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

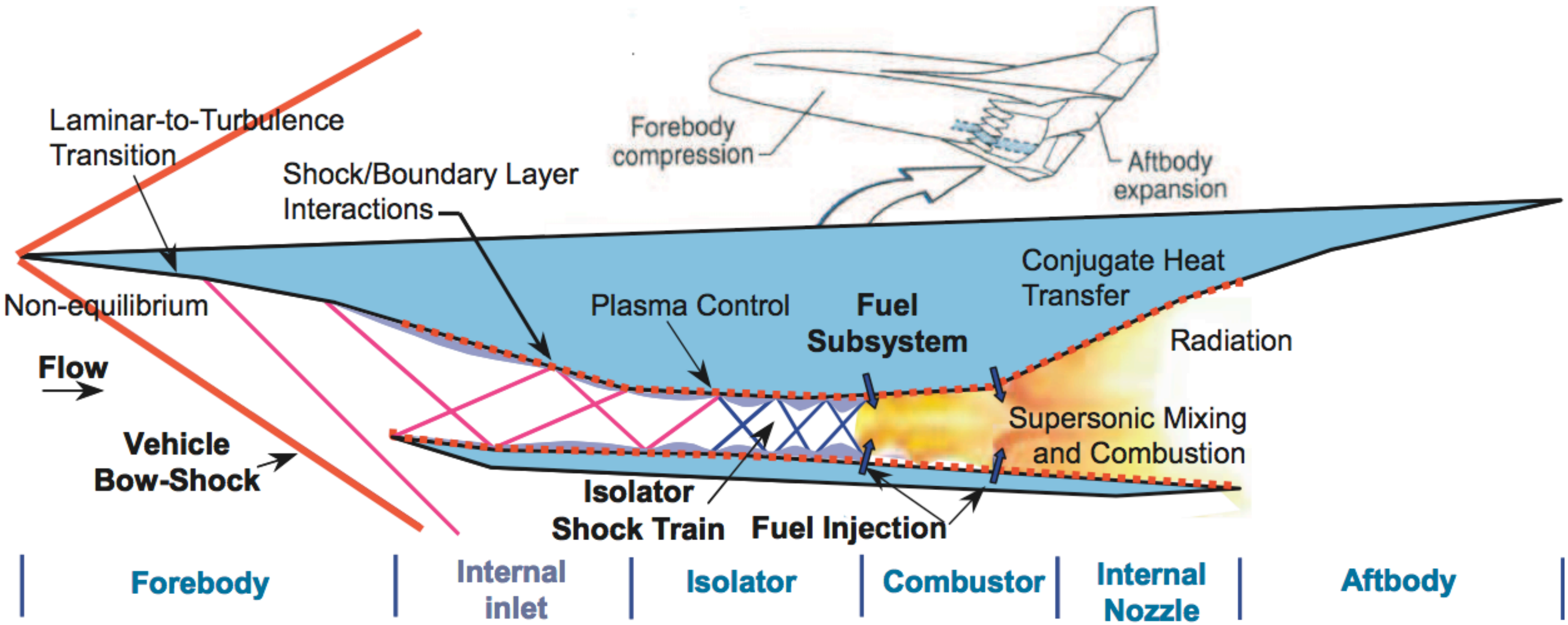
Overarching problem

Predictive simulation of the coupled physics of the unstart problem of the propulsion system of a hypersonic cruise vehicle

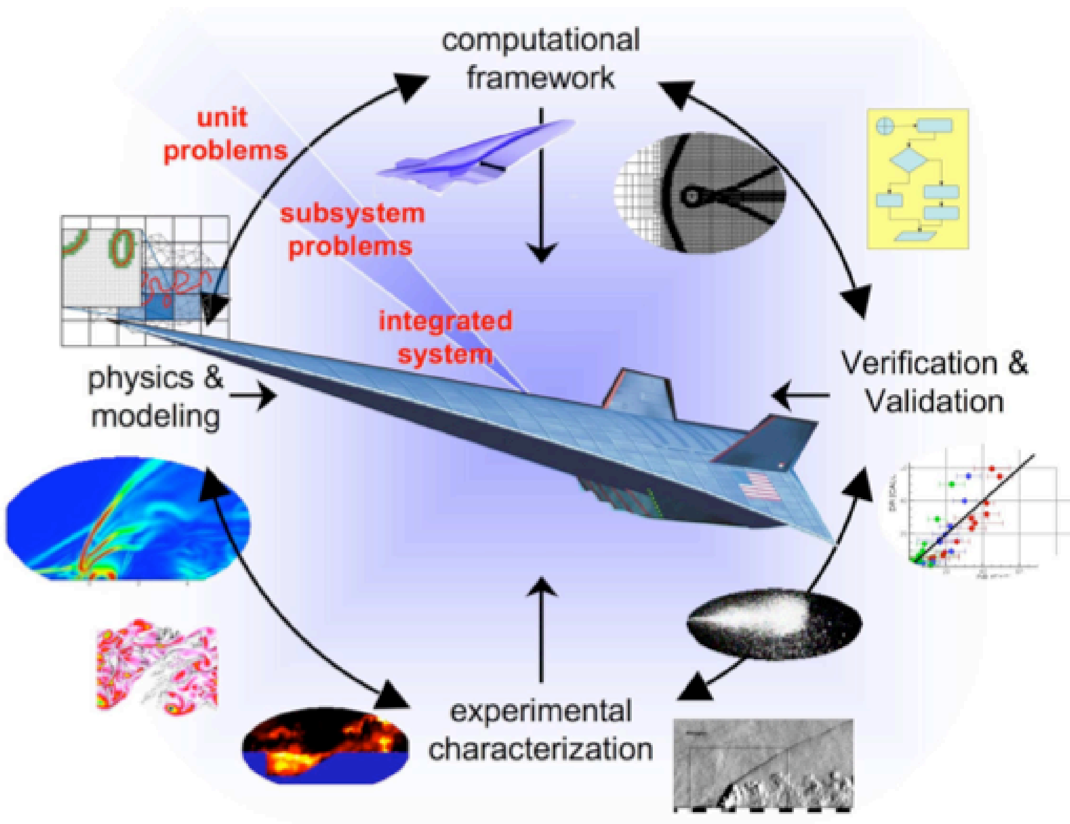
- Build a mixed fidelity, multidisciplinary, V&V'd computational infrastructure for the simulation of this complex, highly integrated engineering system

- Components
  - Code Development and Deployment
  - Numerical Analysis and Algorithms
  - Physical Modeling
  - Simulation
  - Verification & Validation
  - UQ Strategy

Integrated Physics of a Hypersonic Vehicle



Towards prediction...



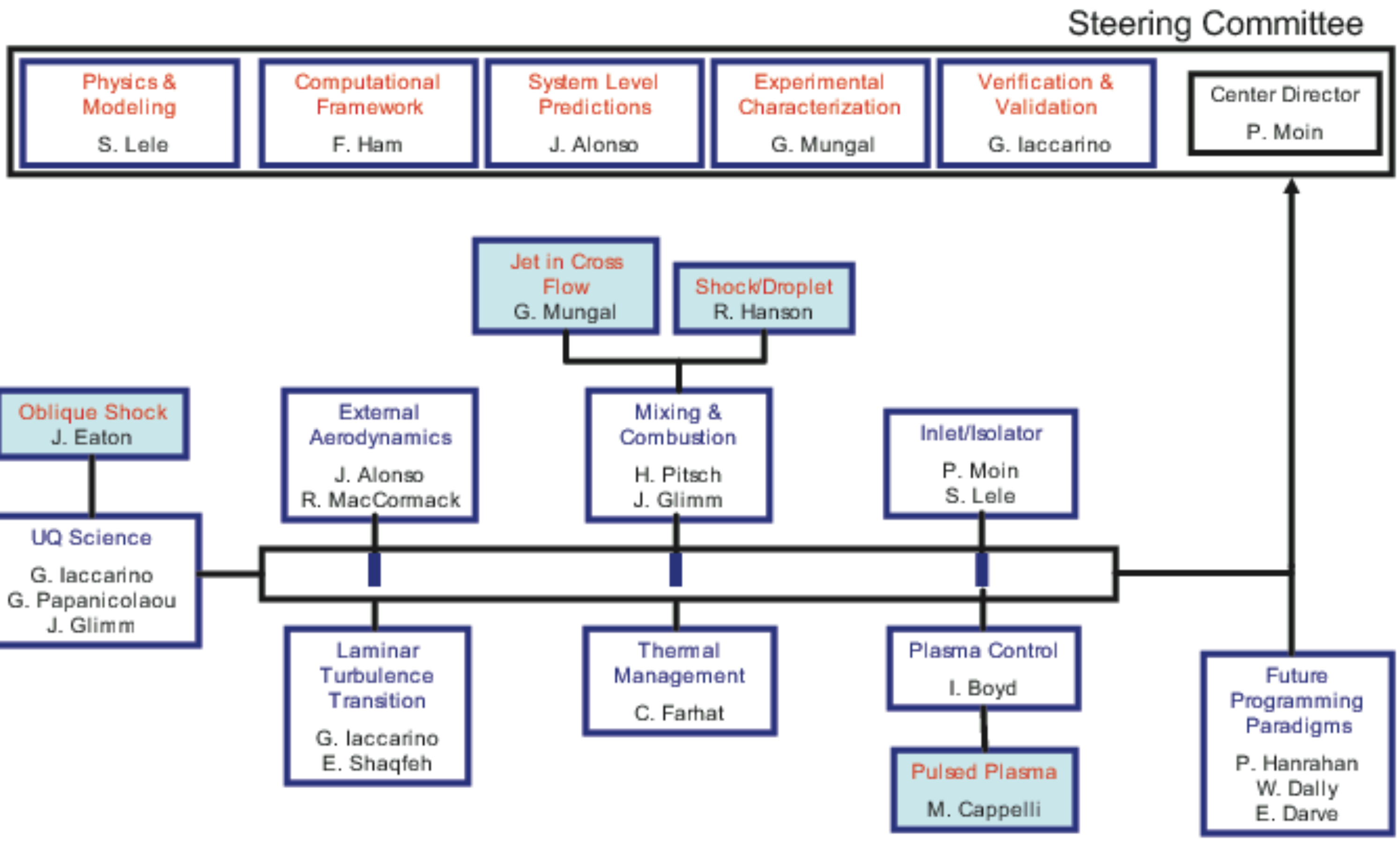
- The successful development of a predictive simulation capability will require the tight coupling of these 4 research areas
- The Center's organization structure reflects this vision

The Center

- 16 Stanford faculty members from 5 departments (Computer Science, Mechanical Engineering, Aeronautics and Astronautics, Chemical Engineering, Mathematics, and the Institute for Computational and Mathematical Engineering).

- 2 collaborators from the State University of New York at Stony Brook (led by James Glimm) and the University of Michigan (led by Iain Boyd)

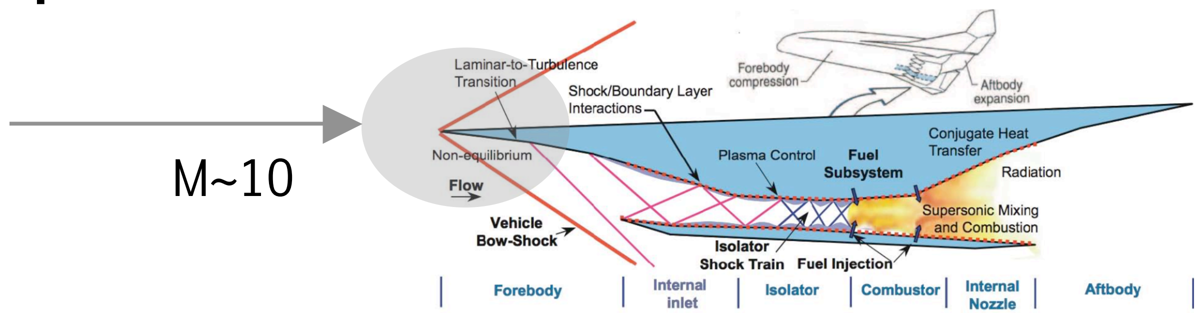
Center's Organizational Structure



- 7 topical groups distinguished by their simulation codes
  - Important sub-system linkages identified by vertical blue lines
- 4 experiments
- Steering committee with representation from all disciplines

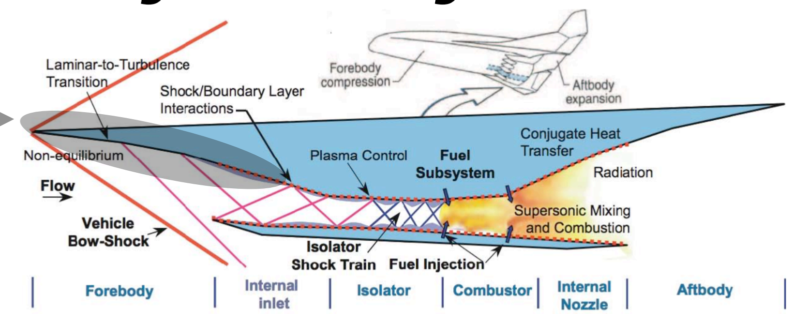
Physics Components and Challenges

External Hypersonic Flow



- High-speed flow creates shock waves:
  - Significant increase in temperature and pressure
  - Real gas effects (internal energy, nonequilibrium thermal processes)
  - Separate vibrational energy equation
  - Coupling with heat transfer in the structure

