Hypersonic Task-based Research solver

A finite-difference tool for compressible reacting flow simulations

Legion Project Virtual Retreat

June 14, 2021

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Design objectives

- Creating an **open-source** tool for studying hypersonic turbulence at high enthalpies
- Begin able to consider multicomponent reacting gas mixture
- Perform direct numerical simulations with **minimal numerical dissipation**
- Achieve high scalability and efficiency to tackle problems with billions of degrees of freedom
- Being portable on CPU and GPU based HPC facilities

The Hypersonic Task-based Research solver

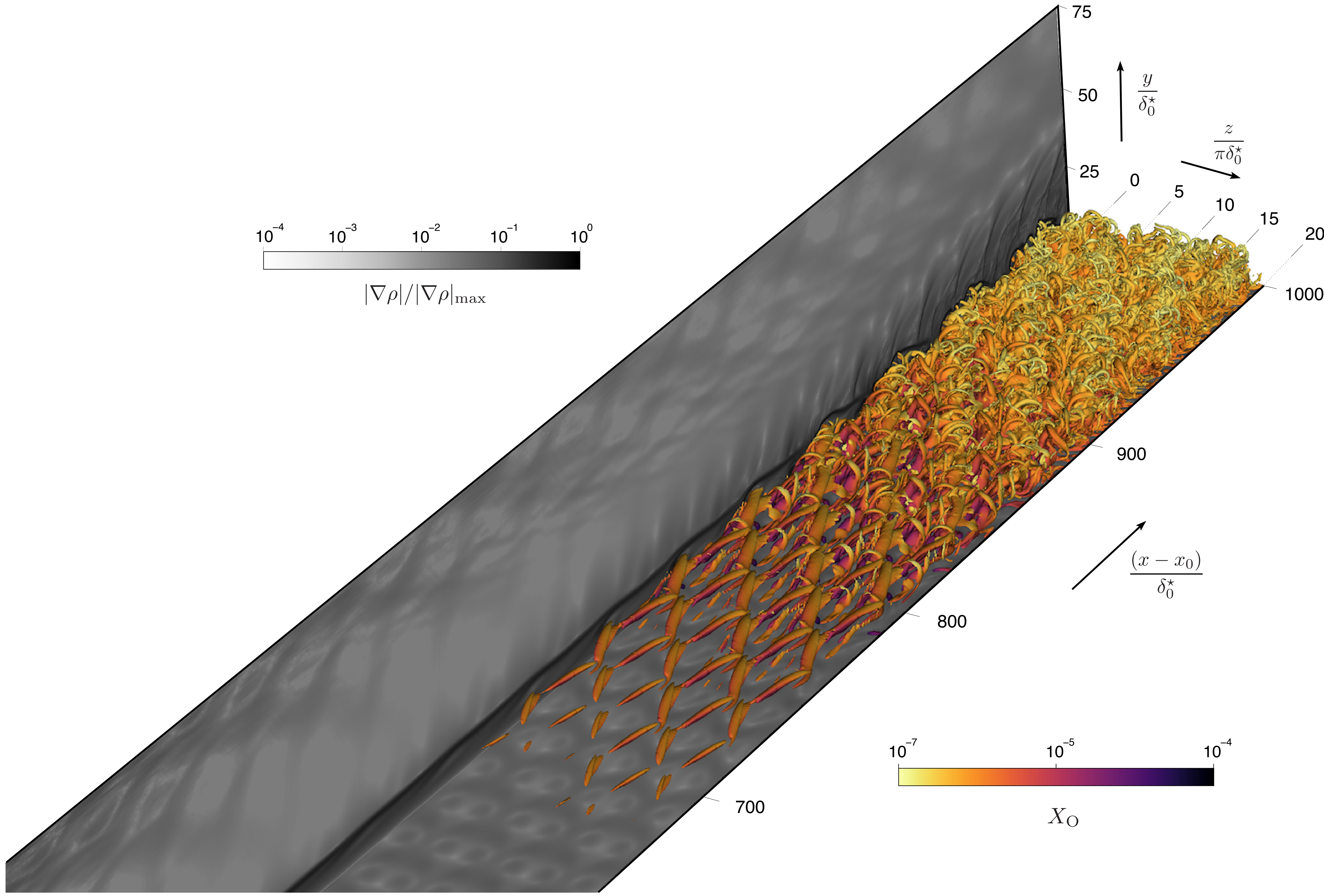
Considered physics

- Compressible Navier—Stokes solver
- Multicomponent species transport
- Curtiss-Hirschfelder approximation for species diffusion
- Arrhenius finite-rate chemistry computed at runtime

Numerics

- Cartesian orthogonal grids
- Sixth-order low-dissipation schemes for Euler fluxes
  - TENO6-A
  - Skew-symmetric
  - Hybrid scheme
- Second-order conservative scheme for diffusion fluxes
- Explicit and semi-implicit time advancement

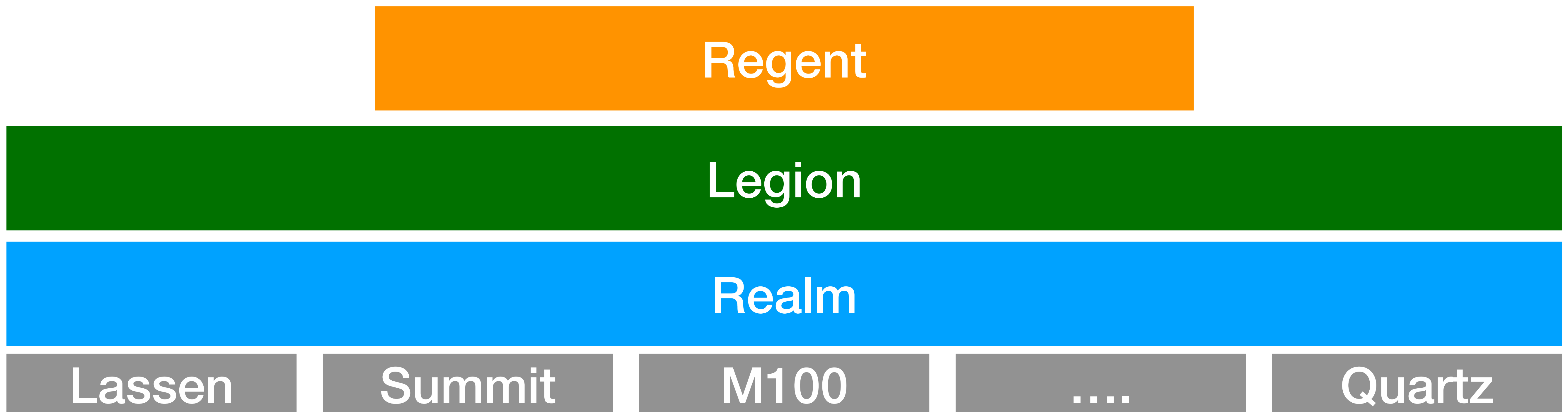
Snapshot of an hypersonic high-enthalpy transitional boundary layer computed with the HTR solver



Further reading:

Di Renzo, M., Fu, L. & Urzay, J. 2020 "HTR solver: An open-source exascale-oriented task-based multi-GPU high-order code for hypersonic aerothermodynamics." Computer Physics Communications 255, 107262

HTR solver and the Legion library



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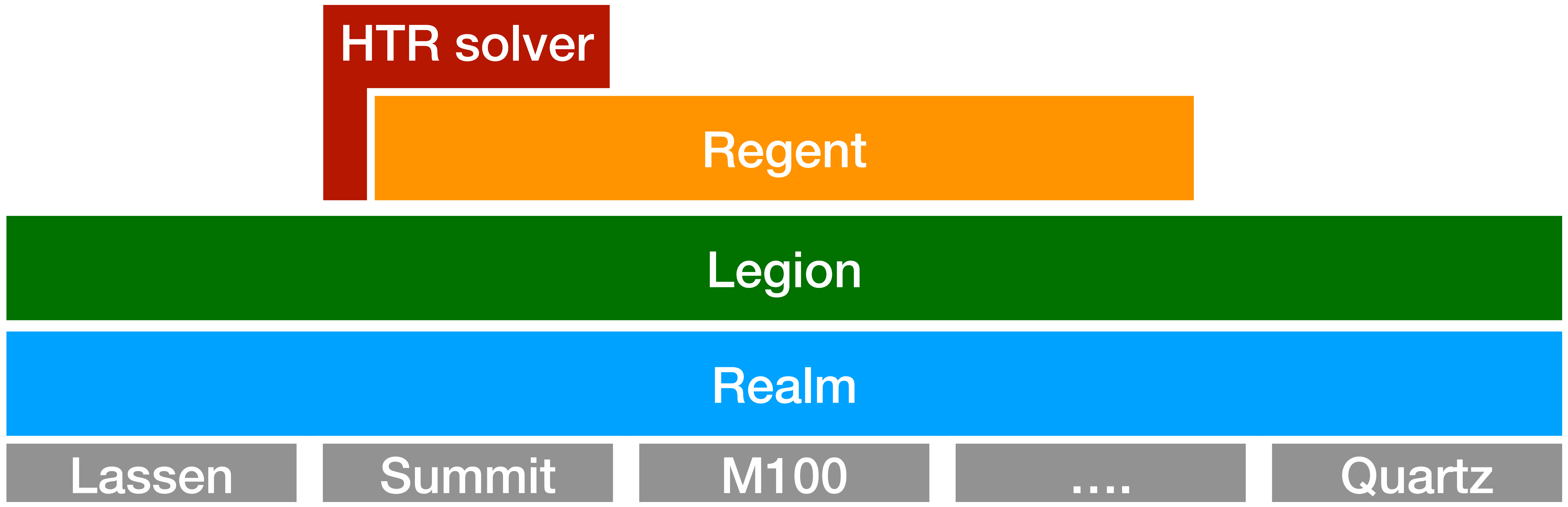


