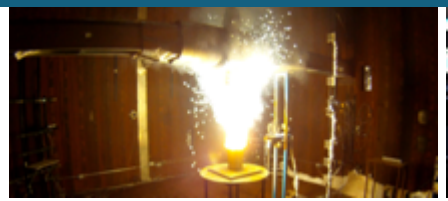
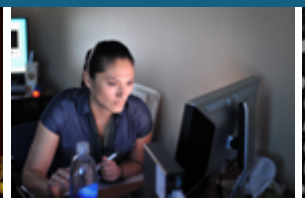
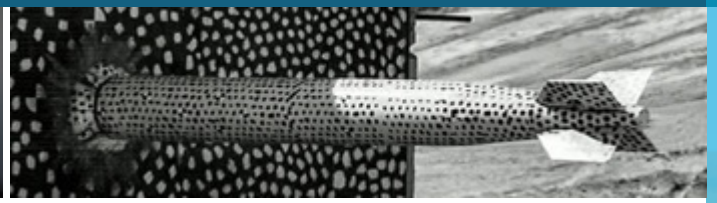
SAND2021-4751C

Sandia National Laboratories

Concurrent V&V/UQ and Code Capability Development: Hypersonic Reentry Analysis with SPARC







PRESENTED BY

Sarah L. Kieweg, SNL

U.S. DEPARTMENT OF ENERGY | NNSA

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Acknowledgements

Slide Material Acknowledgments: **Brian Carnes, Derek Dinzl, Micah Howard, Erin Mussoni, Jaideep Ray, Greg Weirs**

SPARC and Hypersonics V&V/UQ Team: Victor Brunini, Brian Carnes, Derek Dinzl, Travis Fisher, Brian Freno, Mike Hansen, Micah Howard, Ryan Keedy, Sarah Kieweg, Erin Mussoni, Jaideep Ray, Ross Wagnild, Greg Weirs, and Justin Winokur

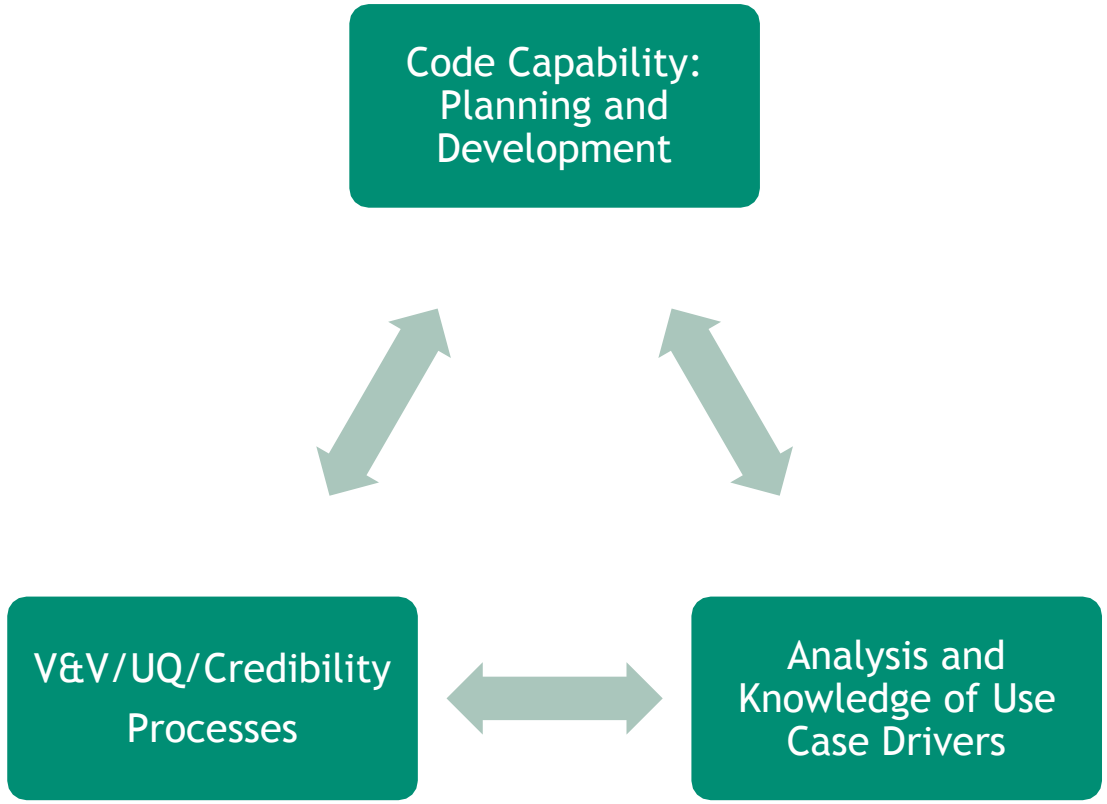
Managers, PMs, and PIs: Paul Crozier, Amanda Dodd, Mike Glass, Bill Rider, Justin Smith, Jim Stewart, and Angel Urbina

Funding:

- ATDM FY20 L1 Milestone (PI/PMs: Paul Crozier, Jim Stewart)
- ASC V&V (PMs: Lauren Beghini, Justin Smith, Amanda Dodd)

Outline

- Introduction:
  - SPARC
  - Concurrent V&V and Code Development
  - V&V and Credibility Processes
- Recent ATDM L1 Milestone: Aero-thermal Analysis Reentry V&V/UQ Workflow
- Challenges in Concurrent V&V and Code Development in Hypersonic Reentry:
  - UQ in Coupled/Combined Environments
  - V&V Suites
  - Limited Validation Data
  - Code Verification in Coupled/Combined Environments
- Example: Hypersonic Wind Tunnel V&V
- Summary of Benefits and Challenges



Introduction | **Hypersonic Reentry Simulations**

SPARC = **S**andia **P**arallel **A**erodynamics and **R**eentry **C**ode

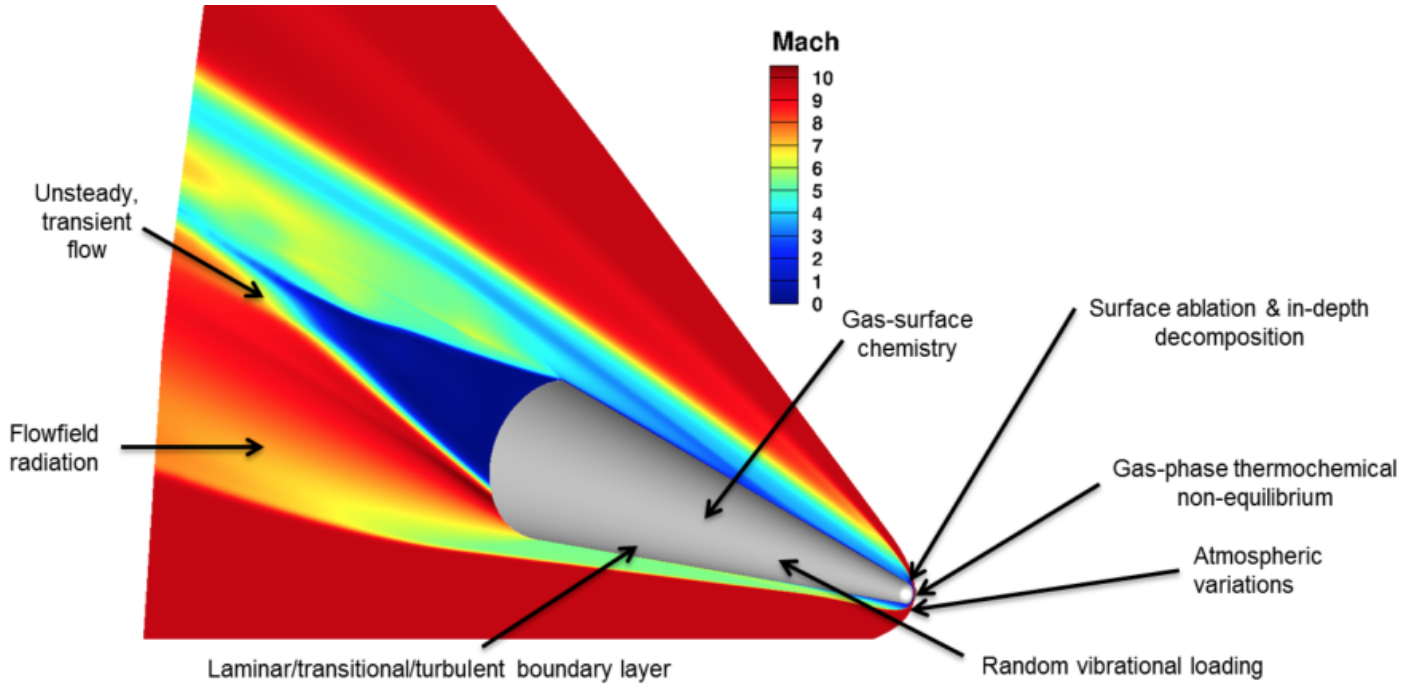
Atmospheric reentry of flight vehicles:

- Compressible flow from subsonic to hypersonic
- Turbulence
- Thermochemical nonequilibrium

Vehicle performance predictions require estimates of aerodynamic forces and heat transfer.

