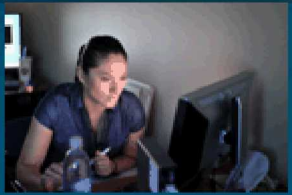
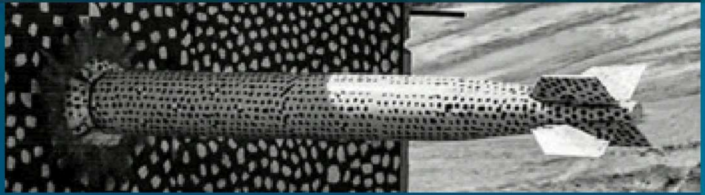
SAND2019-10876C

Recent Developments in Modeling of Ablation Physics at Sandia National Laboratories





PRESENTED BY

Derek Dinzl, Micah Howard

Aerosciences Department, Sandia National Laboratories

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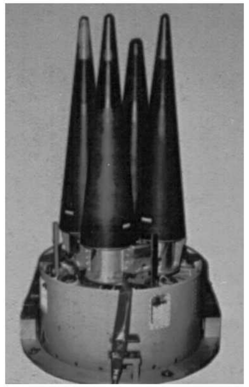
Outline

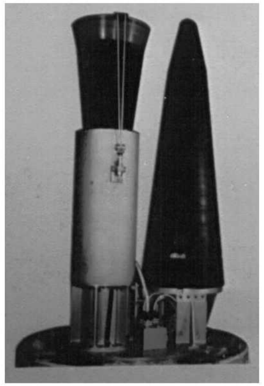
- SPARC Development and V&V Progress
  - Fluids
  - Ablation
- Next year's effort: "Virtual Flight Test"
- Sneak Peeks:
  - Materials Testing and Modeling at Sandia
  - Mesoscale Modeling at Sandia



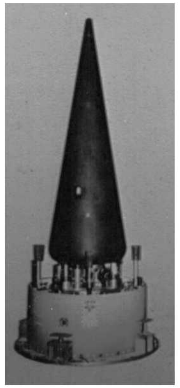
A.N.T. I

NASA SHARP-B01

SAMAST/MINT



PAS II



LBRV I

MaST

GRANITE

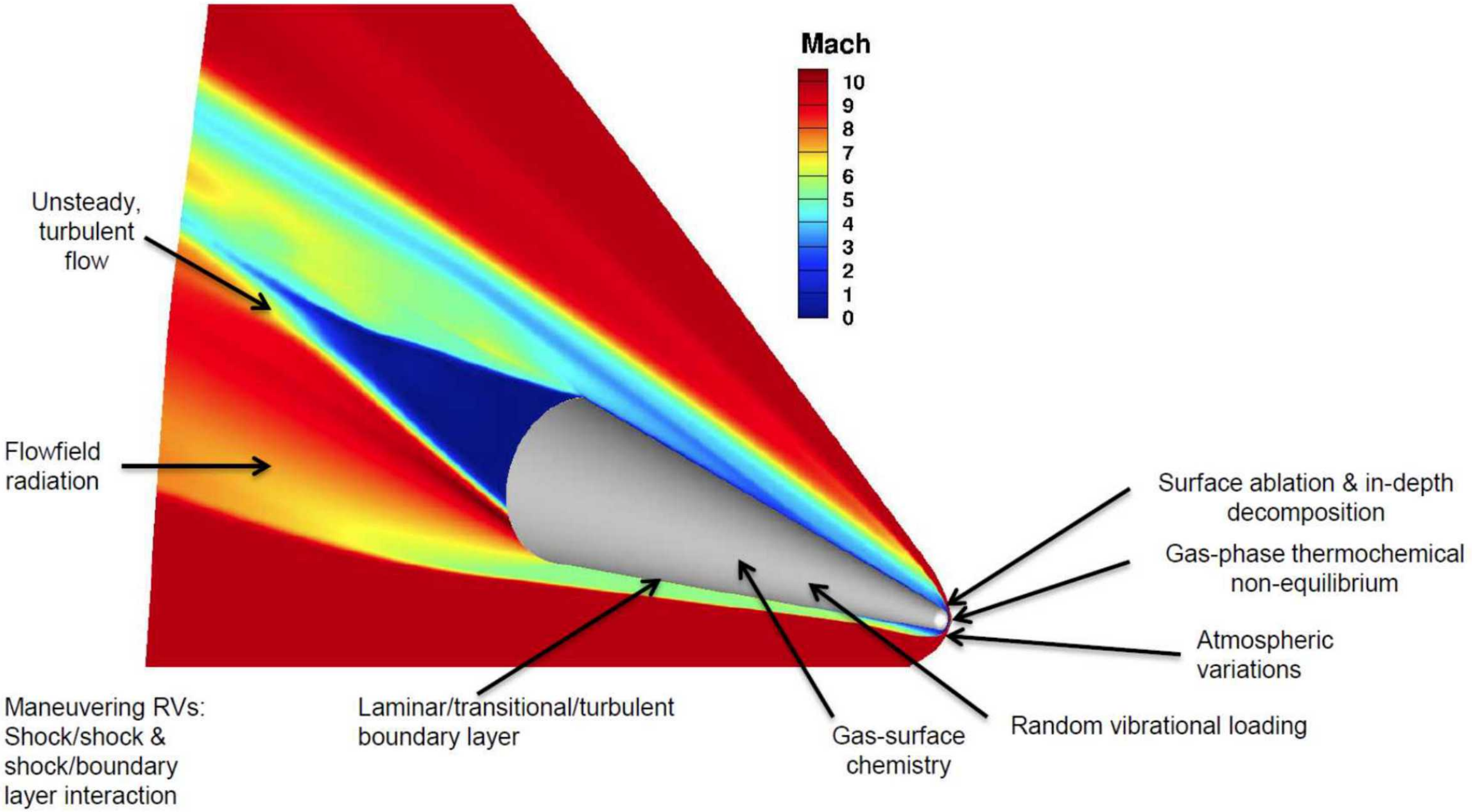
Sandia Parallel Aerodynamics and Reentry Code (SPARC)

SPARC is an aero-ablation code targeting reentry problems.

Consists of:
- Finite-rate compressible Navier-Stokes solver
- 3D Material thermal response solver
- Interfaces to other libraries

Quantities of Interest:
- Aerodynamic forces and moments
- Heat transfer
- Material thermal/structural response

Critical features:
- Development prioritizes scalability and portability
- Supports multiple discretizations



Acknowledgements – SPARC Team

PM: Paul Crozier
PI: Micah Howard

Dev Team: Matt Bopp, Steve Bova, Andrew Bradley, Sam Browne, Brian Carnes, Derek Dinzl, Jeff Fike, Travis Fisher, Mark Hoemmen, Micah Howard, Ryan Keedy, Robert Knaus, Brad Maeng, James Overfelt, Eric Phipps, Tom Smith, Ross Wagnild, et al.

