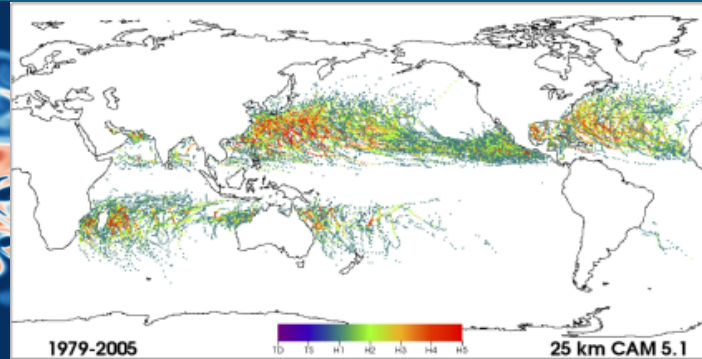
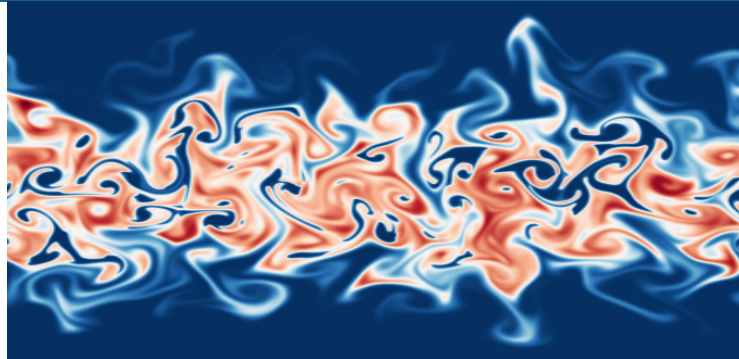




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In-Situ Machine Learning for Intelligent Data Capture on Exascale Platforms



PRESENTED BY

Warren L. Davis IV

Collaborators: Hemanth Kolla, Tim Shead, Irina Tezaur, Philip Kegelmeyer, Gabriel Popoola

Platform for Advanced Scientific Computing (PASC) Conference 2021
July 9, 2021

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U.S. DOE Base Computer Science Research



U.S. DEPARTMENT OF
ENERGY

Office of
Science



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- DOE Office of Science - ASCR funded research
- Phase 1: Three-year research, Collaborative research with Stony Brook University
- Phase 2: Recently renewed as a 4-year project

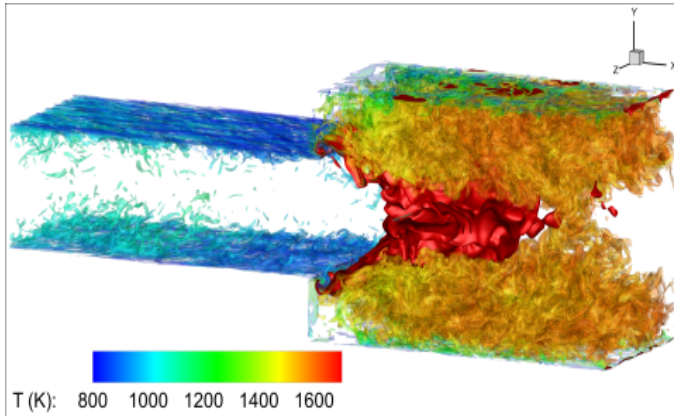
SNL: Warren Davis (PI), Hemanth Kolla, Tim Shead, Irina Tezaur, Philip Kegelmeyer, Gabriel Popoola

Past Members: Kevin Reed (Stony Brook University), Danny Dunlavy (SNL), Julia Ling (Citrine Informatics),
Aditya Konduri (Indian Institute of Science)

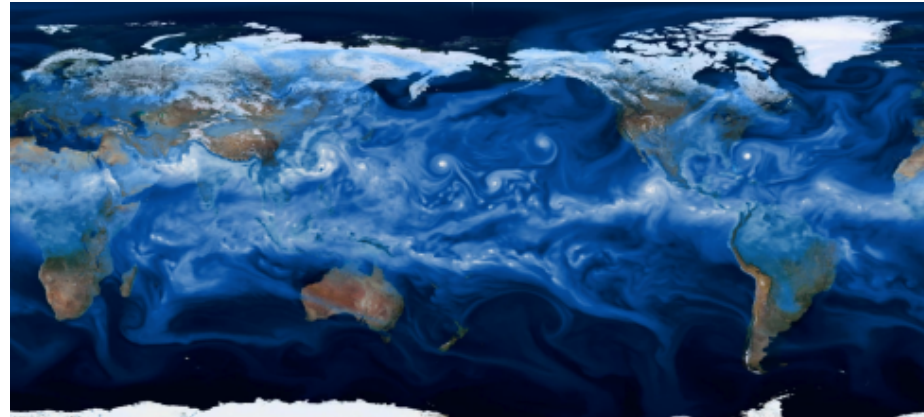
Motivation and Context



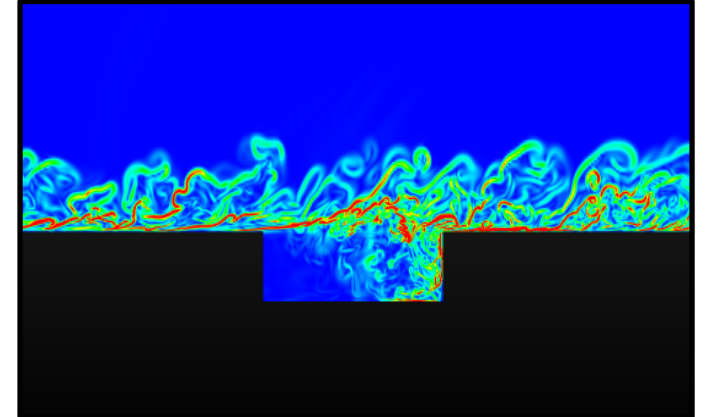
- DOE is interested in many problems that require high-fidelity physics-based HPC simulations



Combustion



Climate Modeling



Fluid Dynamics

- Want to find “interesting” events, anomalies, state changes, etc.
 - Examples may include cyclones, onset of combustion, or other things that the scientists may not prescribe *a priori* and may be difficult to perform via rule-based detection
- Desired solution would be to take all the data and run the appropriate detection algorithms (e.g., LOF, isolation forests, clustering)
- These simulations produce massive amounts of data (problems for storage capacity, data access, etc.)

Current state-of-the-art for HPC simulation analysis



- Take “snapshots” in space and time ($1/1000^{\text{th}}$ or $1/10000^{\text{th}}$)
- Post-process snapshot data with standard algorithms

Problems with the current methods:

- Interesting events may happen between or outside of these snapshots
- Important information leading up to the captured event could be lost
- Rerunning simulations to capture lost information is expensive
- This problem will only get worse as the amount of data and fidelity of the simulations increases

Is there a way to detect the anomalies *in-situ*,
thus facilitating more precisely targeted event capture?