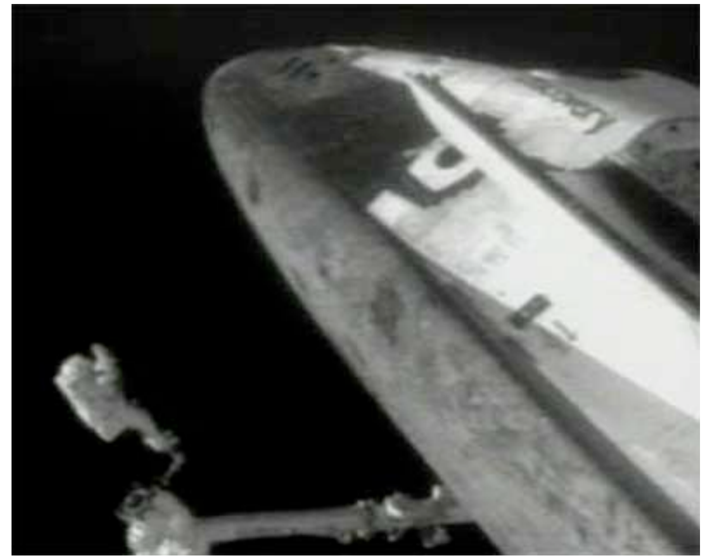
Hypersonic Boundary Layer Physics



- Boundary layer formed on external vehicle surfaces:
  - Determines critical element of thermal load
  - Strongly affected by laminar/turbulent transition
  - Few reliable experiments (tunnel noise)
  - Affects flow entering the scramjet
  - Shock-boundary layer interactions
  - Critical element of engine unstart phenomenon

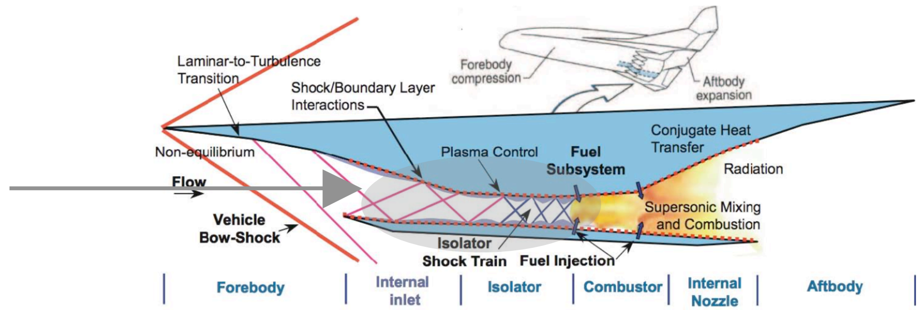
Laminar to Turbulence Transition

- Predicting heat loads is of critical importance to hypersonic systems, heat loads depend strongly on the transition to turbulence



- Current transition simulation capability not predictive
  - During STS-114 gap-filler problem, Simulations could not agree on transition prediction

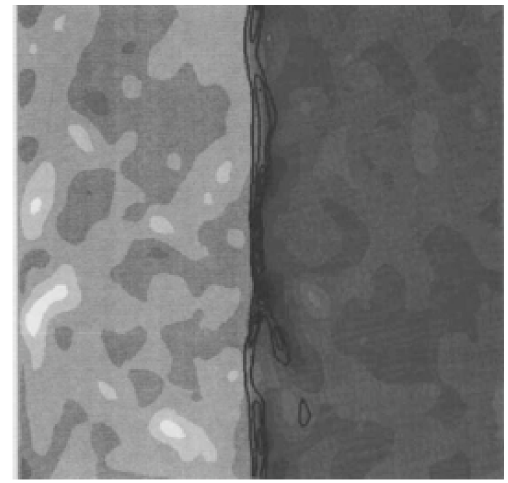
Inlet/Isolator Physics



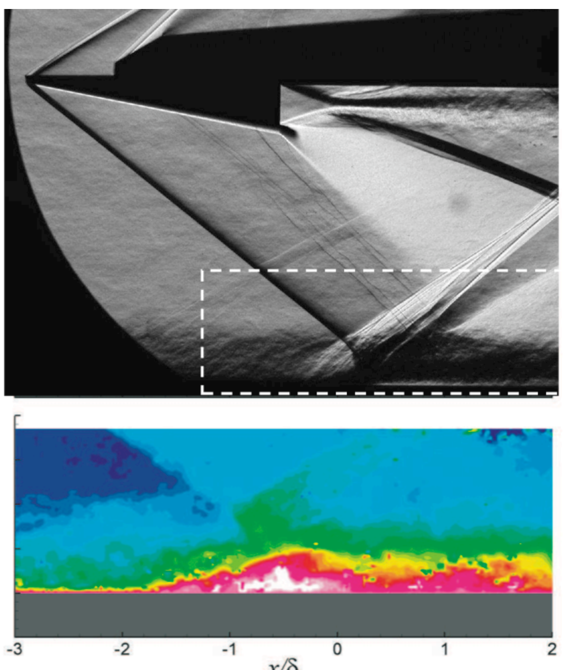
- Complex flow patterns (shock train):
  - Shock-shock and shock-boundary layer interactions
  - Moving shocks
  - Boundary layer separation (leading to unstart) due to adverse pressure gradient from combustor
  - Resolution of complex turbulent flow structures
  - Plasma flow control

Shock/Turbulence Interaction

- Conflicting requirements of low-dissipation numerics for broad-band turbulence and high-Ma shock capturing



Simulation of S. Lee, Moin,& Lele, JFM 1993

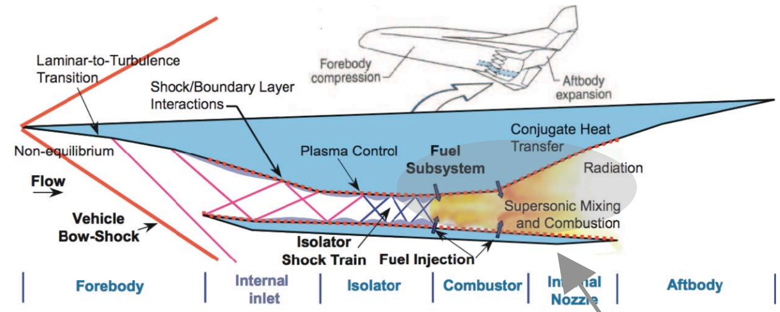


PIV from Humble et al., AIAA 2006

Shock/Boundary Layer Interaction

- Leads to highly unsteady, separated flows. RANS modeling cannot reliably predict the resulting interactions

Combustor Flow Physics

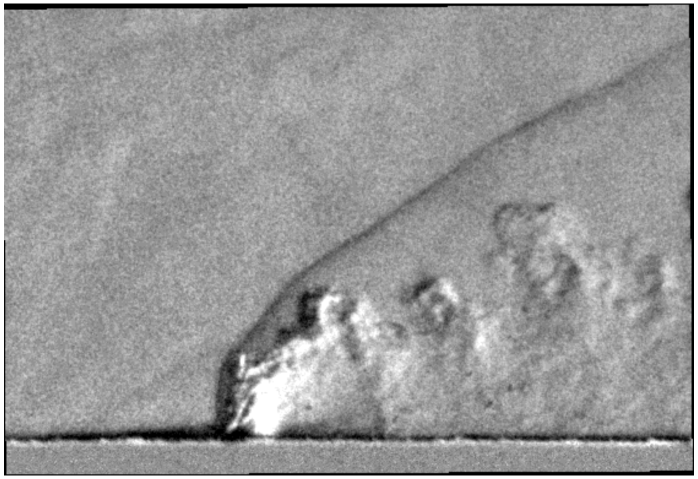


- Fuel mixing and combustion at supersonic speeds
- Potential for multiphase flow
- Turbulent and unsteady flow with intermittent ignition and quenching

- Simulation requirements:
  - Low-fidelity combustor model
  - High-fidelity combustor model (LES)
  - Multiphase combustion
  - Chemical modeling for surrogate fuels

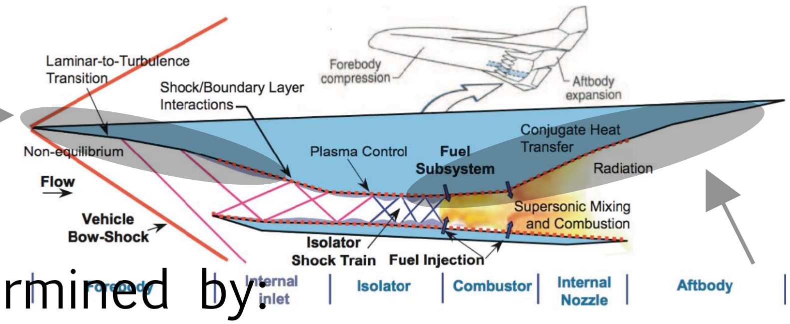
Supersonic mixing and combustion

- Thermodynamic and (even) chemical state of fuel uncertain, and tightly coupled with heat transfer to vehicle
- Transient and highly non-linear flow/chemistry interaction
- Flame stabilization very sensitive to complex interaction of local rate of molecular mixing and chemistry
  - Potential importance of density driven instabilities (RT/RM)



Supersonic Jet in Crossflow, G. Mungal

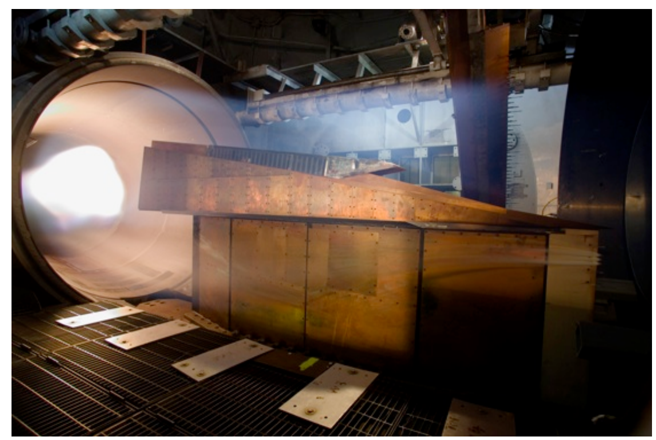
Heat Loads to Vehicle



- Internal thermal environment determined by:
  - Combustion flow processes
  - Convective heating
  - Radiation heating (nozzle)
  - Conductivity and physical properties
  - Thermal state of inhomogeneous structures
  - Conjugate heat transfer

The deformed state of the vehicle due to thermal loads can itself lead to unstart

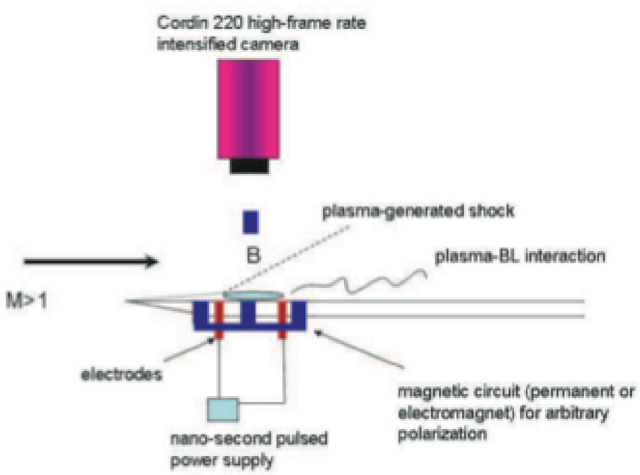
Active cooling controls the state of the fuel