Quantities of Interest (QOIs) from experiments and simulations:

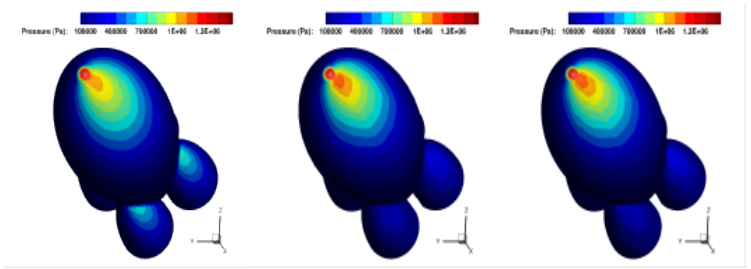
- Heat flux at surface
- Pressure on surface
- Separation length, separation point, and reattachment point
- Temperature on and inside the re-entry vehicle
- Surface recession



Illustrative image created by Ross Wagnild and Micah Howard (SNL)

Introduction | **SPARC Capability Development – A Spectrum**

Increasing CFD Fidelity

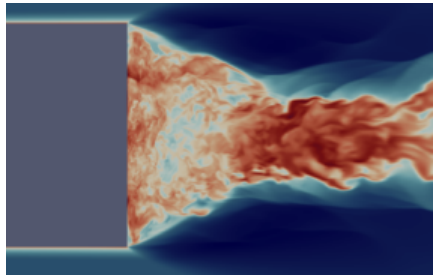


Modified Newtonian Aero
Runtime ~10 seconds,
1 core

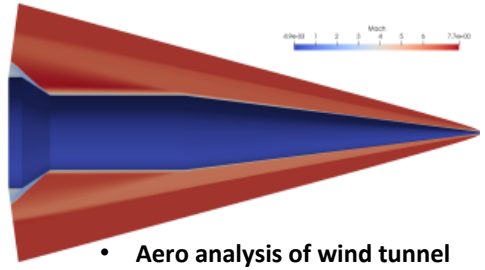
Euler
Runtime ~10 minutes,
8 cores

RANS
Runtime ~100 minutes,
288 cores

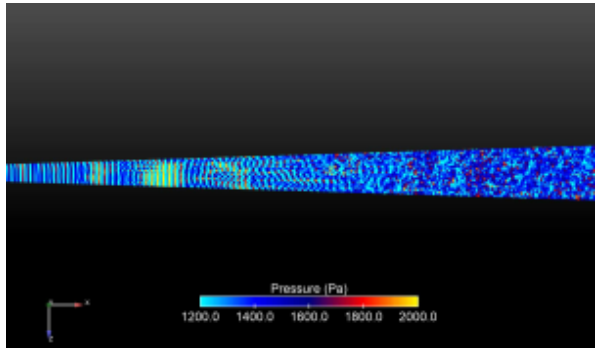
"RocketShip" geometry: Increasing CFD Fidelity



Unsteady cylinder wake



- **Aero analysis of wind tunnel**
- **Aerothermal coupled analysis**



Mach 8 transitional boundary layer

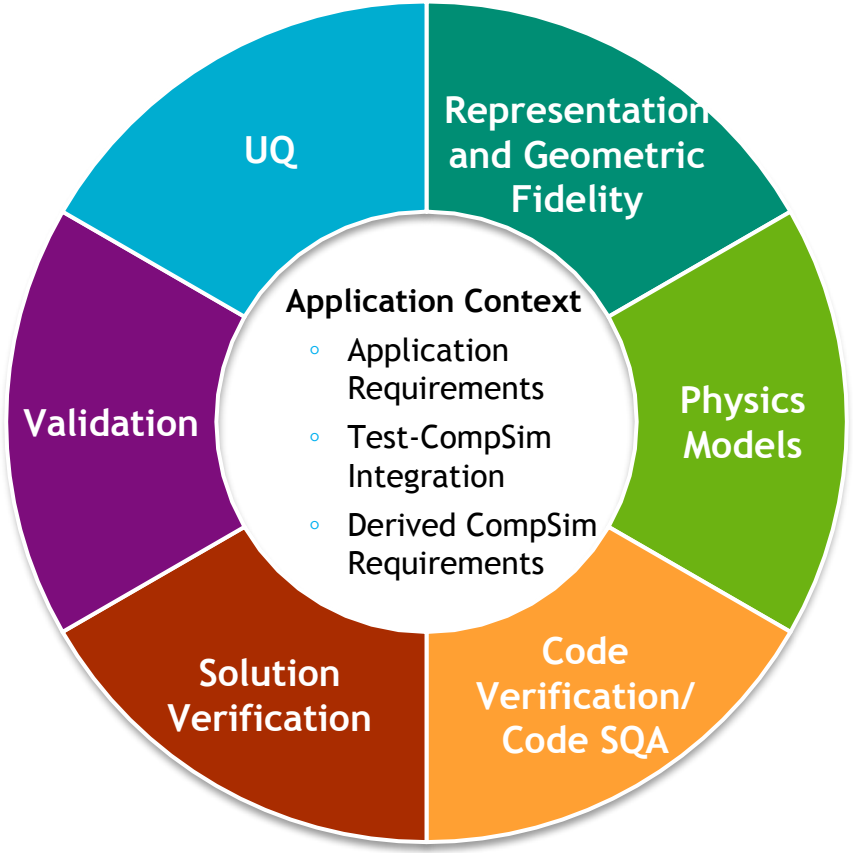
Increasing Computational Cost

Runtime:	seconds	minutes	hours	days	weeks
Resources:	1 core	10-100 cores	100's to 1000's of cores	1000's of cores	1000's to millions of cores
Uses:	**Conceptual design**		**Engineering analyses**	**Qualification**	**Research**

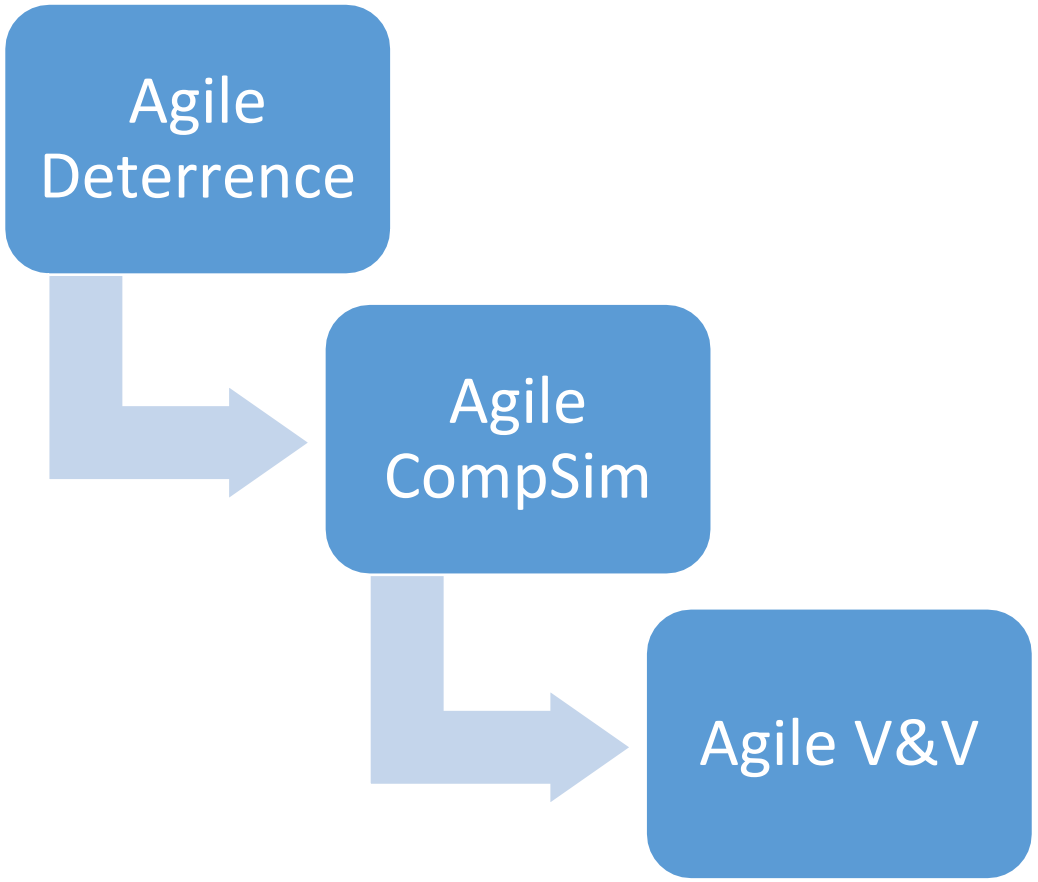
Slide Acknowledgement: Derek Dinzl

Introduction | **V&V/UQ and Credibility Processes**

The computational simulation (CompSim = ModSim) **credibility process** assembles and documents **evidence** to ascertain and communicate the **believability** of **predictions** that are produced from computational simulations.

