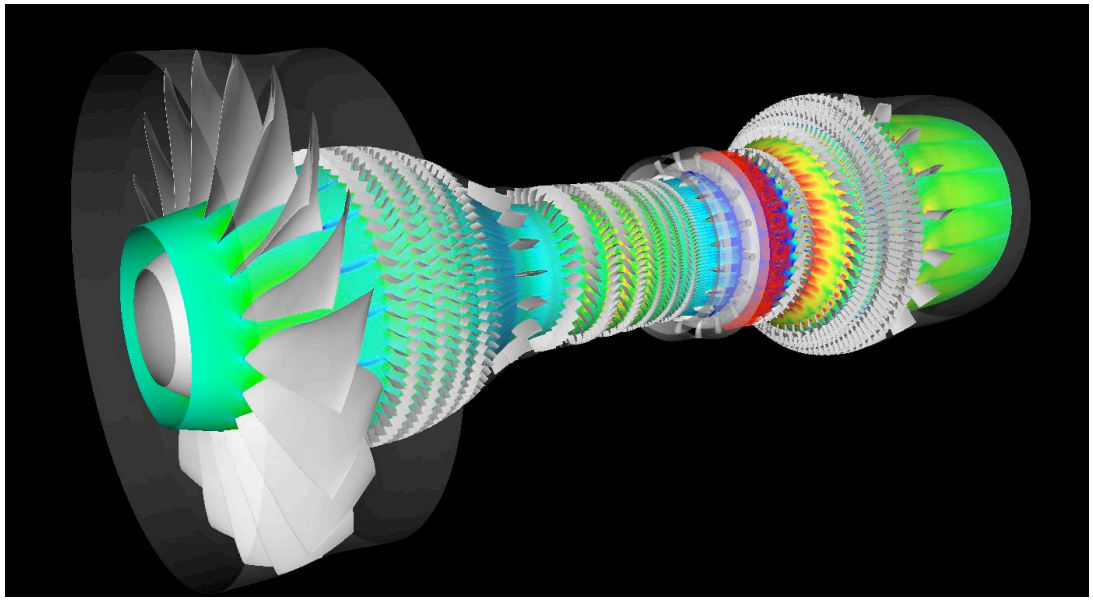
Stanford ASC Alliance Legacy

- Development of Large Eddy Simulation methodology for multi-physics flows in complex geometry (CDP)
- Code integration Environment (CHIMPS)
- Numerical Analysis of Multi-code Coupling, Streaming Architectures and Programming Paradigms, pioneering GPU computing
- Transition of codes and active collaborations with industry: GM, UTRC (now doing integrated simulations), P&W, Boeing, Bosch,…
- ICME
  - E.g. Q. Wang (MIT)
- PPL
- Commercialization
  - CUDA, VMWare,
  - Coverity
- OpenSource Software
  - Chromium, BrookGPU



Sample end-to-end simulation of a PW6000 jet engine

Predictive Simulations of Multi-Physics Flow Phenomena, with Application to Integrated Hypersonic Systems