Changing the Paradigm with *In-Situ* Event Detection



- **Develop techniques to detect interesting spatial and temporal events *in-situ* for HPC physics simulations**
- **Scalable** : Can't significantly hinder the runtime of the application
- **Unsupervised** : To enable discovery, should not require labeling of interesting events
- **Generalizable** : Not focused on one specific event or domain
- **Online** : Don't require having access to all the data from every time step (post-processing)

This is foundational research, with a focus on algorithms that can motivate changes to simulation code and facilitate more intelligent, focused data capture

Related Research is in the Early Stages



•Domain-specific

- J. Bennett, A. Bhagatwala, J. Chen, A. Pinar, M. Salloum, and C. Seshadhri. 2016. Trigger Detection for Adaptive Scientific Workflows Using Percentile Sampling. *SIAM Journal on Scientific Computing* 38, 5 (2016), S240–S263. <https://doi.org/10.1137/15M1027942>
- P. Malakar, V. Vishwanath, C. Knight, T. Munson, and M. E. Papka. 2016. Optimal Execution of Co-analysis for Large-Scale Molecular Dynamics Simulations. In *SC '16: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. 702–715. <https://doi.org/10.1109/SC.2016.59>

•Non *In-Situ*

- Bo Zhou and Yi-Jen Chiang. 2018. Key Time Steps Selection for Large-Scale Time-Varying Volume Datasets Using an Information- Theoretic Storyboard. *Computer Graphics Forum* (2018). <https://doi.org/10.1111/cgf.13399>

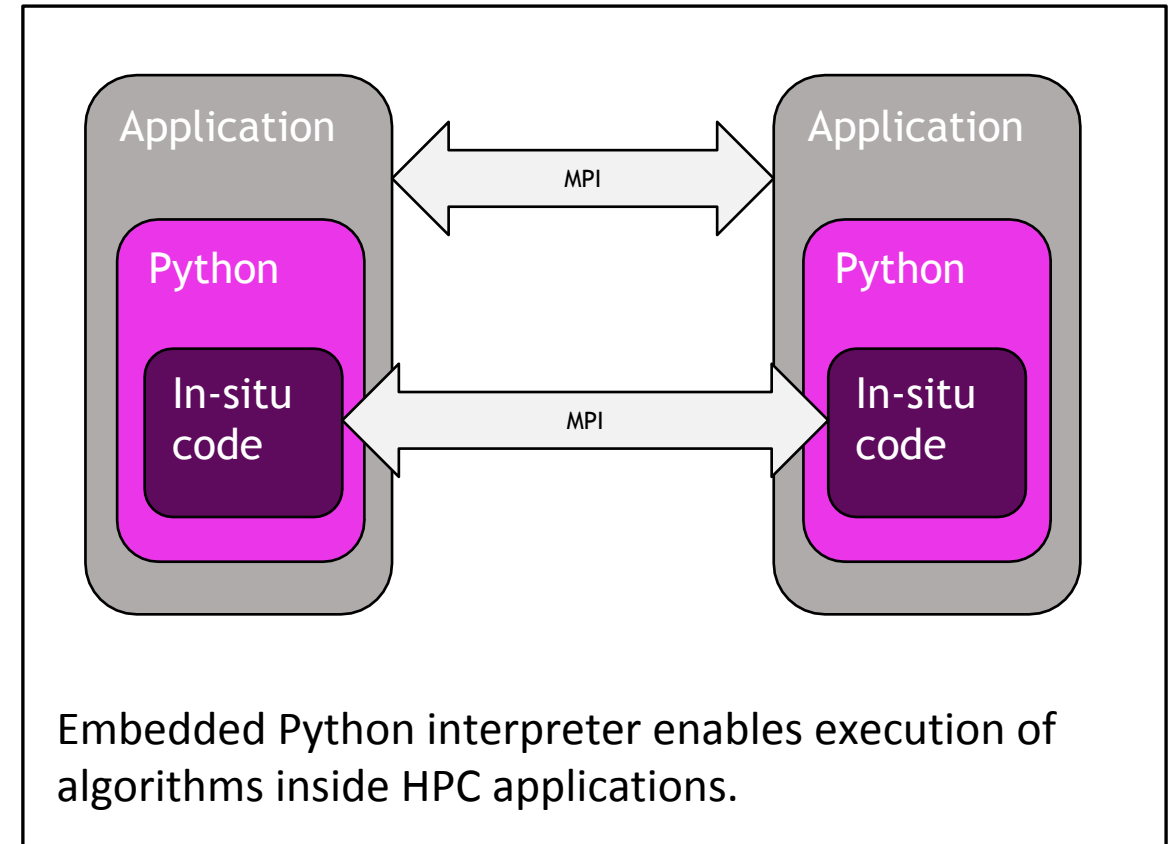
•Domain Agnostic/*In-Situ*

- K. Myers, E. Lawrence, M. Fugate, C. McKay Bowen, L. Ticknor, J. Woodring, J. Wendelberger, and J. Ahrens. 2014. Partitioning a Large Simulation as It Runs. *ArXiv e-prints* (Sept. 2014). [arXiv:stat.ME/1409.0909](https://arxiv.org/abs/1409.0909)
- Larsen, M., Woods, A.L., Marsaglia, N., Biswas, A., Dutta, S., Harrison, C., & Childs, H. (2018). A flexible system for in situ triggers. *ISAV@SC*.

Vehicles for Exploration and Experimentation

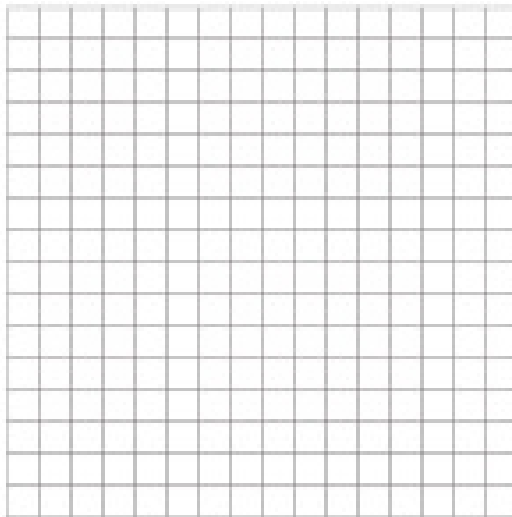


- Sandia 3D Direct Numerical Solver (S3D)
 - Used for reacting flows (e.g., combustion)
- Python Interpreter
- *In-Situ* code has access to state variables.
- Enabled immediate use of OTS algorithms and facilitated the development of new algorithms
- Tested algorithms on combustion *in-situ*, climate offline (e.g., LOF, DBSCAN, i-Forests)

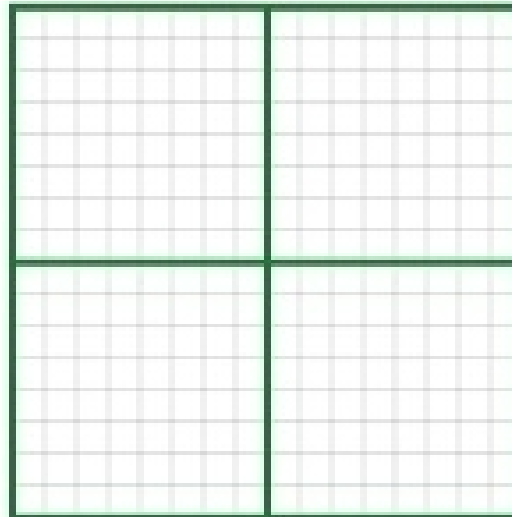


Timothy M. Shead et al. "Embedding Python for In-Situ Analysis." SAND2018-9009. August 2018.