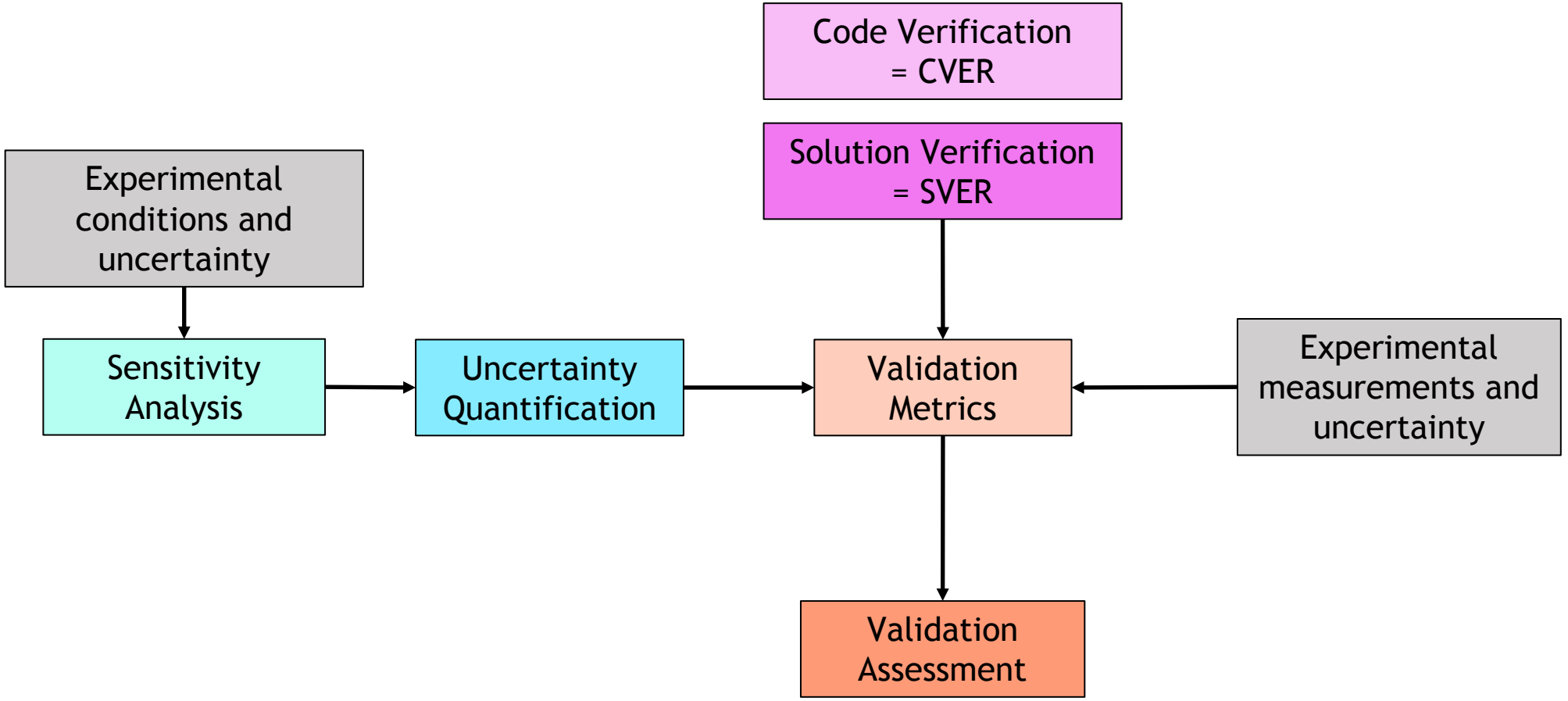


Introduction | **Concurrent V&V/UQ with Code Development**



- Approach: Use concurrent code development and V&V to be more agile.
  - In contrast, V&V has often been left until after it is a production code
- How can we achieve agile V&V along with code development?
  - Address challenges with validation data
  - Create and maintain verification and validation suites
  - Create UQ and code verification plans in challenging combined environments

Introduction | **V&V/UQ Workflow**



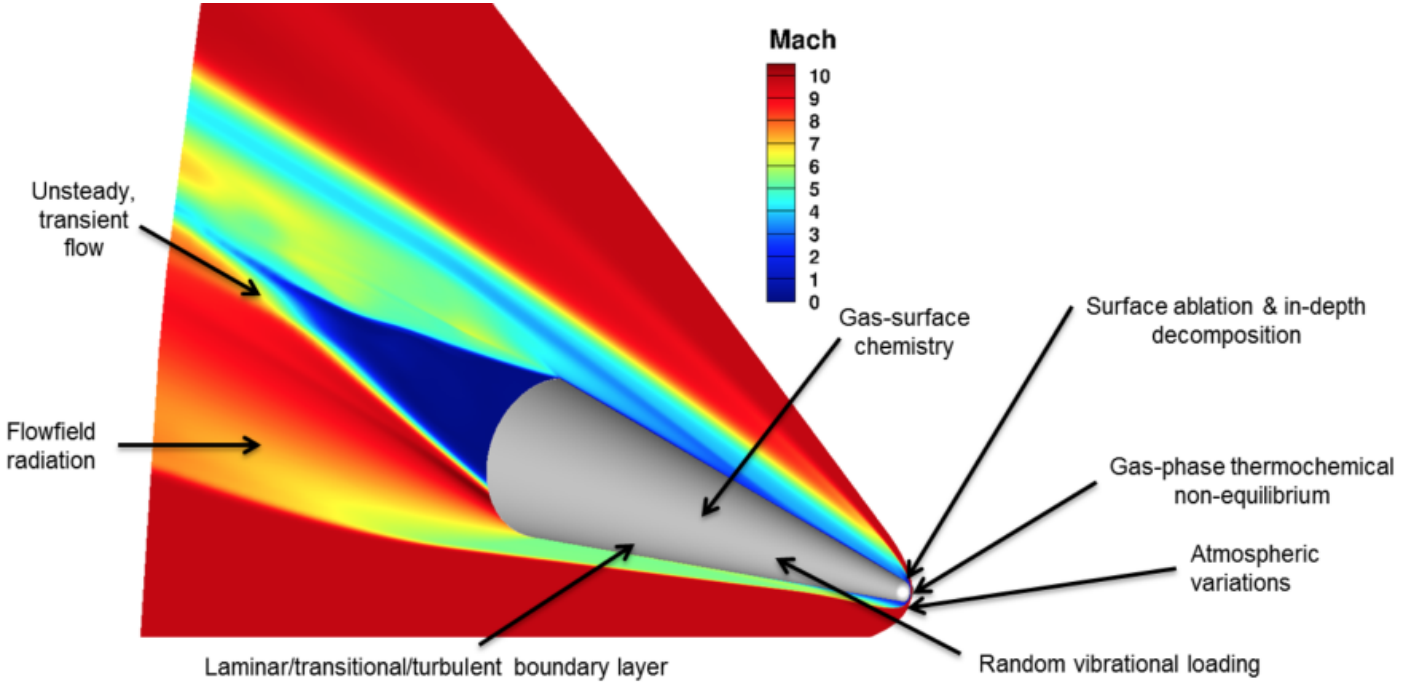
Experimental uncertainty of <u>both</u> inflow conditions and measured outputs is important part of the validation assessment.

FY20 L1 ATDM Milestone | **Recent Accomplishment**

ATDM L1 Milestone Goal		Metric	Minimum criteria	Stretch criteria	L1 status
1(a)	**Mission Impact**	Hypersonic flight test V&V assessment	Demonstrate physical models and workflow with SPARC	Validation assessment of SPARC simulations against flight test	Completed

Accomplishments:

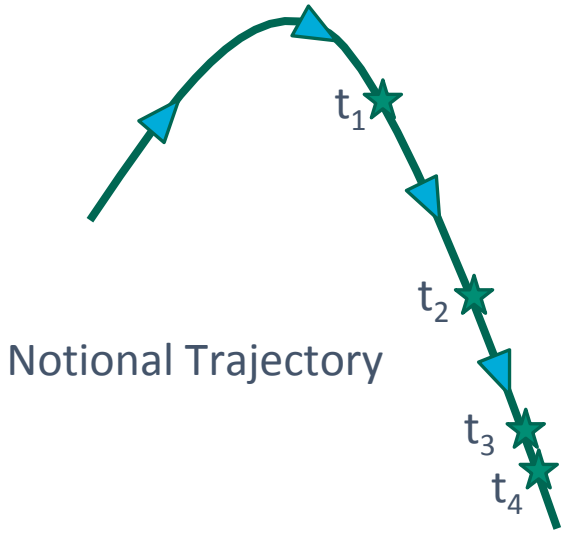
- Demonstrated analysis and UQ workflow on HPC ARM computing platform (Astra)
- Demonstrated Benefits of Concurrent Code Development and V&V/UQ
- Developed new V&V/UQ Approaches for Coupled/Combined Environments
- Found Advantages of WFH during COVID
- Established V&V Foundation as Further Capabilities Continue