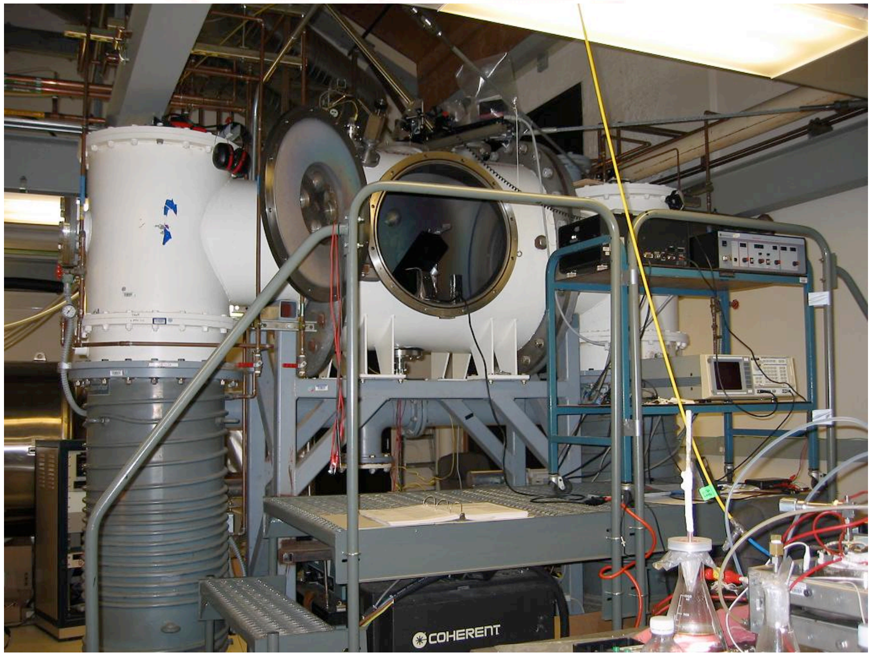
X-1 engine test for X-51

Pulsed Plasma Control

- Can plasma actuators control unstart?
- Development of a hybrid fluid/particle method for pulsed plasmas

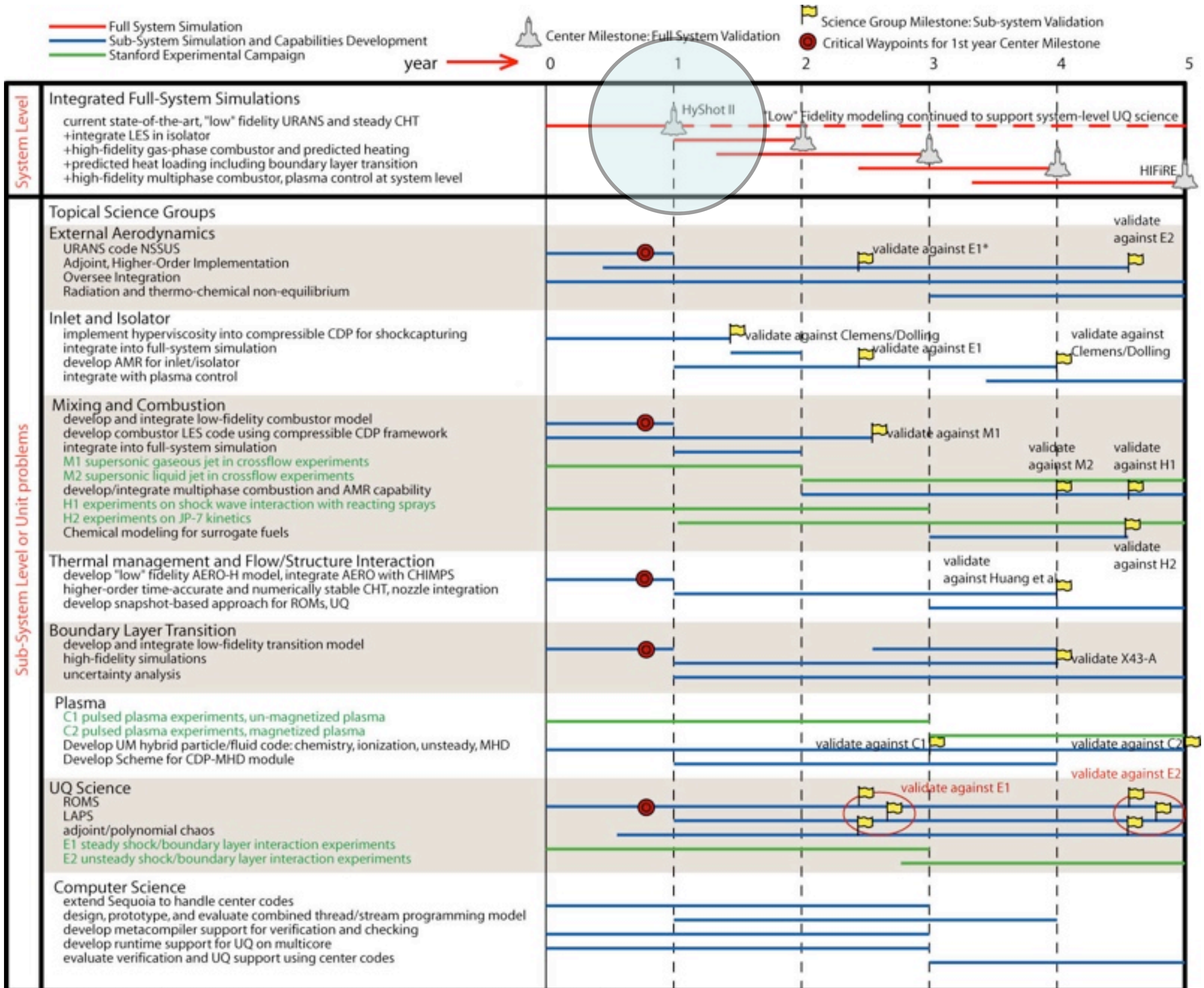


Proposed plasma experiments



Stanford's Plasma Physics Laboratory, Prof. Cappelli

Ultimate Predictability Goals and Intermediate Goals

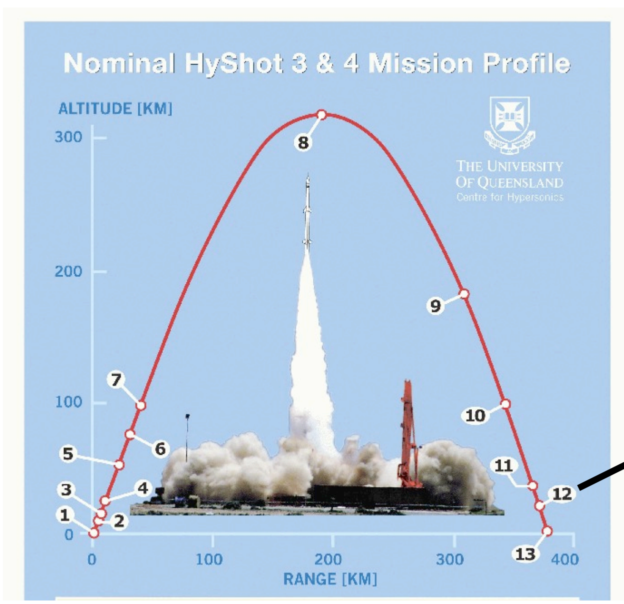


* Stanford's experiments are denoted as E1, E2, M1, M2, C1, C2, H1 and H2. For details see left column.

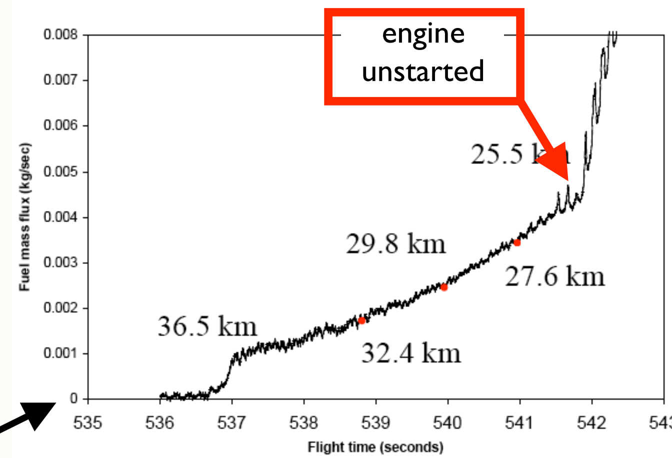
Overarching problem

- Initial system-level experimental data: HyShot II flight test
- Complete flight dataset already received from University of Queensland