Most of the HTR solver is implemented in Regent

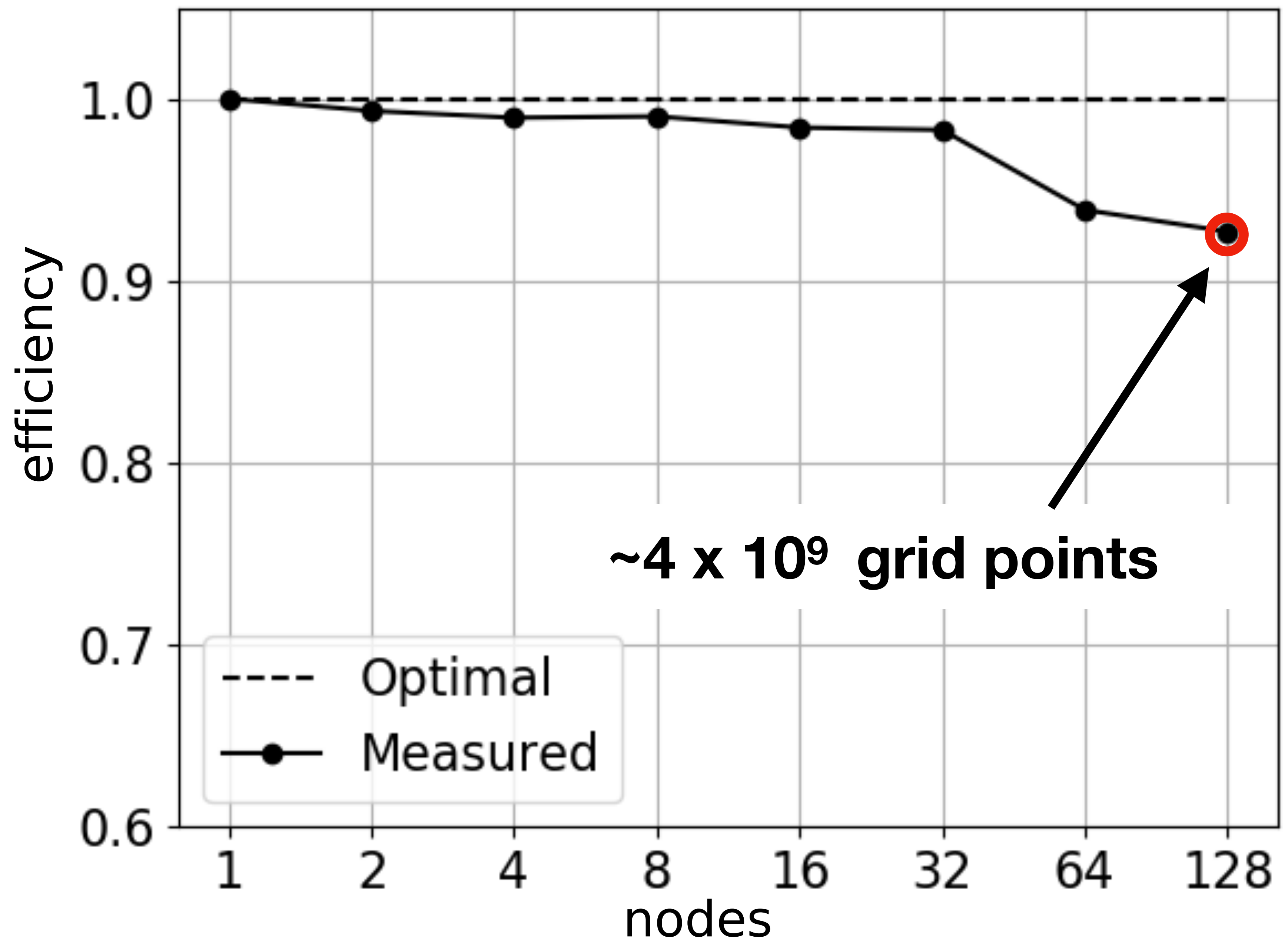
- Very friendly for new users
- Generates CPU and GPU ready binaries from the same sources
- Limited number of available libraries

Some leaf tasks are implemented in C++ and CUDA using Legion C++ API

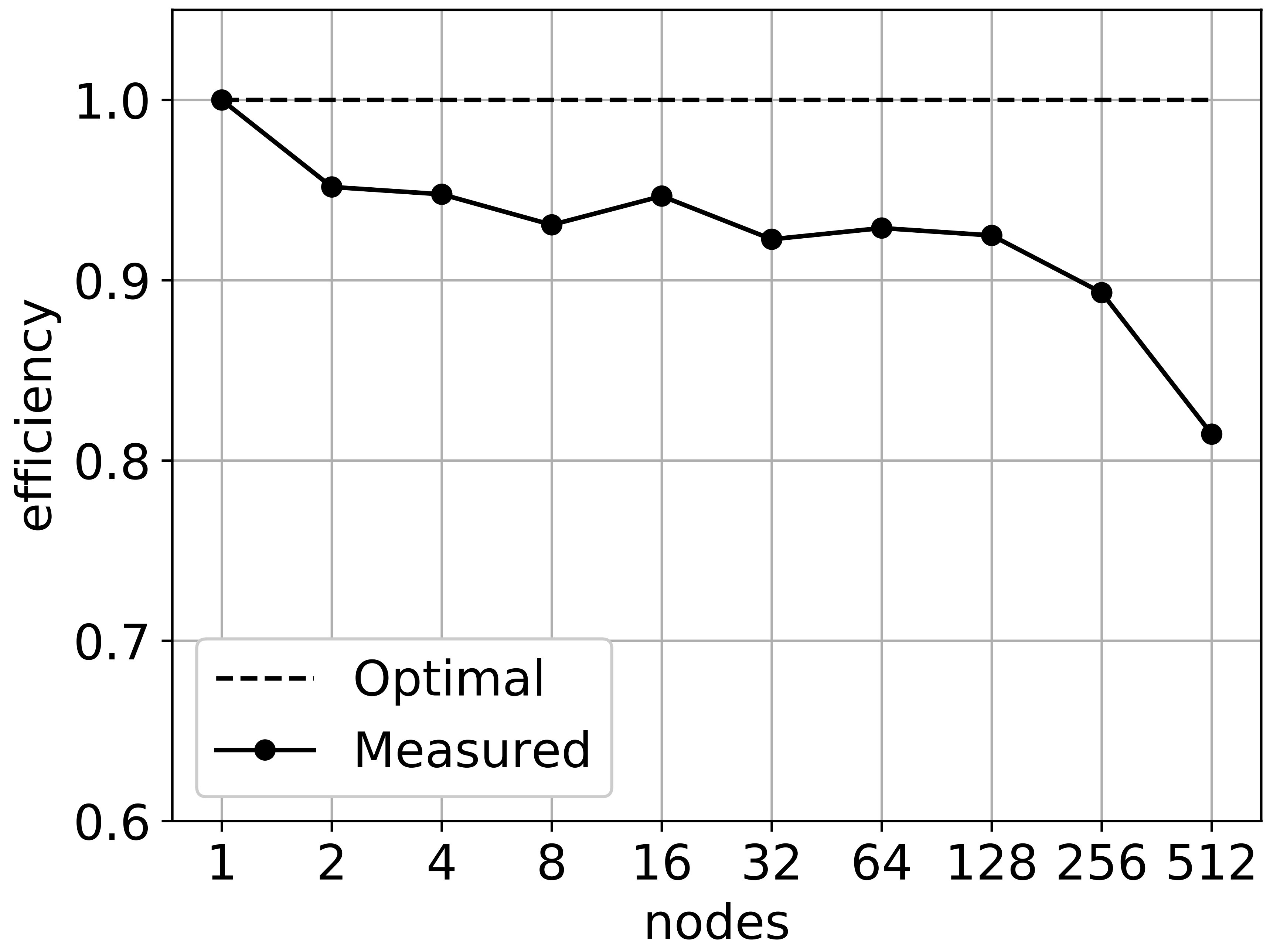
- Large community and established libraries
- Requires better knowledge of the Legion runtime

Scalability and portability of HTR

Lassen (@ LLNL)
4 GPUs per node



Quartz (@ LLNL)
40 CPU cores per node



Main tested systems:

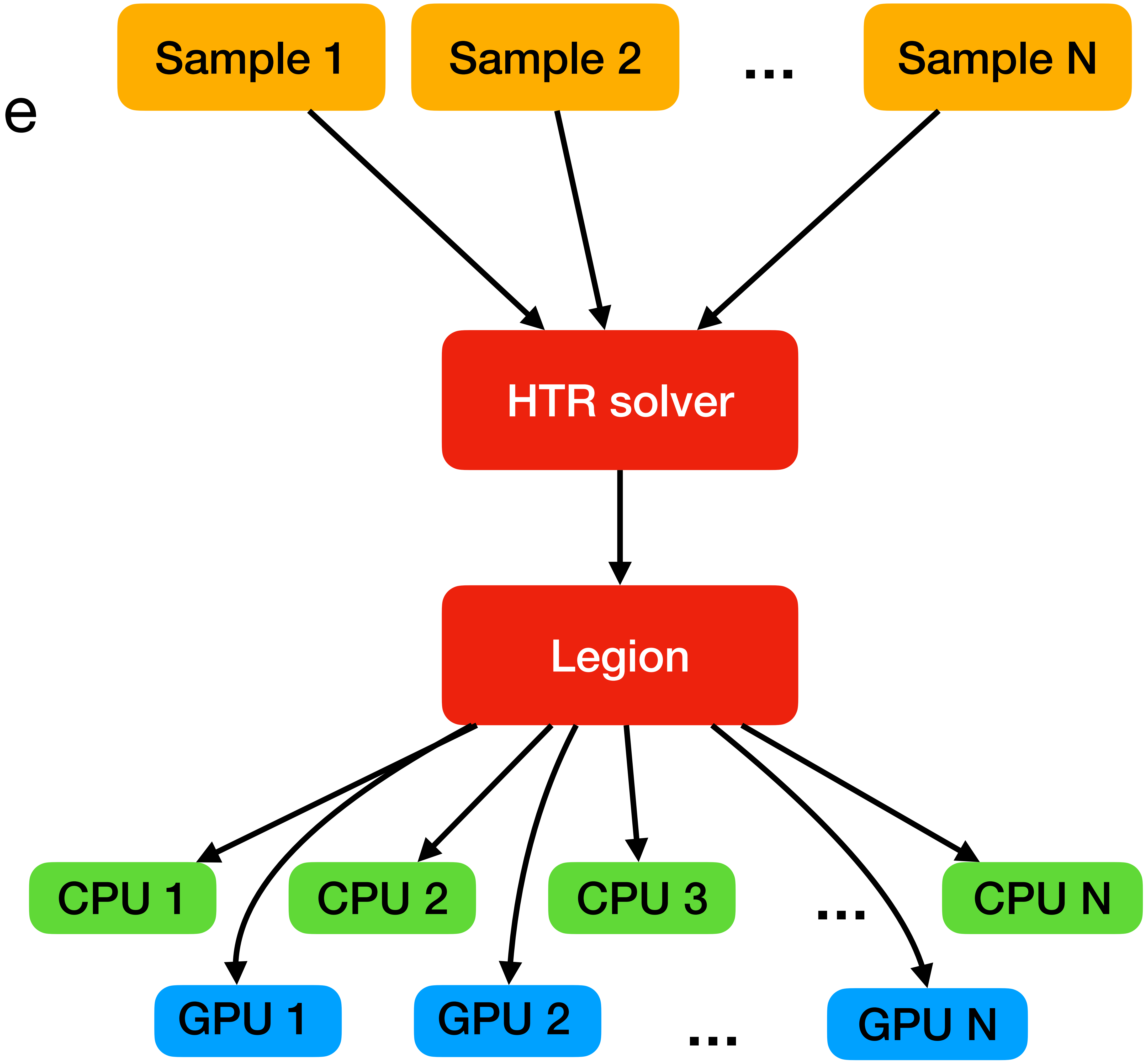
GPU based
- Lassen (@ LLNL, USA)
- Marconi 100 (@ CINECA, Italy)
- Juwels (Germany)

