Pressure Gain, Stability, and Operability of Methane/Syngas Based RDEs Under Steady and Transient Conditions

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DOEDE-FE0031773 with Dr. Mark Freeman as Program Monitor

Outline

- **Programmatic overview and introduction to the problem**
- **Experimental activities**
- **Computational activities**

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Overarching objectives

- **Objective 1:**
  Develop and demonstrate a low-loss fully axial injection concept, taking advantage of stratification effects to alter the detonation structure and position the wave favorably within the combustor

- **Objective 2:**
  Obtain stability and operability characteristics of an RDE at fixed and transient operating conditions, and determine performance rules for full-scale operations

- **Objective 3:**
  Develop quantitative metrics for performance gain, as well as quantitative description of the loss mechanisms through a combination of diagnostics development, reduced-order modeling, and detailed simulations

Expected outcomes: RDE physics advancements

- **Outcome 1:**
  A comprehensive study of the stability and operability of high AAR designs under engine-relevant conditions:
  - Air inlet design is critical to limit losses and manage secondary effects;
  - Generally limits operability of devices.

- **Outcome 2:**
  A low-loss inlet design with optimal placement of detonation wave to promote efficiency gain:
  - Needs to be coupled to optimal design of
    - Fuel/air stratification
    - Detonation channel shape
    - Exit nozzle shape

Expected outcomes: RDE methods advancements

- **Outcome 3:**
  Methods for estimating effective pressure gain realized
  - Basis is measurements, reduced-fidelity models, and laser diagnostics.
  - A Bayesian optimization framework to combine experimental data, simulations and reduced-fidelity models to design practical RDEs

- **Outcome 4:**
  A suite of computational tools for modeling full-scale RDEs, including an AI-based acceleration for long duration simulations
  - Based on classification-learning approach, with automatic model reduction from high fidelity simulation
  - Implementation into U-M solvers
  - Transfer of detonation computational models to industry

Expected outcomes: RDE technology advancement

- **Outcome 5:**
  Demonstration of efficiency improvement (gain) using a 12-in methane/syngas mixture RDE
  - Ultimate goal of the program
  - Based on cumulative progress under DOE UTSR program
  - Achieved through balancing and management of loss mechanisms
  - CFD aided optimization of current designs

Objectives and tasks

Pressure Gain, Stability, and Operability of Methane/Syngas Based RDEs Under Steady and Transient Conditions

Objective 1
Low-loss injector based RDEs for methane/syngas operation at elevated pressure/temperature

- **Task 2.1** Effect of stratification/fuel composition on detonation structure
- **Task 2.2** Injector design for minimizing parasitic/commensal combustion
- **Task 2.3** Develop design rules for performance and scalability

Objective 2
Stability and operability characteristics of RDEs at fixed and transient conditions

- **Task 3.1** Operating map of RDEs and transition between different operating conditions
- **Task 3.2** Stability of system to perturbations in boundary and/or operating conditions
- **Task 3.3** Develop design rules for operability and stability for integrated systems

Objective 3
Develop tools for quantitative diagnostics, estimation of performance, and design optimization

- **Task 4.1** Development of validated quantitative tools for estimating pressure gain based on measurements
- **Task 4.2** Imaging-based quantification of RDE losses
- **Task 4.3** Development of AI-based accelerated models for long term computations
- **Task 4.4** Development of CFD-based design tool using Bayesian optimization

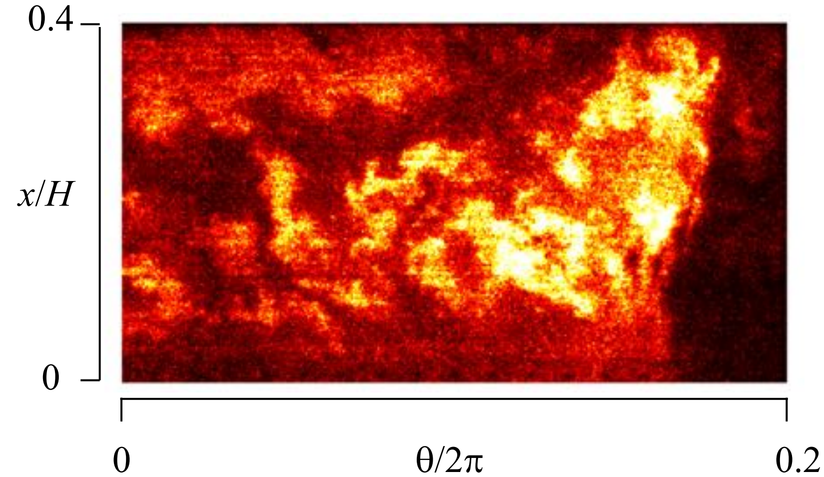
AIR INLET / FUEL INJECTOR DESIGN

FIXED AND TRANSIENT OPERATION & PERFORMANCE

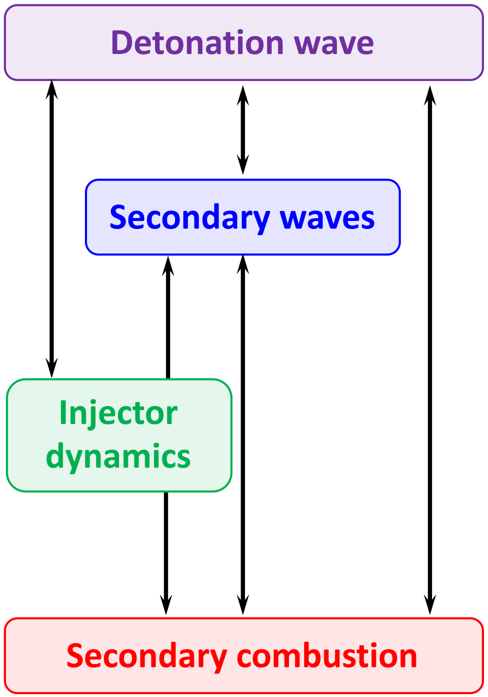
METHODS DEVELOPMENT

ADVANCING PHYSICAL UNDERSTANDING SOURCES OF GAIN AND LOSS
&
INVESTIGATING REALIAZABLE GAIN IN FIXED AND TRANSIENT CONDITIONS

Physics of RDEs and current challenges



- **Prior work has identified non-ideal behaviors that alter the operation of RDEs**
  - Secondary combustion is a dominant phenomena, controlling the structure, dynamics and properties of the detonation;
    - Need and can be managed.
  - Secondary waves exist, and can affect the propagation of the primary detonation wave
    - Non-linear coupling with deflagration and detonation
    - Need and can be managed
  - Non-uniform mixing may not be a limiting factor
    - On the contrary, stratification can serve to stabilize wave
  - Response of air inlet / fuel injector is key, but can be managed by tuning relative responses



- **Based on what learnt so far:**
  - Develop new inlet / injector configurations that provide strong detonation, minimizes deflagration and secondary waves;
    - End goal: raise the understanding of the device and TRL
  - **Focus is on understanding the impact of losses on achieving gain**

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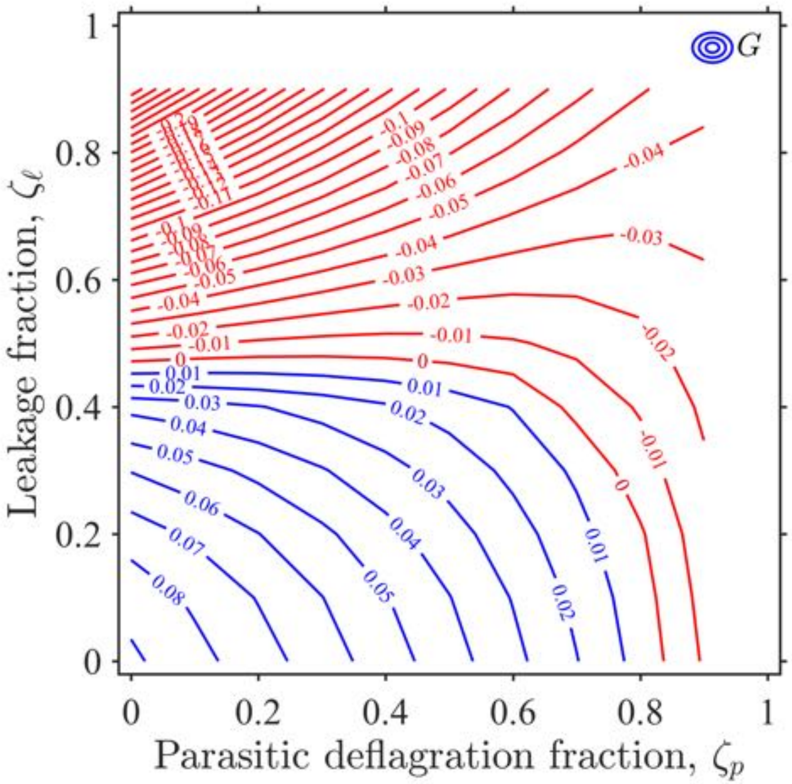
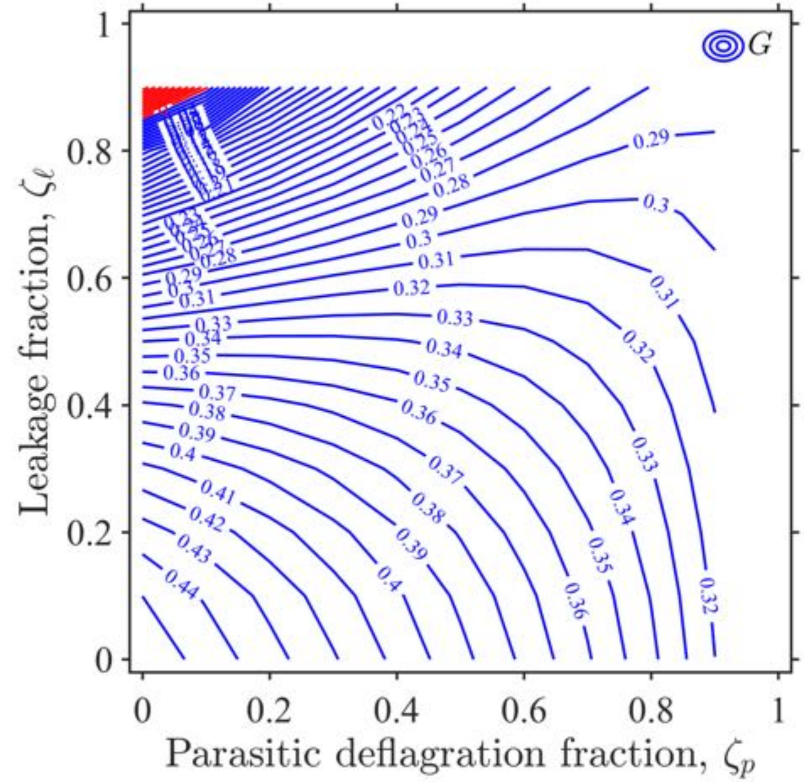
o Gain, where art thou?