HyShot II Launch
Japan/US/Australia

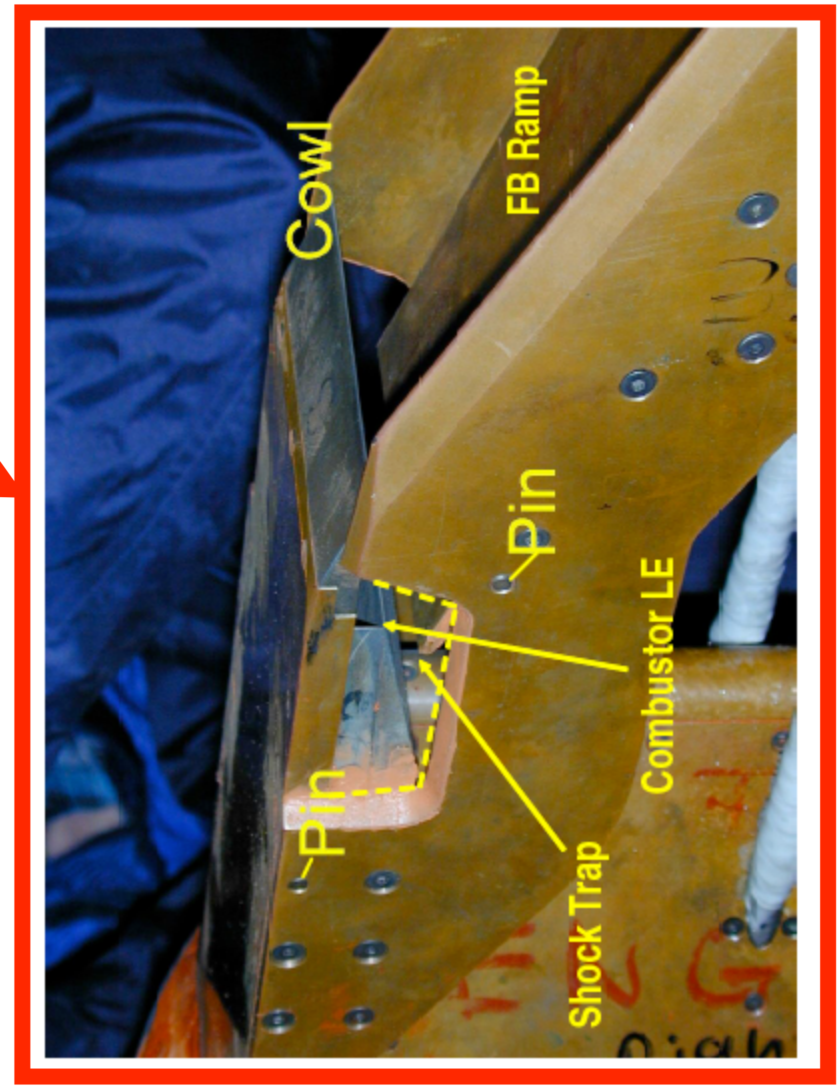


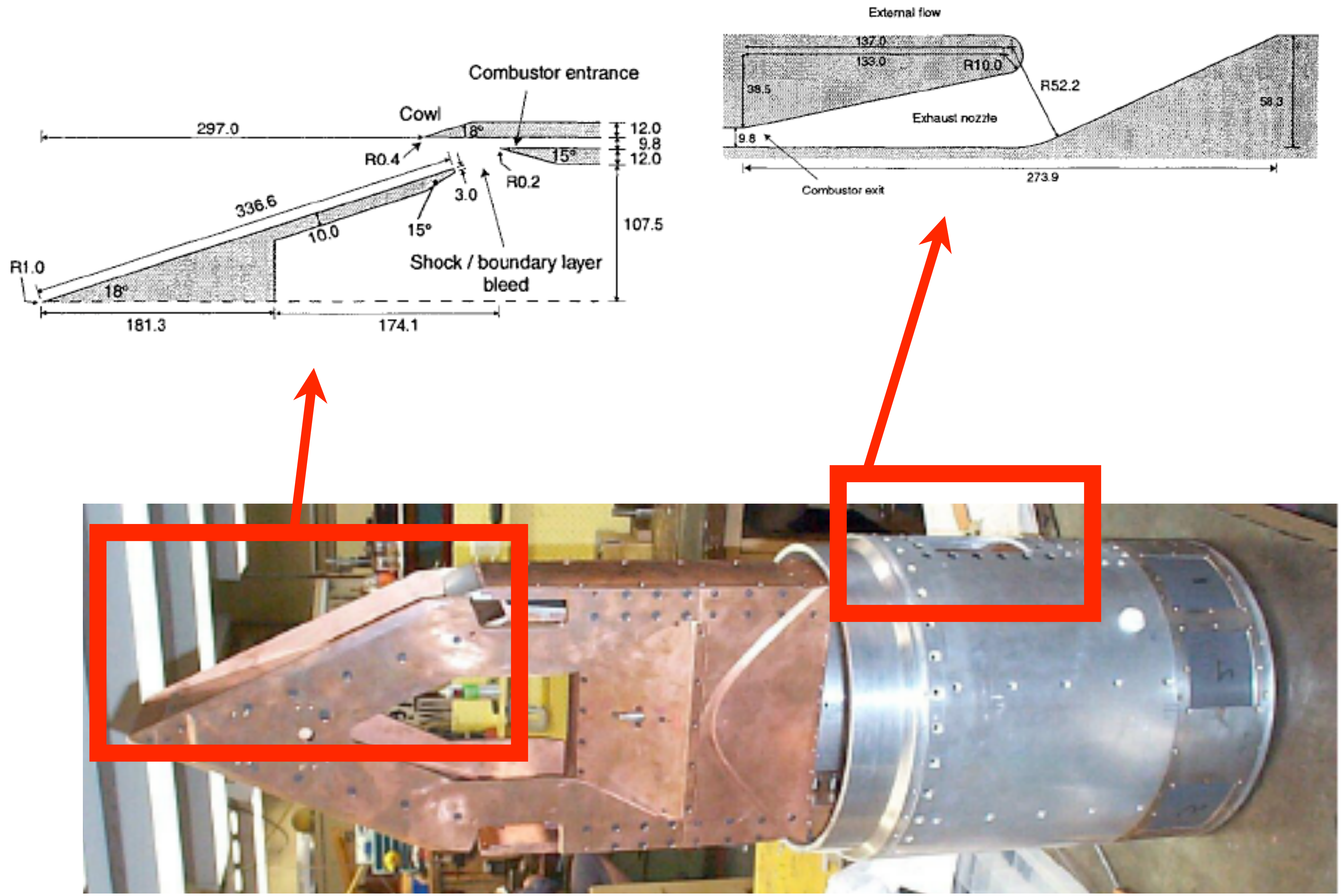
Flight Trajectory



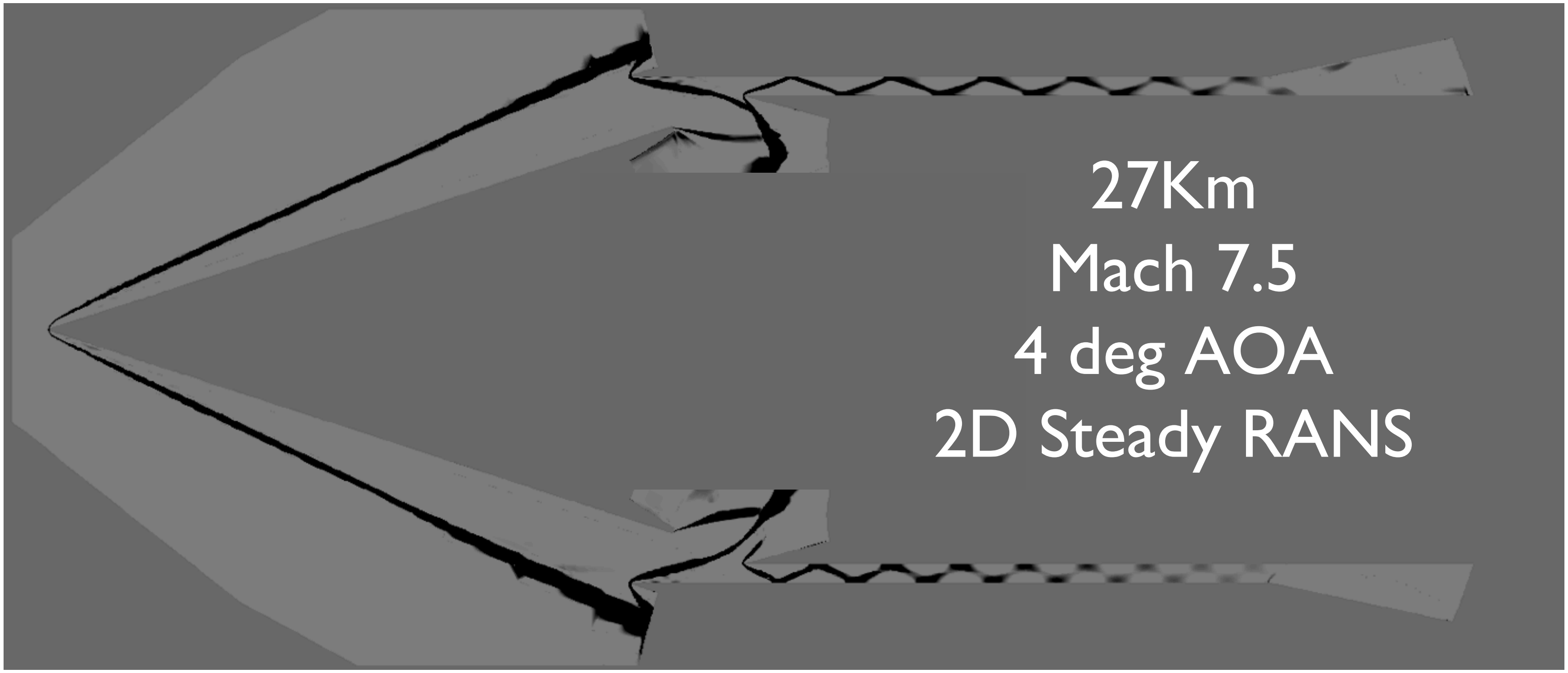
Thermal choking induced by an increase of the injected fuel

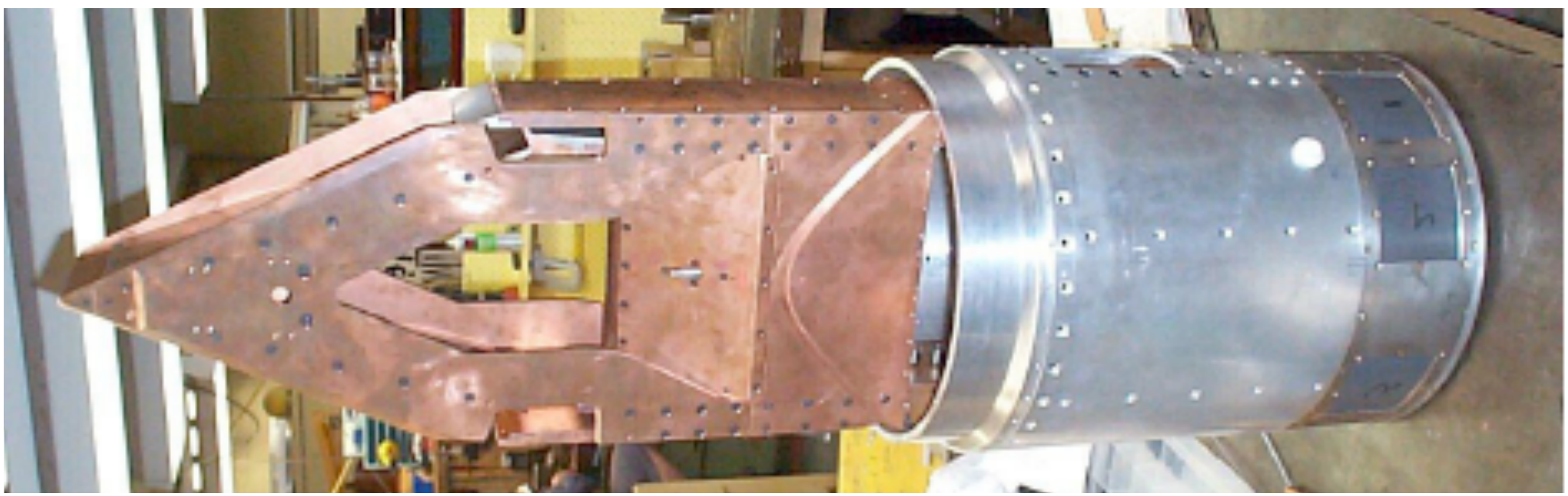
HyShot - U. Queensland

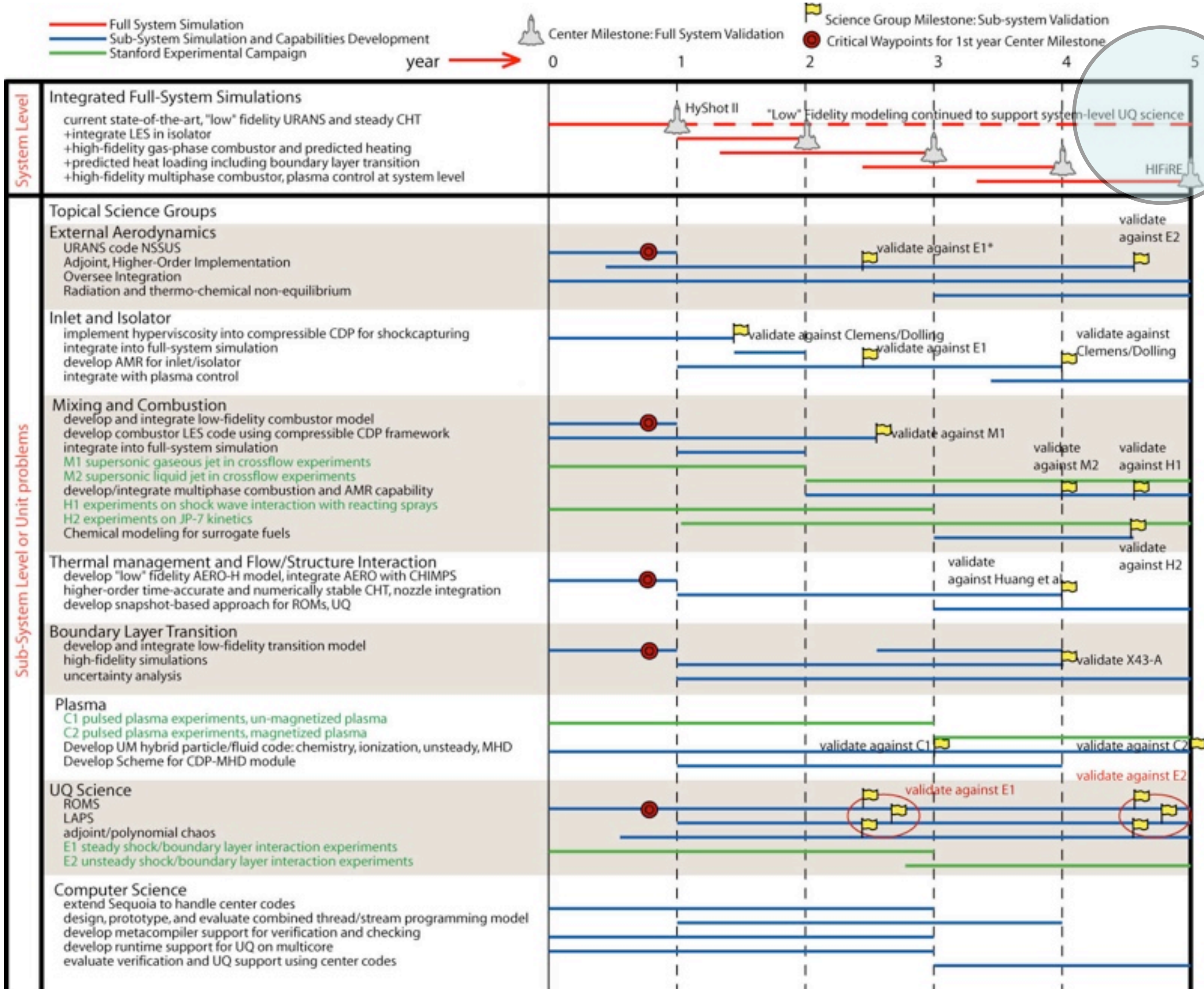




Combustor entrance
Cowl
297.0
18°
12.0
9.8
12.0
R0.4
15°
R0.2
336.6
3.0
10.0
15°
107.5
R1.0
18°
Shock / boundary layer bleed
181.3
174.1
External flow
137.0
133.0
R10.0
39.5
R52.2
Exhaust nozzle
58.3
9.8
Combustor exit
273.9


27Km
Mach 7.5
4 deg AOA
2D Steady RANS





* Stanford's experiments are denoted as E1, E2, M1, M2, C1, C2, H1 and H2. For details see left column.