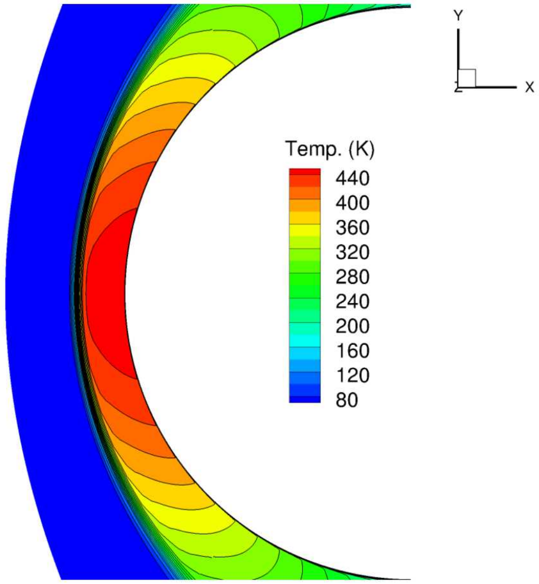
V&V/UQ Team: Brian Carnes, Derek Dinzl, Brian Freno, Micah Howard, Ryan Keedy, Sarah Kieweg, Erin Mussoni, Eric Phipps, Jaideep Ray, William Rider, Denis Ridzal, Thomas Smith, Greg Weirs

Collaborators: NASA JSC and ARC, DoD HPCMP/CREATE-AV, U of Minnesota and Wyoming

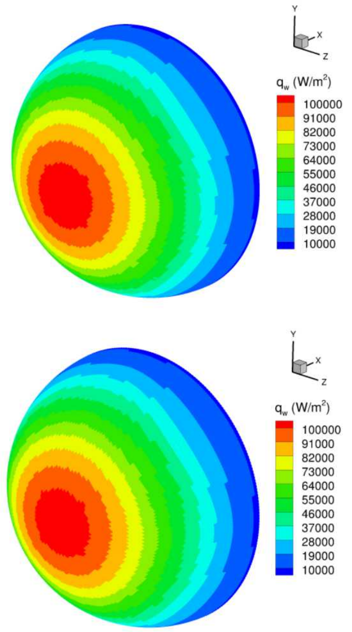
And others!