Phenomenological model to guide design selection

Application of model to understanding impact of
various losses and design conditions



Geometry 1
Operating condition A
Assumes parameter set B



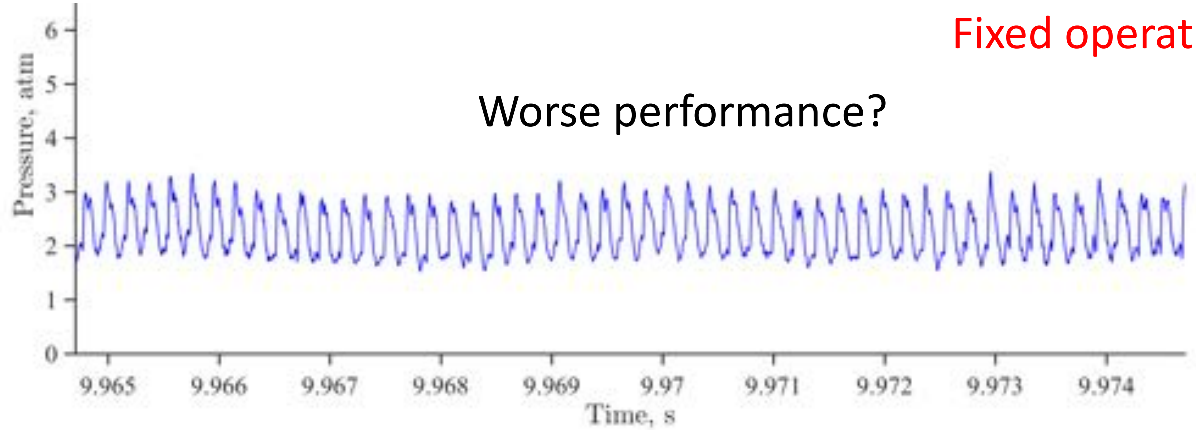
Geometry 2
Operating condition A
Assumes parameter set B

Such a model can allow us to evaluate designs

Fixed operating condition

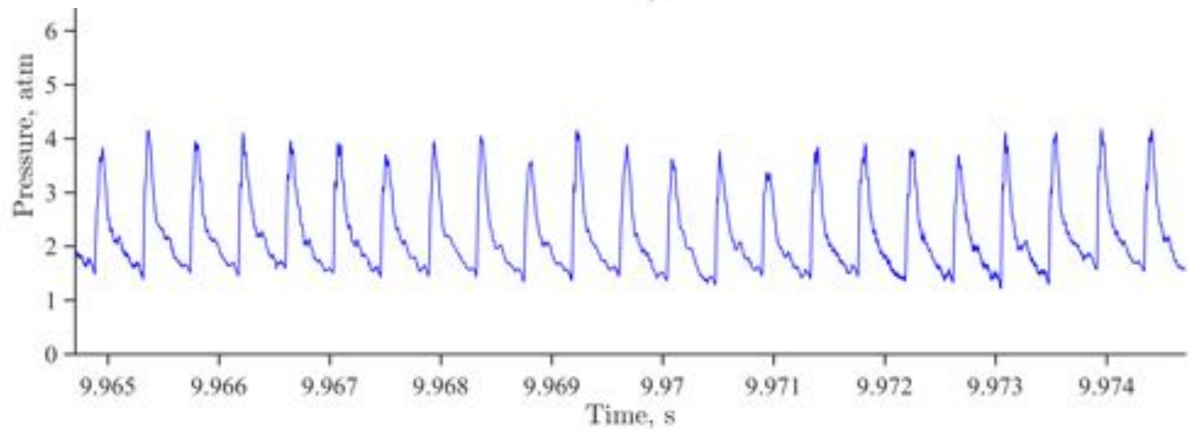
Worse performance?

Geometry 1



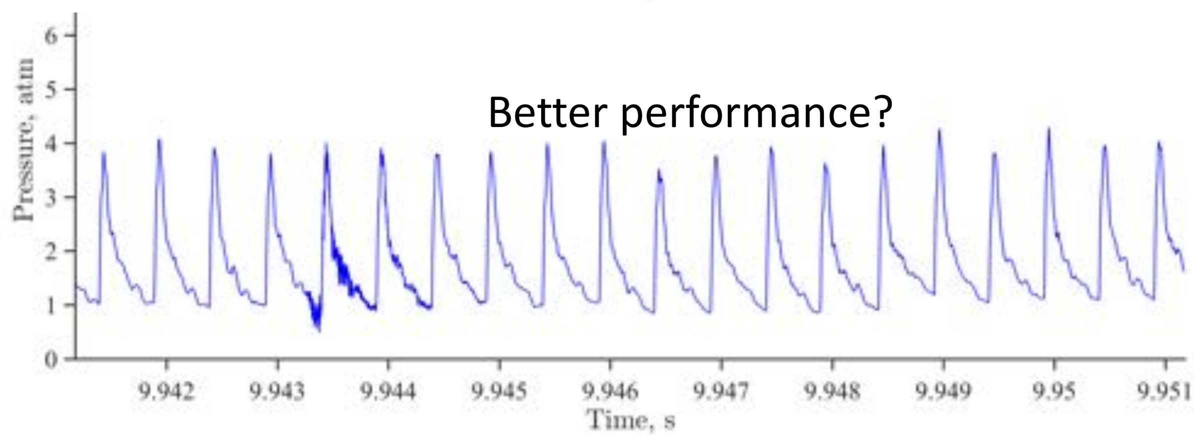
Faster wave

Geometry 2



Better performance?

Geometry 3



Slower wave

Outline

- Programmatic overview
- Experimental activities
- Computational activities

Future of Modeling for Gas Turbines

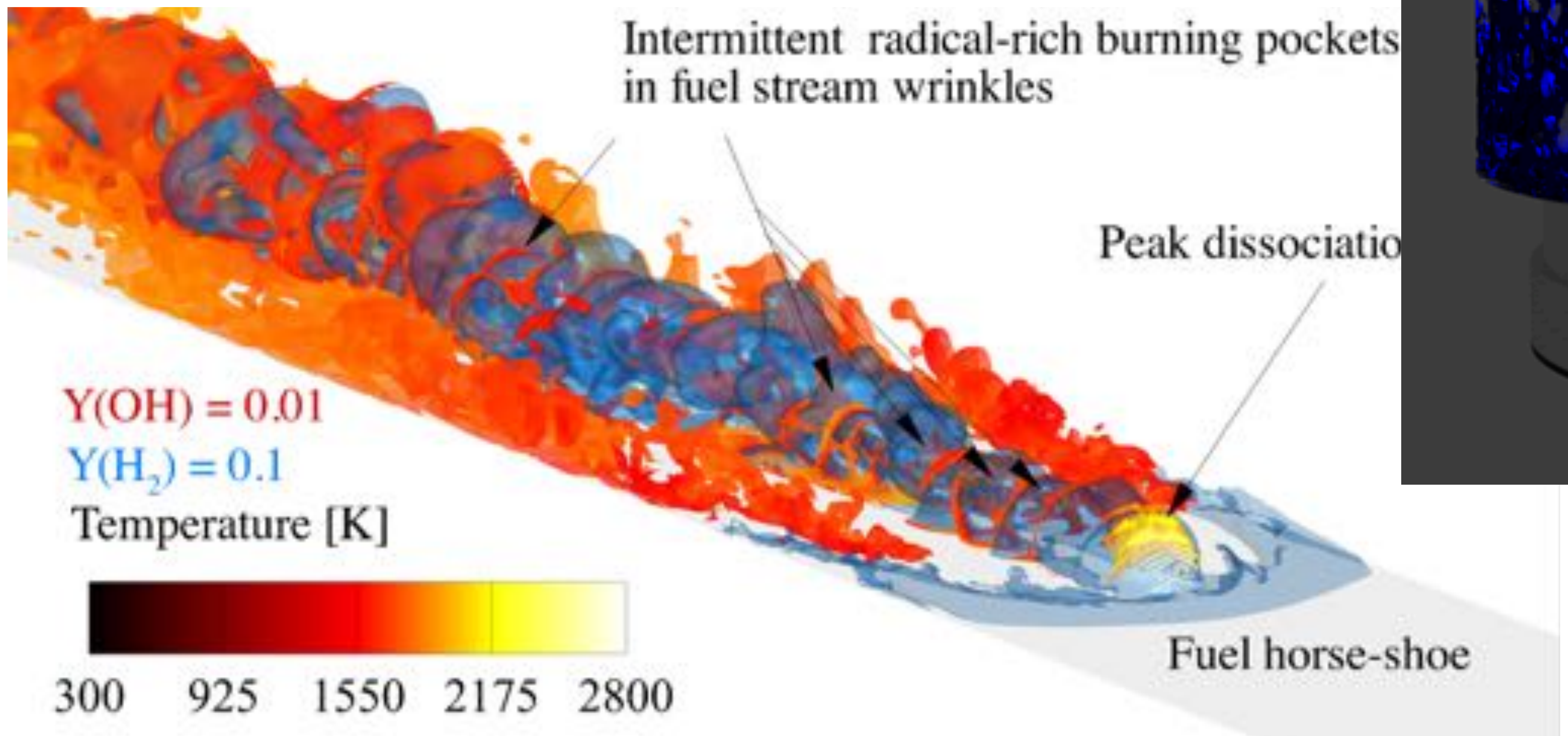
Venkat Raman

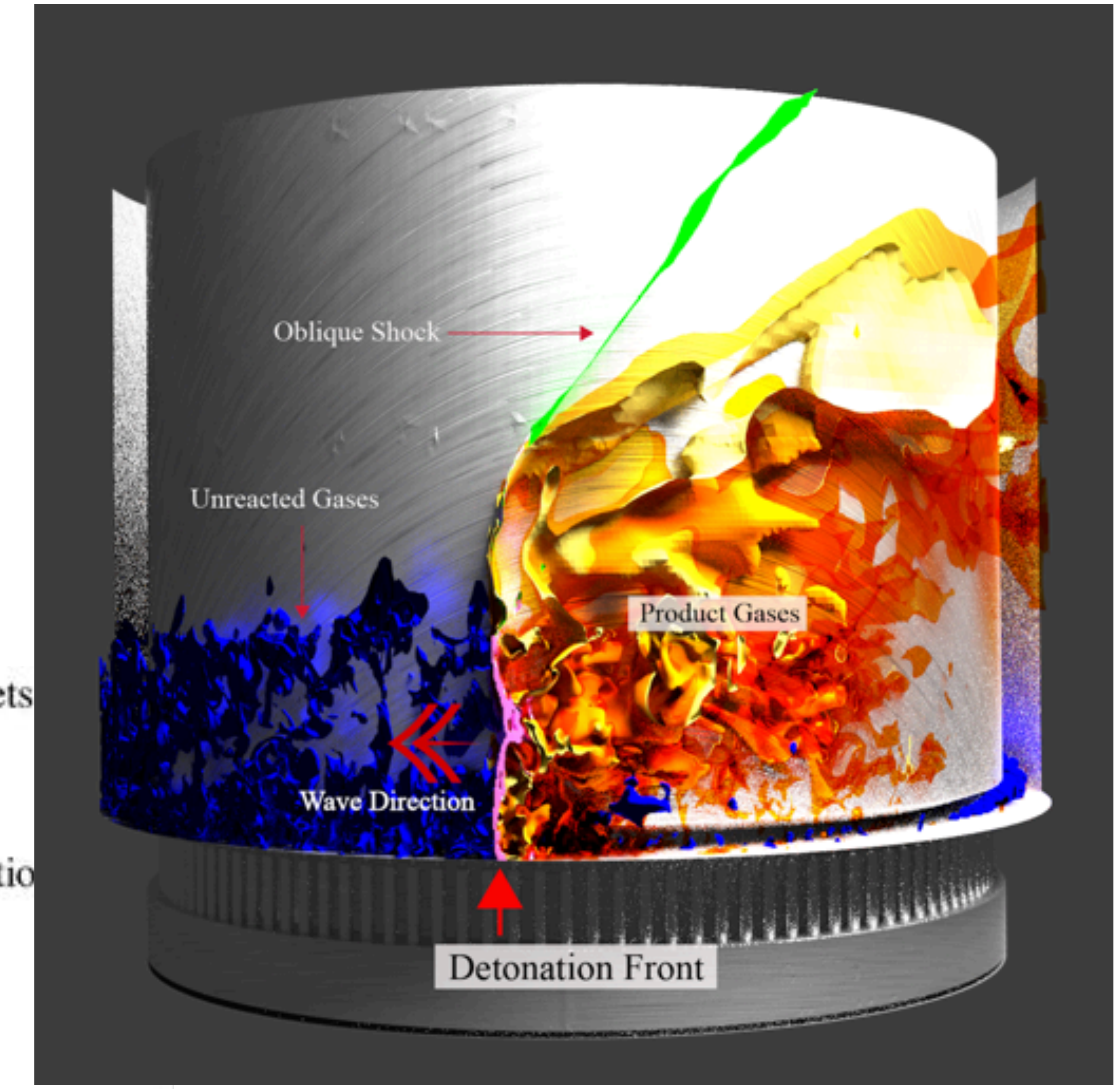
University of Michigan, Ann Arbor
Department of Aerospace Engineering

APCL

Progress in Modeling

APCL





NETL-funded Research

Is This All There is To Modeling?