CPU based
- Quartz (@ LLNL, USA)
- Galileo (@ CINECA, Italy)

Credit: Thiago Teixeira @ Stanford University

Ensamble calculations

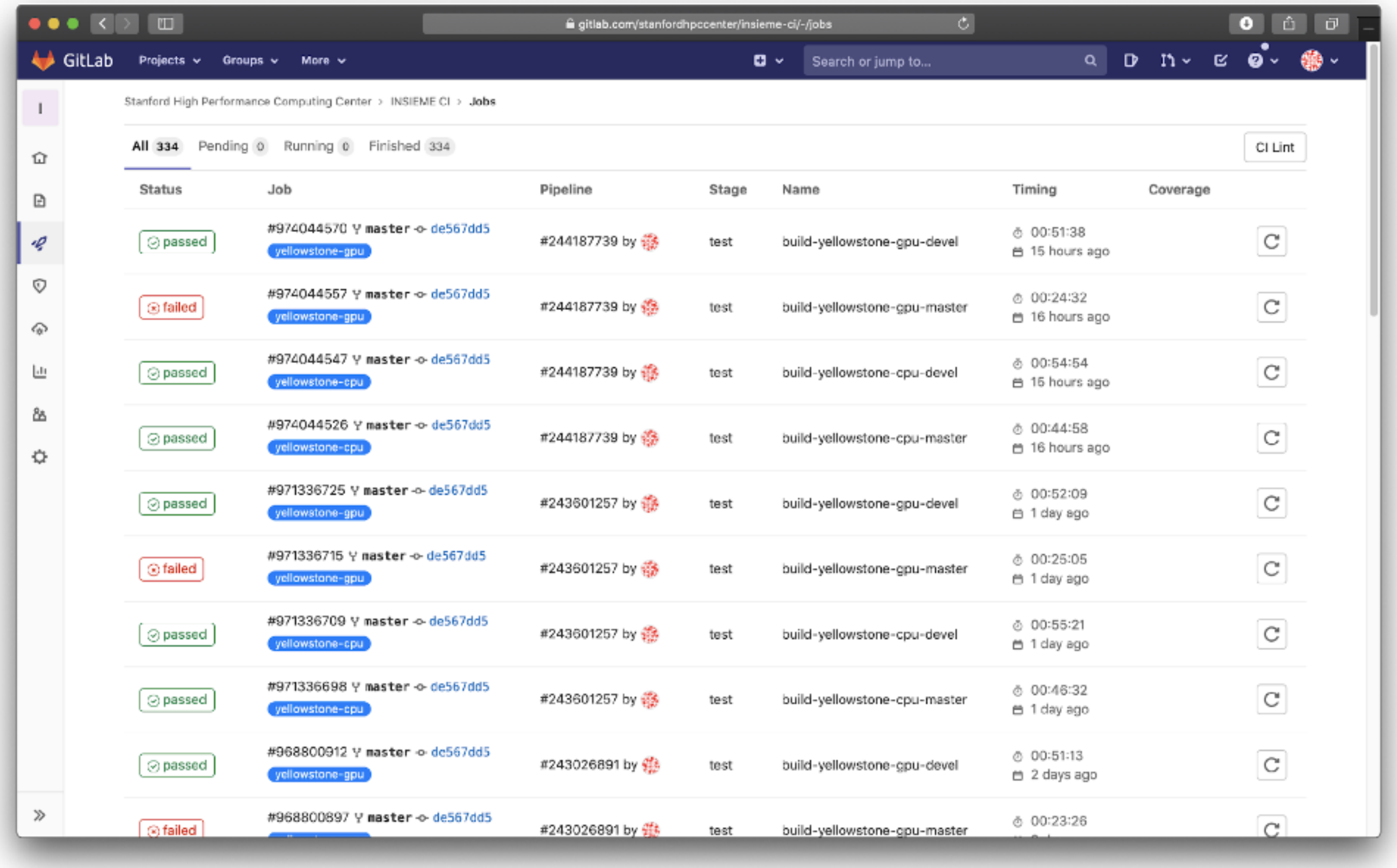
- HTR can manage multiple samples in the same execution
- The task graphs of every sample are made available to the runtime
- The mapper assigns them to the machine components taking into account user defined priorities



Further discussion at 2:45 pm during Gianluca Iaccarino's speed talk

Continuous integration and deployment

- The correctness of the solver is tested at every push in our repository. We check:
  - each module of the solver separately
  - the whole solver with physically relevant setups



- Compatibility with HPC systems is checked every night with builds of executables and unit test executions

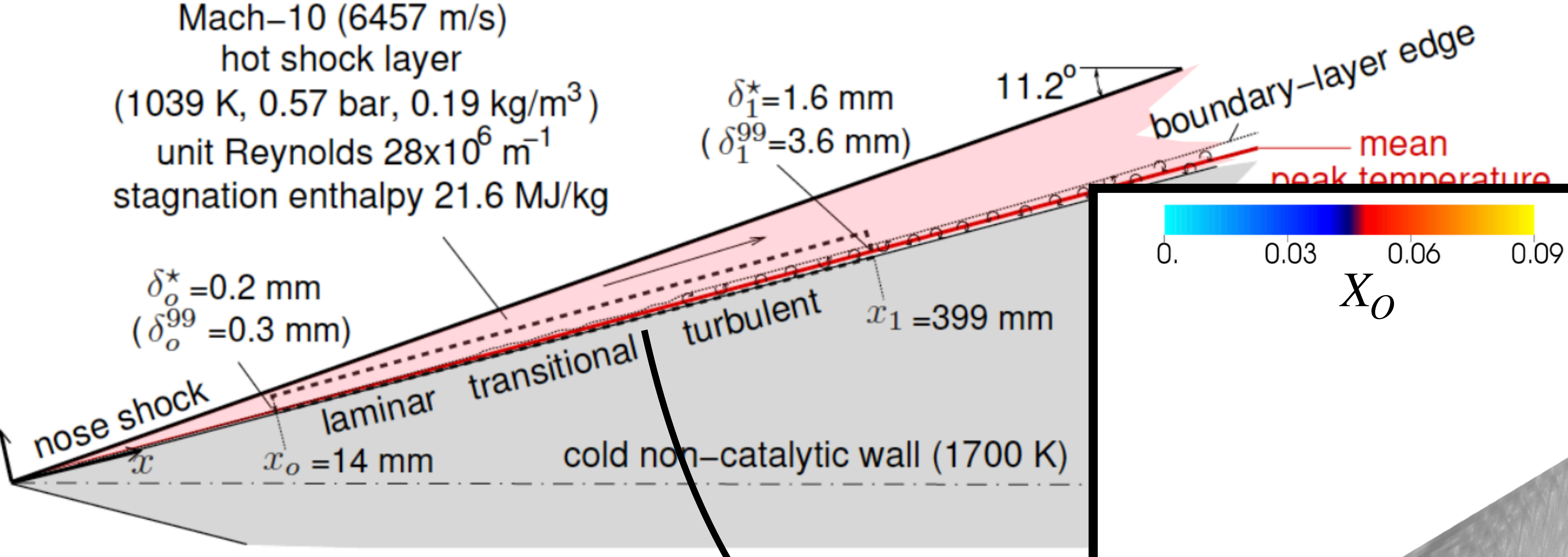
- Nightly builds are executed on
  - Lassen (@LLNL)
  - Quartz (@LLNL)
  - Yellowstone (@ Stanford HPC center)

Credit: Steve Jones, Caetano Melone, Sophie Opferman, Paul Mure, Dellarontay Readus

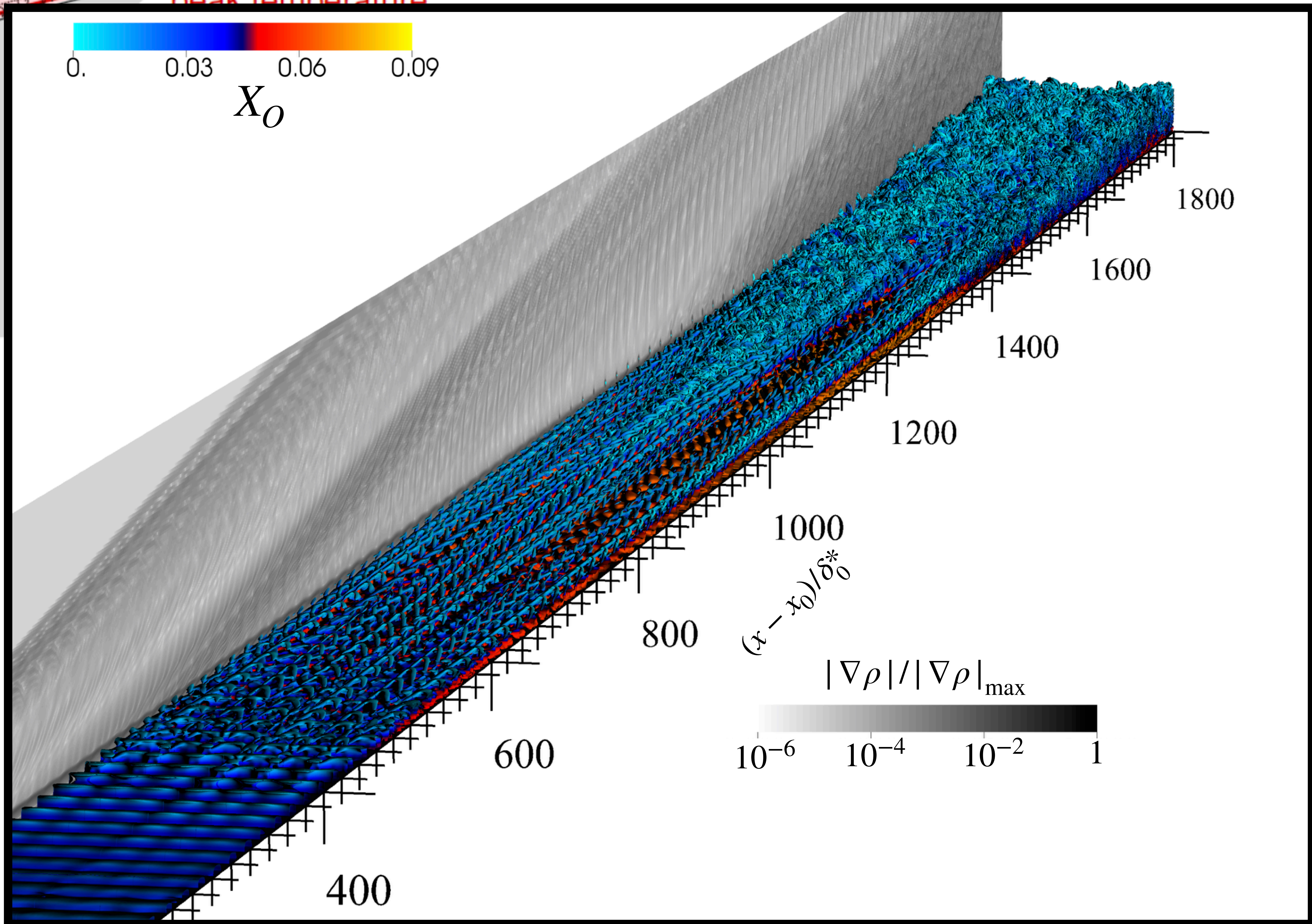
Studying transitional hypersonic boundary layers