Previously… at Ablation Workshop 2016

SPARC vs. US3D
Mach 5 flow over sphere
Coarse grid

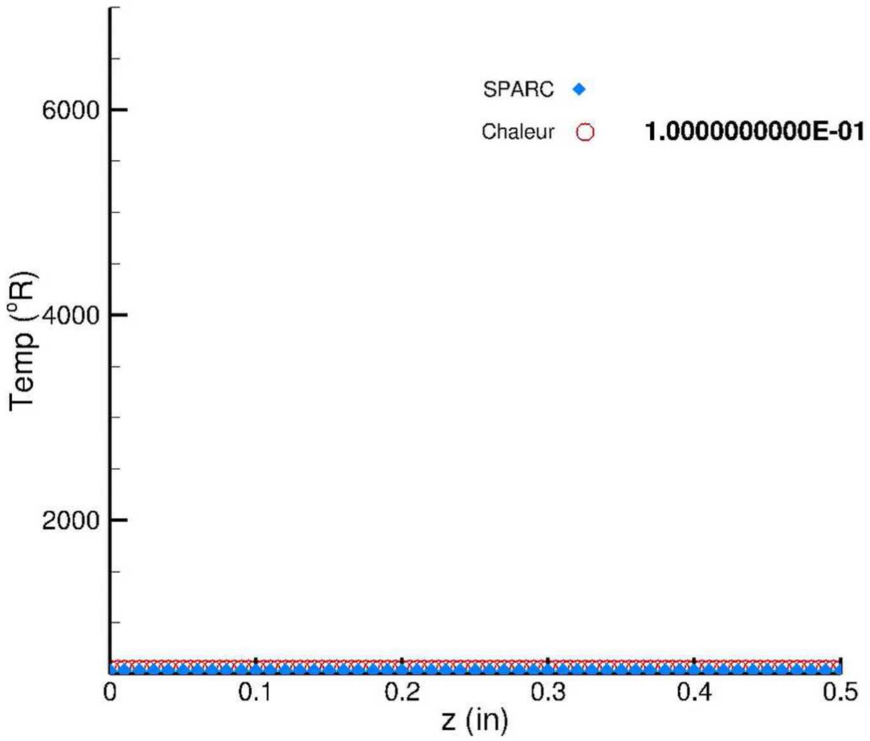


Slice of flowfield
Lines: US3D
Contours: SPARC



Surface heat flux
Top: US3D
Bottom: SPARC

SPARC vs. Chaleur
1-D carbon-carbon ablation



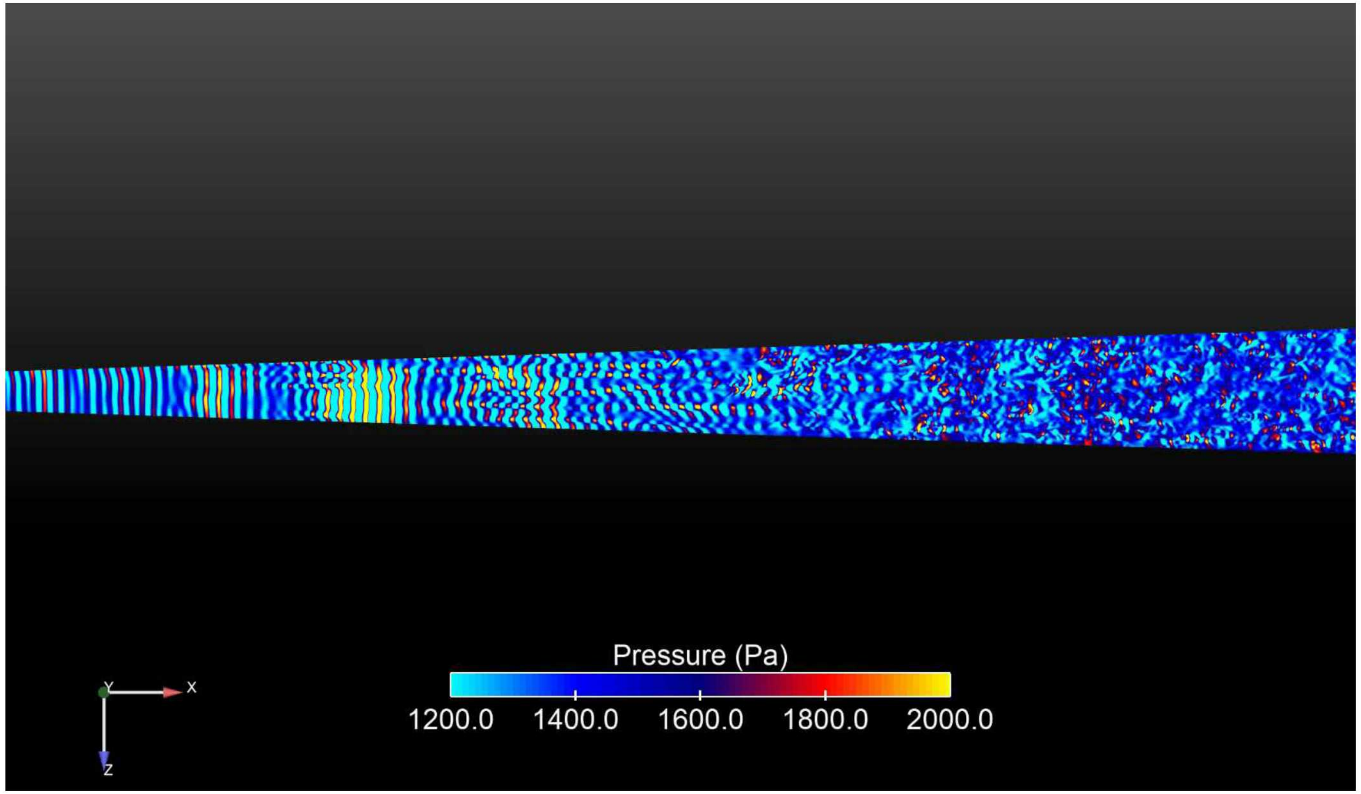
Since…

Development for fluid solver:

- Reacting gas models
- SA and SST RANS models (both perfect and RG), WMLES
- Periodic, farfield, subsonic BCs
- Refactored input parser – YAML, informative error checking, standalone validation
- Greatly expanded surface/volume postprocessing capabilities
- HOFD/DG numerics

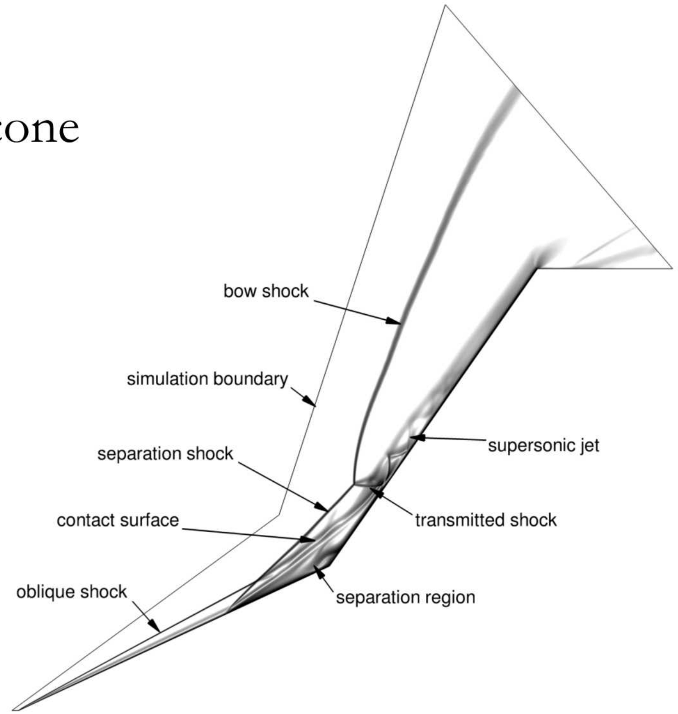
V&V Efforts for both fluid and ablation solvers

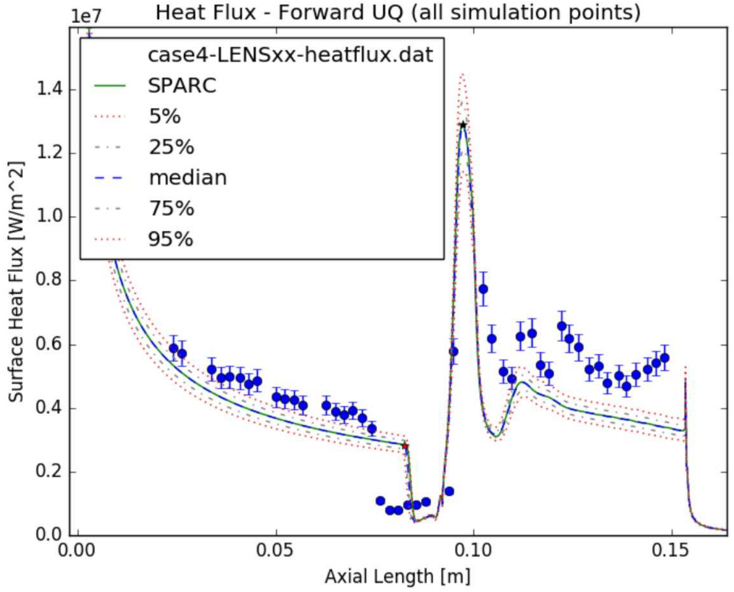
DNS of Hypersonic Transitional Boundary Layer, ~2.7B Cells