HIFiRE Flight Manifest

Technology Area	FLIGHT									
	1 US Sep 07	2 US Aug 08	3 AUS Aug 08	4 AUS Jan 09	5 US Nov 10	6 US Nov 10	7 AUS Nov 10	7a US TBD	8 AUS Mar 11	9 US Jun 11
✓ Primary Experiment ✓ Secondary Experiment	Captive Cone Cylinder	Captive Flowpaths	Captive Flowpaths	Flyer Elliptic Cone	Flyer Waverider	Captive Flowpaths	Flyer Flowpaths	Flyer Elliptic Cone	Powered Waverider Flowpath	Flyer Waverider Flowpath
Aerosciences	BLT, SBLI ✓ (primary)			Aero, S&C ✓ (primary)	S&C, BLT ✓ (primary)		S&C ✓ (secondary)	BLT, SBLI, Aeroheat ✓ (primary)	TBD ✓ (secondary)	S&C ✓ (primary)
Propulsion		HCSJ, Isolator ✓ (primary)	H2SJ ✓ (primary)			HCSJ Dual Mode ✓ (primary)	SJ Thrust Measure ✓ (primary)		TBD ✓ (primary)	
Materials & Structures		Materials Survival ✓ (secondary)				Materials Survival ✓ (secondary)		Materials Survival ✓ (secondary)		
Sensors	RF Attenuat'n ✓ (secondary)				RF Attenuat'n ✓ (secondary)	RF Attenuat'n ✓ (secondary)		GPS, Aero Optics, RF Attenuat'n ✓ (secondary)		
Space Environment	Plasma Dynamics ✓ (secondary)				Plasma Dynamics ✓ (secondary)	Plasma Dynamics ✓ (secondary)		Plasma Dynamics ✓ (secondary)		
Instrumentation & Measurements	OMC ✓ (secondary)	OMC ✓ (secondary)	OMC ✓ (secondary)			OMC ✓ (secondary)				

Source: Dolvin, kickoff meeting, Nov. 2006

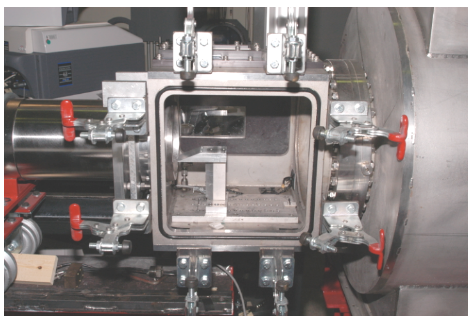
Tightly Coupled Experimental Characterization

Subsystem and Unit Problems

In-house Experimental Campaign

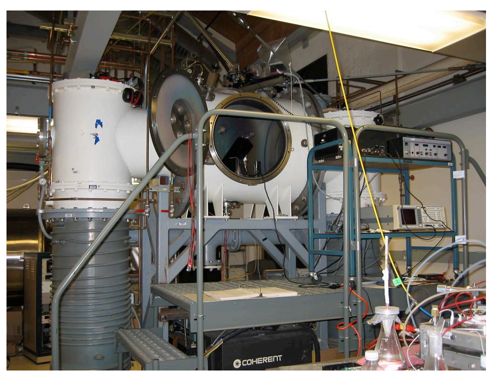
- 4 new experiments
  - 3 in support of model development and validation activities
  - 1 in support of sensitivity analysis and uncertainty quantification
- Leverage "world-class" facilities
- Employ advanced diagnostics

Supersonic mixing and combustion (Prof. Mungal)

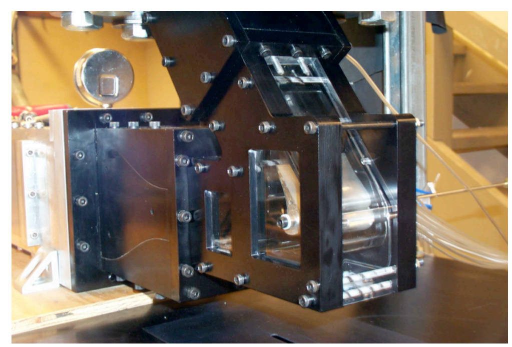


Shock/fuel droplet interaction and kinetics (Prof. Hanson)

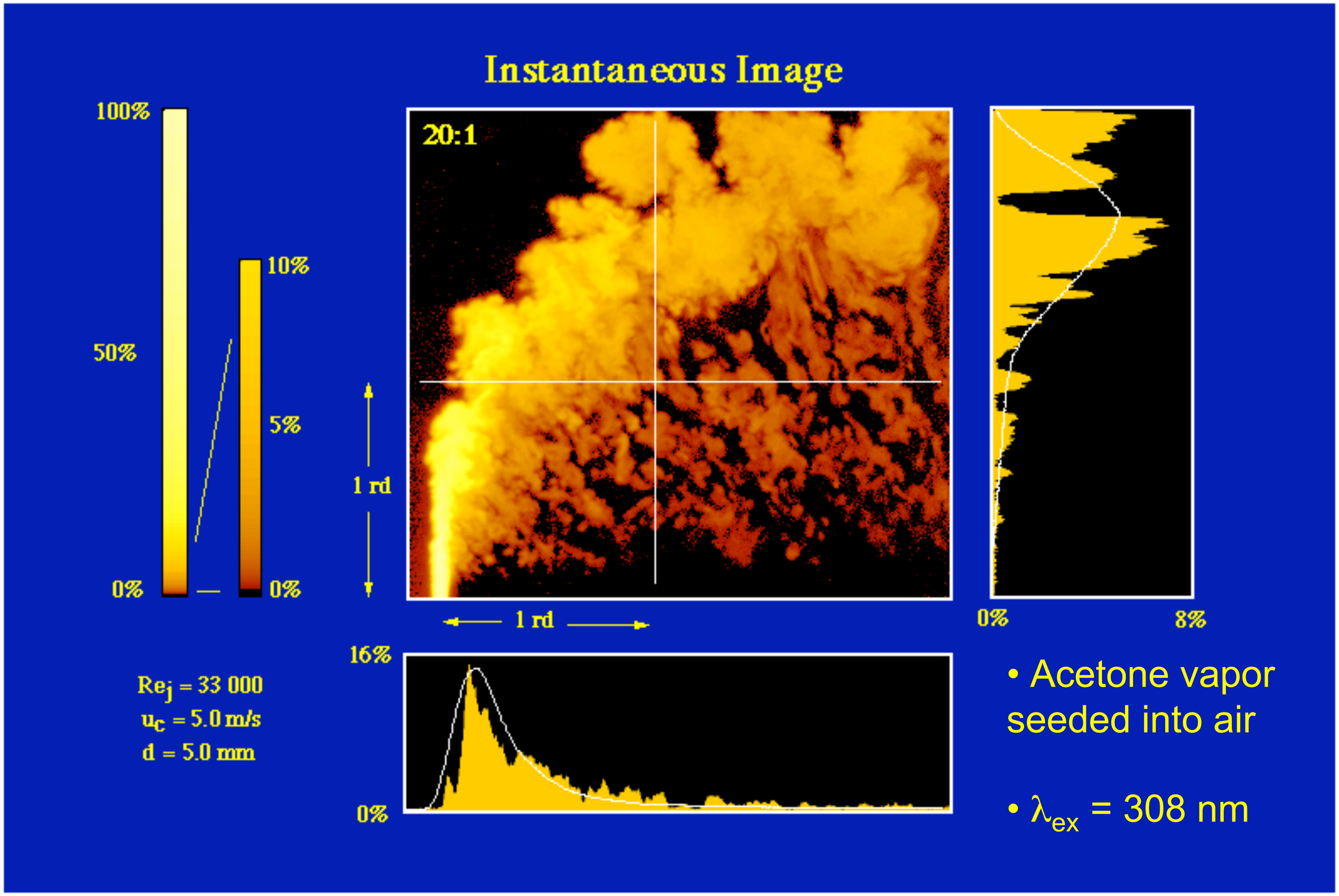
Plasma/shock/boundary layer interaction (Prof. Cappelli)



Shock/BL interaction (Prof. Eaton)

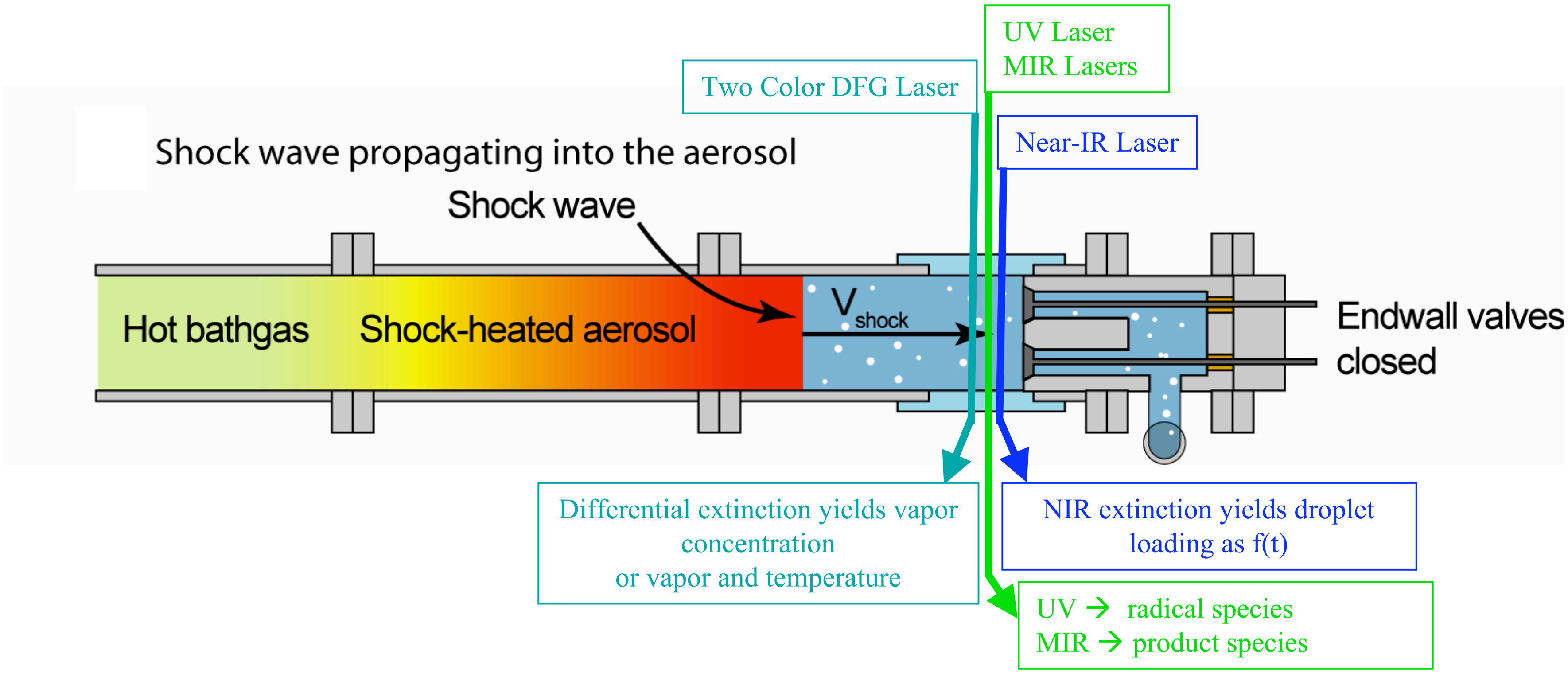


Isothermal Mixing Study:
An Example of Acetone PLIF to Investigate Jet in Crossflow



Since initial work of Lozano (1992), acetone PLIF has been popular for studying mixing in a variety of flow configurations: data here is jet in crossflow from (Smith & Mungal 1998)

Stanford's Unique Aerosol Shock Tube Facility



- Enables fundamental studies of shock-wave interactions with droplets
- Enables studies of kinetics of low-vapor pressure fuels
- Enables studies of shock-wave interactions with bio-aerosols

Experimental support for UQ

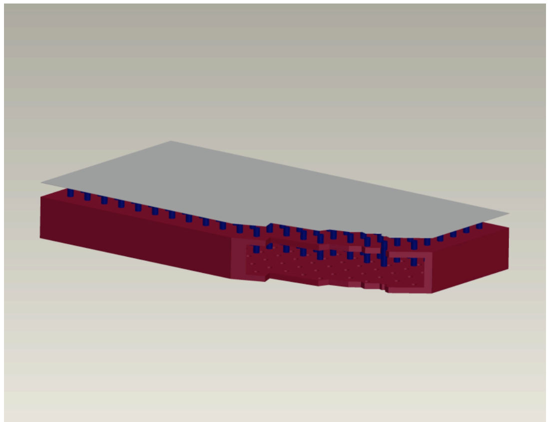
One of the Stanford's experiments has been specifically designed to assess the quality of various UQ propagation methods

This is a unique component of this program

Prof. Eaton's Shock/Boundary layer interaction test will include features to accurately control the inflow turbulence and boundary geometry.

Physical Monte Carlo
100 to 1000 repeated measurements
will be used to build detailed sensitivity maps and PDFs of important quantities such as separation length, shock locations.