Illustrative image of phenomena in hypersonic reentry. Created by Ross Wagnild and Micah Howard (SNL)

Challenges | **Aero-thermal Re-entry Analysis Workflow**

Solve **Aero Analysis** at Snapshots along Trajectory

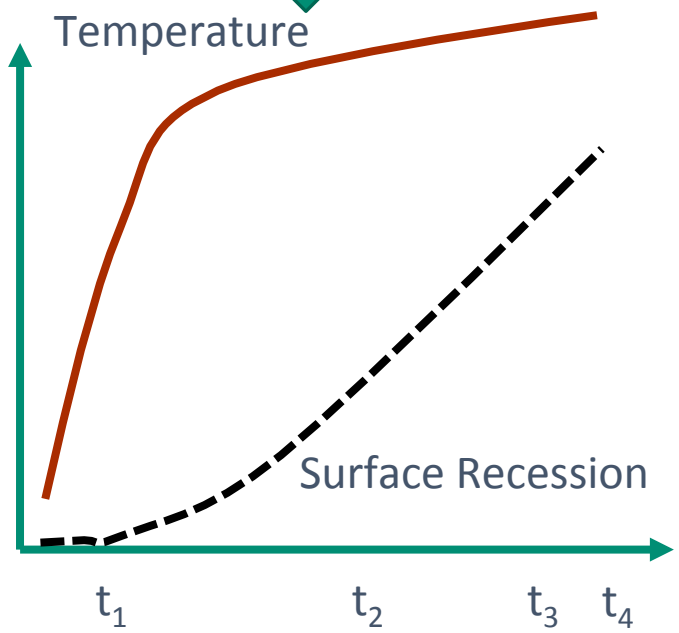


Map aeroheating information from trajectory CFD solution to surface mesh

Solve **Thermal/Ablative Response** over time for temperature and recession as function of time and location

Map aeroheating load to surface of thermal model

Model/code coupling choices:
- One-way
- Two-way



Coupled Analysis:
- **Uncoupled Snapshot**
- **Coupled Snapshot**
- **Coupled Unsteady**

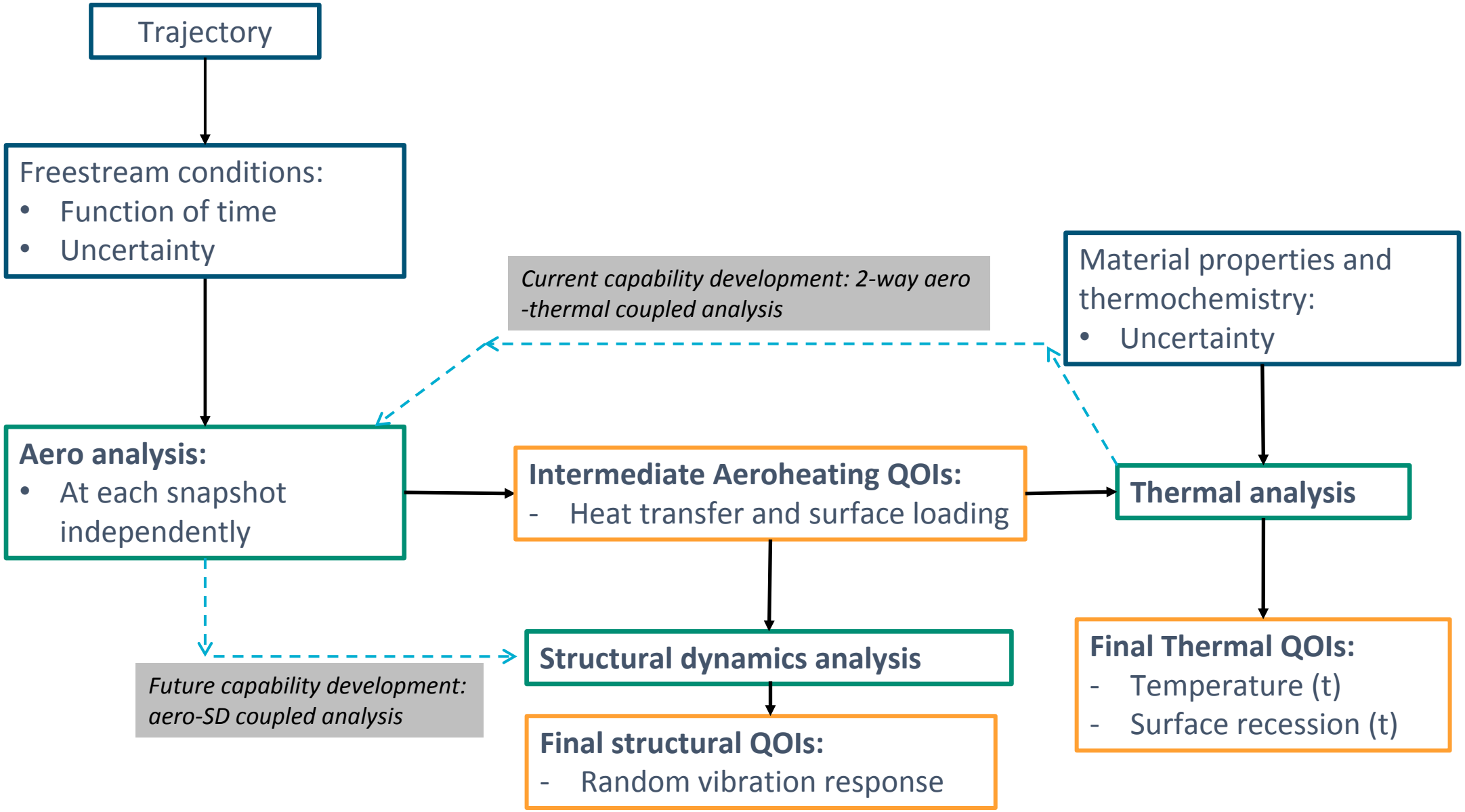
Coupled Analyses include:
Aero→Thermal and Aero→ SD

Challenges | **Outline**

Challenges for Concurrent V&V/UQ and Code Development in Hypersonic Reentry:

- **Uncertainty quantification (UQ)** and **validation** in a coupled analysis with combined environments
- Creating and maintaining **V&V suites**
- Limited **validation data** available
- **Code verification** in a coupled analysis with combined environments

Challenges | 1. **Coupled Analyses and Combined Environments**



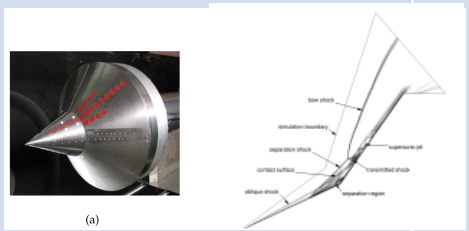
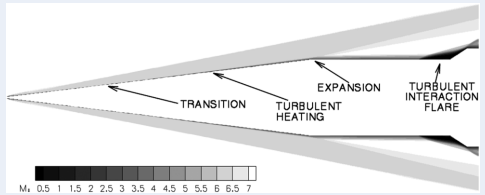
Challenges | 2. **Creating and Maintaining V&V Suites**

- PIRT = Phenomena Identification Ranking Table
- Challenges:
  - How summarize and update code capability and credibility?
  - How document verification and validation evidence in the context of phenomena?
  - How translate V&V cases completed in our work to verification and validation suites?
  - Repositories
  - Framework to create credibility evidence for mission driver use cases

Application: Double-cone laminar, reactive gas mixture		LENS XX: thermochemically quiescent high-enthalpy freestream gas				
Quantity of Interest: heat flux, pressure, separation			match (or over-adequate)			
Contact: Sarah Kieweg			adequacy one notch too low			
Assessment Team: SPARC VVUQ team			adequacy two notches too low			
Date: 10/19/17						
			Adequacy for Intended Use			
ID	***Phenomena***	***Importance***	**Math Model**	**Code**	**Validation**	**Model Parameter**
A	**Hypersonic Flow**					
A1	Shock structure	H			L	
A2	Nonequilibrium vibrational energy	H			M	
A3	Molecular viscosity model for thermochem neq	L/M			M	
A4	uniform, equilibrium freestream and inflow	L			L	
A5	transient effects	L			L	
B	**Laminar Boundary Layer + interactions**					
B1	Attached laminar BL	M			M	
B2	shock standoff at bdry layer	L			L	
B3	Shock-BL interaction at cone junction	H			H	
B4	Shock train downstream of corner	M			M	
B5	detachment and reattachment of laminar BL	H			H	
C	**Gas Models**					
C1	reacting gas mixture (air)	H			M	
D						
D1	surface catalycity	H			L	

Note: Here, the validation adequacy column indicates the adequacy of the available validation case (LENS XX double) cone to capture a particular phenomena (row). It does not reflect SPARC capability or validation of a SPARC simulation.