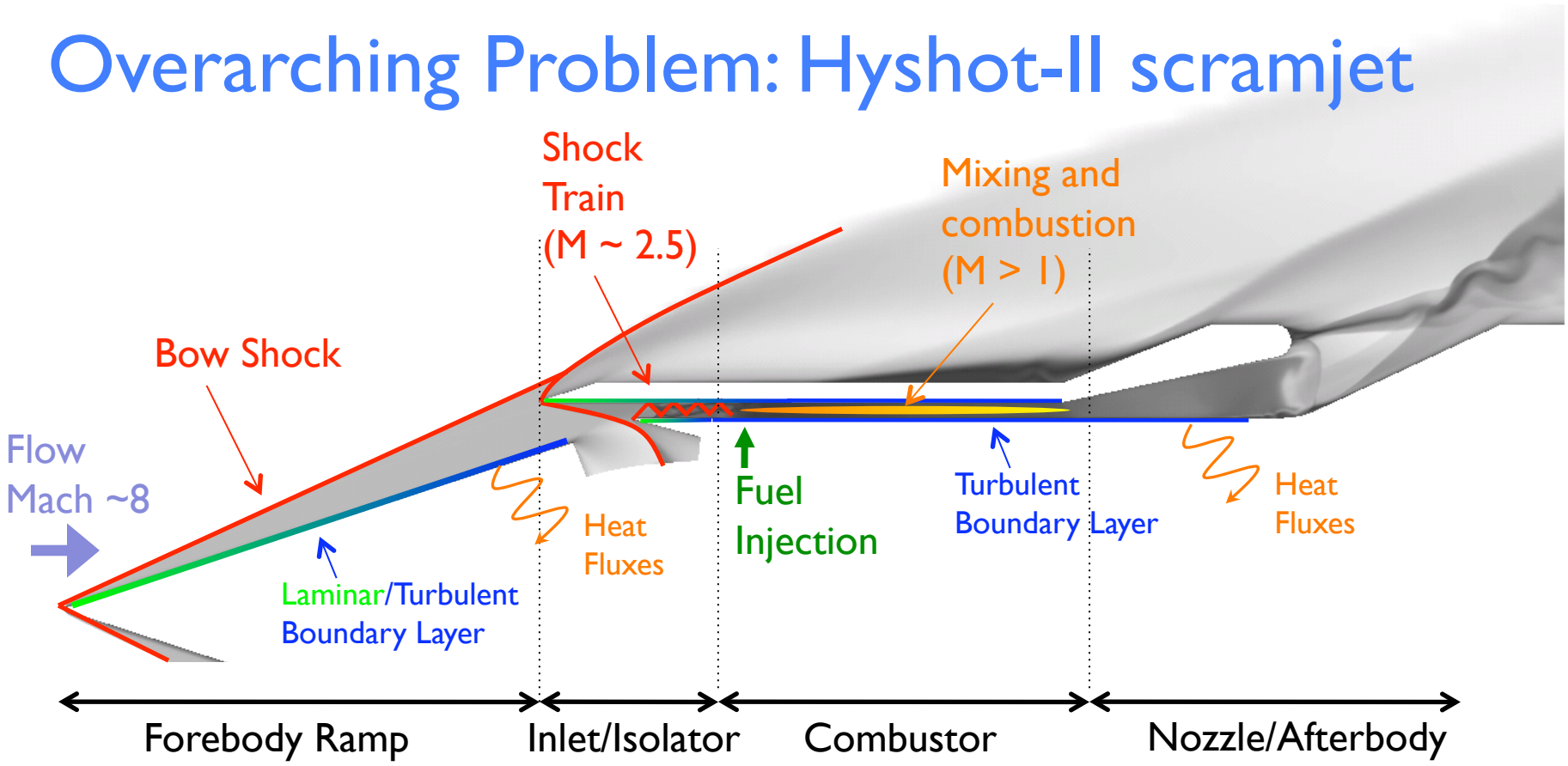
Parviz Moin

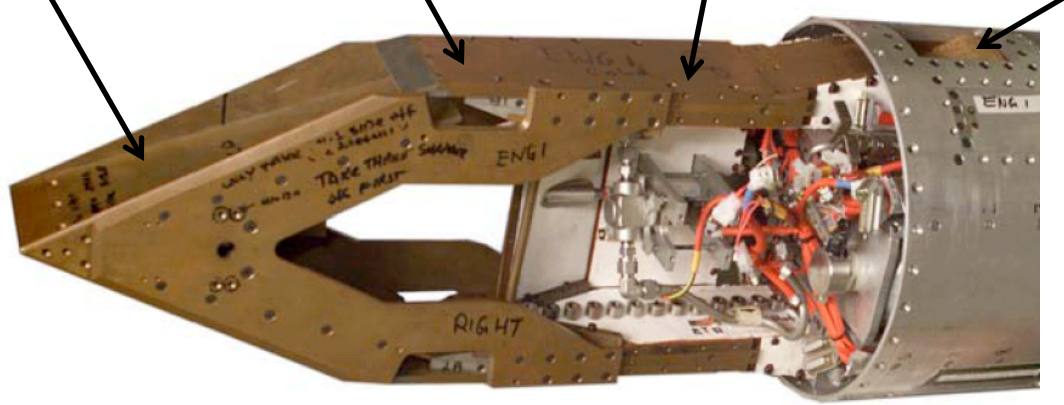
Stanford PSAAP Center

University of Michigan

STONY BROOK
STATE UNIVERSITY OF NEW YORK

Overarching Problem: Hyshot-II scramjet





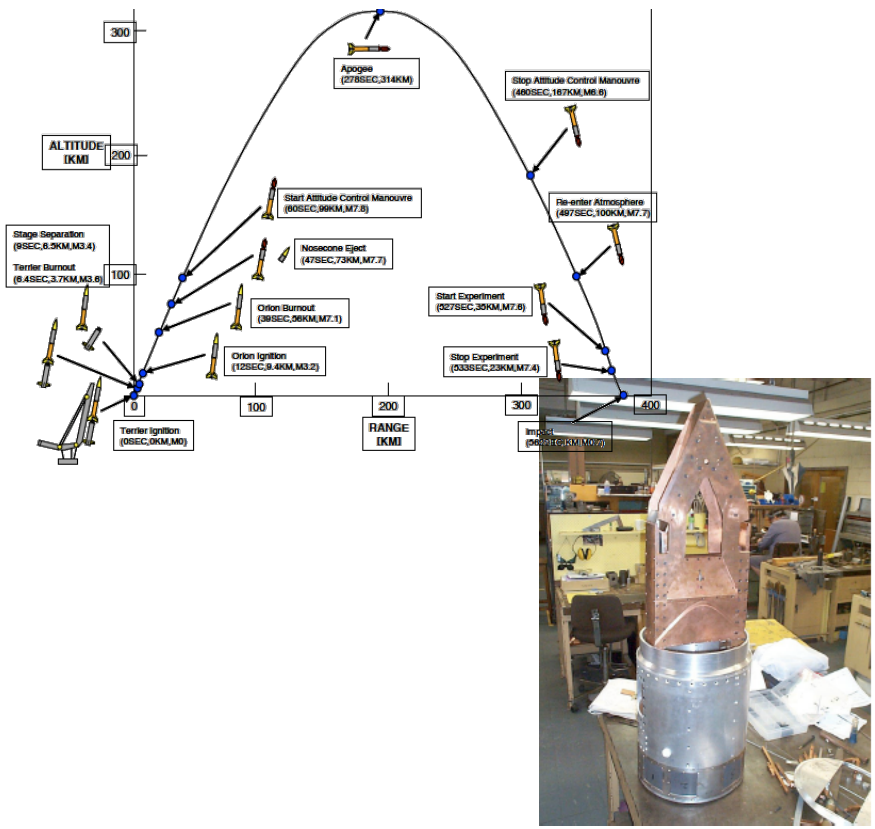
"Hot" side: hydrogen fueled scramjet

"Cold" side: unfueled inlet isolator

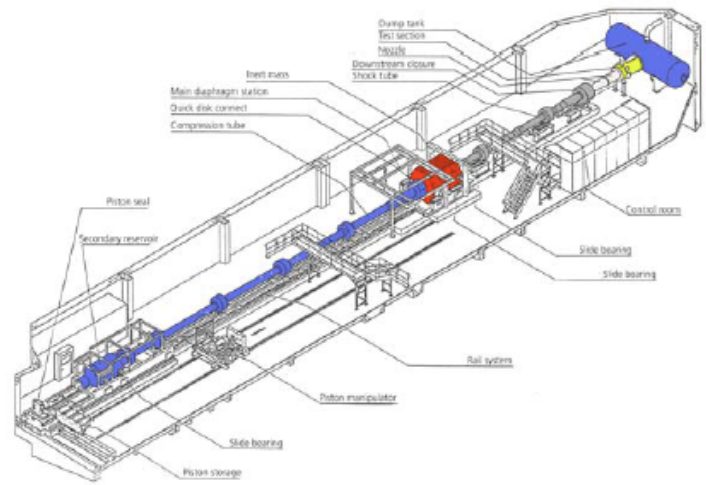
Full System Experimental Data: HyShot II

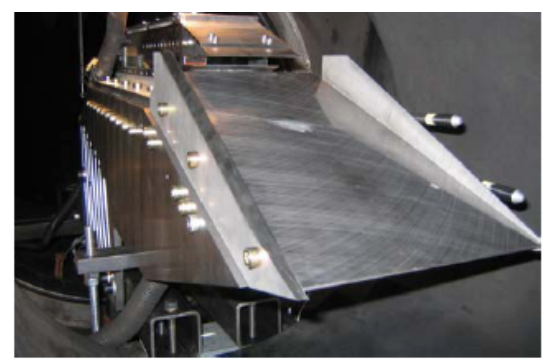
There are 2 sources of system-level experimental data, plus the potential for additional tests at DLR

Flight Test
U. Queensland, Australia, 2002



High Enthalpy Shock Tunnel
Göttingen, DE, 2008



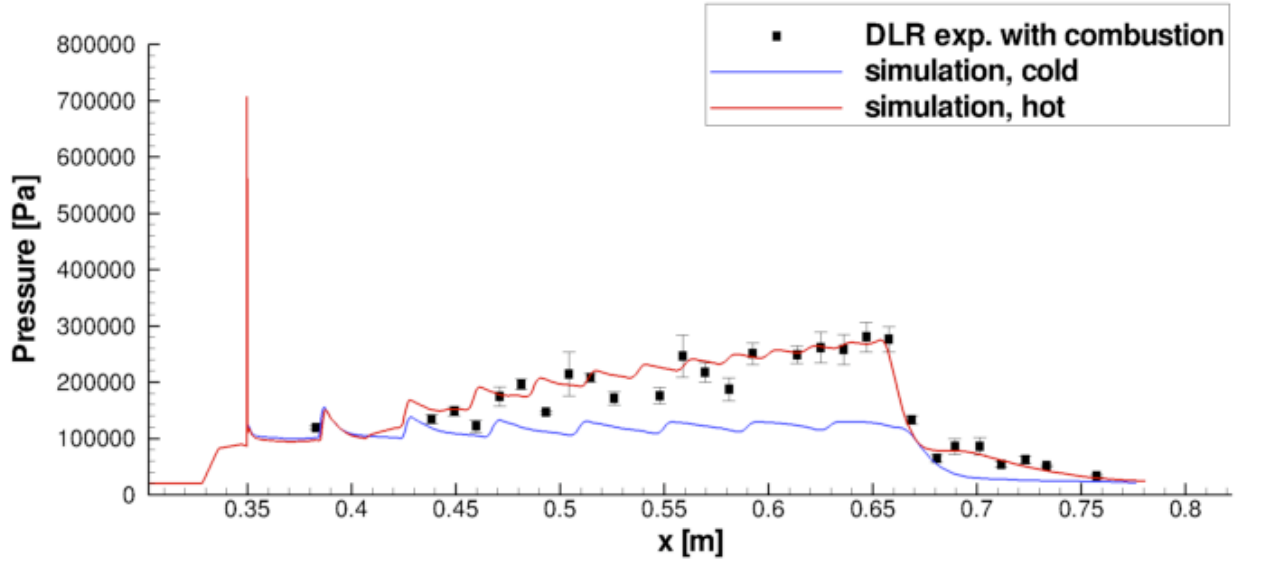


What exactly are we going to predict?

- Quantify the Margin (with uncertainty) to a particular failure mode: Unstart induced by thermal choking

Excessive heat addition in the combustor can lead to a violent ejection of the shock system from the started engine.

Result is a loss of oxygen for combustion, excessive scramjet pressures



We are a "Physics-based" Center

Because of the complex physical phenomena involved, we recognize that epistemic uncertainties (model, model form) will be major factors in the reliability of our predictions.

Can we use first-principles simulations to solve this problem?