- **Modeling has focused on ever-increasing complexity to improve accuracy**
  - ➡ Faster computers mean more complicated models
  - ➡ Does not necessarily decrease total compute cost
  - ➡ **May not be all that accurate either!**
- **Can we re-imagine modeling?**
  - ➡ **What is the purpose of computational models?**
  - ➡ **Do we need models only for design?**
- **How can models overcome time-to-solution limitation?**

Purpose of Models

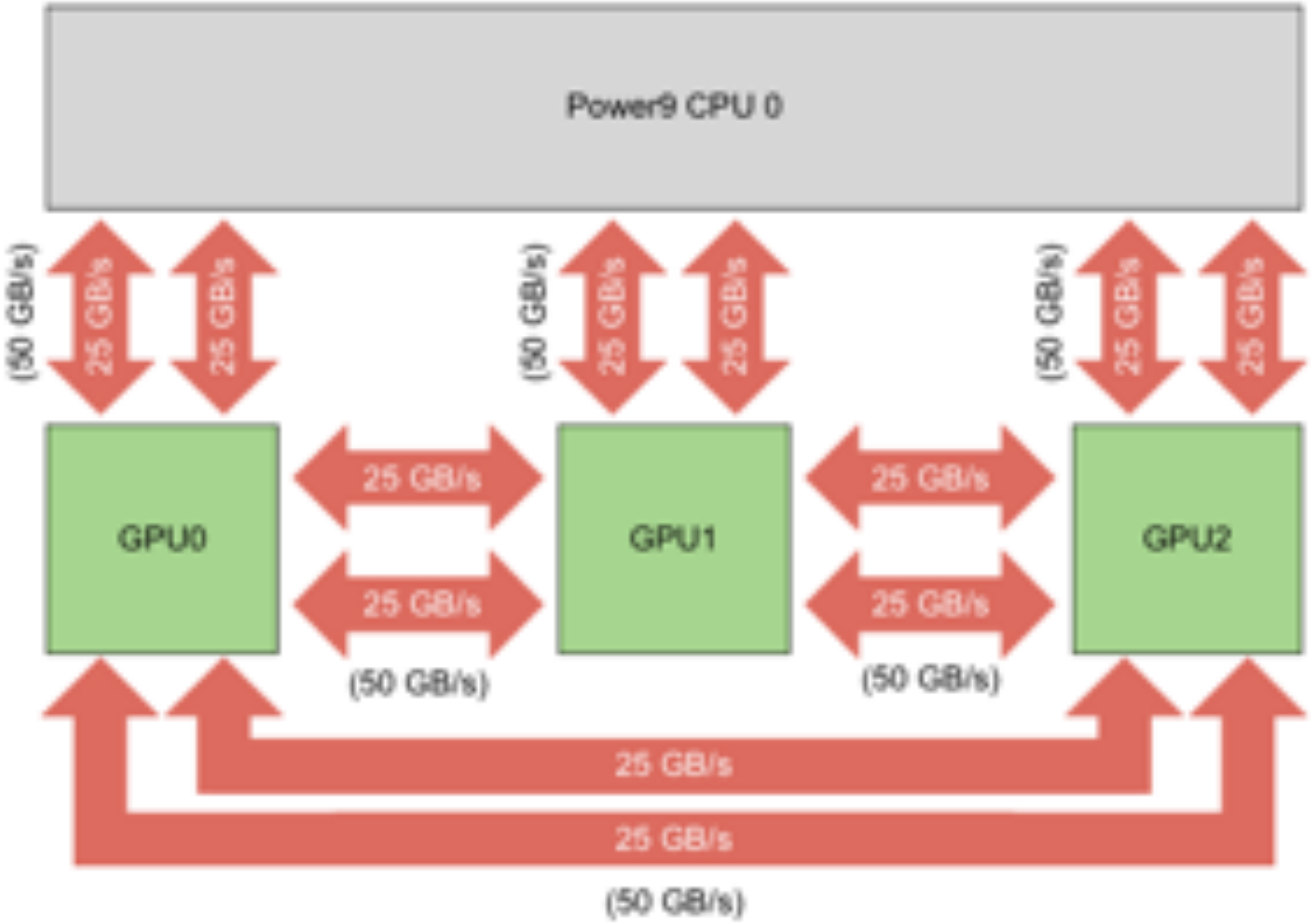
- **Acceleration of modeling for gas turbine applications**
- **Models for real-time prediction**
- **Models for augmenting experiments**

Pre-exascale Machine - SUMMIT

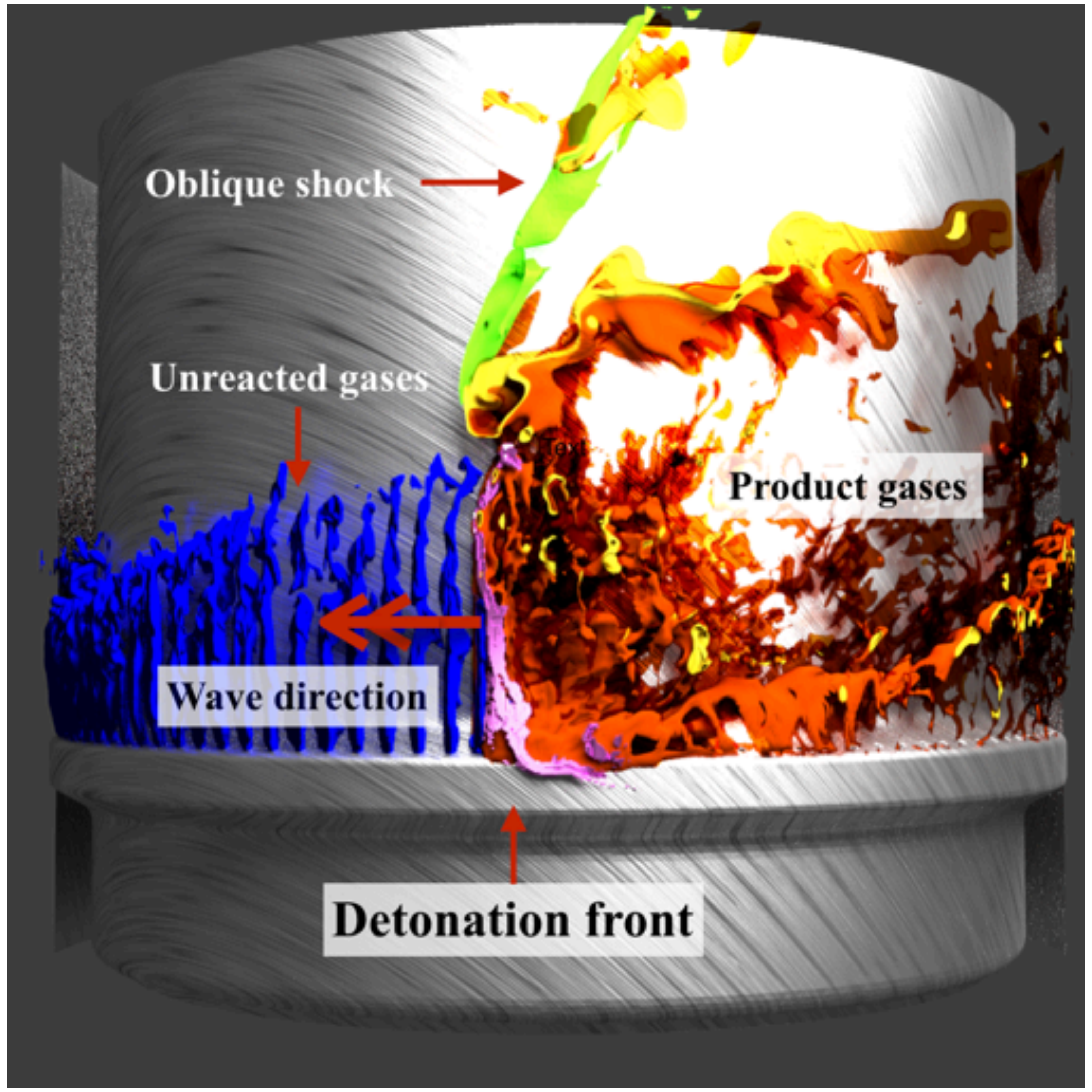
GPU-Centric Design

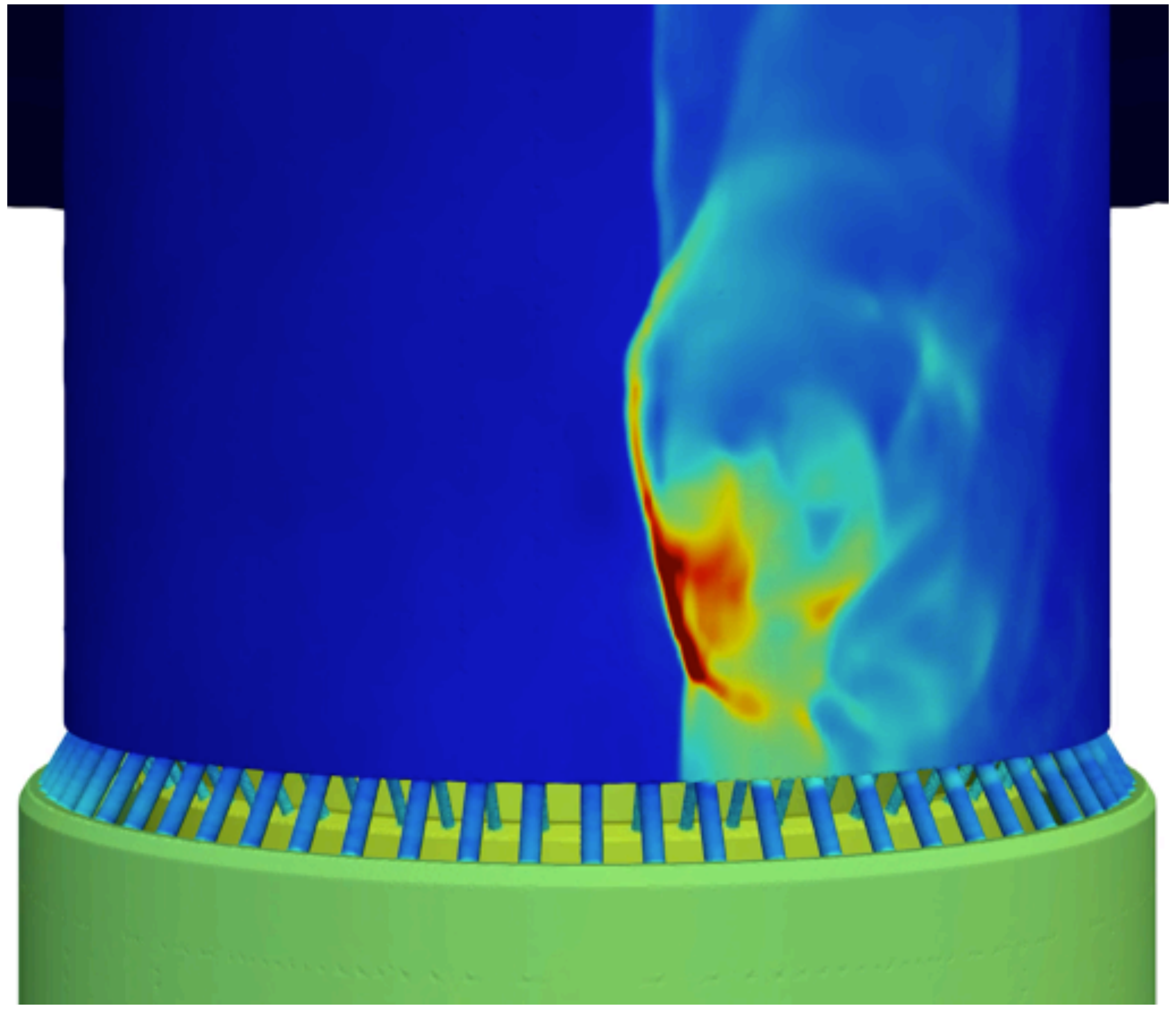
90% of compute power on GPUs

200 Pflops



What can SUMMIT do?