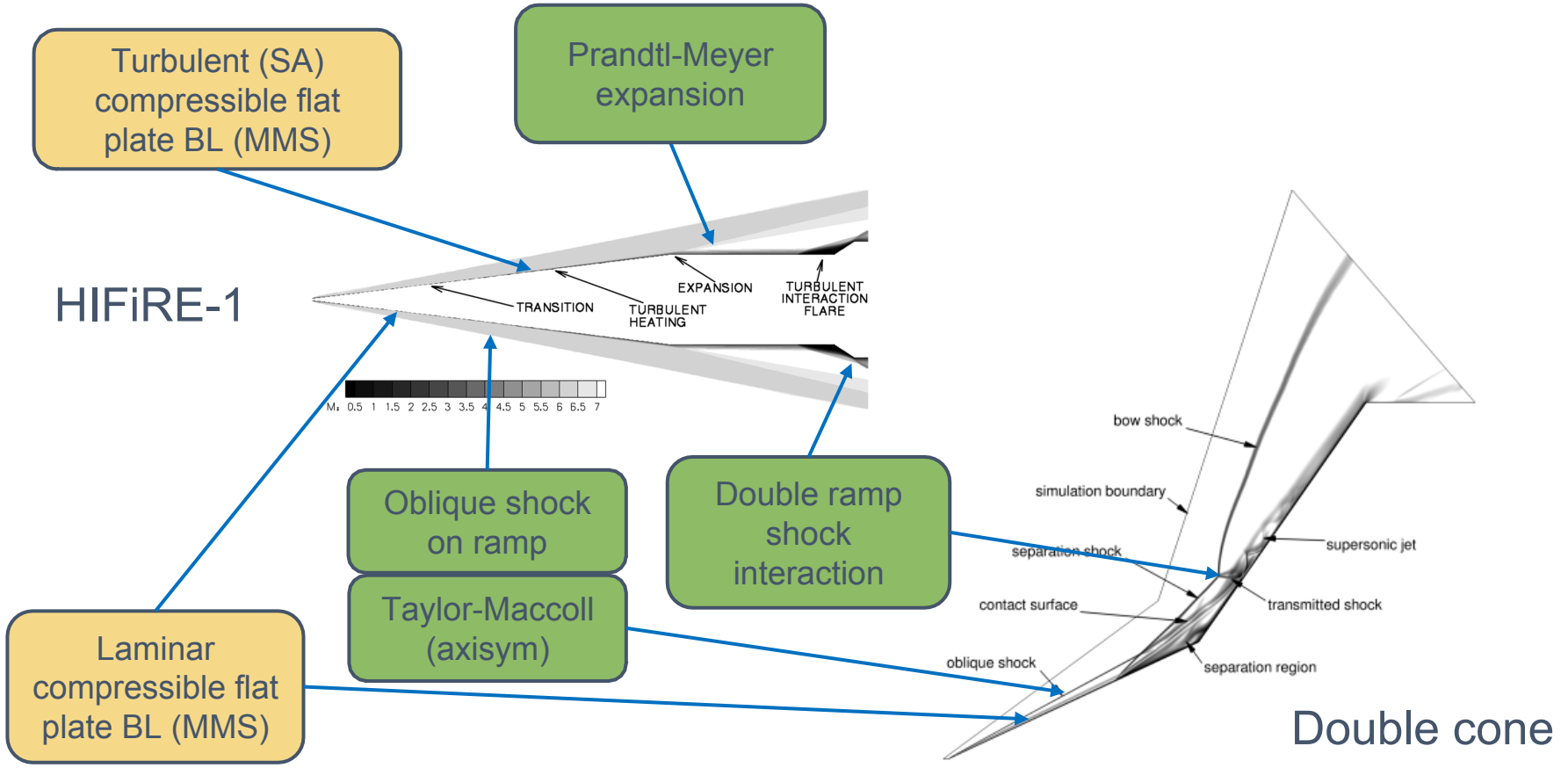
Challenges | 3. **Limited Validation Data**

Use Cases → / Validation Cases ↓	Steady-State Aerodynamic Analysis	Ablation / Thermal Response	Trajectory Aerothermal Analysis	Reentry Random Vibration Analysis
Double-cone (wind-tunnel) 	**FY18**			
HI-FiRE-1 (wind-tunnel) 	**FY18, FY19**			
Arcjet ablation 		**FY19 – FY21**	**FY22**	
Flight Test		**FY19 – FY21**	**FY19 – FY21**	
Other Flight Tests				**FY21, FY22+**

Code verification activities also selected to isolate phenomena present in these hierarchical validation cases and use cases

Challenges | 4. **Code Verification in Coupled Analyses and Combined Environments**

- Code verification activities, such as exact solutions, often driven by phenomena in hierarchical validation cases.
- **Challenge and Research Need:** How best design code verification cases applicable to 2-way coupled analyses and combined environments?
  - Aero-thermal
  - Aero-SD



Double cone image computed using SPARC

HIFiRE-1 image: MacLean, Wadhams, et al., JSR 45(6), 2008.

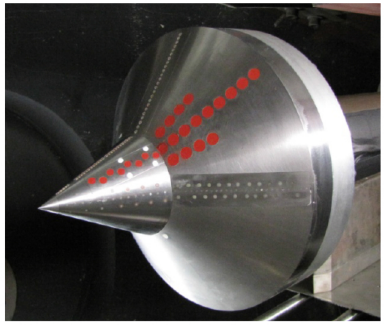
Example of V&V Approach| **Hypersonic Wind Tunnel Validation**

Hypersonic Wind Tunnel with Double Cone

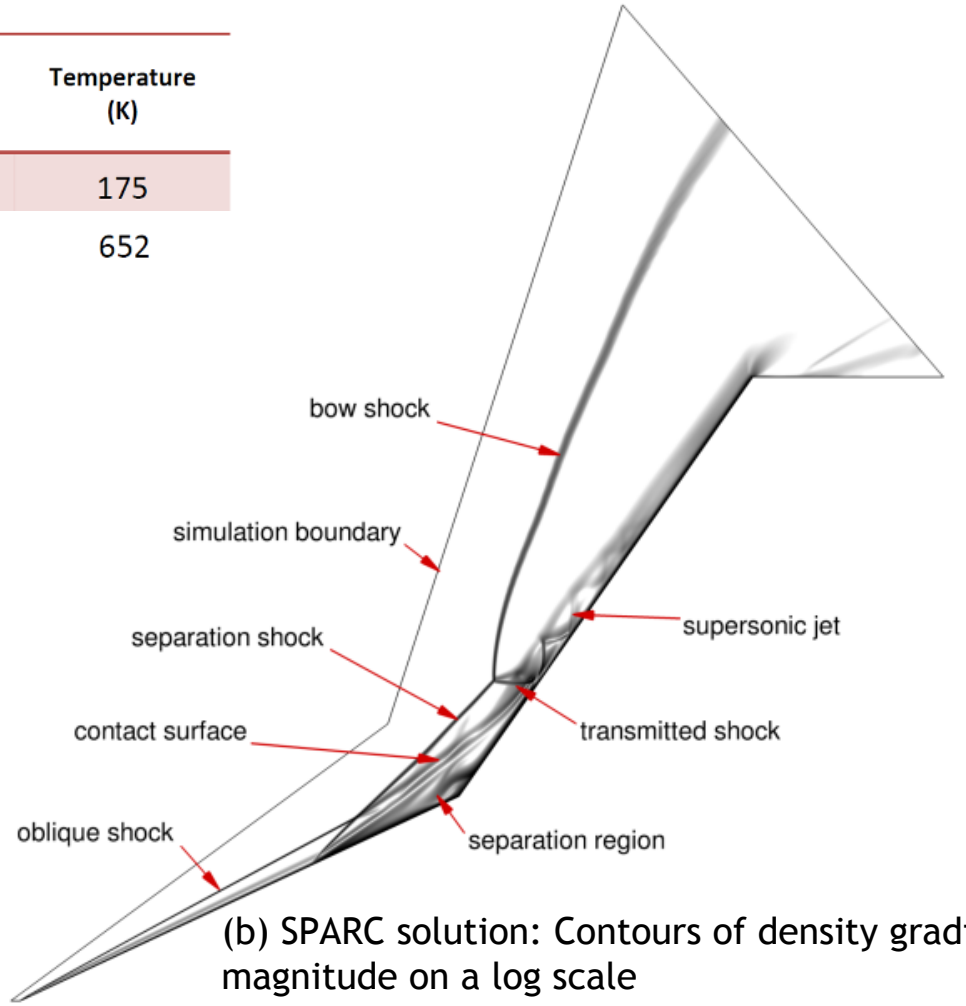
Run #	Total Enthalpy (MJ/kg)	Mach Number	Pitot Pressure (kPa)	Unit Reynolds Number /10^6 (1/m)	Velocity (km/s)	Density (g/m^3)	Temperature (K)
1	5.44	12.2	5.1	0.14	3.246	0.499	175
4	21.77	12.82	39.5	0.20	6.497	0.964	652

Validation data set provides a focus on specific phenomena:

- Laminar flow of an air mixture
- Strong thermochemical non-equilibrium
- Shock – boundary layer interactions.