- Compressible, Navier-Stokes equations for a reactive mixture of air and hydrogen
  - turbulence length scales = $\Delta y+$=1E-6 m
  - reaction time scales = 1E-9 to 1E-8 s
  - number of species = 10 species, 30 reactions
  - spatial scales (combustor flow path) = 0.5 m x 0.1 m x 0.01 m
  - duration of unstart = 0.001 to 0.1s

Cost of an unstart simulation ~1E+14 zones x 15 dof x 1E+8 steps,
~ 1 year on 1 million 2009 cores

We are a "Physics-based" Center

But that is not enough…

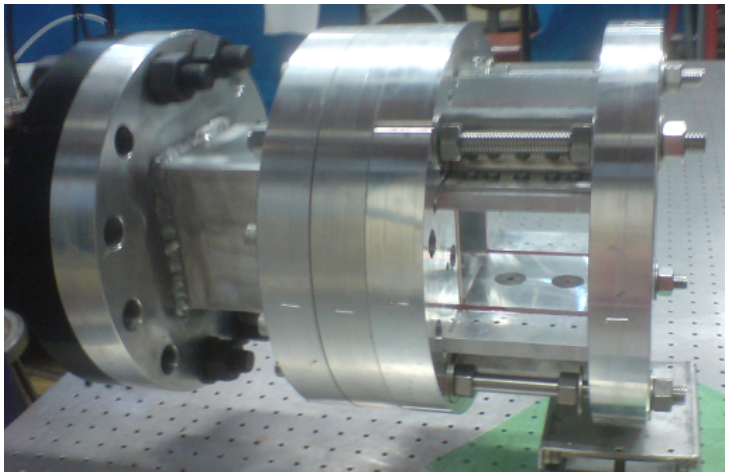
- Still need to propagate irreducible (aleatory) uncertainties through our first-principles simulations: angle of attack, inflow conditions, geometry, etc…
- Not possible!
- Reduced-order models and inevitable epistemic uncertainties will be part of our simulations and must be characterized (and reduced if necessary)

Our Solution: a multi-fidelity approach that leverages our strengths in experiments, high-fidelity simulation, and physics-based modeling.

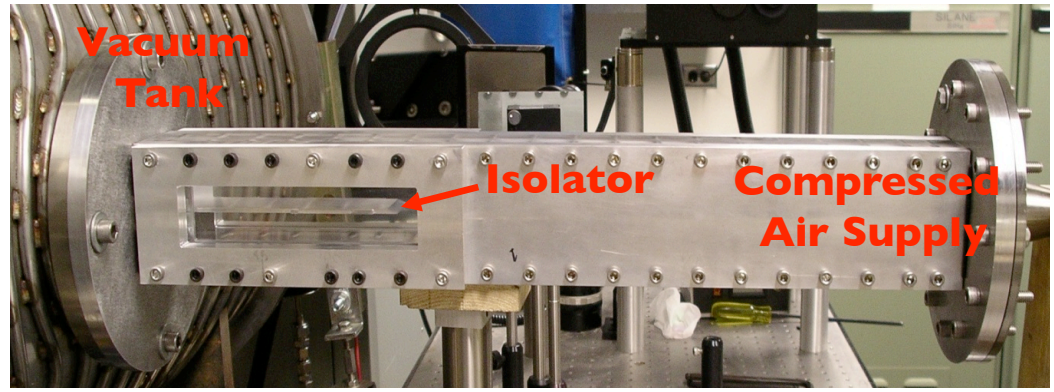
Center Ingredients

- Experimental Validation
  - In-house & external: full system, sub-system, component level
- Simulation Infrastructure
  - Both high-fidelity and lower-fidelity
  - Numerical Analysis and Methods
  - Verification
  - Future computing paradigms
- Physics-based Reduced-order Modeling
- UQ
  - Research in algorithms and methods

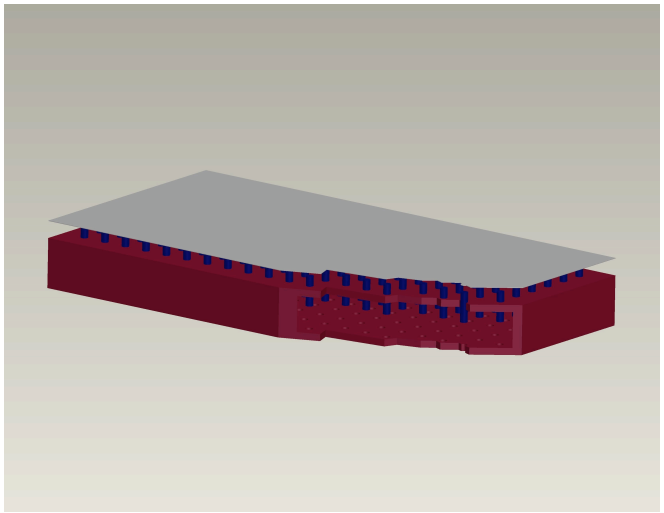
In-house Experimental Campaign



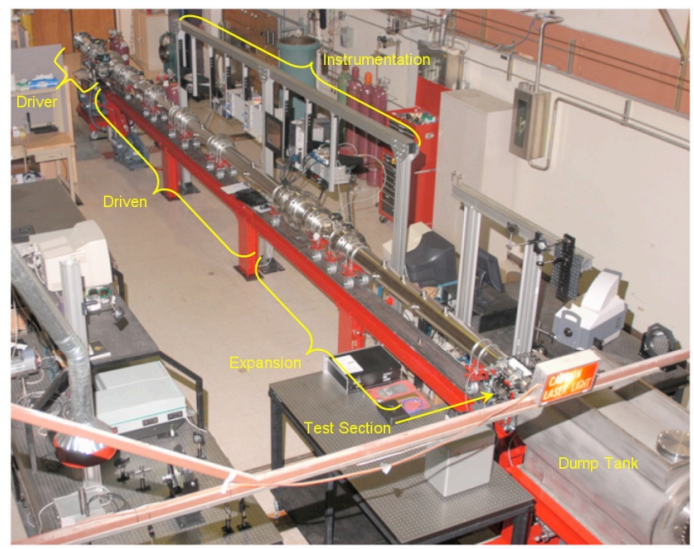
Hanson Shock Tube/Laser Studies: Chemical kinetics and flow imaging



Cappelli: Unstart induced by mass injection in a model isolator



Eaton: UQ of shock/boundary layer interaction



Mungal: Mixing and combustion in supersonic flows

Meet the center solvers

Joe

- Multi-physics integrated code for full system simulation
- unstructured steady and unsteady RANS
- Flamelet-based chemistry

