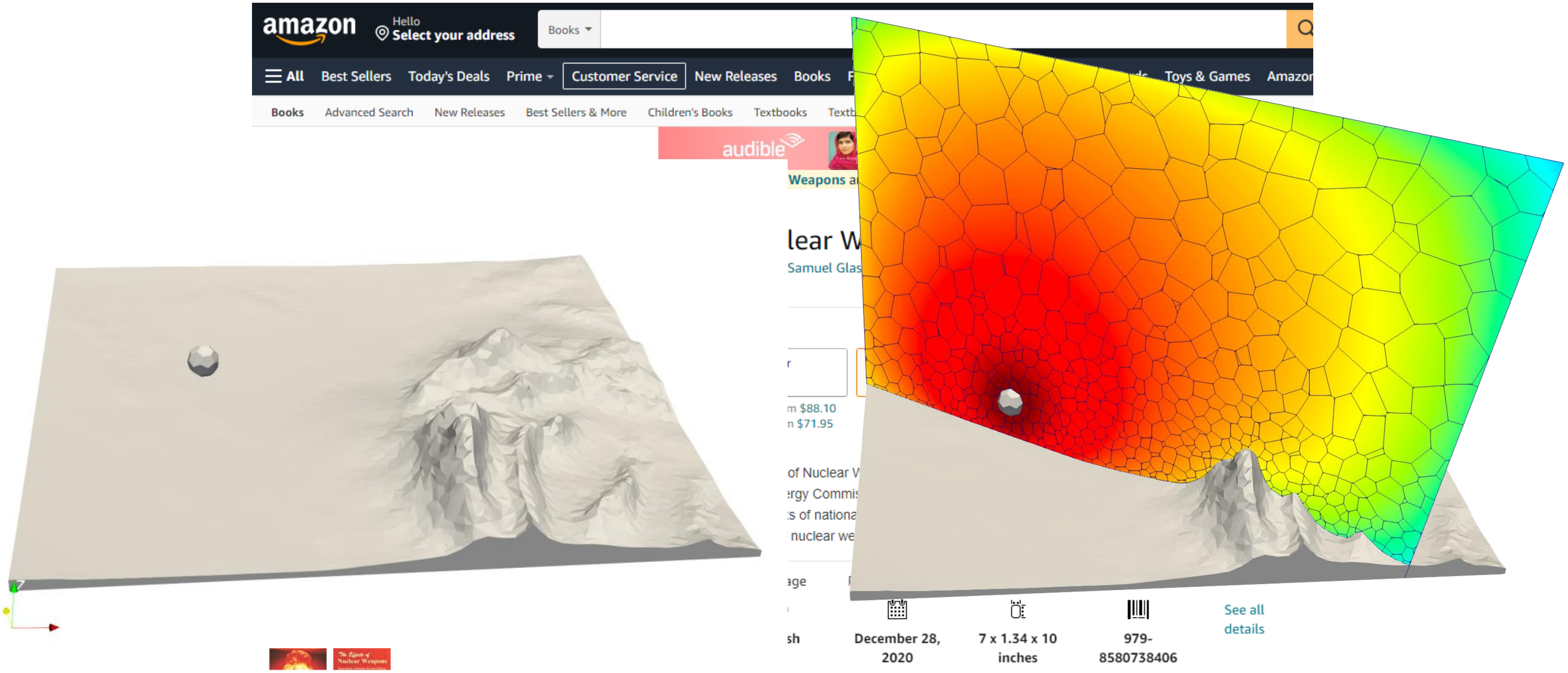

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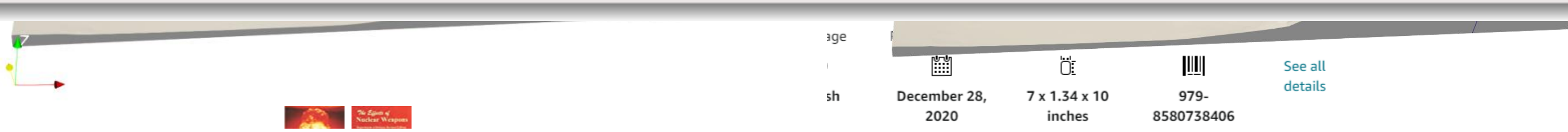
Quantities of Interest, QoI

- Functionals of the computed solution:

$$\text{QoI} = \int_0^\infty dE \int_{\text{RoI}} d^3r\, \varrho(\boldsymbol{r}, E) \int_{4\pi} d\Omega\, \Psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$$

- Examples: dose, dose rates, fluence, fluence rates, radiation fluxes through boundaries, SREMP and SGEMP fields.
- Usually defined on a subset of the computational domain (= Region of Interest)
- Can be transferred to other physics models to compute important effects (bio., electronic, etc.).



Outline

1. High-performance computing (HPC)
   - *A. Some history*
   - *B. Some well-recognized software used in nuclear engineering*
   - *C. A few application examples*
2. Fast Data-driven Surrogate Models
   - *A. Motivations for parametric Reduced-Order Modeling (ROM)*
   - *B. What is model-order reduction?*
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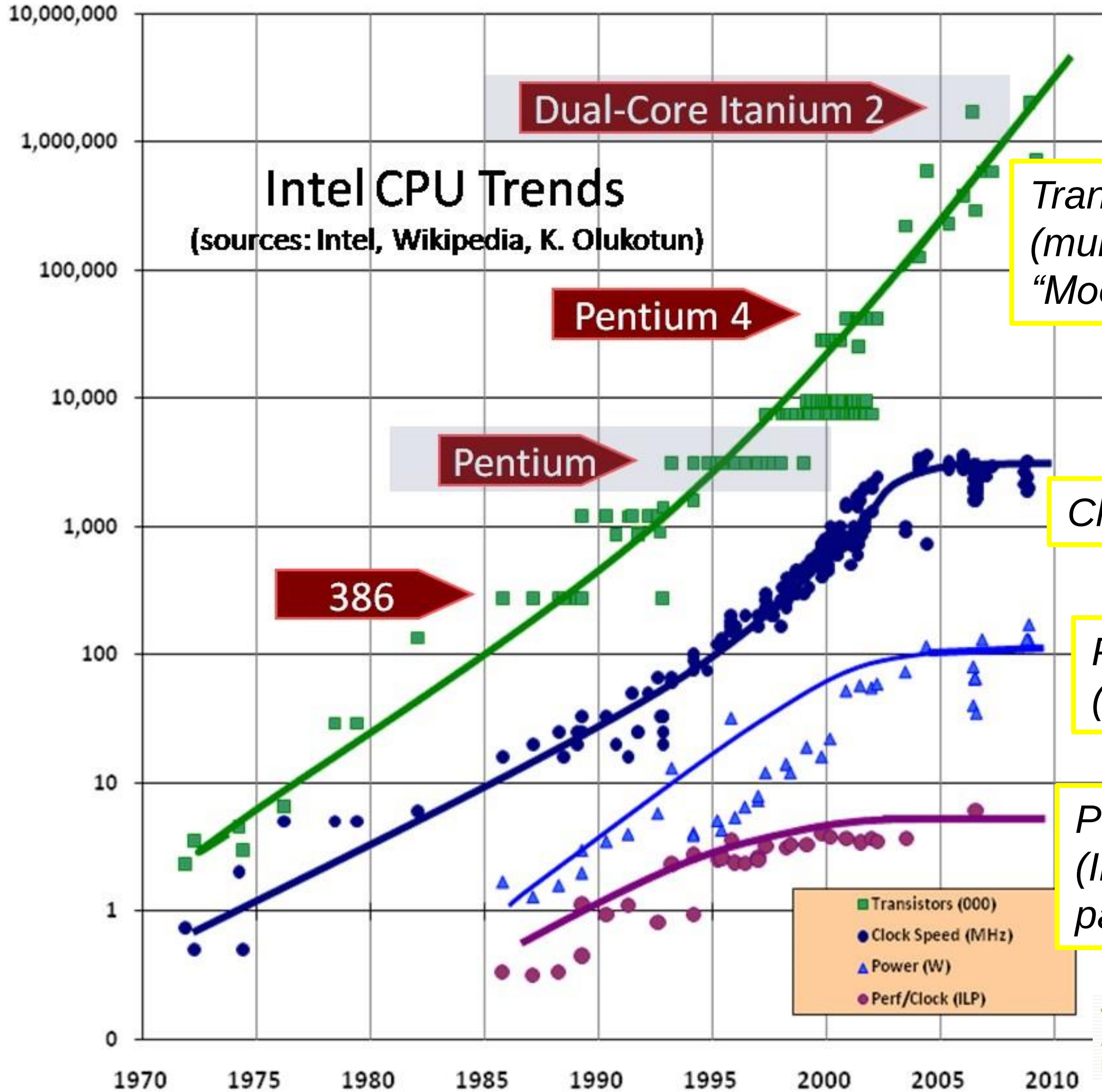
3. Reduced-Order Models for Reactor Physics
   - *A. Projection-based ROM for LWR neutronics*
   - *B. Projection-based ROM for Molten Salt Reactor Applications*
     - i. Methods
     - ii. Examples (MSFR / MSRE)
4. Reduced-Order Models for Transport
5. Summary and Outlook

Evolution of processor speeds



Transistor count still rising (multi-core designs); "Moore's law re-interpreted"

Clock speed has flattened

Power consumption (W/cc is the issue)

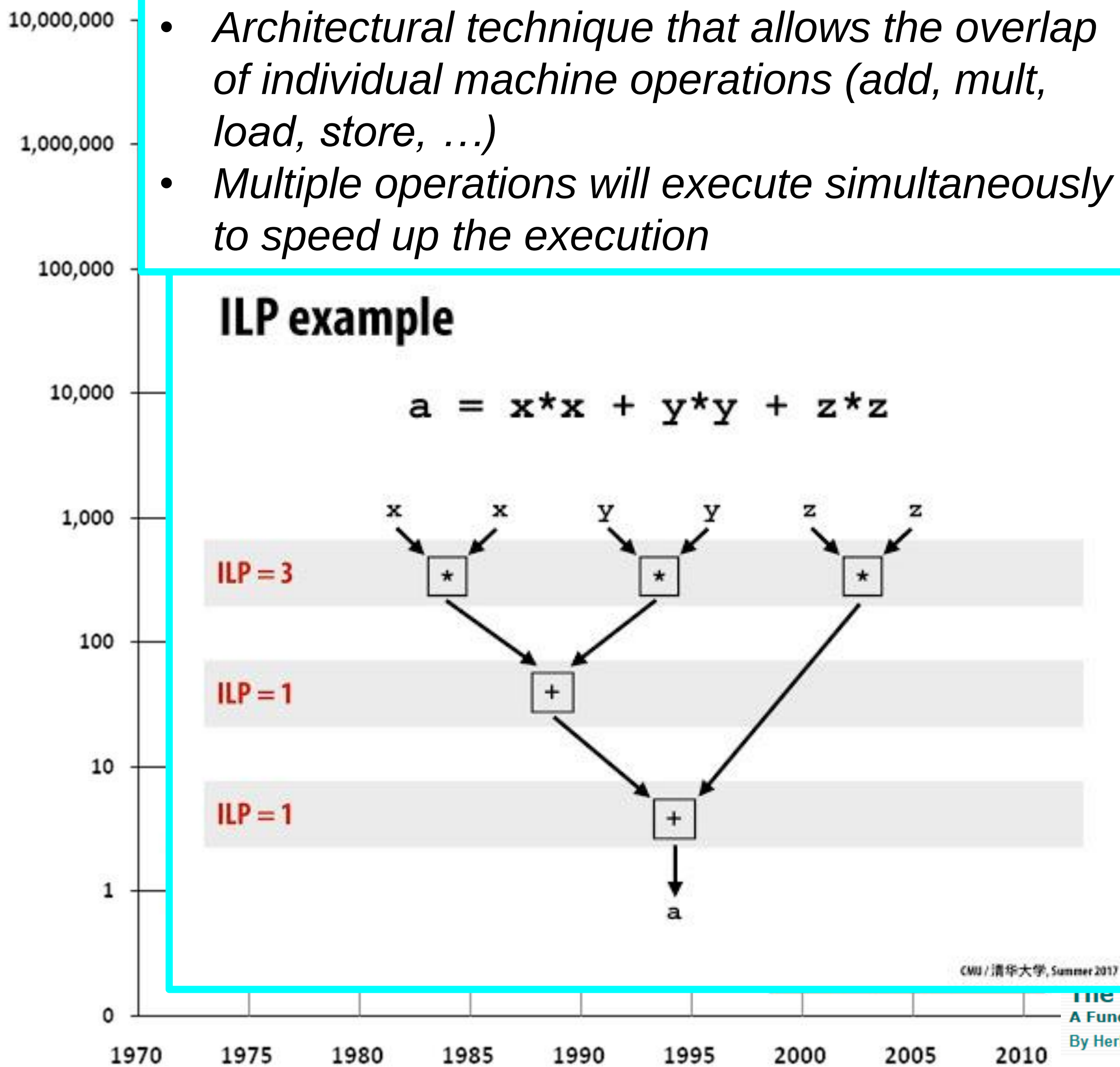
Parallel instructions (Instruction-level parallelism or ILP)

The Free Lunch Is Over
A Fundamental Turn Toward Concurrency in Software
By Herb Sutter

Evolution of processor speeds

Instruction-level parallelism:

- *Architectural technique that allows the overlap of individual machine operations (add, mult, load, store, …)*
- *Multiple operations will execute simultaneously to speed up the execution*



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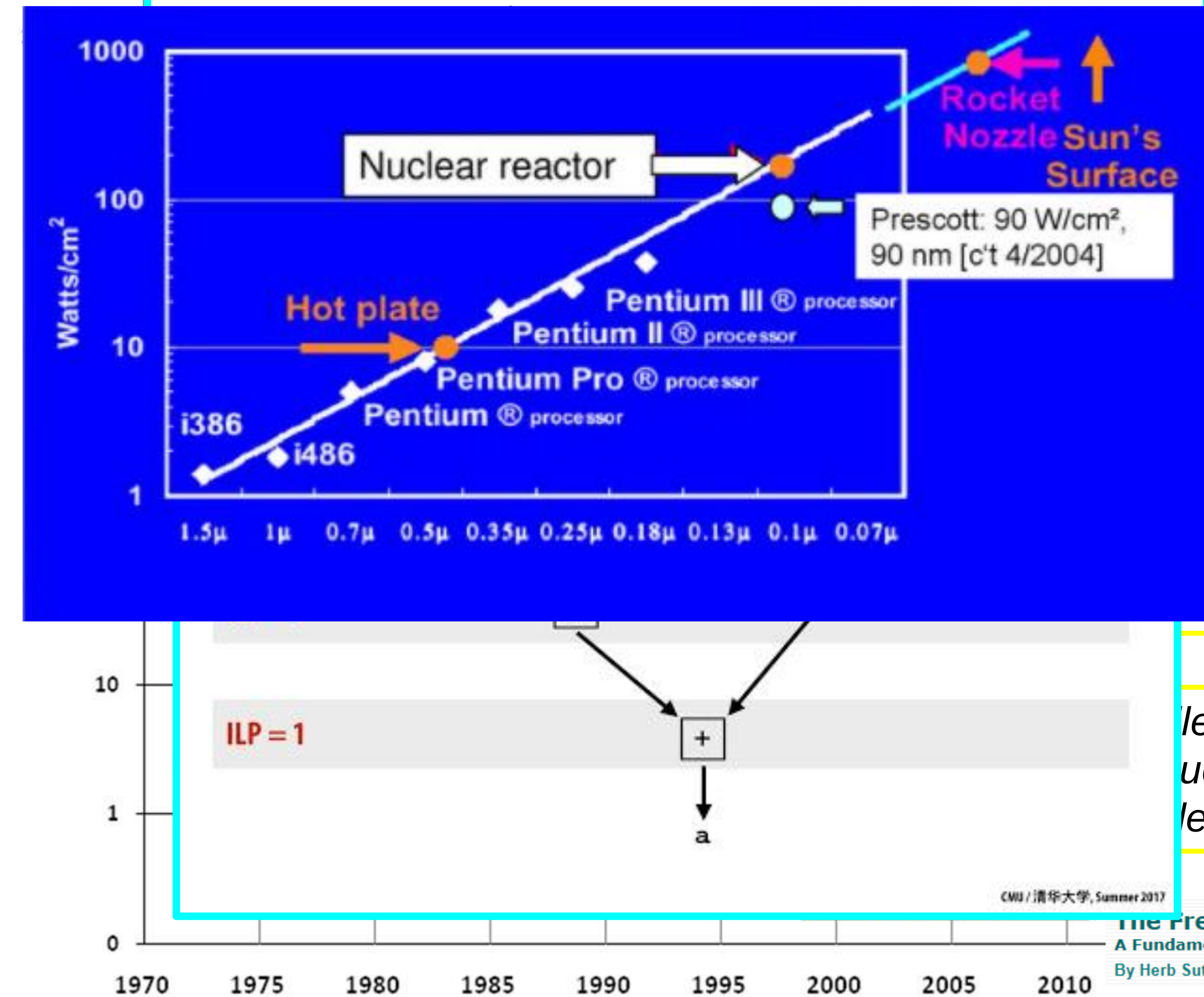

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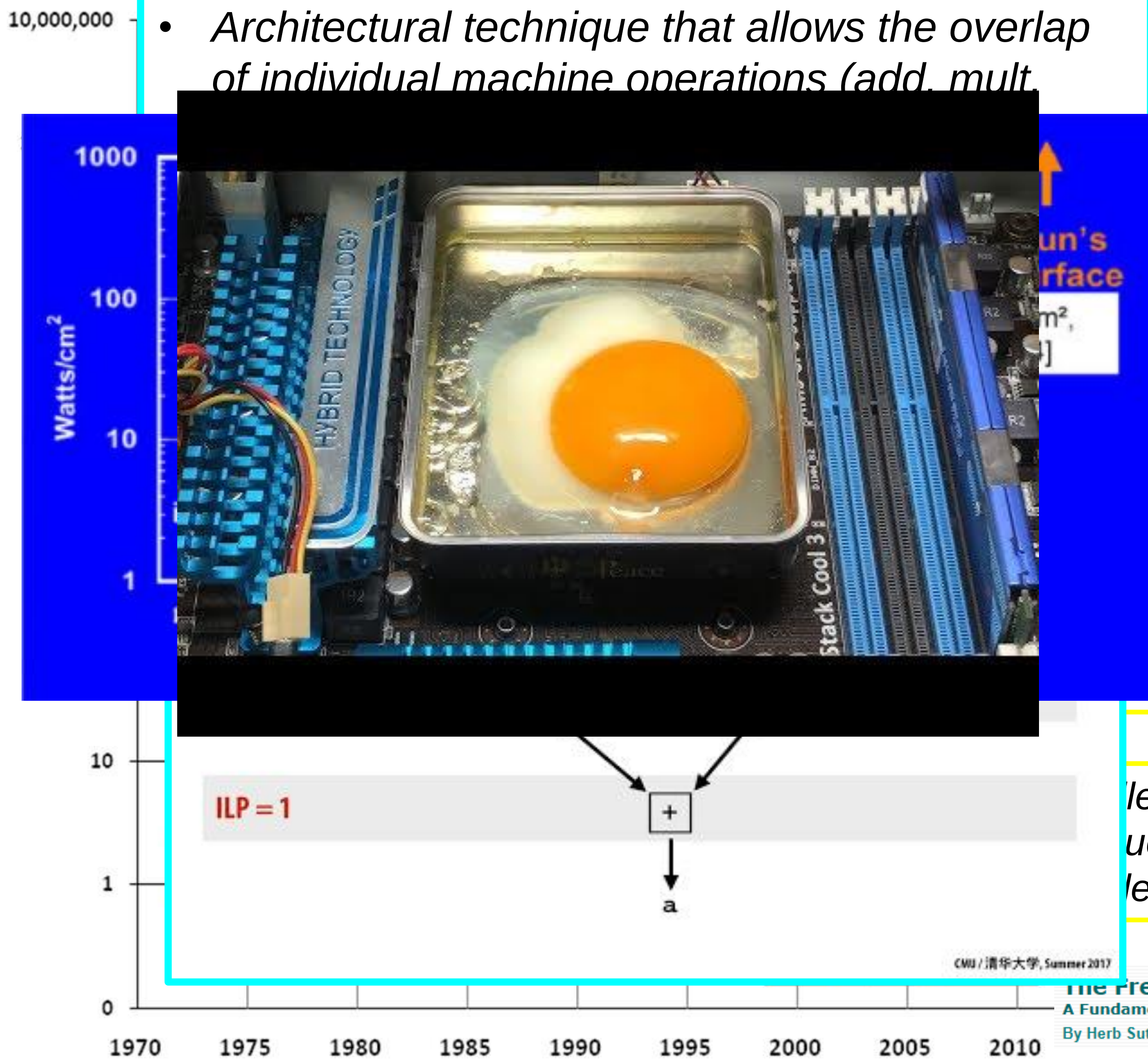

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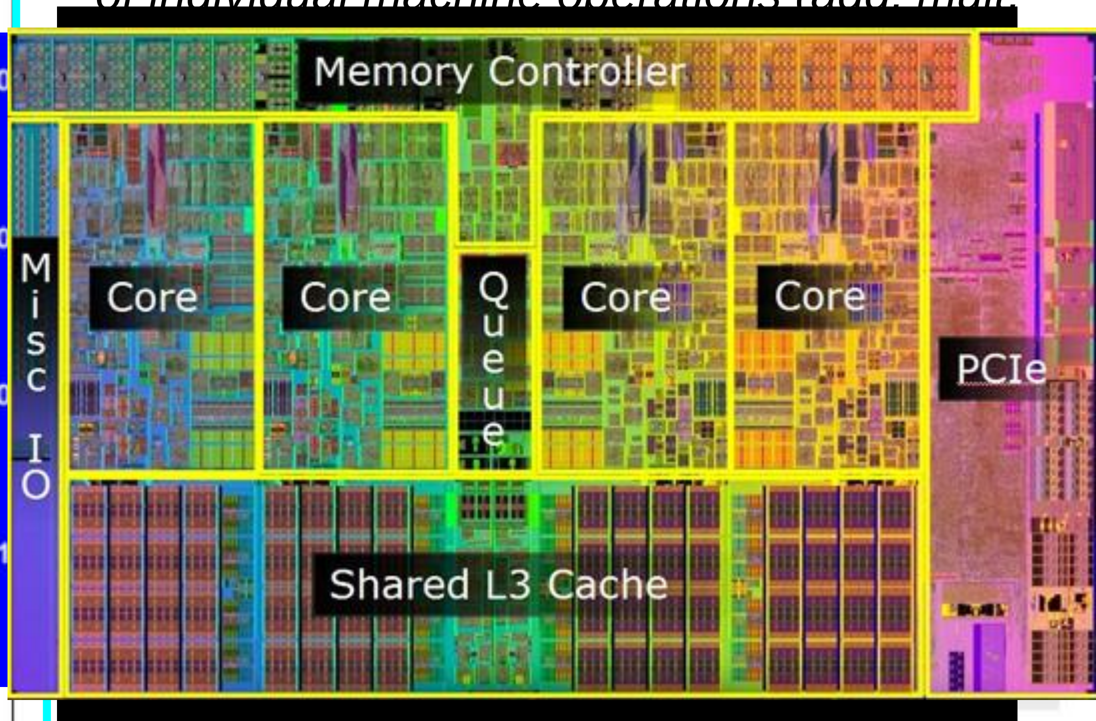

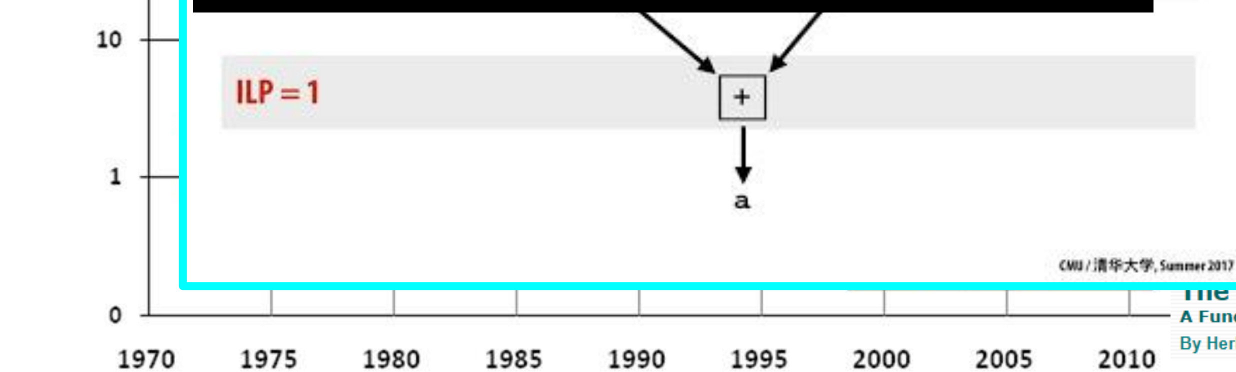

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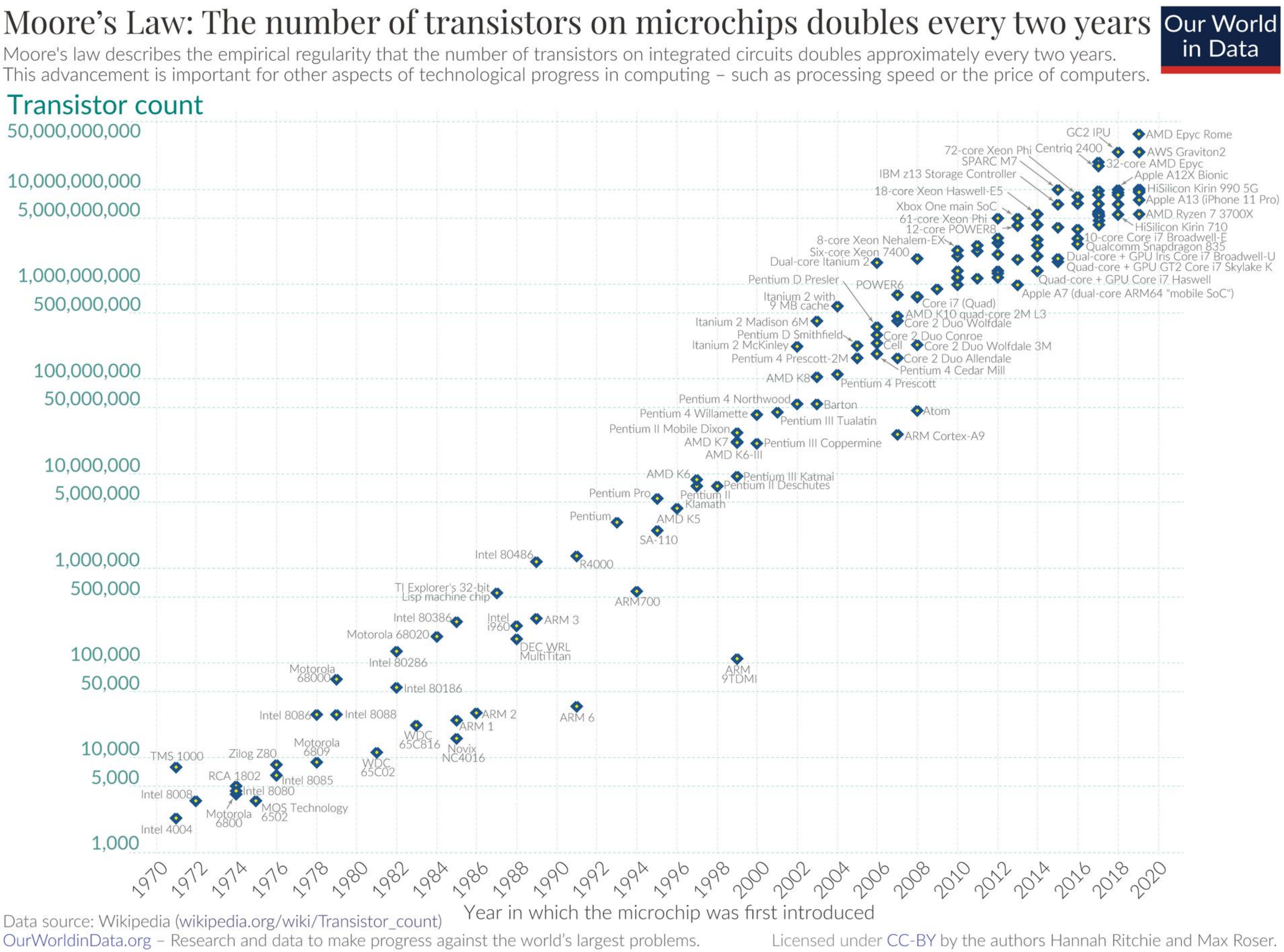
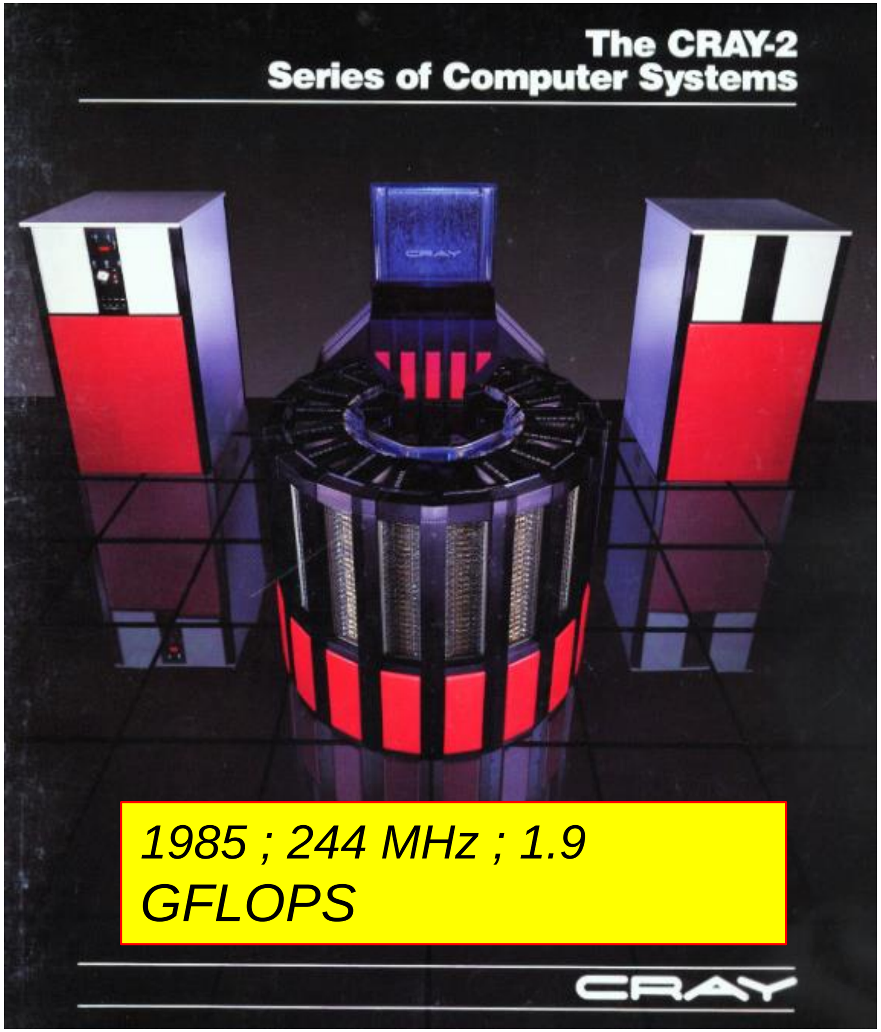
Moore’s law: ~straight line on semilog scale



Perspective



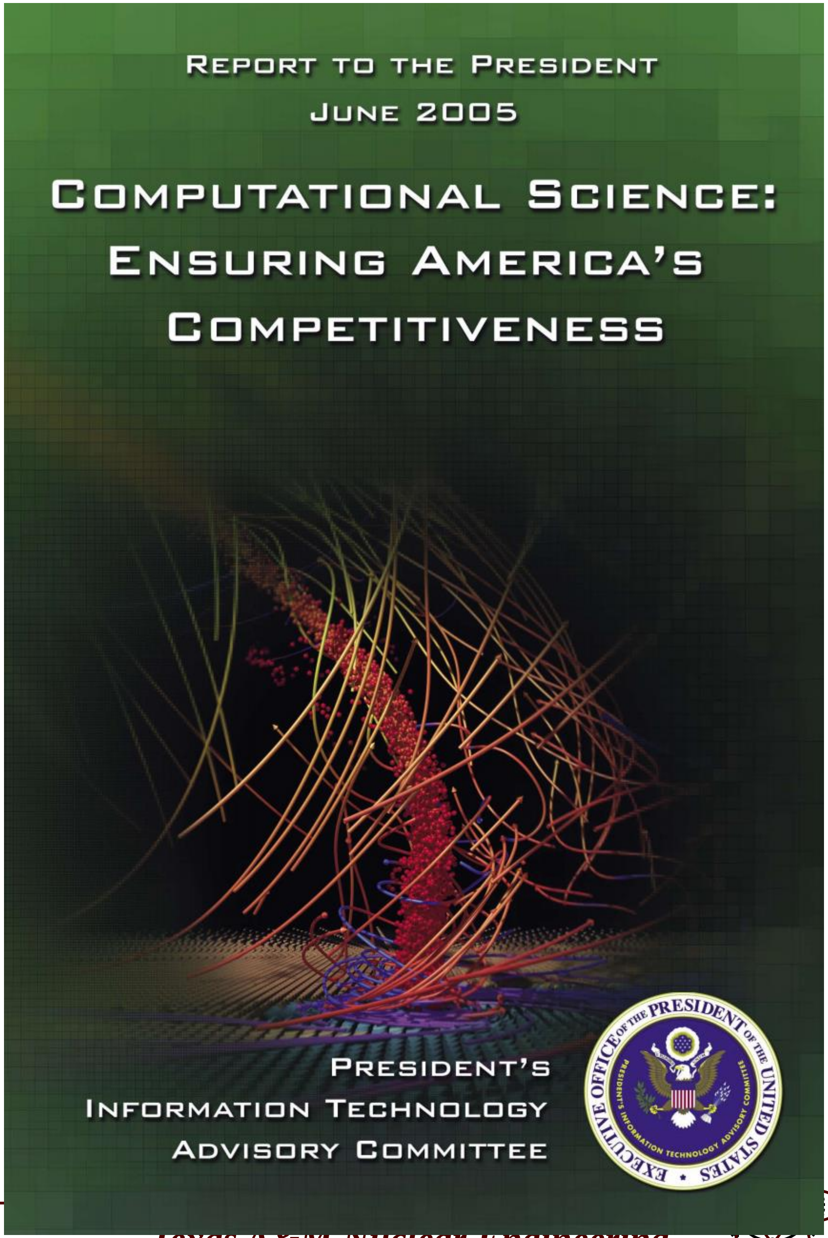
1985 ; 244 MHz ; 1.9 GFLOPS

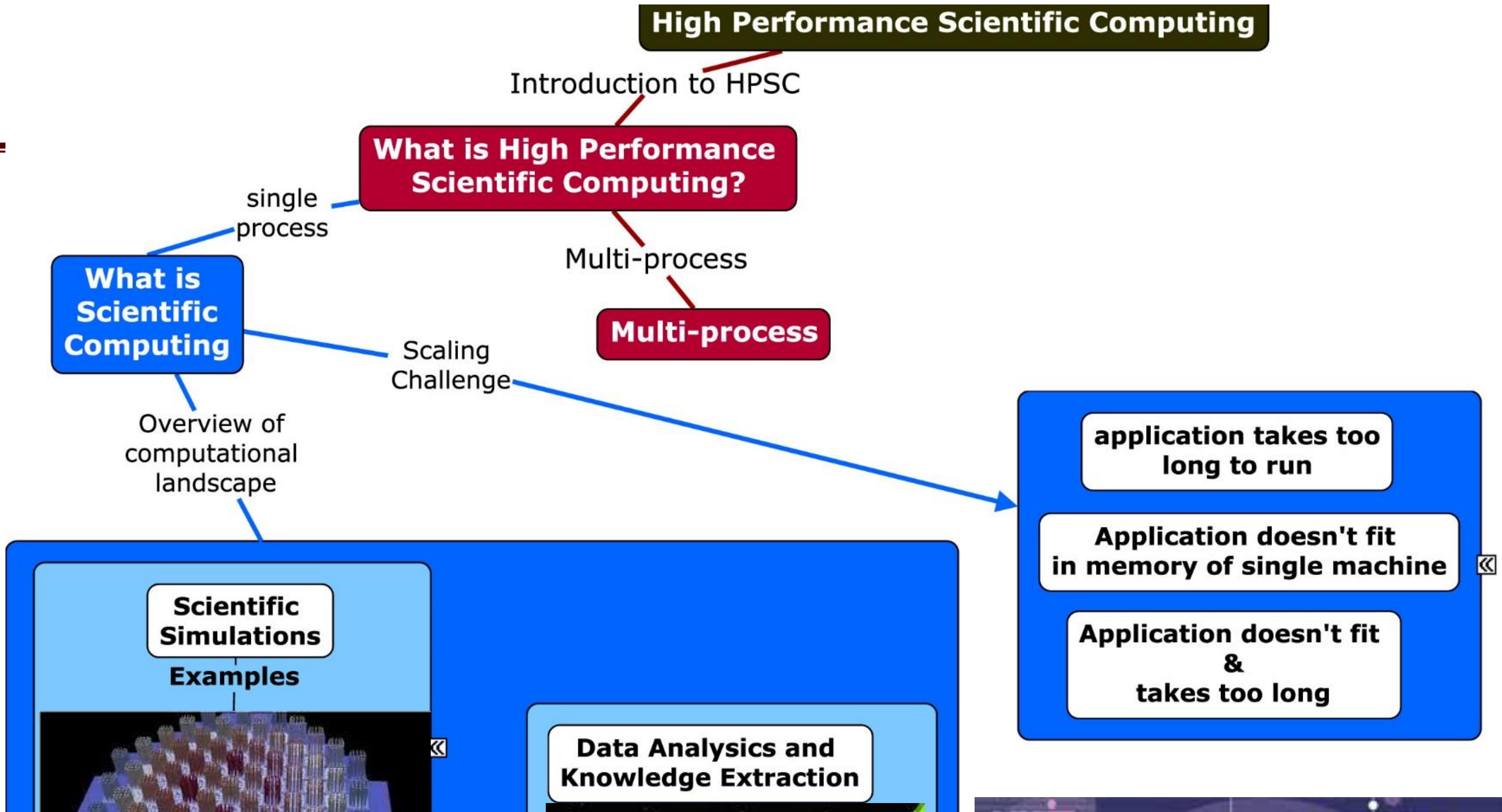
2010; 800 MHz ; 1.6 GFLOPS

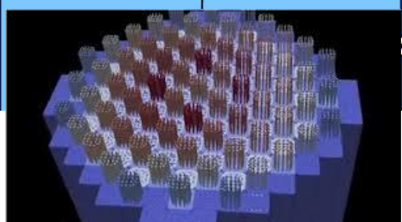
2015; 1,000 MHz ; 3 GFLOPS

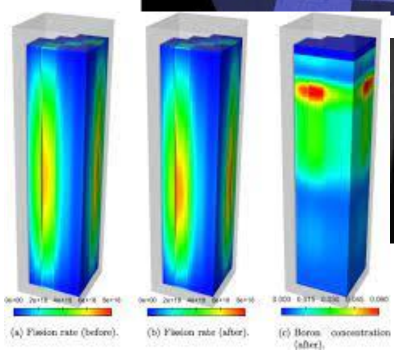
U.S. Presidential Information Technology Advisory Committee (PITAC)

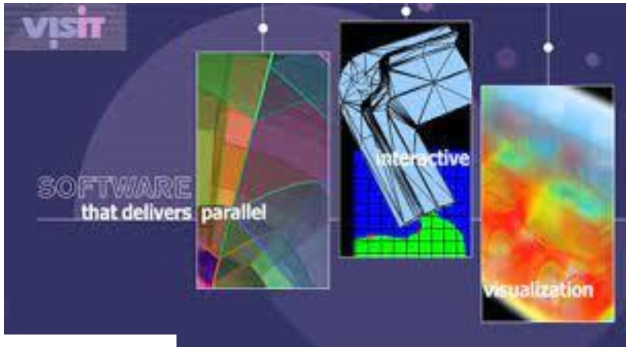
- Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems.
- Requires advances in hardware and software.