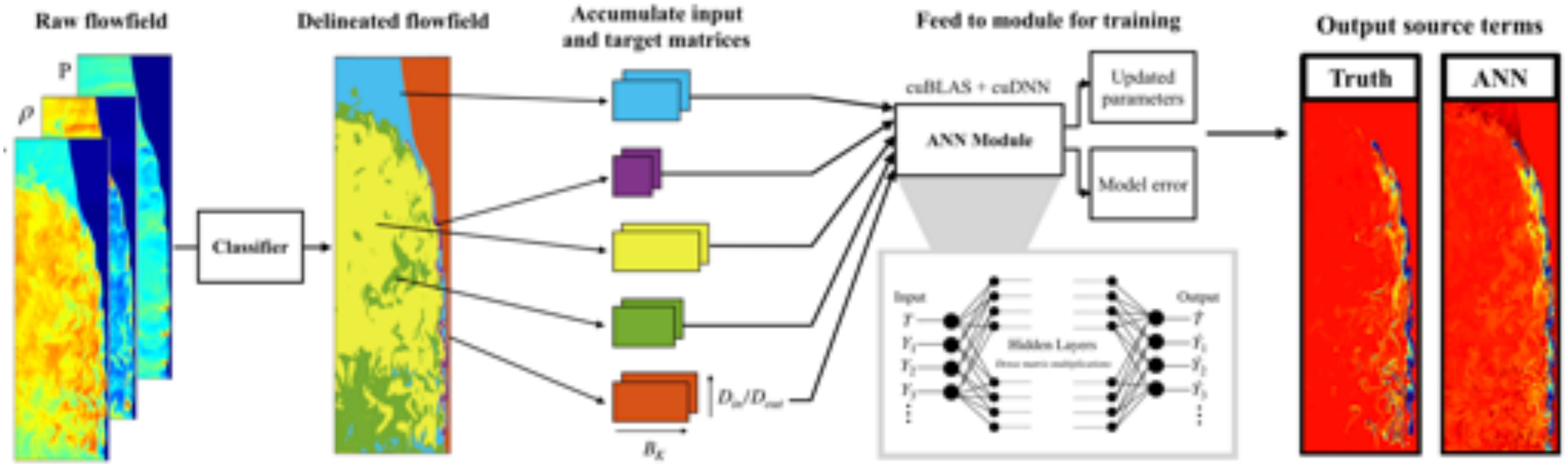


4000 Cores on NASA → **GPU Conversion** → 200 GPUs on Summit → **Code Optimization** → 50 GPUs on Summit

SUMMIT has 27,000 GPUS!

AI-based Acceleration

- Use machine learning to minimize cost of chemistry computations



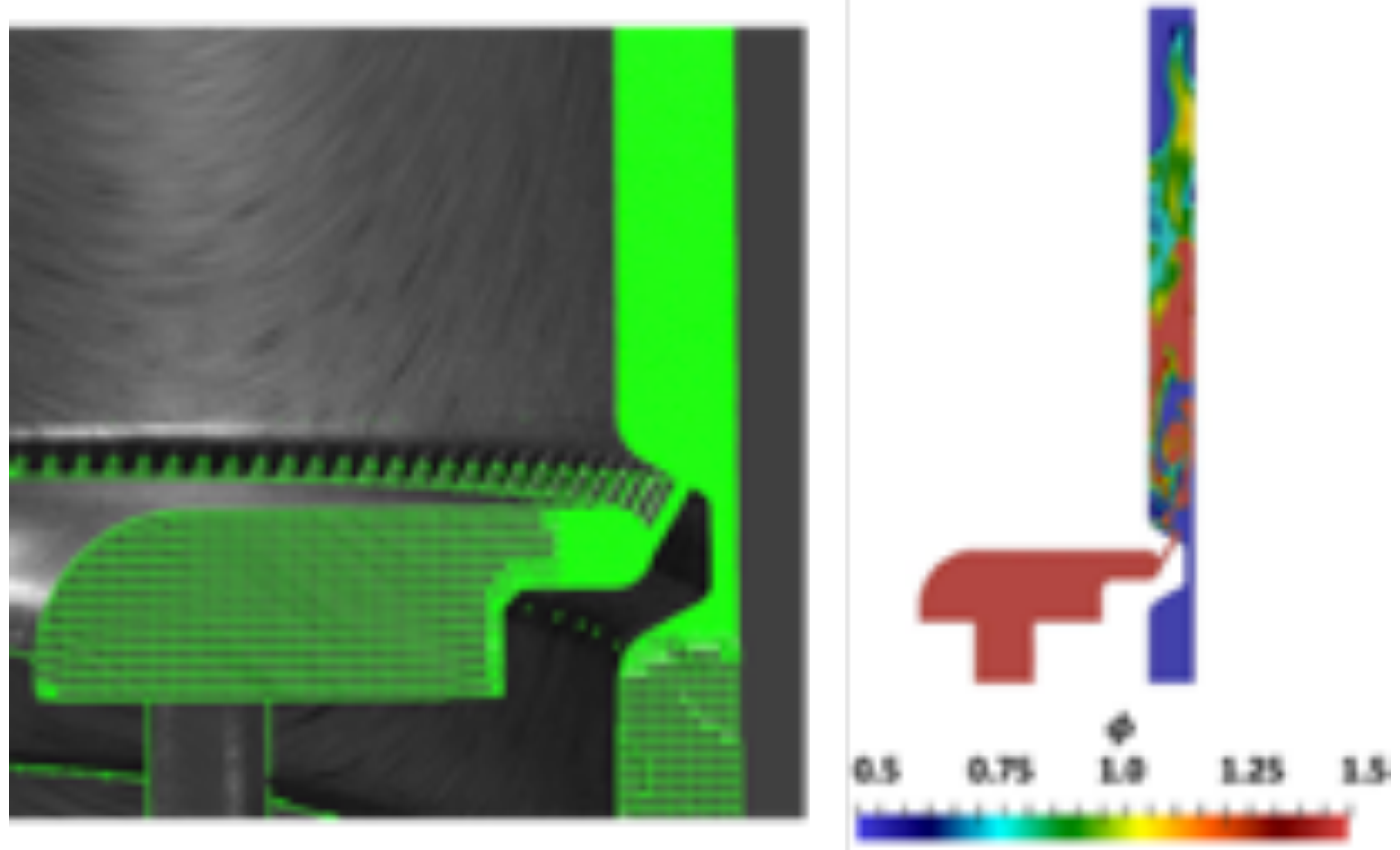
100-1000X Speedup

AI For Improving Detonation-Driven Gas Turbine Technology

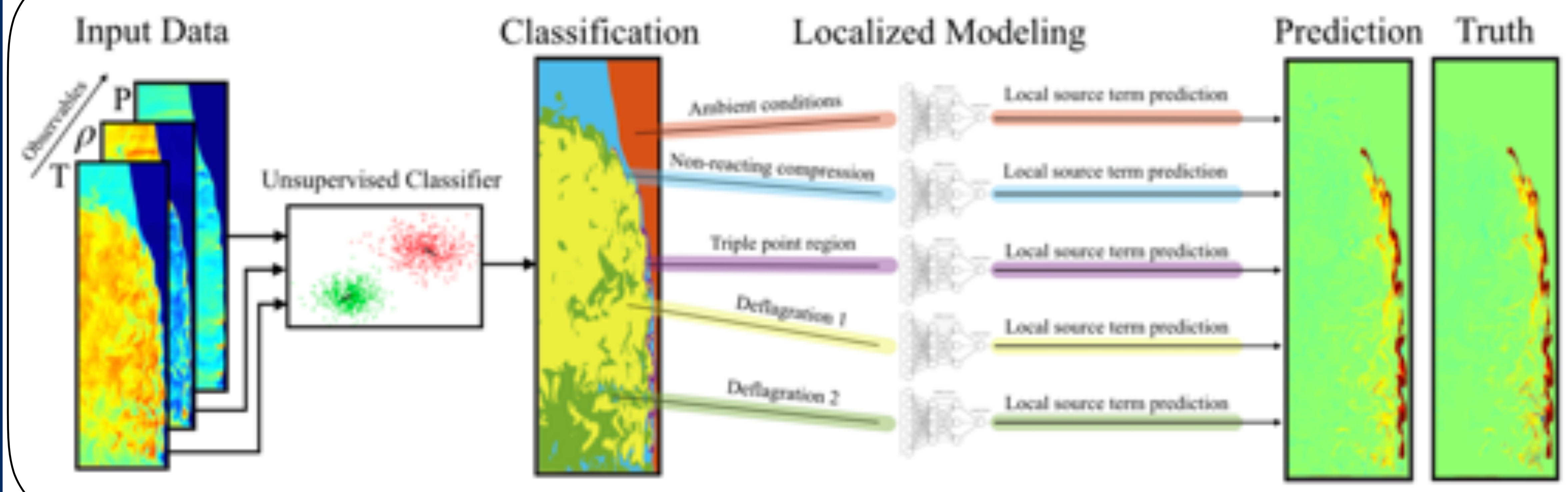
DOE Summit — 200 PetaFLOP Machine

UM-GE-NETL Collaboration

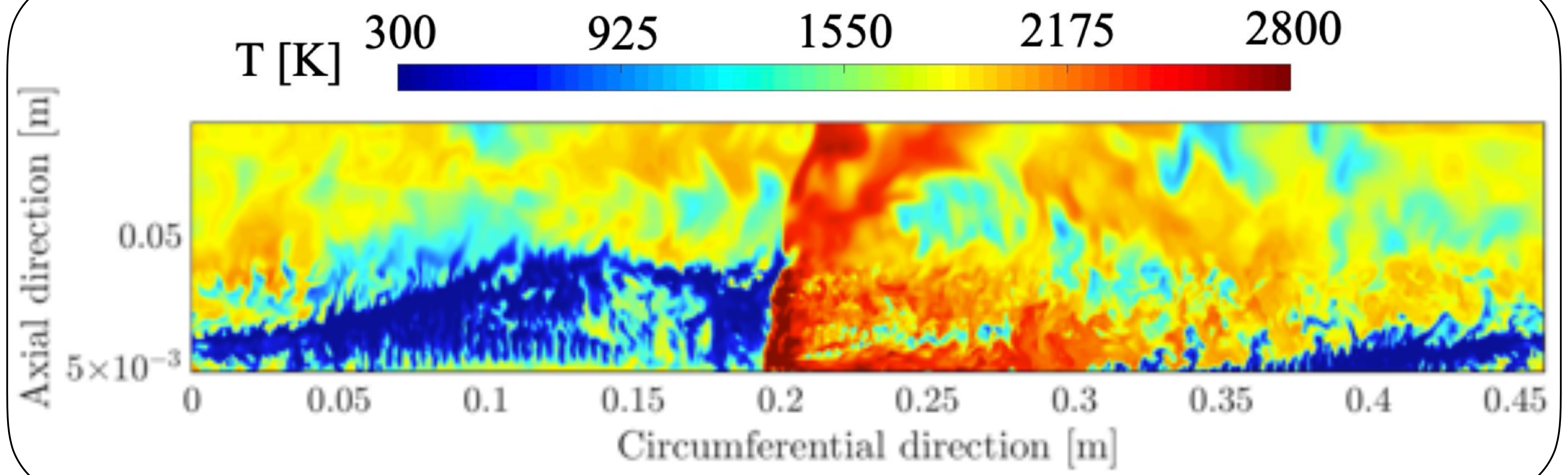
UTSR Funded Detonation Engine



Machine Learning Applied to Combustion Modeling (1000X Speed up Potential)