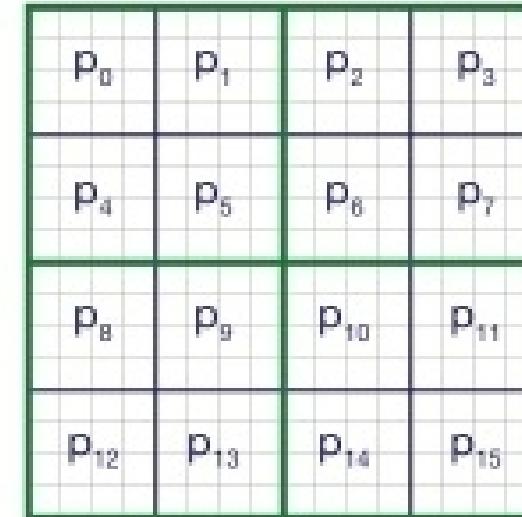
Communication is a constraint for In-Situ HPC Anomaly Detection



Simulation Domain

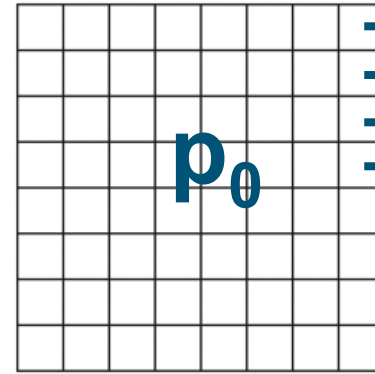
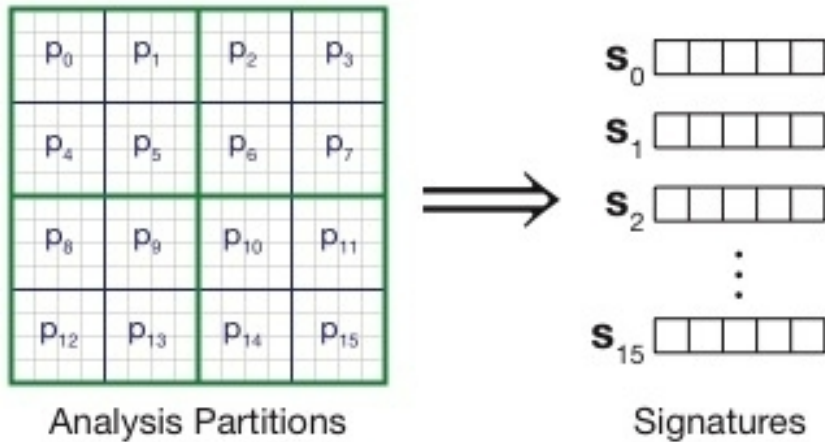


Processors



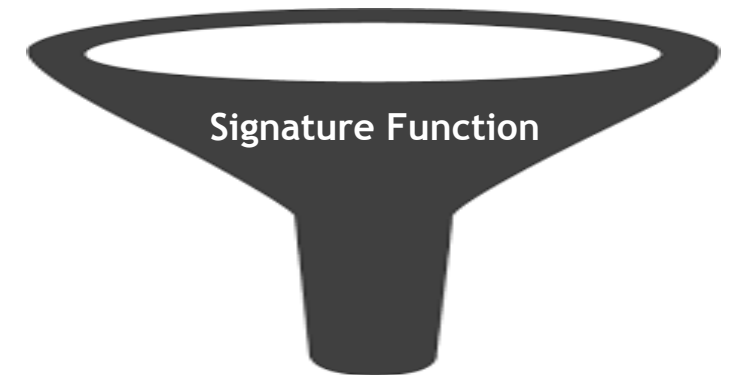
Analysis Partitions

Signatures Represent the Data on a Partition



Individual mesh attributes for P_0

Density	Pressure	Vx	Vy
10	4	2	4
20	10	8	8
30	8	8	12
40	6	2	16
40	6	2	16



P_0 signature

25	7	5	10
----	---	---	----

m Number of mesh points
 a Attributes per mesh point

t $m*a$, the total number of values on a partition


Signatures can be shorter or longer than a , as long as they are shorter than t



- Mean

- *Ling et al. "Using feature importance metrics to detect events of interest in scientific computing applications." *2017 IEEE 7th Symposium on Large Data Analysis and Visualization (LDAV)* (2017): 55-63.

Individual mesh attributes for P_0



Signature Function

P_0 signature

25	7	5	10
----	---	---	----

Measures Indicate the Distance of a Signature From Neighbors



Measures take as input a list of $T P \times S$ matrices where T is the number of elapsed timesteps and each $P \times S$ matrix contains the signatures for the partitions at a given timestep.

Measures can be specific to a type of signature, or general measures, including typical anomaly detection algorithms

Examples

- Mean-Squared Distance
- DBSCAN
- FIEDA M1*

*Ling et al. "Using feature importance metrics to detect events of interest in scientific computing applications." *2017 IEEE 7th Symposium on Large Data Analysis and Visualization (LDAV)* (2017): 55-63.

Decisions Allow for Customization



Measures are scalar values that do not, by themselves, answer whether something is anomalous.

Different applications can decide an appropriate anomalousness point

Examples

- Threshold
- Percentile-Change
- Memory / Feathering

Decision functions are meant to be adjustable to fit application needs and are the final arbiter of what is “interesting” in a simulation.

New, Effective *In-Situ* Anomaly Detection Algorithms



Using Feature Importance Metrics to Detect Events of Interest in Scientific Computing Applications

Julia Ling¹, W. Philip Kegelmeier^{2*}, Kondu Aditya³, Hemant Kolla⁴, Kevin A. Reed⁵
¹Crane Informatics¹, ²Sandia National Labs, ³Sandia National Labs, ⁴Sandia National Labs, ⁵Energy Research University
 Timothy M. Shaw⁶, Warren L. Davis IV⁶
⁶Sandia National Labs

Abstract

With current high performance scientific computing applications, data are typically recorded at regular intervals (e.g., seconds) and stored on tape. Data are not saved at every time step to prevent excessive time and space costs. Some data (e.g., location) may exist in the workflow. However, in some domains, systems (e.g., nuclear reactors) are highly in-situ and time critical, e.g., real-time data acquisition, processing at regular intervals is both inefficient and ineffective. It is not this data being used for diagnosis where a lack of interest is concerning, but it will cause interest if interest that occurs at irregular intervals in data. When a series of interest events occur, it is not clear if they are of interest or not. This is a difficult task to be performed on the existing processes. We propose a method of identifying such events by using feature importance metrics. This method requires very little communication between processes, thereby leading to a more efficient and high performance computing solution.