$Re_{x,max}$	$Re_{\tau,max}$	$Re_{\theta,max}$	$Re_{\delta*,max}$	$B_{q,max}$	$Ma_{\tau,max}$
11×10^6	900	3000	3.6×10^4	0.28	0.23

Studying transitional hypersonic boundary layers



Snapshot of the Q-criterion iso-surface colored with atomic oxygen molar fraction.
Side surface of the domain colored with "pseudo-schlieren"



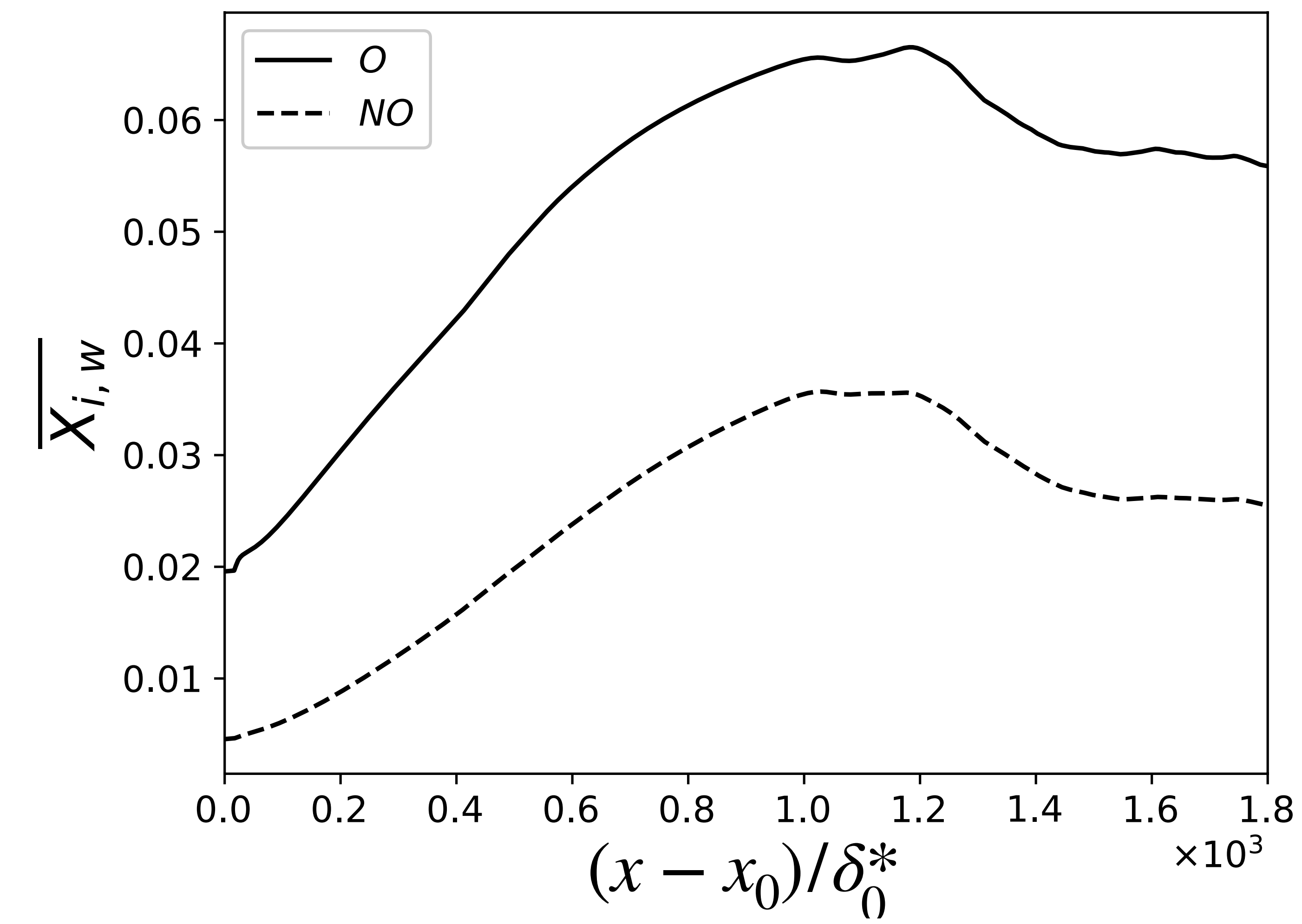
Main calculation parameters
- About 2 billion grid points
- 5 transported species
- About 18 billion DOF
- Run on 512 GPUs on Lassen at LLNL

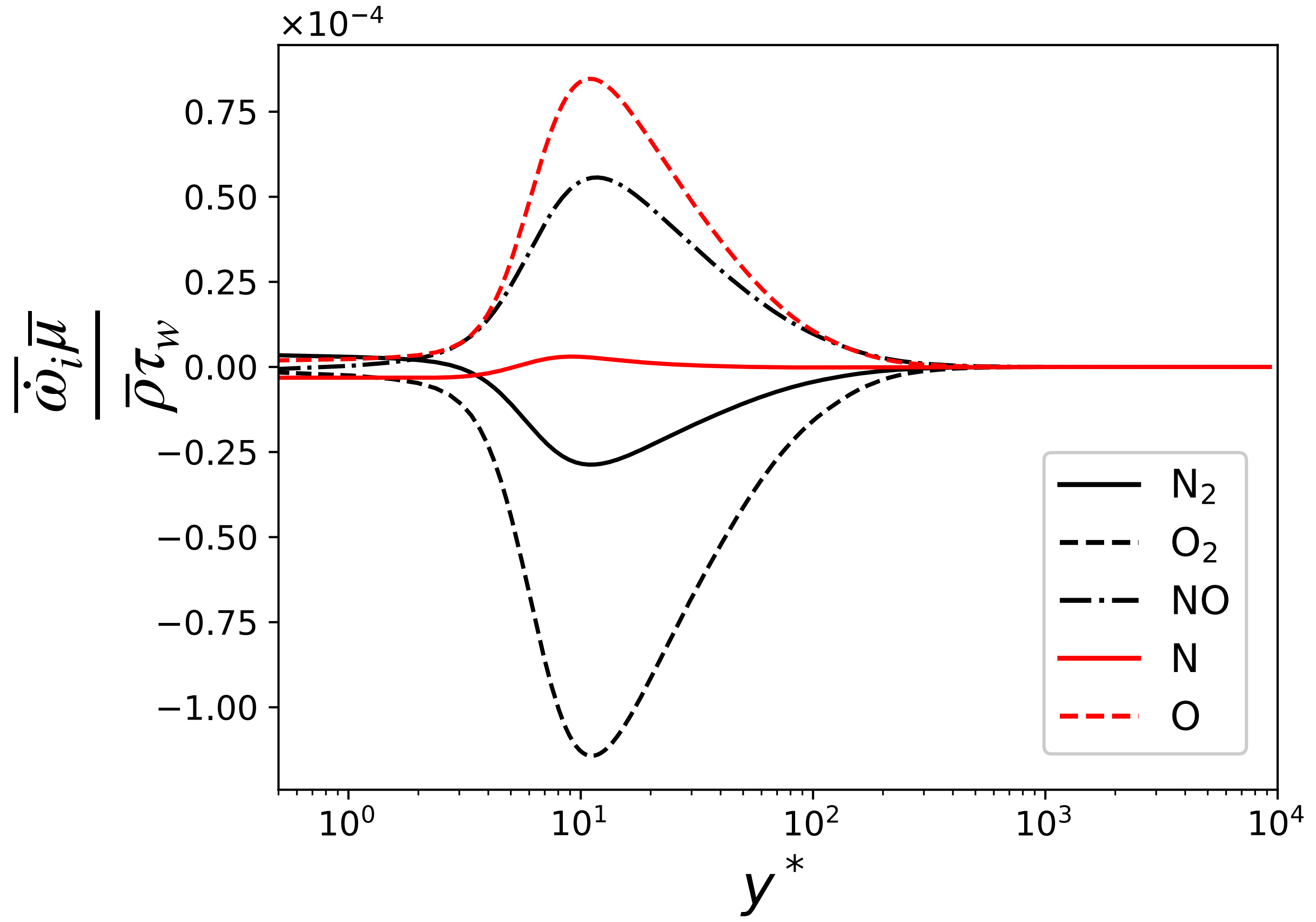
Studying transitional hypersonic boundary layers

Main results

- The concentration of dissociated species tends to increase in the laminar boundary layer
- The increased transport due to turbulence suddenly diminishes the concentration of atomic oxygen and nitrogen oxide at the wall
- Chemical production is much slower than the flow time scales, particularly in the turbulent section
- Morkovinian correlation between the species transport and the velocity field are observed away from the wall