ParaView
Parallel Visualization Application

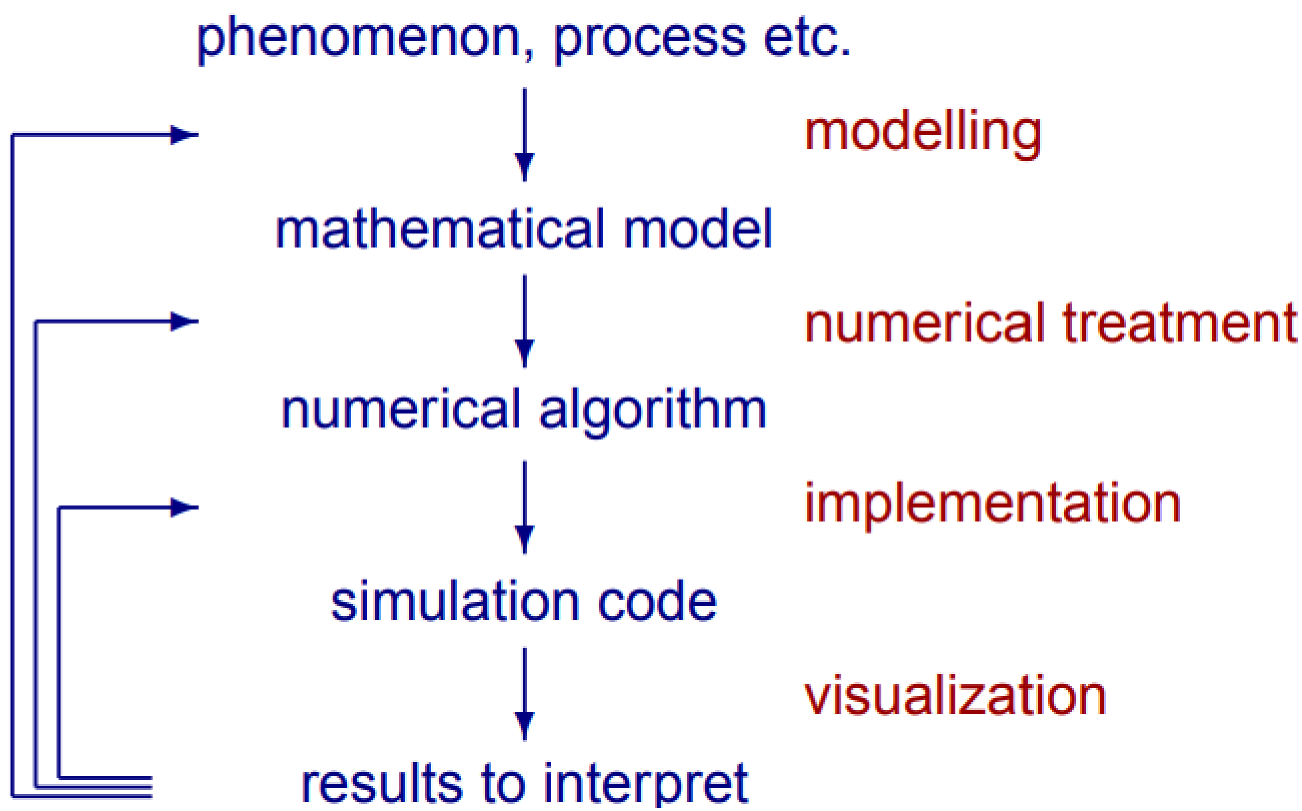
Partially adapted from the Lincoln Laboratory Supercomputing Center (MIT)

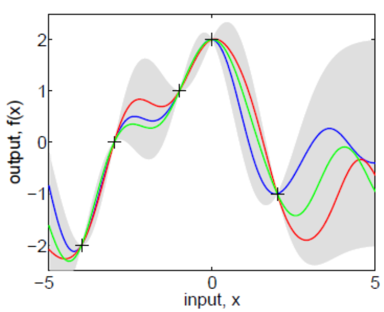
HPC for Scientific computing (SC)

Verification
(Am I solving the equations correctly?)

Validation
(Am I solving the correct equations?)

Uncertainty Quantification
(What is the goal of my simulation? What are the QoI's?)



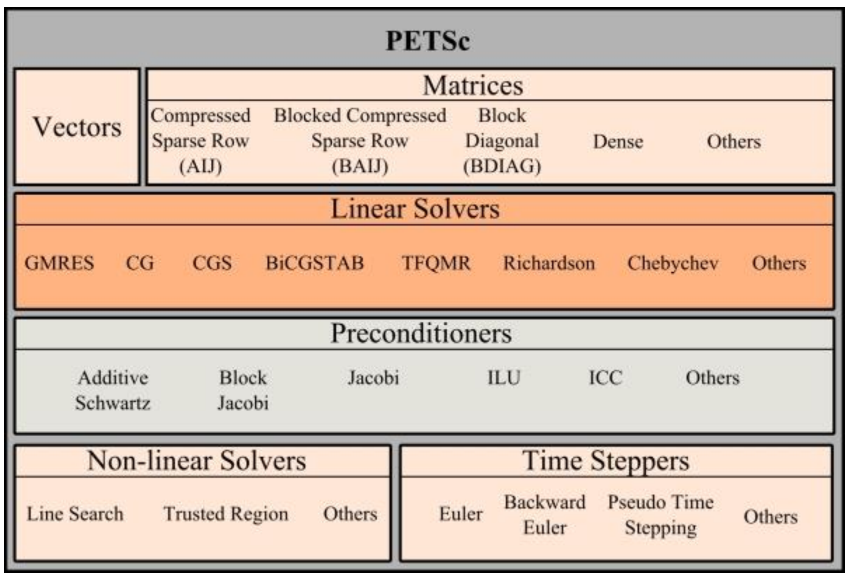


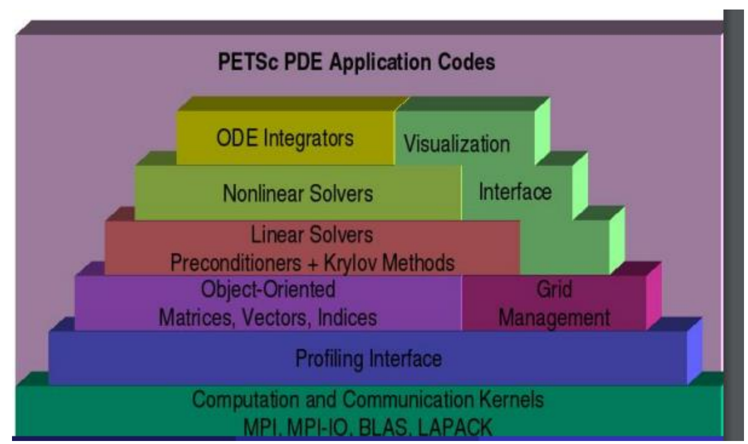
FastMath: Frameworks, Algorithms and Scalable Technologies for Mathematics

PETSc TAO

Portable, Extensible Toolkit for Scientific Computation

Toolkit for Advanced Optimization





FastMath: Frameworks, Algorithms and Scalable Technologies for Mathematics

FASTMATH

RESEARCH | APPLICATION PARTNERSHIPS | SOFTWARE CATALOG | OUTREACH | TEAM | PROJECT HIGHLIGHTS

Applied mathematics algorithms, tools, and software for HPC applications

PETSc TAO

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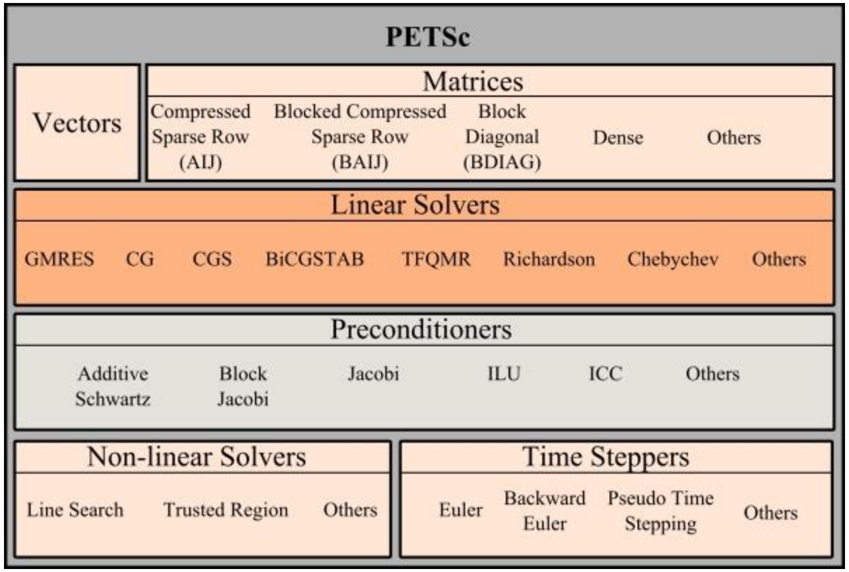
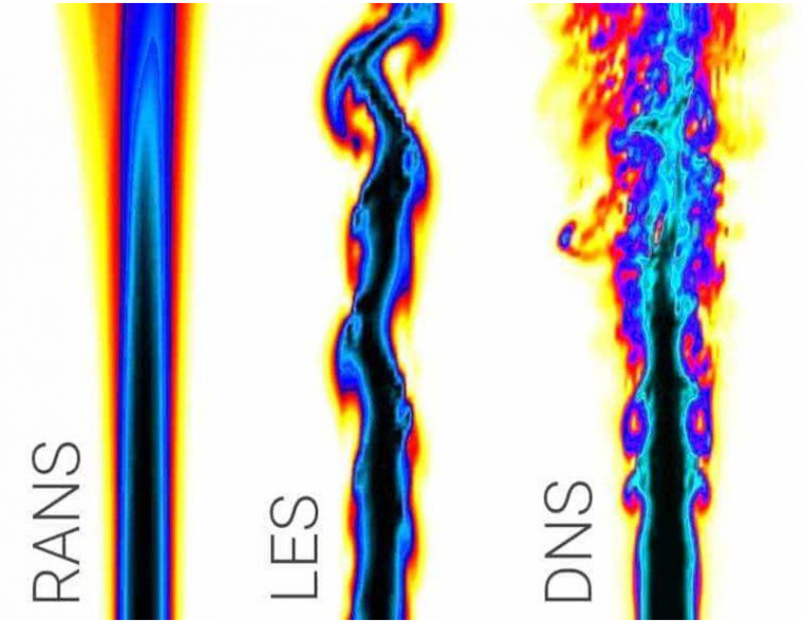
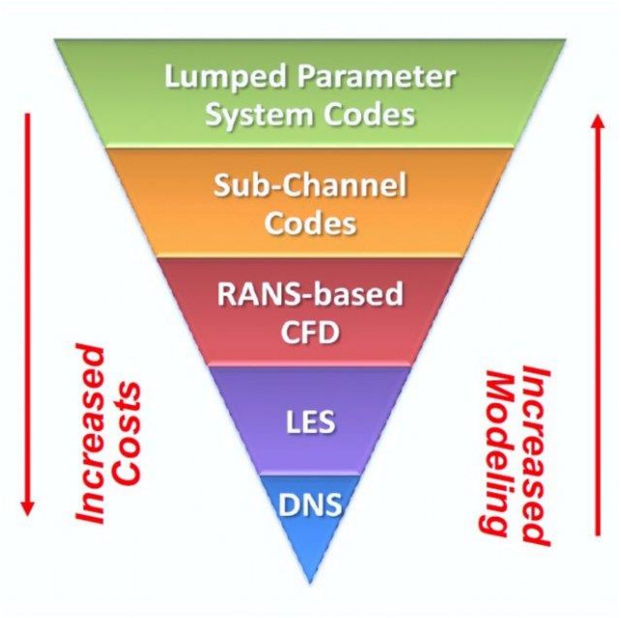


Example-1: Computational fluid dynamics





Example-1: Computational fluid dynamics

U.S. DEPARTMENT OF ENERGY

Nuclear Energy

Nek5000: Open Source Spectral Element Code

Spectral Element Discretization:
High accuracy at low cost

- Highly respected code in Fluid Dynamics Community. > **300 registered users**. Europe and United States mostly.
- Open source.
- Portable: runs on a laptop as well as a supercomputer.

Particularly well suited to LES and DNS of turbulent heat and flow transfer

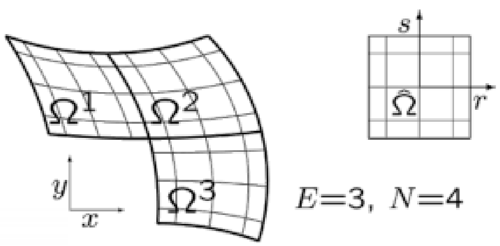
- Incompressible and Low-Mach, combustion, MHD, conjugate heat transfer, moving meshes, RANS, two-phase, CHT, buoyancy, adjoints,...
- New features in progress: compressible flow (GE), LBM, AMR, other meshing options.

Exceptional **scaling**

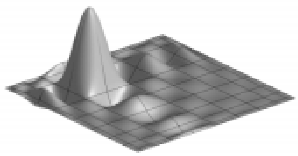
- 1999 Gordon Bell Prize.
- recently run with > 106 MPI processes.
- R&D100 awards in 2016.

High order method

- Local Polynomial Nodal Basis: Lagrange polynomials on Gauss-Lobatto-Legendre (GLL) quadrature points. for stability (not uniformly distributed points). **Implies a 2 level mesh.**
- Exponential convergence (100x reduction in error for 2x increase in resolution).
- Fast operator evaluation.



Example of the "2-level" mesh typical of Nek5000



2D basis function, N=10

NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Example-1: Computational fluid dynamics

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

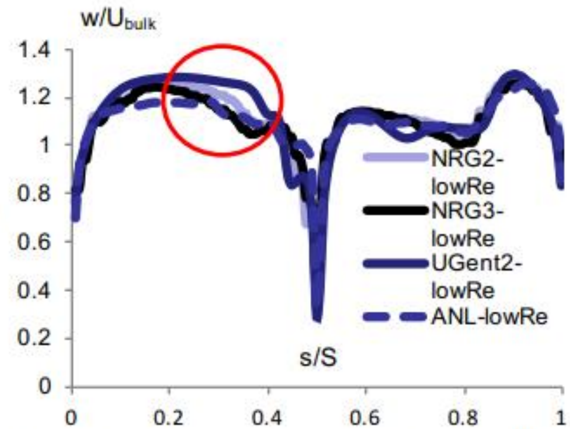
User case: Using higher-resolution approaches to inform lower-resolution methods - 1

For complex geometries CFD-grade data is often not available.

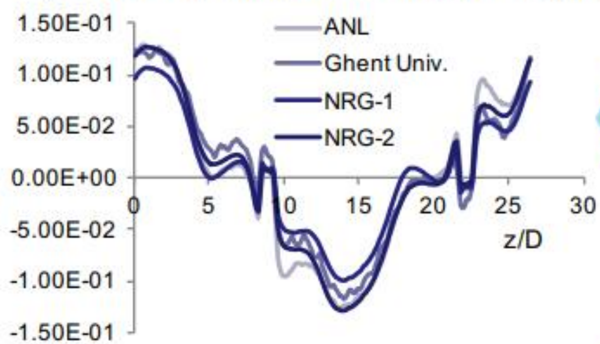
- RANS approaches can benefit from comparison with DNS/LES

International collaboration (INERI) centered on wire-wrappers.

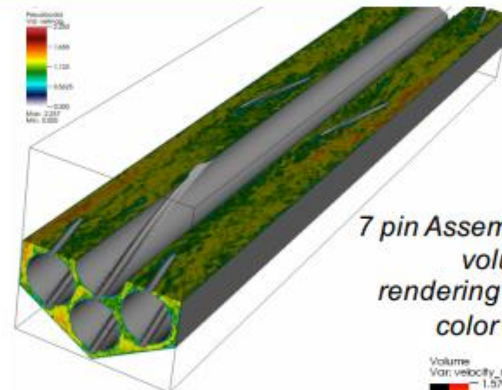
- Comparison between commercial codes and Nek5000
- Results are being used in the design of advanced reactors in Europe



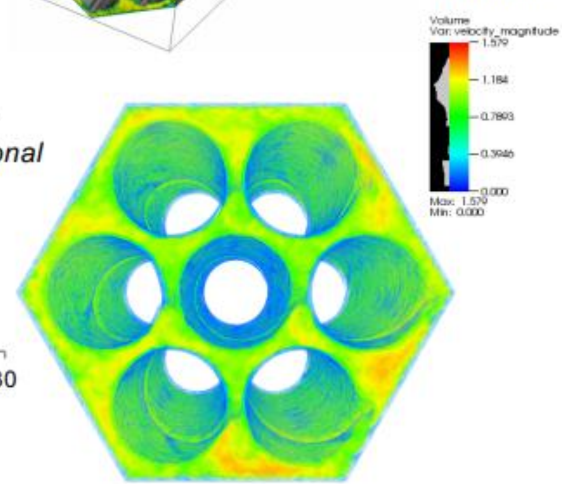
7 pin Assembly: streamwise velocity on diagonal



7 pin Assembly: Average Cross-flow



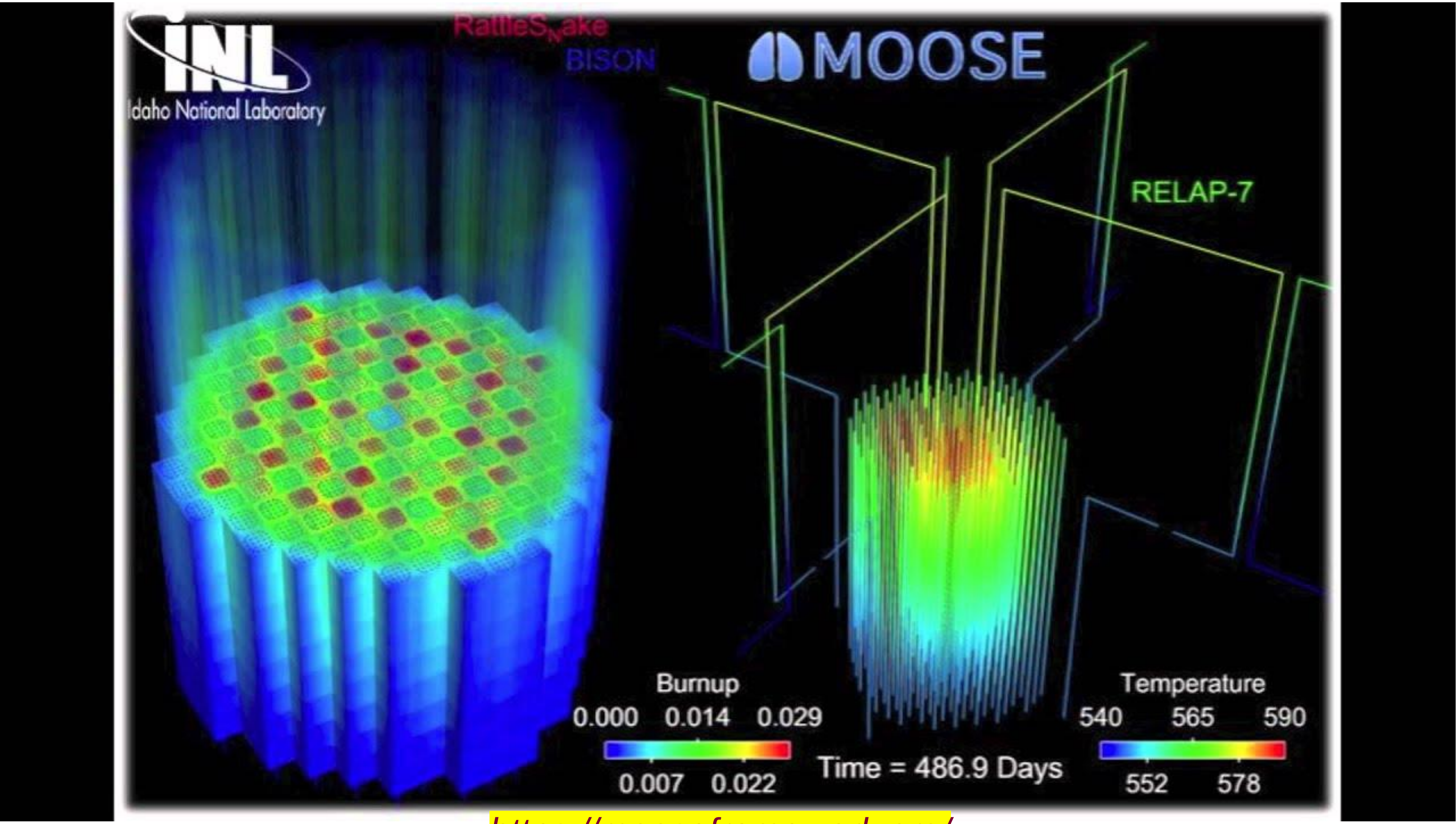
7 pin Assembly: volume rendering and color cuts



NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

[SFR]

Example-2: MOOSE, a Multiphysics HPC platform



https://mooseframework.org/

Example-3: Massively parallel radiation transport

- neutron, thermal radiation, gamma, electron
- steady-state, time-dependent, criticality, adjoint, etc.
- advanced solution techniques
- discretization in space/angle/energy
  - *Largest problem we have done: 20.8 Trillion unknowns*

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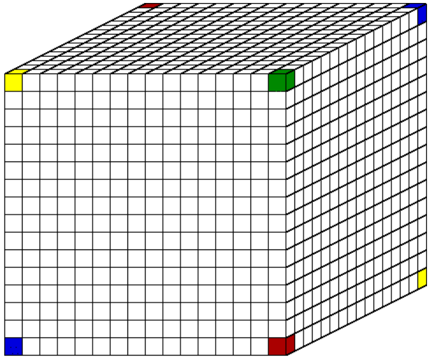
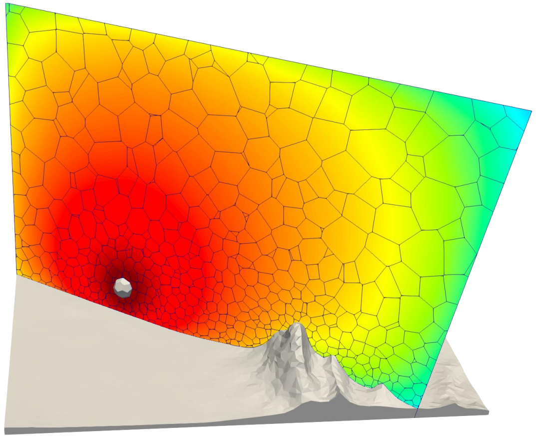
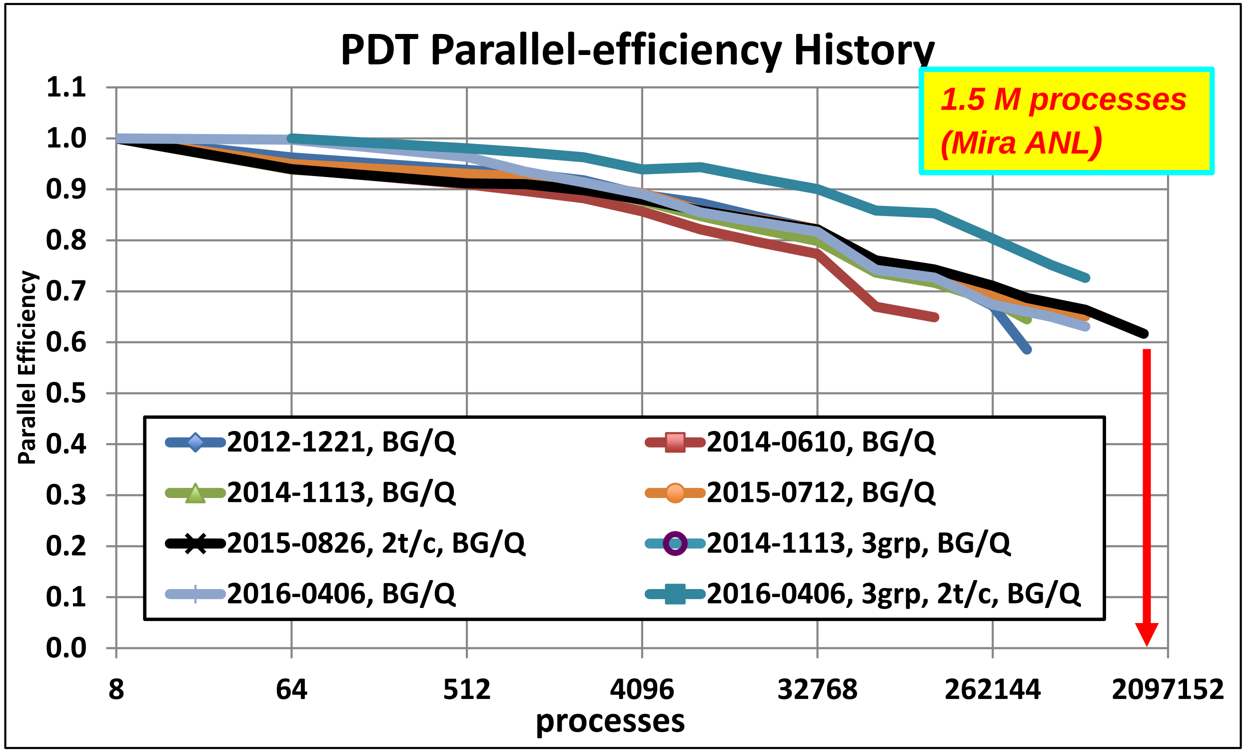
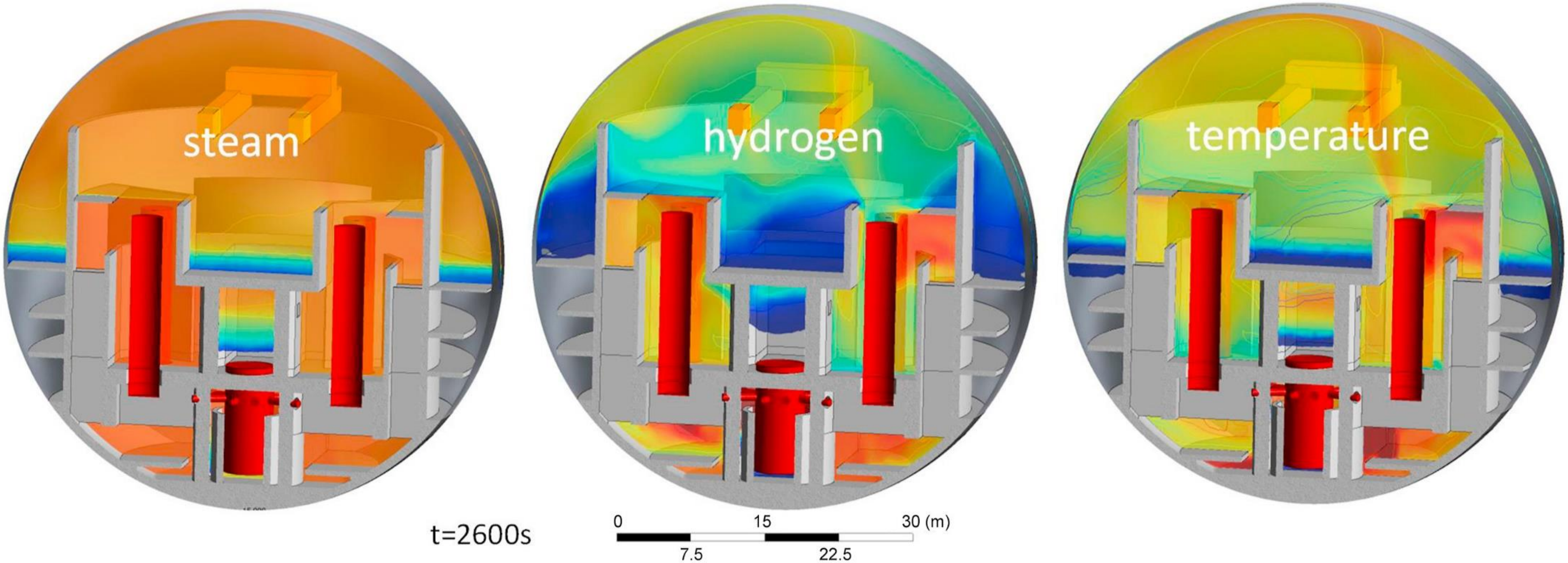






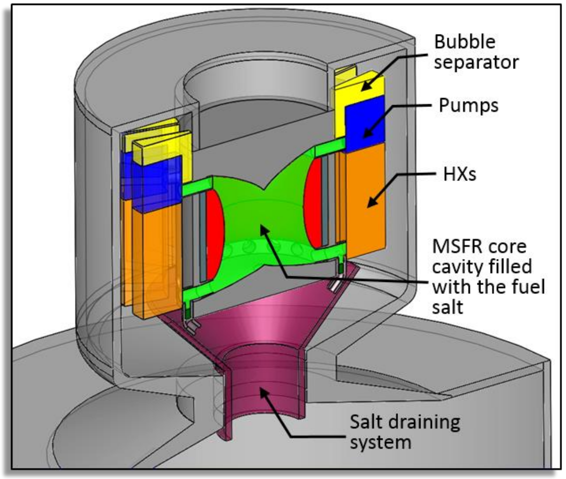
Example-4: Reactor containment



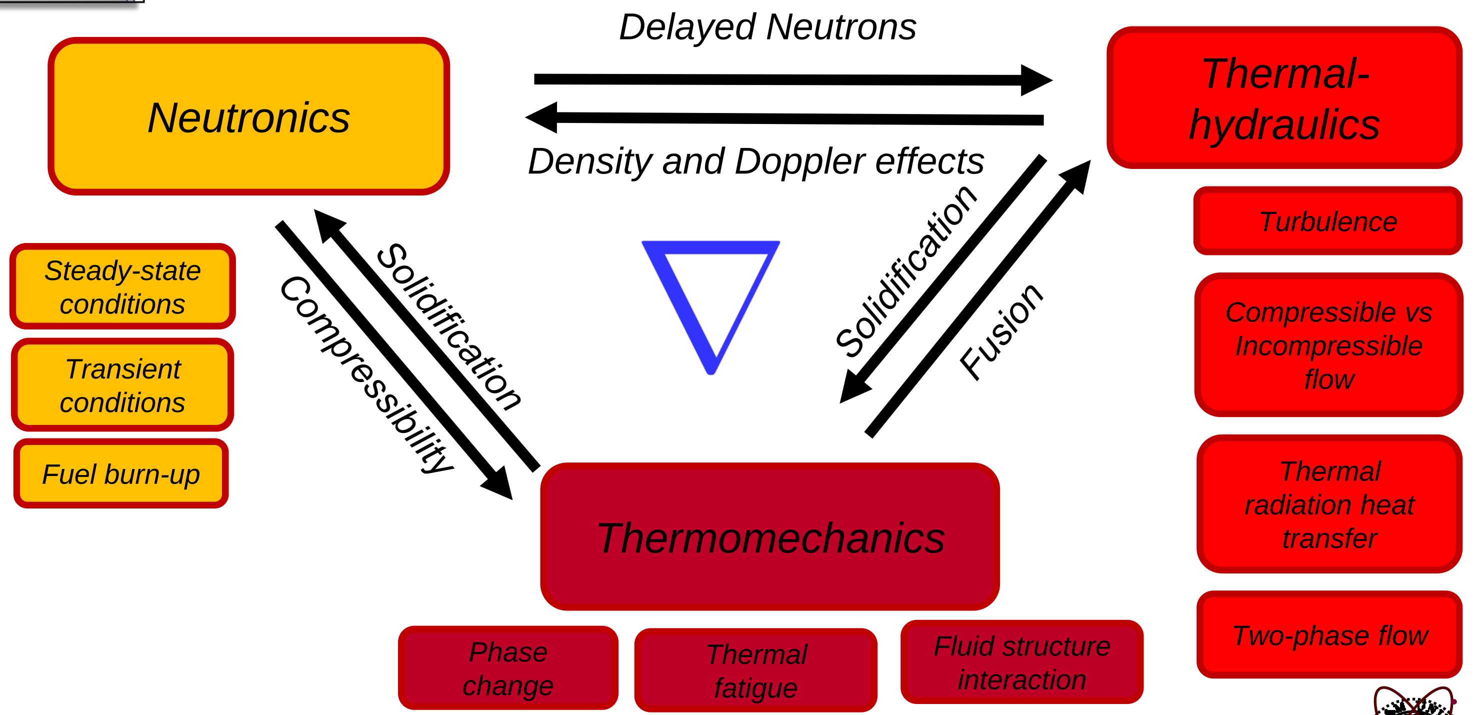
Gas distribution and pressurization inside the containment during an SB-LOCA (Julich, Germany, Kelm et al.).

Based on OpenFOAM for CFD

Example-5: Multiphysics of molten salt reactor



Conceptual Design of the MSFR core cavity



(CNRS, Tano)

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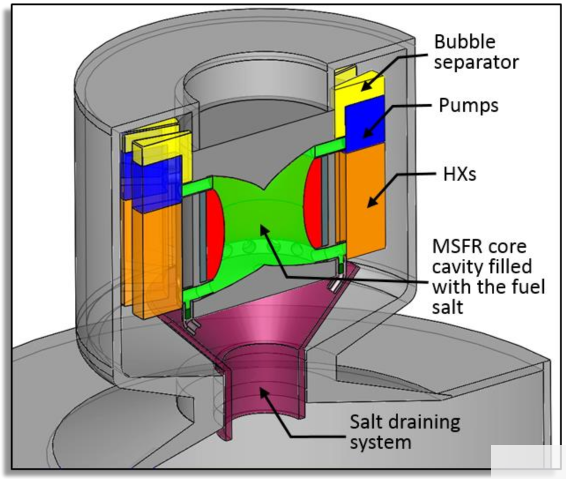

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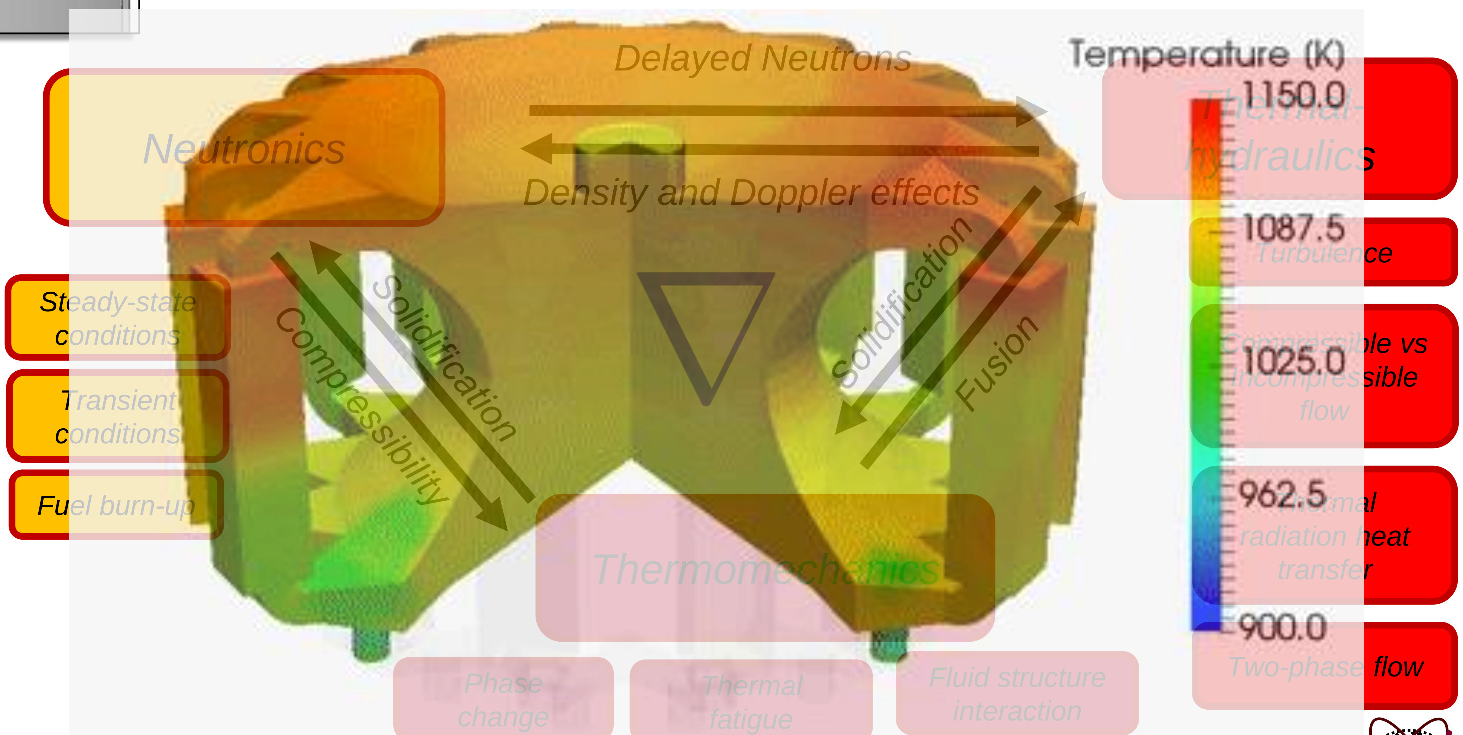

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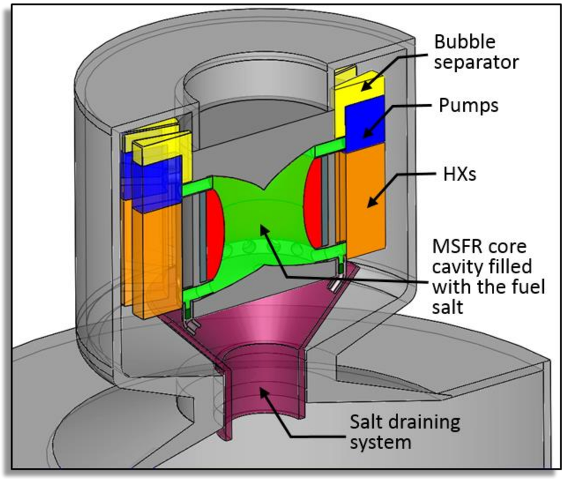
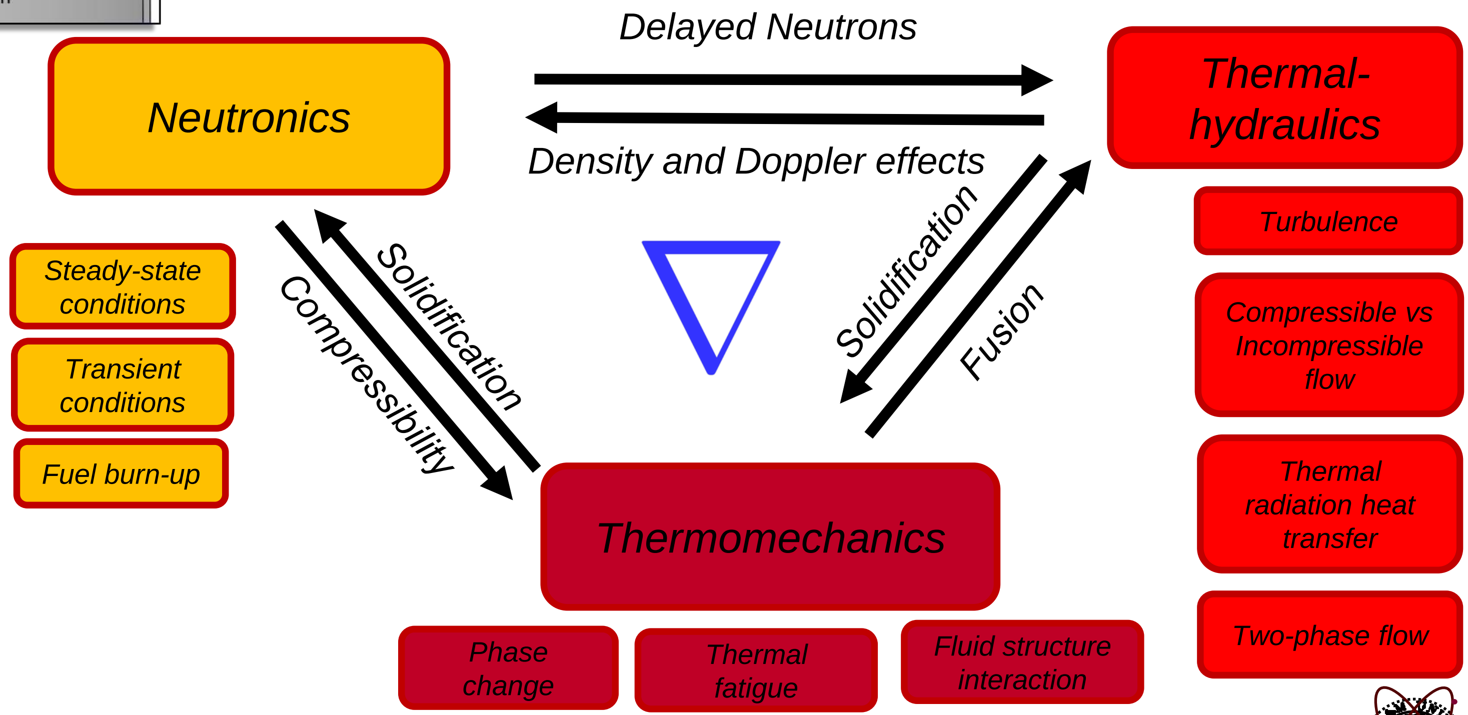
5. Summary and Outlook

Is there a need for fast yet accurate surrogate models?

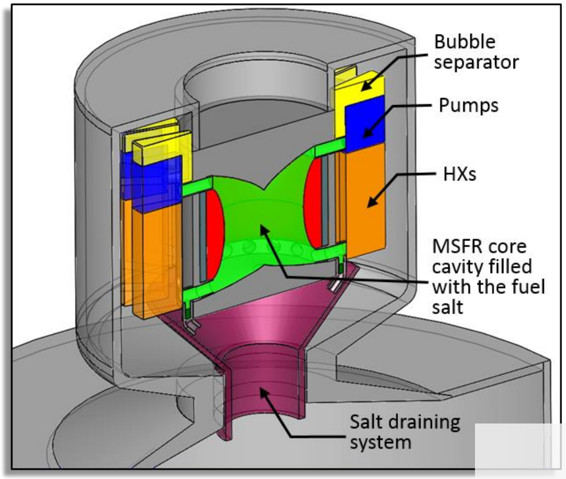
- **Multiphysics of molten salt reactor**

Conceptual Design of the MSFR core cavity





Is there a need for fast yet accurate surrogate models?