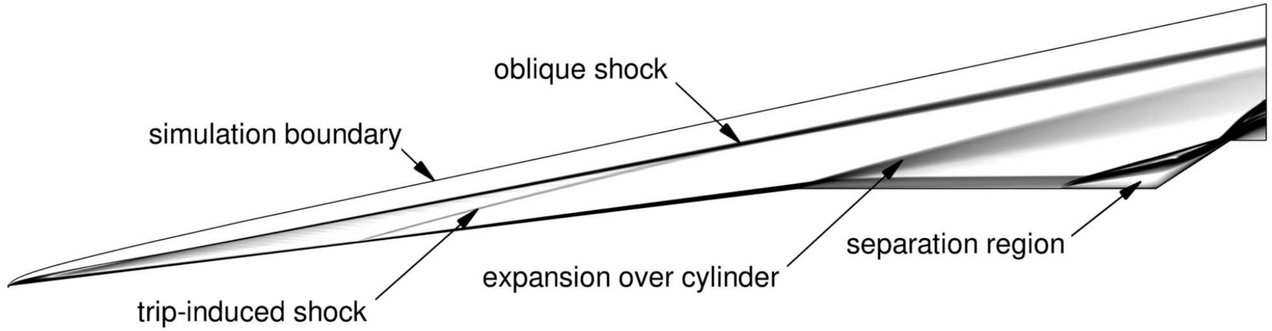
Fluids Validation Work

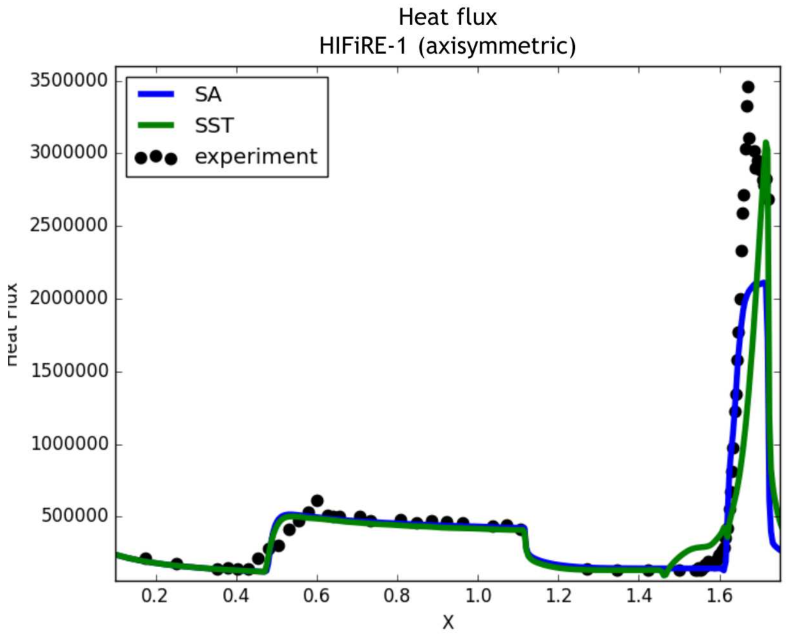
LENS I, II, XX double cone experiments





LENS HIFiRE-1 experiments

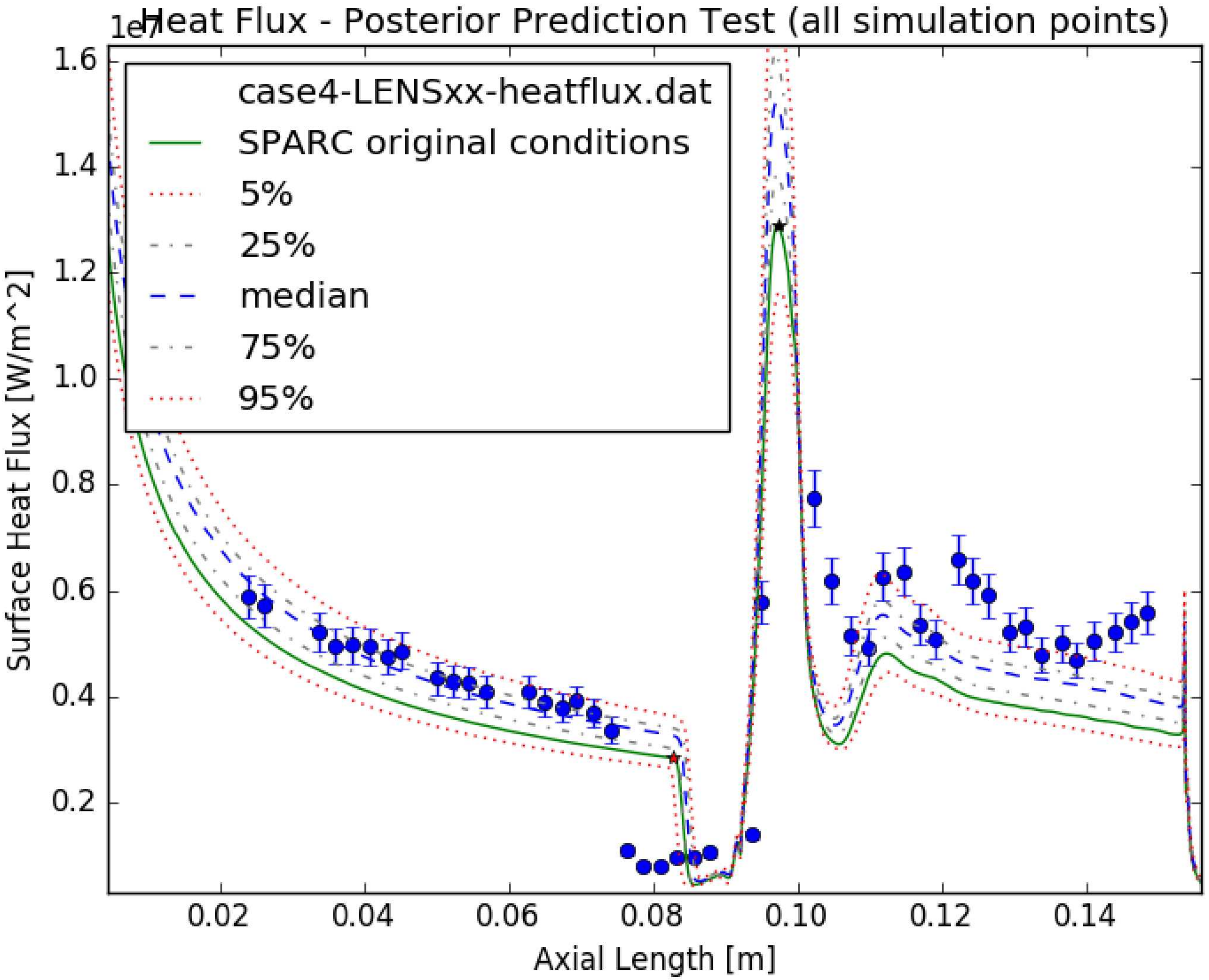




Fluids Validation Work

Rigorous analysis including:
- Sensitivity analysis
- Forward UQ
- Bayesian Calibration

Several conference and journal articles covering this work



Ablation Model Development: Monolithic Solve

SPARC solves set of 3 equations

Total Energy

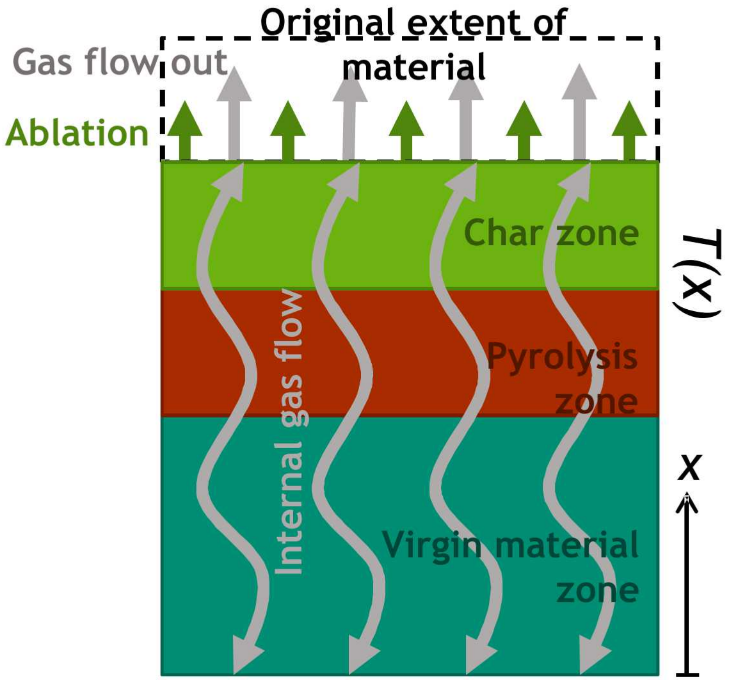
$$\frac{\partial \rho_b e_b}{\partial t} - \frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial T}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\rho_b h_b v_{m_i}) + \frac{\partial}{\partial x_i}(\phi \rho_g h_g v_{g_i}) - \dot{Q} = 0$$

Gas Continuity

$$\frac{\partial \phi \rho_g}{\partial t} - \dot{\omega}_g + \frac{\partial}{\partial x_i}(\phi \rho_g v_{g_i}) - \frac{\partial}{\partial x_i}(\phi \rho_g v_{m_i}) = 0$$

Mesh Motion

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0$$



The previous solution approach solves the equations separately and then iterates until convergence