Mean species molar fraction at the wall along the streamwise coordinate





Wall-normal distribution of the normalized air dissociation rates

Further reading:

Di Renzo, M. & Urzay, J. 2021 "Direct numerical simulation of a hypersonic transitional boundary layer at suborbital enthalpies" Journal of Fluid Mechanics 912, A29

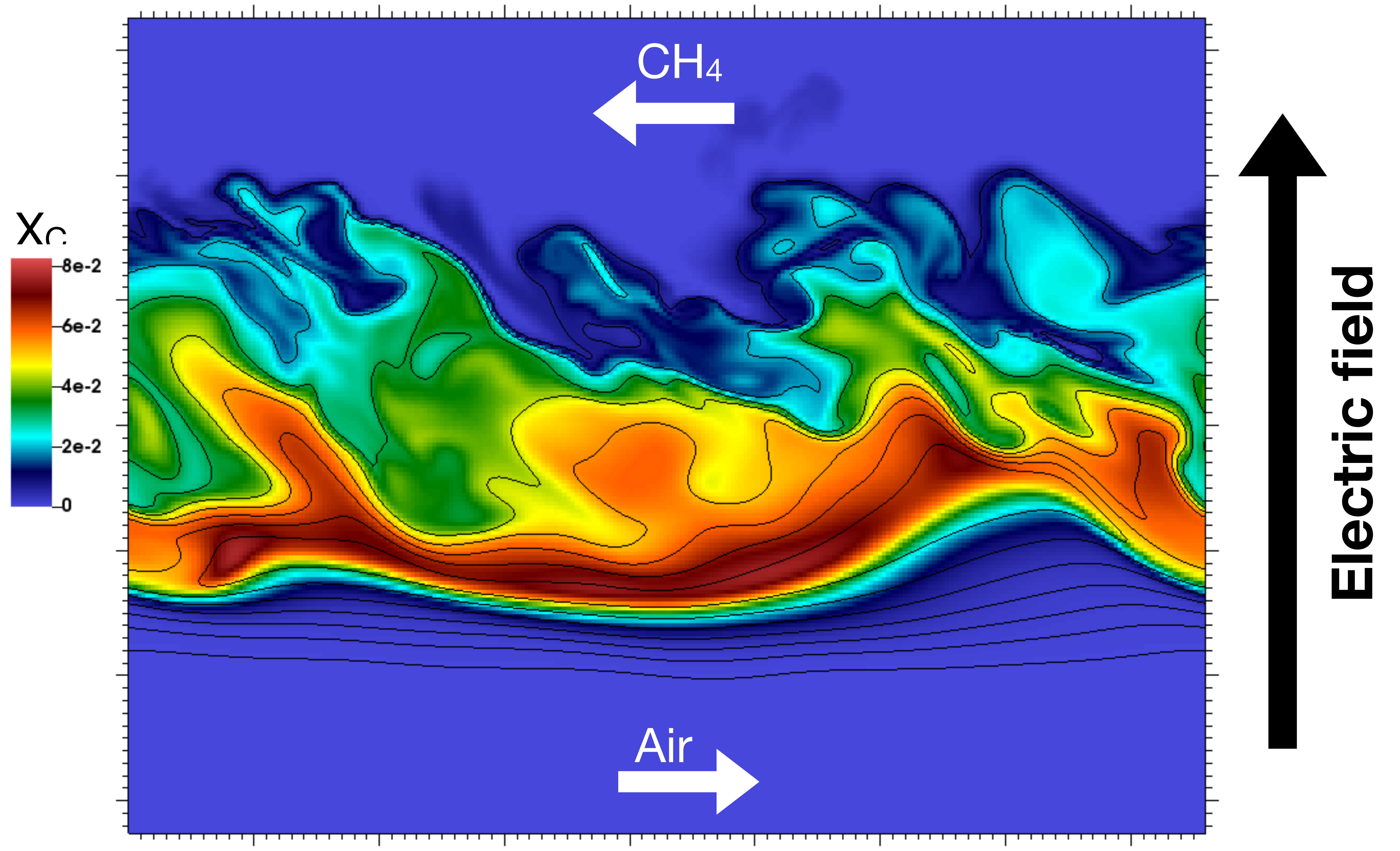
Interaction of turbulent flame with electric fields

Investigated problem

This projects aims at computing the effects of electric fields on turbulent methane/air flame

The investigation will be carried out performing DNS of a reacting temporal mixing layer

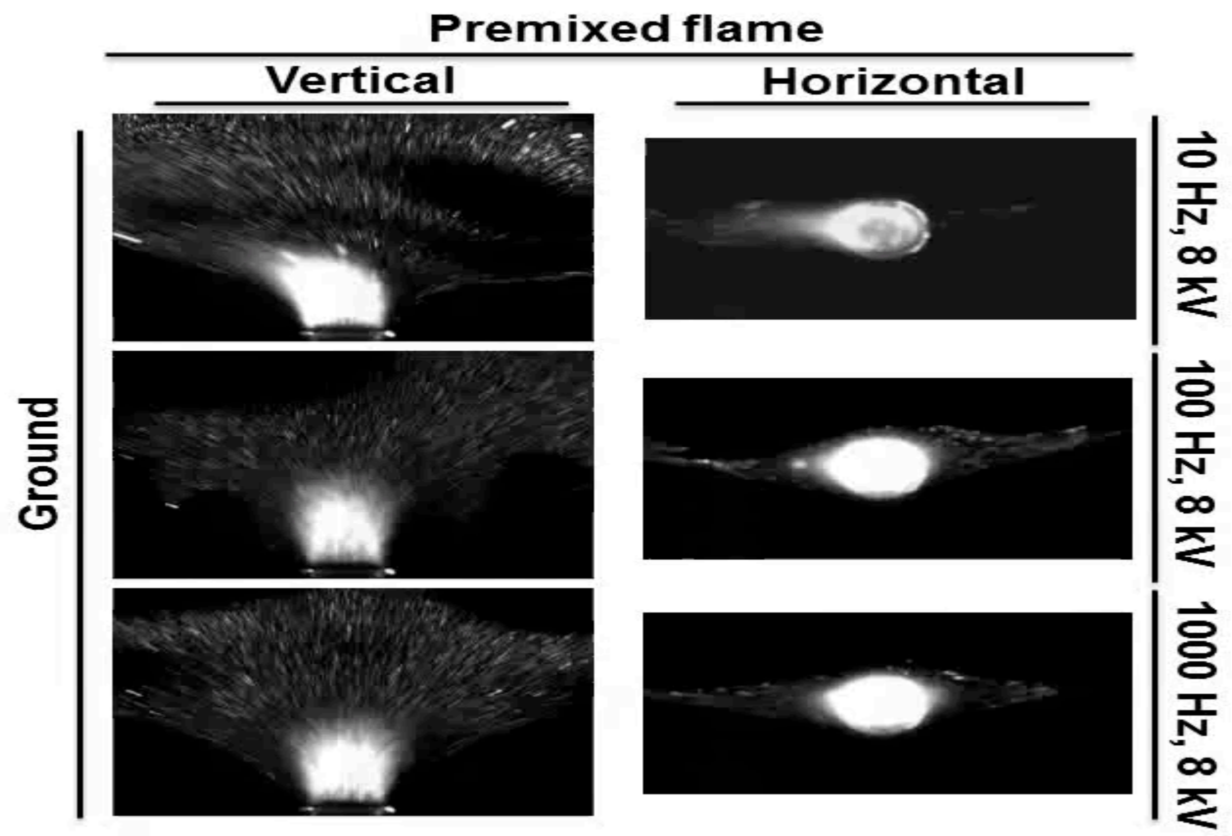
A multi-GPU task-based elliptic solver is required to solve the Gauss law at during the flow advancement



Credit: GM Whitesides (Harvard)

Known benefits of impinging electric fields

- Flame speed augmentation
- Decrease of pollutant emissions
- Mitigation of flame instabilities
- Electrically-induced flame extinction
- Enhanced jet-flame anchoring



Credit: Park et al. C&F (2017)

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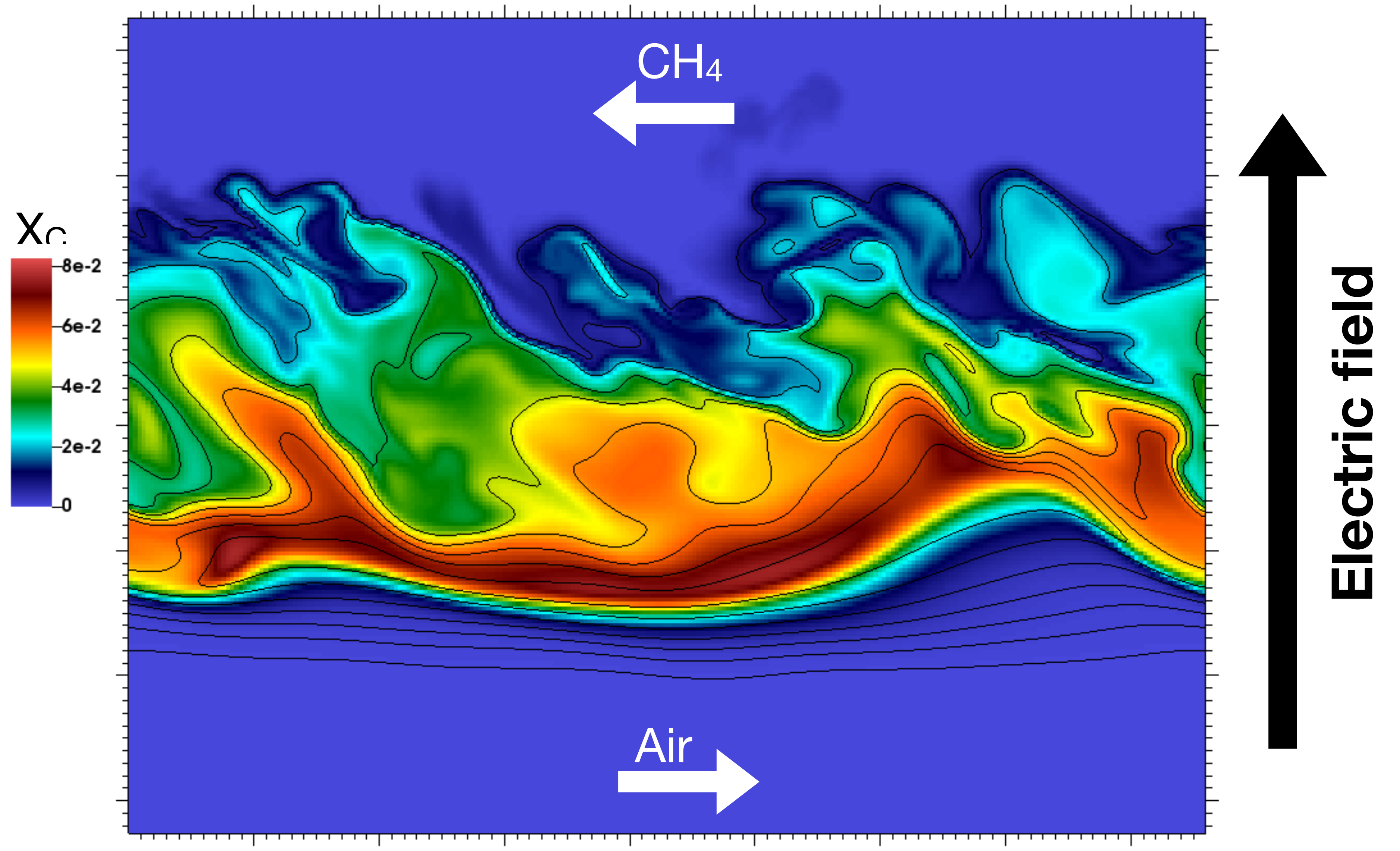