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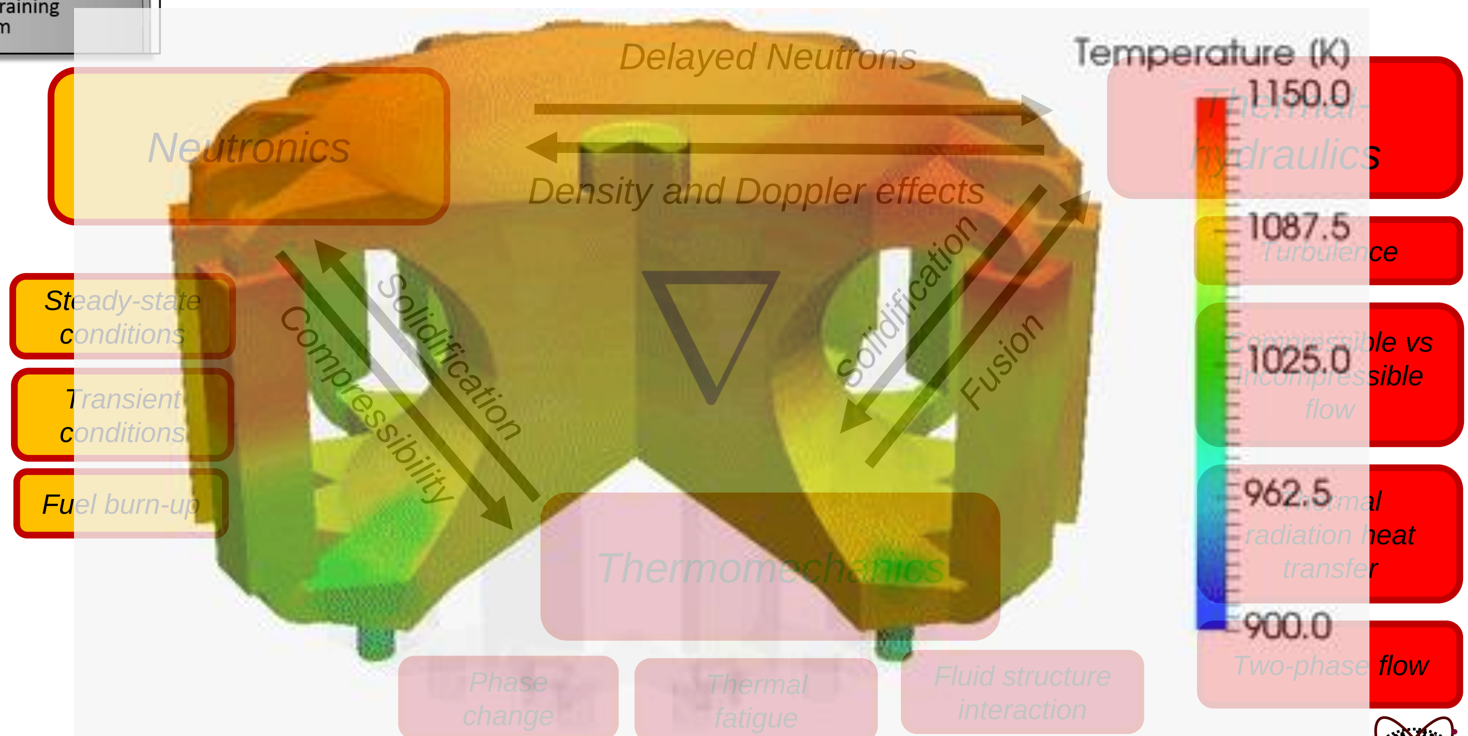

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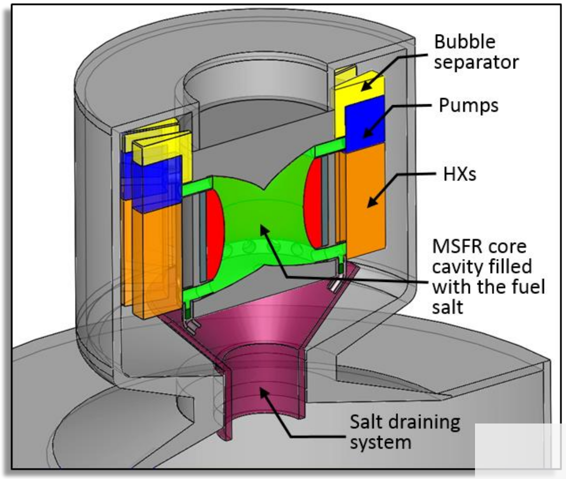
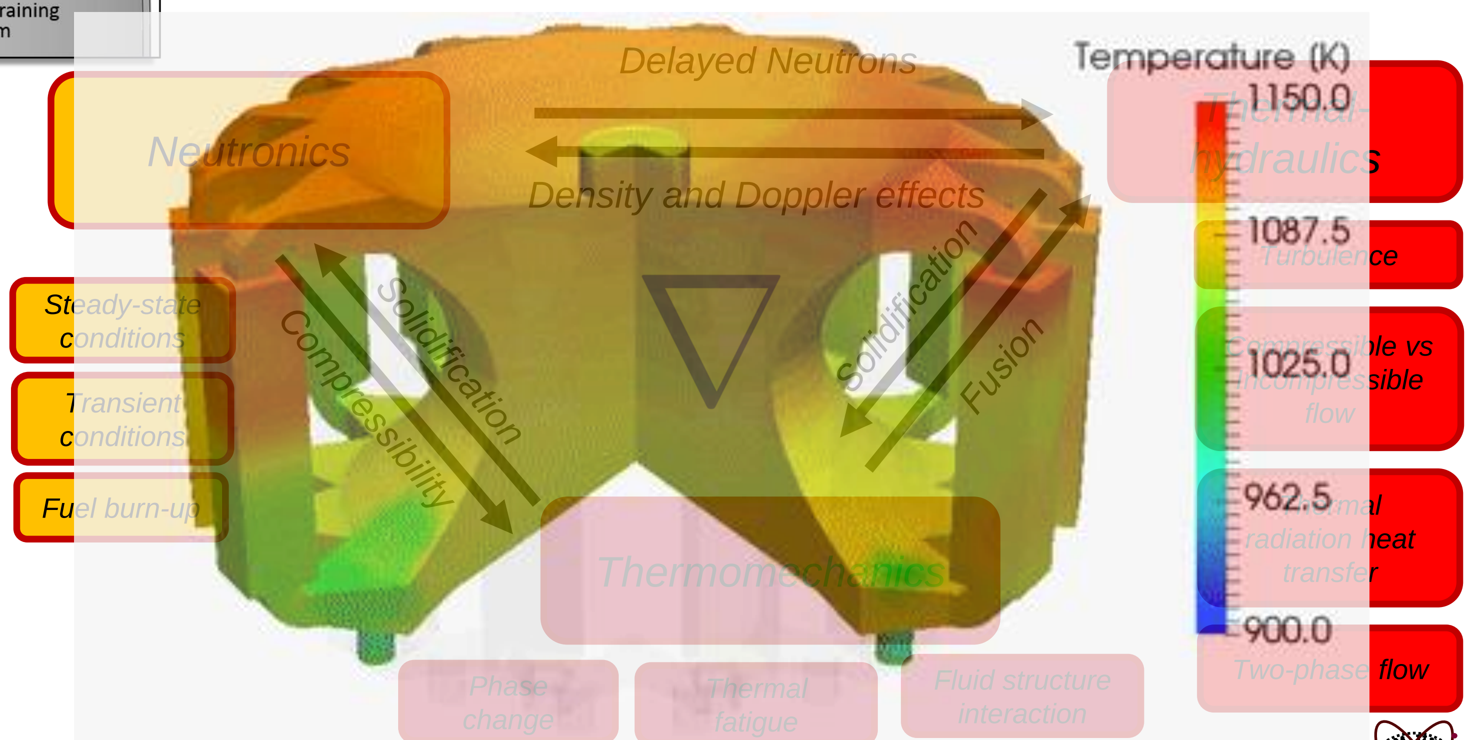


- **Multiphysics of molten salt reactor**

Conceptual Design of the MSFR core cavity

- ***64 cores. 3 days of simulation***
- *Pump characteristics not finalized*
- *HX characteristics not finalized*
- *Freeze plug characteristics not finalized*



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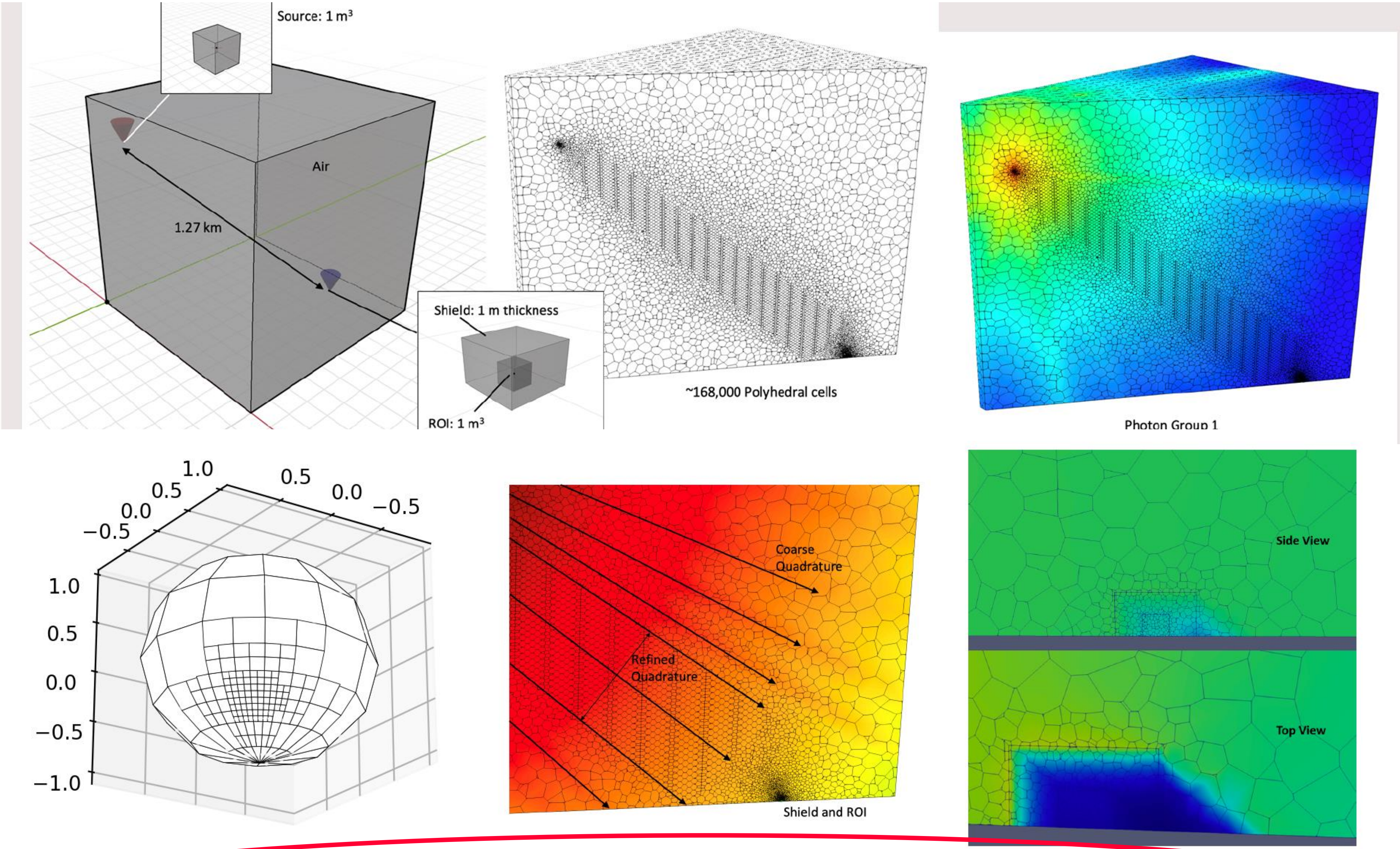

⟨FEM-unk⟩/cell	spatial cells	angles	groups	total unkws	CPU processes	wall-clock
22	$\sim 168,000$	~ 600	42	94B	320	60 min.

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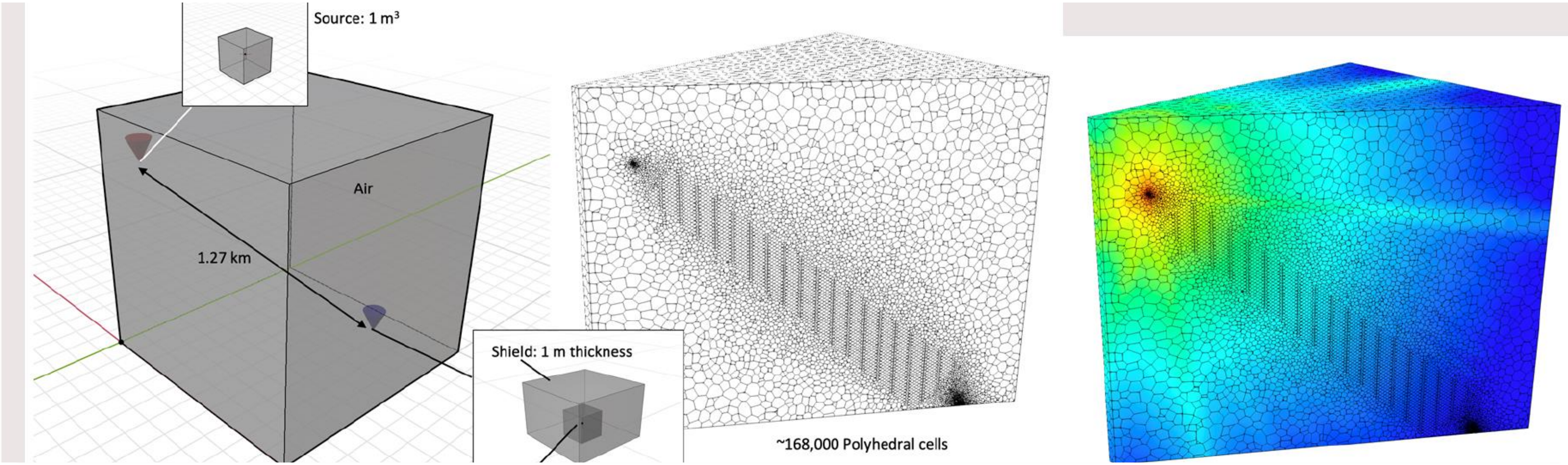
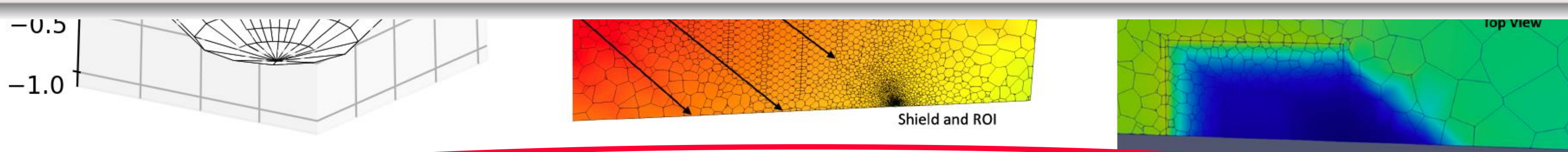


Sources of Uncertainty in QoIs for NWrE:

1. Source position (altitude, slant).
2. Source spectrum (fraction of fission spectrum + fusion spectrum, for n and γ).
3. Air Humidity (in addition to air density variation wrt to z).
4. Ground Composition.
5. Location and orientation of RoI (Region of Interest).



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Parametric full-order models

- **Full-order models:**
  - *Little comprise on the selection of the governing laws (first-principle models, HiFi models, few physics approximations; e.g., transport, not diffusion)*
  - *Models resulting from the discretization of governing laws (PDEs)*
  - *Relatively fine resolution of the phase space (3D space but also energy, angle)*
  - *Thus costly in CPU+RAM (clusters, supercomputers)*

- **Parametric full-order models:**
  - *Input data (model parameters) can change*
    - Design of Experiments
    - Design optimization
    - Uncertainty Quantification
  - *Thus, not a hero-calculation !*
  - *Multi-query problems*

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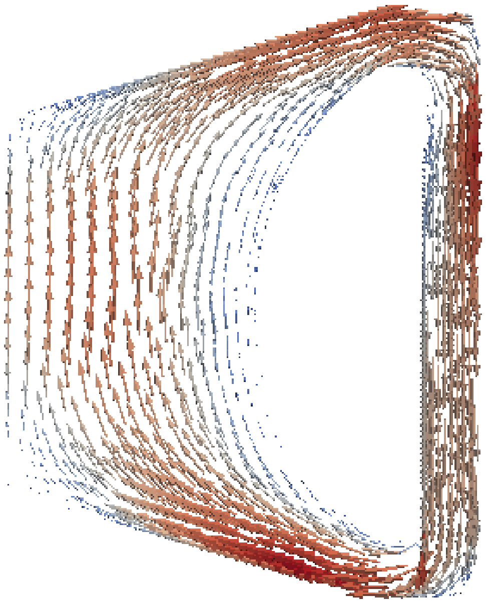

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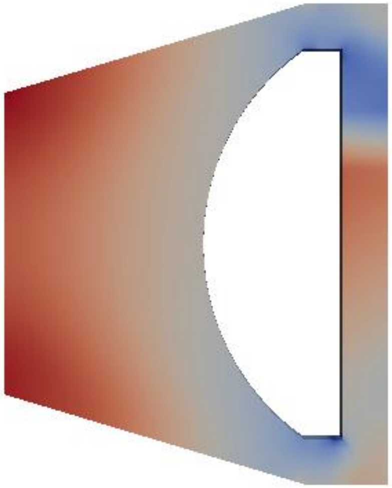

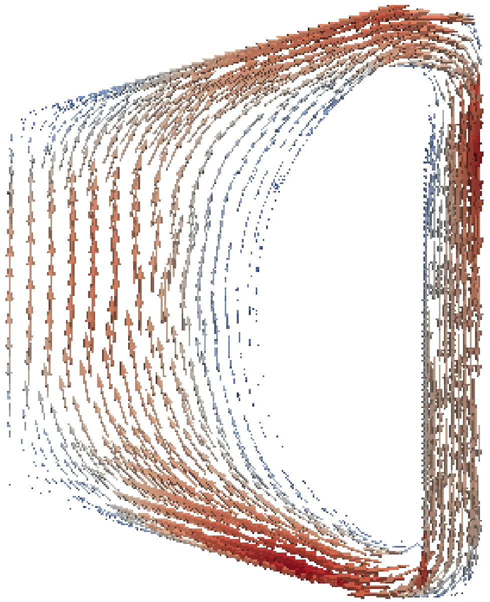

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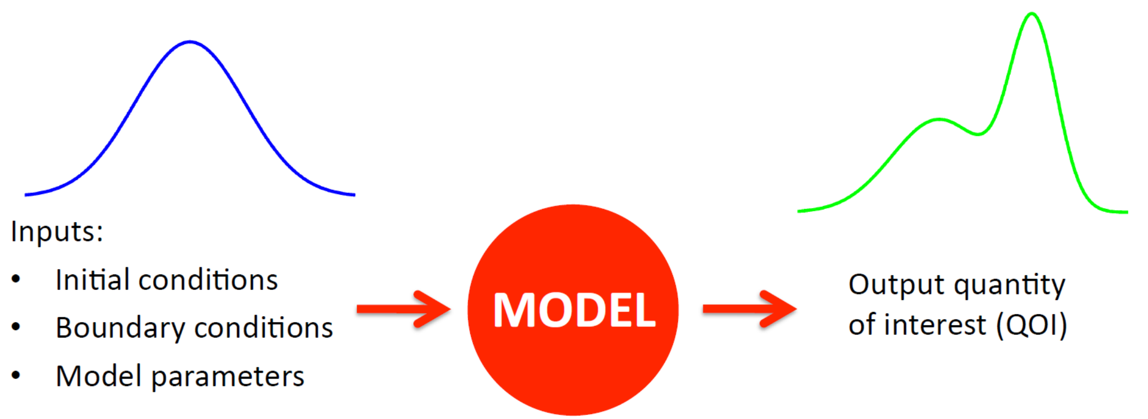
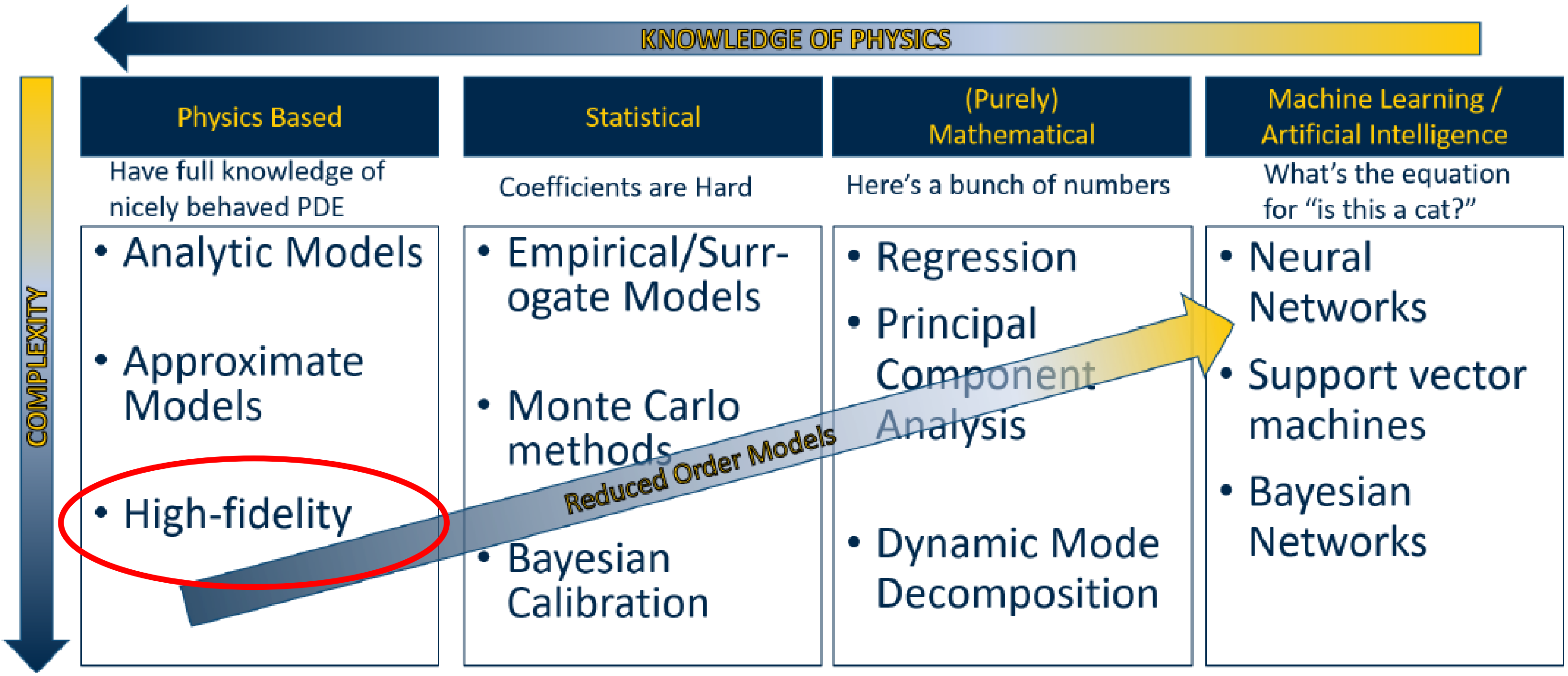


- Quantify the impact of input uncertainties on output QOI
- Propagate input uncertainty through the computational model
- Nonlinear transformation of input uncertainty

Taxonomy of reduced-order models



Energies 2021, *14*, 4235. https://doi.org/10.3390/en14144235

Taxonomy of reduced-order models

Model Order Reduction

- MOR techniques:
  - Requires data for training?

    Data-driven (Scientific Machine Learning): Polynomial regression, Polynomial Chaos Expansion, Gaussian Processes, Neural Networks, Reduced Basis Methods, ...

    Not data-driven: Balanced Truncation, Krylov Subspace methods, Proper Generalized Decomposition...
  - Requires the operators of the FOM for training?

    Non-intrusive: Polynomial regression, Polynomial Chaos Expansion, Gaussian Processes, Neural Networks, ...

    Intrusive (physics based): Balanced Truncation, Krylov Subspace methods, Reduced Basis Methods, Proper Generalized Decomposition...

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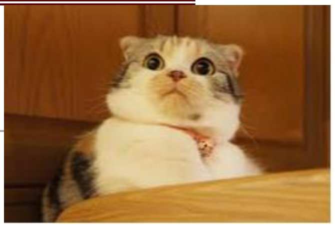
MOR

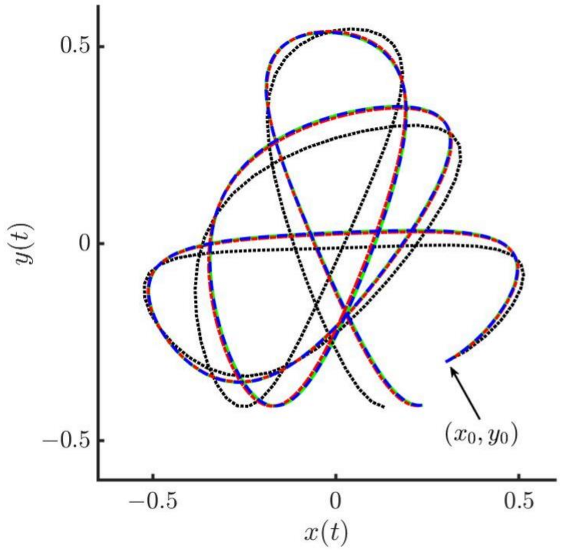
Model order reduction

From Wikipedia, the free encyclopedia



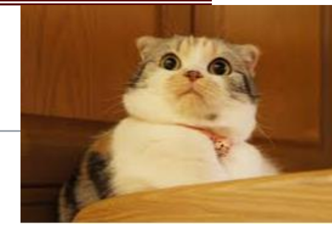
Model order reduction (MOR) is a technique for reducing the computational complexity of mathematical models in numerical simulations. As such it is closely related to the concept of metamodeling with applications in all areas of mathematical modelling.

- **Simple but powerful observation:**
  - ***very often, the trajectory of a large-scale discrete system belongs to an affine subspace whose dimension is significantly lower than that of the original system.***
  - ***for this reason, MOR methods search for the solution of a set of governing equations in a subspace, thereby offering a potential for significant CPU time reductions***



Purpose of MOR : solve many times a given problem under parametric variations (UQ, design opt.)

MOR



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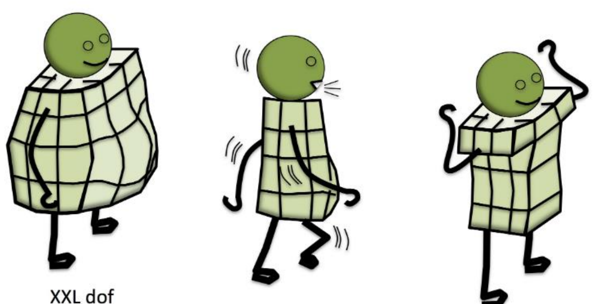

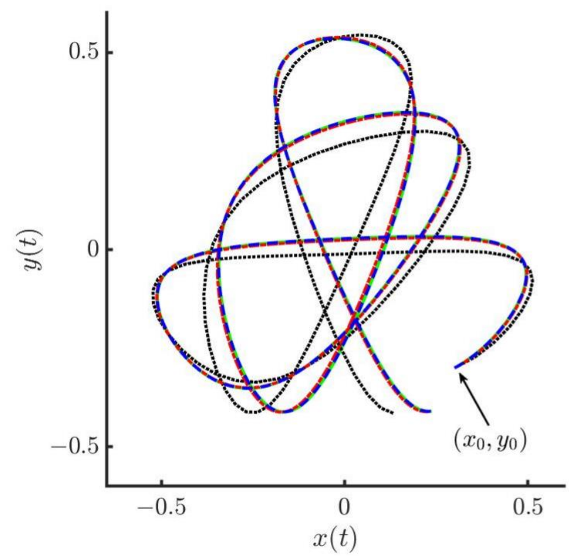

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Model Order Reduction: to reduce the computational complexity

Definition

- Model order reduction (MOR) is a set of techniques aimed at reducing the computational complexity of mathematical models in numerical simulations.
- Description of reality (model) + problem input data (in) $\longrightarrow$ PDEs $\longrightarrow$ discretization $\longrightarrow$ large-scale model with a large number of unknowns (degrees of freedom, DoFs) N.

$$\text{Full Order Model (FOM): Solve} \quad \dot{x} = f(x(t), in(t)) \quad \text{with} \quad \boxed{x \in \mathbf{R}^N}$$

- Model order reduction aims at lowering the computational complexity of such problems by reducing the # of DoFs ($r \ll N$)

$$\text{Reduced Order Model (ROM): Solve} \quad \dot{c} = f_r(c(t), in(t)) \quad \boxed{c \in \mathbf{R}^r \quad \text{with } r \ll N}$$

such that

$$\|x - Uc\| \leq C_r \|in\| \quad \text{with} \quad \lim_{r \to N} C_r = 0$$

U: reconstruction operator.

Key points:

- Full Order Model (FOM) $\boxed{x \in \mathbf{R}^N}$
- Reduced Order Model (ROM) $\boxed{c \in \mathbf{R}^r \quad \text{with } r \ll N}$
- Reconstruction: $\boxed{x \approx Uc}$ where U (size $N \times r$) is a data-driven discovered basis.

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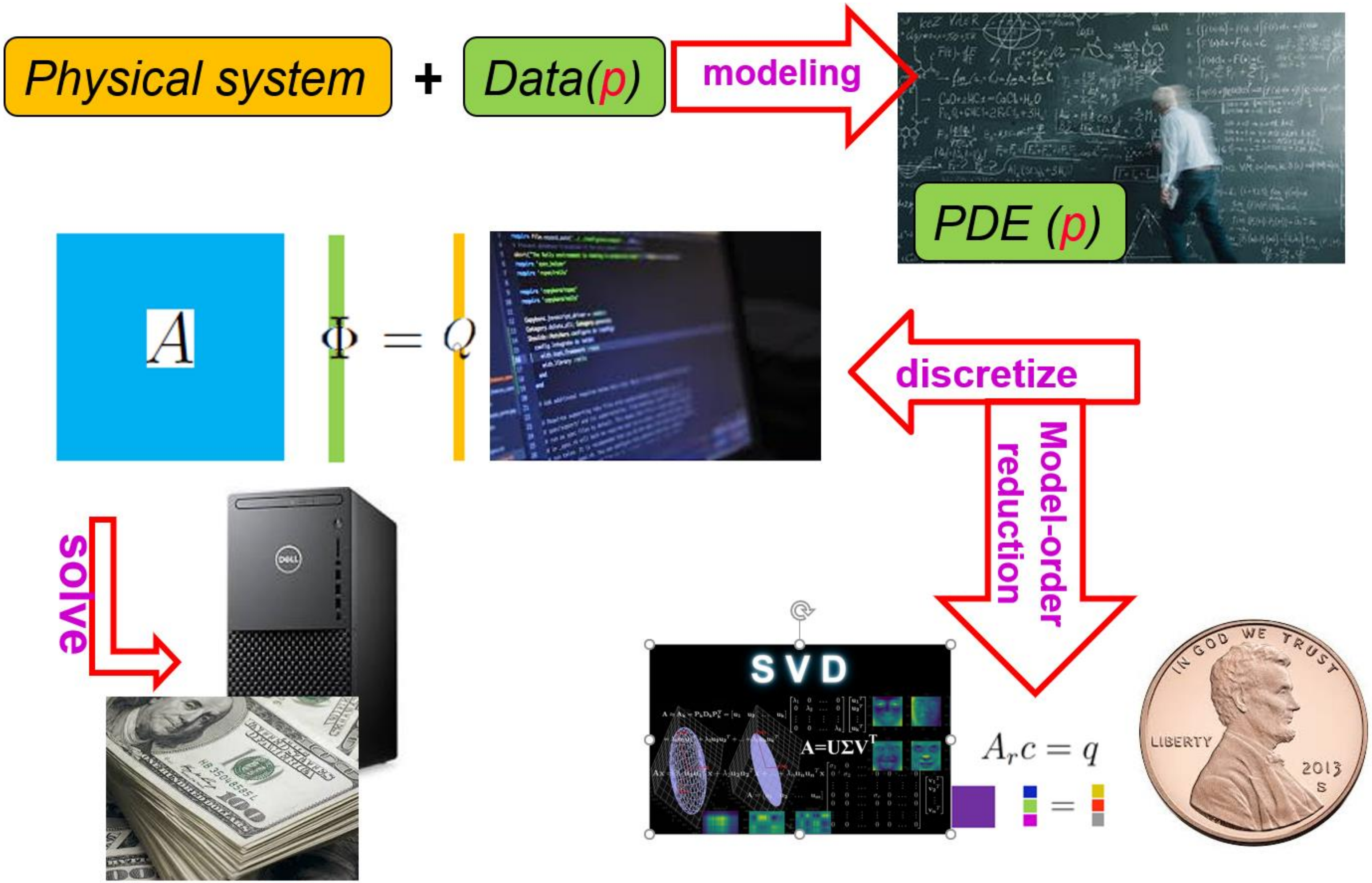
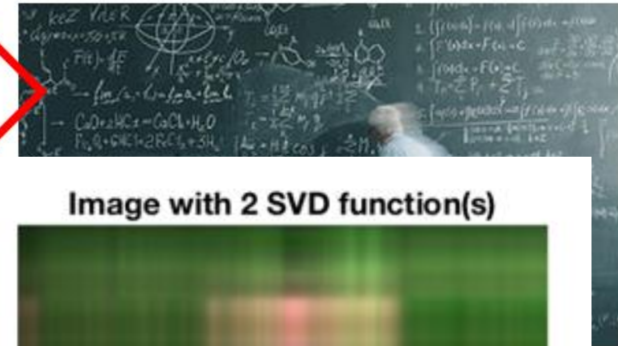
Need to determine the expansion coefficients c (as functions of the input parameters)

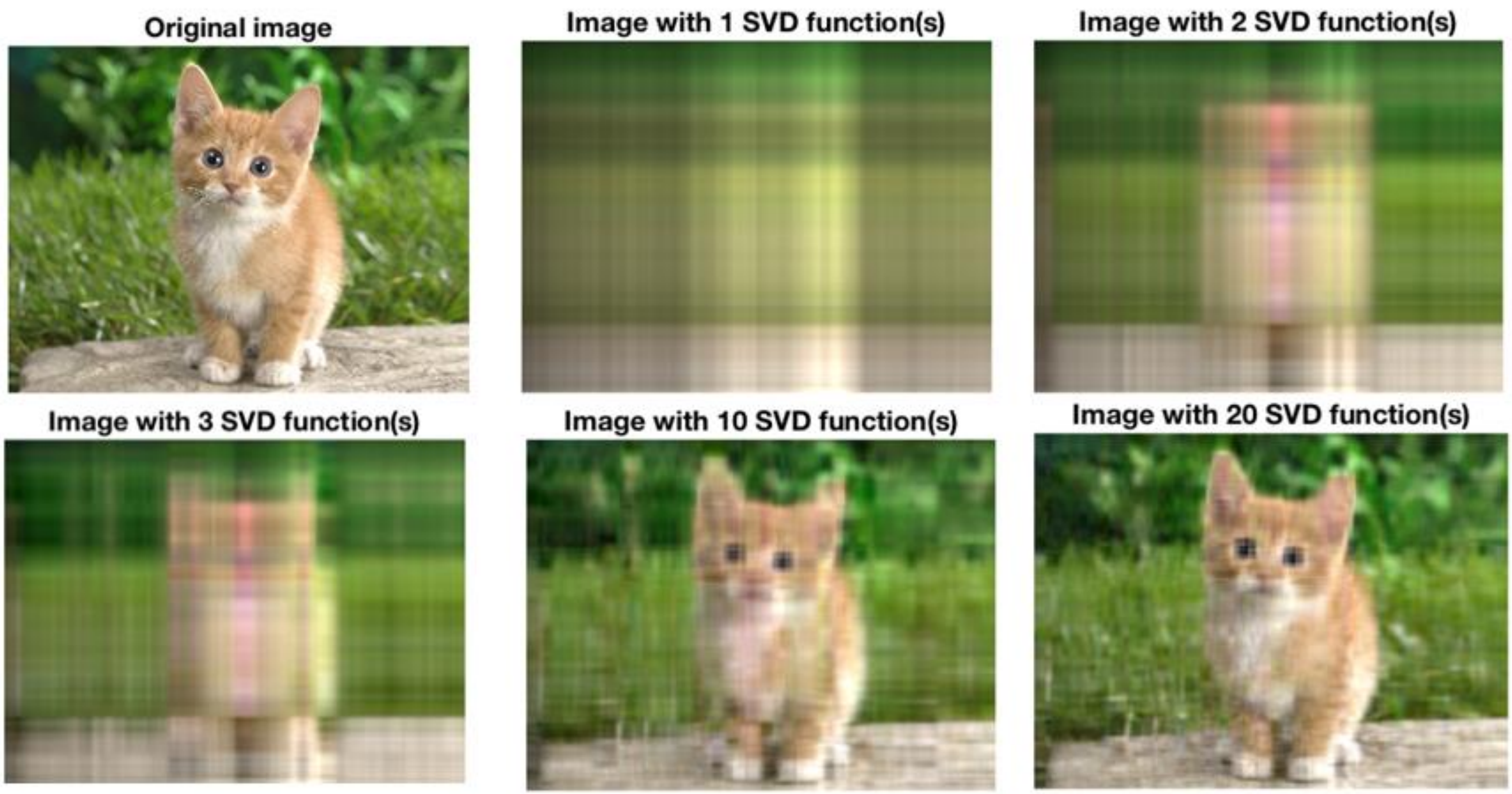
Data-driven sub-space discovery



Data-driven sub-space discovery

Physical system + *Data(p)* → **modeling**





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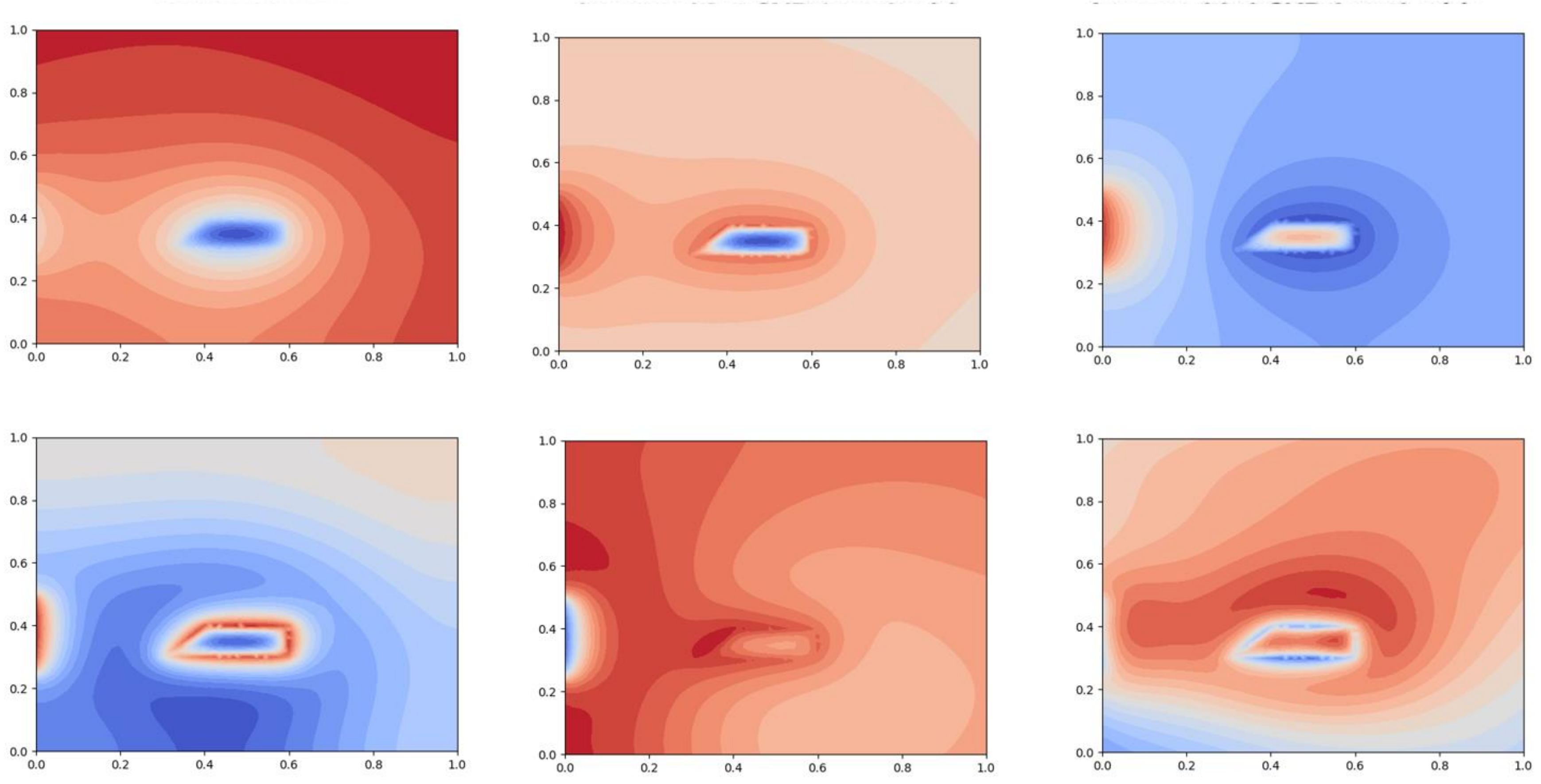