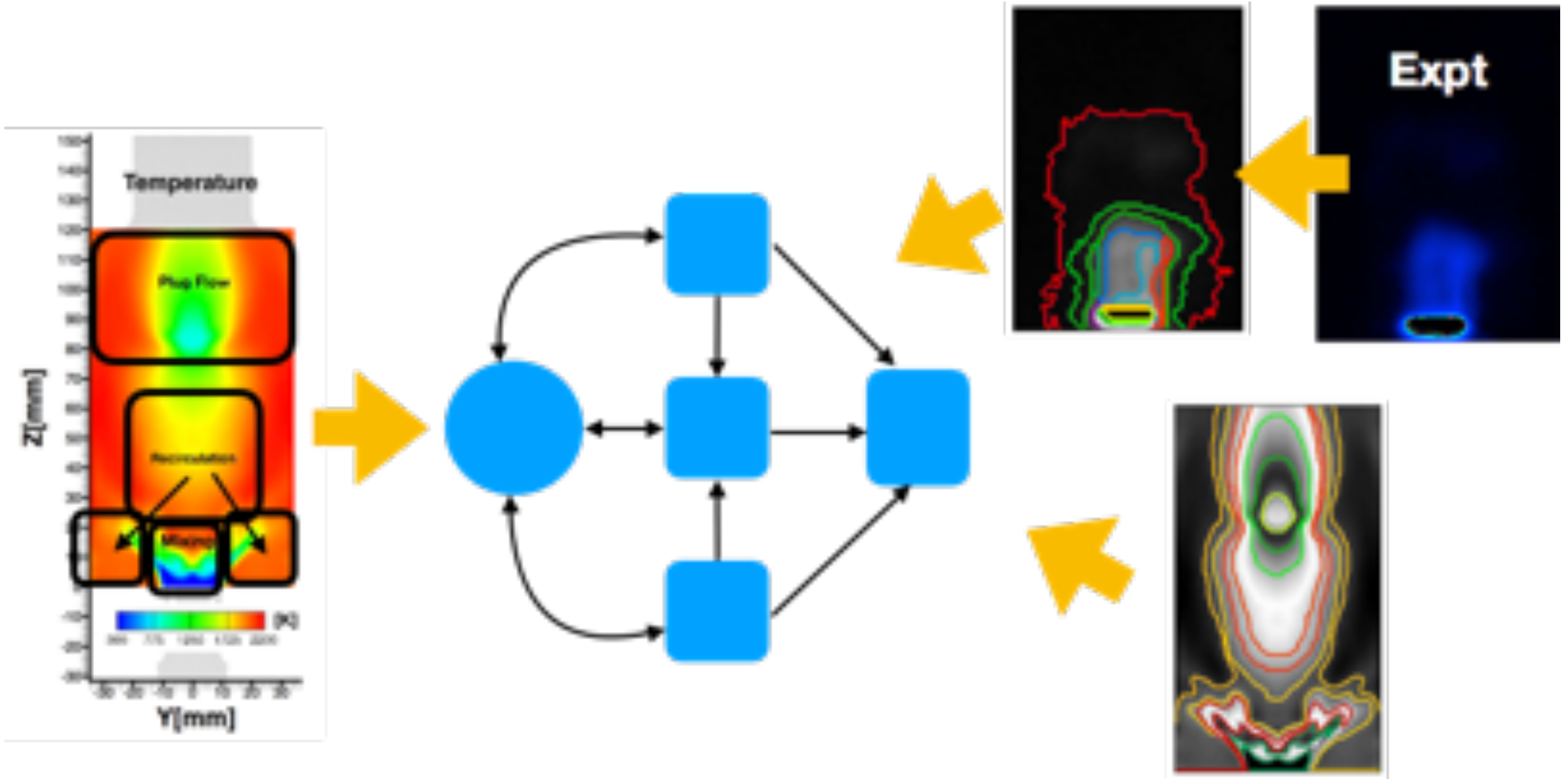
- First Full Scale Simulation of RDEs with Axial Injection
- Capable of simulating 100-1000 cycles in 1 day

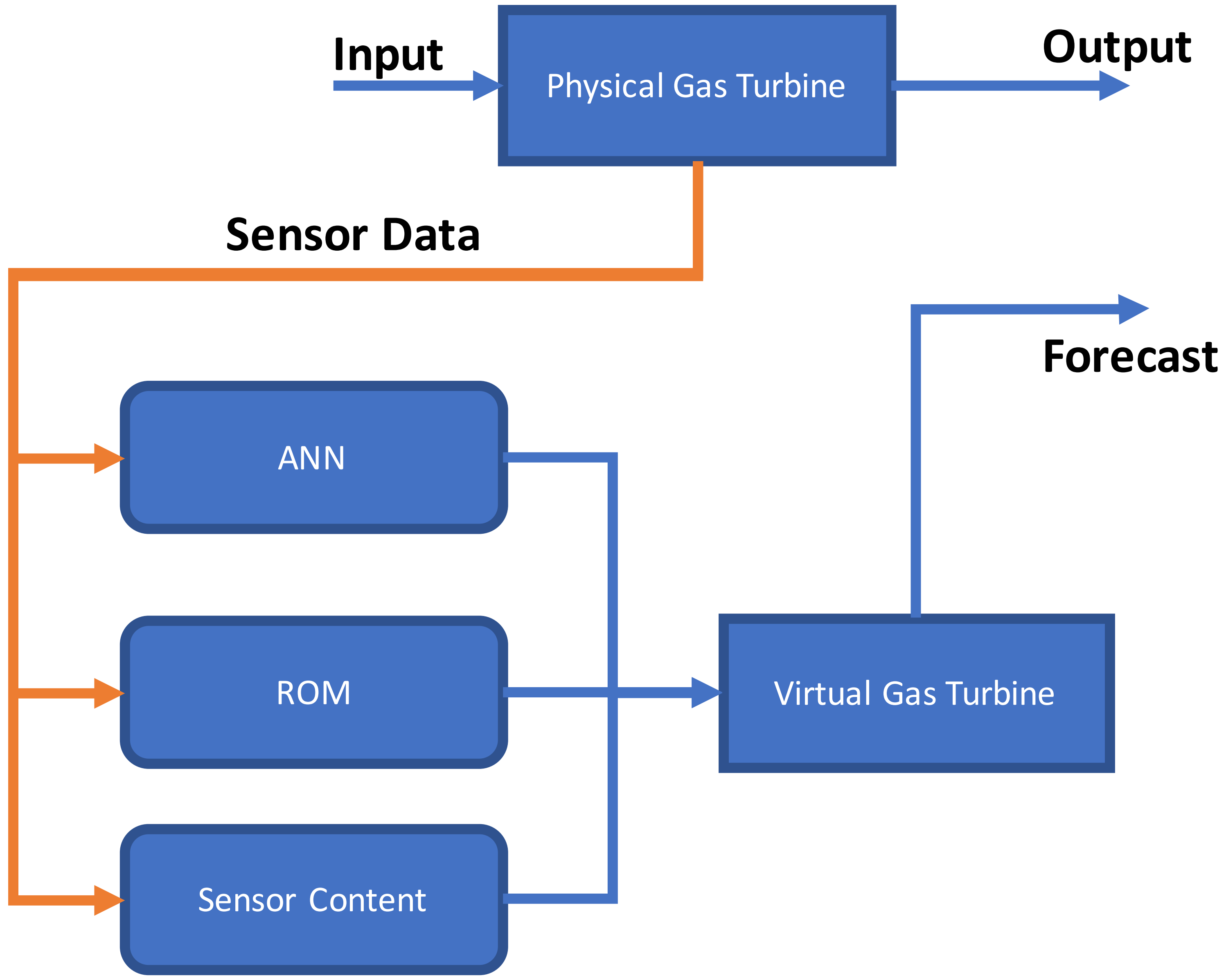


Virtual machine

➡ Consists of layers of descriptors

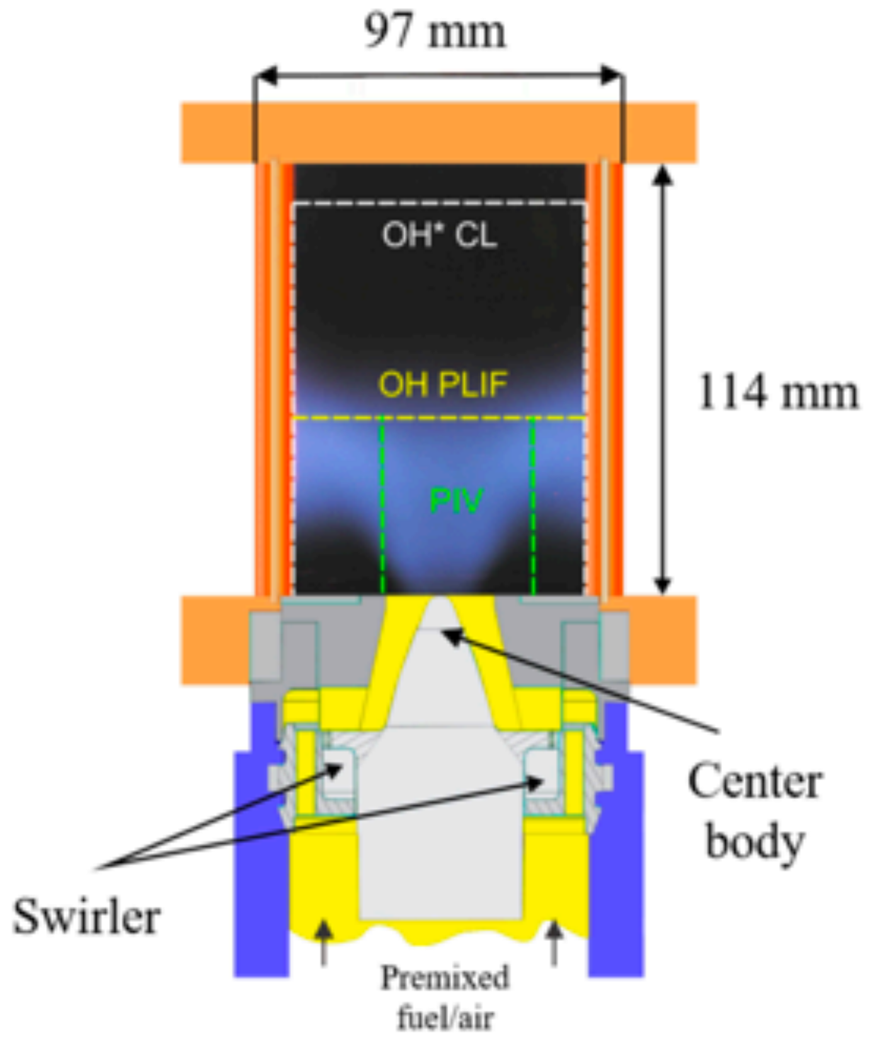
- Descriptor enables particular input-output relation