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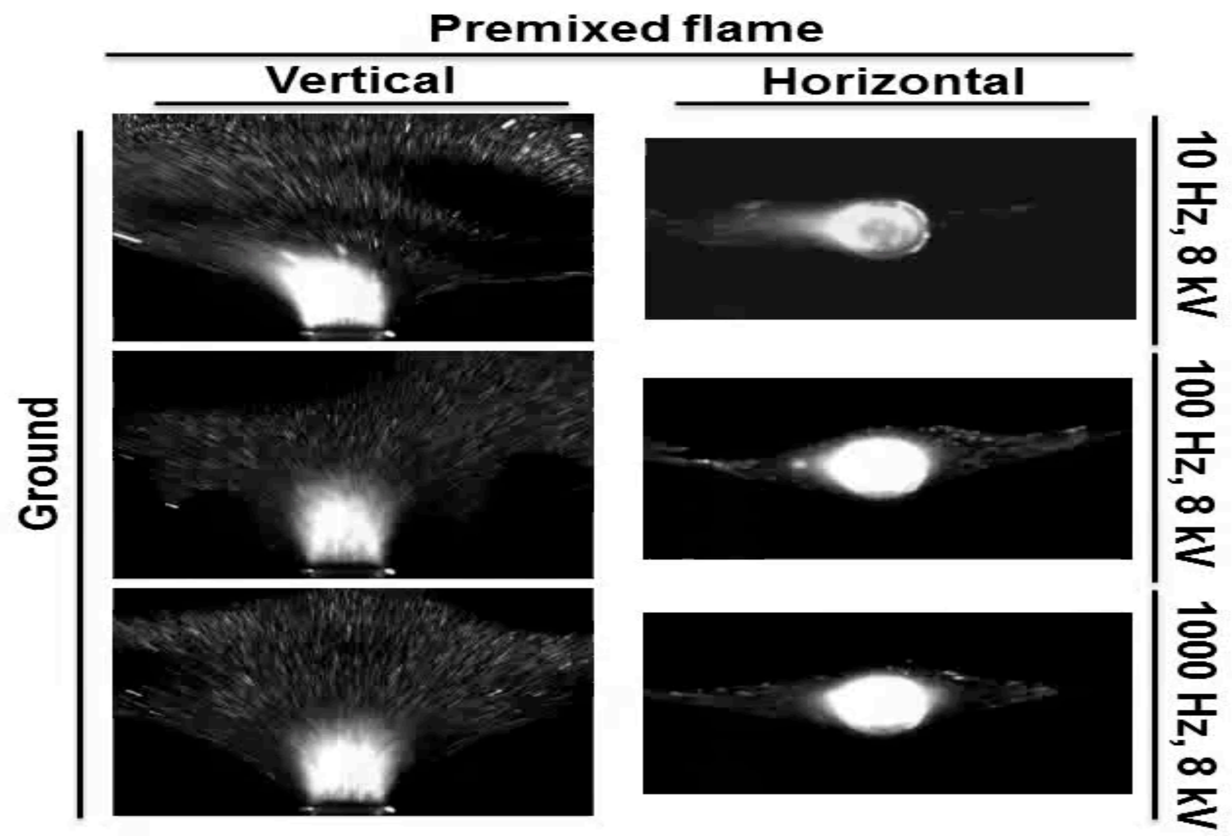

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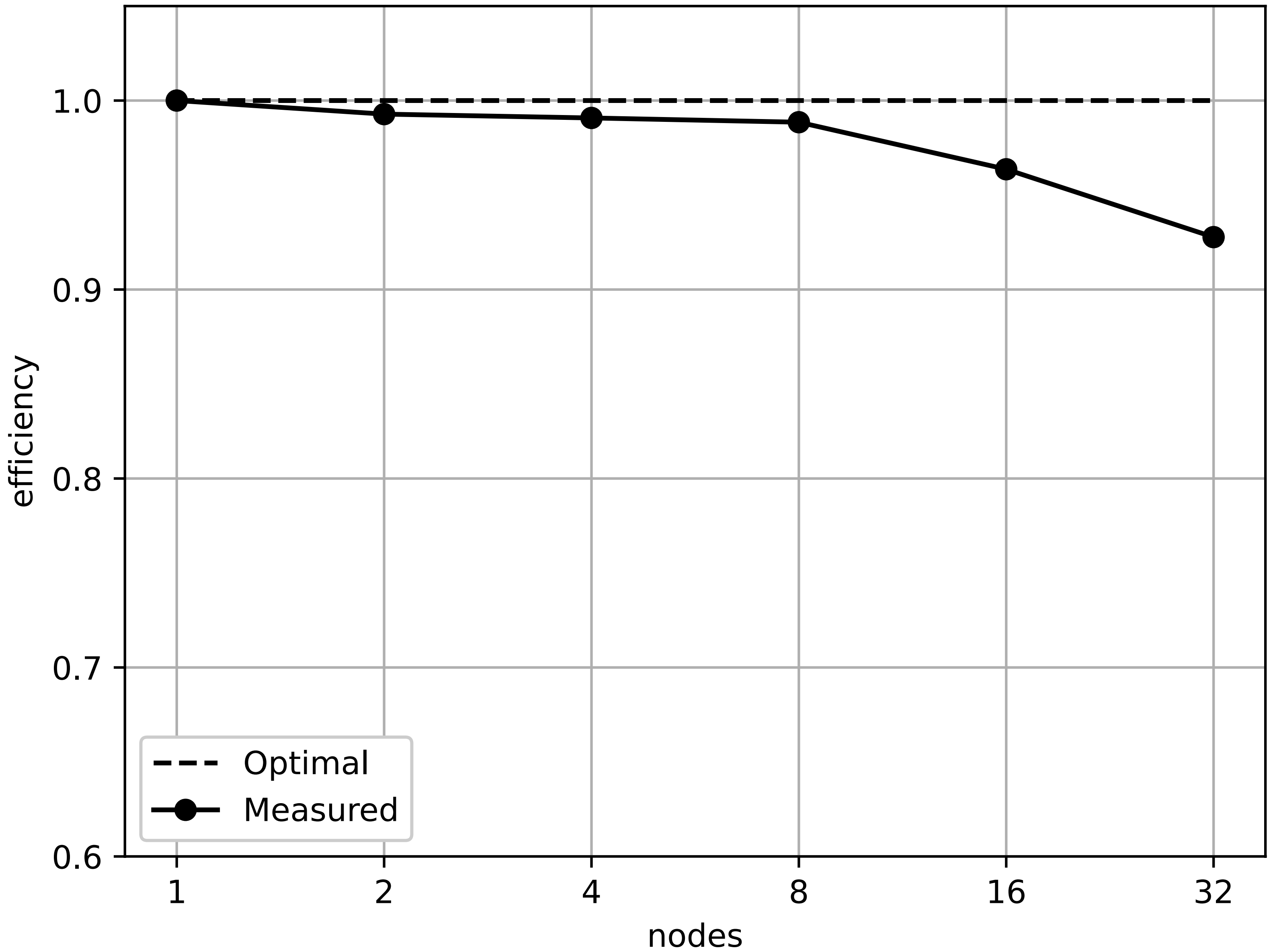
Elliptic solver for heterogeneous architectures

Main characteristics of the Poisson solver

- Uses FFTs along periodic directions, and 2nd order finite differences along inhomogeneous directions.
- Compatible with GPUs (CUDA) and CPUs (OpenMP)
- Legion manages the data communications and organization among the domain partitions at runtime

Weak scaling on Marconi100



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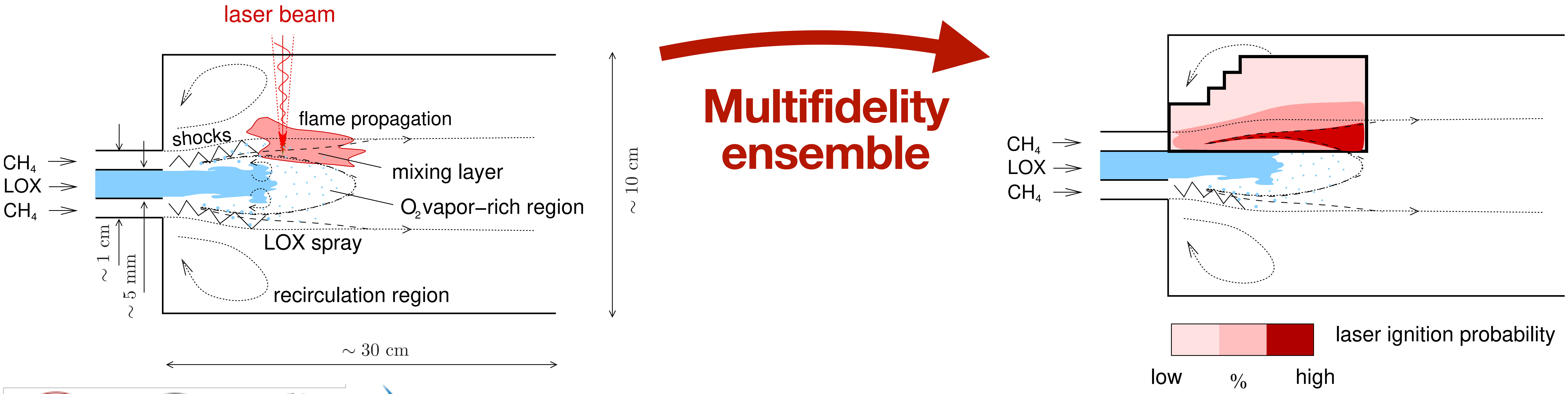
Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Overarching problem

The prediction of reliability of in-space ignition of cryogenic methane and liquid oxygen propellants in a rocket combustor by using pulsed high-energy lasers.