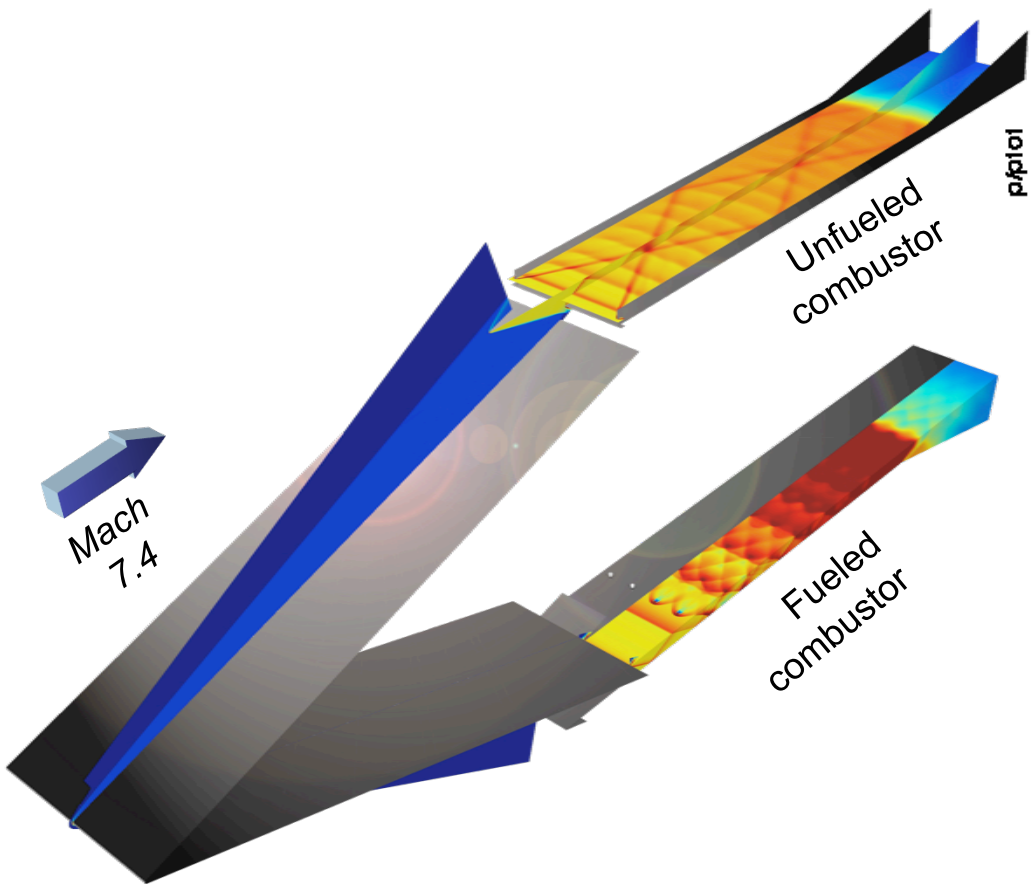
Ray

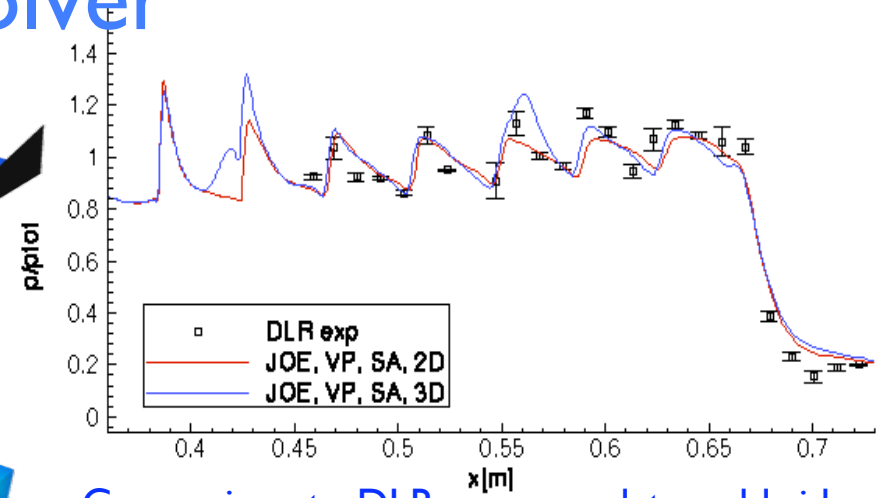
- Facilitates non-intrusive UQ for Joe
- Eventual support for weakly-intrusive UQ methodologies

Charles

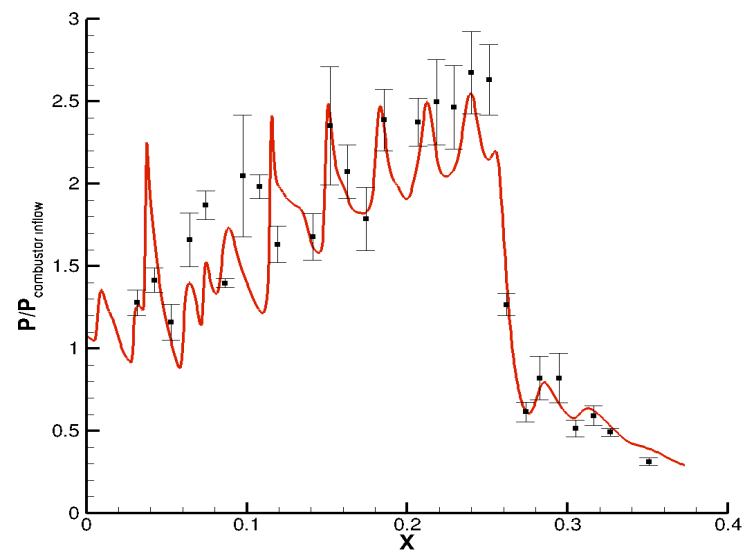
- unstructured compressible LES solver
- Low-dispersion and dissipation grid-sensitive operators

Sample Joe Simulation: Full System integrated RANS solver





- Comparison to DLR pressure data: cold side 2D and 3D



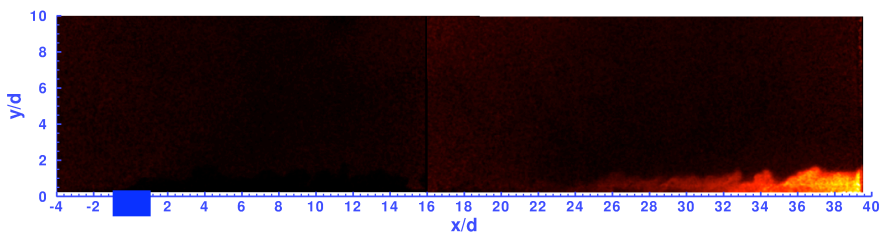
- Comparison to DLR pressure data: hot side

Comparison with jet-in-crossflow experiment

Jet-in-crossflow experiment

- OH-PLIF measurements
- External flow
- Free stream conditions:
  - M = 2.4
  - P = 35 kPa
  - T = 1500-1600 K
- J = 0.2

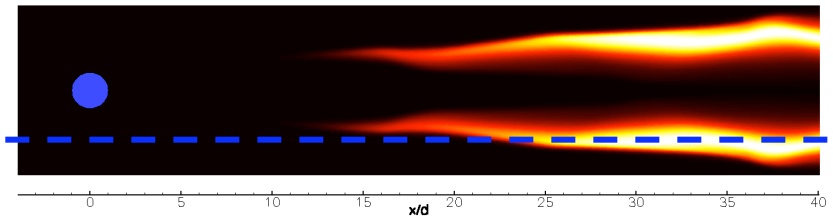
OH-PLIF in x-y plane at z/d* = 5



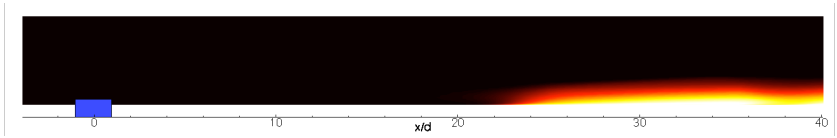
HyShot II simulation

- Internal flow (shock reflections, symmetry)
- Combustor inflow conditions:
  - M = 2.4
  - P = 100 kPa
  - T = 1100-1200 K
- J = 0.3