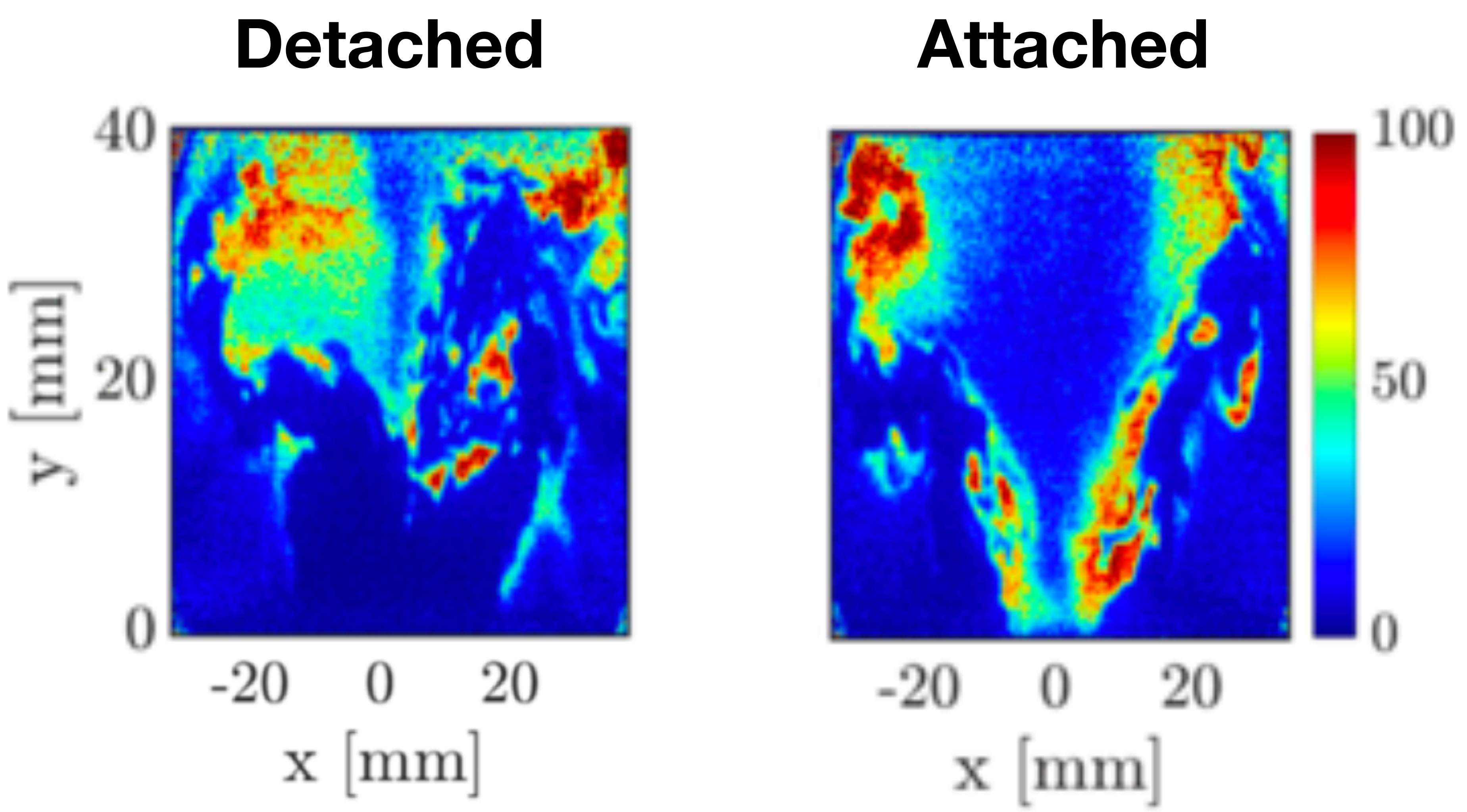




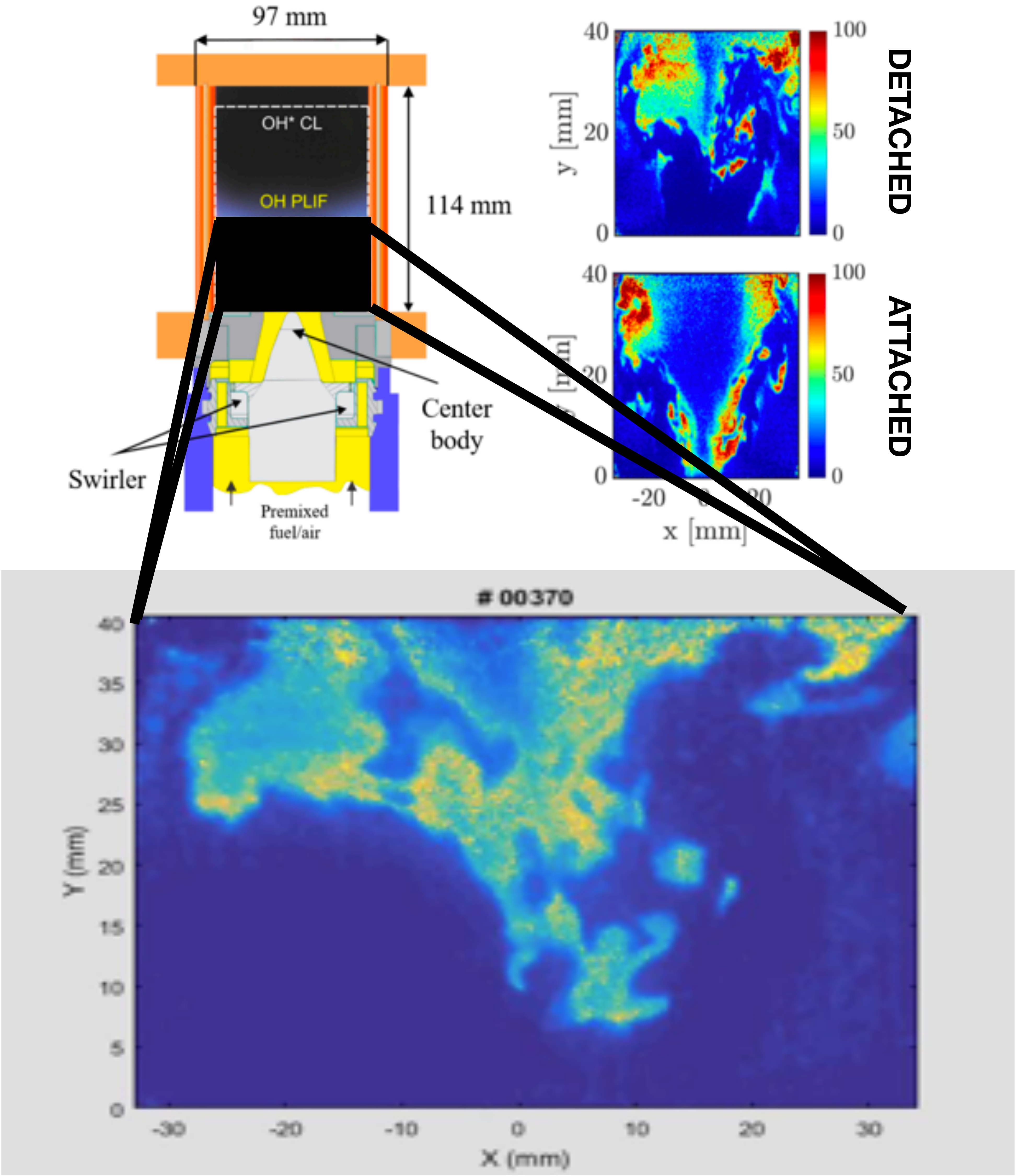
Application: Flame Transition

- **Swirl-stabilized premixed combustor**
- **Experimental dataset:**
  - ➡ Fuel: 60% CH_4 and 40% CO_2.
  - ➡ Equivalence ratio: 0.60
  - ➡ Preheat temperature: 400 K.
  - ➡ Air flow rate: 400 SLPM.
- **Time-resolved 2D measurements**
  - ➡ OH-PLIF, PIV
  - ➡ Total time: 1.5 sec at 10 kHz
- **<u>Objective</u>: Predict flame transition using data**





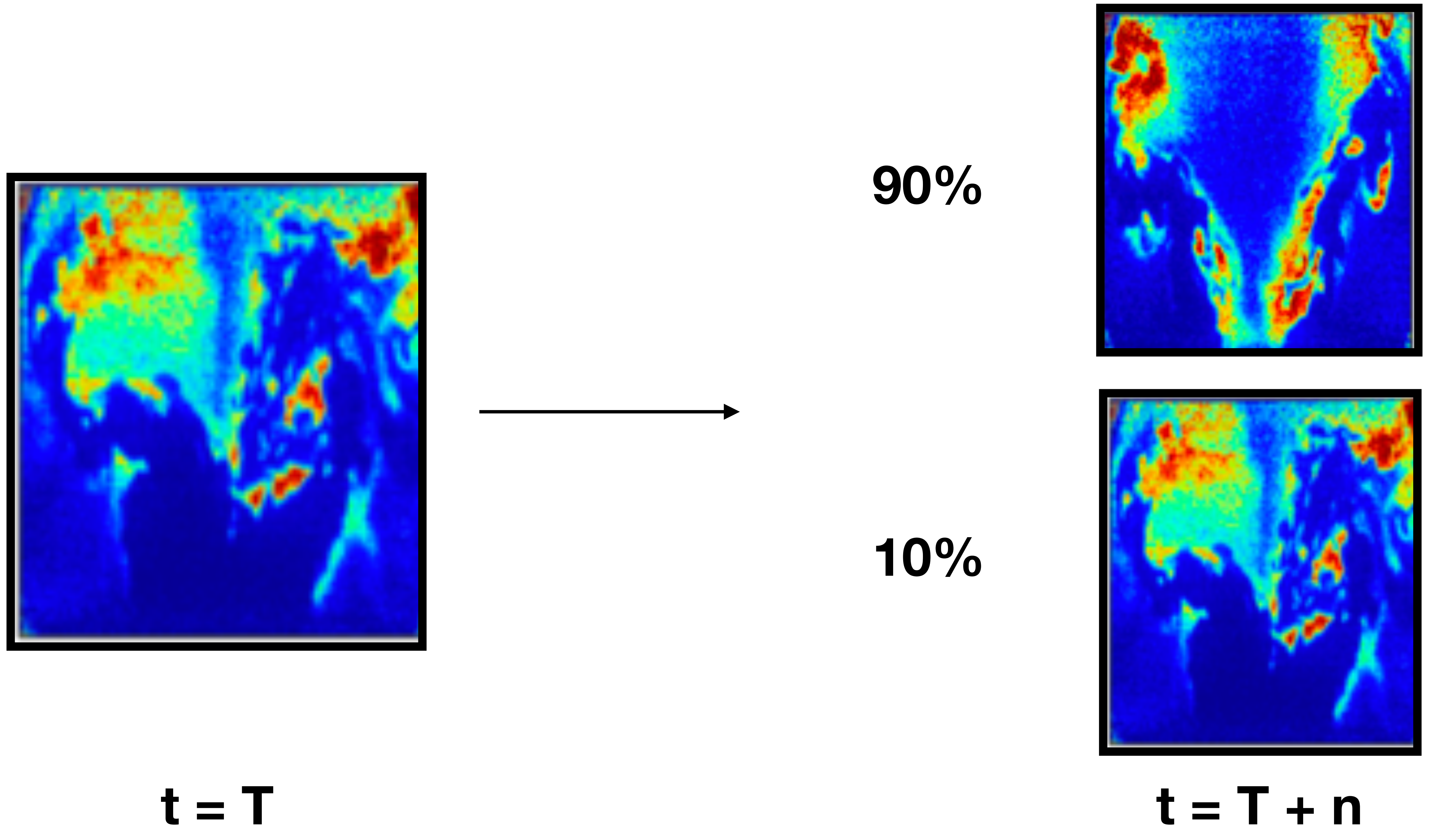
Application: Flame Transition



Dataset courtesy of Q. An (U. Toronto), A. Steinberg (Ga. Tech.)

Probabilistic Forecasting

- **Probabilistic forecasting**

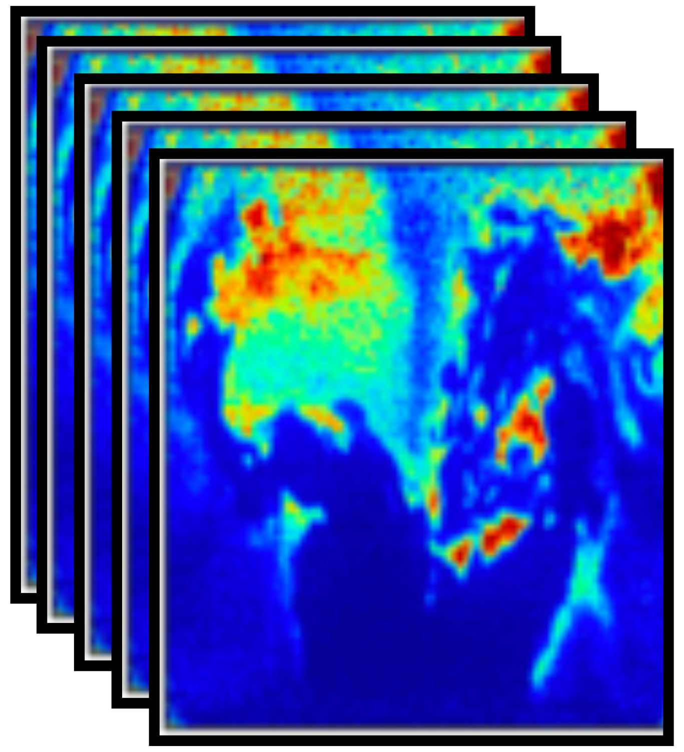


- **Approximate transport of probability density function (PDF) of the observables**