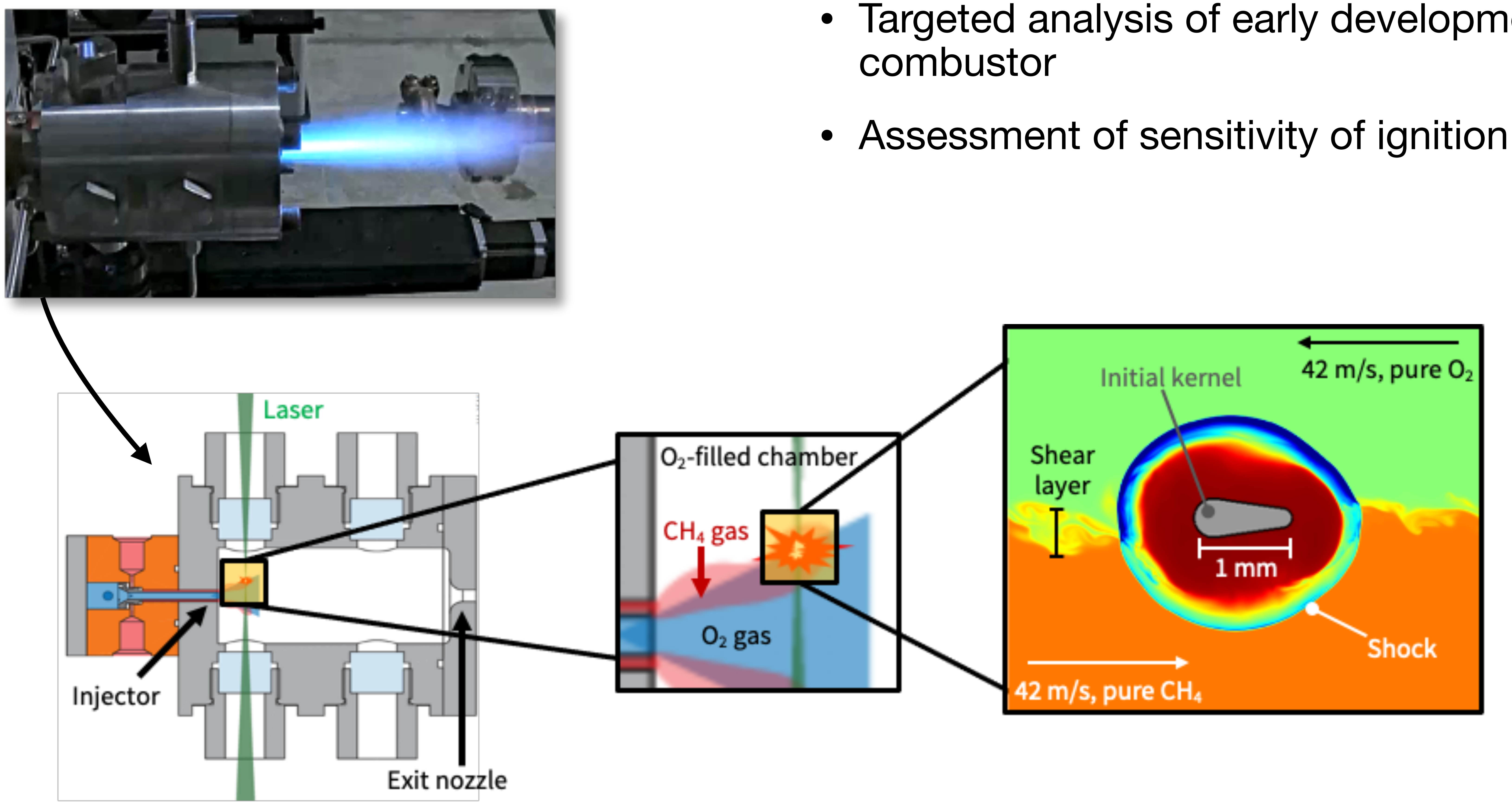
https://insieme.stanford.edu

Credit: Jonathan Wang @ CTR, Stanford

Simulation of laser induced ignition

Goals

- Targeted analysis of early development of ignition kernel in a rocket combustor
- Assessment of sensitivity of ignition and flow dynamics to physics modeling



Results

- Kernel expands supersonically and generates a shock wave
- Peak temperature relaxes down to flame temperature
- Radical species produced in quantities comparable to combustion products
- Products located only along kernel perimeter due to high temperature in core

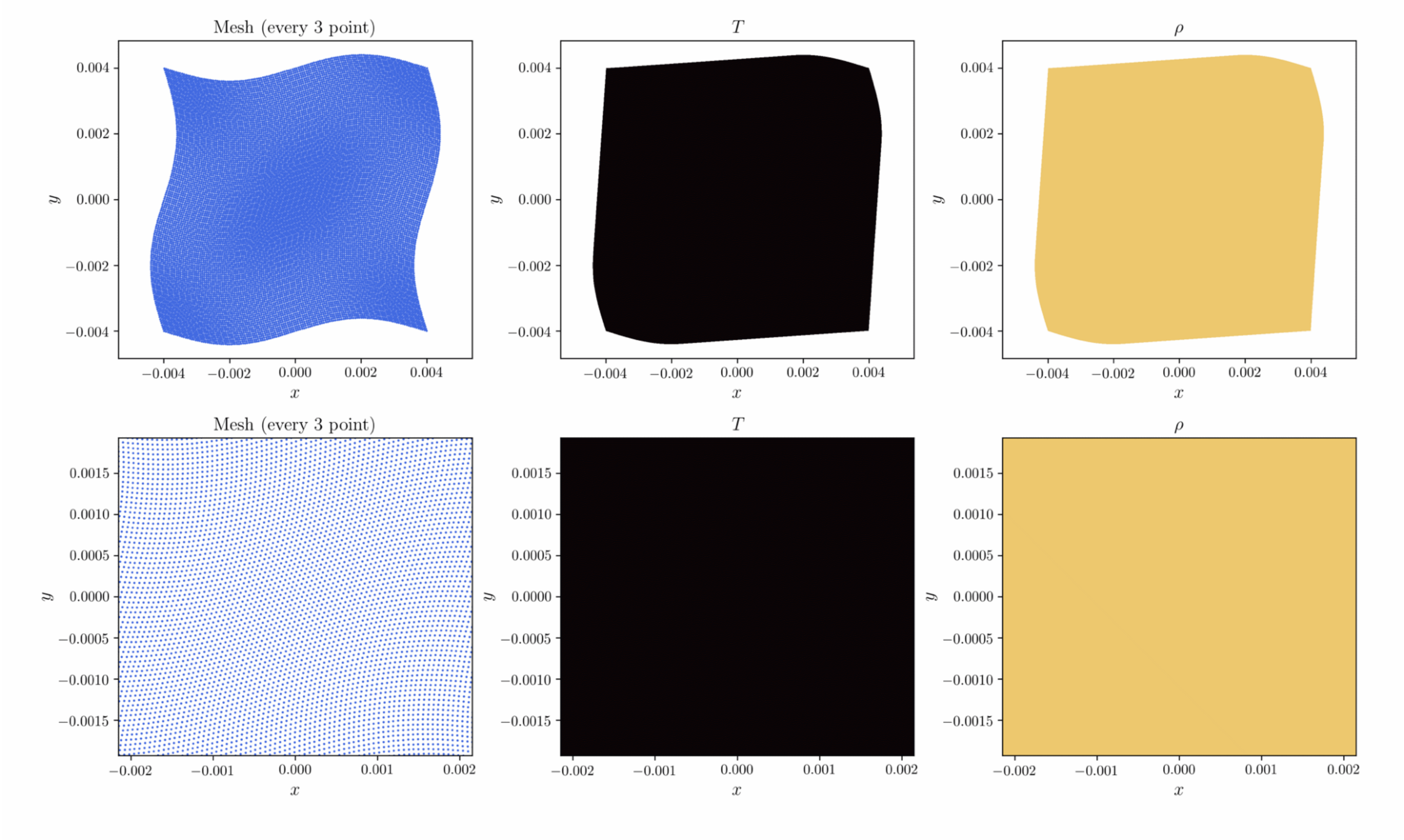
Funded by the Predictive Science Academic Alliance Program III center at Stanford University