OH mass fraction in x-z plane at y/d* = 0.05

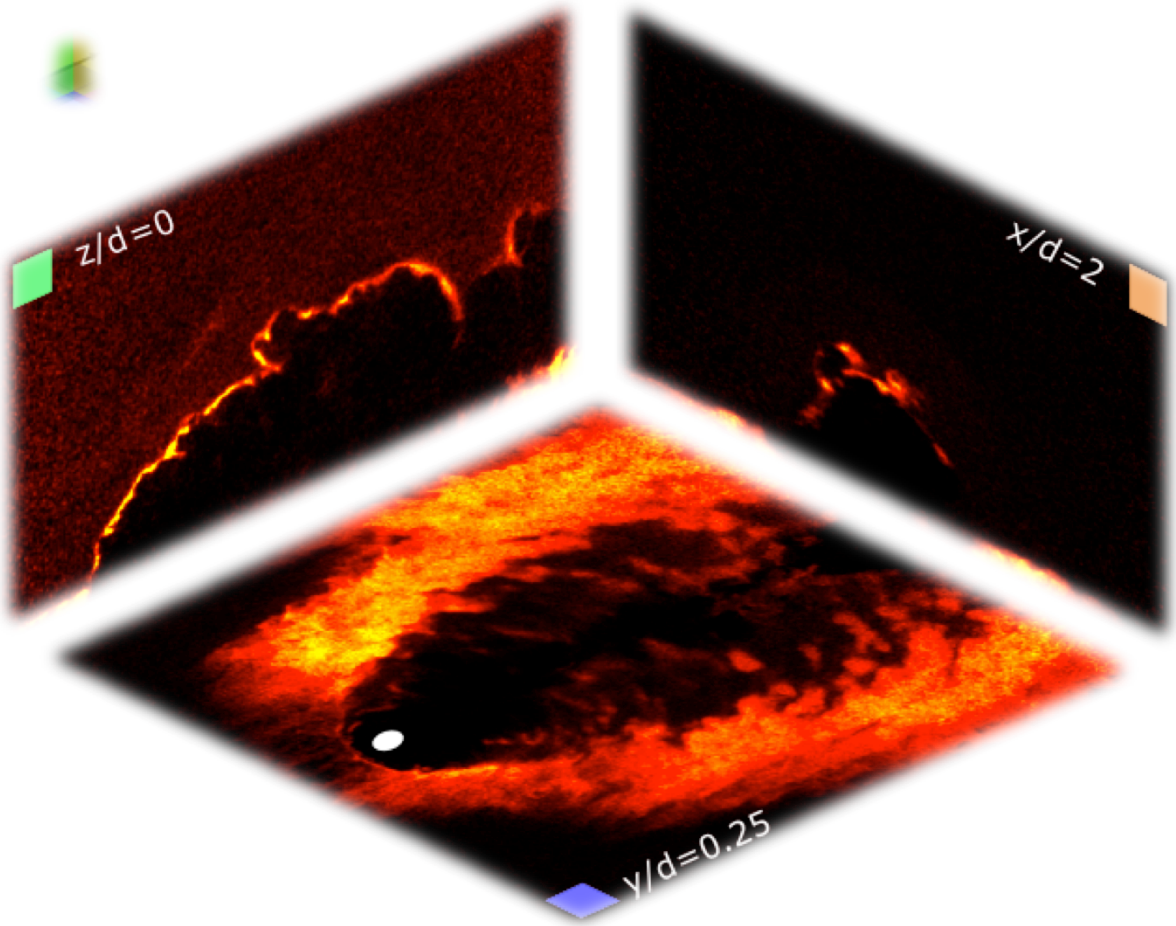


OH mass fracion in x-y plane at z/d* = 2.5



* d = 2mm

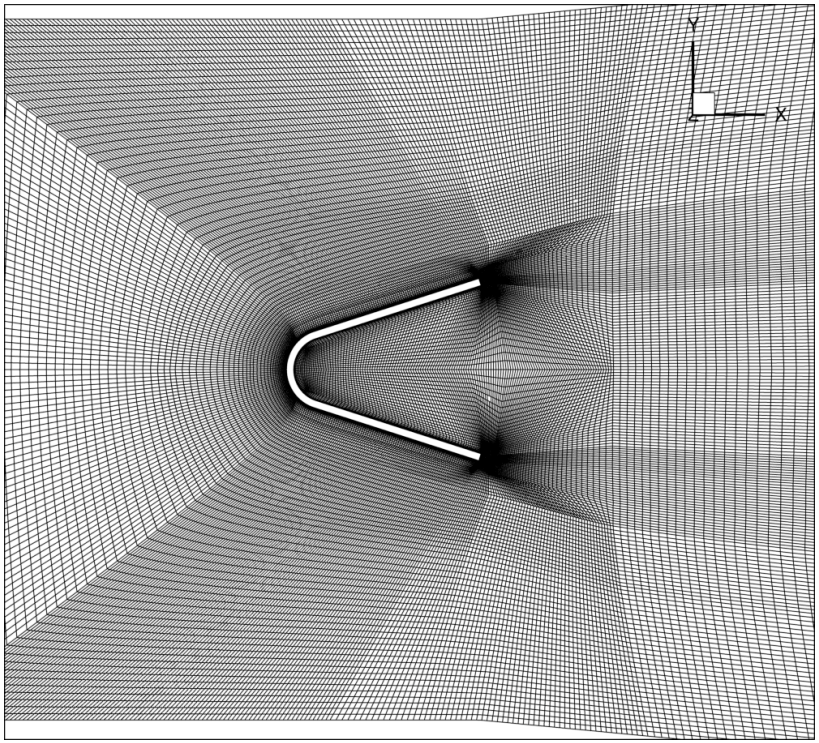
Surprise: Experimental results at higher J



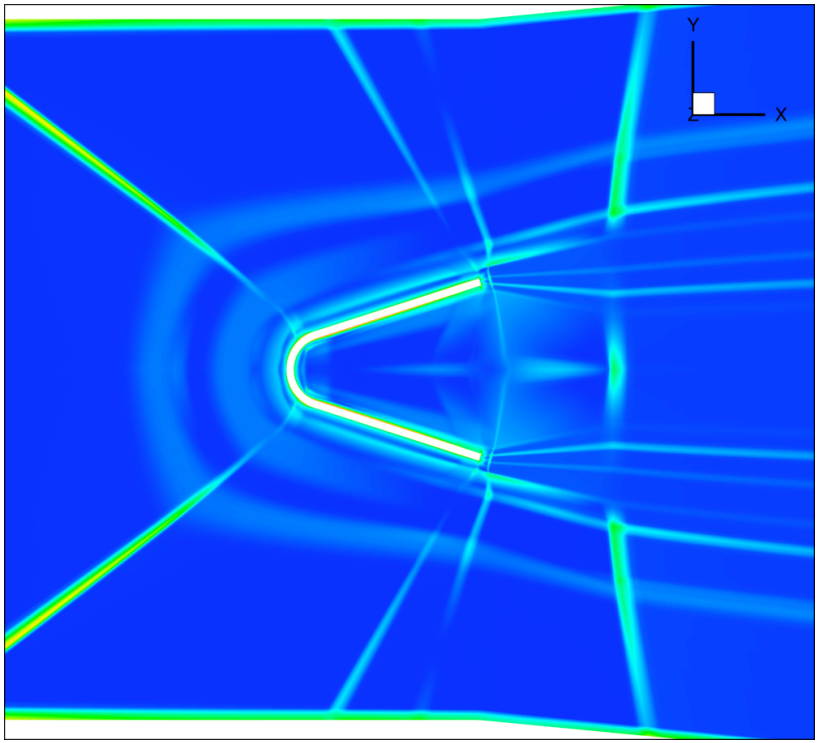
Composite image showing the instantaneous reaction zone on three orthogonal planes for the transverse hydrogen injection at J=2.4 (freestream conditions: T=1500 K, To=2800 K, M=2.4, p=40 kPa.

Charles: Compressible LES on Unstructured Grids

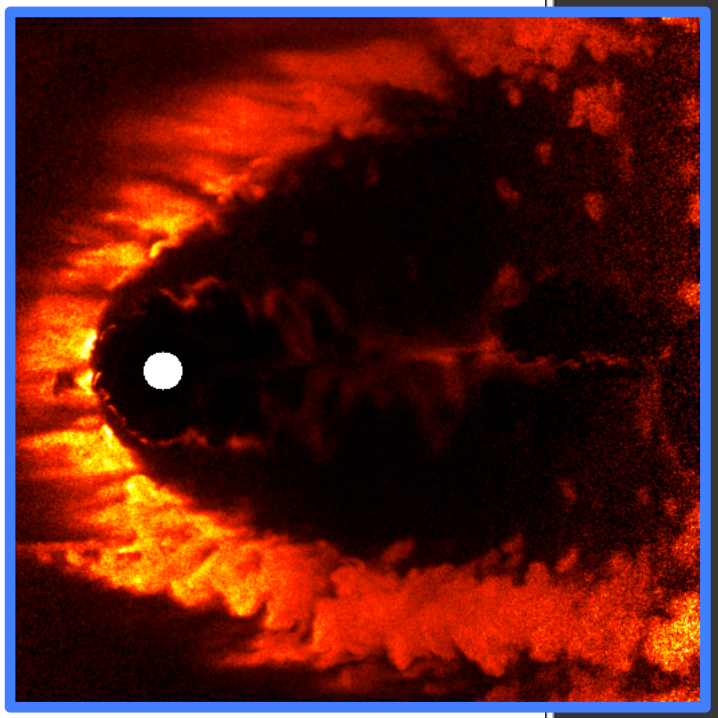
- Minimal dissipation and dispersion is critical
- Developing grid-sensitive methods that use Summation-by-Parts ideas to modify operators in regions of lower mesh quality