Index Terms: Data Mining, Methodology, Simulation, and Modeling, Statistical, Output Analysis, Data Mining, Methodology, Pattern Recognition, General

1 Introduction

1.1 Motivation

In many cases, including a linear process, fluid mechanics, combustion, and materials science, high performance computing clusters are used to produce simulations to make scientific and engineering predictions. In these scientific computing workflows, it is common to record the simulation state at every time step, every several hundred time steps. Recording the data every time step can cause excessive memory usage and/or network bandwidth that is typically not desired [1].

However, in many domains, systems (e.g., nuclear reactors) are highly in-situ and time critical. In the case of nuclear reactors, data can be recorded at a few time steps, often after many hundreds of time steps (e.g., minutes of interest) [2]. In such cases, simulating sub-critical events can occur over a long time scale, but can be detected during short time intervals. In such cases, it is not clear if they are of interest or not. This is a difficult task to be performed on the existing processes. We propose a method of identifying such events by using feature importance metrics. This method requires very little communication between processes, thereby leading to a more efficient and high performance computing solution.

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 978-1-5386-0675-5/17/\$31.00 ©2017 IEEE

the event of interest is limited to a small fraction of the domain. Data recorded at regular intervals can miss important events of interest. In order to capture such events, a more powerful method, the system must capture the simulation data at every time step, which is not feasible for high frequency data. During this period, it is not clear if they are of interest or not. This is a difficult task to be performed on the existing processes. We propose a method of identifying such events by using feature importance metrics. This method requires very little communication between processes, thereby leading to a more efficient and high performance computing solution.

1.2 Problem statement

We suggest that a modeling learning approach could be used to automatically detect events of interest. In this context, interest of a time is defined as any time when a system process that diverges significantly from its nominal or expected behavior. In this context, the divergence is defined as a change in the principal values and vectors of kurtosis. Obtaining the principal kurtosis vectors requires decomposing a fourth order joint moment tensor for which we use a simple, computationally less expensive approach that involves performing a singular value decomposition (SVD) over the matrixized tensor. We demonstrate the efficacy of this approach on synthetic data, and develop an algorithm to identify the occurrence of a spatial and/or temporal anomalous event in scientific phenomena. The algorithm decomposes the data into several spatial sub-domains and time steps to identify regions with such events. Feature importance metrics, based on the alignment of the principal kurtosis vectors, are computed at each sub-domain and time step for all features to quantify their relative importance towards the overall kurtosis in the data. Accordingly, spatial and temporal anomaly metrics for each sub-domain are proposed using the Hellinger distance of the feature moment metric distribution from a suitable nominal distribution. We apply the algorithm to two turbulent auto-ignition combustion cases and demonstrate that the anomaly metrics reliably capture the occurrence of auto-ignition in relevant spatial sub-domains at the right time steps.

The desired behavior of the machine learning algorithm would be to detect the processes on which an event of interest is occurring, so that those processes can store the data at a high time step. Such an approach would require storing a high time and computational resources, and also identifying the data. The desired attributes of such a machine learning algorithm are as follows:

- **Generalizability:** The algorithm should be deployable on a variety of different scientific computing applications without need of application-specific tuning.
- **Unsupervised:** The algorithm should be able to operate in an unsupervised manner without bias or examples of events of interest.
- **Low communication overhead:** The algorithm should require minimal communication between processes.
- **Online capability for streaming data:** The algorithm should be able to make online predictions during streaming data, without having to store data from previous time steps.

Anomaly detection in scientific data using joint statistical moments

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¹Sandia National Laboratories, Livermore, CA 94550, United States

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Abstract

We propose an anomaly detection method for multi-variate scientific data based on analysis of high order joint moments. Using kurtosis as a reliable measure of outliers, we suggest that principal kurtosis vectors, by analogy to principal component analysis (PCA) vectors, signify the principal directions along which outliers appear. The inception of an anomaly, then, manifests as a change in the principal values and vectors of kurtosis. Obtaining the principal kurtosis vectors requires decomposing a fourth order joint moment tensor for which we use a simple, computationally less expensive approach that involves performing a singular value decomposition (SVD) over the matrixized tensor. We demonstrate the efficacy of this approach on synthetic data, and develop an algorithm to identify the occurrence of a spatial and/or temporal anomalous event in scientific phenomena. The algorithm decomposes the data into several spatial sub-domains and time steps to identify regions with such events. Feature importance metrics, based on the alignment of the principal kurtosis vectors, are computed at each sub-domain and time step for all features to quantify their relative importance towards the overall kurtosis in the data. Accordingly, spatial and temporal anomaly metrics for each sub-domain are proposed using the Hellinger distance of the feature moment metric distribution from a suitable nominal distribution. We apply the algorithm to two turbulent auto-ignition combustion cases and demonstrate that the anomaly metrics reliably capture the occurrence of auto-ignition in relevant spatial sub-domains at the right time steps.

Keywords:

Anomaly detection, Scientific computing, Co-Kurtosis, Tensor decomposition, Hellinger distance, Auto-ignition

1. Introduction

Anomaly detection is such a widely studied topic, and has found numerous applications in various contexts, that it defies easy generalization. Nonetheless, the vast majority of applications that have embraced anomaly detection methods have characteristics that may not be representative of scientific data. Chandola *et al.* [1] emphasize that the key aspects of anomaly detection include the nature of input data, type(s) of anomaly and output of anomaly detection. In all these aspects, scientific data have distinctly different attributes compared to all other domains. As the scale or scientific investigations keeps ever increasing, robust anomaly detection is becoming increasingly critical. One of the key findings of a Department of Energy Workshop on mathematics of data [2] is “near real-time identification of anomalies in streaming and evolving data is needed in order to detect and respond to phenomena that are either simulated or real”.

Some of the challenges of anomaly detection in scientific data stem from the following attributes:

- **Multi-variate, multi-physics phenomena:** The observations are of numerous variables (tens to hundreds) that represent coupled non-linear physics and hence elude easy assumptions about statistical (in)dependence.

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February 26, 2019

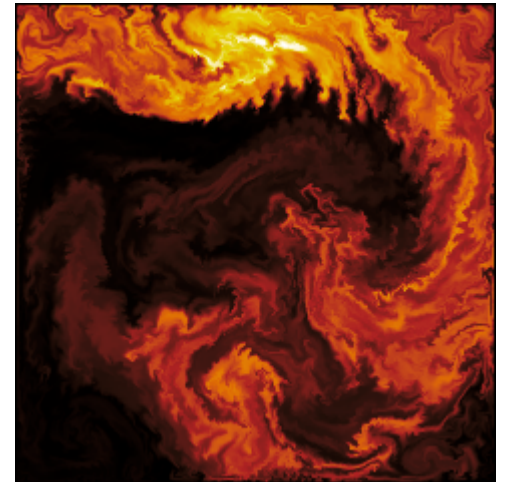
Ling et al. “Using feature importance metrics to detect events of interest in scientific computing applications.” *2017 IEEE 7th Symposium on Large Data Analysis and Visualization (LDAV) (2017)*: 55-63.

Aditya et al. “Anomaly detection in scientific data using joint statistical moments”, *Journal of Computational Physics*, Vol 387, June 15 2019, pp. 522-538.