These are known to be challenging to obtain using conventional UQ methods



Individually adjustable pins for surface geometry perturbation

Discussion on V&V of Turbulent Flow Simulations

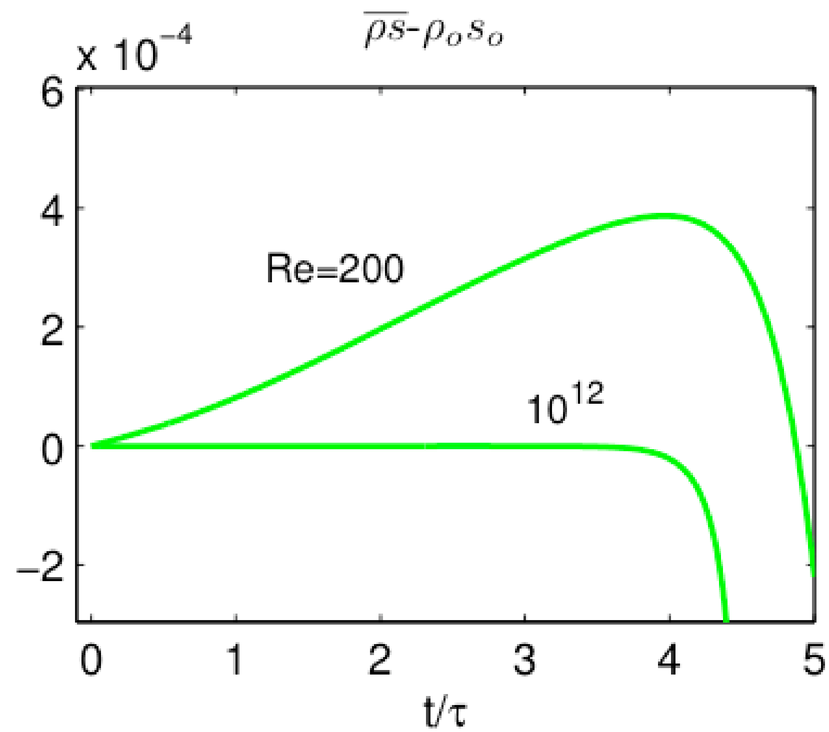
Algorithms for High-fidelity Turbulence Simulations

- Critical to separate numerics and sub-filter modeling errors
  - This is contrary to "Implicit LES", where dissipation of the numerical scheme is used as an implicit SGS model
  - Our own investigations show Implicit LES results are extremely grid and scheme dependent, even for simple, canonical flows
- Numerical dissipation is NOT good for turbulence!
  - Higher conservation principles enable the development of stable, non-dissipative schemes

Existing Compressible Schemes

$M_t = 0.07$, 32^3, 6th-order compact, no model

Second law violation



HEC Scheme

- Extension of conservation ideas for discrete low-Ma number equations to compressible flows
  - We have shown the higher-conservation principles involving entropy are critical
  - Formulated numerical discretizations that discretely conserve second-moments of entropy flux (Honein & Moin, JCP 2004)

- Entropy equation: $\frac{\partial \rho s}{\partial t} + \frac{\partial \rho s u_j}{\partial x_j} = \frac{1}{T}\left[\tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\right]$

  multiply by $2s$: $\frac{\partial \rho s^2}{\partial t} + \frac{\partial \rho s^2 u_j}{\partial x_j} = \frac{2s}{T}\left[\tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\right]$

- Nonlinear terms should not spuriously contribute to $\overline{\rho s}$ and $\overline{\rho s^2}$

  Use the conservative skew-symmetric form:

$$\frac{\partial \rho s u_j}{\partial x_j} \longrightarrow \frac{1}{2}\frac{\delta \rho s u_j}{\delta x_j} + \frac{s}{2}\frac{\delta \rho u_j}{\delta x_j} + \frac{\rho u_j}{2}\frac{\delta s}{\delta x_j}$$

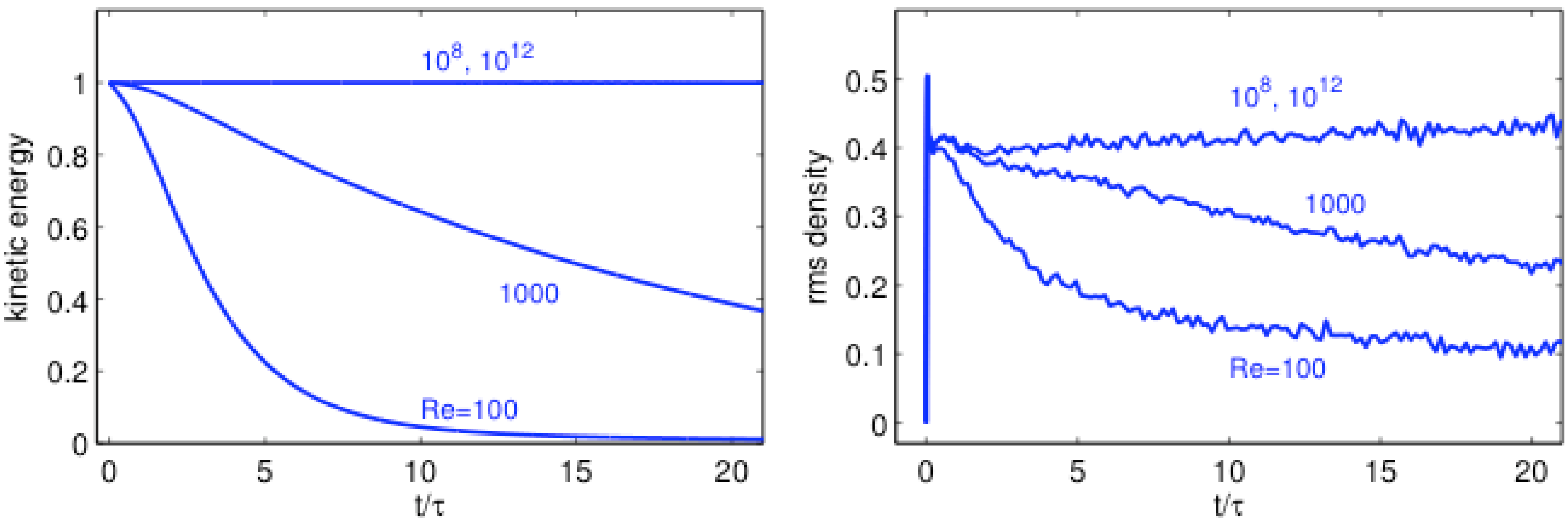
- Equivalent energy equations can also be derived

$$\frac{\partial \rho e}{\partial t} + e\left(\gamma - \frac{s}{2C_v}\right)\frac{\delta \rho u_j}{\delta x_j} + \frac{e}{2C_v}\frac{\delta \rho s u_j}{\delta x_j} + \frac{\rho e u_j}{2C_v}\frac{\delta s}{\delta x_j} = \tau_{ij}\frac{\delta u_i}{\delta x_j} - \frac{\delta q_j}{\delta x_j}$$

New formulation results: HEC

$M_t = 0.07$, 32^3, 6th-order compact, no model

Stable for all Re



Computation of flows with shocks

Classical low order Godunov Schemes (Roe, Lax-Friedrichs, ...)

- Too dissipative for turbulent flows

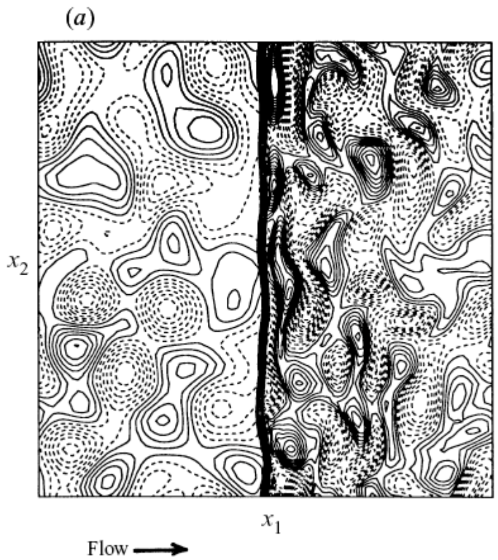
High-order methods (ENO/WENO)

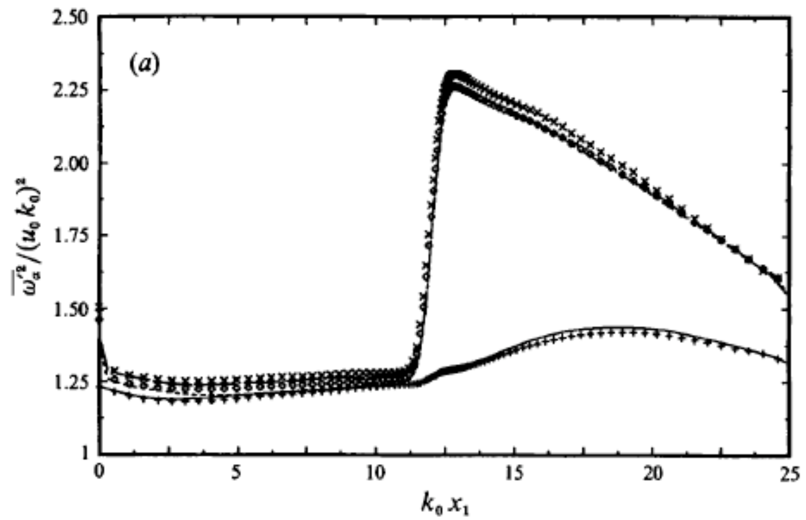
- Selects the optimal stencil for flux calculations
- High cost
- Dissipative for turbulent flows (can be overcome if used in a hybrid scheme together with a central scheme)
- Difficult to implement for unstructured grids

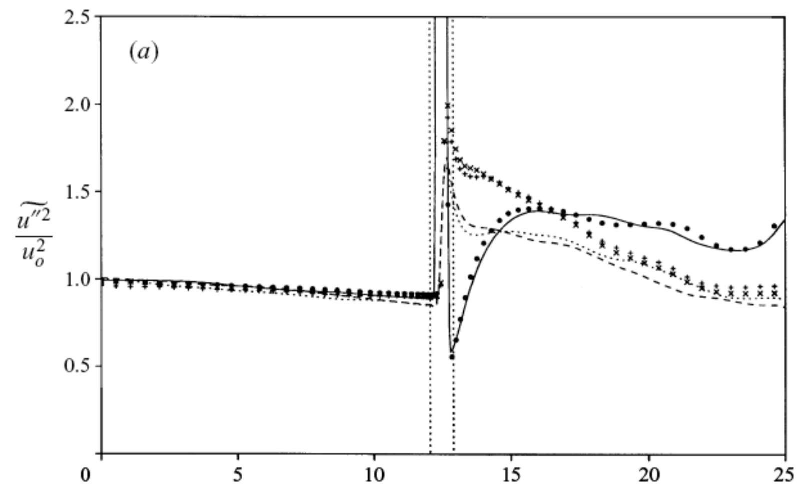
Artificial viscosity (Cook and Cabot JCP 2004)

- Employs a local bulk viscosity for treating shocks
- The model does not influence the vortical structures
- Easy implementation for both structured and unstructured grids.

Shock Turbulence Interaction



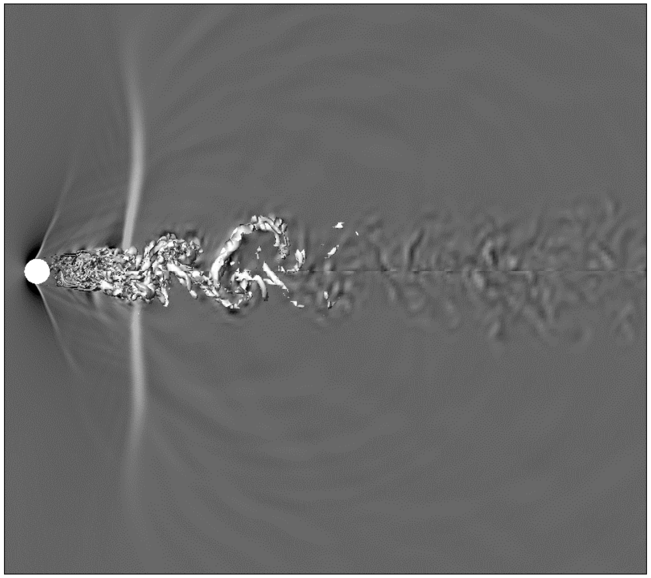




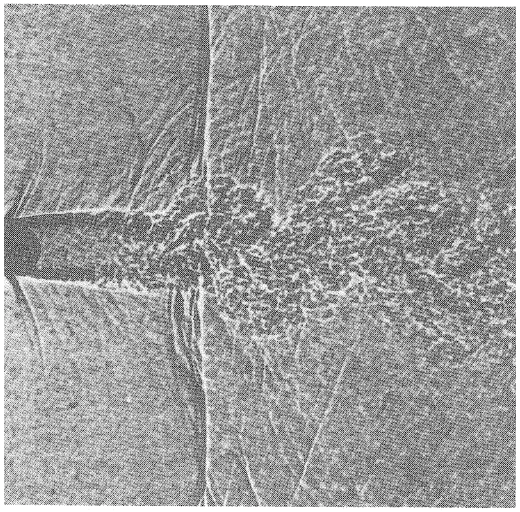
“Interaction of isotropic turbulence with shock waves: effect of shock stength ”, Lee et all. , 1997