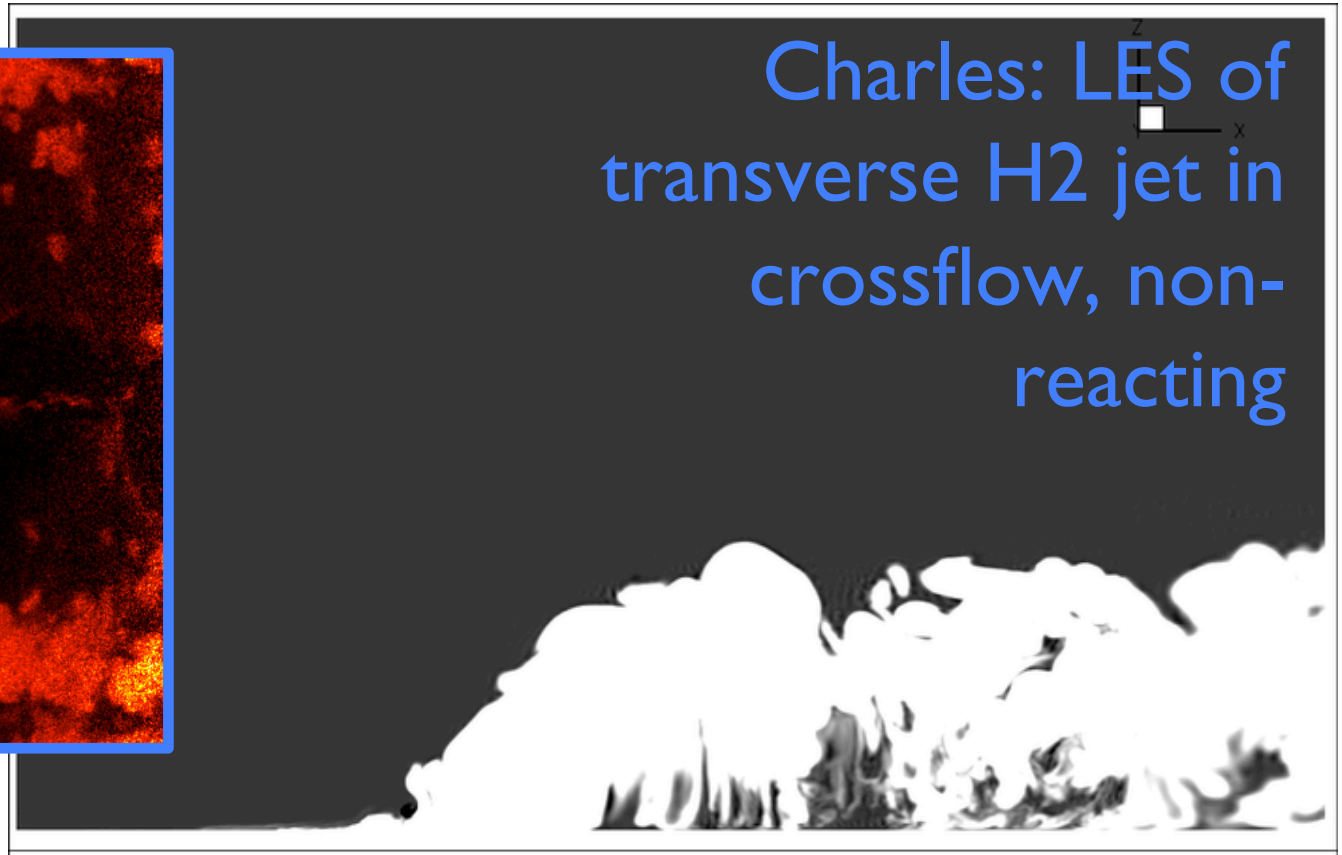
Sample Mesh detail in plane through flameholder geometry