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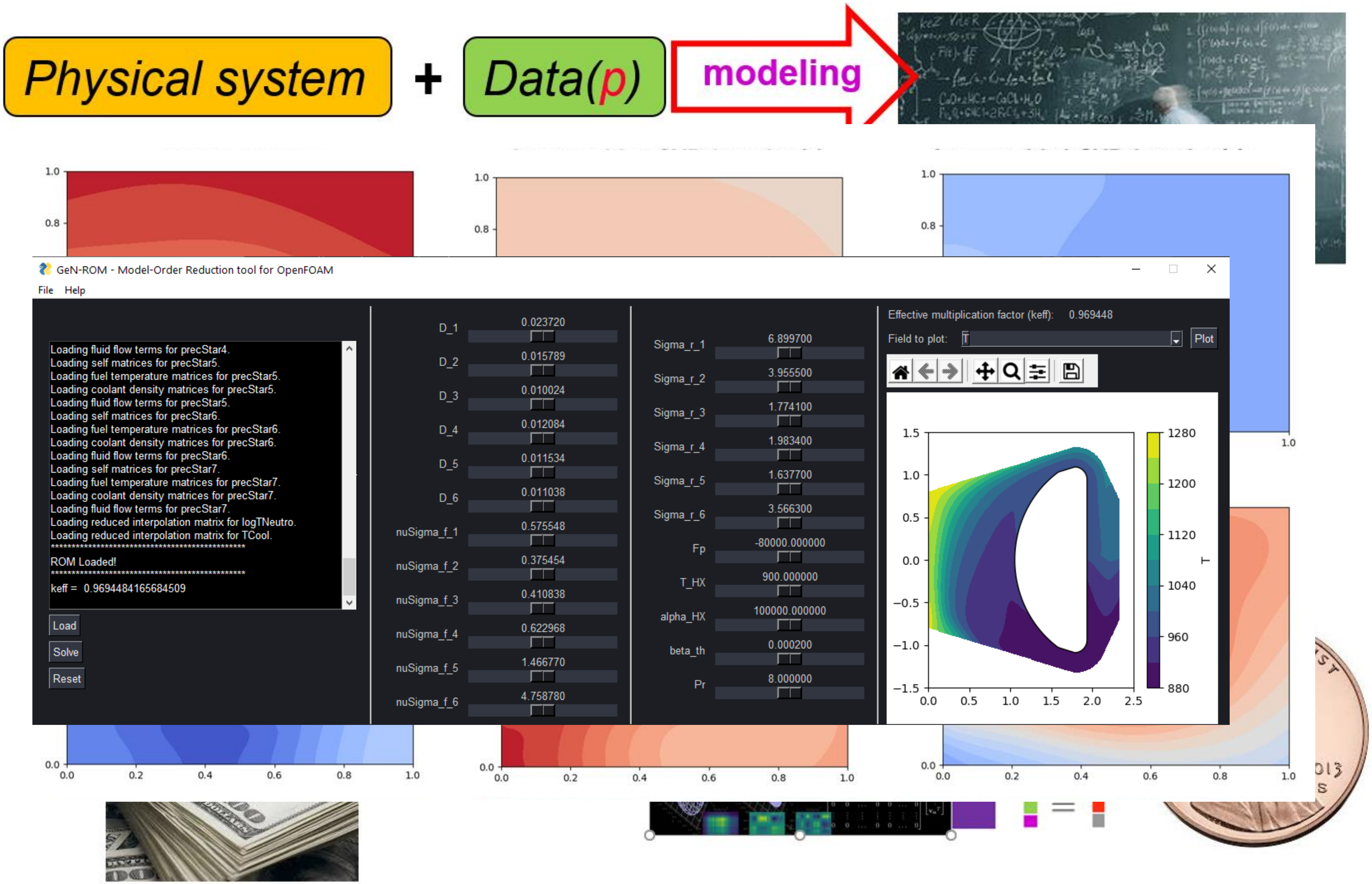
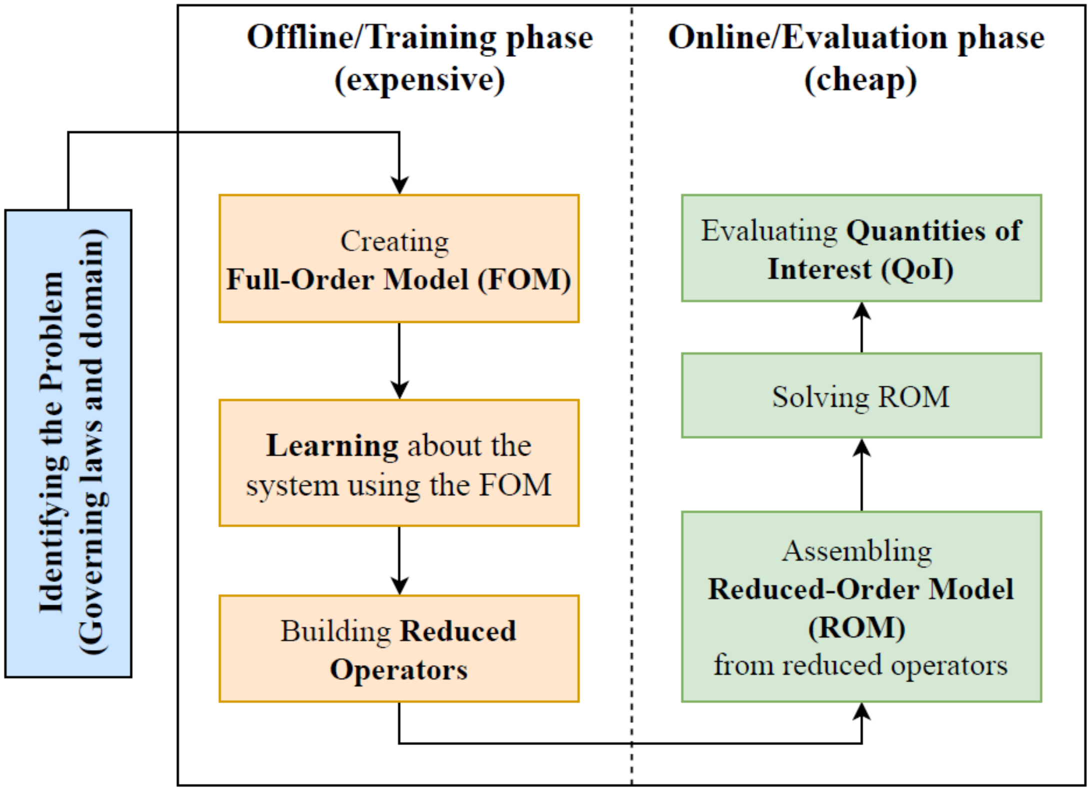


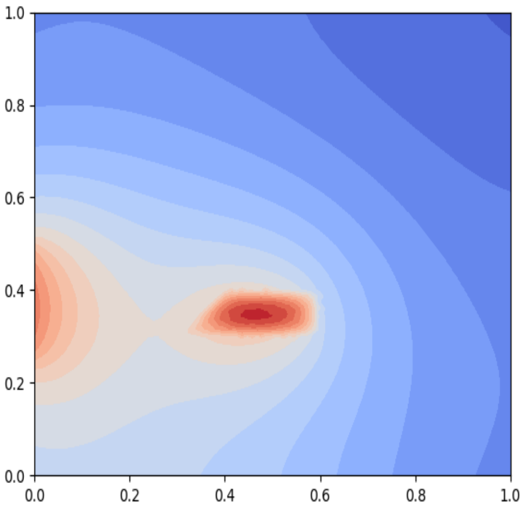
Flow chart

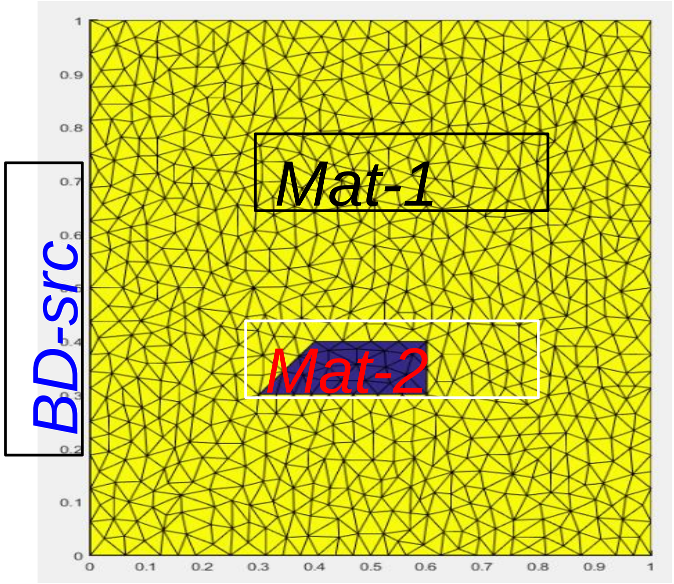


Important

Generating a ROM is only viable if the Training phase can be justified!

Many simulations with parametric variations





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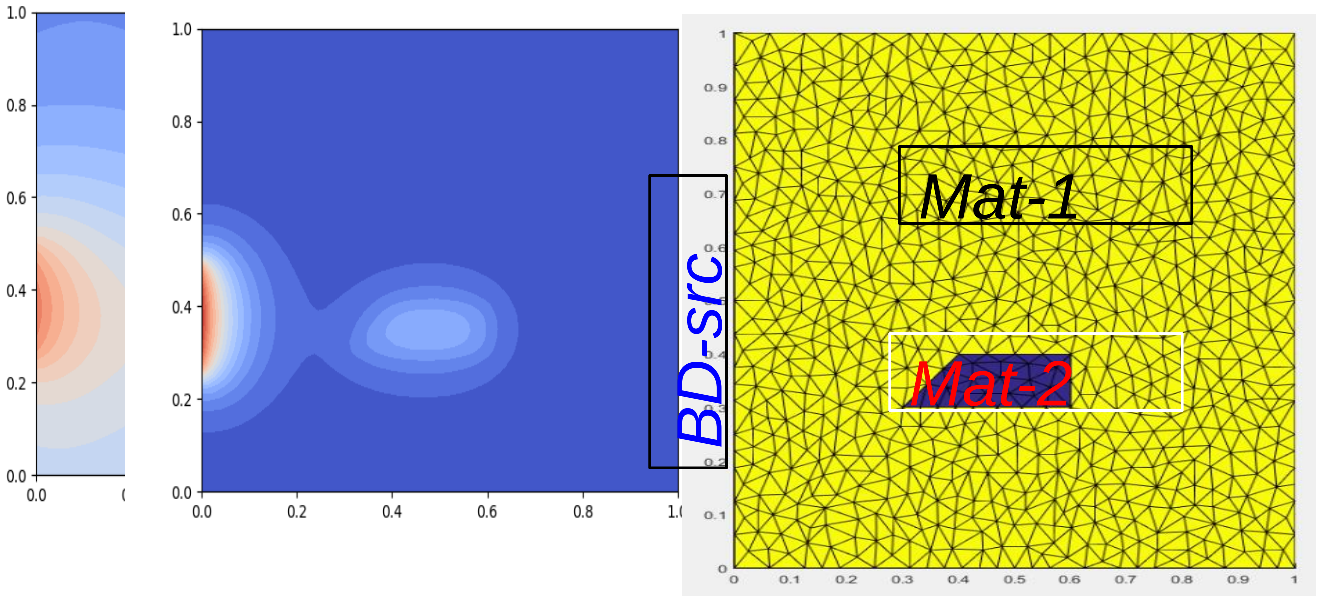

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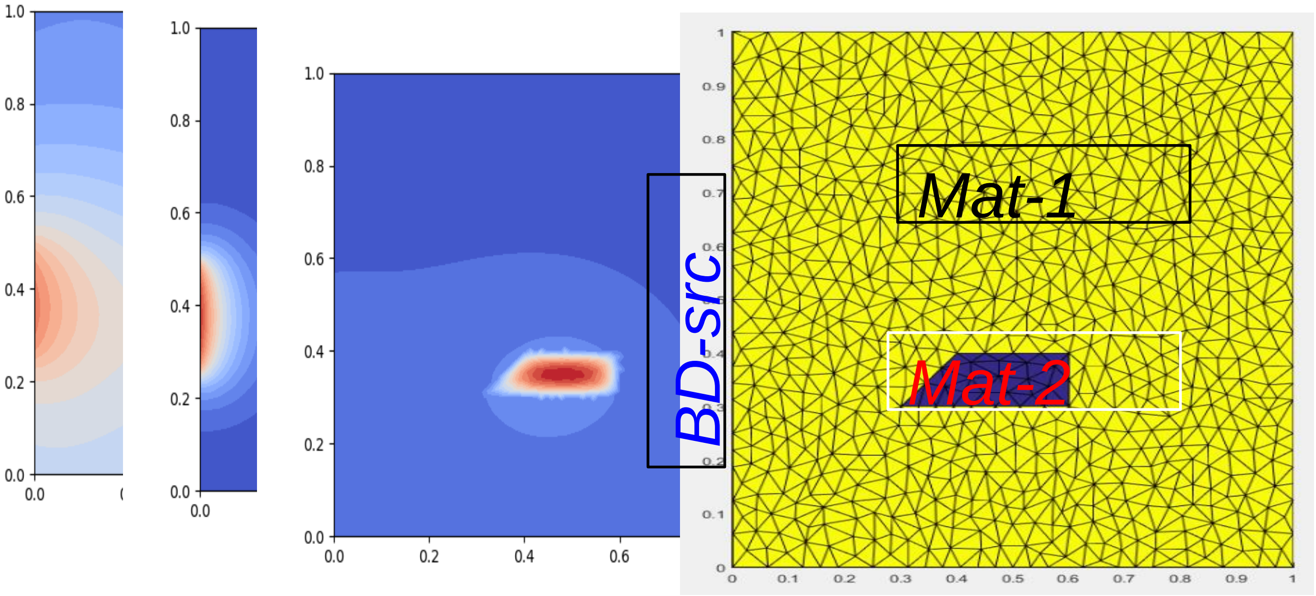

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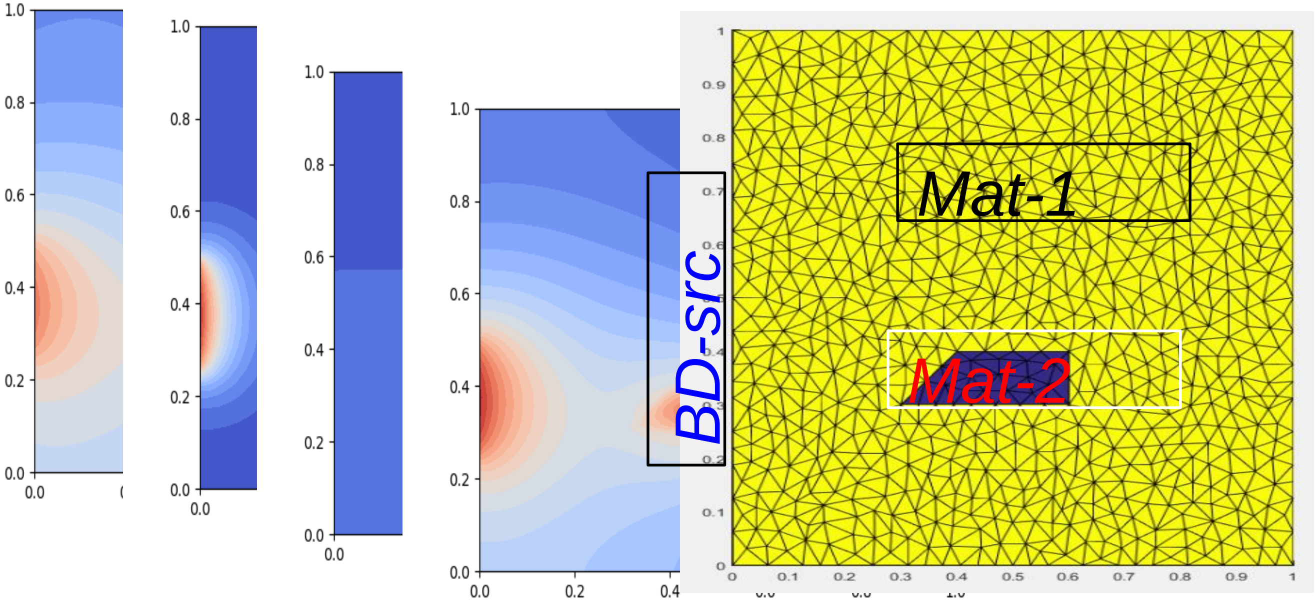

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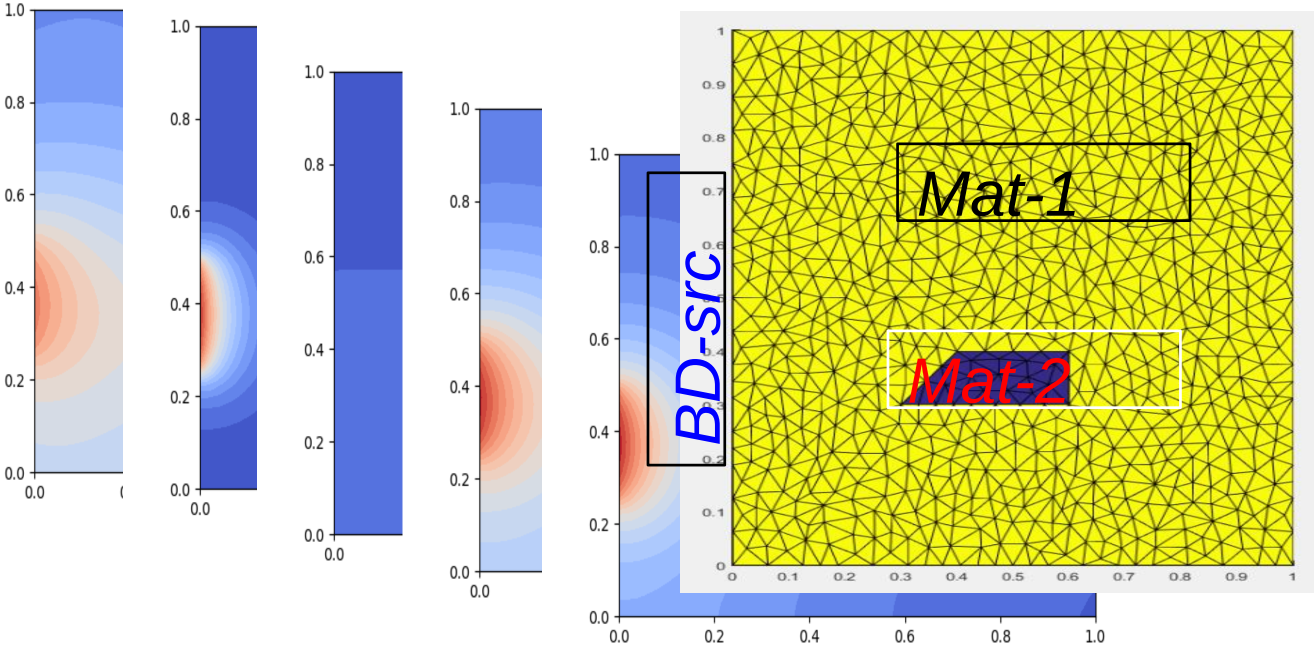

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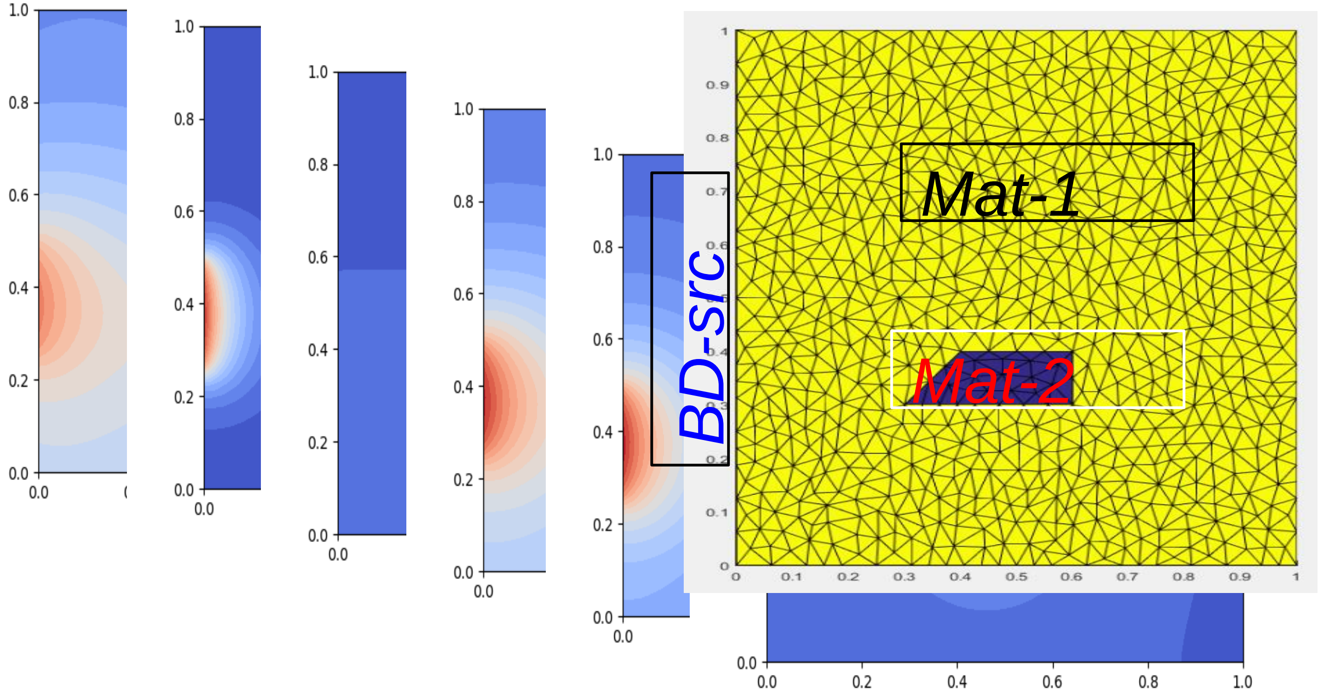

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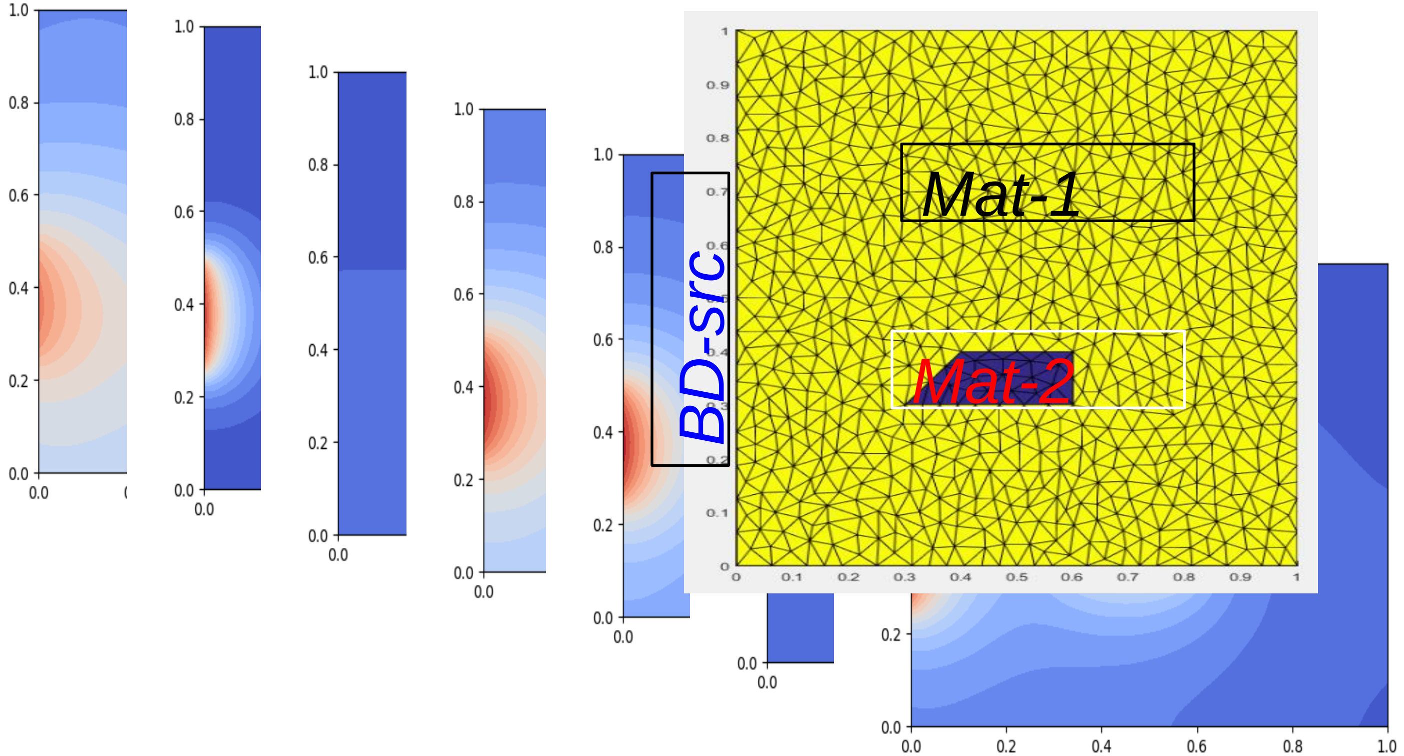

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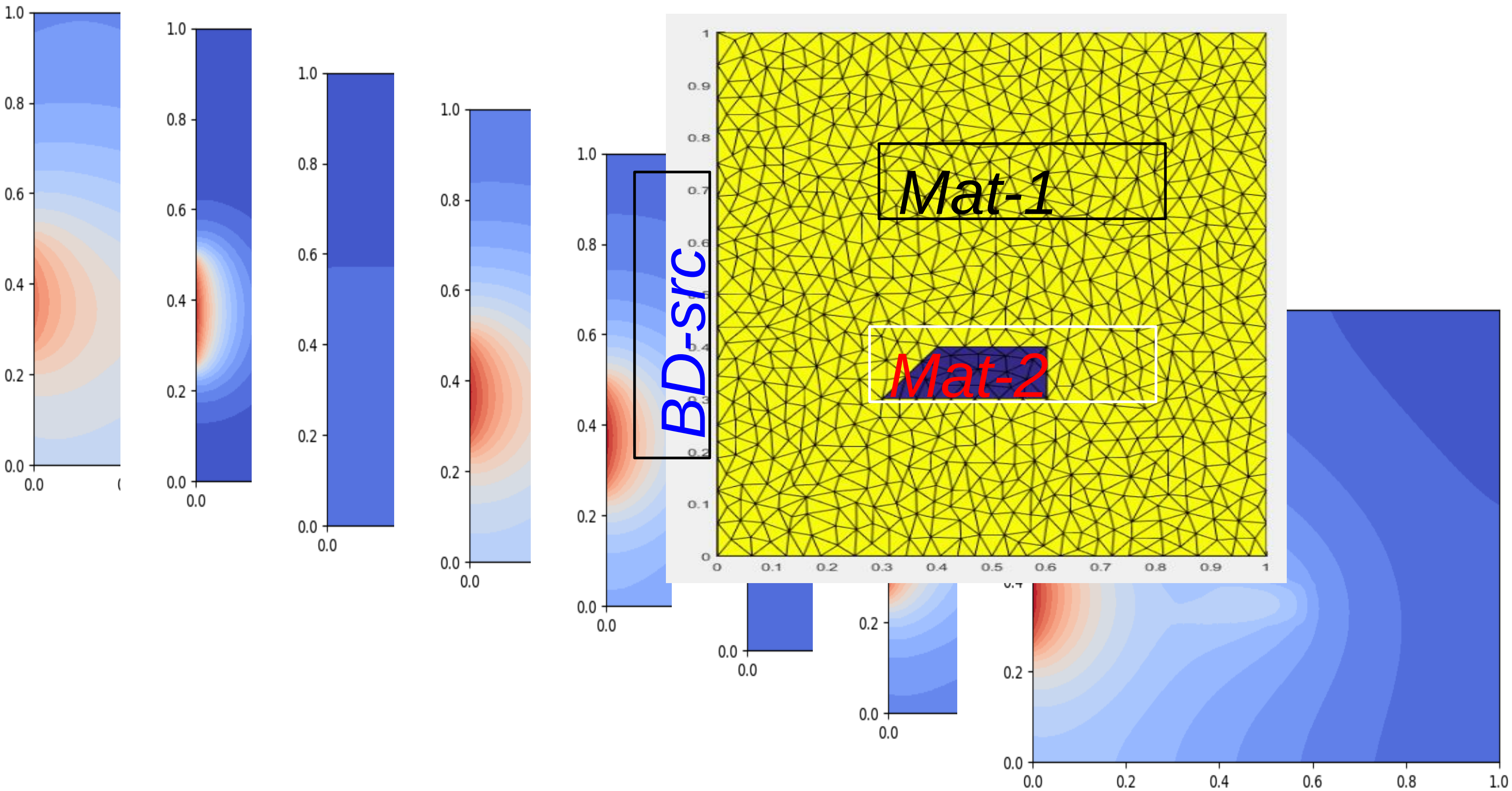

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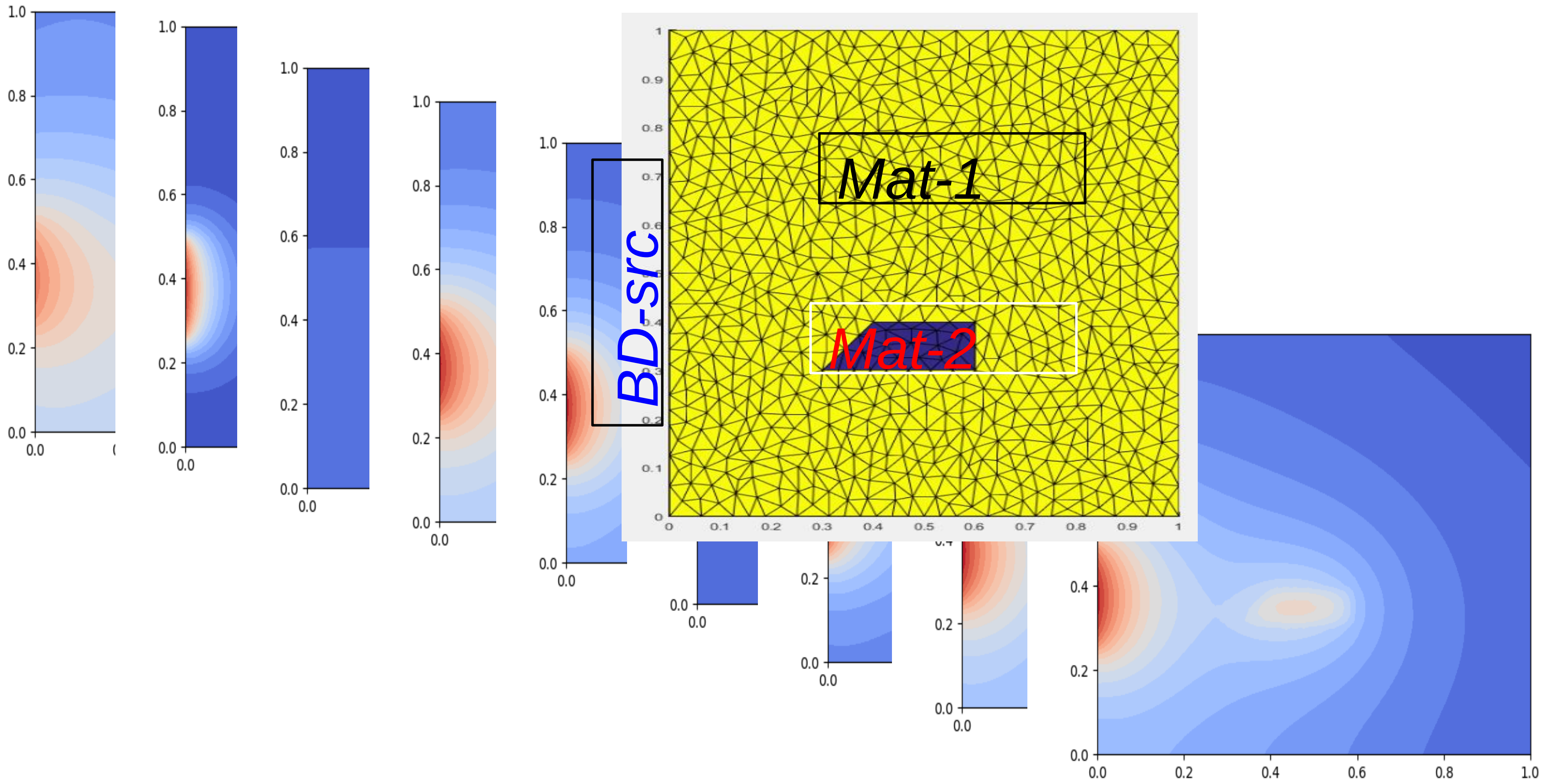

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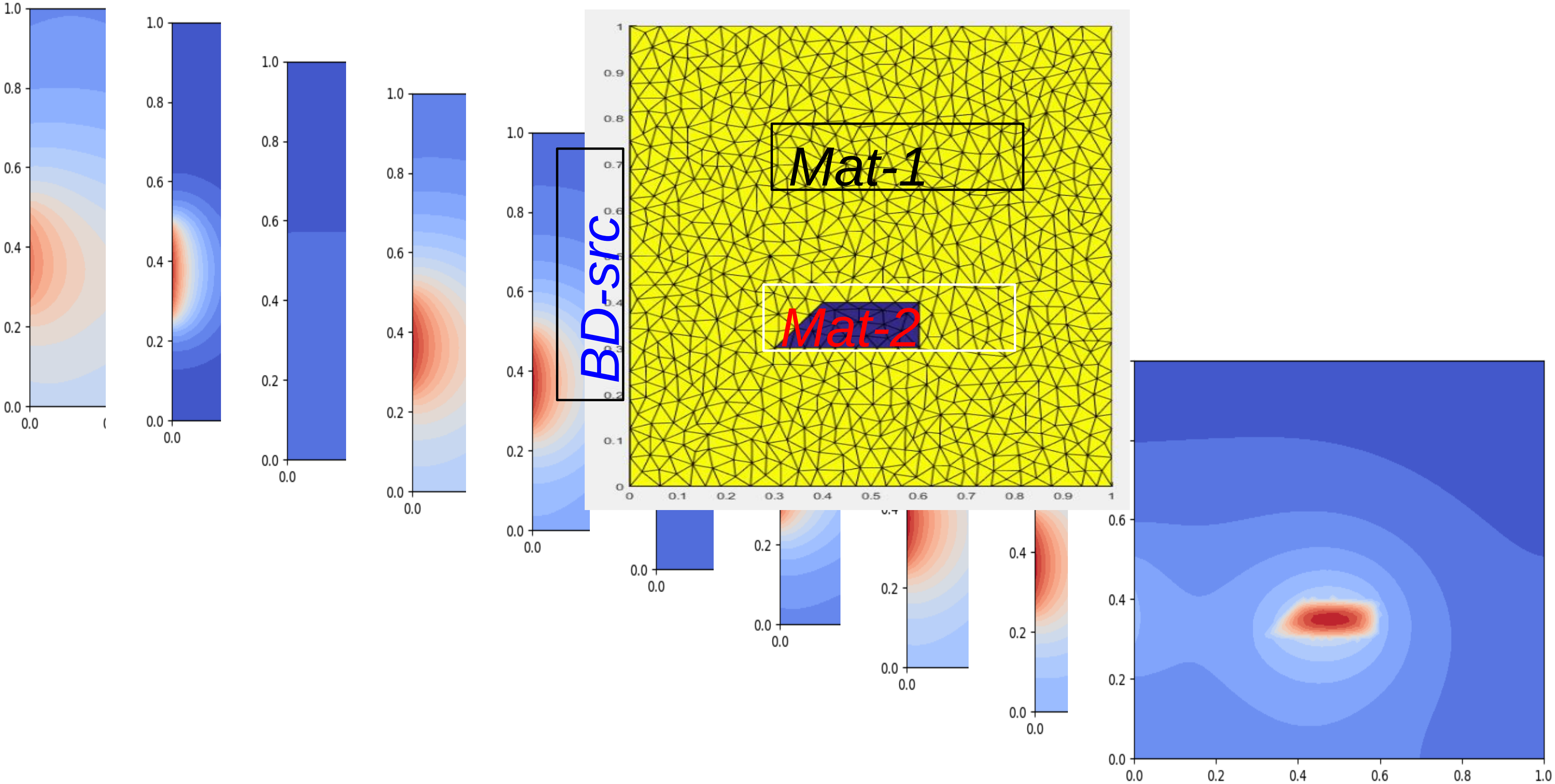

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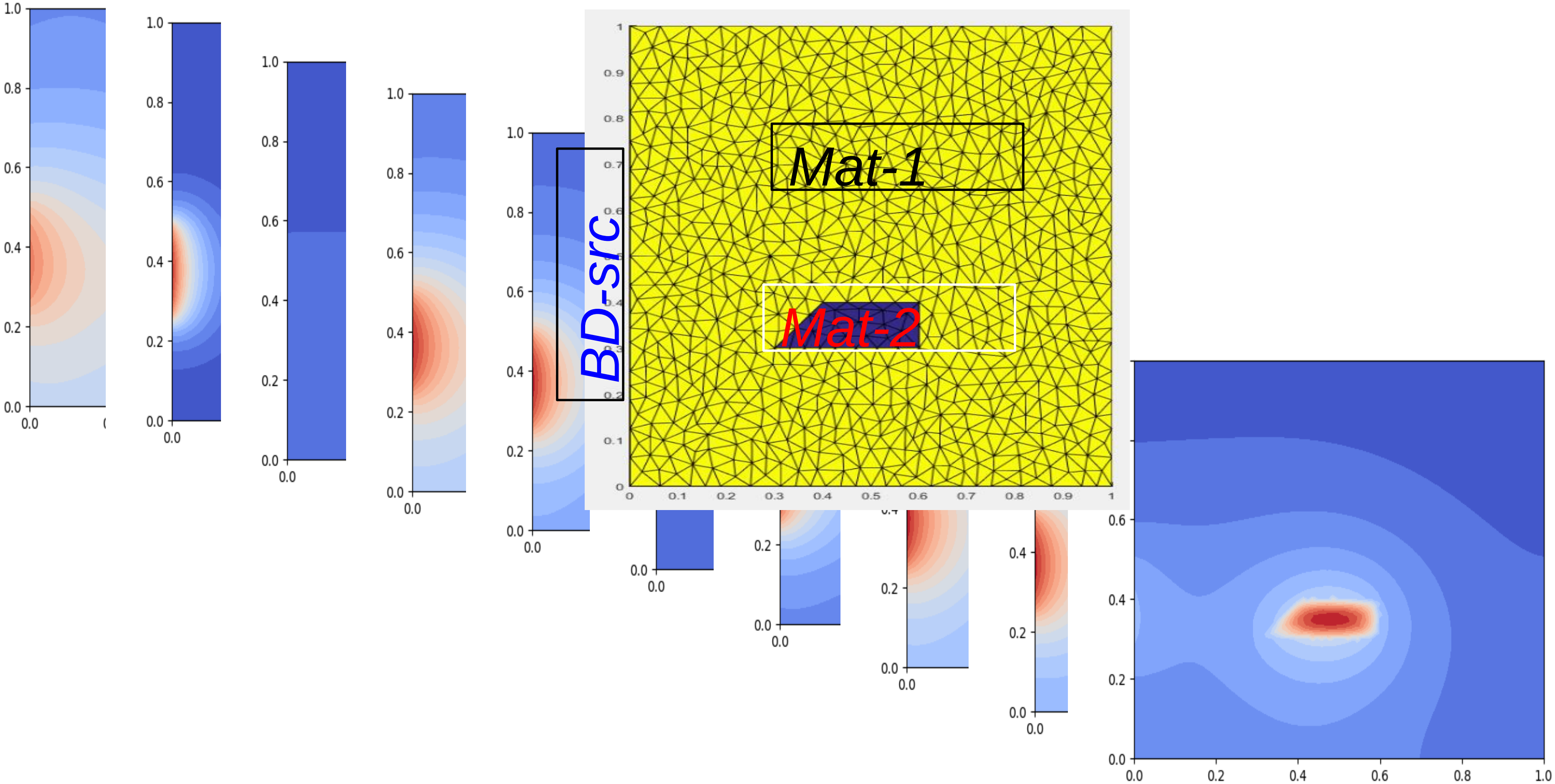
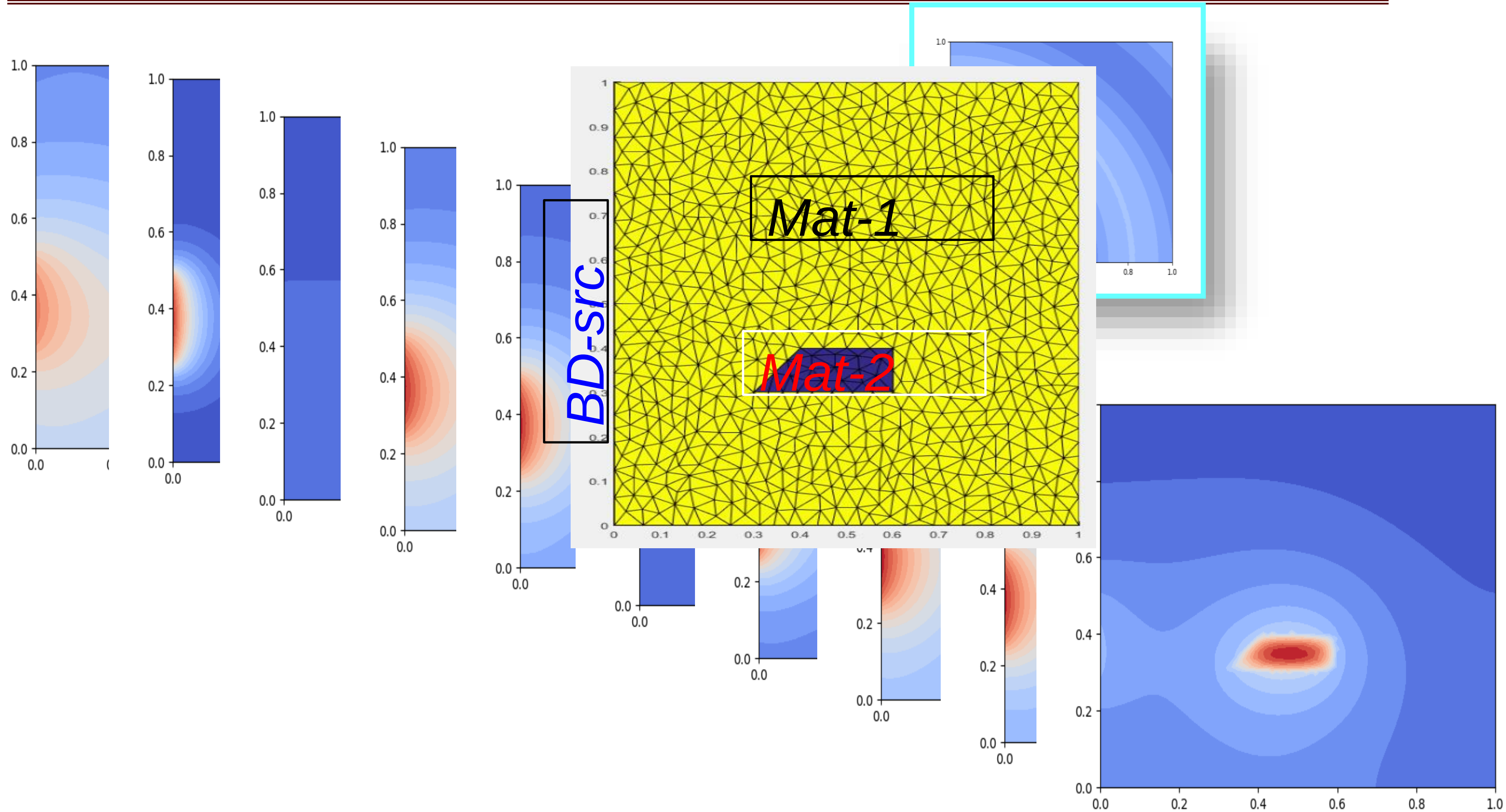