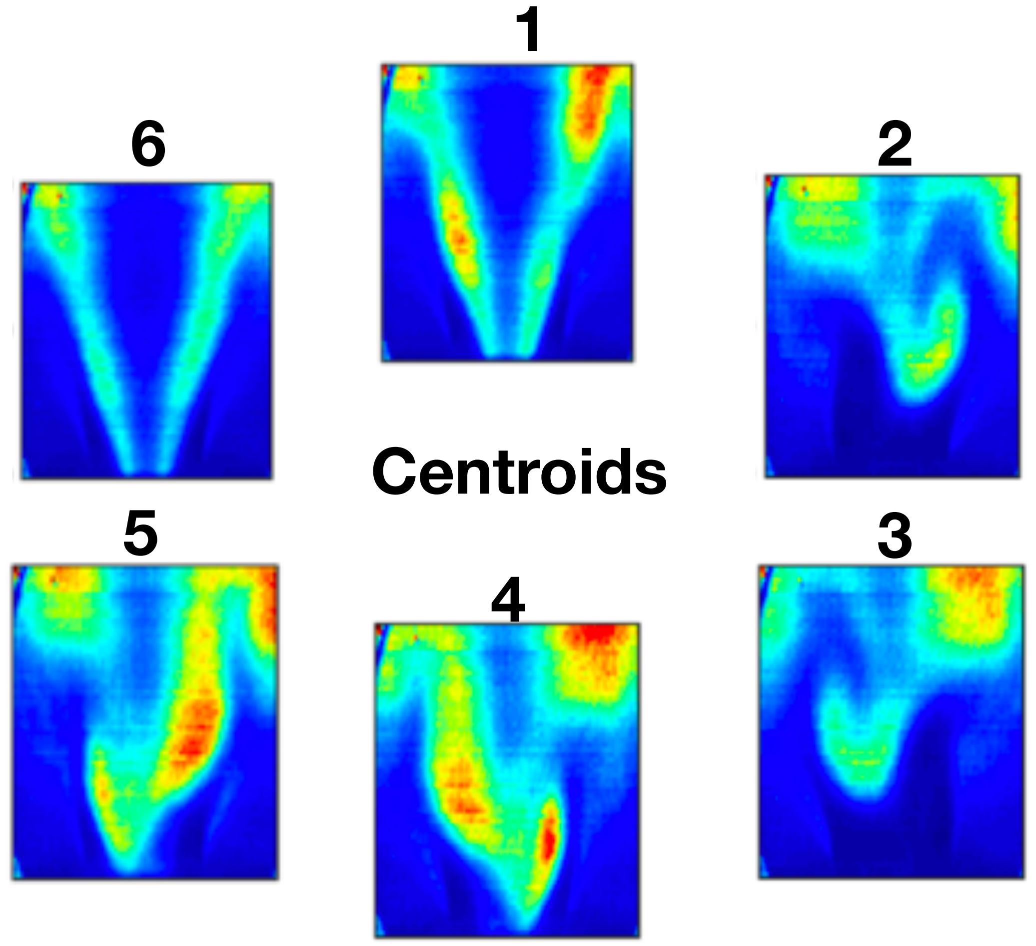
➡ Keep the forecasting affordable for real-time applications