Rapid Development and Testing



- S3D is useful but too unwieldy for rapid experimentation
- Mantaflow (ETH Zurich, Technical University of Munich)
 - Mini-app that can be run on the desktop
 - Modified to simulate HPC environment (partitioning, inter-partition communication model)



Approximately 30 new viable algorithms, some of which perform better than our previous published algorithms

Experiments and the Complexity of Measuring Performance



- Buoyant fluid injections simulated in Mantaflow
- Various algorithms capture different aspects of the simulation
 - Hard to get a crisp definition of accuracy vs. data efficiency
 - We devised a way of adding anomalies independent of the flow simulation
 - Modifications to mesh attributes that wouldn't be congruent with the simulation
 - Determining *recall* in relation to data export is now possible

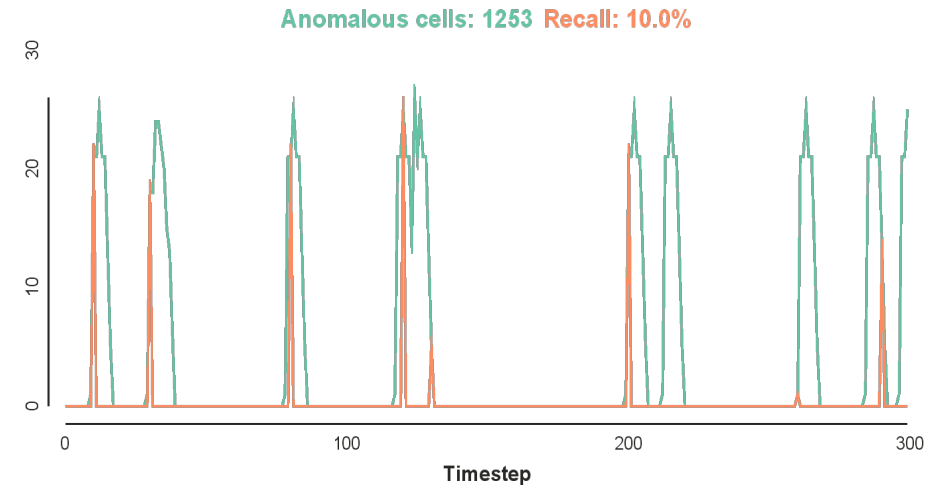
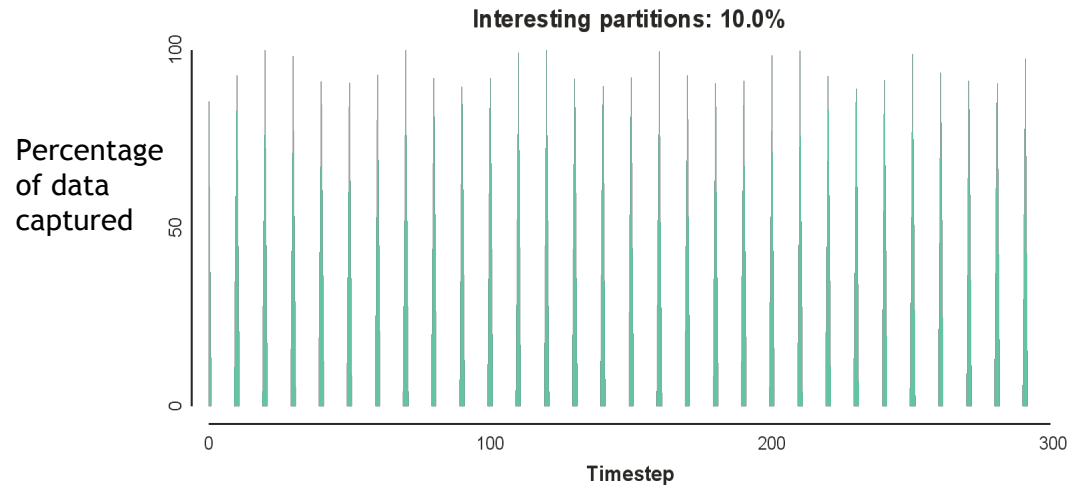


We can measure the accuracy of our methods along with the data savings and compare to “snapshotting” and other approaches.

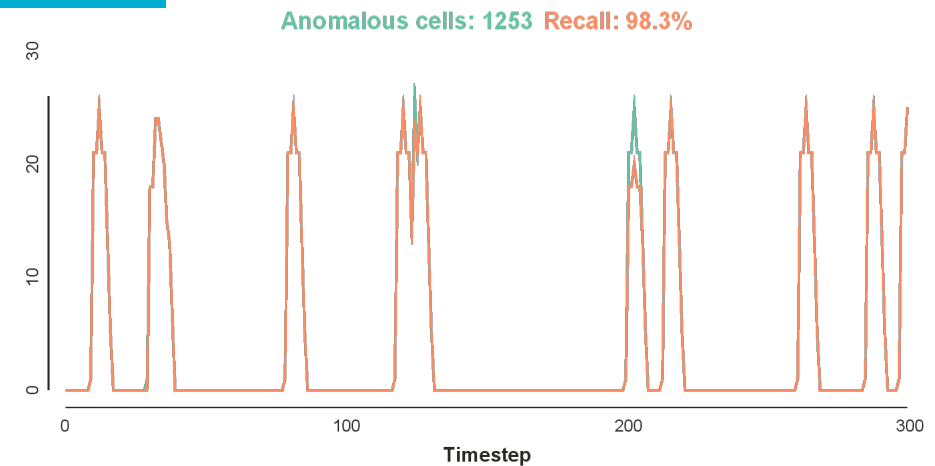
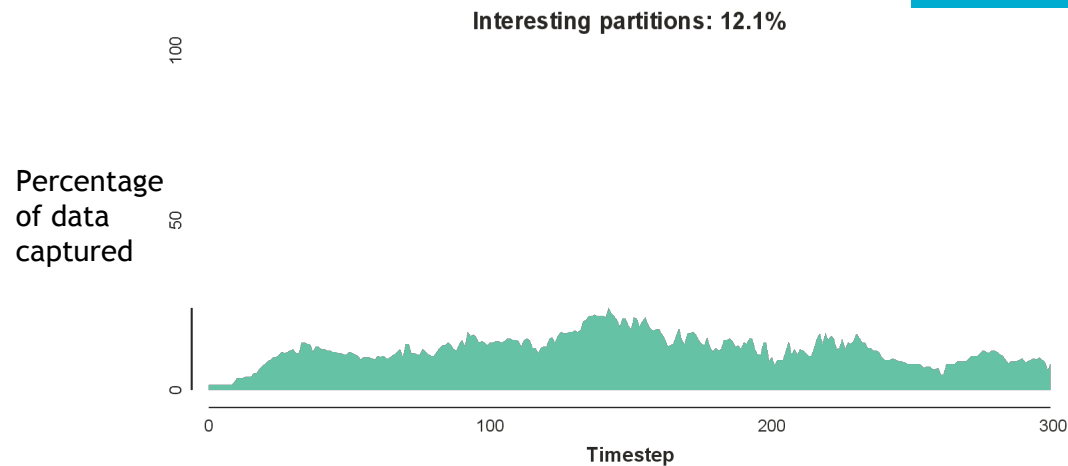
In-Situ Detection is More Accurate and Efficient