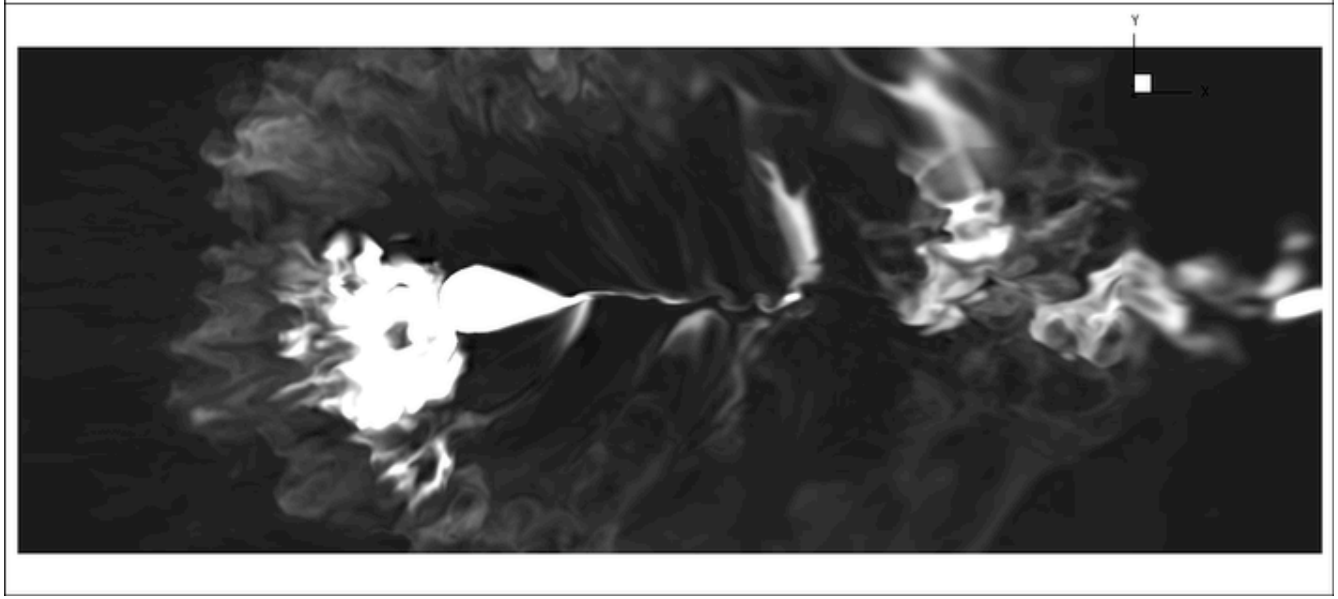


Quality indicator: Row-norm of the symmetric part of differencing matrix D

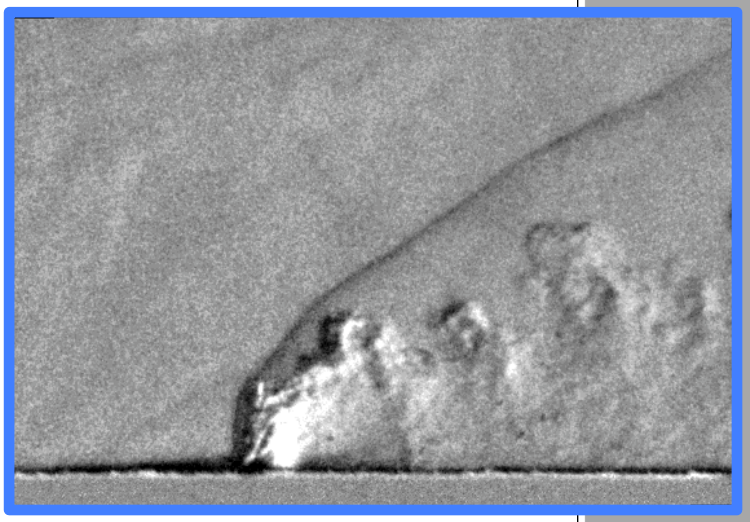


OH PLIF of Will Heltsley, PhD Dissertation, Stanford University, 2009

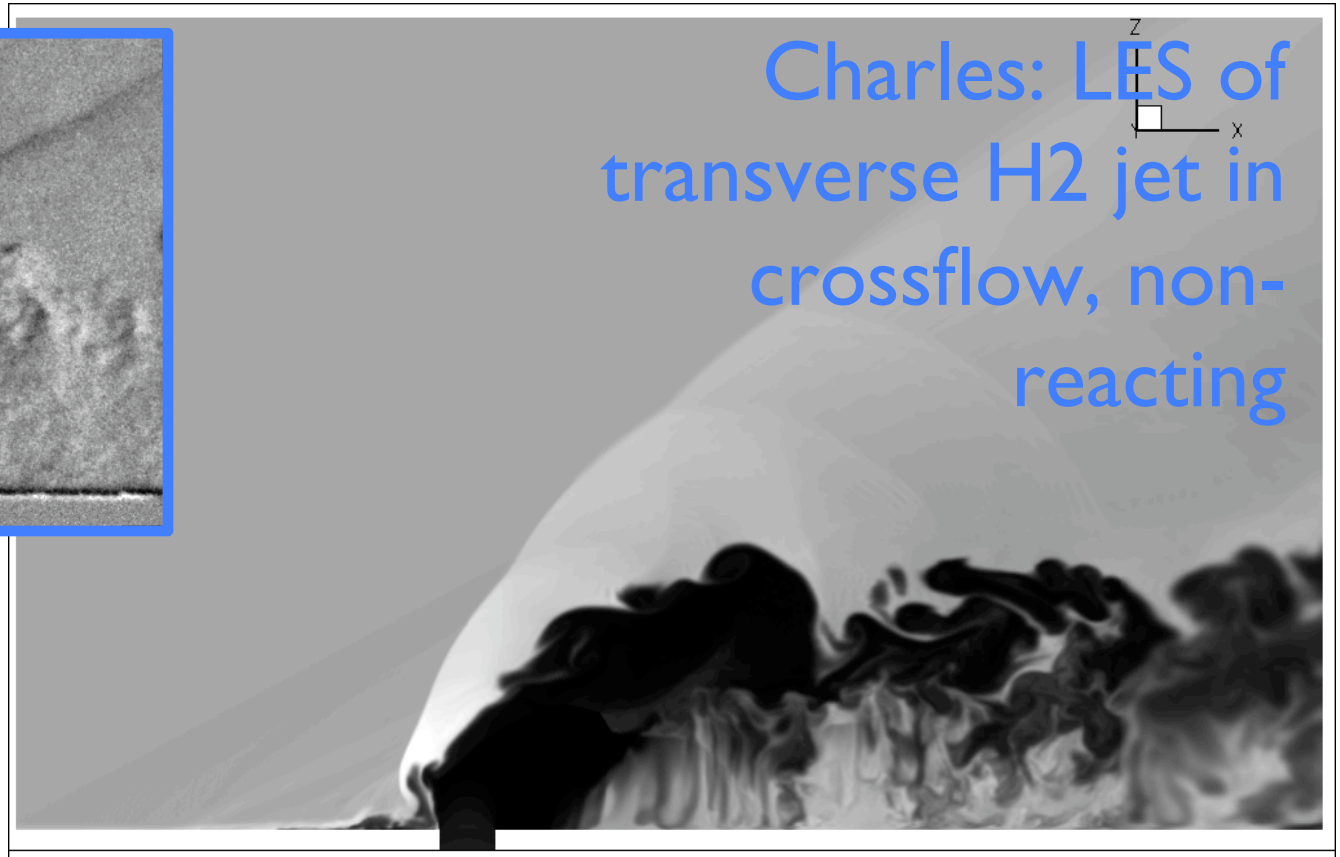




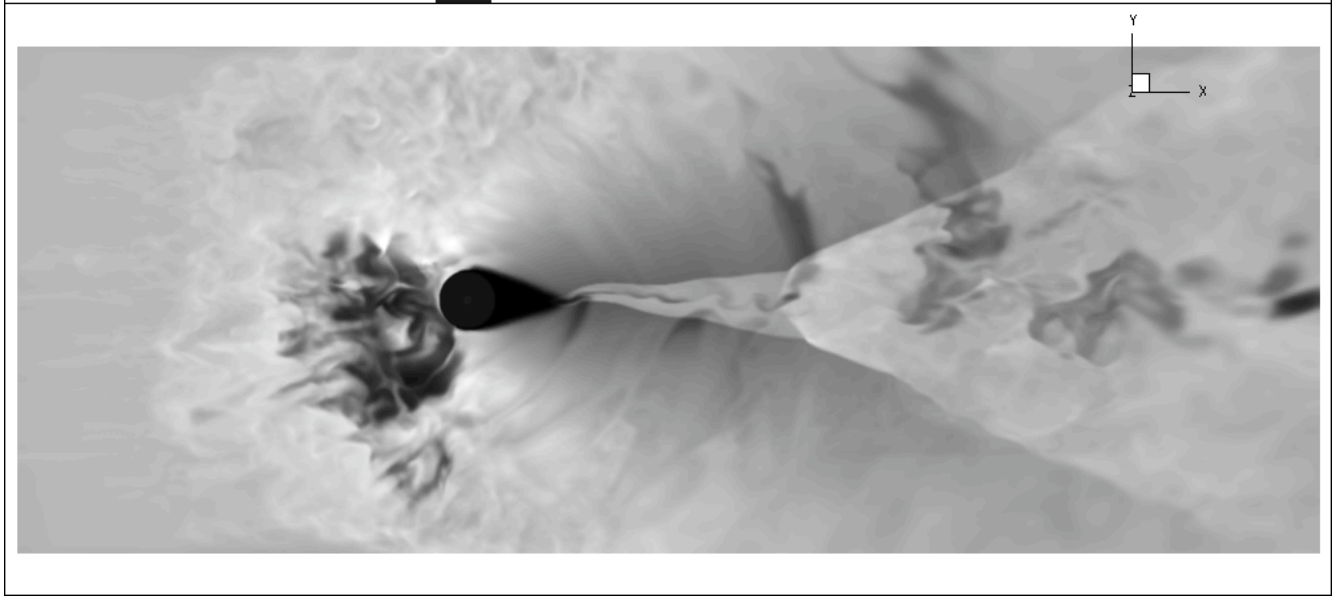
Instantaneous H2 mass fraction from non-reacting Charles simulation



HTGL Experiments: Schlieren of Non-reacting flow

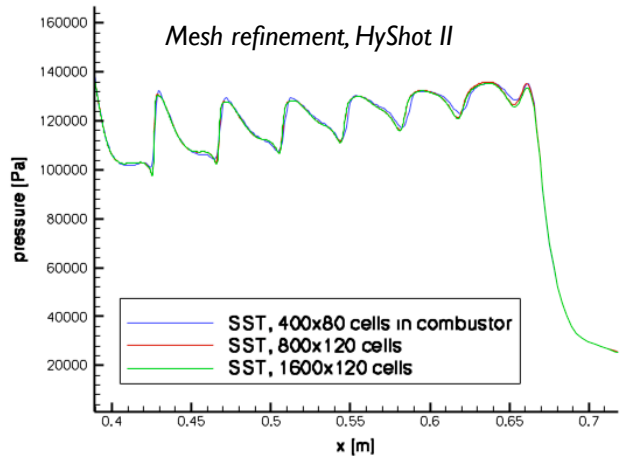


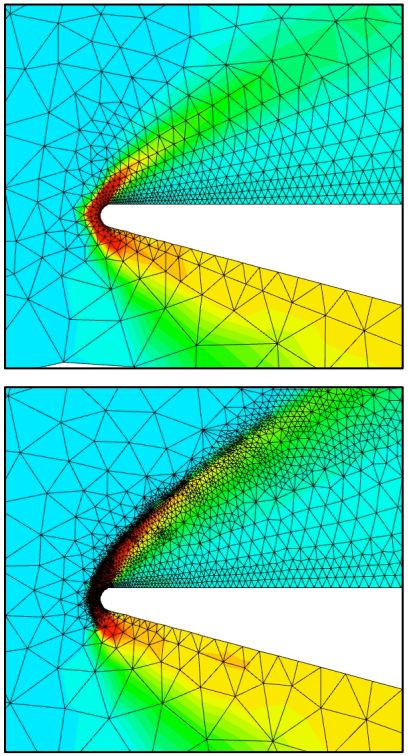
Temperature from a Charles simulation of non-reacting H2 jet in supersonic crossflow