Clustered Reduced Order Model

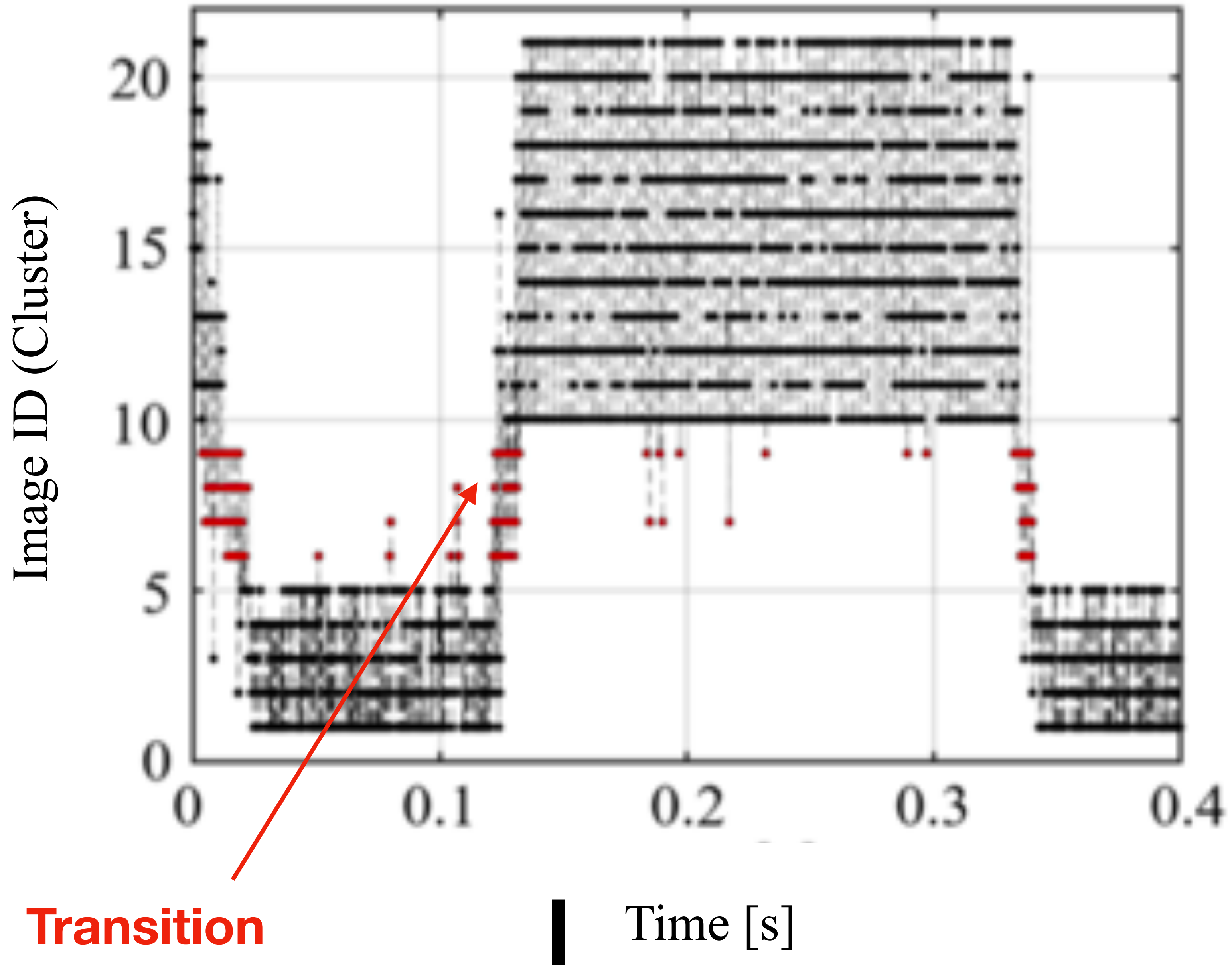
Snapshots



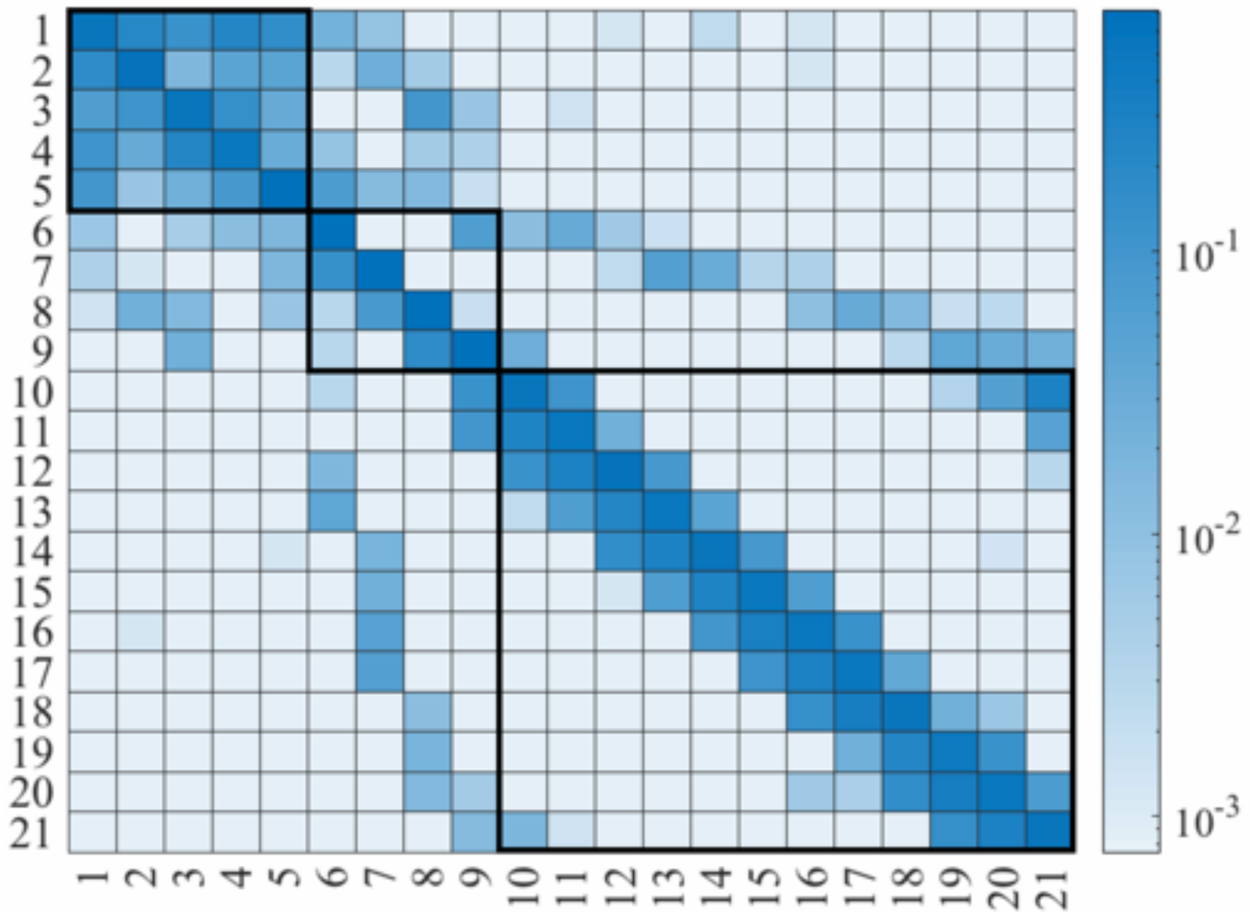
Classification →



Time Series →

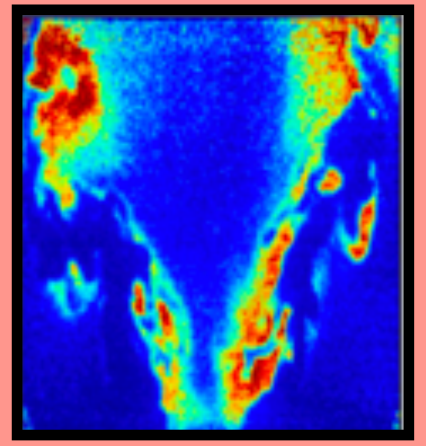


Transition Matrix A



Prediction Step

Snapshot at t = 0

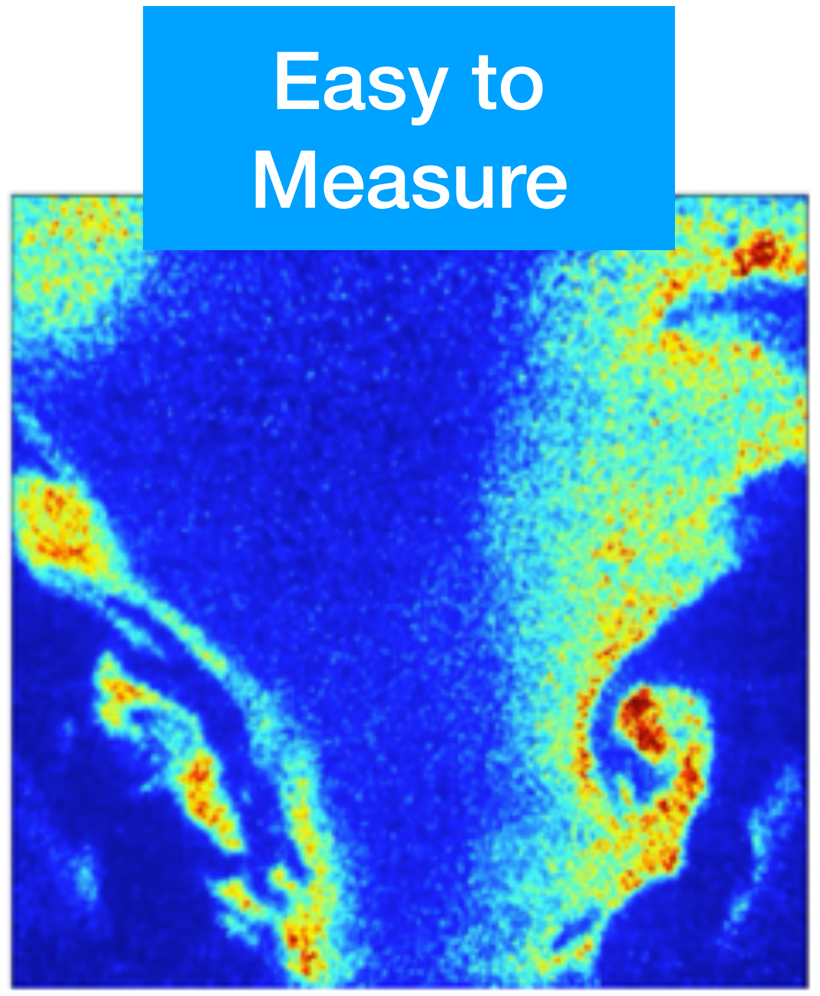


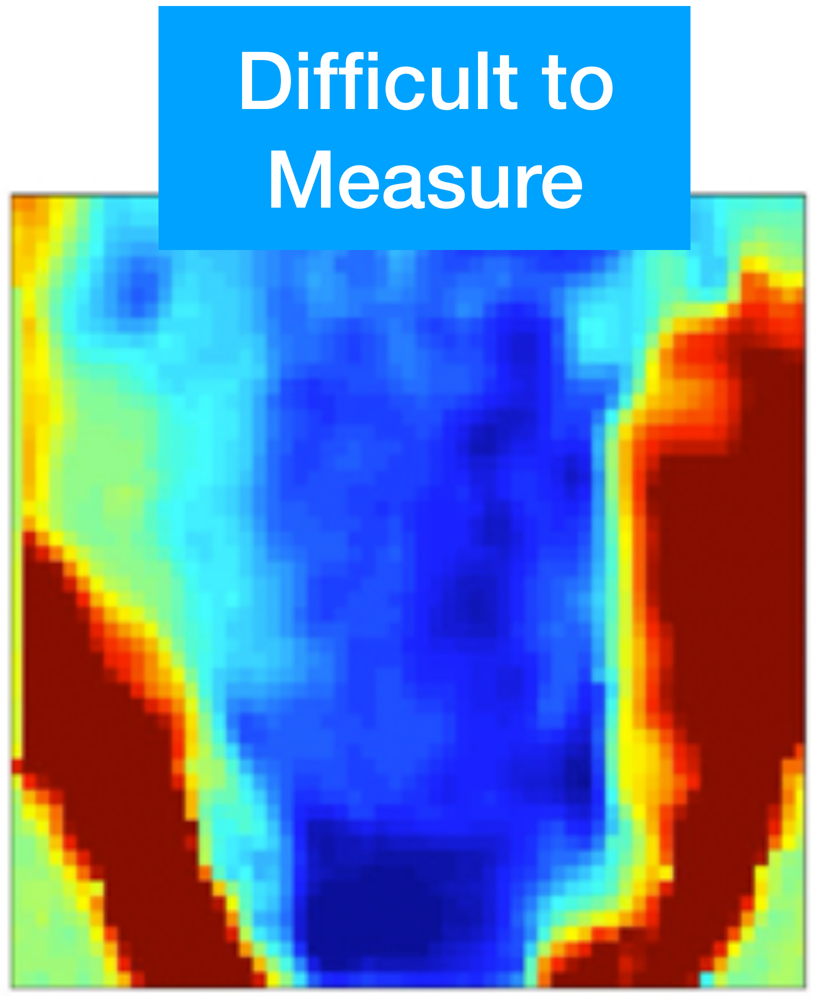
→ In first cluster: $r^0 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ → Transition matrix → $r^f = \begin{bmatrix} 0.2 \\ 0.1 \\ 0.1 \\ 0.4 \\ 0.1 \\ 0.1 \end{bmatrix}$

Assign to cluster

Future PDF

Generating Data





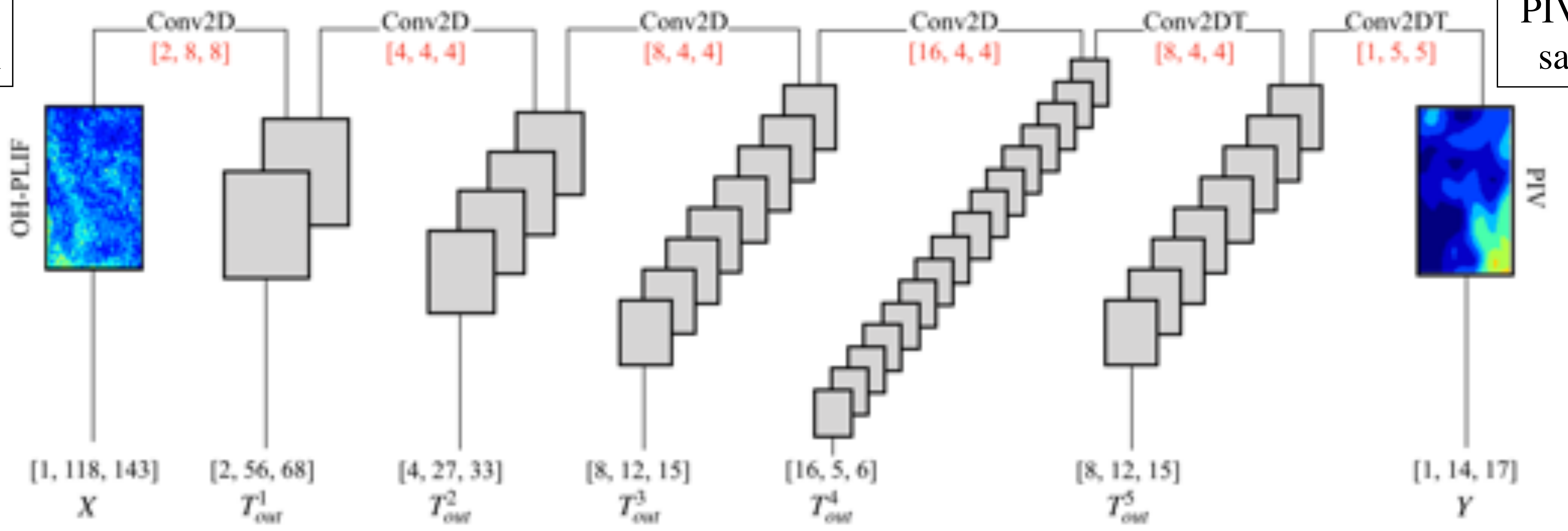
- **Can data be constructed by training?**

Network architecture

Fully convolutional network

Input is PLIF field in one box

Output is PIV field in same box

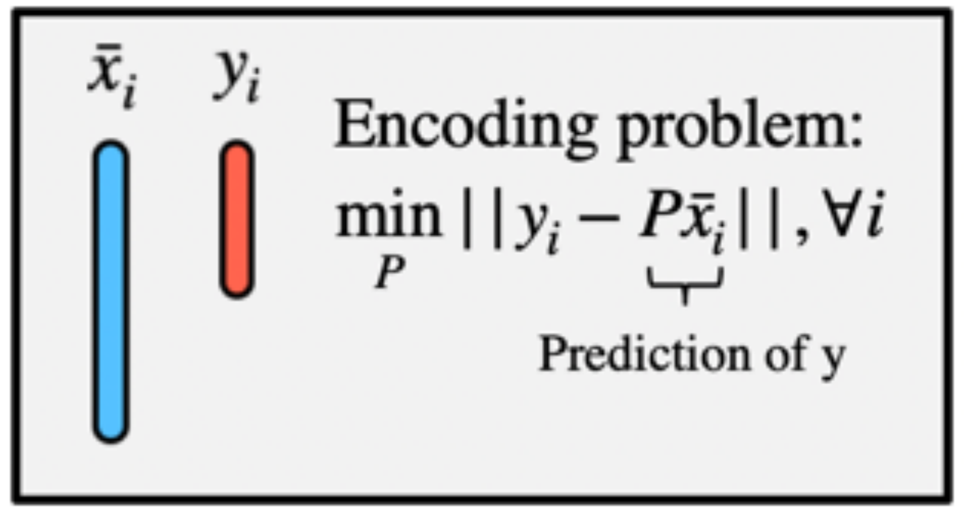


Downsampling phase

Reduces dimensionality of PLIF image

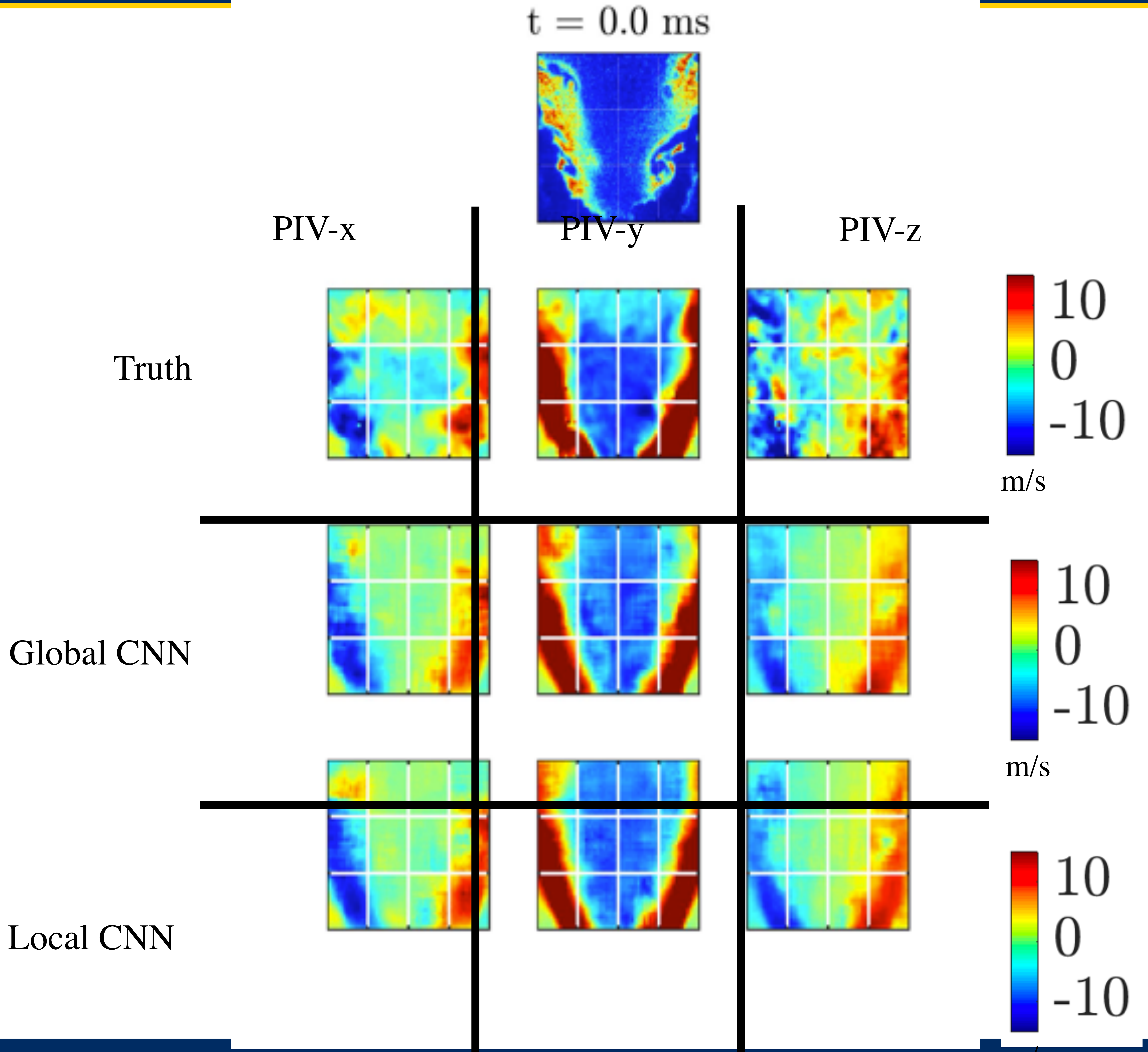
Upsampling phase

Decodes reduced PLIF image into PIV image



Recall encoding problem: $P\bar{x}_i = CNN(\bar{x}_i; \phi) \approx y_i$

Velocity field in time



Comparison with OH-PLIF Data

End Goal

- **We want to build J.A.R.V.I.S**

Planned Activities

- **AI-based simulation of RDEs**
  - ➡ 6 hour turnaround time for 100 cycles
  - ➡ Ability to execute on in-house clusters
- **Design using multi-fidelity tools**
  - ➡ Reduced-order models using high-fidelity simulations
  - ➡ Design cycle tools for optimization
- **Data assimilation from experiments**
  - ➡ Can we use canonical experiments to generate full scale experimental data?
  - ➡ Where does this transferability come from/break?

Questions?