Common features among the family of solutions

Can we learn from that? → data-driven subspace discovery

Many simulations with parametric variations



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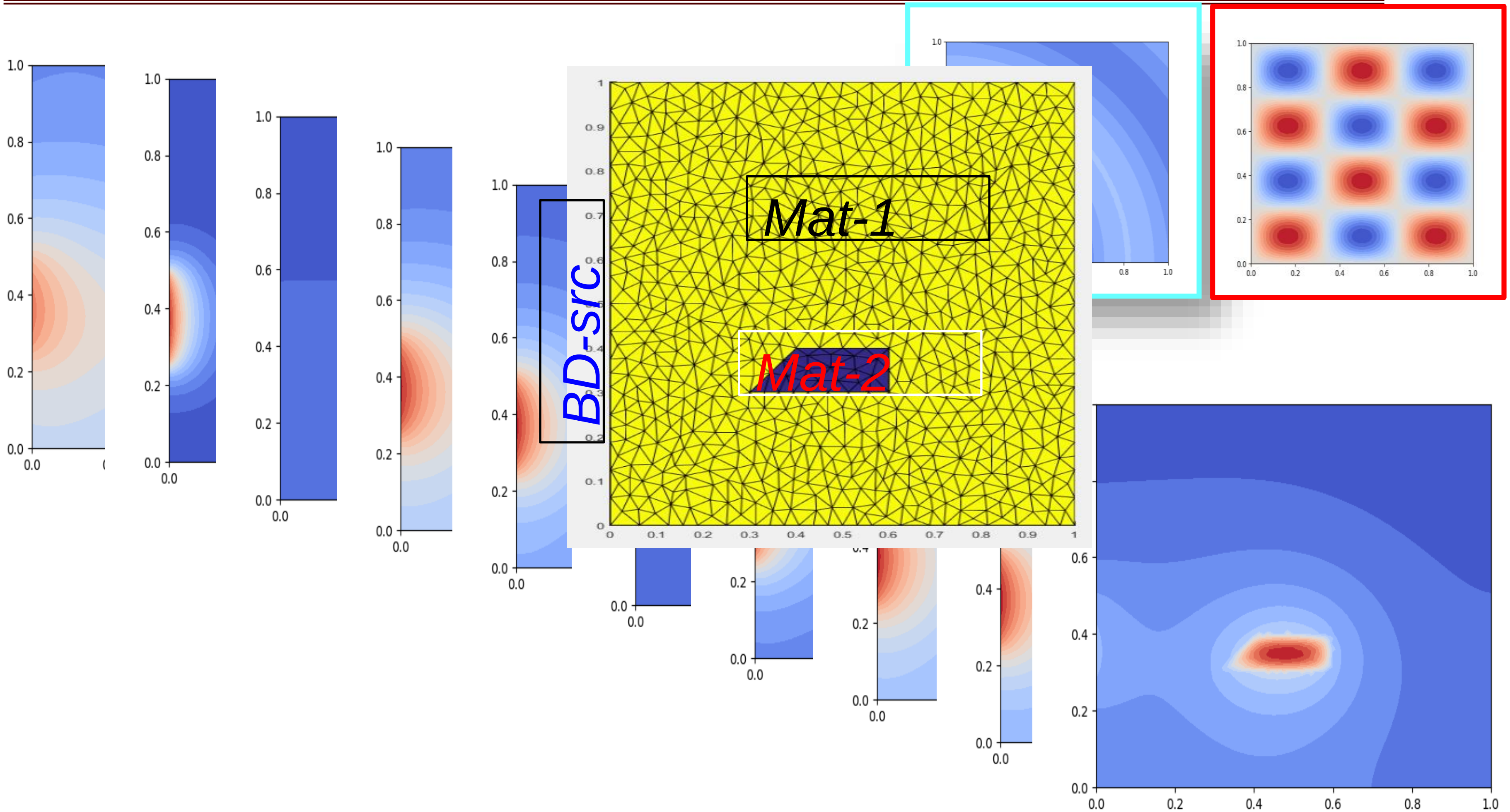

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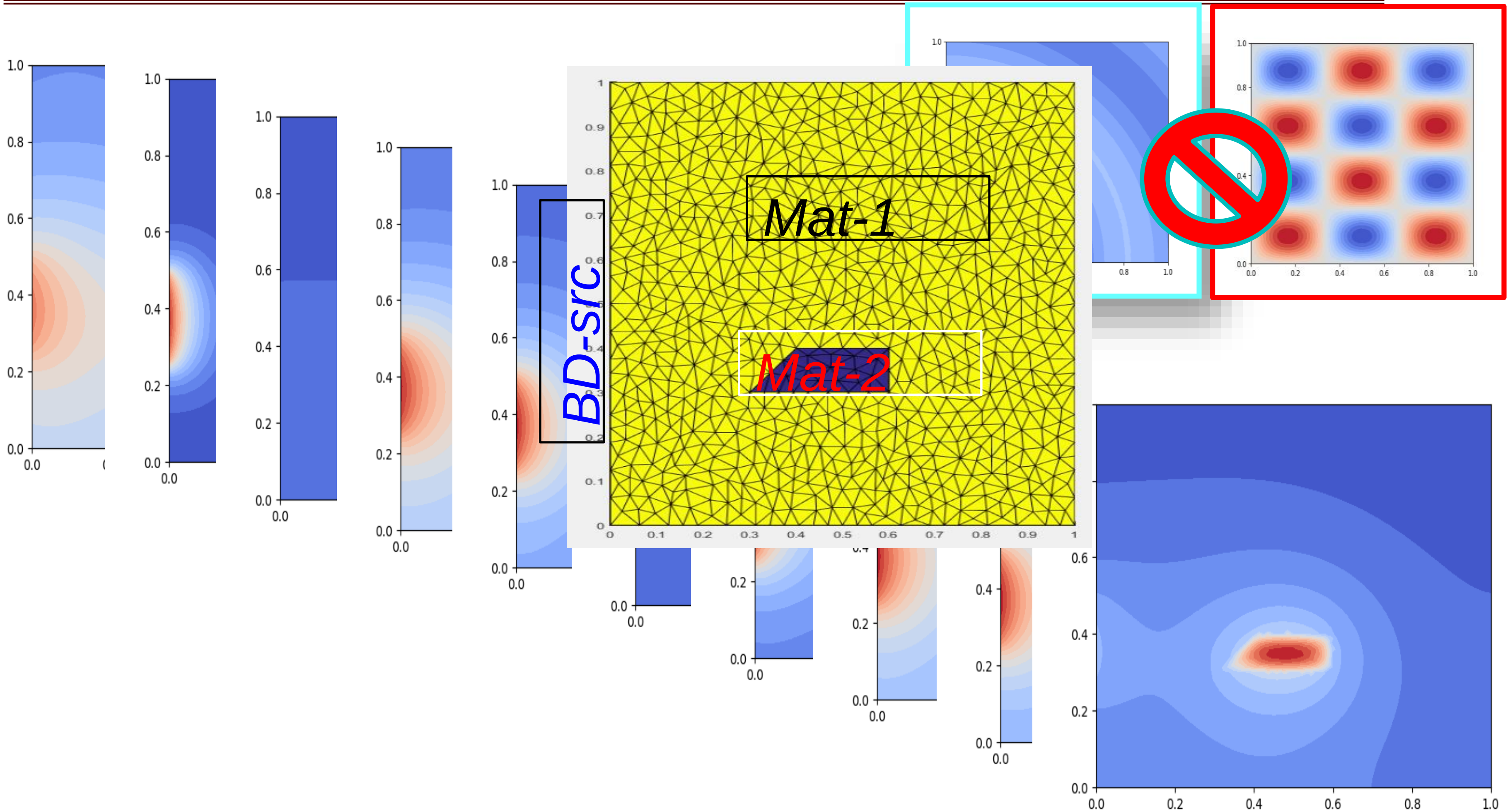

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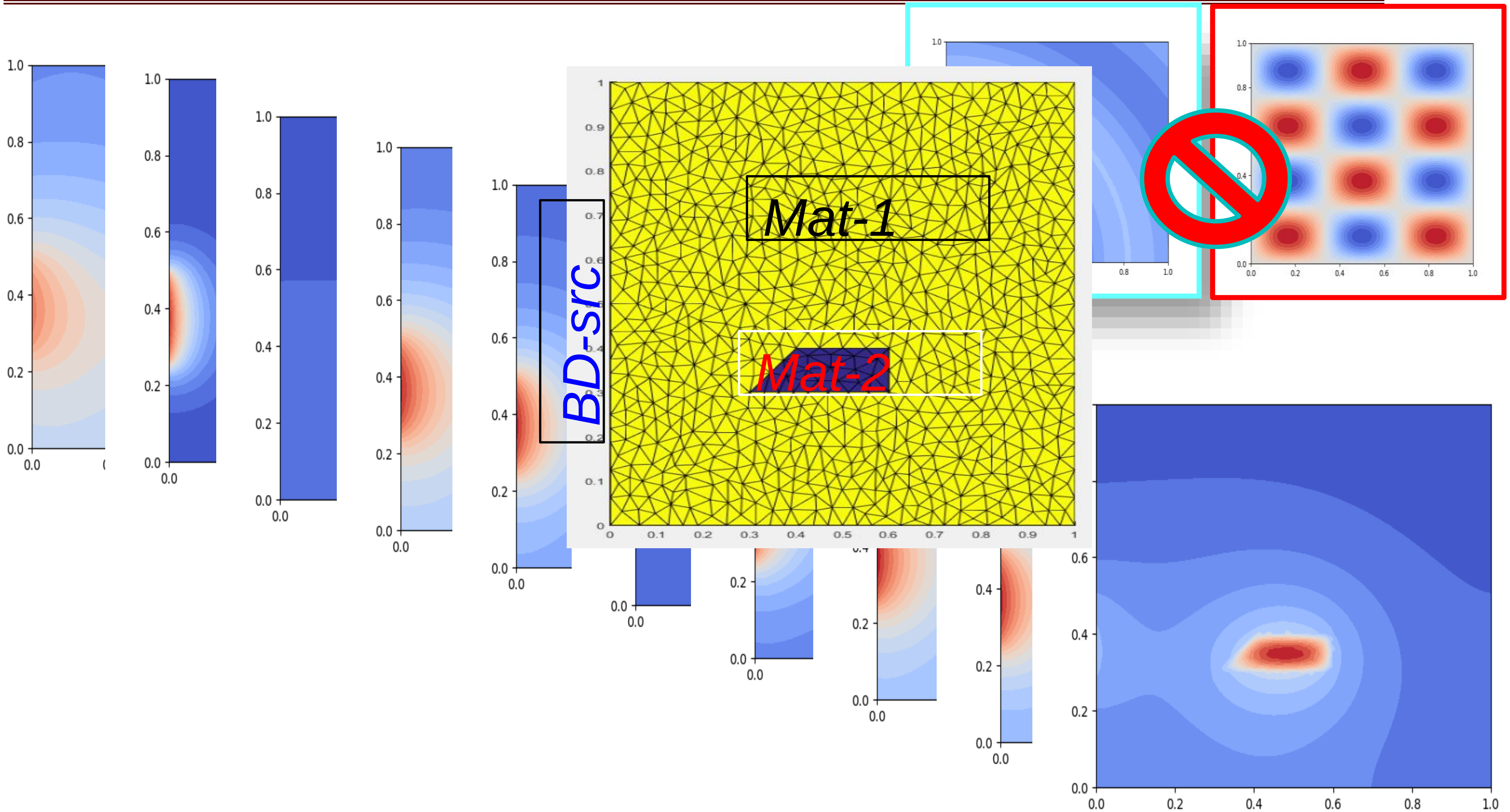

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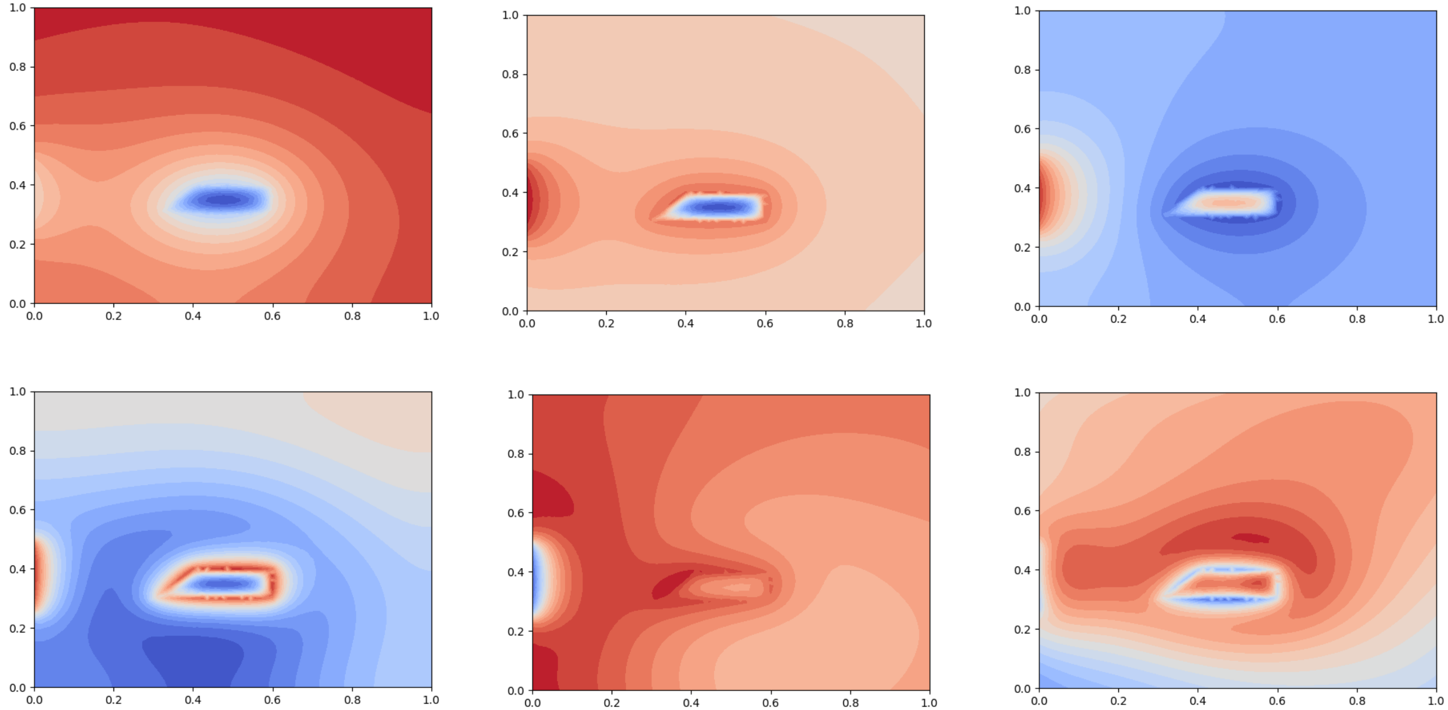
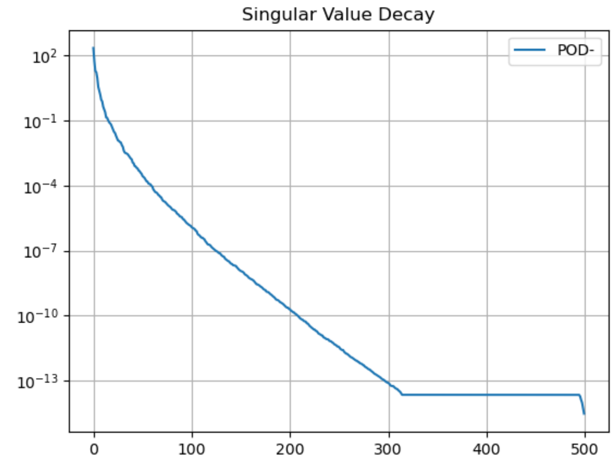
Discovered subspace from training data



- *Obtained via **Singular Value Decomposition** of the snapshots (learned data)*
- *Reduction comes from the low number of modes needed*



Not teaching SVD in UG linear algebra? A big mistake in the 21st century

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We Recommend a Singular Value Decomposition

Posted August 2009.

In this article, we will offer a geometric explanation of singular value decompositions and look at some of the applications of them.

...

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David Austin
Grand Valley State University
david at merganser.math.gvsu.edu

Introduction

The topic of this article, the *singular value decomposition*, is one that should be a part of the standard mathematics undergraduate curriculum but all too often slips between the cracks. Besides being rather intuitive, these decompositions are incredibly useful. For instance, Netflix, the online movie rental company, is currently offering a $1 million prize for anyone who can improve the accuracy of its movie recommendation system by 10%. Surprisingly, this seemingly modest problem turns out to be quite challenging, and the groups involved are now using rather sophisticated techniques. At the heart of all of them is the singular value decomposition.

A singular value decomposition provides a convenient way for breaking a matrix, which perhaps contains some data we are interested in, into simpler, meaningful pieces. In this article, we will offer a geometric explanation of singular value decompositions and look at some of the applications of them.

The geometry of linear transformations

Let us begin by looking at some simple matrices, namely those with two rows and two columns. Our first example is the diagonal matrix

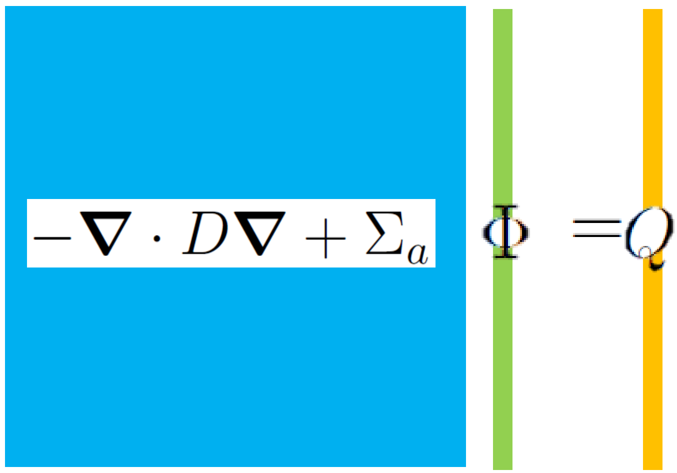
$$M = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$

Full-Order Model: an example

- Consider a neutron diffusion problem

$$-\nabla \cdot D \nabla \Phi + \Sigma_a \Phi = Q$$

- Discretize and obtain a linear system

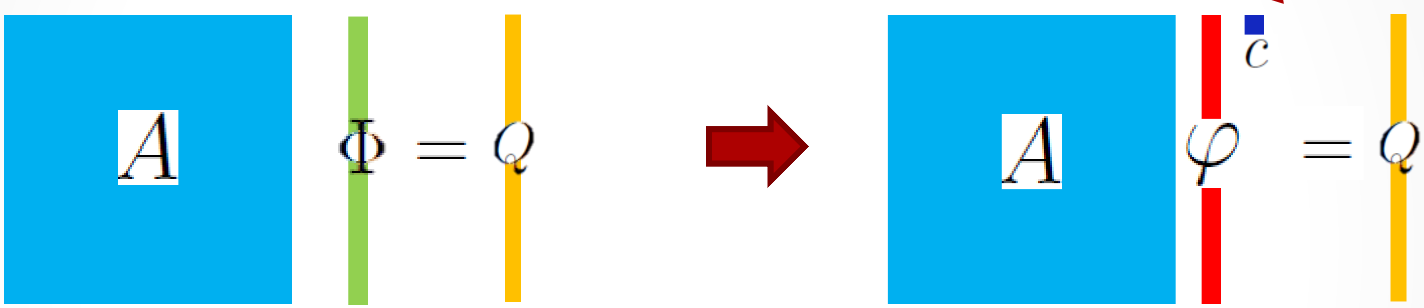


- The linear system can be very **large (size *n* *is* BIG)**
- This is what we call the **Full-Order Model** (which we wish to reduce)
- **Parameters ??** Let's say you do not know *D* and Σ in each region of the problem

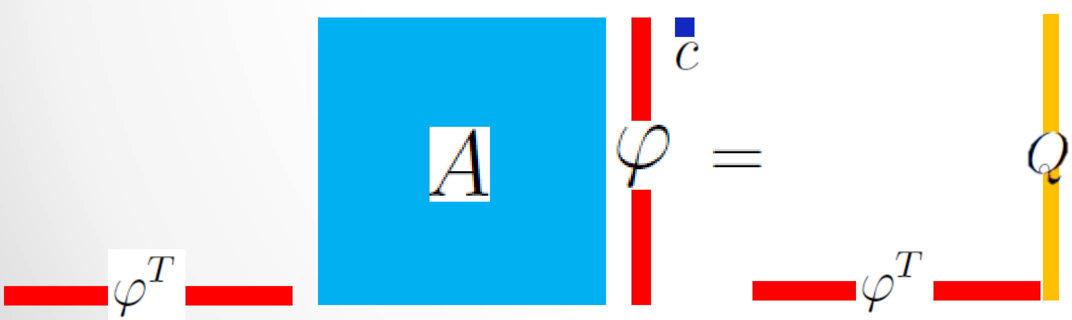
Physics-based model reduction: an example

- Assume the flux is expanded as a **known** spatial shape (basis) and a parametric amplitude $\Phi(\vec{r},\vec{\mu}) = \varphi(\vec{r})c(\vec{\mu})$
- Plug expansion in the linear system:

A single unknown number !!!



- Galerkin-project using known basis function:



$A_r c = q$

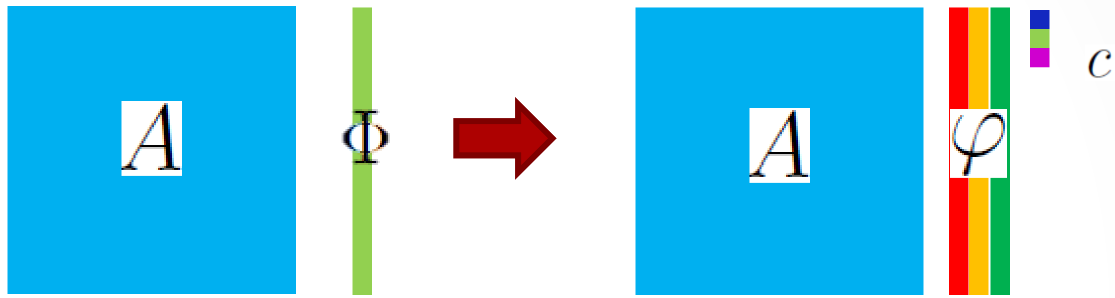
$A_r = \varphi^T A \varphi$

Solve for c

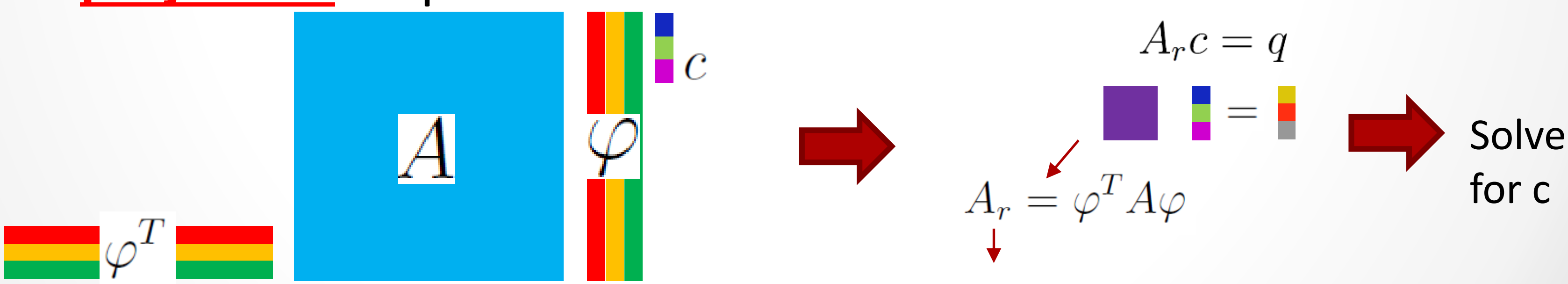
reduced matrix of size 1x1

Building improved reduced-order models

- Question :
  - Why not seek a solution with several basis function $\Phi = \sum_{i=1}^{i=r} \varphi_i(\vec{r})\ c_i(\vec{\mu})$



- The **projection** step is then:



reduced matrix of size *r* x *r* !!!
Goal: r << n

Why use more basis functions?

- We can capture variations in the solutions by using **more basis functions**
  - For instance, if a set of input parameters is uncertain, we can explore how the solution varies

→ reduction of **<u>parameterized</u>** full-order models

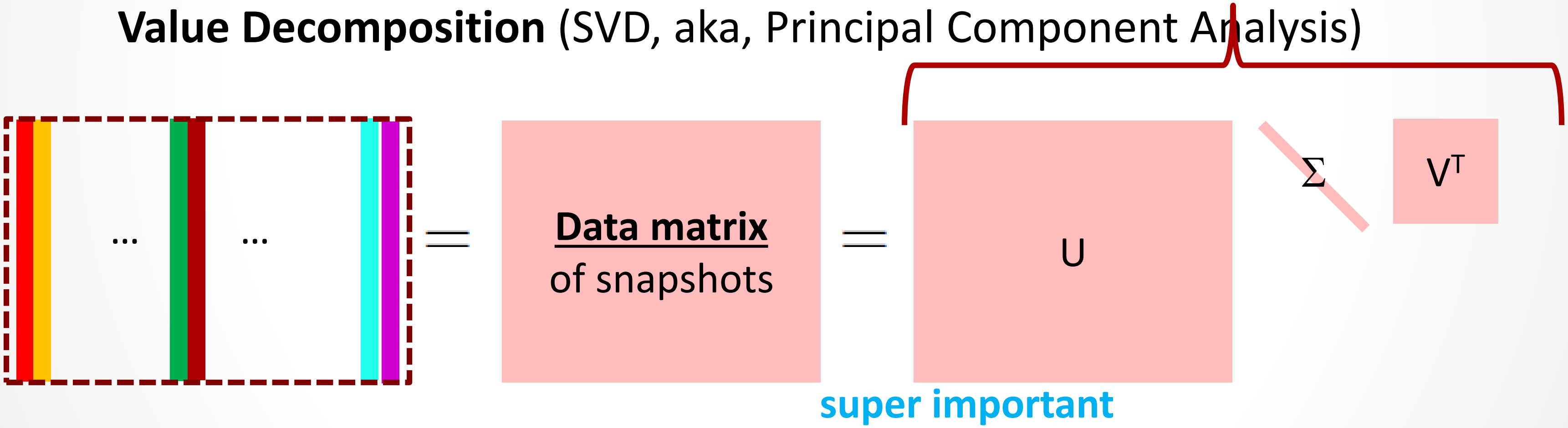
→ uncertainty quantification

→ design optimization

  - Parameter examples:
    - Cross-section variations
    - Geometrical variations
    - Heat removal rate
    - …

How to choose these basis functions ?

- Method of Snapshots
  - Used in CFD for turbulence modeling for a long time
  - Recently started to be popular for particle transport, reactor kinetics, …
- Process:
  - **Explore** the input space (e.g., Latin Hypercube Sampling)
  - **Generate** full-order model solutions (snapshots) and perform **Singular Value Decomposition** (SVD, aka, Principal Component Analysis)



  - Finally, based on the magnitude of the singular values, **down-select the dominant modes**
    - Think of "image compression" for physical solutions

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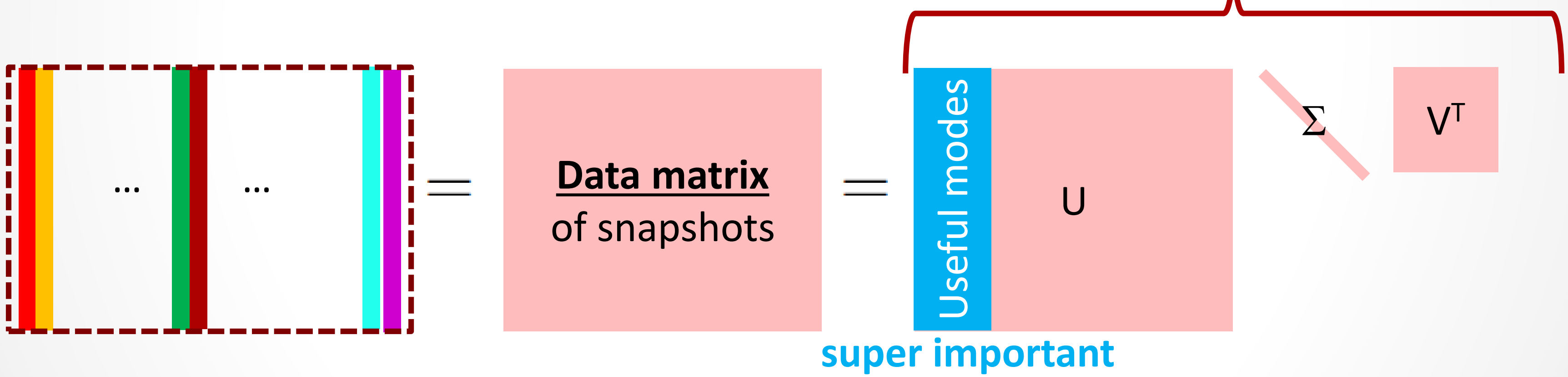
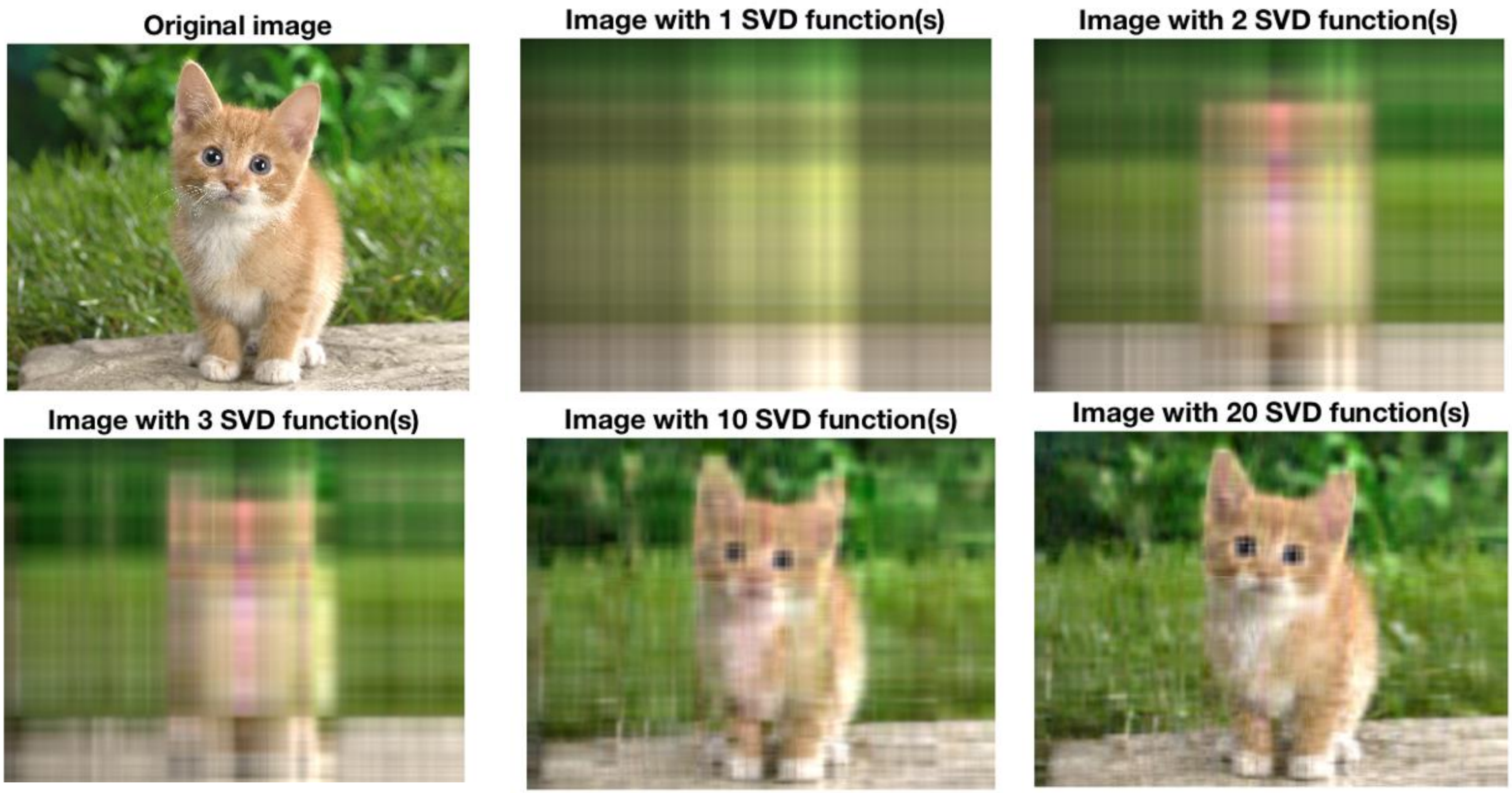


  - Finally, based on the magnitude of the singular values, **down-select the dominant modes**
    - Think of “image compression” for physical solutions

Demonstration of SVD with image compression

- 1200 x 1600 pixels (RGB array)
- Do we need 1600 vectors to have a representative picture ?



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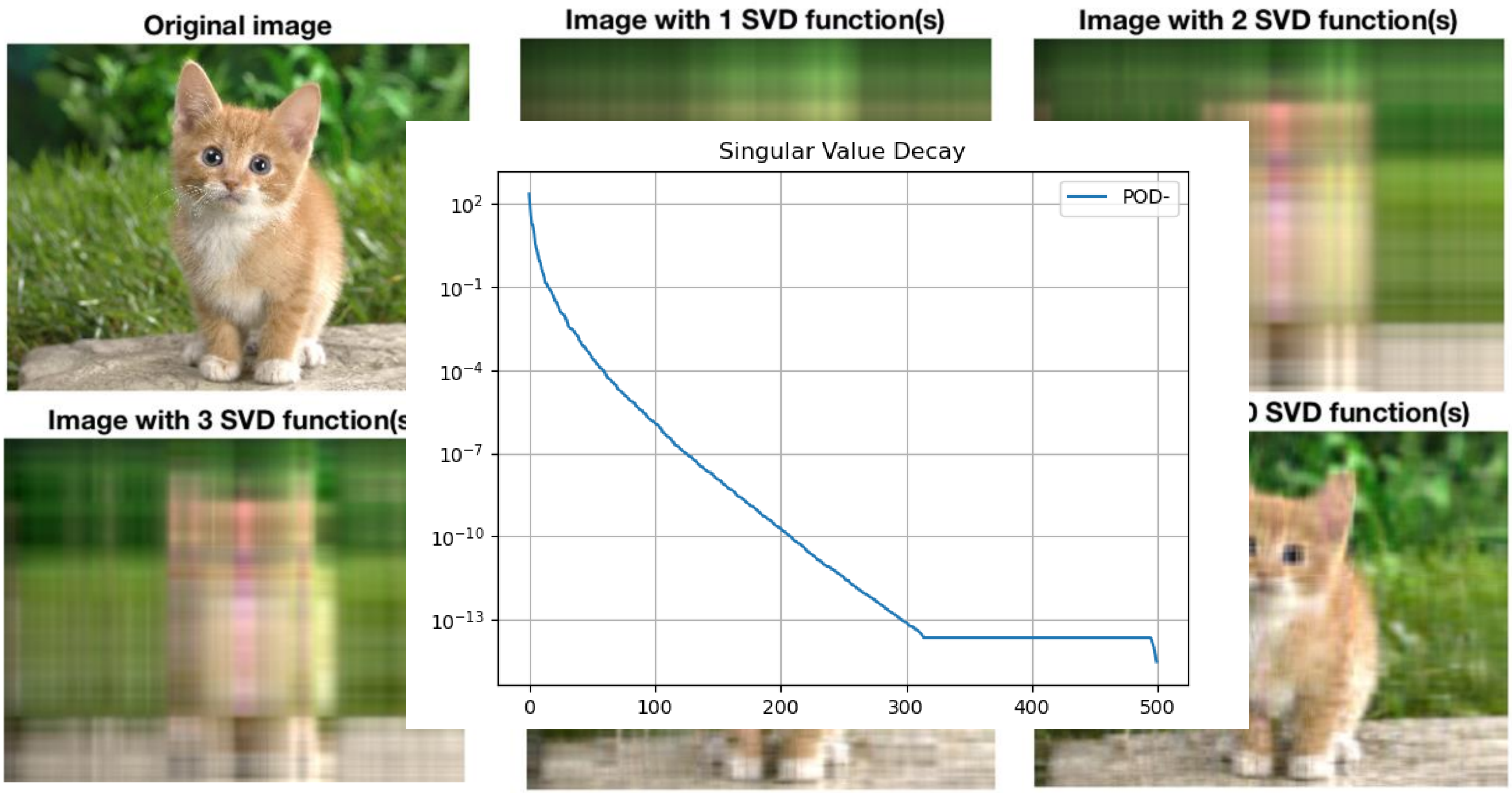


Projection-based ROM: some math …

- **First, the parametric full-order system (FOM):**

Training phase - Creating a Full-Order Model (FOM)

Discretization in space

$$\boldsymbol{M}_{\mathcal{D}} \frac{d\boldsymbol{\theta}(t;\boldsymbol{\mu})}{dt} + \boldsymbol{A}(t;\boldsymbol{\mu})\boldsymbol{\theta}(t;\boldsymbol{\mu}) + \boldsymbol{F}(\boldsymbol{\theta}(t;\boldsymbol{\mu}),t;\boldsymbol{\mu}) = \boldsymbol{S}(t;\boldsymbol{\mu}),$$

Together with appropriate initial and boundary conditions (on Γ)

- $\boldsymbol{\theta}$ discretized solution field
- $\boldsymbol{M}_{\mathcal{D}} \in \mathbb{R}^{N\times N}$ mass matrix
- $\boldsymbol{A}(t;\boldsymbol{\mu}) \in \mathbb{R}^{N\times N}$ discretized linear operator
- $\boldsymbol{F}(\boldsymbol{\theta},t;\boldsymbol{\mu}) \in \mathbb{R}^{N}$ nonlinear function
- $\boldsymbol{S}(t;\boldsymbol{\mu}) \in \mathbb{R}^{N}$ source term

Projection-based ROM: learning about the FOM

Training phase - Learning about the System

Approximating of the solution

The **reduced-basis approximation** of $\boldsymbol{\theta}$ can be expressed as:

$$\boldsymbol{\theta}(t;\boldsymbol{\mu}) \approx \tilde{\boldsymbol{\theta}}(t;\boldsymbol{\mu}) = \sum_{i=1}^{r_\theta} \psi_i^\theta c_i^\theta(t;\boldsymbol{\mu}) = \boldsymbol{\Psi}^\theta \boldsymbol{c}^\theta,$$

Generation of the basis vectors

- **Method of snapshots** is used to collect information about the system $\rightarrow N_s$ instances of $\boldsymbol{\theta}$ is saved into a **snapshot matrix**:

$$\boldsymbol{R}_\theta = [\boldsymbol{\theta}(\boldsymbol{\mu}_1, t_1), \ldots, \boldsymbol{\theta}(\boldsymbol{\mu}_{N_\mu}, t_{N_\tau})] \in \mathbb{R}^{N \times N_S},$$

- The basis functions of the reduced subspace can be obtained by computing the constrained **Singular Value Decomposition (SVD)** of $\boldsymbol{R}_\theta$:

$$\boldsymbol{R}_\theta = \boldsymbol{\Psi}^\theta \boldsymbol{\Delta}^\theta \boldsymbol{V}^\theta.$$

  with enforcing $\boldsymbol{\Psi}^T \boldsymbol{M}_{\mathcal{D}} \boldsymbol{\Psi} = \boldsymbol{I}$. This is equivalent to **Proper Orthogonal Decomposition (POD)** for discrete systems.