Future developments

Handling complex geometries in the HTR solver

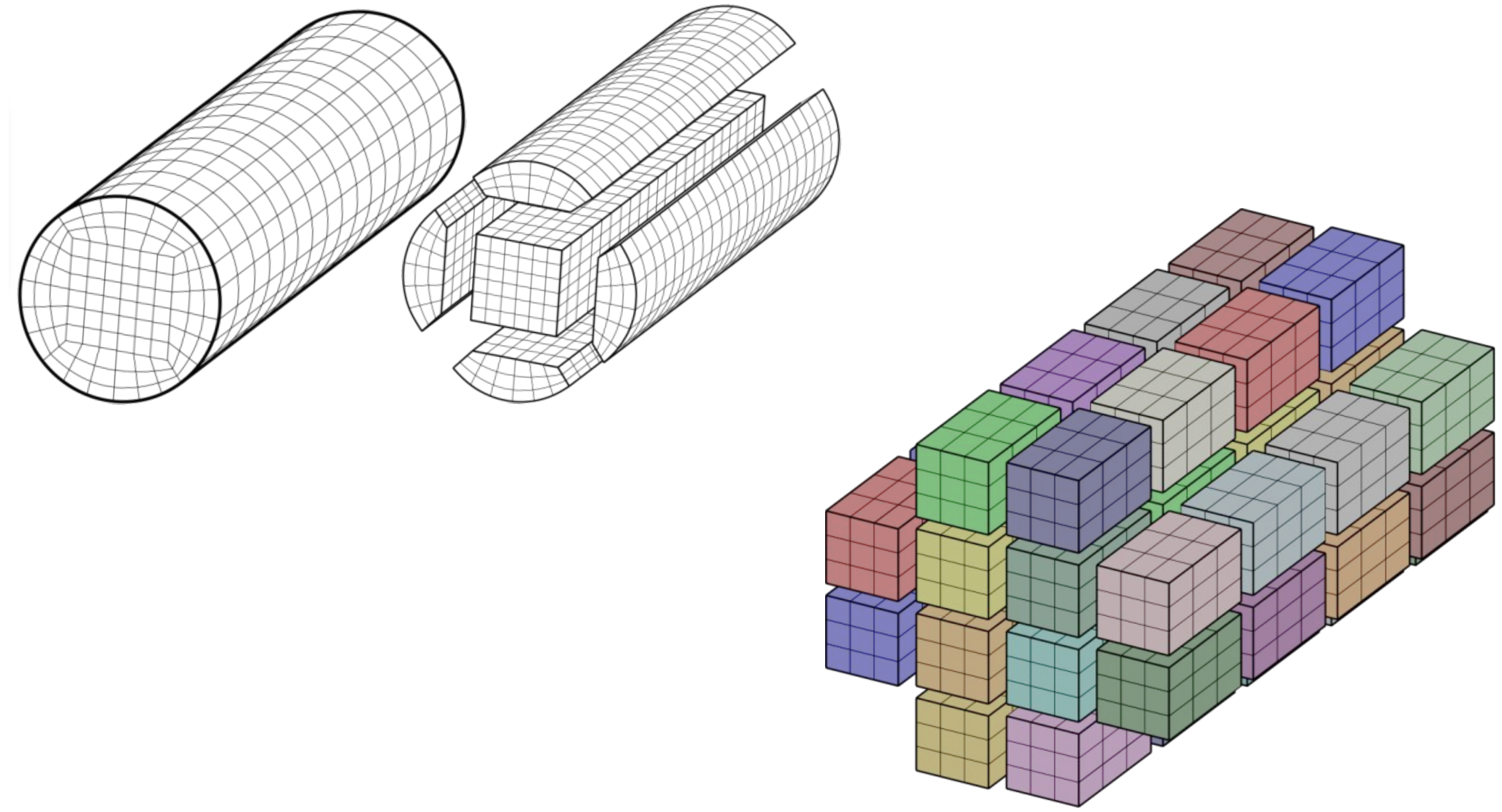
Curvilinear coordinates

We use covariant transformation to transform the transport equations from a Cartesian computational space to a curvilinear physical space



Multi-block domains

Computational grids composed of multiple blocks are handled in a single region in Legion. The runtime will handle the required data communications



Credit: Alboreno Voci @ CTR, Stanford

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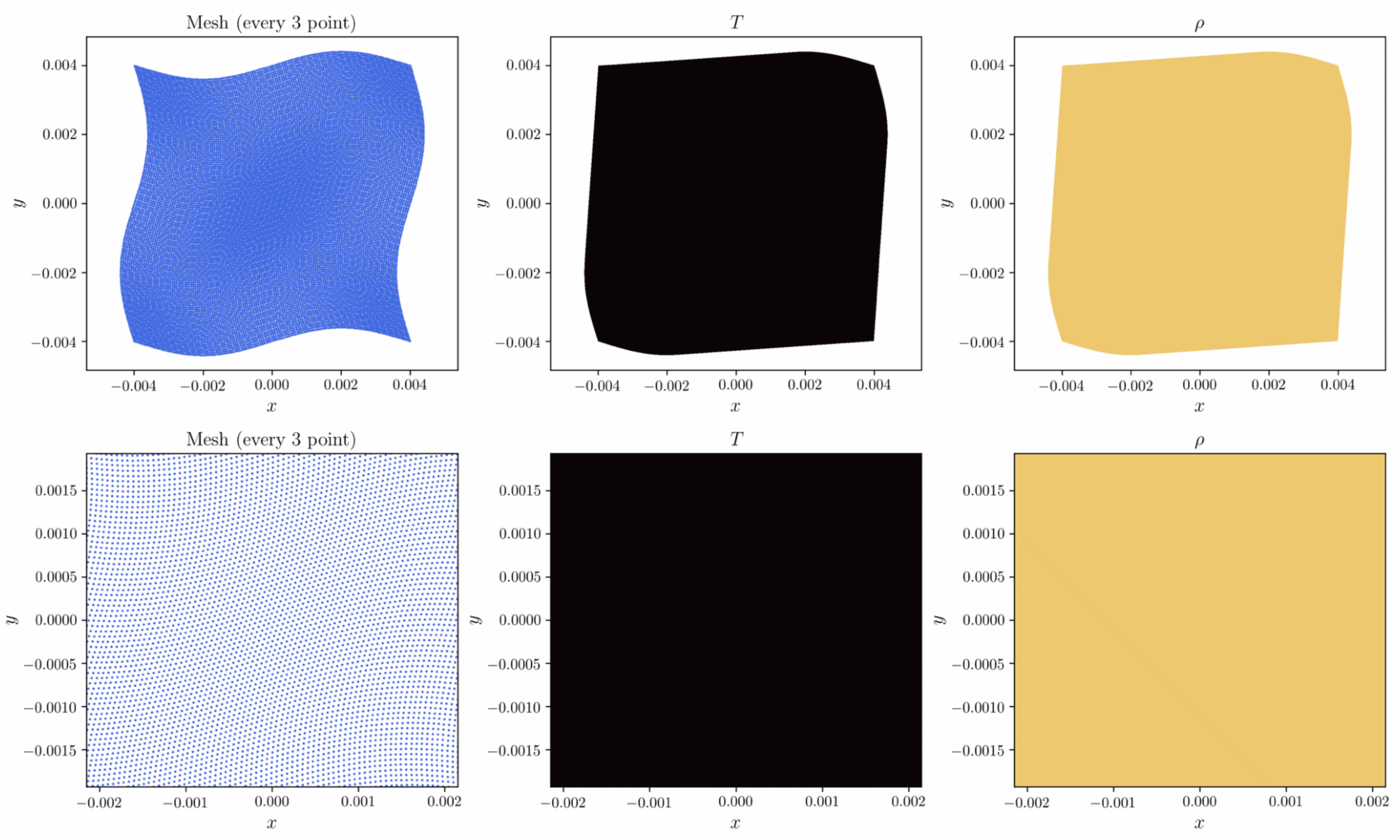

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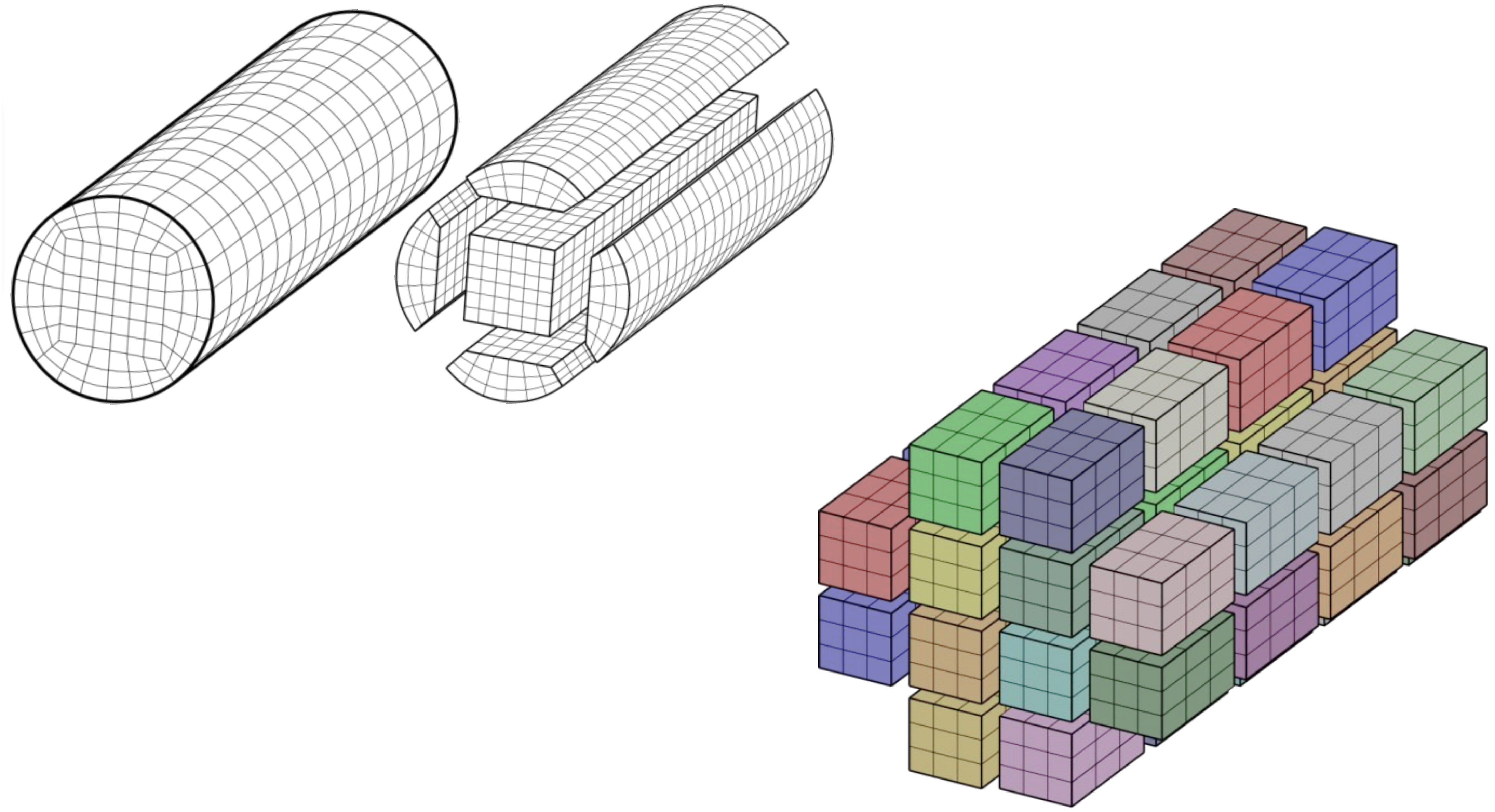

Credit: Alboreno Voci @ CTR, Stanford

Conclusions

- The Hypersonic Task-based Research solver is a flexible open-source tool to study compressible reacting flows
- HTR is mainly implemented in Regent, though the Legion C++ API is utilized to implement some leaf task
- Its implementation has so far shown good portability and scalability of very different HPC systems
- New versions capable of handling electric fields and complex geometries will be released soon