Snapshot (Conventional)



In-Situ Detection





- *density*

- *density (masked)*



density



density (masked)



QBOT

QBOT (masked)

Summary



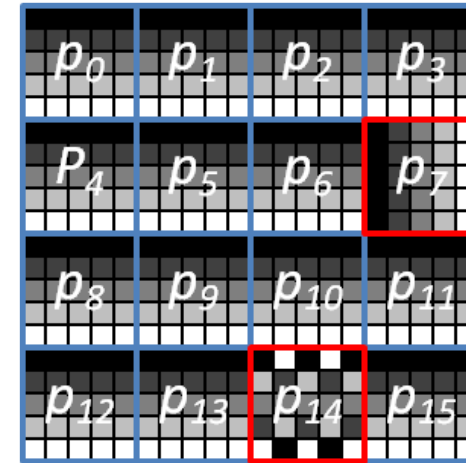
- Conventional approaches to anomaly detection in HPC simulations are insufficient, and this problem will grow
- Experiments have shown that in-situ anomaly detection is possible, both implementation-wise and algorithmically
- In-situ detection is more accurate and efficient
- Developed new algorithms and a framework for rapid development and testing

Towards Exascale

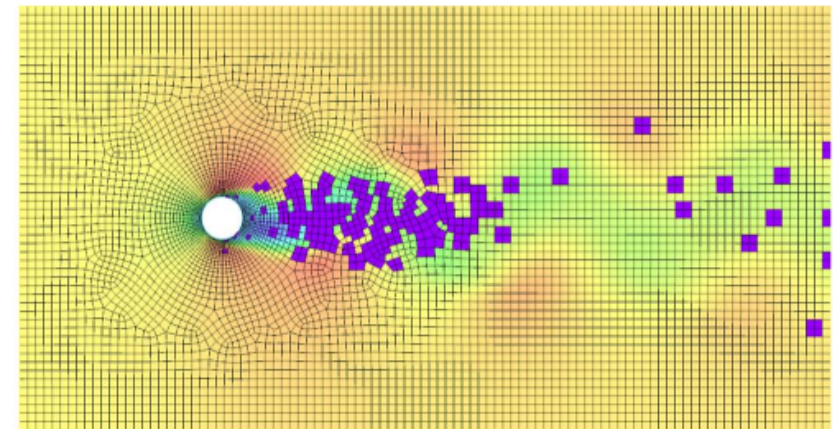


- Signature families
 - Gradient
 - Frequency
 - Simulation-driven error indicators
 - Multi-fidelity/scale signatures
- Partition/time-window effects
- Utilization of simulation data
 - Unsupervised to supervised (e.g., anomaly classification)
 - Creating supervised signatures without event labels
 - Creating supervised signatures with labels
 - Using generative models to *predict* anomalies
- Reduced-order modeling (ROM)

Our research will enhance the utility of machine learning in HPC scientific computation, creating new capabilities and increasing our overall efficacy.



Detection of statistically homogenous anomalous patterns



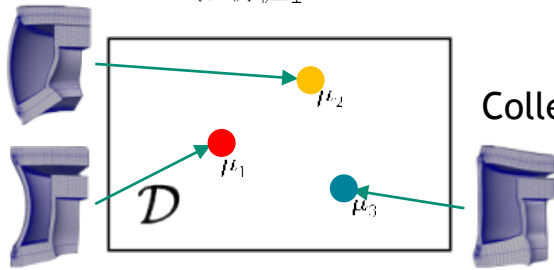
Mesh sampling for ROM refinement

ROMs = physics-based surrogates tied directly to a “full-order model” (FOM) that can enable full-field predictions in real time.

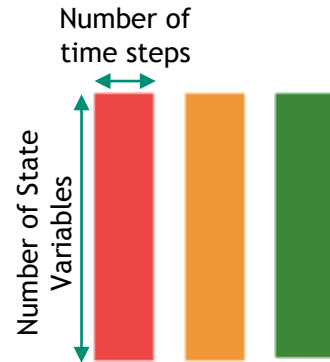
1. Data Acquisition

Sample FOM parameter space,

$$\{\mu_i\}_{i=1}^{n_{\text{train}}} \in \mathcal{D}$$



Collect solutions



2. Manifold Learning

Unsupervised Learning of Reduced Basis
(e.g. via Principal Component Analysis or Nonlinear Methods):

$$\mathbf{X} = \begin{bmatrix} \text{red} & \text{orange} & \text{green} \end{bmatrix} = \Phi \mathbf{U} \quad \Sigma \quad \mathbf{V}^T$$

3. Projection and Reduction

Choose ODE
Temporal
Discretization

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \mu)$$

\Downarrow

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

Reduce the
Number of
Unknowns

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \Phi \hat{\mathbf{x}}(t)$$

Minimize the Residual
(Galerkin or Petrov-
Galerkin Projection)

minimize $\|\hat{\mathbf{v}}\|$

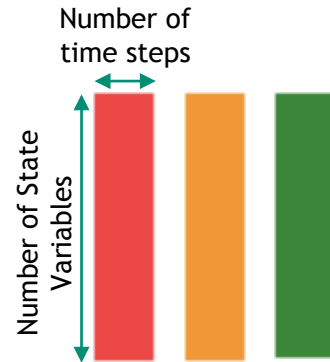
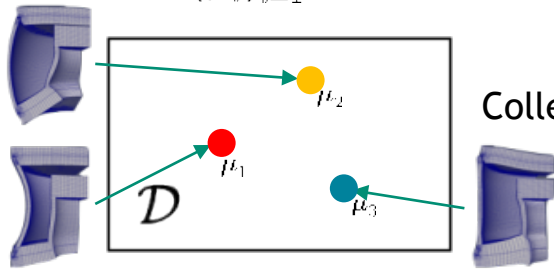
$$\left\| \mathbf{r}^n(\Phi \hat{\mathbf{v}}; \mu) \right\|_2$$

Challenge: for non-linear problems, residual minimization requires operations scaling like FOM.

1. Data Acquisition

Sample FOM parameter space,

$$\{\mu_i\}_{i=1}^{n_{\text{train}}} \in \mathcal{D}$$



2. Manifold Learning

Unsupervised Learning of Reduced Basis
(e.g. via Principal Component Analysis or Nonlinear Methods):

$$\mathbf{X} = \begin{bmatrix} \text{red} & \text{orange} & \text{green} \end{bmatrix} = \begin{bmatrix} \text{brown} & \text{blue} \end{bmatrix} \Phi \mathbf{U} \quad \Sigma \quad \mathbf{V}^T$$