(a) Double cone photograph with sensor locations



(b) SPARC solution: Contours of density gradient magnitude on a log scale

Table and Figure (a): LENS XX CUBRIC double cone wind tunnel, MacLean *et al.*, 2014. Figure (b) : SPARC solution of Run 35 (LENS I) by Derek Dinzl. Shown here to demonstrate phenomena.

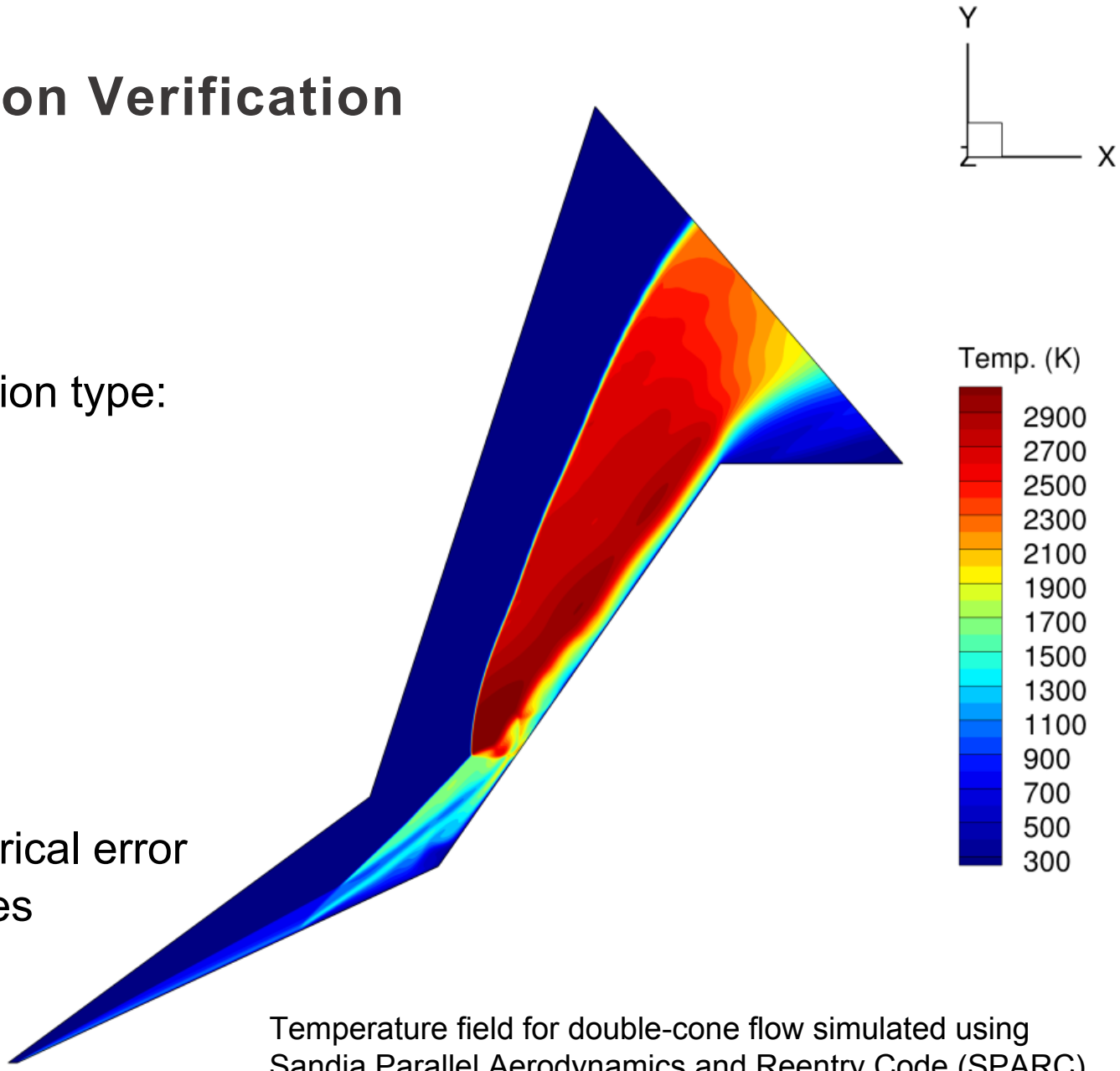
Example | **Code and Solution Verification**

Code verification

- Planning for test development
- Organized by physics and solution type:
  - Manufactured
  - Exact
  - Benchmark

Solution verification

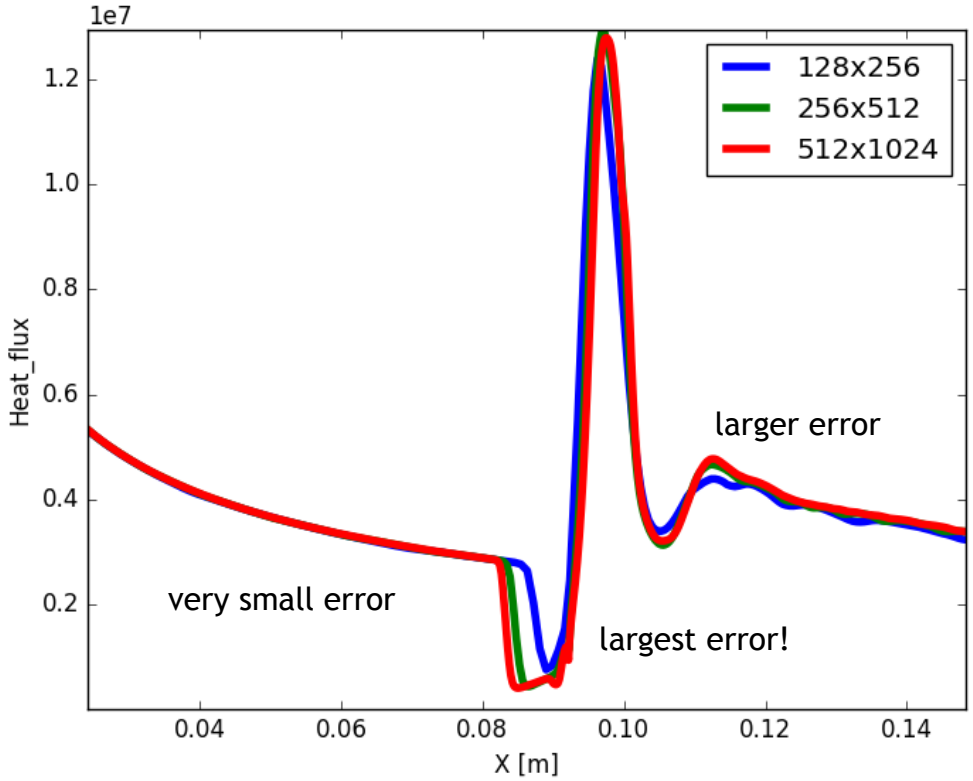
- Nominal discretization
- Iterative convergence
- Robust extrapolation and numerical error
- Combining multiple error sources

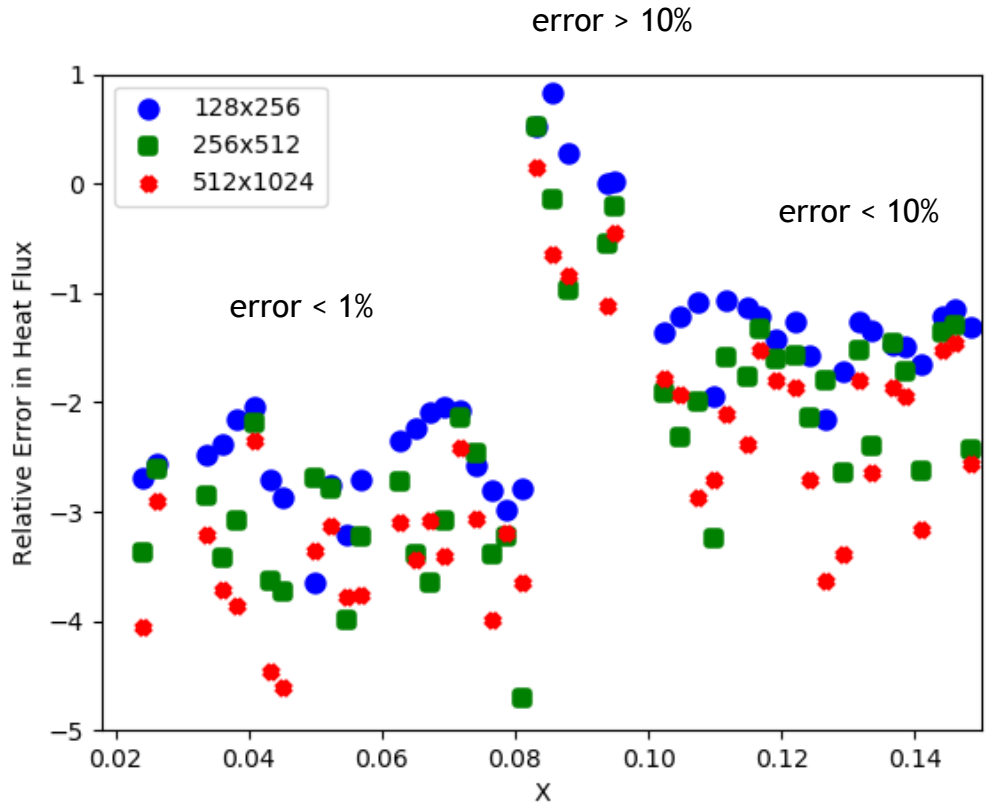


Temperature field for double-cone flow simulated using Sandia Parallel Aerodynamics and Reentry Code (SPARC)