Projection-based ROM: building the ROM

Training phase - Building Reduced Operators

- Using the spatially discretized formulation in Eq. (2) and the approximation in Eq. (3) together with a **Galerkin projection** (left multiplication by $\boldsymbol{\Psi}^{\theta,T}$):

$$\boldsymbol{\Psi}^{\theta,T}\boldsymbol{M}_{\mathcal{D}}\boldsymbol{\Psi}^{\theta}\frac{\partial \boldsymbol{c}^{\theta}(\boldsymbol{\mu},t)}{\partial t}+\boldsymbol{\Psi}^{\theta,T}\boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{\Psi}^{\theta}\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t)+\boldsymbol{\Psi}^{\theta,T}\boldsymbol{F}(\boldsymbol{\Psi}^{\theta}\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t),\boldsymbol{\mu})=\boldsymbol{\Psi}^{\theta,T}\boldsymbol{S}\,, \tag{6}$$

- where $\boldsymbol{\Psi}^{\theta,T}\boldsymbol{M}_{\mathcal{D}}\boldsymbol{\Psi}^{\theta}=\boldsymbol{I}$, $\boldsymbol{A}^{r}(\boldsymbol{\mu})=\boldsymbol{\Psi}^{\theta,T}\boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{\Psi}^{\theta}\in\mathbb{R}^{r_\theta\times r_\theta}$ and $\boldsymbol{S}^{r}=\boldsymbol{\Psi}^{\theta,T}\boldsymbol{S}\in\mathbb{R}^{r_\theta}$ can be used to get

$$\frac{\partial \boldsymbol{c}^{\theta}(\boldsymbol{\mu},t)}{\partial t}+\boldsymbol{A}^{r}(\boldsymbol{\mu})\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t)+\boldsymbol{\Psi}^{\theta,T}\boldsymbol{F}(\boldsymbol{\Psi}^{\theta}\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t),\boldsymbol{\mu})=\boldsymbol{S}^{r}\,. \tag{7}$$

- It is visible that at this point the only unknowns in the system are the elements of $\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t)$, which means that **the number of spatial unknowns is reduced from N to $r_\theta \ll N$.**

Projection-based ROM: building the ROM

About the Nonlinear Term

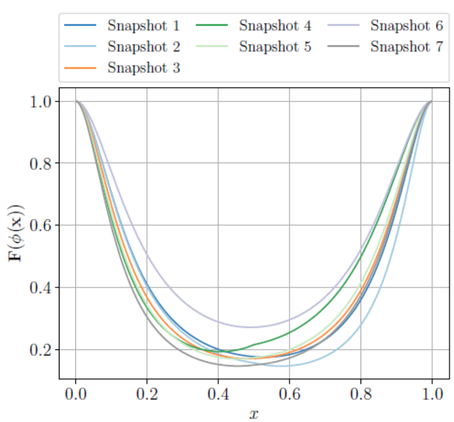
Discrete Empirical Interpolation Method (DEIM) [2]

Discrete Empirical Interpolation Method (DEIM) is used to approximate the "reduced" nonlinear operator as:

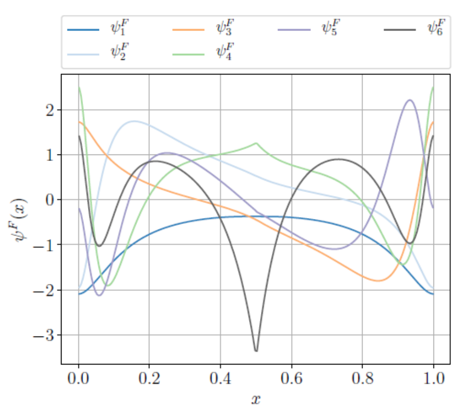
$$\boldsymbol{\Psi}^{\theta,T}\boldsymbol{F}(\boldsymbol{\Psi}^{\theta}\boldsymbol{c}^{\theta}(\boldsymbol{\mu},t),\boldsymbol{\mu}) \approx \boldsymbol{\Psi}^{\theta,T}\boldsymbol{\Psi}^{\boldsymbol{F}}\boldsymbol{c}^{F}(\boldsymbol{c}^{\theta},\boldsymbol{\mu},t) \tag{8}$$

- $\boldsymbol{c}^F(\boldsymbol{c}^\theta,\boldsymbol{\mu},t)$ - coefficient vector for the nonlinear term
- $\boldsymbol{\Psi}^{\boldsymbol{F}}$ - **spatial basis built for the nonlinear term**

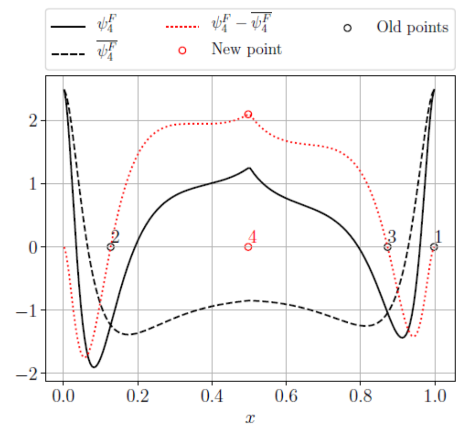
Snapshots



Basis functions



Interpolation points



Projection-based ROM: building the ROM

- **Quadratic terms, as in Navier-Stokes eqs, for instance:**

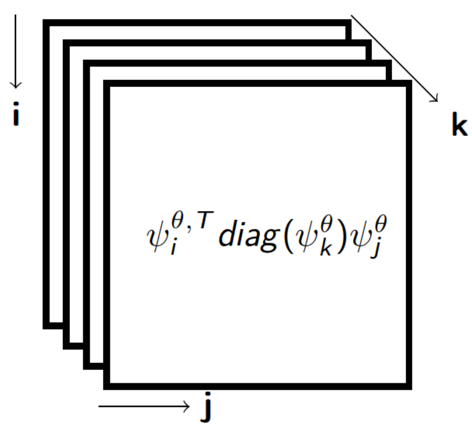
About the Nonlinear Term

Other option (for polynomial nonlinearities)

$$\boldsymbol{\Psi}^{\theta,T}(\boldsymbol{\Psi}^{\theta}\boldsymbol{c}^{\theta})^2 = \left(\sum_{k=1}^{r_\theta} c_k^{\theta}\boldsymbol{\Psi}^{\theta,T} diag(\psi_k^{\theta})\boldsymbol{\Psi}^{\theta}\right)\boldsymbol{c}^{\theta} = \boldsymbol{c}^{\theta,T}\underline{\underline{T}}\boldsymbol{c}^{\theta} \qquad (9)$$

This is commonly used for convection terms.

$\underline{\underline{T}} =$



What about the parameter dependence of the operators?

- Often, your operator (matrix) is linear (**affine**) in the ``parameters''.

$$A = \sum_i f_i(p) A_i$$

$$A = \sum_m D_m \hat{S}_m + \Sigma_m \hat{M}_m$$

- So the reduced operators can be pre-computed

$$A_r = \sum_m D_m \varphi^T \hat{S}^m \varphi + \Sigma_m \varphi^T \hat{M}^m \varphi = \sum_m D_m \hat{S}_r^m + \Sigma_m \hat{M}_r^m$$

- Obtaining them can be a little intrusive to the FOM code but can yield huge speed-ups

Projection-based ROM: Online phase of ROM

Online/evaluation Phase

Assembling ROM

Operations do not scale with N $\rightarrow$ **this step is fast**. (Summation/multiplication with scalar of small matrices/vectors)

Solving ROM

- Size of the system is $r_\theta \times r_\theta$ $\rightarrow$ **Even direct solvers can be used.**
- Time-dependent problems: **time integration is at reduced-order level**
- Nonlinear problems: **fixed-point iteration** is needed.

Computing Quantities of Interest (QoIs)

- Reconstruct approximate $\widetilde{\theta}$ $\rightarrow$ compute the QoIs. This scales with N **(slow)**.
- In **certain cases the QoI can be directly computed using $\boldsymbol{c}^\theta$**: point/average values can be stored for each basis function. **(really fast)**

Projection-based ROM: Online phase of ROM

Online/evaluation Phase

Assembling ROM

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Computing Quantities of Interest (QoIs)

- Reconstruct approximate $\widetilde{\theta}$ → compute the QoIs. This scales with N *not really*
- In **certain cases the QoI can be directly computed using c^θ**: point/average values can be stored for each basis function. **(really fast)**

Outline

1. High-performance computing (HPC)
   - *A. Some history*
   - *B. Some well-recognized software used in nuclear engineering*
   - *C. A few application examples*
2. Fast Data-driven Surrogate Models
   - *A. Motivations for parametric Reduced-Order Modeling (ROM)*
   - *B. What is model-order reduction?*

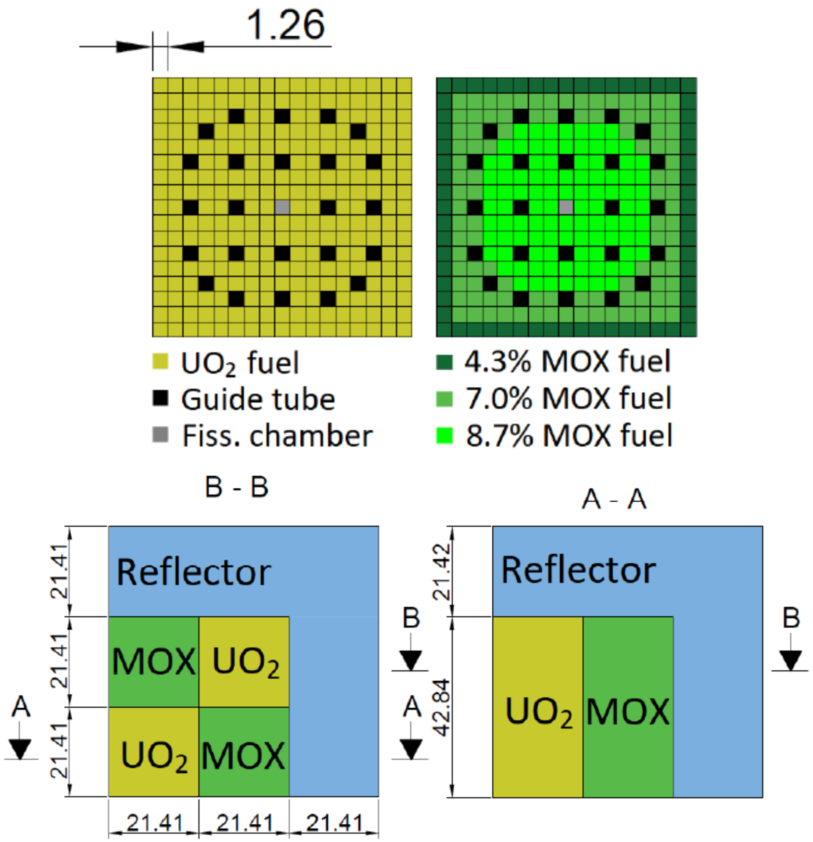
     Sub-space learning in a nutshell (or a coconut shell)
3. Reduced-Order Models for Reactor Physics
   - *A. Projection-based ROM for LWR neutronics*
   - *B. Projection-based ROM for Molten Salt Reactor Applications*
     - i. Methods
     - ii. Examples (MSFR / MSRE)
4. Reduced-Order Models for Transport
5. Summary and Outlook

Application example-1

Multi-group diffusion k-eigenvalue problem

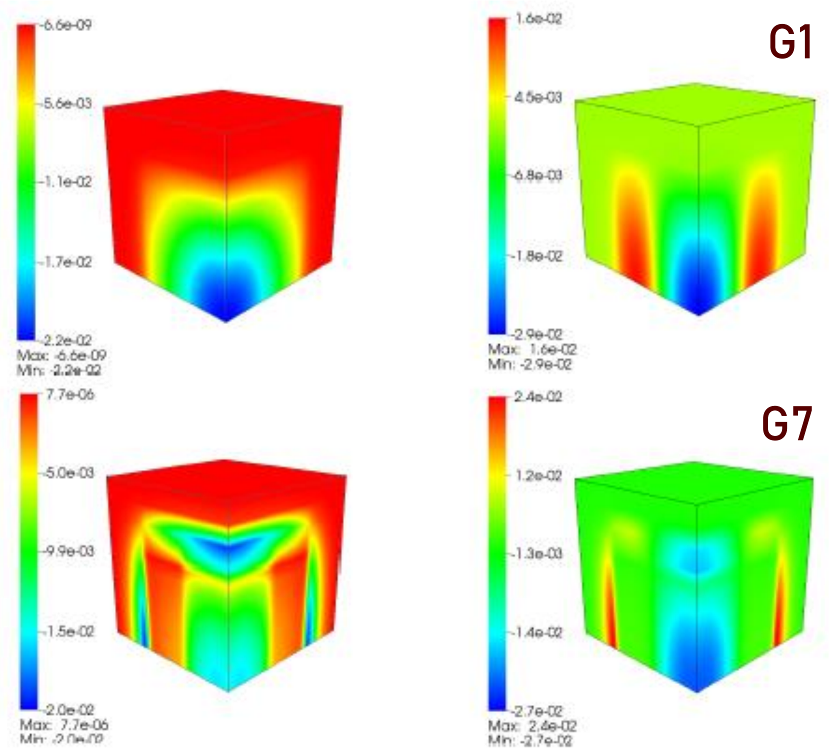
Example: C5G7 benchmark: UO_2 + MOX mini core

- 7 energy groups
- 7 material regions
- **Uncertain parameters**:
  - Diffusion coefficients
  - Absorption cross sections
  - Scattering matrix
  - Fission cross section
- Altogether 287 uncertain parameters
  - Perturbed in a ± 20% interval around the mean
- Original problem size: 231,000 unknowns



Application example-1

- ROM built using **50** snapshots only
- New, group-wise reduction technique published in [1].
- Using 21-34 modes per group
- Robust method
- Altogether 194 unknowns
- **2500 x faster than the FOM**

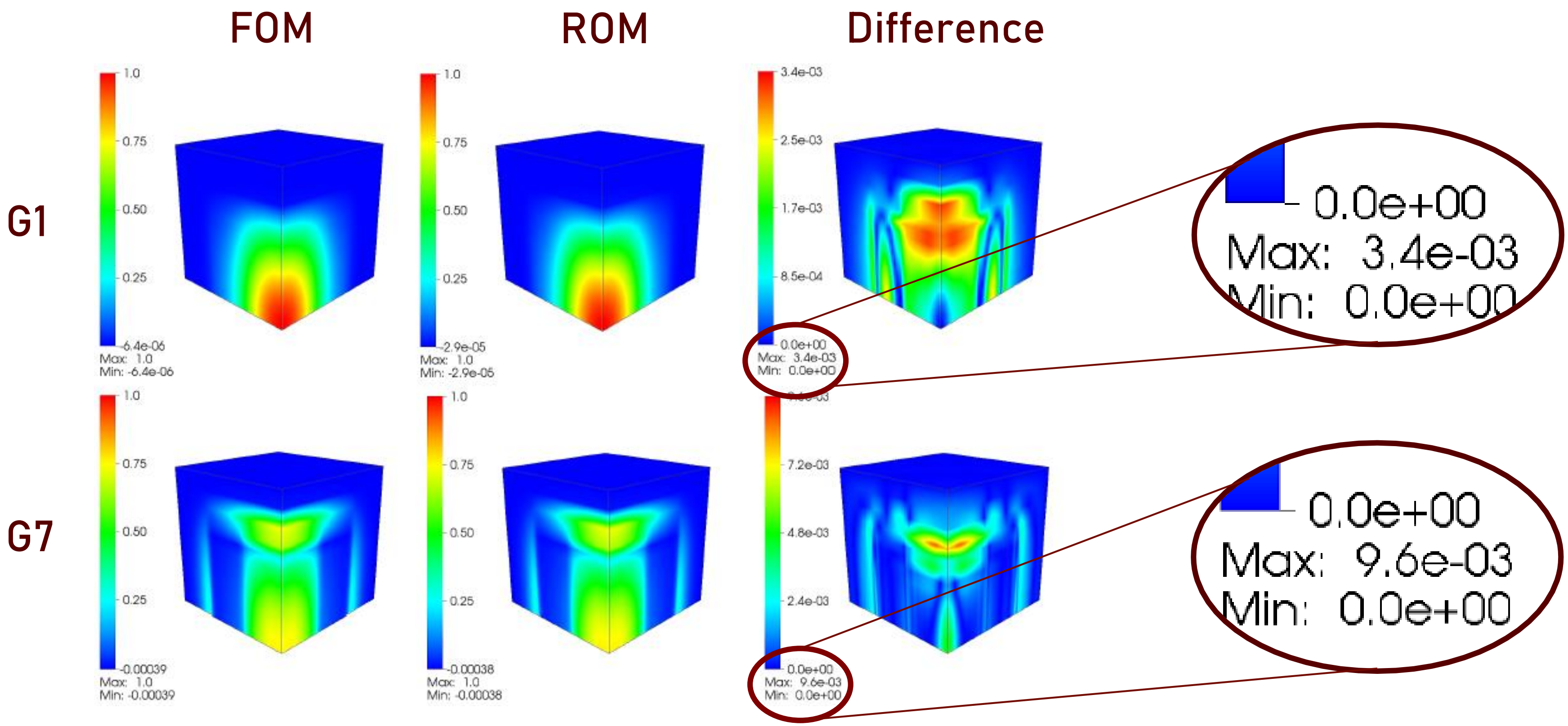


The first two POD modes of the scalar flux in group 1 and group 7

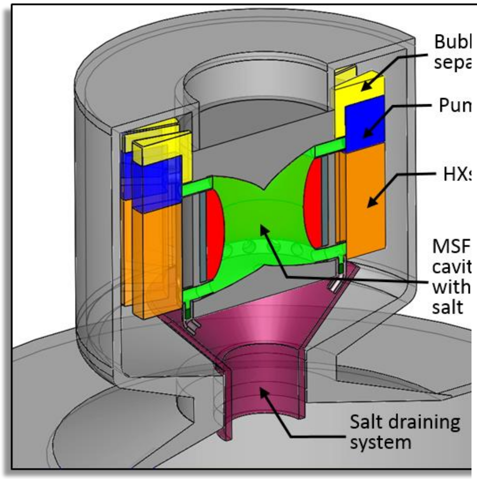
[1] Peter German, Jean C. Ragusa, *Reduced-Order Modeling of Parameterized Multi-group Diffusion k-Eigenvalue Problems*, Annals of Nuclear Energy, **134**, pp. 144-157.

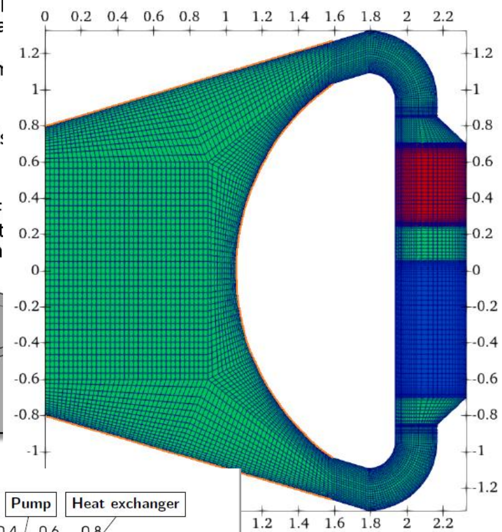
Application example-1

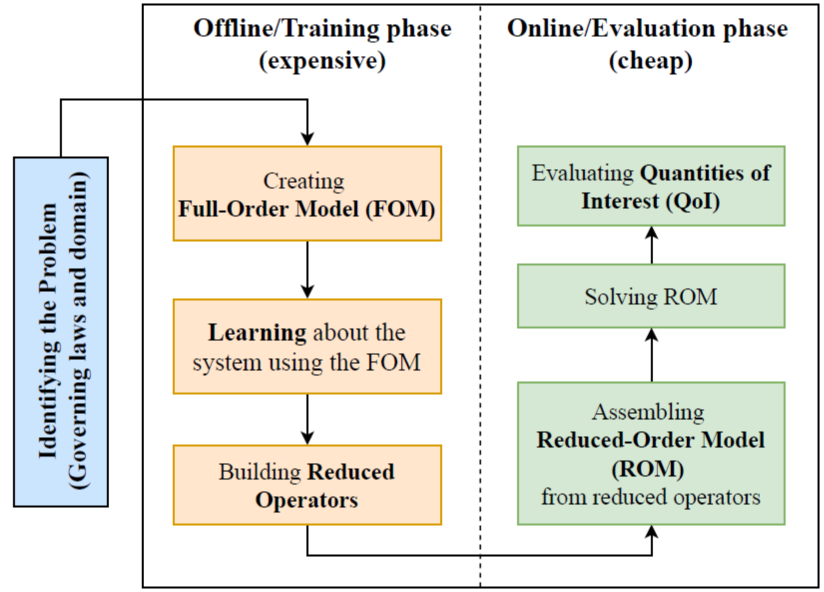
- **200 test samples** (not included in the training set):
  - Average difference in k_{eff} : 10 pcm
  - Maximum difference in k_{eff} : 98 pcm
  - Average difference L2 norm: G1: 0.47%, G7: 1.48%

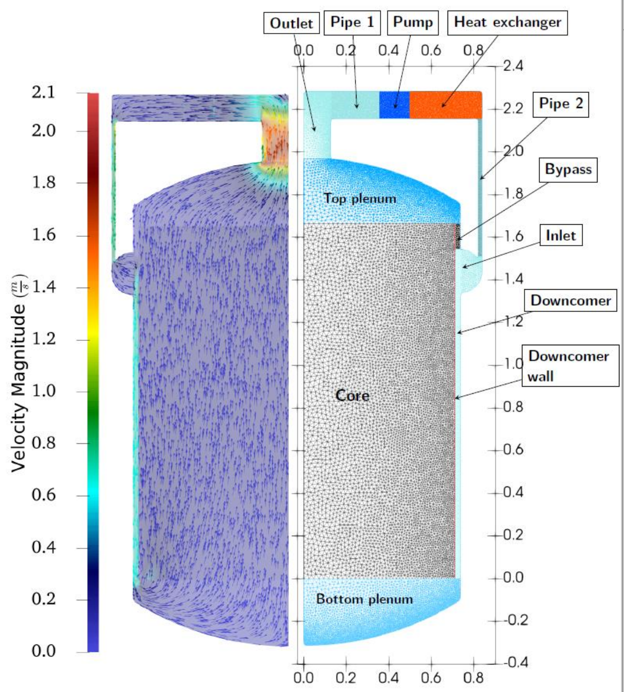


Model-order reduction for advanced reactors









The reduced equation system

$$\rho \boldsymbol{M}\dot{\boldsymbol{c}}^{\boldsymbol{u}_D} + \rho \boldsymbol{c}^{\boldsymbol{u}_D,T}\underline{\underline{\boldsymbol{C}}}\boldsymbol{c}^{\boldsymbol{u}_D} - \boldsymbol{c}^{\eta,T}\underline{\underline{\boldsymbol{T}}}\boldsymbol{c}^{\boldsymbol{u}_D} - \eta \boldsymbol{D}\boldsymbol{c}^{\boldsymbol{u}_D} + \boldsymbol{P}\boldsymbol{c}^{p} + \Gamma\left(\boldsymbol{B}\boldsymbol{c}^{\boldsymbol{u}_D} - |\boldsymbol{u}_{D,in}|\boldsymbol{S}_r^{BD}\right) - \sum_{z=1}^{Z}\left(|\boldsymbol{F}_{p,z}|\boldsymbol{S}_{p,z} - \boldsymbol{S}_{fr,z}\boldsymbol{c}_z^{F_{fr}}\right) - \rho\beta_e\left(\boldsymbol{A}\boldsymbol{c}^{T} - T_{ref}\boldsymbol{S}_T\right) = 0, \quad (16)$$

$$\rho \boldsymbol{G}\boldsymbol{c}^{\boldsymbol{u}_D} = 0 \quad (17)$$

Some of the reduced operators

$$\boldsymbol{M}_{i,j} = \left\langle \psi_i^{\boldsymbol{u}_D}, \psi_j^{\boldsymbol{u}_D} \right\rangle_{\mathcal{D}} \qquad \underline{\underline{\boldsymbol{C}}}_{i,j,k} = \left\langle \psi_j^{\boldsymbol{u}_D}, \frac{1}{\gamma}\nabla \cdot \left(\psi_i^{\boldsymbol{u}_D} \otimes \psi_k^{\boldsymbol{u}_D}\right) \right\rangle_{\mathcal{D}}$$

$$\boldsymbol{D}_{i,j} = \left\langle \psi_i^{\boldsymbol{u}_D}, \nabla \cdot \left[\nabla \psi_j^{\boldsymbol{u}_D} + \left(\nabla \psi_j^{\boldsymbol{u}_D}\right)^T\right] \right\rangle_{\mathcal{D}} \qquad \boldsymbol{P}_{i,j} = \left\langle \psi_i^{\boldsymbol{u}_D}, \gamma \nabla \psi_j^{p} \right\rangle_{\mathcal{D}}$$

$$\boldsymbol{B}_{i,j} = \left\langle \psi_i^{\boldsymbol{u}_D}, \psi_j^{\boldsymbol{u}_D} \right\rangle_{\Gamma_{in}} \qquad \boldsymbol{S}_{p,z,i} = \left\langle \psi_i^{\boldsymbol{u}_D}, \gamma \frac{\delta_z(\boldsymbol{r})\boldsymbol{F}_{p,z}}{|\boldsymbol{F}_{p,z}|} \right\rangle_{\mathcal{D}}$$

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Projection-based ROM for the MSR : Fluid flow

Fluid Dynamics

The equations describe the mass and linear momentum conservation for a liquid in a porous medium with homogenized structural elements:

$$\nabla \cdot \rho \boldsymbol{u}_D = 0 \, , \tag{10}$$

$$\frac{\partial \rho \boldsymbol{u}_D}{\partial t} + \frac{1}{\gamma} \nabla \cdot (\rho \boldsymbol{u}_D \otimes \boldsymbol{u}_D) = \nabla \cdot \left((\eta + \eta_t) \left[\nabla \boldsymbol{u}_D + (\nabla \boldsymbol{u}_D)^T \right] \right) - \gamma \nabla p + \gamma \boldsymbol{F}_p + \gamma \boldsymbol{F}_{fr} + \gamma \rho \boldsymbol{g} \beta_e (T - T_{ref}) \, , \tag{11}$$

- γ - porosity (fraction of fluid in the structure)
- $\boldsymbol{u}_D \equiv \gamma \boldsymbol{u}$ - Reynolds-averaged Darcy velocity vector field
- η_t - turbulent viscosity (only used for turbulent flows)
- $\boldsymbol{F}_p$ - volumetric linear momentum sources (e.g pump)
- $\boldsymbol{F}_{fr}$ - volumetric linear momentum sources and sinks (e.g. flow resistance)

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Projection-based ROM for MSR: Neutronics

Balance of neutrons

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} = \nabla \cdot [D_g \nabla \phi_g] - \Sigma_{t,g}\phi_g + \frac{(1-\beta)\chi_{p,g}}{k_{\text{eff}}}\sum_{g'=1}^{G_e} \nu_{g'}\Sigma_{f,g'}\phi_{g'} + \sum_{g'=1}^{G_e}\Sigma_{s,g'\to g}\phi_{g'} + \chi_{d,g}\sum_{i=1}^{G_d}\lambda_i\gamma C_i^*, \quad (18)$$

- ϕ_g neutron scalar flux in group $g \in [1,...,G_e]$
- C_i^* corrected delayed neutron precursor in group $i \in [1,..,G_d]$ (computed from real concentration as $C_i^* = C_i/\gamma$)

Balance of delayed neutron precursors

$$\frac{\partial \gamma C_i^*}{\partial t} + \nabla \cdot [\boldsymbol{u}_D C_i^*] = \nabla \cdot \left(\left[\frac{\alpha_l}{\rho} + \frac{\alpha_t}{\rho} \right] \nabla C_i^* \right) + \frac{\beta_i}{k_{\text{eff}}}\sum_{g'=1}^{G_e}\nu_{g'}\Sigma_{f,g'}\phi_{g'} - \lambda_i\gamma C_i^* \quad i \in [0,...,G_d] \quad (19)$$

Temperature-dependent group constants

The group constants in the neutron and precursor balance equations depend on the temperature. It is handled by an interpolation between different data bases:

$$\Sigma(\boldsymbol{r},T) \approx \Sigma(\boldsymbol{r},T_{ref},\rho_{ref}) + \delta_{FT}\left(\sqrt{T} - \sqrt{T_{ref}}\right) + \delta_{FD}\rho_{ref}\beta_e\left(T - T_{ref}\right). \quad (20)$$

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- C_i^* corrected delayed neutron precursor in group $i \in [1,..,G_d]$ (computed from real concentration as $C_i^* = C_i/\gamma$)

Balance of delayed neutron precursors

$$\frac{\partial \gamma C_i^*}{\partial t} + \nabla \cdot [\boldsymbol{u}_D C_i^*] = \nabla \cdot \left(\left[\frac{\alpha_l}{\rho} + \frac{\alpha_t}{\rho} \right] \nabla C_i^* \right) + \frac{\beta_i}{k_{\text{eff}}} \sum_{g'=1}^{G_e} \nu_{g'}$$

Temperature-dependent group constant

The group constants in the neutron and
temperature. It is handled by an interpo

$$\Sigma(\boldsymbol{r},T) \approx \Sigma(\boldsymbol{r},T_{ref},\rho_{ref}) + \delta_{FT}\left(\sqrt{T}\right.$$

$$\left\langle \psi_k^{\phi_g}, \frac{1}{v_g}\frac{\partial \widetilde{\phi}_g}{\partial t} - \nabla \cdot \left[D_g \nabla \widetilde{\phi}_g \right] + \Sigma_{t,g}\widetilde{\phi}_g - \frac{(1-\beta)\chi_{p,g}}{k_{\text{eff}}} \sum_{g'=1}^{G_e} \nu_{g'}\Sigma_{f,g'}\widetilde{\phi}_{g'} - \sum_{g'=1}^{G_e}\Sigma_{s,g'\to g}\widetilde{\phi}_{g'} - \chi_{d,g}\sum_{i=1}^{G_d}\lambda_i\gamma \widetilde{C}_i^* \right\rangle_{\mathcal{D}} = 0, \quad k = 1,\ldots,r_{\phi_g} \quad (21)$$

$$\left\langle \psi_k^{C_i^*}, \frac{\partial \widetilde{C}_i^*}{\partial t} + \nabla \cdot \left[\widetilde{\boldsymbol{u}}_D \widetilde{C}_i^* \right] - \nabla \cdot \left(\left[\frac{\alpha_l}{\rho} + \frac{\widetilde{\alpha}_t}{\rho} \right] \nabla \widetilde{C}_i^* \right) - \frac{\beta_i}{k_{\text{eff}}} \sum_{g'=1}^{G_e} \nu_{g'}\Sigma_{f,g'}\widetilde{\phi}_{g'} + \lambda_i \widetilde{C}_i^* \gamma \right\rangle_{\mathcal{D}} = 0, \quad k = 1,\ldots,r_{C_i^*} \quad (22)$$

Heat Transfer

To be able do determine the temperature of the system, a porous medium enthalpy equation is solved:

$$\frac{\partial \gamma \rho c_p T}{\partial t} + \nabla \cdot (\boldsymbol{u}_D \rho c_p T) = \nabla \cdot (\gamma [k_l + c_p \alpha_t] \nabla T) - h A_V (T - T_{ext}) + \gamma \sum_{g=1}^{G_e} \Sigma_{p,g} \phi_g ,$$

Projection-based ROM for the MSR : Heat Transfer

Heat Transfer

To be able do determine the temperature of the system, a porous medium enthalpy equation is solved:

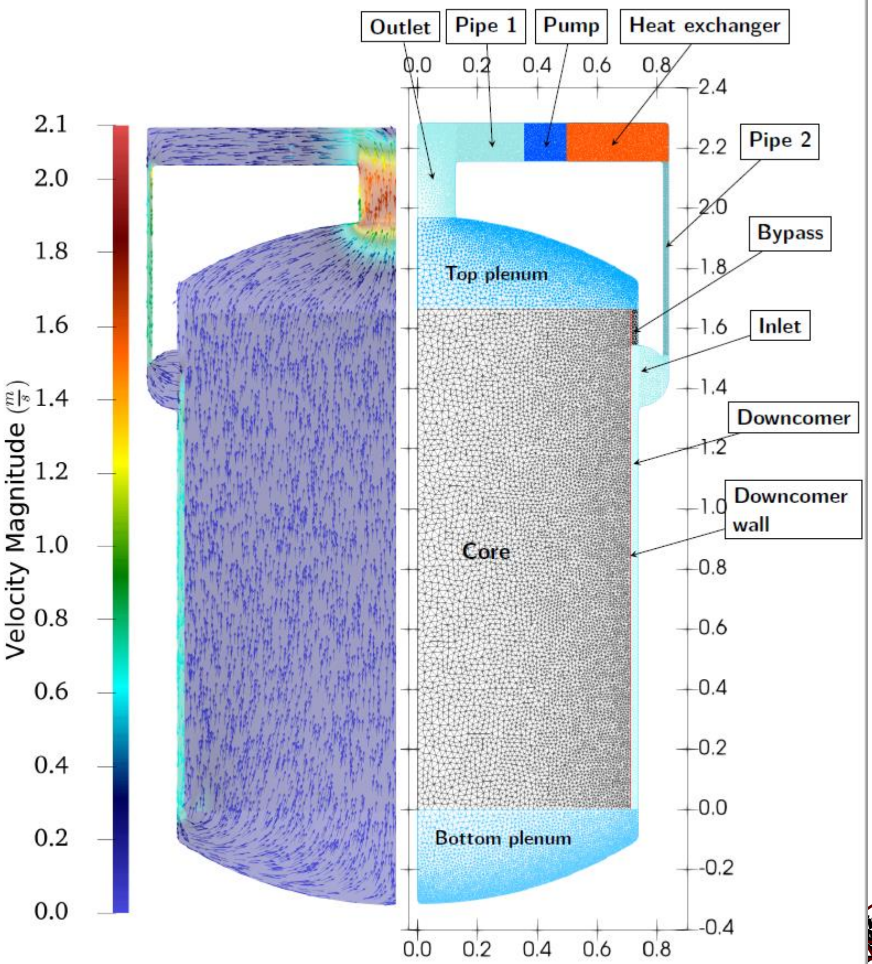
$$\frac{\partial \gamma \rho c_p T}{\partial t} + \nabla \cdot (\boldsymbol{u}_D \rho c_p T) = \nabla \cdot (\gamma \left[k_l + c_p \alpha_t\right] \nabla T) - hA_V (T - T_{ext}) + \gamma \sum_{g=1}^{G_e} \Sigma_{p,g} \phi_g ,$$

$$\left\langle \psi_k^T, \frac{\partial \gamma \rho c_p \widetilde{T}}{\partial t} + \nabla \cdot (\widetilde{\boldsymbol{u}_D} \rho c_p \widetilde{T}) = \nabla \cdot \left(\gamma \left[k_l + c_p \widetilde{\alpha_t}\right] \nabla \widetilde{T} \right) - hA_V (\widetilde{T} - T_{ext}) + \gamma \sum_{g=1}^{G_e} \Sigma_{p,g} \widetilde{\phi_g} \right\rangle, \quad k = 1, \ldots, r_T$$

MSRE ROM: some results

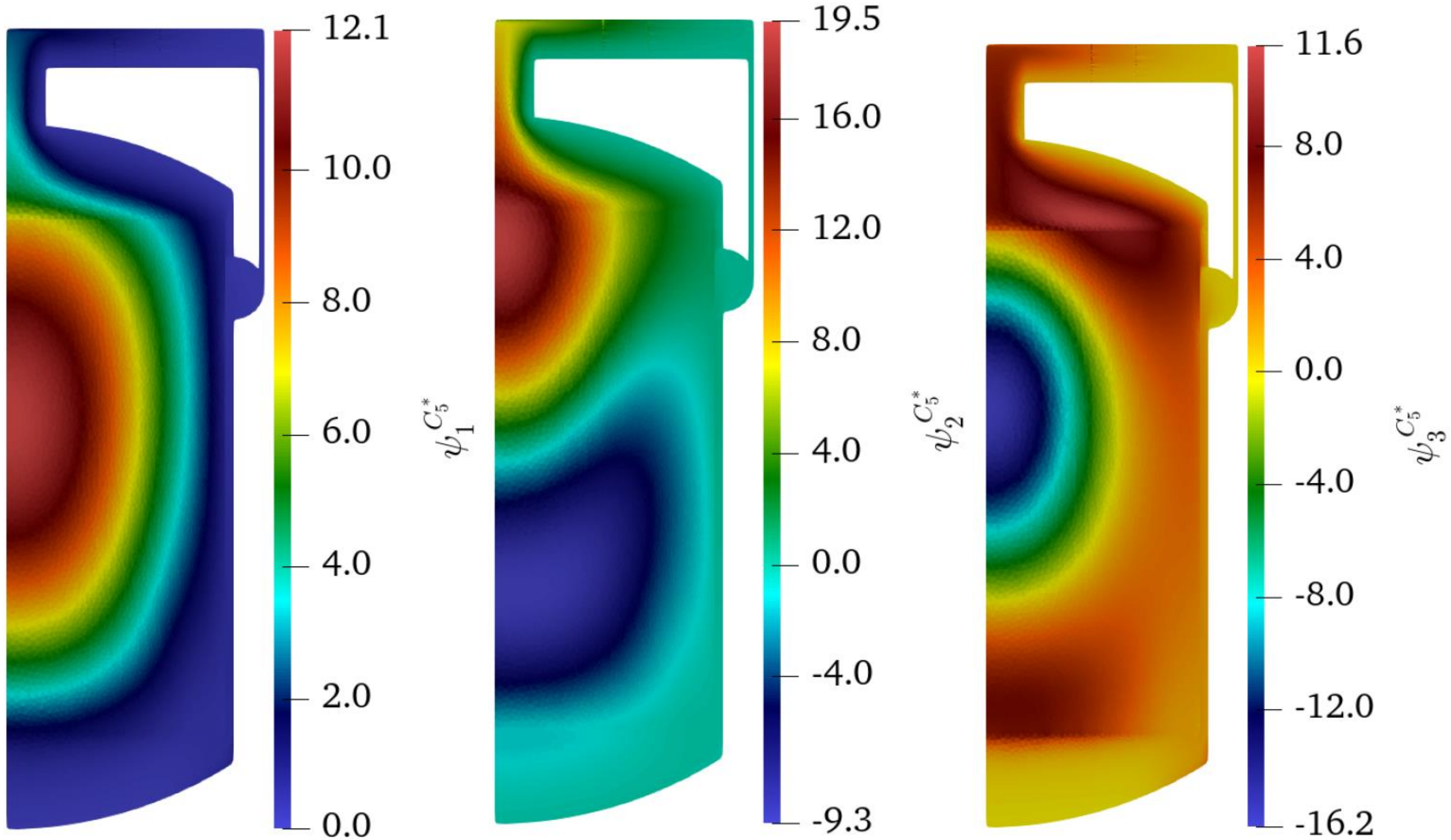
Results - Molten Salt Reactor Experiment

- Test case for neutronics-heat tr. DEIM
- 2D axysymmetric model (Jun Shi, UC Berkeley)
- Fixed (precomputed) $\boldsymbol{u}_D$, α_t
- Number of cells: 38,562
- Energy groups: 2
- Precursor groups: 6
- Porous media: Core, Top/bottom plenum, Heat exchanger
- FOM Solver: GeN-Foam (EPFL)
- ROM Solver: GeN-ROM (TAMU)



MSRE ROM: some results

Examples of Basis Functions



MSRE ROM: some results

Results - Molten Salt Reactor Experiment

- Uncertain parameters (6 total):
  Parameters of the heat exchanger (A_V, h, T_{ext}), Prandtl number (Pr), Reactor power (P_{th}), Thermal expansion coefficient (β_e)
- Number of snapshots: 20
- Number of test samples: 30
- Error definition: $e_X = ||X_{FOM} - X_{ROM}||_{L^2} / ||X_{FOM}||_{L^2}$

Field	**Rank**	**Field**	**Rank**
ϕ_1	4	C_4^*	4
ϕ_2	4	C_5^*	4
C_1^*	3	C_6^*	4
C_2^*	3	T	5
C_3^*	4	$\sqrt{T}$	4

max(Δk_{eff}) (pcm)	**max(e_{ϕ_2}) (%)**
0.36	0.001

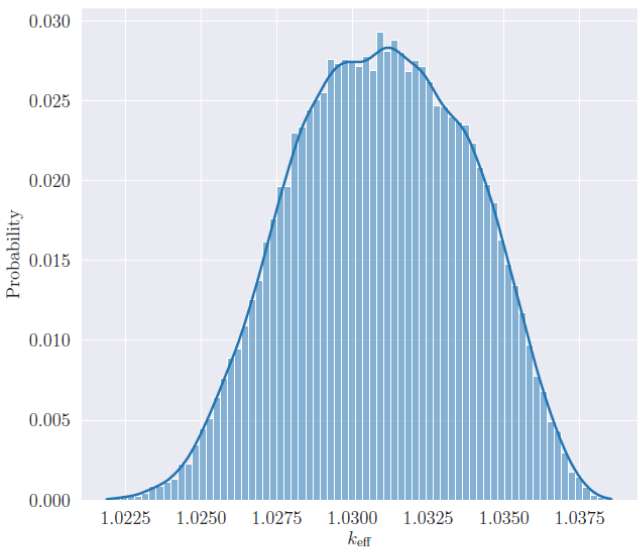
max($e_{C_5^*}$) (%)	**max(e_T) (%)**
0.001	0.012