3. Projection and Reduction

Choose ODE
Temporal
Discretization

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \mu)$$

\Downarrow

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

Reduce the
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Minimize the Residual
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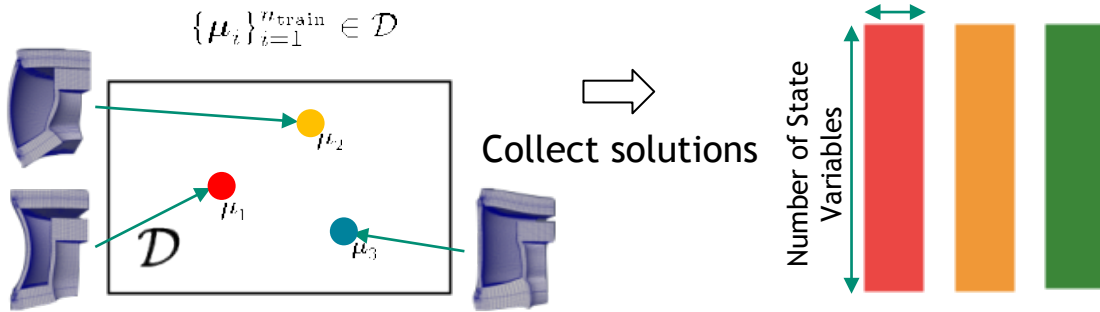
minimize $\|\mathbf{r}^n(\Phi \hat{\mathbf{v}}; \mu)\|_2$

$$\left\| \begin{pmatrix} \text{brown} & \text{grey} & \text{black} \end{pmatrix} \right\|_2$$

Solution is hyper-reduction: compute the residual on a small subset of the mesh, represented by matrix A

1. Data Acquisition

Sample FOM parameter space,



2. Manifold Learning

Unsupervised Learning of Reduced Basis
(e.g. via Principal Component Analysis or Nonlinear Methods):

$$\mathbf{X} = \begin{bmatrix} \text{red bar} & \text{orange bar} & \text{green bar} \end{bmatrix} = \begin{bmatrix} \text{brown bar} & \text{blue square} \end{bmatrix} \begin{bmatrix} \text{blue square} \end{bmatrix}^T$$

Σ

3. Projection and Reduction

Choose ODE
Temporal
Discretization

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \mu)$$

\Downarrow

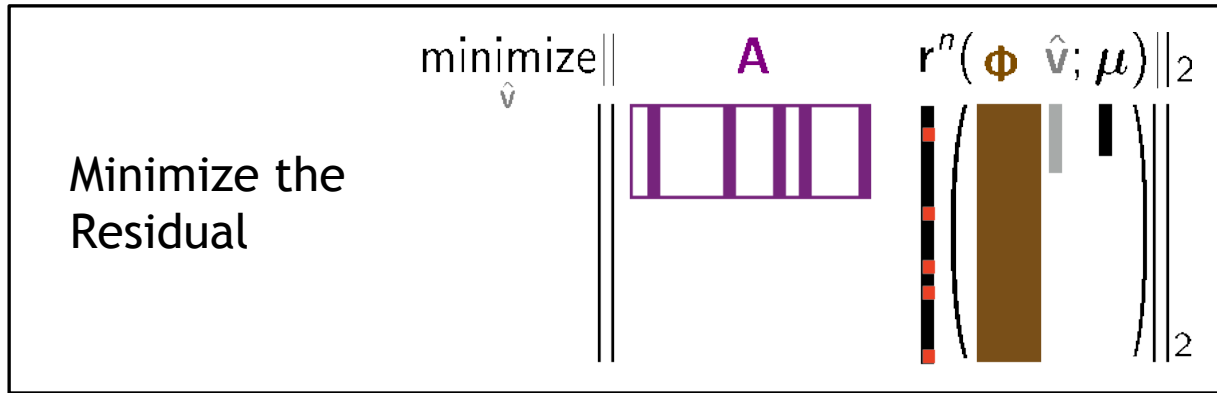
$$\mathbf{r}^n(\mathbf{x}^n; \mu) = \mathbf{0}, \quad n = 1, \dots, T$$

Reduce the
Number of
Unknowns

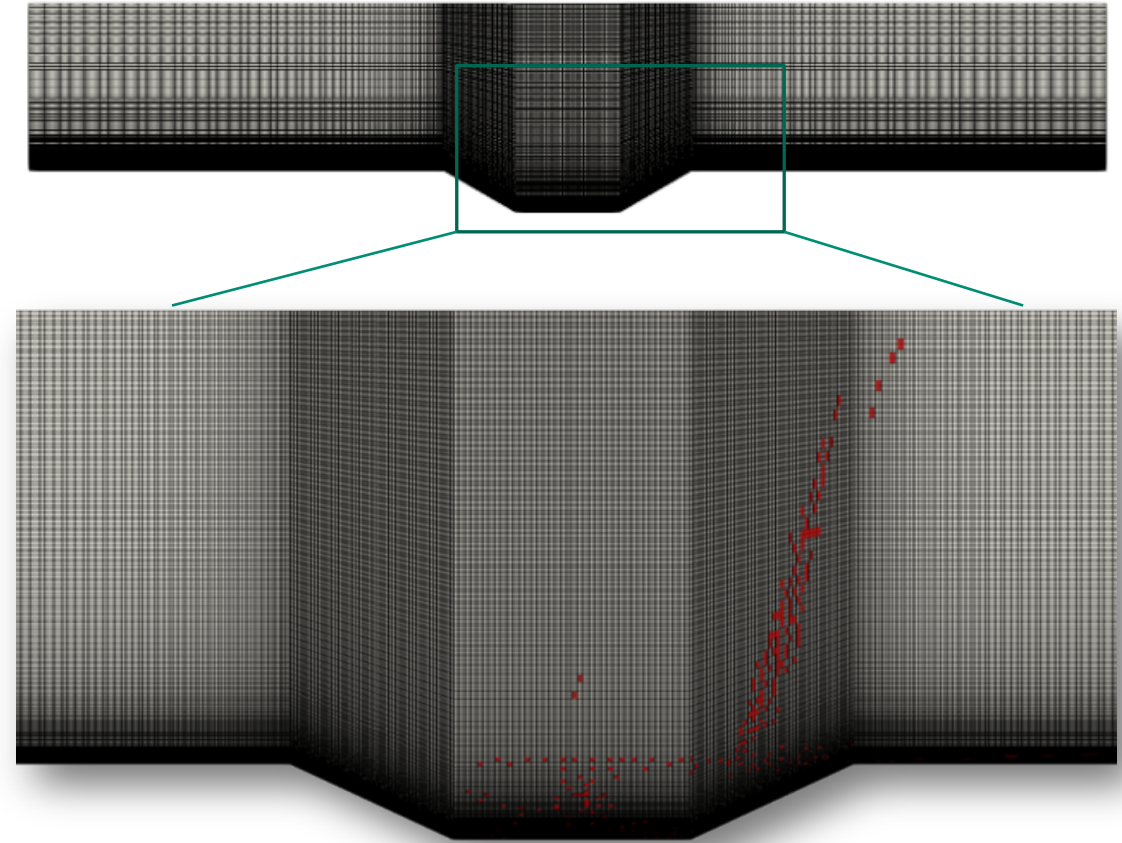
$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \Phi \hat{\mathbf{x}}(t)$$

Minimize the Residual
(Galerkin or Petrov-
Galerkin Projection)

$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \left\| \begin{bmatrix} \text{purple matrix } A \end{bmatrix} \mathbf{r}^n(\Phi \hat{\mathbf{v}}; \mu) \right\|_2$$