- Energy and mesh displacement equations
- Gas continuity equations

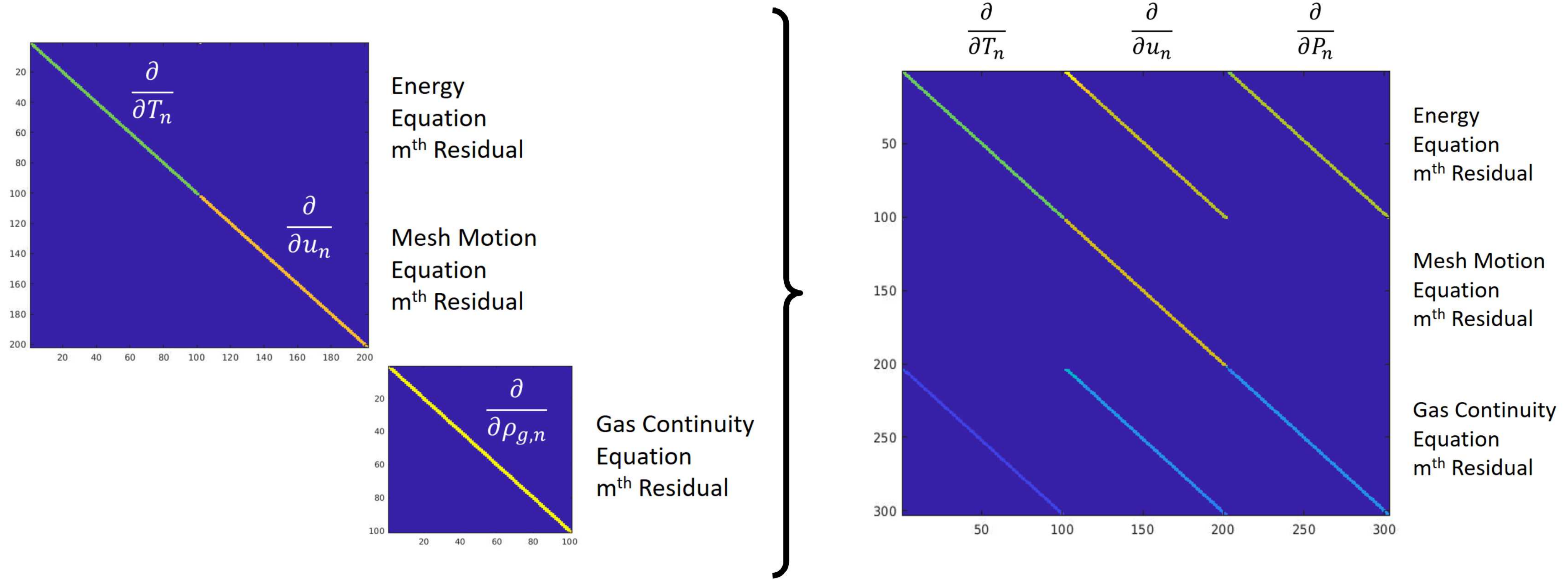
Many of the Jacobian entries were not required or incomplete

$$\boldsymbol{J} = \begin{bmatrix} \frac{\partial R_e}{\partial T} & \boxed{\frac{\partial R_e}{\partial u}} & \boxed{\frac{\partial R_e}{\partial \rho_g}} \\ \boxed{\frac{\partial R_m}{\partial T}} & \frac{\partial R_m}{\partial u} & \boxed{\frac{\partial R_m}{\partial \rho_g}} \\ \boxed{\frac{\partial R_g}{\partial T}} & \boxed{\frac{\partial R_g}{\partial u}} & \frac{\partial R_g}{\partial \rho_g} \end{bmatrix}$$

Ablation Model Development: Monolithic Solve

We are undertaking a monolithic approach to the equation system, solving them all simultaneously

- This should make the solution more stable and accurate
- The remainder of the Jacobian entries must be calculated



Ablation Model Development: Monolithic Solve

We are undertaking a monolithic approach to the equation system, solving them all simultaneously

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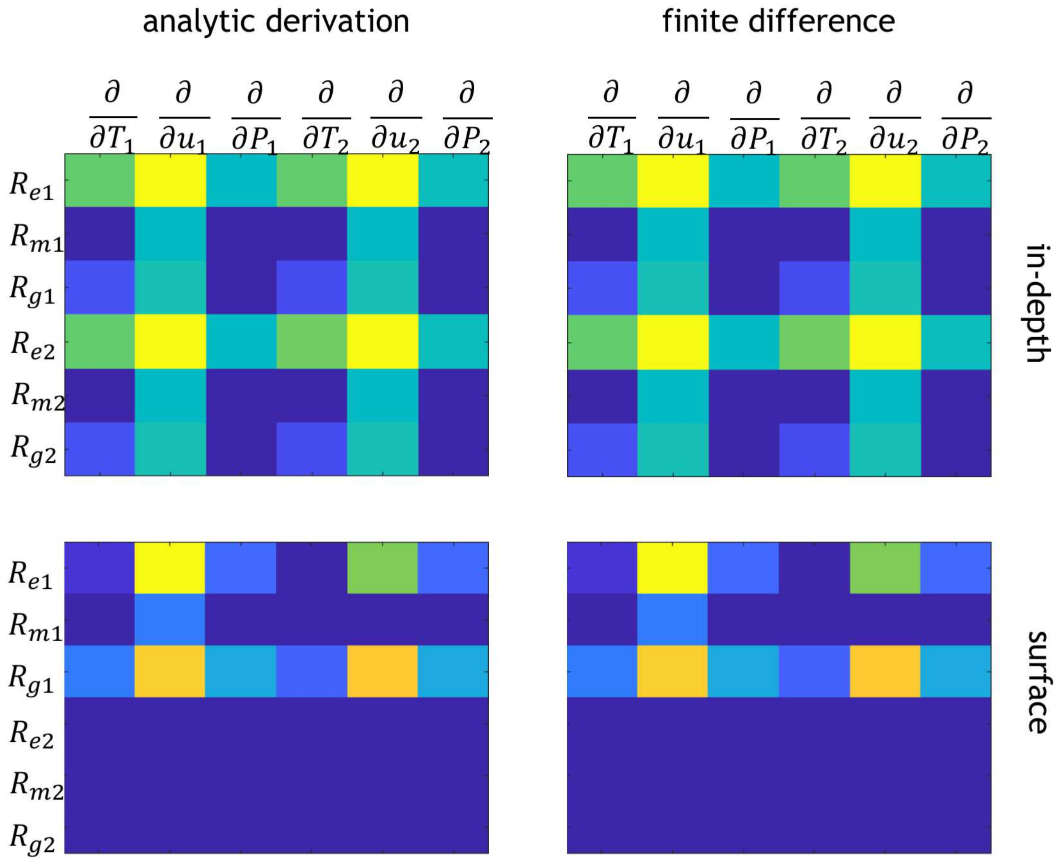
Verification of the analytic Jacobians show all entries of the element matrices agree for both surface and in-depth equations