Transonic Flow over Cylinder

$Re = 10^4$ and $Ma_\infty = 0.85$



$Re = 10^5$ and $Ma_\infty = 0.9$



"An album of fluid motions", M. Van Dyke, 1982

Combined Dynamic Smagorinsky for subgrid shear viscosity and artificial bulk viscosity with the variation (Mani, et al. 2008):

$$\text{replace S with } \nabla.\vec{u}$$

$$\beta_{art.} = C_\beta \Delta^{r+2} \overline{\rho |\nabla^r \nabla.\vec{u}|}$$

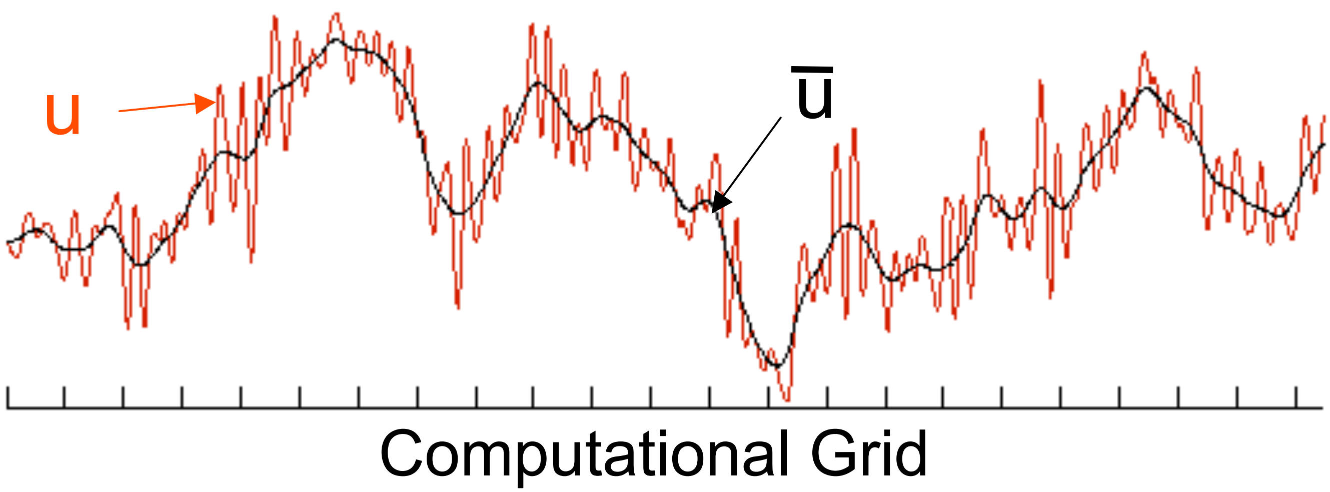
Verification & Validation

Verification Strategy

- Strict separation of mathematics and physics
  - Filtering for multi-scale problems
  - Proper numerical convergence of simulation results
- Exact and Manufactured solutions
  - Multi-physics problems: across disciplines and “codes”
  - Non-smooth solutions: for example, shock physics
  - Parameter coverage: robustness
- Error estimates and control
  - A posteriori estimates using duality principle
  - Adaptive mesh refinement
- Code-embedded verification
  - Static/dynamic property checks: conservation, SBP, etc.
  - Code coverage and testing

Verifiable LES

$$\overline{u}_i(x, \Delta, t) = \int_D G(x, x', \Delta) u_i(x', t) dx'$$



- Explicit filtering is used rigorously to derive the constitutive equations for the large-scale field
- Allows "true" grid-converged LES; LES should not converge to DNS

LES with Explicit Filtering

- Use filters that commute with differentiation
- Filter width should not be tied to grid spacing. Preferably,

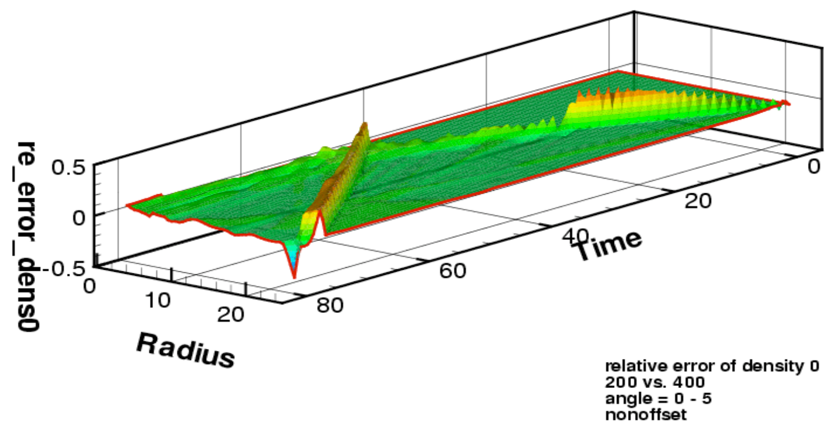
$$\Delta_{\text{filter}} > \Delta_{\text{grid}}$$

- Makes LES more expensive, but necessary

Genuine Discontinuous Solutions

- Shocks and discontinuities introduce difficulties in assessing code and solution accuracy
- Discontinuity position mismatch generates *error-ridges* in grid convergence analysis
- Glimm et al. have developed error analysis and filtering/averaging approaches for complex shock interactions
- Also of interest the generation of manufactured solutions with (unsteady) strong curved shocks: cross derivatives, entropy/vorticity gradients

Circular RM instability: converging shocks
Interacting with perturbed density interface



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1. Glimm, J. et al. "Statistical Riemann Problems and a Composition Law for Errors in Numerical Solutions of Shock-Physics Problems". LANL report UR-03-2921, 2003.
2. Glimm, J. & Sharp, D. H. "Prediction and the Quantification of Uncertainties", Physica D. Vol. 133, 1999.

UQ Methodology

At unit and subsystem level

- Comprehensive probabilistic models feasible
- Use problem-dependent technique: MC, PCE or others
  - Intrusive PCE for structural thermal loading
  - Pade-Legendre for isolator/inlet shock dominated region
  - PCE colocation for reaction zone and supersonic mixing
  - MC typically for unit problems only

At full system level

- no clear winner
- Need *agile* approach - ability to focus on functional of interest
- ROMs and LAPS (likelihood averaging in probability space). Comparison of the uncertainty bounds will provide increased insights and confidence
- UQ in multi-physics environments

Combined ROM and LAPS

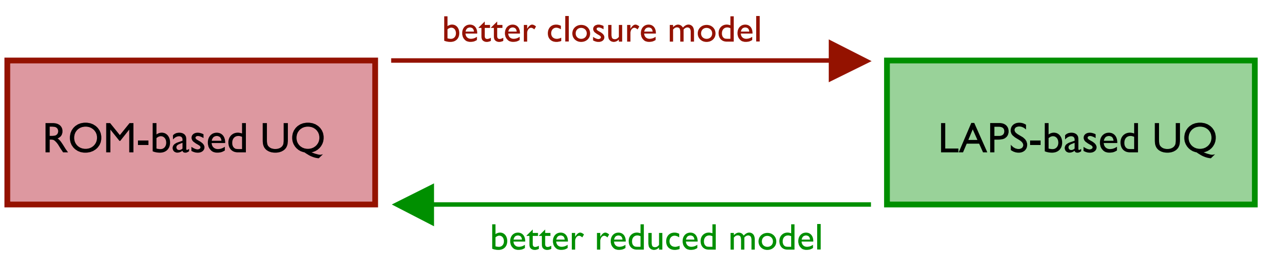
Total analysis error = physical space errors + probability space errors

ROM-based UQ : small probability-space errors

- Accurate identification of the cliffs in probability space
- Provide information for improving the closure models in LAPS

LAPS-based UQ : small physical-space errors

- Improve the accuracy of the physics reduction in ROMs



Successive use of ROMs and LAPS is a path towards “converged” high-fidelity predictions

Expected impact of the new center

Numerical Analysis and Algorithms

- Verified LES - explicit filtering
- UQ for full-system, unsteady problems
- the science of integration
- Numerical methods for turbulent flows with shocks

Validation Experiments

- highly-compressible, all unsteady, high-temperature regime, advanced diagnostics

Computer Science

- Exaflop computing paradigm: pervasive parallelism, multicore/manycore challenge

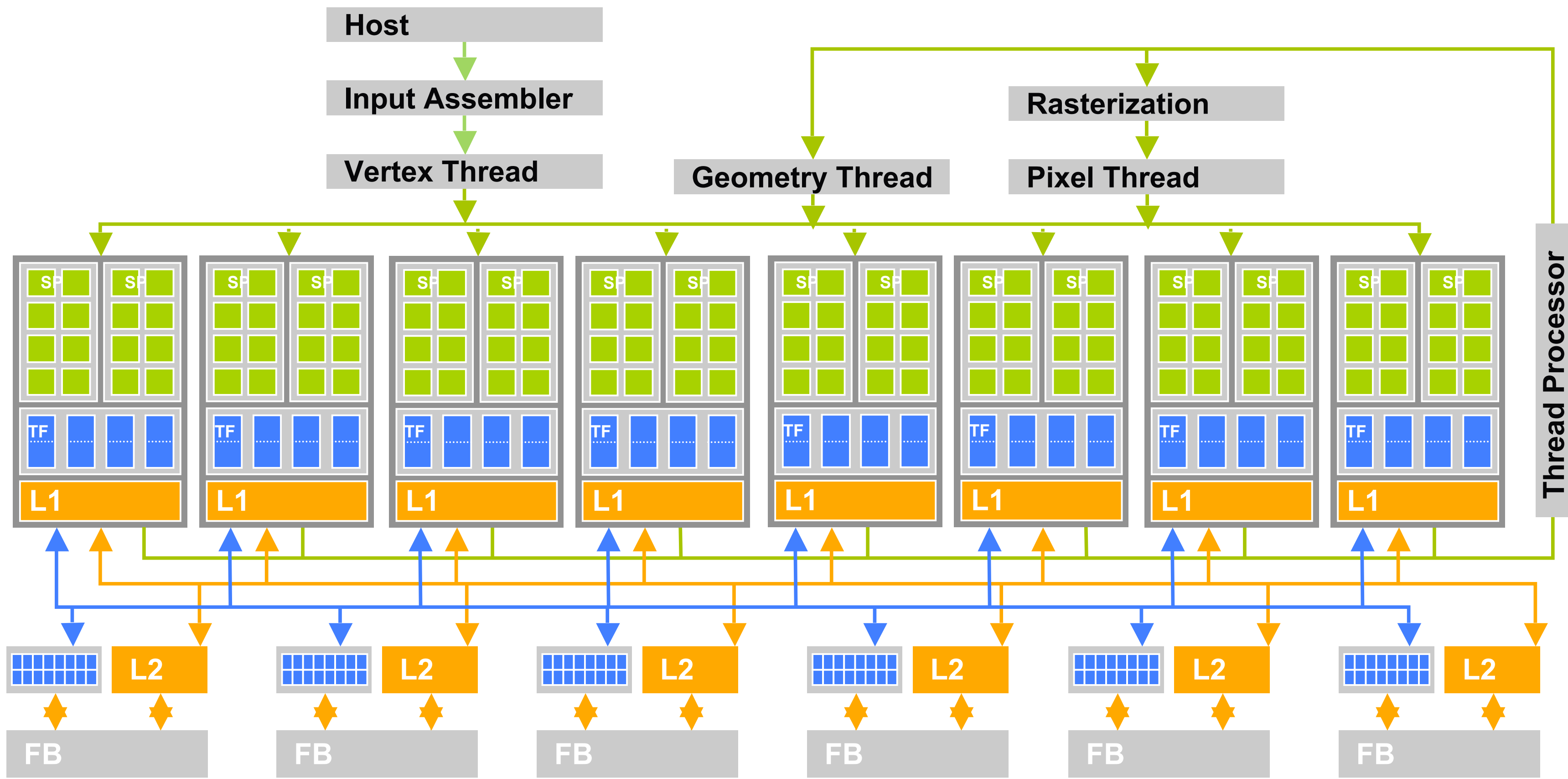
Stanford's HTGL will perform validation experiments

New and Innovative

- Focus on unsteady, high-consequence, truly multidisciplinary failure mode of a complex system: unstart
- LES of turbulence, supersonic mixing and combustion in the propulsion system
- Parameter-free sub-grid scale modeling
- Grid converged LES - explicit filtering
- High-fidelity numerical treatment of shock/turbulence interaction
- Formal verification process and development MMS and proper grid convergence criteria for flows with shocks
- Unique facilities and diagnostics in Stanford's HTGL for sub-filter model development and validation
- UQ and sensitivity analysis, with experiments specifically designed for UQ
- Major advances in the mathematical coupling of multiple codes: integration science
- Leveraging CS advances for scientific code development for future platforms, verification and UQ