Single-run speedup: 3,000

MSRE ROM: performing UQ with ROM

Results - Molten Salt Reactor Experiment

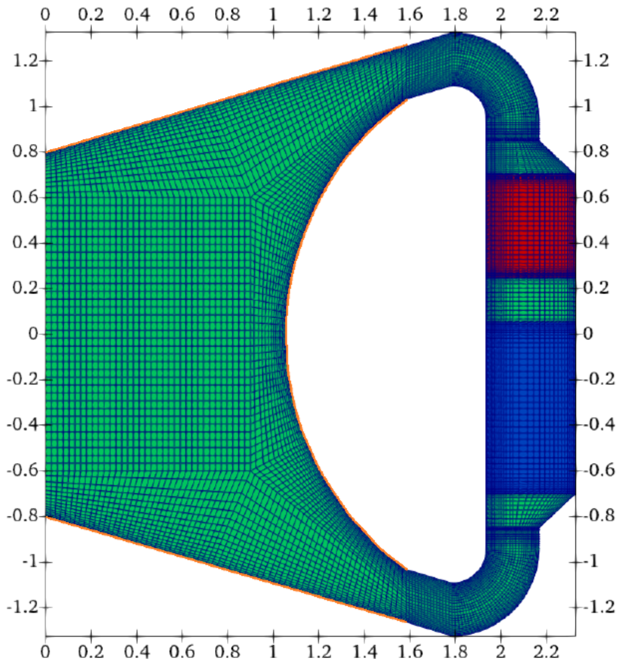
- Quantity of Interest: Effective multiplication factor (k_{eff})
- Propagating uncertainties from model parameters to QoI (Monte Carlo)
- Sobol Index analysis: contributions to the variance of the QoI
- Overall speedup: 1,300 (including training)



MSFR ROM: some results

Results - Molten Salt Fast Reactor

- Three examples considered:
  - zero-power steady-state
  - zero-power transient
  - nominal-power steady-state
- Number of cells: 16,140
- Number of energy groups: 6
- Number of precursor groups: 8
- Porous medium zones:
  - Pump (red): volumetric momentum source
  - Heat exchanger (blue): flow resistance, volumetric heat sink
- Full-Order Solver: GeN-Foam (EPFL)
- Reduced-Order Solver: GeN-ROM (TAMU)



MSFR ROM: some results

Results - Molten Salt Fast Reactor

- Zero-power assumption: buoyancy effects and the temperature-dependence of the neutronics group constants are not considered
- Uncertain parameters (13 total):
  - Diffusion coefficients, fission cross sections ($\pm$ 10% around the nominal values)
  - Pumping force in the momentum equation
- Number of snapshots: 20
- Number of test samples: 30
- Error definition: $e_X = ||X_{FOM} - X_{ROM}||_{L^2} / ||X_{FOM}||_{L^2}$

$\max(\Delta k_{\text{eff}})$ (pcm)	$\max(e_{\phi_5})$ (%)	$\max(e_{C_6^*})$ (%)	$\max(e_{u_D})$ (%)
0.93	0.05	0.28	0.68

$\max(\Delta \beta_{\text{eff}})$ (pcm)	$\max(e_{\phi_5^\dagger})$ (%)	$\max(e_{C_6^{\dagger,*}})$ (%)	$\max(e_p)$ (%)
0.30	0.03	0.28	0.92

MSFR ROM: some results

Results - Molten Salt Fast Reactor

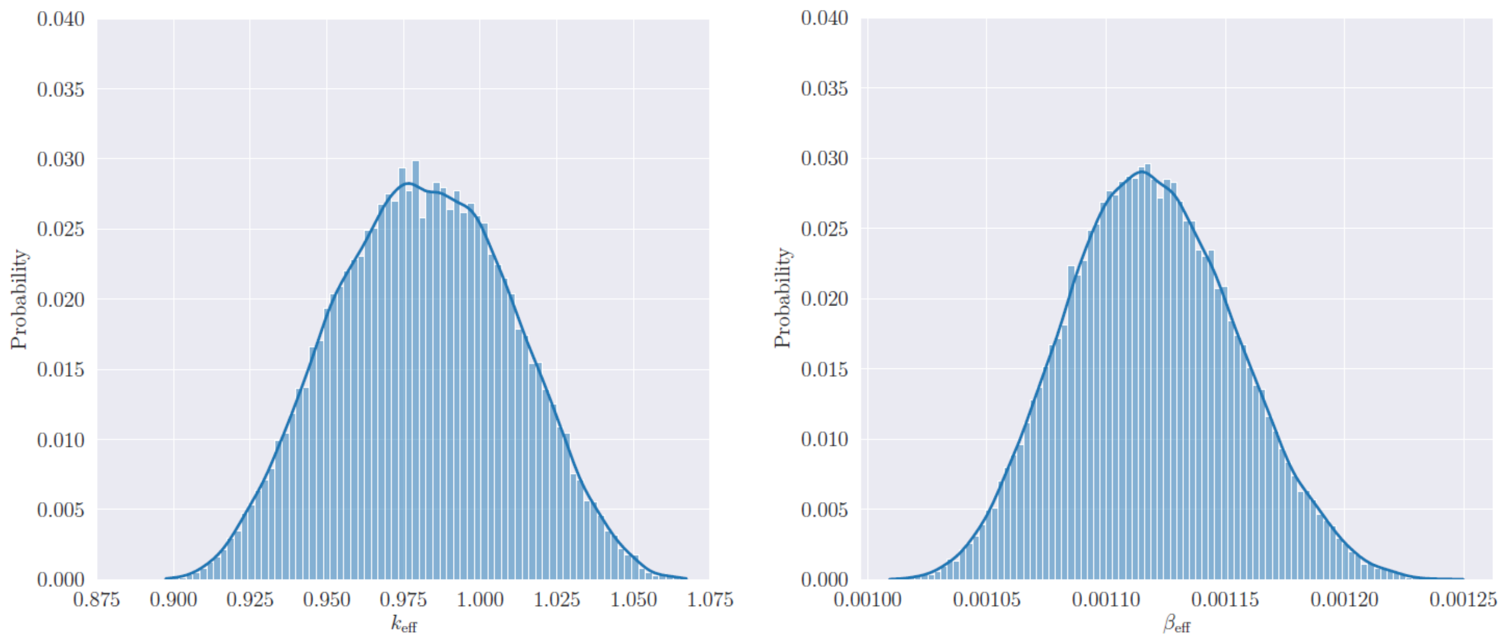
- Used basis functions per field of interest: 1-10
- Acceleration: approximately 2×10^5

Field	Rank	Field	Rank	Field	Rank	Field	Rank	Field	Rank
ϕ_1	3	C_2^*	2	$\phi_1^\dagger$	3	$C_2^{\dagger,*}$	2	$\boldsymbol{u}_D$	3
ϕ_2	3	C_3^*	3	$\phi_2^\dagger$	3	$C_3^{\dagger,*}$	3	p	1
ϕ_3	3	C_4^*	3	$\phi_3^\dagger$	3	$C_4^{\dagger,*}$	4	$\boldsymbol{F}_{fr}$	3
ϕ_4	3	C_5^*	5	$\phi_4^\dagger$	3	$C_5^{\dagger,*}$	5	η_t	10
ϕ_5	3	C_6^*	6	$\phi_5^\dagger$	3	$C_6^{\dagger,*}$	6	α_t	10
ϕ_6	3	C_7^*	5	$\phi_6^\dagger$	3	$C_7^{\dagger,*}$	5		
C_1^*	2	C_8^*	5	$C_1^{\dagger,*}$	2	$C_8^{\dagger,*}$	5		

MSFR ROM: some results

Results - Molten Salt Fast Reactor

- Quantities of interest:
  - Effective multiplication factor (k_{eff})
  - Effective delayed neutron fraction (β_{eff})
- Propagation of uncertainties: Monte Carlo approach with 50,000 samples
- Speedup in the UQ including training: approximately factor of 2,000



MSFR ROM: some results

Results - Molten Salt Fast Reactor

- Buoyancy effects and the temperature-dependence of the neutronics group constants are considered
- Uncertain parameters (23 total):
  - Diffusion coefficients, fission and removal cross sections ($\pm$ 10% around the nominal values)
  - Pumping force, external coolant temperature, Heat transfer coefficient, Pr-number, thermal expansion coefficient
- Number of snapshots: 30
- Number of test samples: 20

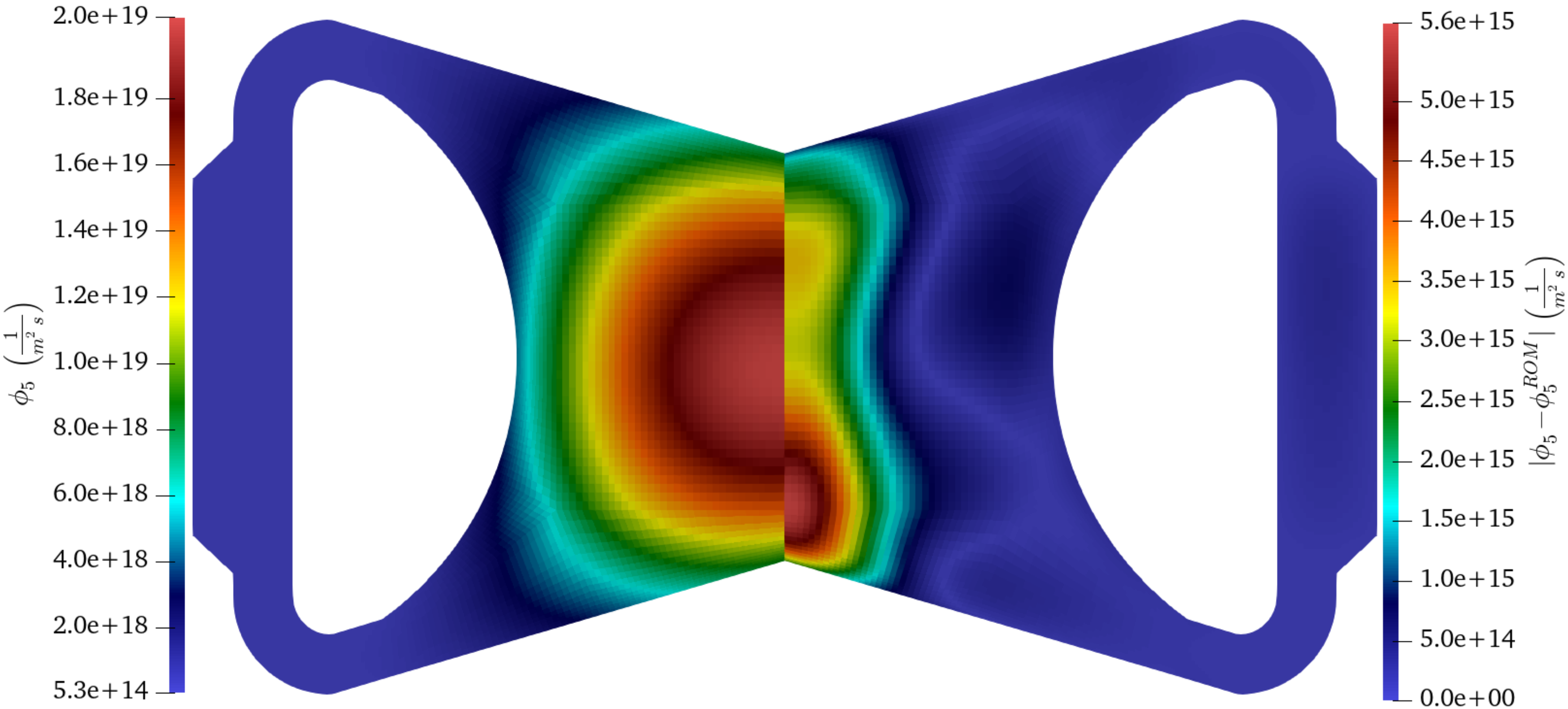
$\max(\Delta k_{\text{eff}})$ (pcm)	$\max(e_{\phi_5})$ (%)	$\max(e_{C_7^*})$ (%)
9.10	0.40	0.38
$\max(e_{\boldsymbol{u}_D})$ (%)	$\max(e_p)$ (%)	$\max(e_T)$ (%)
0.21	0.16	0.13

Results - Molten Salt Fast Reactor

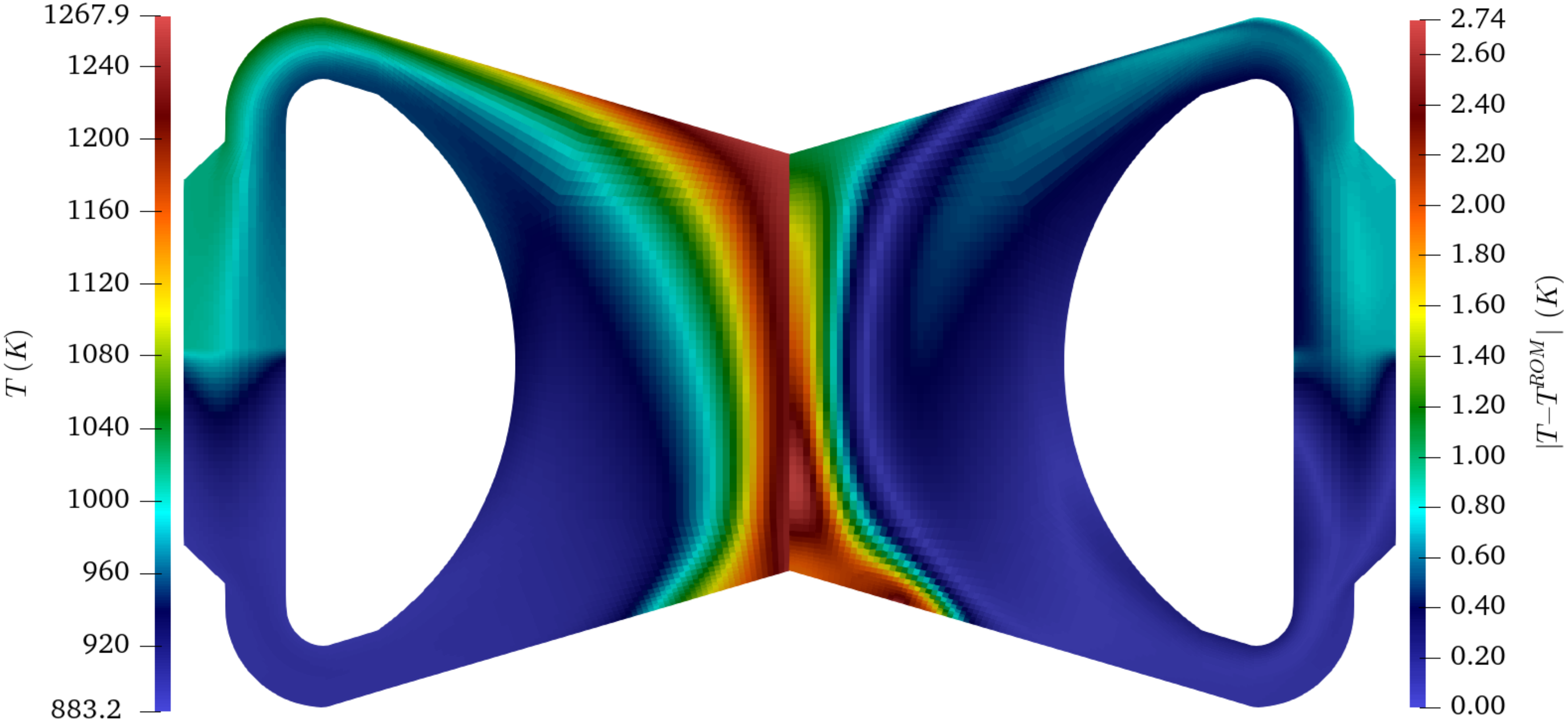
- Used basis functions per field of interest: 2-18 (more than the zero-power scenario)
- Acceleration: approximately $1 \times 10^4 - 2 \times 10^4$

Field	Rank	Field	Rank	Field	Rank	Field	Rank	Field	Rank
ϕ_1	15	ϕ_6	16	C_5^*	16	p	2	$\log(T)$	6
ϕ_2	15	C_1^*	9	C_6^*	17	$\boldsymbol{F}_{fr}$	4		
ϕ_3	14	C_2^*	11	C_7^*	18	η_t	8		
ϕ_4	15	C_3^*	12	C_8^*	17	α_t	8		
ϕ_5	15	C_4^*	14	$\boldsymbol{u}_D$	6	T	10		

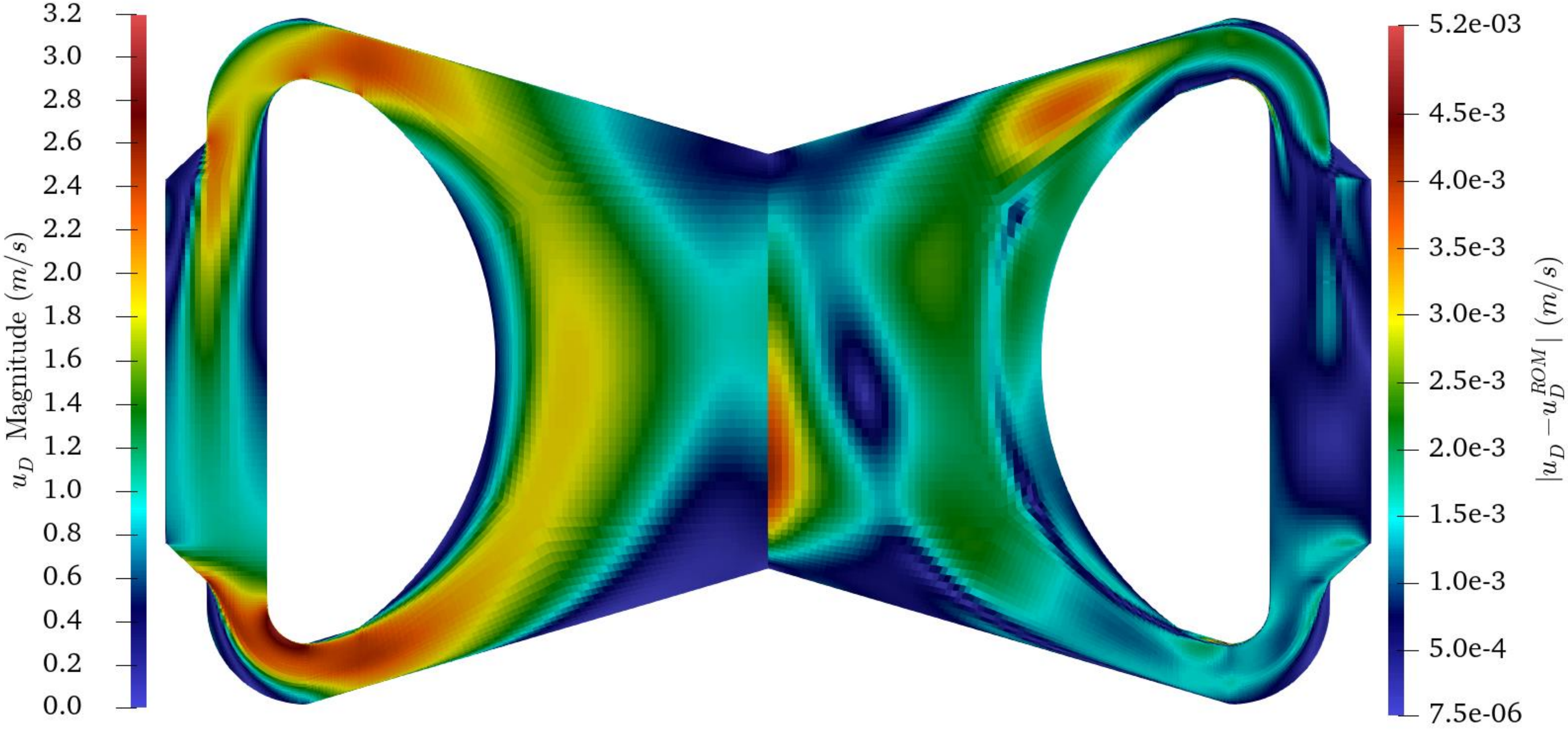
Reconstructed Flux (left) - Reconstruction Error (right)



Reconstr. Temperature (left) – Reconstr. Error (right)

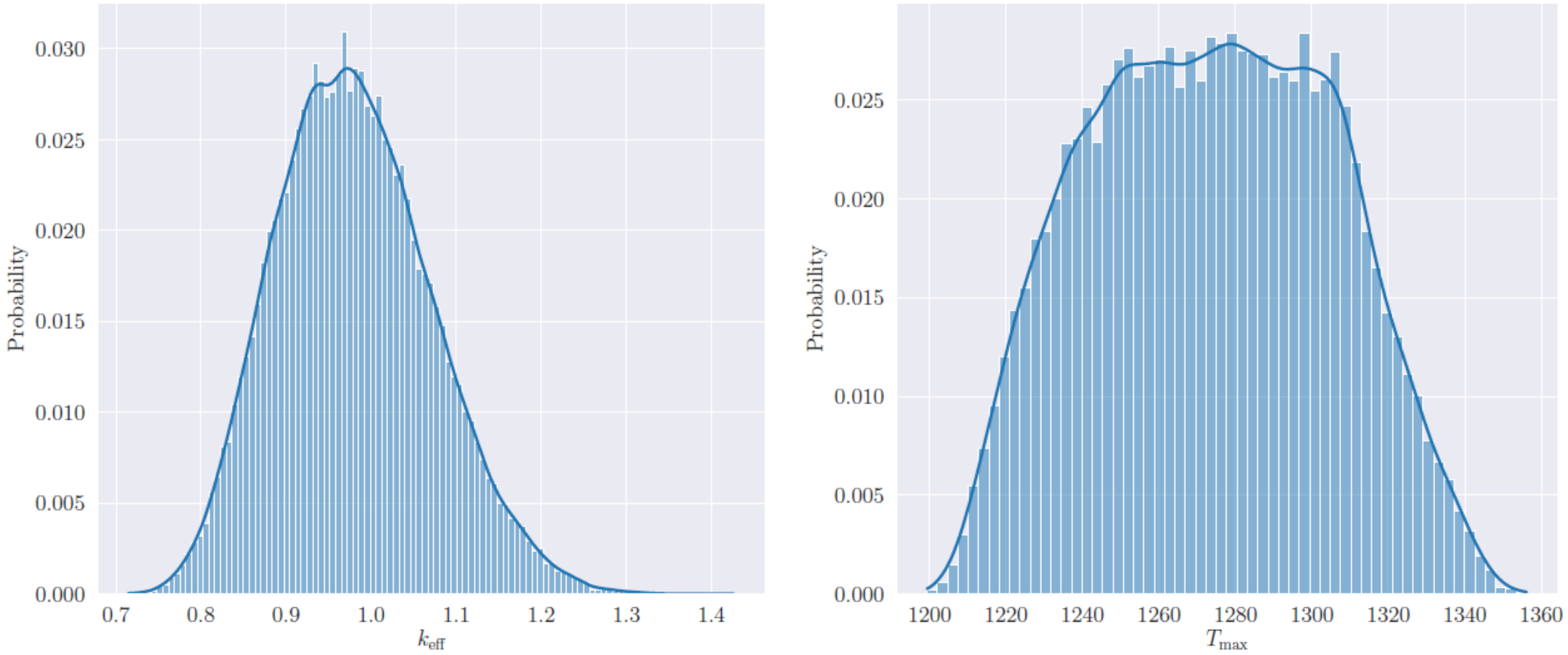


Reconst. Velocity (left) - Reconstruction Error (right)

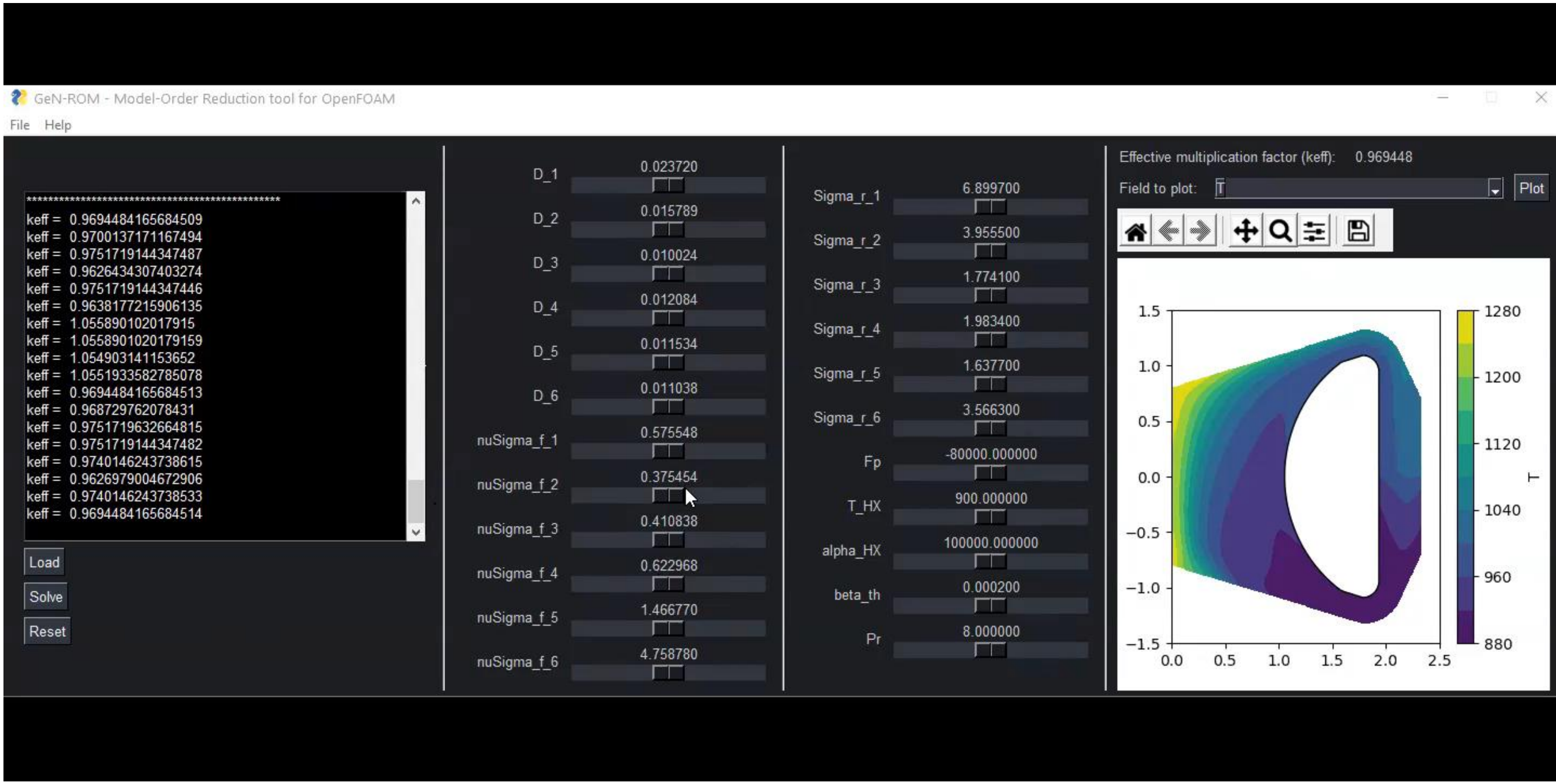


Model-order Reduction: huge speed ups

- Quantities of interest:
  - Effective multiplication factor (k_{eff})
  - Maximum temperature of the system (T_{max})
- Propagation of uncertainties: Monte Carlo approach with 50,000 samples
- Speedup in the UQ including training: approximately factor of 1,500



Graphical User Interface Demo



MSFR: What do some basis functions look like?

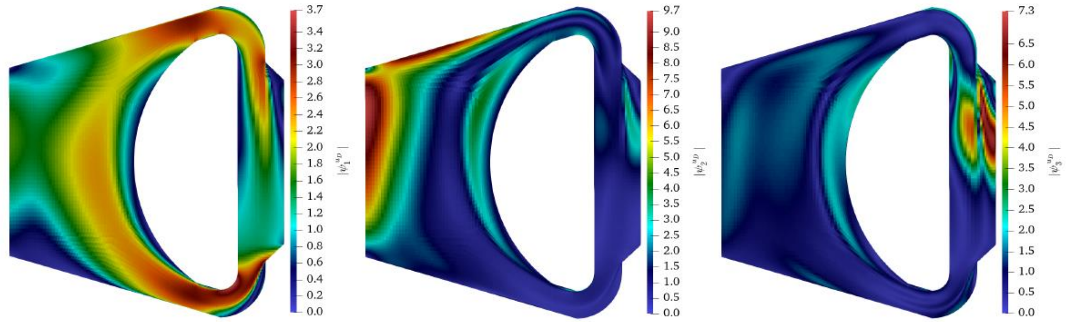


Figure A4. First three (left to right) POD modes of $\boldsymbol{u}_D$ in the case of the transient numerical example.

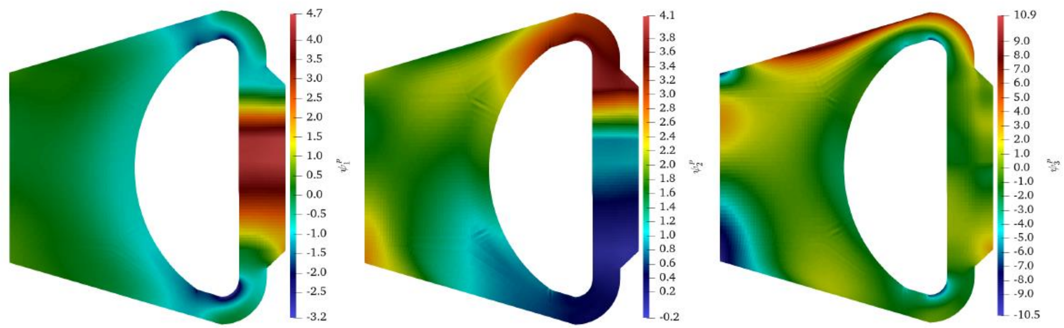


Figure A5. First three (left to right) POD modes of p in the case of the transient numerical example.

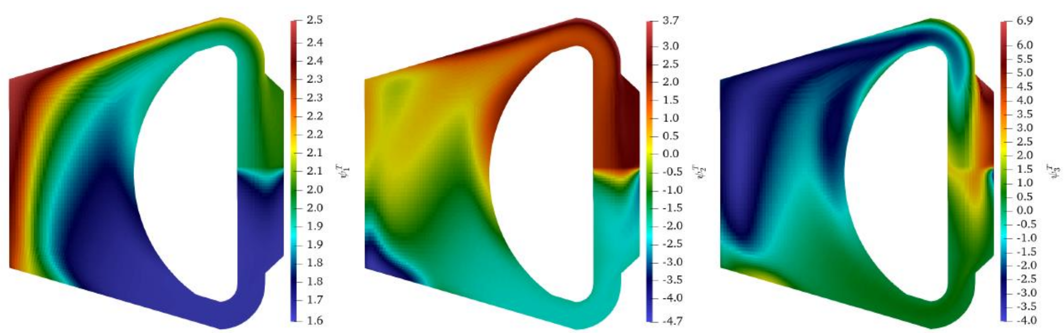


Figure A6. First three (left to right) POD modes of T in the case of the transient numerical example.

Outline

1. High-performance computing (HPC)
   A. *Some history*
   B. *Some well-recognized software used in nuclear engineering*
   C. *A few application examples*
2. Fast Data-driven Surrogate Models
   A. *Motivations for parametric Reduced-Order Modeling (ROM)*
   B. *What is model-order reduction?*
   Sub-space learning in a nutshell (or a coconut shell)
3. Reduced-Order Models for Reactor Physics
   A. *Projection-based ROM for LWR neutronics*
   B. *Projection-based ROM for Molten Salt Reactor Applications*
      i. Methods
      ii. Examples (MSFR / MSRE)
4. Reduced-Order Models for Transport
5. Summary and Outlook

Brief review of linear Boltzmann transport

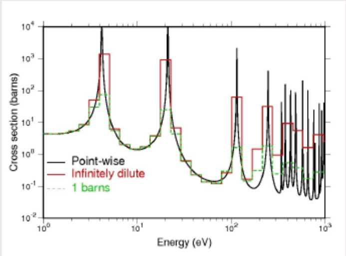
Neutral-particle transport: losses = gains

$$(\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}+\sigma_t(\boldsymbol{r},E))\,\Psi(\boldsymbol{r},\boldsymbol{\Omega},E)=\int_{4\pi}d\Omega'\int dE'\,\sigma_s(\boldsymbol{r},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}',E'\to E)\Psi(\boldsymbol{r},\boldsymbol{\Omega}',E')+S_{\text{fixed}}(\boldsymbol{r},\boldsymbol{\Omega},E)$$

$\Psi(\boldsymbol{r},\boldsymbol{\Omega},E)$ = angular "flux"

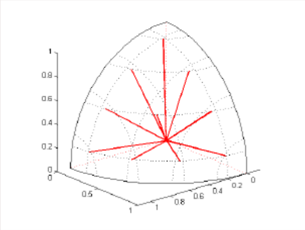
- neutral particles = neutrons; photons; coupled neutrons/photons
- can be amended to include time dependence, production from fission
- can be amended (Boltzmann-Fokker-Planck) for charged particles and coupled charged particles/photons
- 6-dimensional phase-space: space($\boldsymbol{r}$,3)+energy(E,1)+angle($\boldsymbol{\Omega}$,2)

Multigroup in Energy



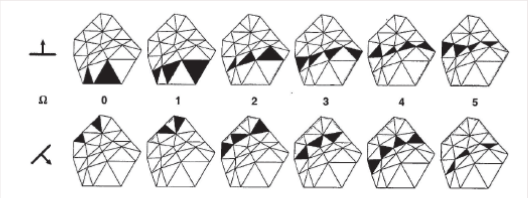
Coupled G equations.

Discrete Directions (S_N method)



Coupled $G\times N_{\text{dir}}$ equations.

Discontinuous Finite Elements (DFE) in Space



Coupled $G\times N_{\text{dirs}}\times N_{\text{cells}}$ equations.

Solution Techniques for LBT

Solving the Linear Boltzmann/Radiation Transport Equation

Basic unit of work: $L\Psi = q_{\text{tot}}$

Solve

$$\underbrace{\left(\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} + \sigma_t(\boldsymbol{r})\right)}_{=L} \Psi(\boldsymbol{r}, \boldsymbol{\Omega}) = q_{\text{ext+scatt}}$$

for each direction, for each energy group, as many times as needed for convergence

Performing L^{-1} by sweeping the mesh is **matrix-free**

Formidable computational problem:

- Space: $N_x \times N_y \times N_z$ cells (say $100 \times 100 \times 100 = 1$ million spatial cells)
- Angle: 50 - 5,000 directions (say 1,000)
- Groups: several dozens and up (say 100)
- 8 spatial degrees of freedom/cell (discontinuous finite elements)
- Total: about 1 trillion (10^{12}) unknowns, (figures $>$ 1 trillion are not infrequent ...)

Key Points:

- Radiation transport is a linear problem $\boxed{Ax = b}$
- The number of unknowns per vertex of a mesh is gigantic ($> 10,000$)
- Due to the size of the problem, matrix A is not available (not built nor stored)

Motivations for parametric reduced-order models for radiation transport

Quantities of Interest, QoI

- Functionals of the computed solution:

$$\text{QoI} = \int_0^\infty dE \int_{\text{RoI}} d^3r\, \varrho(\boldsymbol{r}, E) \int_{4\pi} d\Omega\, \Psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$$

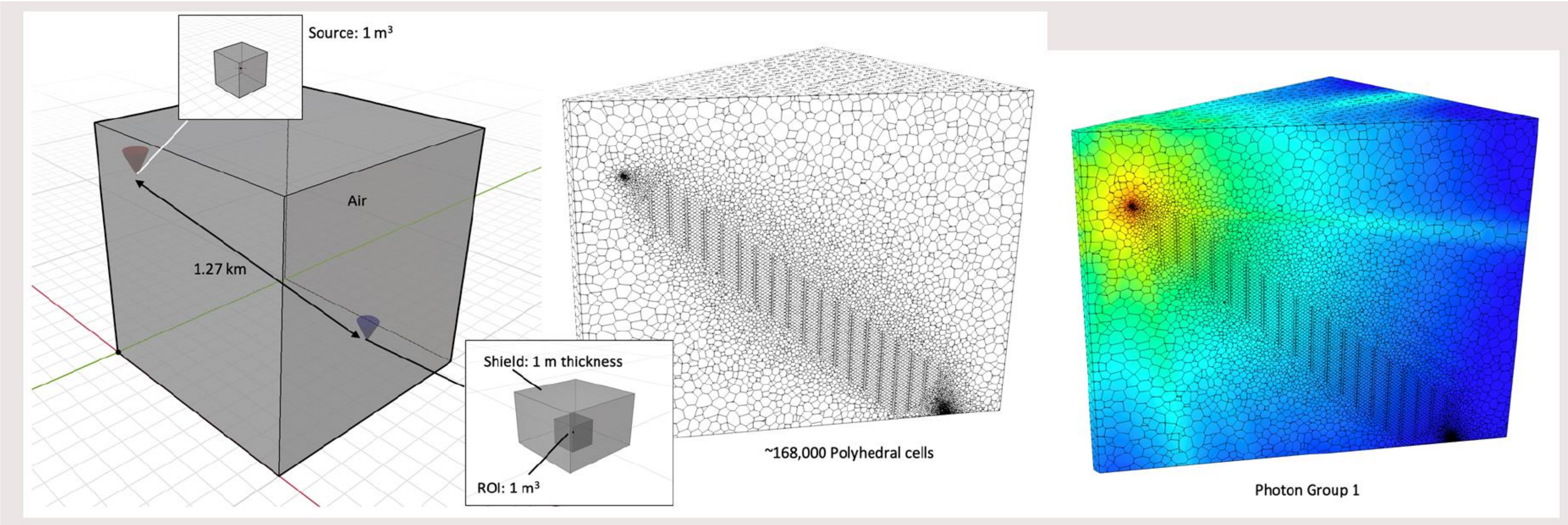
- Examples: dose, dose rates, fluence, fluence rates, radiation fluxes through boundaries, SREMP and SGEMP fields.

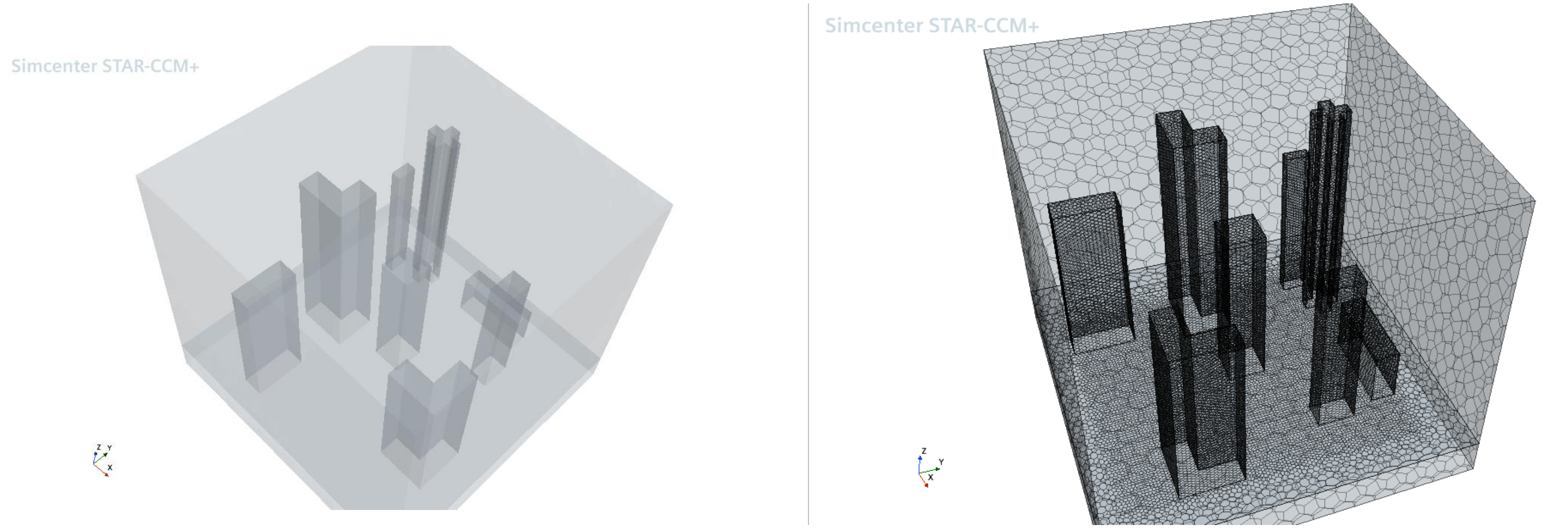
Sources of Uncertainty in QoIs for NWrE:

1. Source position (altitude, slant).
2. Source spectrum (fraction of fission spectrum + fusion spectrum, for n and γ).
3. Air Humidity (in addition to air density variation wrt to z).
4. Ground Composition.
5. Location and orientation of RoI (Region of Interest).