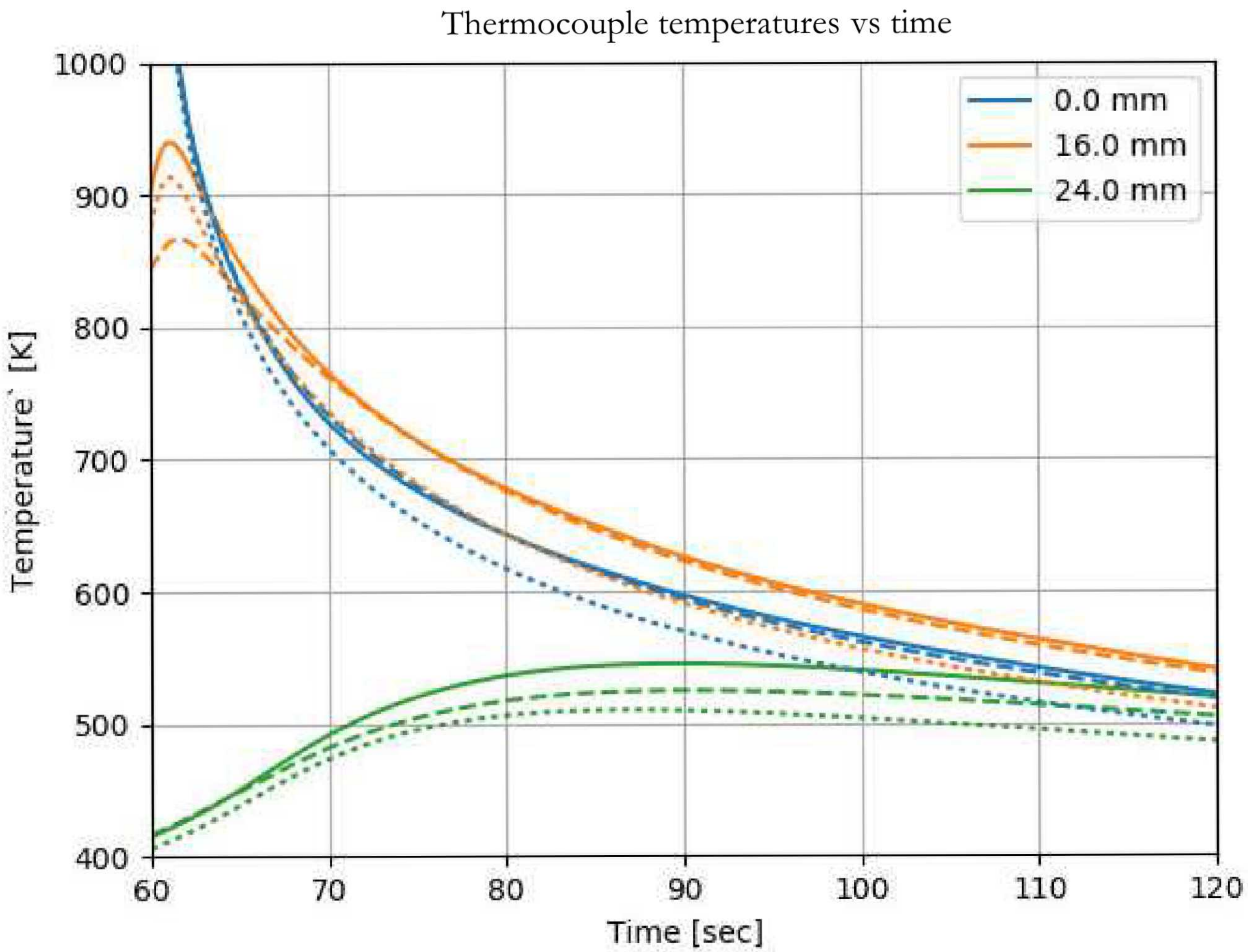
Jacobians colored by the log of the matrix entry value for a single element

Ablation Model Development: Monolithic Solve

Workshop #5, problem 2.2

- 1-D decomposing ablator (TACOT) subject to a constant BC (turns off at 60 sec)

- In-depth equations show improvement
- Investigating other sources of inconsistency with Chaleur
- Work is ongoing



Solid: MTRFEM
Dotted: SPARC
Dashed: Chaleur

Ablation Validation Effort: Arcjet Cases

Also this past year…

- Q* ablation model in both 1D and 3D
- Code comparison work for carbon phenolics
- Coupled solve simulation hardening
- Some flight test validation
- More…

Goal:

Validate both decomposing and nondecomposing ablation models experimental data from arcjets.

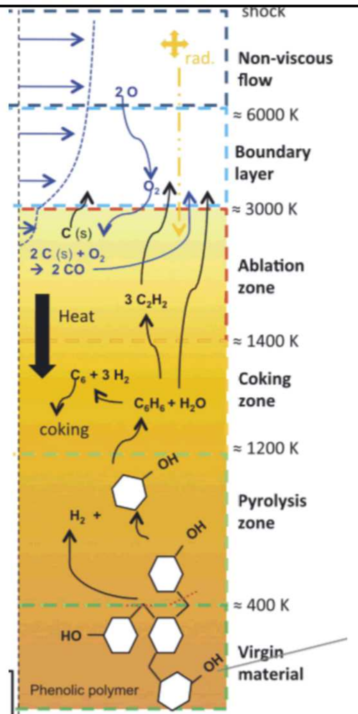
- Can SPARC reproduce experimental data, conditional on uncert
- Can we assess the model-form errors?

Steps:

- Identify influential SPARC inputs $\vec{p}$ for each of the experimental observables
- Model $\vec{p}$ as uncertain (random) variables and predict the experimental data
- Infer $\vec{p}$ from experimental data and assess how plausible it is

Identifying influential SPARC inputs

- Model all 17 SPARC inputs ($\vec{p}$) as uniform distributions ($\pm 20\%$ variation about mean/nominal value)
- Using 2500 samples in 17-dimensional space, compute thermocouple, recession and pyrometer readings at 2 time-instants
- Compute correlation between predictions and elements of ($\vec{p}$)



Rivier et al, AST, 2019

Chemistry mechanisms (simplified illustration)

Next Year's Effort: "Virtual Flight Test"