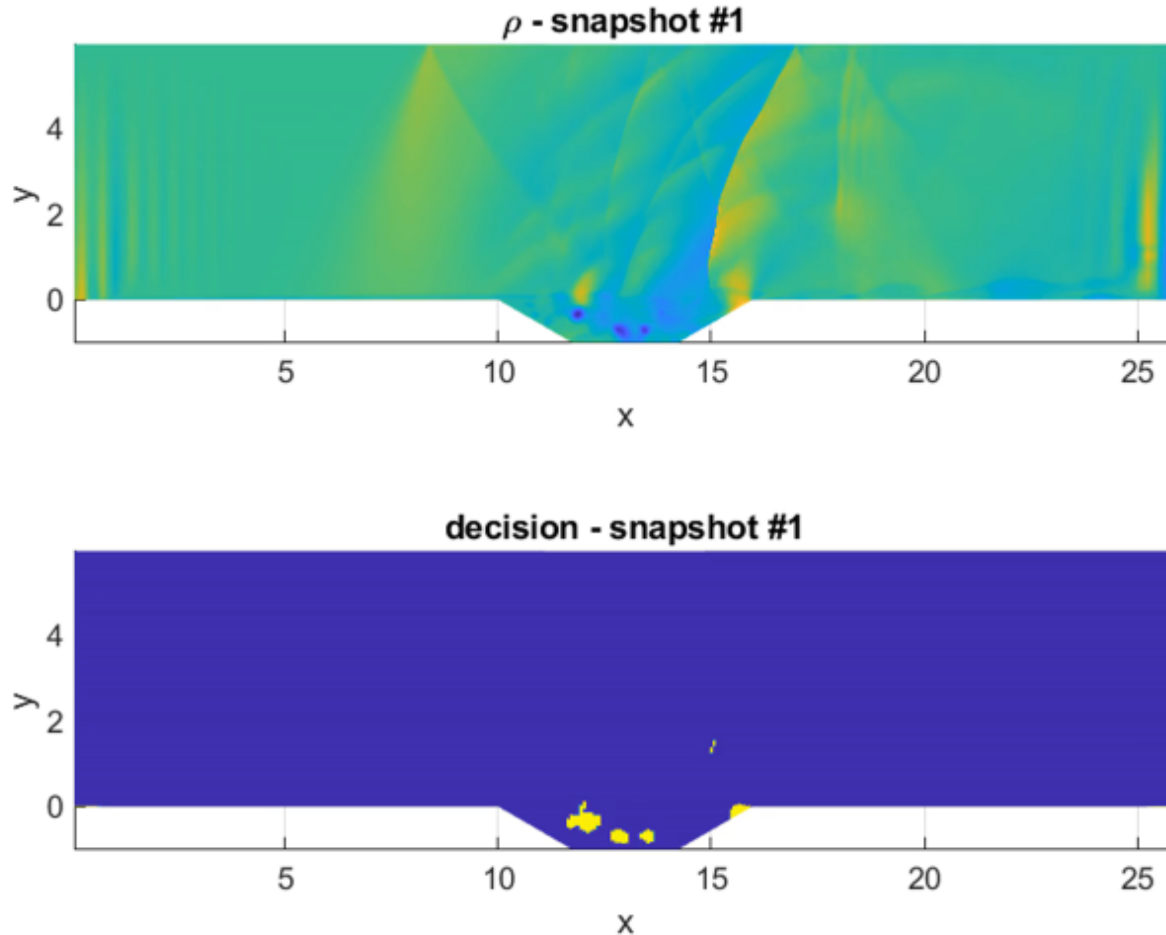


- A *single “sample mesh”* is typically computed using a simple greedy algorithm that minimizes reconstruction error of the non-linear function being approximated and *that same sample mesh is used for hyper-reduction at all time-steps*.

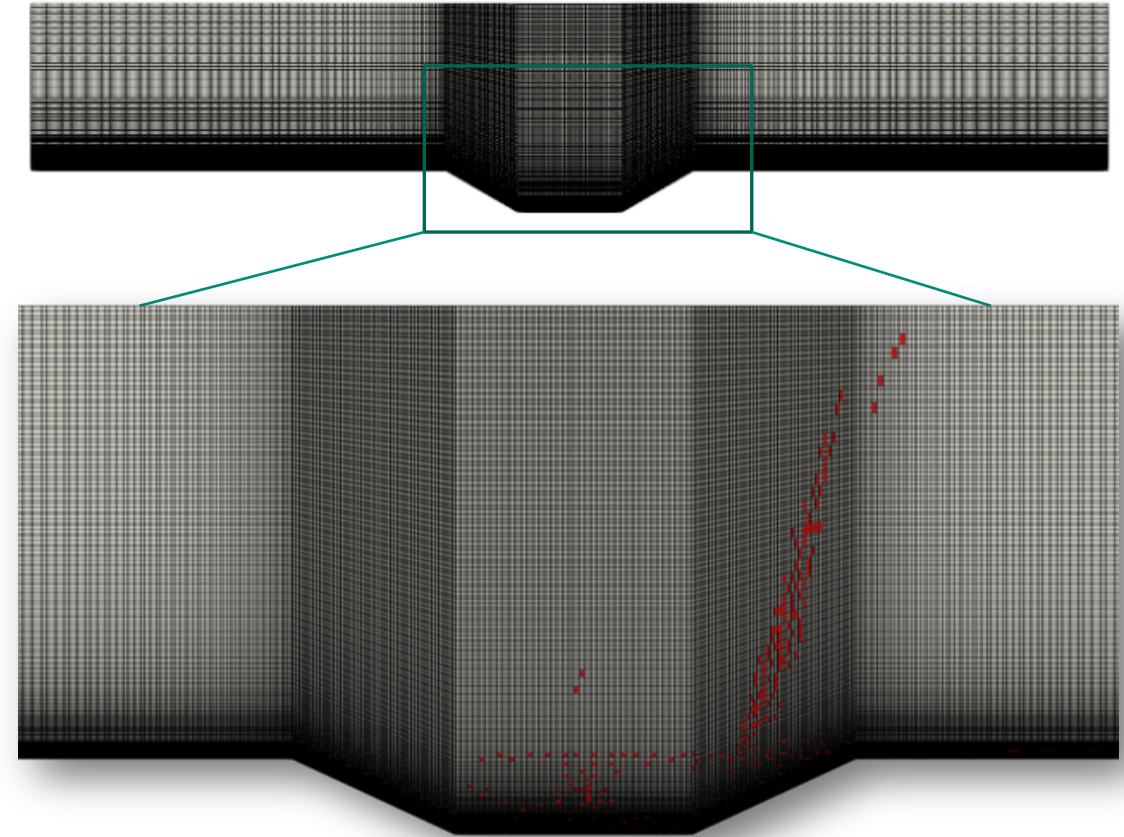


Static sample mesh obtained using q-sampling (Parish et al. 2020)

ISML algorithms have potential for revolutionizing hyper-reduction by calculating an *evolving* sample mesh!



Dynamic sample mesh containing ~4% of the total mesh points, obtained using ISML algorithms



Static sample mesh obtained using q-sampling (Parish et al. 2020)

Publications and Presentations



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