Example | **Solution Verification**

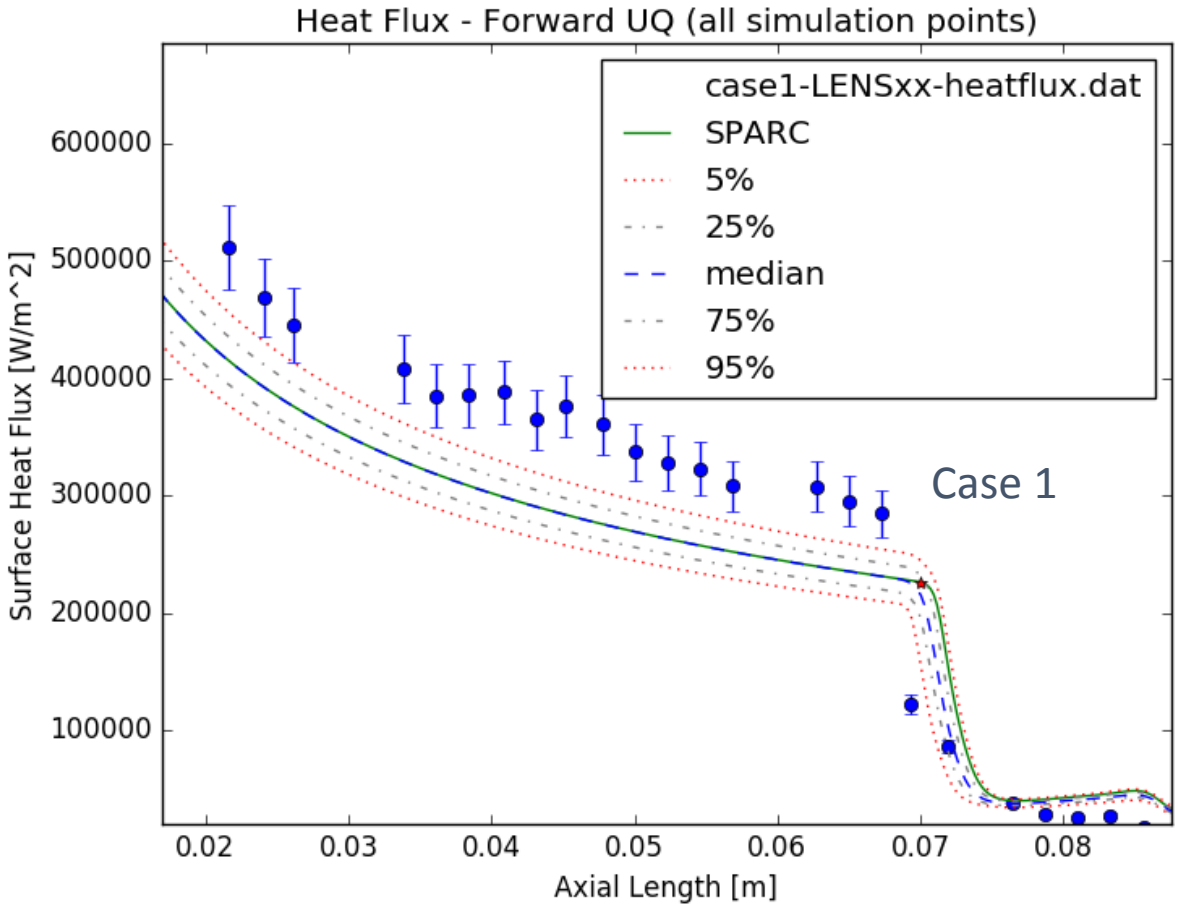
- Quantitative estimation of mesh error
- Ask: is the mesh converged? Should it be 10% or 1%?
- Use in quantitative validation metrics