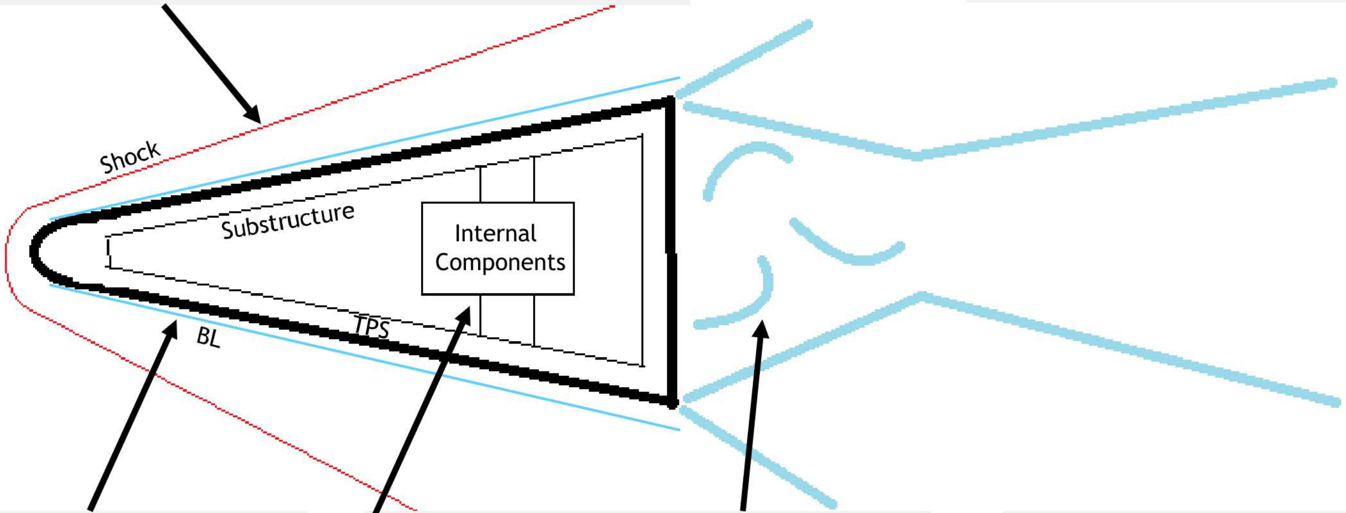
- The physics are coupled: fluid, ablation, material response, and trajectory
- Historically, we have uncoupled them and attempted to correct using engineering assumptions
- Legacy approach is not viable for some classes of problems
- Always striving to reduce assumptions and increase predictive power

Now: formal V&V
Next: formal and embedded V&V/UQ

Now: 100-ish M cell grids
Next: 5-ish B cell grids

Now: Petascale, Xeon-based HPCs
Next: Exascale, ???-based HPCs

Now: Sequence of steady RANS snapshots along a trajectory
Next: Unsteady full-trajectory analysis with WMLES
Impact: prediction of reentry random vibrational loading



Now: correlation based transition prediction
Next: in-situ transition methods

Now: 1-way couplings
Next: 2-way 6 DOF, thermal & structural coupling
Impact: more accurate prediction of flight dynamics, recession, heating and vibrational loading

Now: No wake flow
Next: Full wake flow
Impact:
prediction of base pressure and heating fluctuations

Now: 2^{nd}-order FV scheme
Next:
a) high-res, low-diss. FV scheme
- and/or -
b) high-order FD or DG scheme
Impact: numerical schemes appropriate for unsteady turbulent flows

SPARC Virtual Flight Test Requirements

RANS snapshots → HRLES snapshots → Time accurate HRLES → WRLES

(Lower fidelity) ⟷ Fidelity based on customer/program requirements ⟷ (Higher fidelity)

	RANS snapshots	HRLES snapshots	Time accurate HRLES	WRLES
Size & Quantity	▪ ~100-500 M cells ▪ >10 TB RAM ▪ 1000's of snapshots	▪ ~5-25 B cells ▪ >500 TB RAM ▪ 20's of snapshots	▪ ~5-25 B cells ▪ >500 TB RAM ▪ 5 full simulations	▪ ~50-100 B cells ▪ >2 PB RAM ▪ 1 or 2 time windows
Numerical Methods	▪ Implicit, steady-state ▪ 2nd-order hybrid FV scheme ▪ Continuation solvers ▪ Tridiag solver & GMRES/Multigrid solver	▪ Implicit or IMEX, time accurate ▪ High-res, low-order FV scheme -or- high-order entropy-stable FD/FE ▪ Jacobi & SGS solvers & GMRES/ILU(0)		▪ IMEX or explicit, time accurate ▪ HR, LO FV scheme -or- high-order ES FD/FE ▪ Jacobi & SGS
Coupling & Analysis	▪ Ablation/structural one-way coupling ▪ 6 DOF trajectory coupling ▪ Mesh refinement ▪ Parameter UQ	▪ Ablation/structural coupling ▪ 6 DOF trajectory coupling ▪ Mesh refinement ▪ Parameter UQ & In-situ viz		▪ Mesh refinement ▪ In-situ viz
Critical Components	▪ Scalable solvers ▪ Performance portability ▪ Embedded analysis (meshing ▪ V&V	▪ Scalable solvers ▪ Performance portability ▪ Embedded analysis ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V		▪ Performance portability ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V

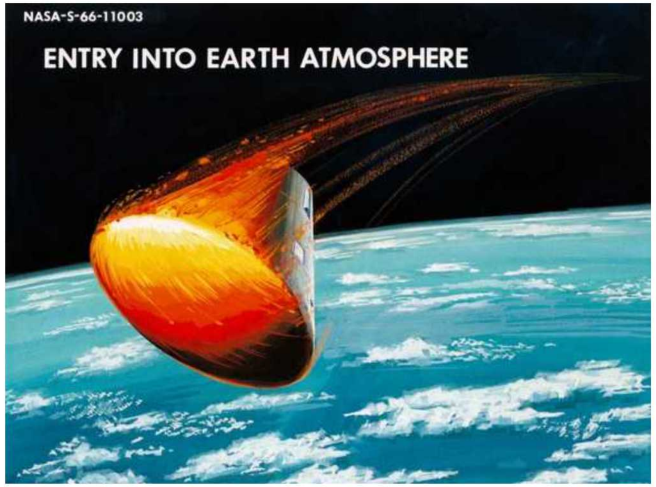
Legacy/Current Capability

FY20 Target

Sneak Peeks: Work at Sandia Impacting Macroscale Modeling

Understanding Materials Under Extreme Environments

Thermal Protection System (TPS) materials must withstand extreme environments



NASA: "Project Fire Redux: Interplanetary Reentery Test (1966)
https://www.wired.com/2012/07/interplanetary-reentry-tests-1966/