Towards Pervasive Parallelism

GeForce 8800 Series GPU



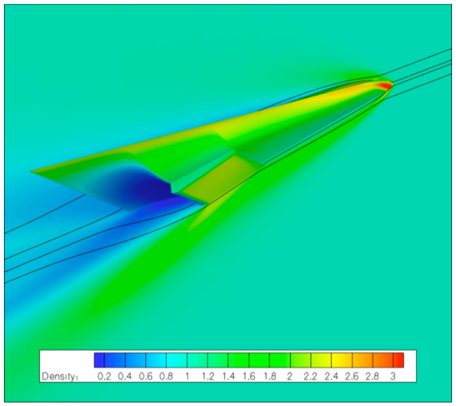
Can view as an 8-core processor with 16-wide SIMD units
Approximately 10,000 threads in flight

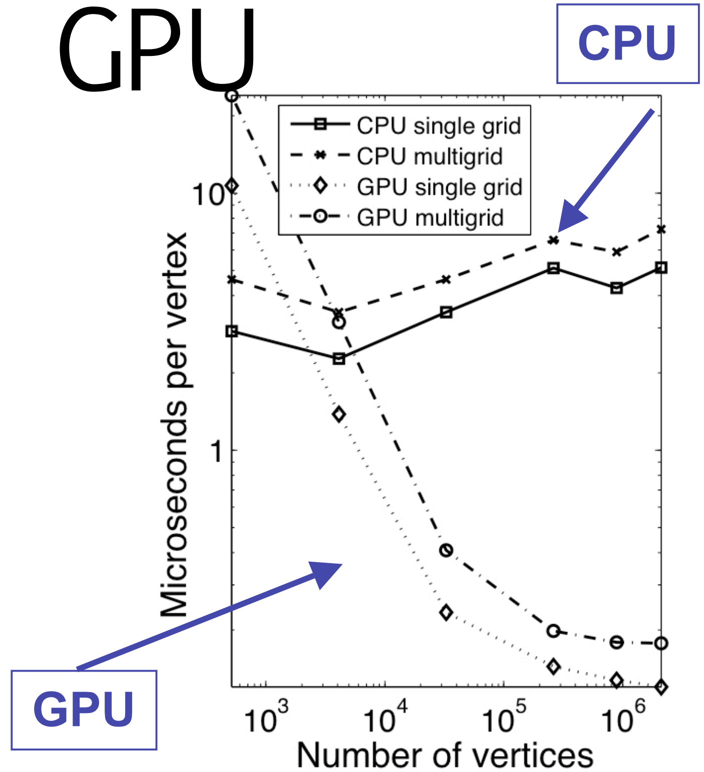
Molecular Dynamics: Folding@Home

Client type	Current TFLOPS*	Active Processors
Windows	201	211,028
Mac OS X/PPC	7	8,404
Mac OS X/Intel	27	8,812
Linux	74	43,802
GPU (ATI/NV)	924	8,404
PS/3	1,331	47,215
Total	2,564	327,665

*TFLOPs is actual folding flops, not peak values [July 7, 2008]

NSSUS on NVIDIA GPU





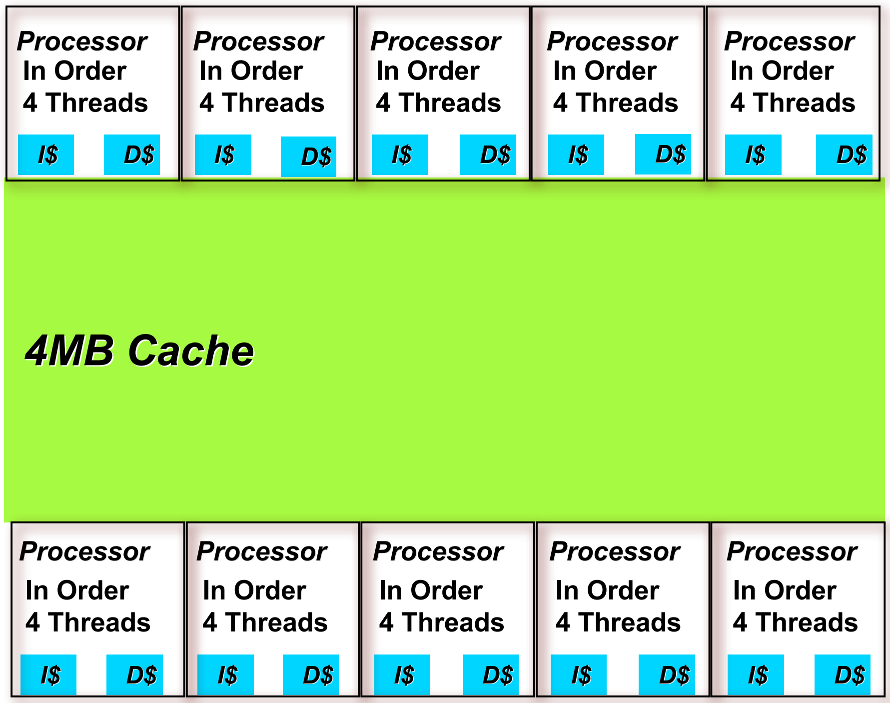
Code was developed to port the compressible Euler solver of NSSUS to model a hypersonic vehicle:

- Code was written using BrookGPU
- Multigrid cycle was implemented

This is a complex CFD code of the center ported to GPU with real physics and engineering accuracy.

Mesh	Multigrid cycle	Overall Speed-up
720k	single grid	**15.4**
720k	2V	**11.2**
1.5M	single grid	**20.2**
1.5M	2V	**15.8**

Intel's Larrabee



- 32 throughput cores
- Cores
  - In-order execution
  - 4 threads
  - 16-wide vector ISA
  - Coherent 4MB cache
- 1 LRB core = 20:1 Duo core
- ½ sequential performance

Larrabee: A many-core x86 architecture for visual computing, D. Carmean, E. Sprangle, T. Forsythe, M. Abrash, L. Seiler, A. Lake, P. Dubey, S. Junkins, J. Sugerman, P. Hanrahan, to appear SIGGRAPH 2008

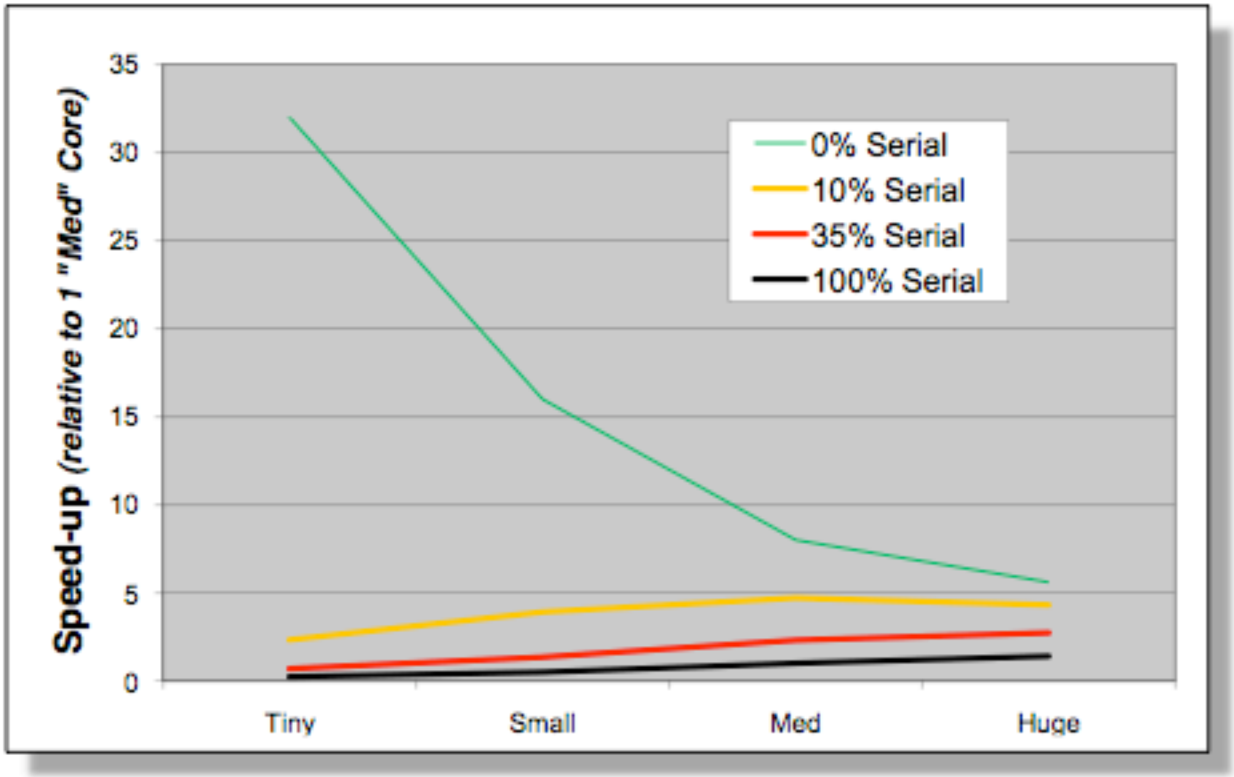
Amdahl's Implication – *Never forget the Uni !!*

Slide courtesy of Chuck Moore

Chip Assumptions:

200mm2 for Cores
80W for Cores

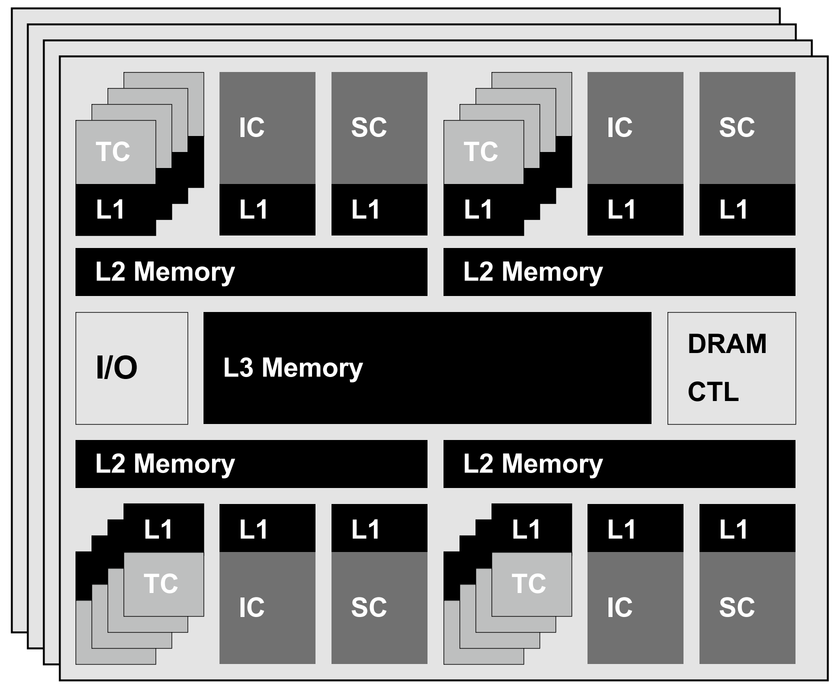
Use as appropriate for each CMP option



Rel. Perf.	P=0.25	P=0.5	P=1	P=1.4
mm^2/Core	1.5 mm^2	6 mm^2	25 mm^2	50 mm^2
# of Cores	128	32	8	4
Power/Core	0.6 W	2.5 W	10 W	20W

Hybrid Architecture in 5 Years

- The many-core chip
  - 100s of cores
  - Multiple types
    - Sequential (ILP) cores
    - Throughput cores
    - Fixed function units (codecs)
  - Hierarchy of shared memories
  - On-chip network
- The system
  - Few many-core chips
  - Per-chip DRAM channels
  - Global address space



Heterogeneous Prog. Env.

Enhance object-oriented language

- Task parallel
  - Semantics of atomic methods in objects using ideas from transactional memory
  - Composition rules for parallel objects
- Data parallel
  - Built-in parallel collections
  - Evolve Sequoia for vertical memory hier.
- Combine both in single environment
- Port to 8-core + GPU
- Current plan is to prototype in Scala

Biggest Challenges

- Mixed scheduling
  - Giga-tasks/second in high-throughput
    - Hardware threads
  - Kilo-tasks/second in sequential core
    - Software threads
- Resource management

Application Driven Projects

- Domain-specific programming environments for scientific computing
  - Fluid flow (structured and unstructured)
  - Carrot: runs on many-core
- Verification and validation
  - Probabilistic programming language

    Random ⟨float⟩ X;

    Random ⟨list⟩ L;
  - Many-core fine-grain V&V approach

Summary

- Emerging class of high-throughput processors
  - “Multi-threaded stream/vector processor machine”
  - Many mainstream applications map to these procs
- Hybrid processor is the next big thing
  - Heterogeneous workload; Amdahl’s law
  - Small number of traditional CPU cores running concurrent object system
  - Large number of high-throughput GPU cores running data-parallel work
  - Fixed-function units for power efficiency
  - Challenges: programming, scheduling, resource management