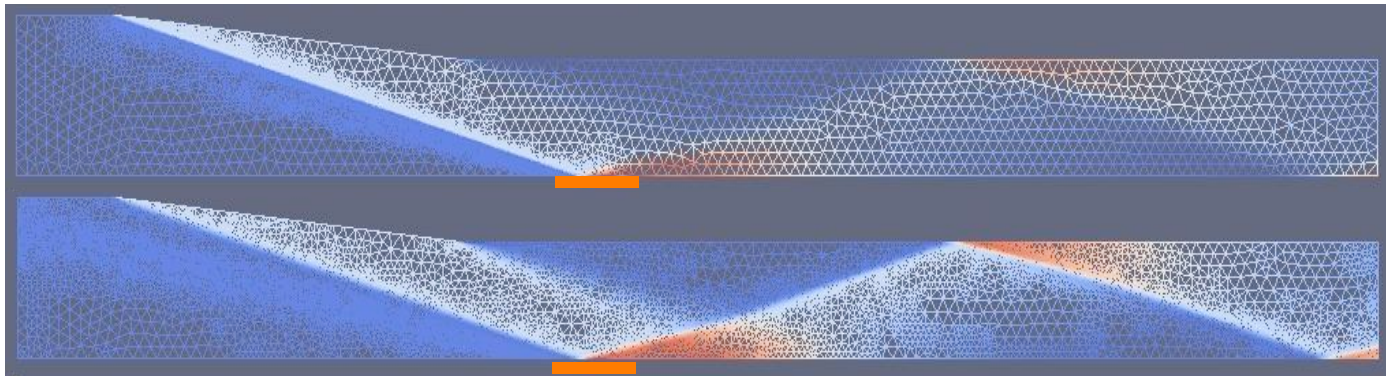
Verification Activities

- Goal: to make numerical error *estimation* and *control* both *automated* and *pervasive* in our simulations
- Many methods pursued simultaneously: mesh refinement, MMS, invariance, mesh-independent LES
- Strong focus on applications of adjoint solvers to verification/UQ activities
- Ultimate question is how to add "numerical error bars" to our simulations and how to adapt a mesh to reduce numerical errors only as much as is needed





HyShot II discrete adjoint Goal-oriented mesh adaptation and error estimation



Adjoint-based (top) and new robust grid adaptation for UQ (bottom) to compute pressure on orange surface

UQ Science

Goals: Develop and implement a range of methodologies to address the direct needs of the Center, as well as fundamental research in UQ Science

- Discontinuous responses:
  - E.g Pade/Legendre Collocation method
- High-dimensional parameter space:
  - Intrusive: Alternating Least Squares
  - Non-Intrusive: Compressing Sensing (in collaboration with CalTech)
  - Risk analysis using adjoints (with Q. Wang, now MIT)
- Ranking of the Uncertainties
  - Variance decomposition (in collaboration with Sandia)
- Multiphysics Coupling
  - Weakly Intrusive Approach (with P. Constantine, now Sandia)

Epistemic "Structural" Uncertainties

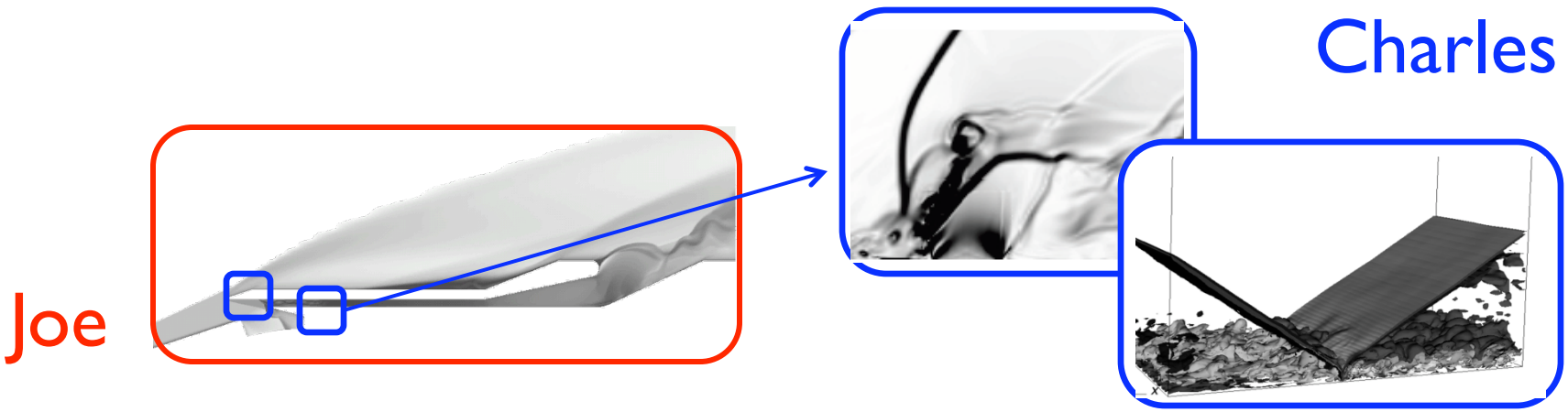
- Important Focus of the Center: *Uncertainty deriving from the use of physical models, e.g. combustion models, turbulence models*

Observations:

- Can dominate overall uncertainties in the predictions
- Not efficiently described by "random" parameters
- Likely intractable: very high-dimensional functional space, non-linear, time-dependent, etc., needs physical insight

Epistemic "Structural" Uncertainties

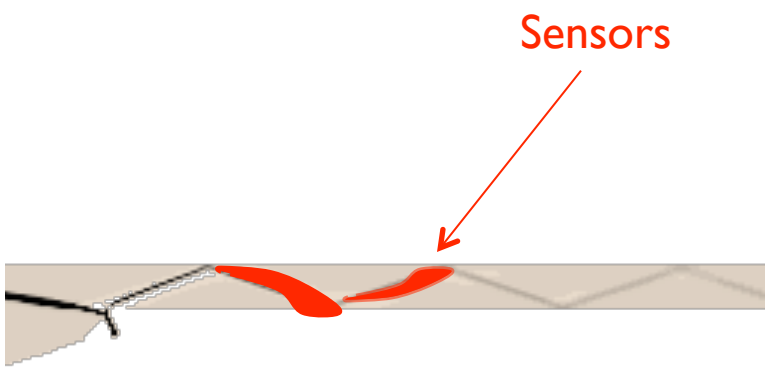
Approach (I): Use sub-system experiments and complementary high-fidelity (first principle) simulations

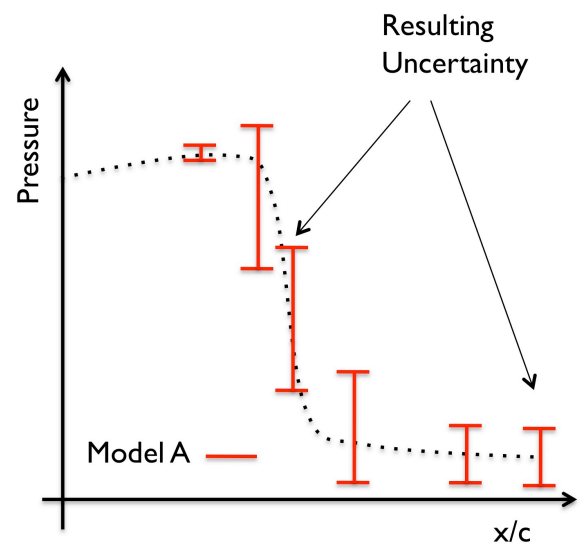


Epistemic "Structural" Uncertainties

Approach (II): Define sensors and bounds

- Sensors: identify regions in physical space where the assumption in the models are questionable or inapplicable
- Bounds: inject uncertainty locally according to known limiting behavior





The uncertainty is "produced" by the models only if some assumptions are "locally" violated

Future Computing Paradigms

PSAAP computational & computer scientists are collaborating to develop a domain-specific language for mesh-based PDE's: Liszt

Productivity & Performance

- Separate domain expertise (computational science) from computer science expertise
- Super-optimize using a combination of domain knowledge and platform knowledge

Portability

- Run on wide range of heterogeneous platforms

Innovation

- Allows vendors to change architecture and programming models in revolutionary ways

We have a simplified Joe solver running in Liszt with both MPI and OpenMP back-ends.