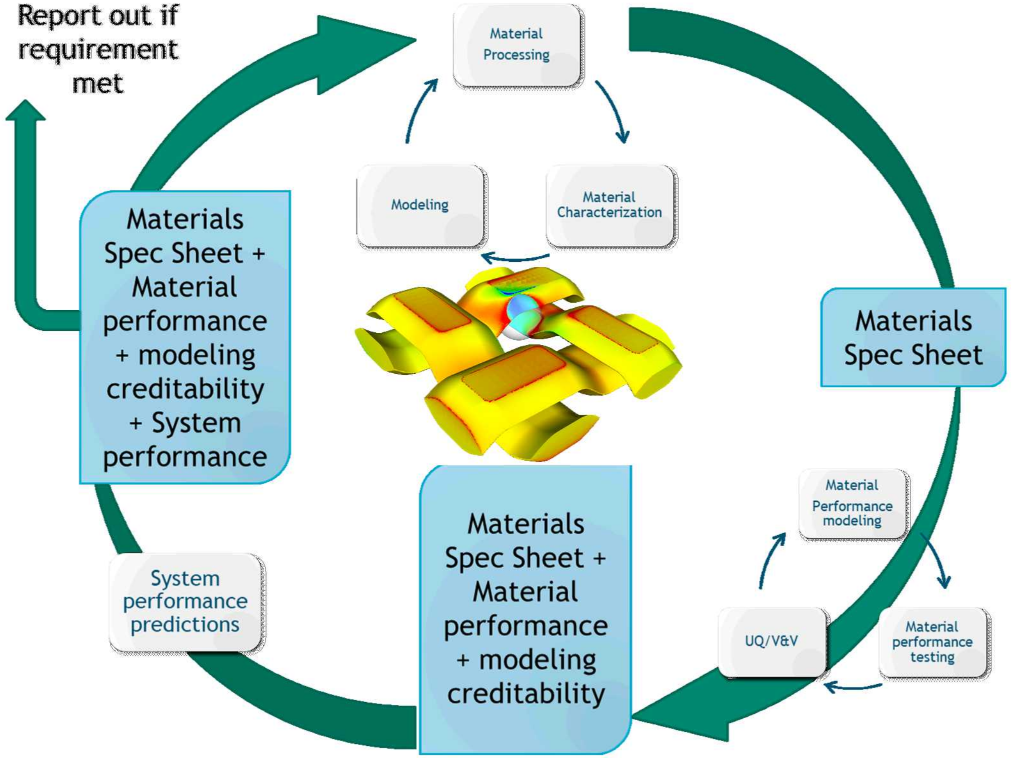
How do we quickly improve our understanding of materials used?

2-fold: computation & performance characterization.

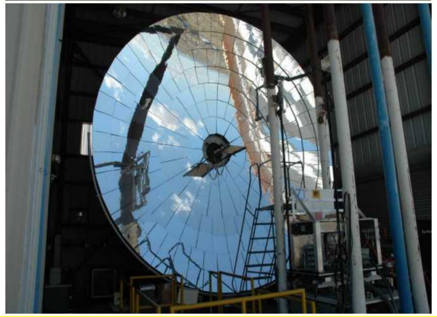
1966 FIRE REUDUX NASA: Complex problem "no substitute for testing specific configurations and materials in the actual environment of interest"

Goal: manufacture materials & improve our understanding of properties under extreme environments through modeling efforts

Models are using data from materials science & environmental performance to improve our understanding



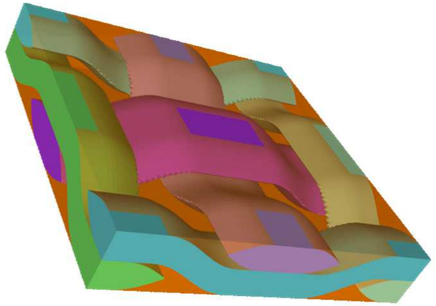
The power of the Sun is used to simulate reentry heating to verify performance behavior

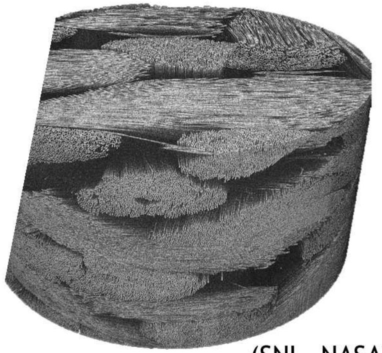


*One of several Sandia testing facilities available to simulate extreme environments

Mesoscale materials and ablation modeling

Geometry

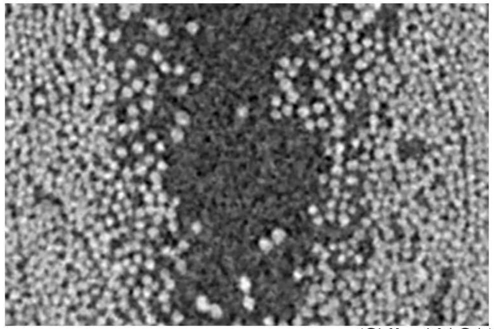




(SNL, NASA)

Analytical + Image-based

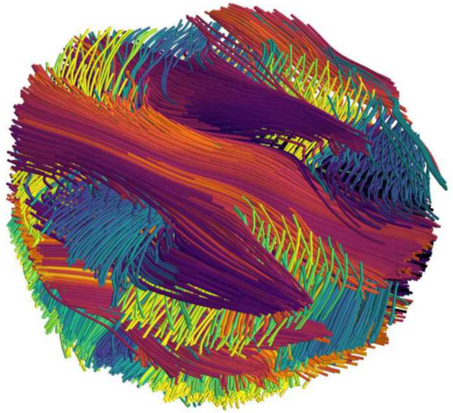
Constituent properties



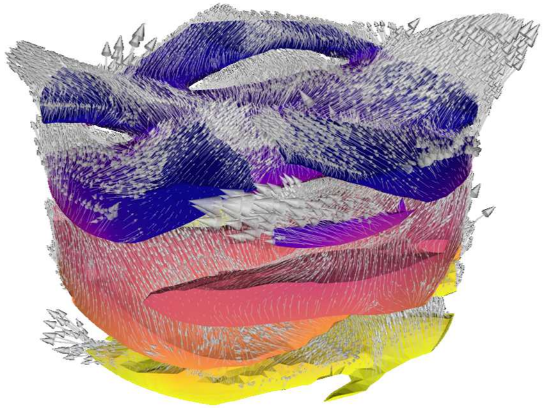
(SNL, NASA)

Microscale + constituent measurements

Mesoscale

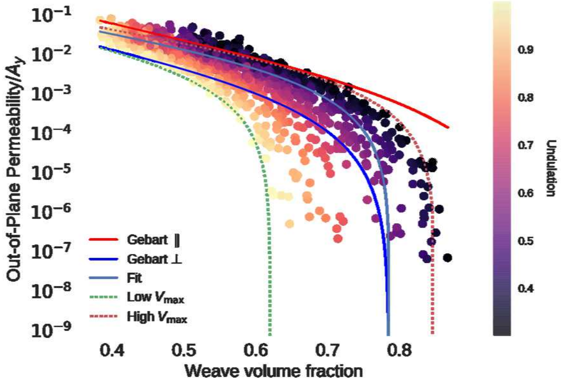


Orientation analysis

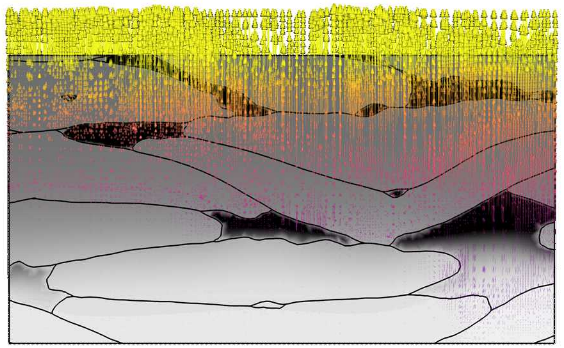


Physics calculations (heat flux)

Macroscale



Effective property distributions and sensitivities



Transient ablation performance

Mesoscale modeling systematically bridges fundamental constituent behavior and macroscale response

Thank You