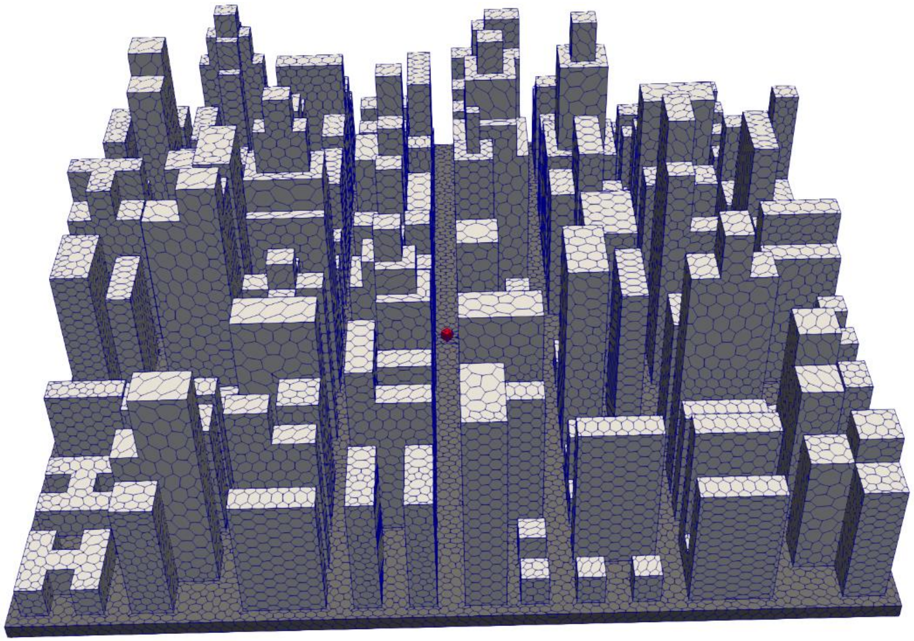
- **Multi-query problems to investigate input parameter space**
- **Boltzmann simulation models are computationally expensive and may not meet mission needs.**
- **→ Need faster but accurate surrogate models**

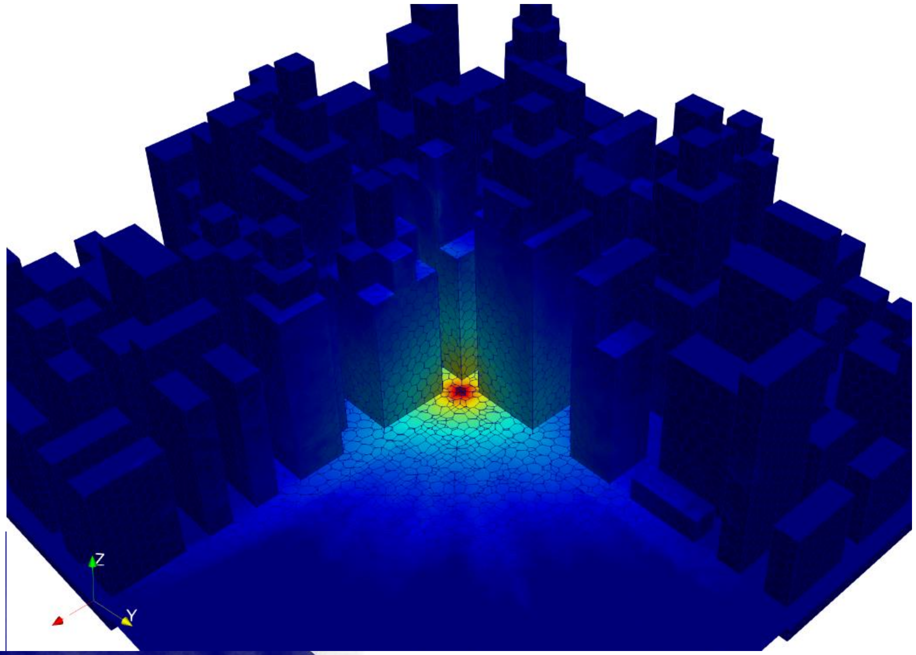
Examples of target applications

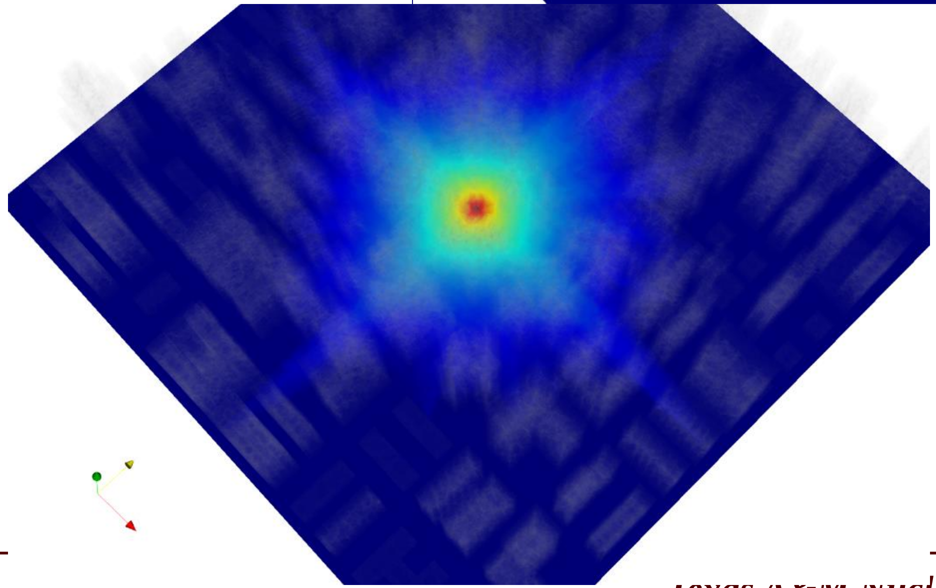




NWrE and Urban Modeling





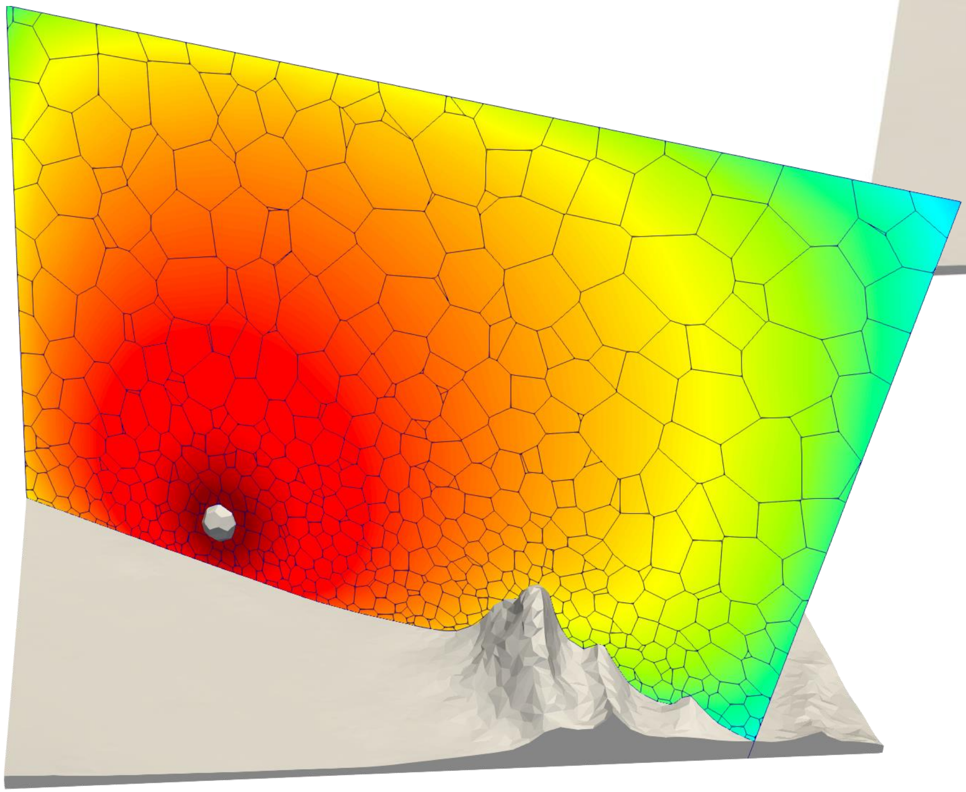


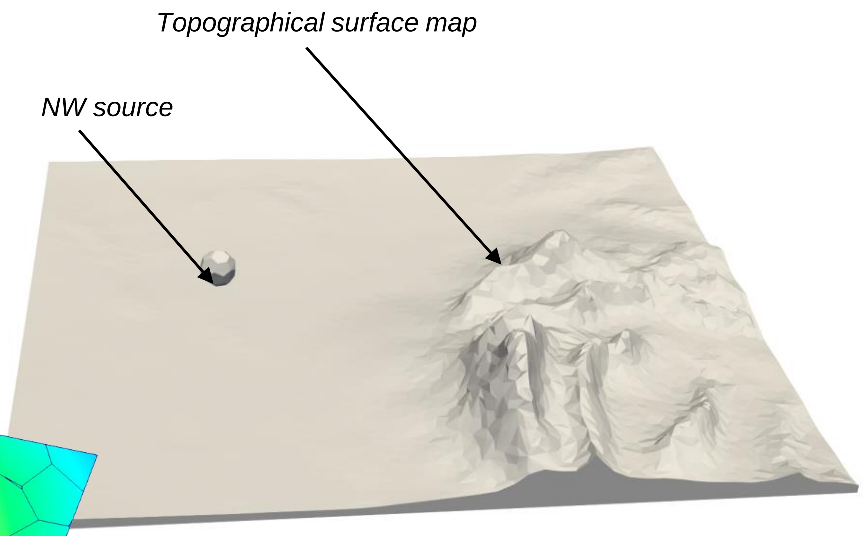
Discretization

- *Spatial cells: 136,633*
- *Vertices per cell: ~19*
- *Energy groups: 116*
- *Angles: 512*
- *DoFs:* ***160 B***

Terrain Geometry

- **Polyhedral mesh**





- **512 angles**
- **1 group problem**
- **~170 M angular unknowns**
- **78,113 nodes, 14,864 cells**
- **Sweep time 43 seconds**
- **6 processors**
- **ParMETIS partitioning**

Projection approach (to be skipped)

Classical ROM approach (Proper Orthogonal Decomposition, POD)

- **Offline stage:**
  1. Investigate the solution space (exercise the Full-Order Model), →data-driven

     Solve $A(\mu_i)x_i = b(\mu_i)$ for $i \in$ training set, $i = 1, .., M$

  2. Accumulate FOM solution in snapshots

     $$S = [x_1, \dots, x_i, \dots, x_M] \in \mathbb{R}^{N \times M}$$

  3. Extract relevant information (Singular Value Decomposition)

     $$S = U \Lambda V^T \quad U \in \mathbb{R}^{N \times N}$$

  4. Compress (solution-space reduction, global bases are now known)

     $$U \to U_r \in \mathbb{R}^{N \times r} \quad \text{with } \boxed{r \ll N}$$

- **Online Stage:**
  1. Given a set of uncertain parameters θ, seek solution as

     $$x^\theta = U_r c^\theta \quad \to \quad A(\theta) U_r c^\theta = b(\theta)$$

  2. Perform (Petrov-)/Galerkin Projection (G: $W = U$, PG: $W = AU$)

     $$\boxed{W_r^T A(\theta) U_r c^\theta = W_r^T b(\theta)} \quad \text{or} \quad \boxed{A_r c^\theta = b_r}$$

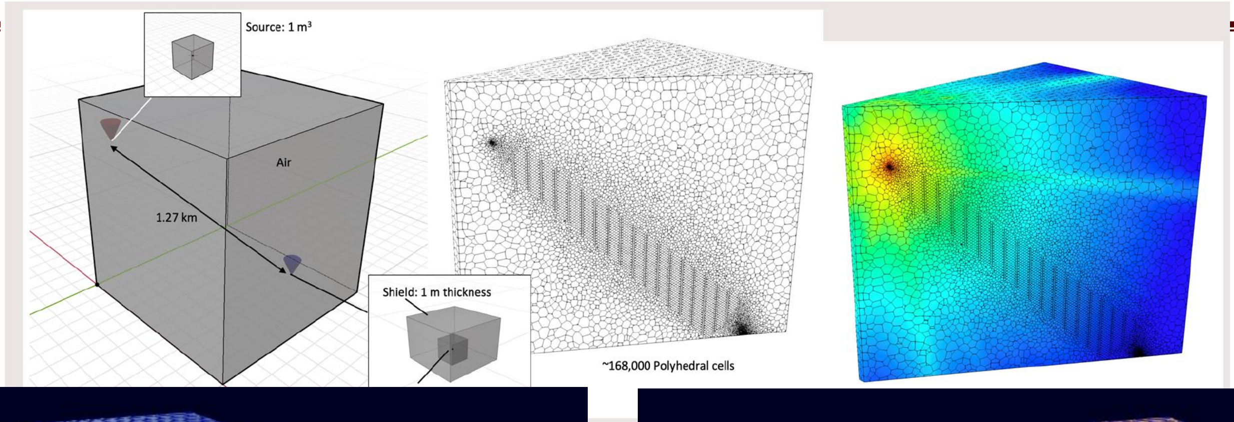
  3. Solve small reduced system:

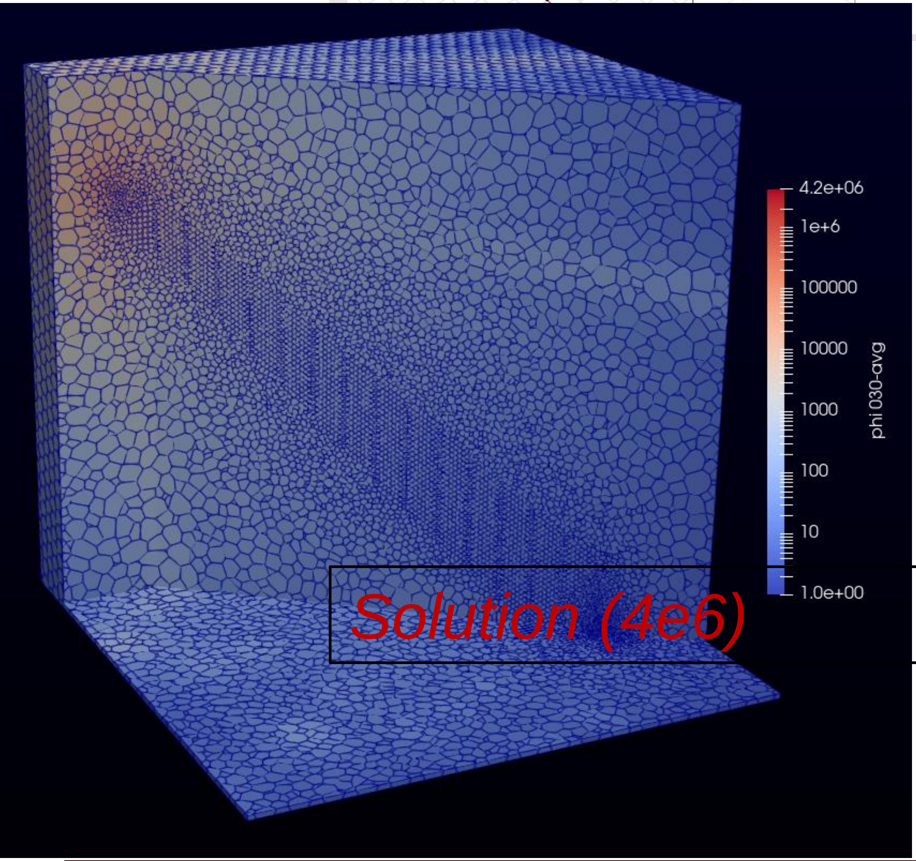
     $$A_r c^\theta = b_r$$

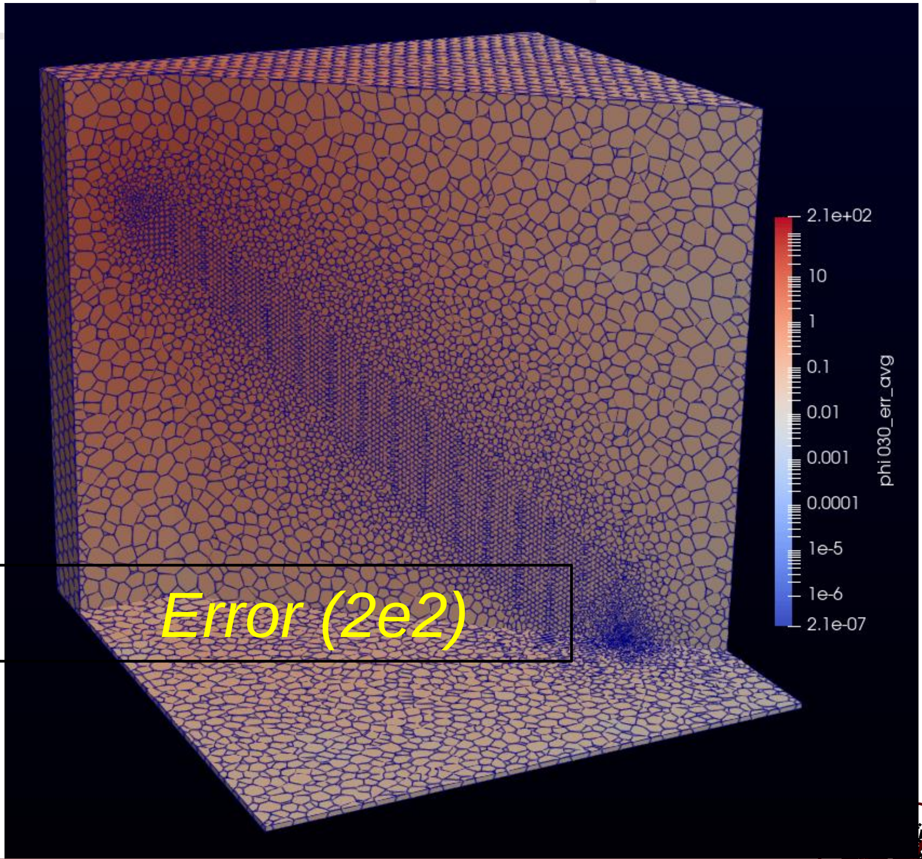
  4. Reconstruct full solution

     $$x^\theta = U_r c^\theta$$

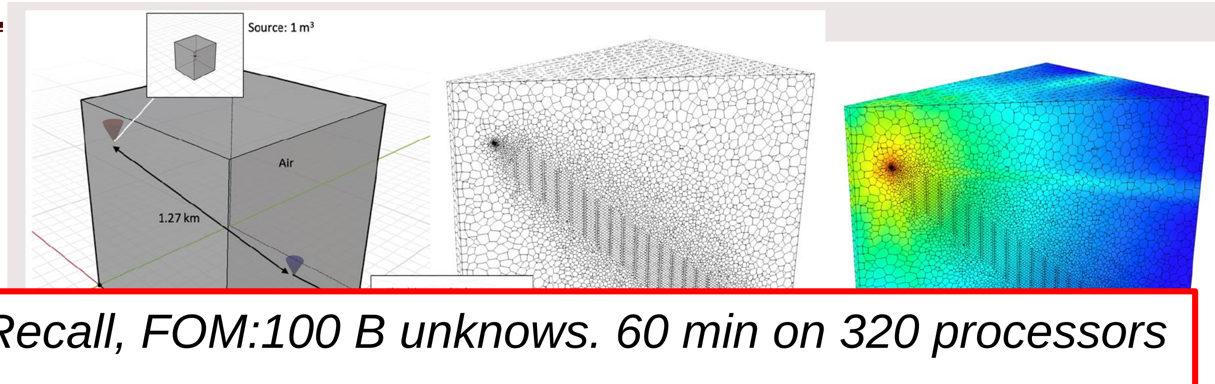
Non-intrusive ROM for Transport using Gaussian Processes





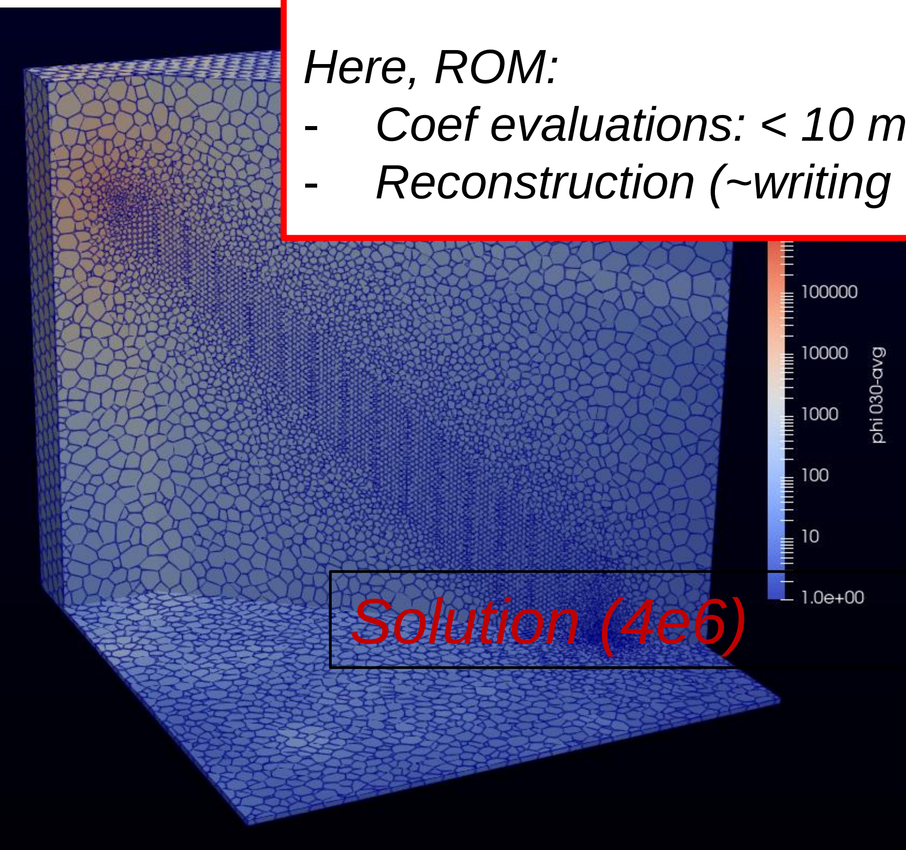


Non-intrusive ROM for Transport using Gaussian Processes

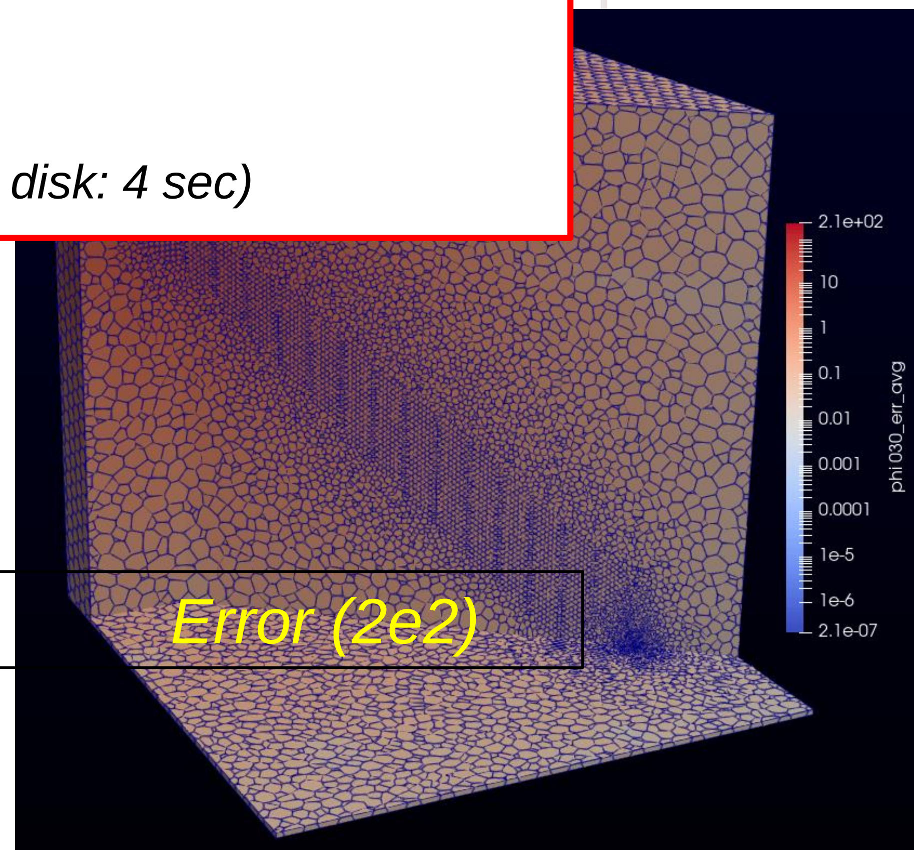


Recall, FOM:100 B unknows. 60 min on 320 processors

Here, ROM:
- *Coef evaluations: < 10 ms*
- *Reconstruction (~writing to disk: 4 sec)*



Solution (4e6)



Error (2e2)

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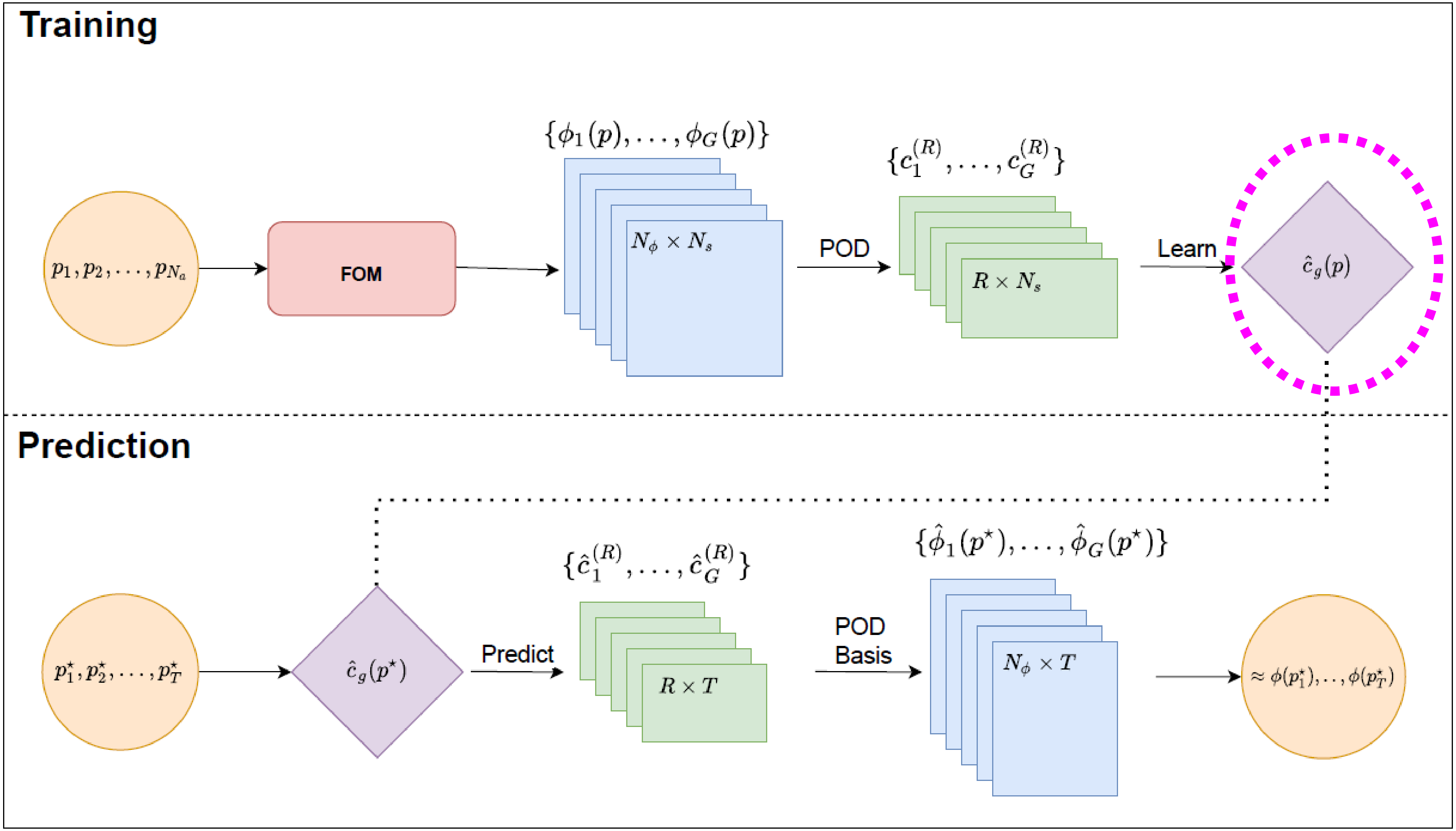
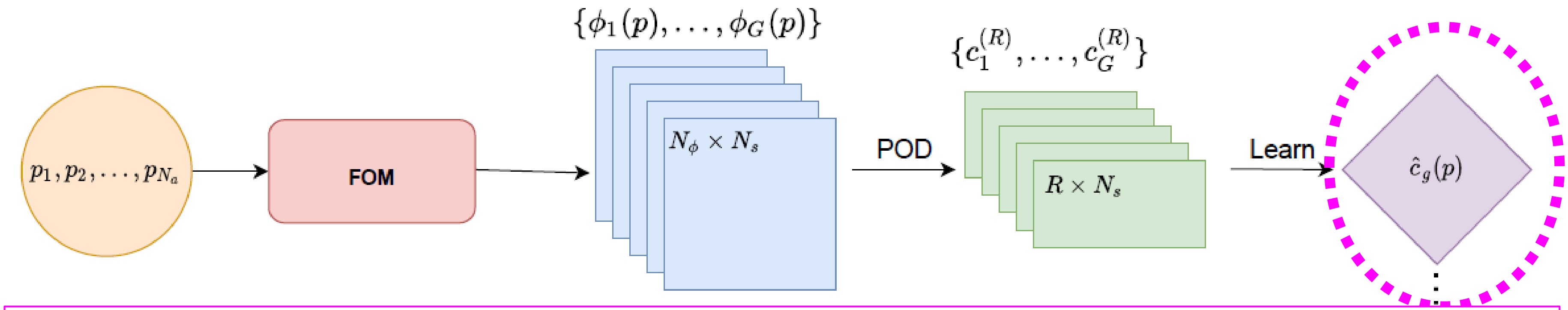
5. Summary and Outlook

High-level view of Model Order Reduction with subspace learning



High-level view of Model Order Reduction with subspace learning

Training



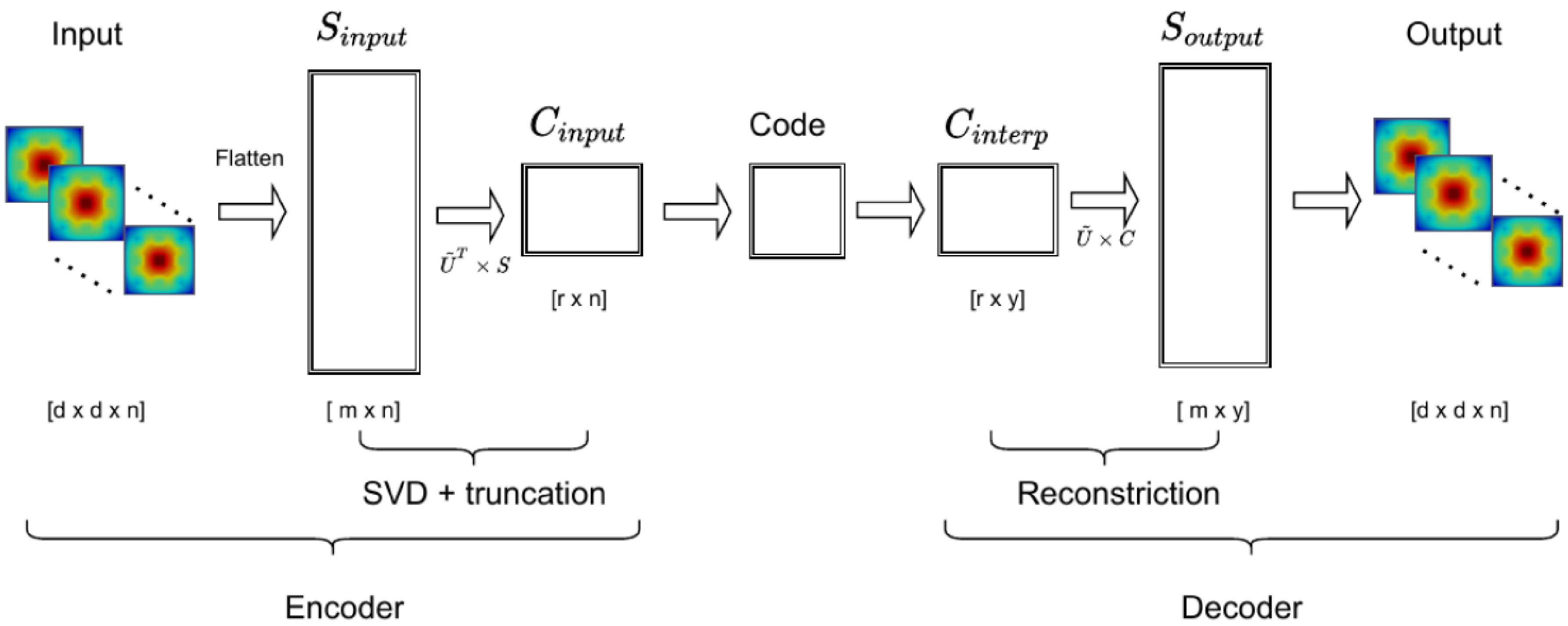
Today, the reduced coordinates were obtained by a projection process

A x = b → the reduced system A_r c = b_r (code invasive)

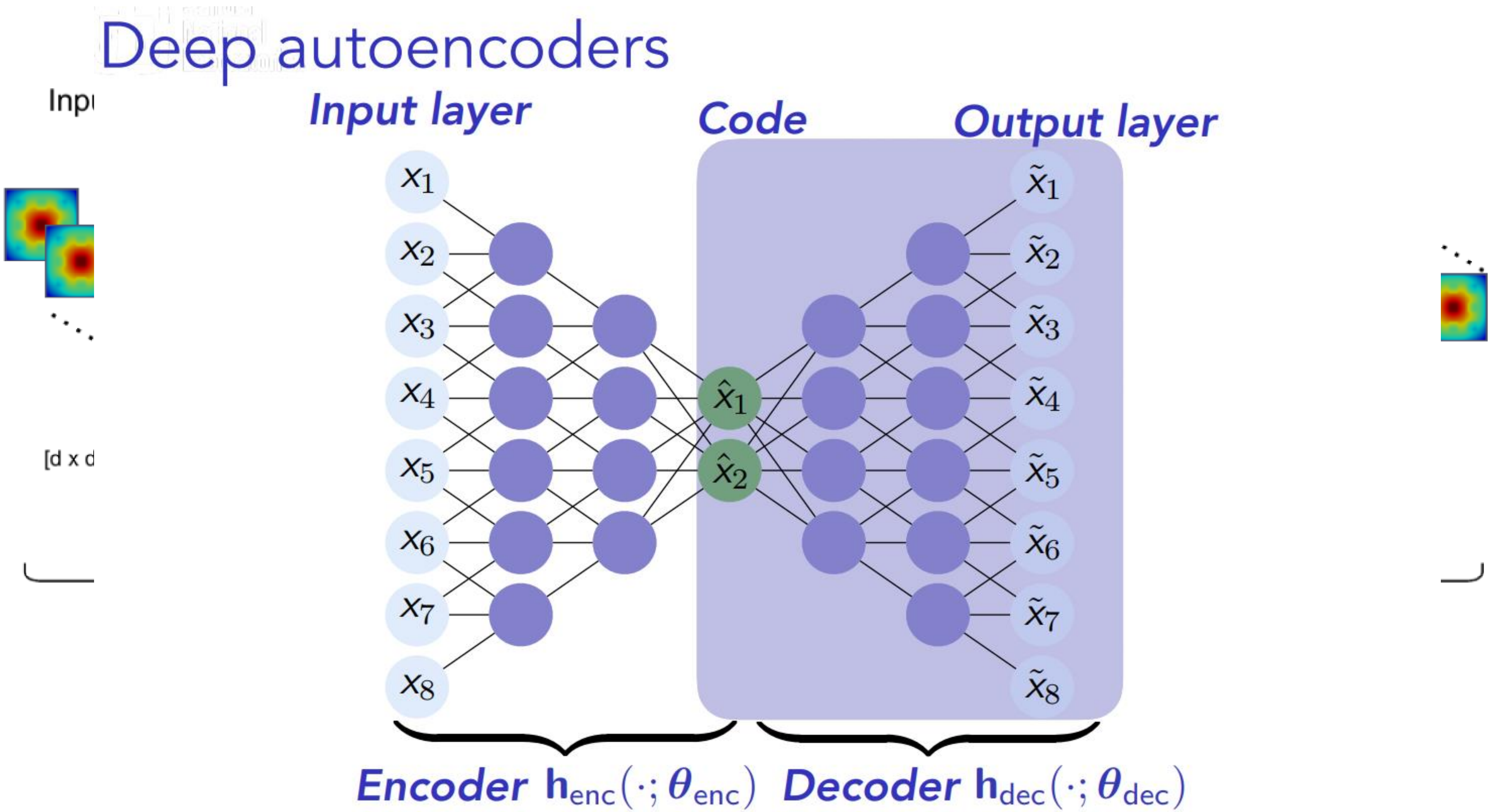
This is not the only option. Non code-invasive possibilities include learning the reduced coordinates with :

1. **Gaussian Processes**
2. **Regression splines**
3. **Neural Networks**
4. **etc. …**

What else is next in MOR?



What else is next in MOR?



$$\tilde{\mathbf{x}} = \mathbf{h}_{\text{dec}}(\cdot;\boldsymbol{\theta}_{\text{dec}}) \circ \mathbf{h}_{\text{enc}}(\mathbf{x};\boldsymbol{\theta}_{\text{enc}})$$

If $\tilde{\mathbf{x}} \approx \mathbf{x}$ for parameters $\boldsymbol{\theta}^{\star}_{\text{dec}}$, $\mathbf{g} = \mathbf{h}_{\text{dec}}(\cdot;\boldsymbol{\theta}^{\star}_{\text{dec}})$ produces an accurate manifold

Conclusions

- HPC for nucl. sci. engr. applications
- Intro to parametric reduced-order modeling
  Data-driven subspace discovery
- Applications to reactor physics (LWRs & MSRs)
- Applications to particle transport

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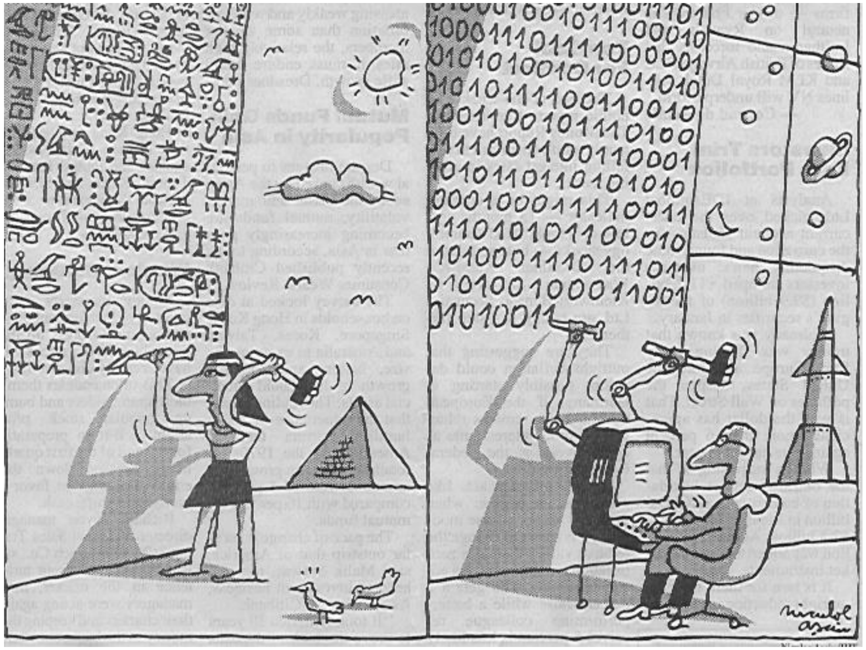

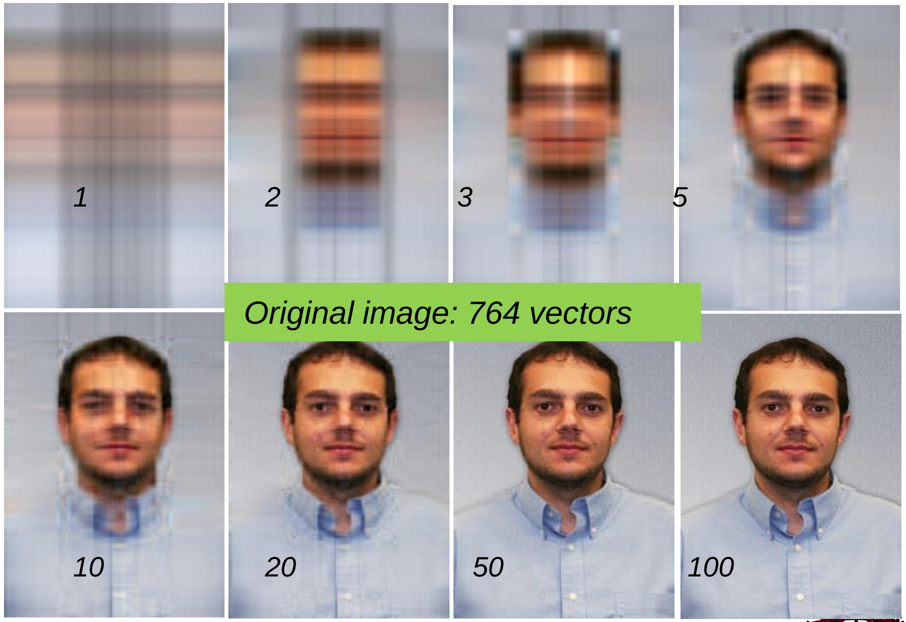

Our papers about POD-ROMs for MSRs

Tano, M., **German, P.**, Ragusa, J., *Evaluation of pressure reconstruction techniques for Model Order Reduction in incompressible convective heat transfer*, Thermal Science and Engineering Progress, Vol. 23, 2021, 100841.

German, P., Tano, M., Ragusa, J. C., Fiorina, C., *Comparison of Reduced-Basis techniques for the model order reduction of parametric incompressible fluid flows*, Progress in Nuclear Energy, 130 (2020), 103551.

German, P., Ragusa, J. C., and Fiorina, C., *Application of multiphysics model order reduction to doppler/neutronic feedback*, EPJ Nuclear Sciences & Technologies 5, ARTICLE (2019): 17.

German, P., and Ragusa, J. C.. *Reduced-order modeling of parameterized multi-group diffusion k-eigenvalue problems*, Annals of Nuclear Energy 134 (2019): 144-157.

German, P., Ragusa, J. C., Tano, M., and Fiorina, C., *Reduced-order modeling of convective flows in porous media*, Fluids

German, P., Ragusa, J. C., Tano, M., and Fiorina, C., *Multiphysics reduced-order modeling of Molten Salt Reactors*, Progress in Nuclear Energy

About GeN-ROM, now published

https://gitlab.com/peter.german/gen-rom