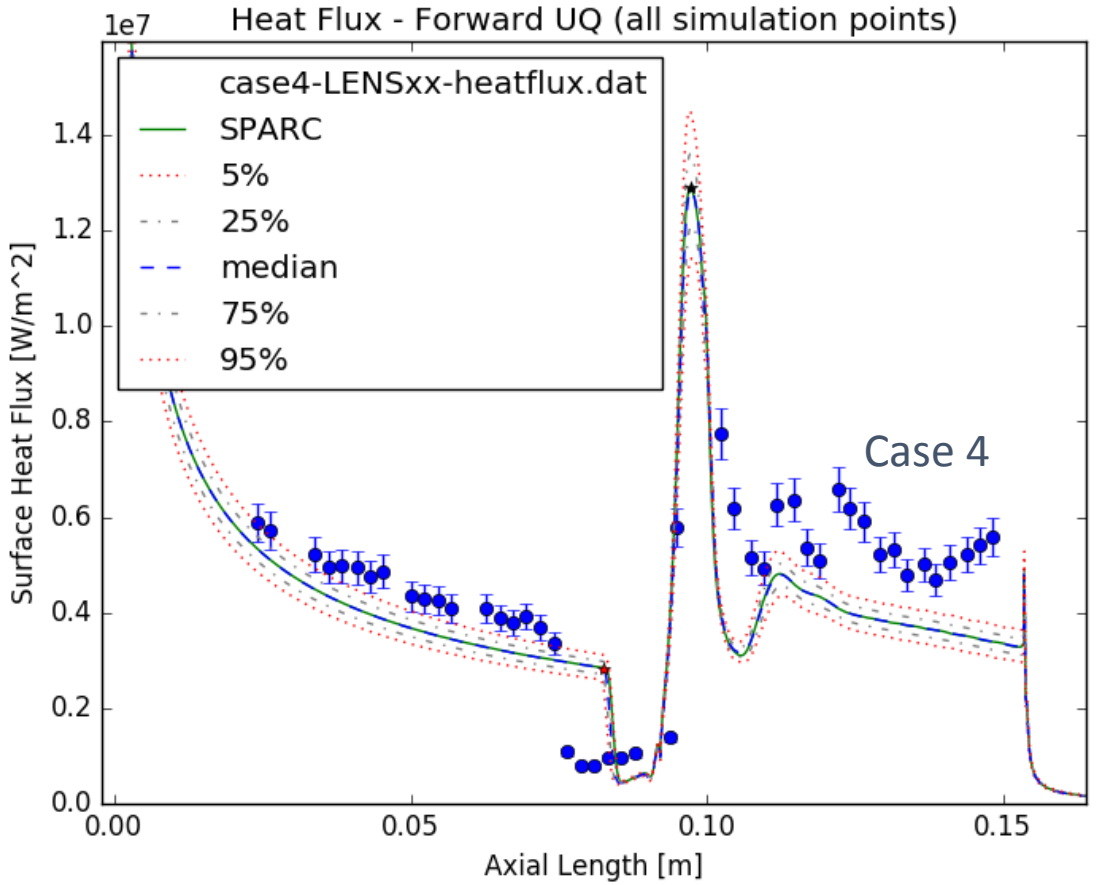




Example | **Validation Assessment with Uncertainty**

Forward Propagation of Uncertainty → parametric (input) uncertainty

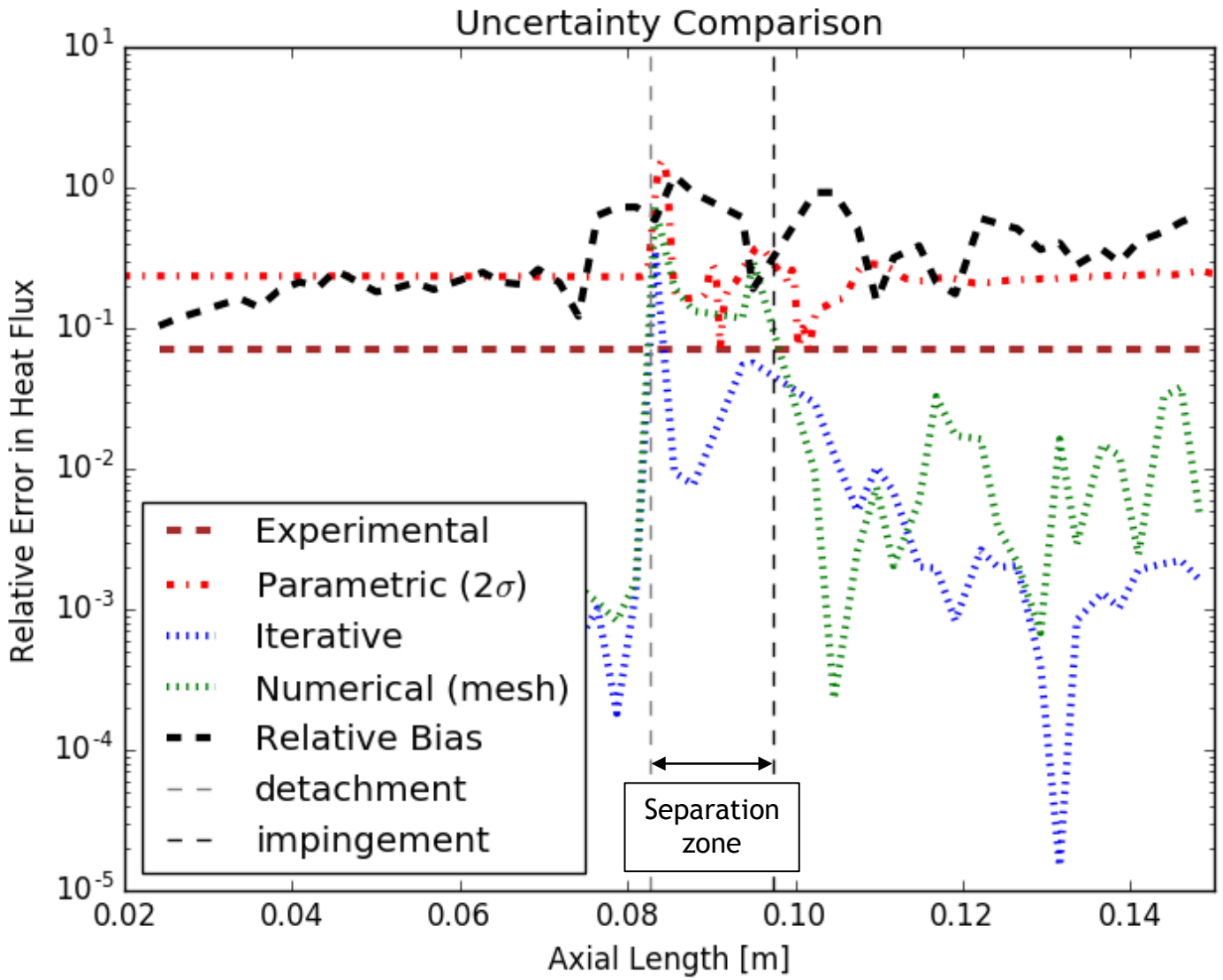




Example of validation using uncertain experiments and probabilistic ensembles of SPARC simulations.

SPARC simulations use “fineR” v2_512x1024mesh, 100,000 iterations. UQ ensemble from PCE Surrogate and inputs: 7, 3, and 3% rho, U, T per CUBRC; Tv = T. PCE = Polynomial Chaos Expansion

Example | **Relative Contributions of Uncertainty**



$$u_{\text{val, rel}} = \sqrt{u^2_{\text{param, rel}} + u^2_{\text{iter, rel}} + u^2_{\text{num, rel}} + u^2_{\text{expt, rel}}}$$

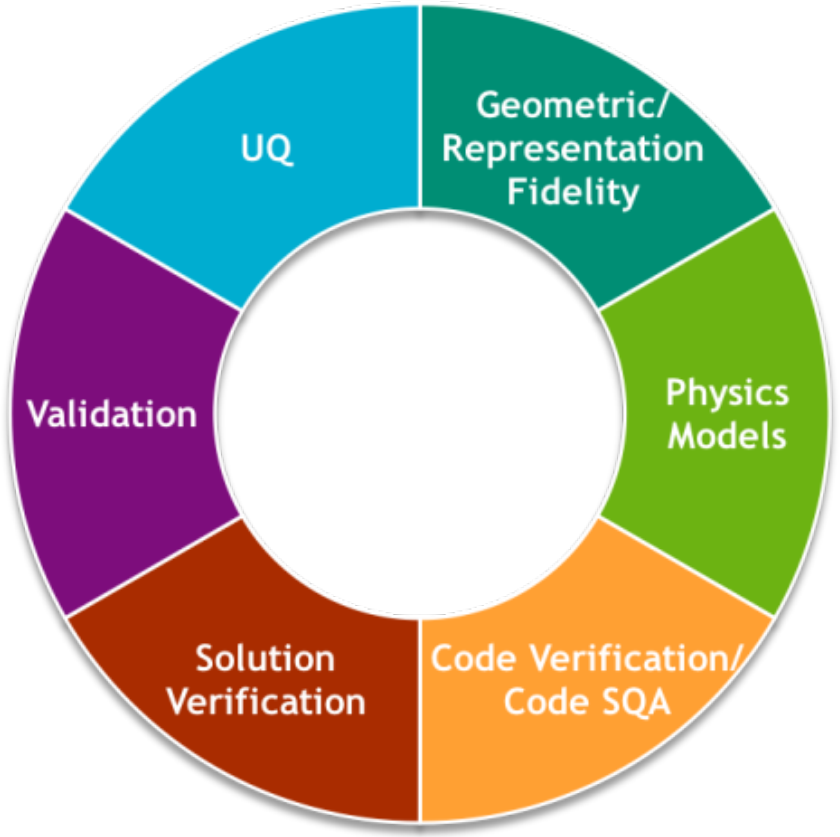
$$u_{\text{val}} = (u_{\text{val, rel}})(\text{median})$$

No Image

SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Expt error bars: heat flux +/- 7 %, pressure +/- 5% per CUBRC.

Summary | **V&V Provides Credibility Evidence and Novel R&D in Combined Environments**

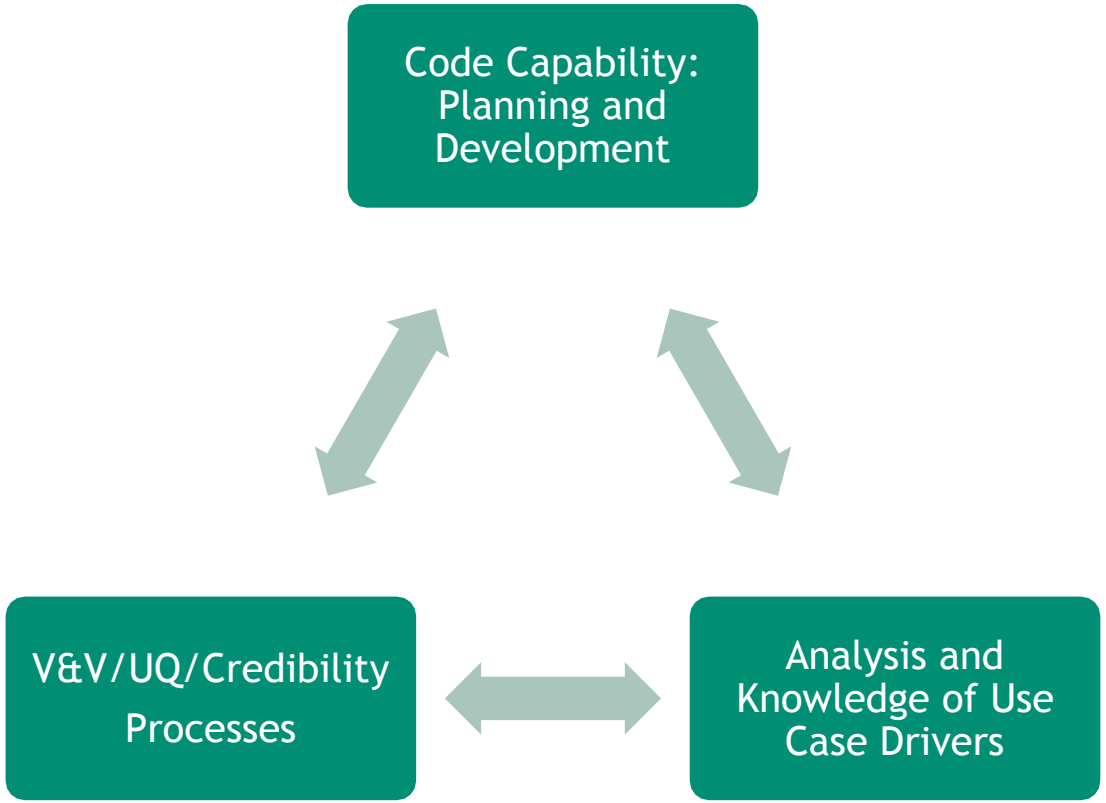
- **R&D for UQ in Coupled Environment Simulations**
  - UQ of trajectory: atmosphere, snapshot selection
  - UQ methodology for 1-way coupled snapshot aero-thermal analysis
- **R&D for Code and Solution Verification**
  - Manufactured solutions for inviscid and reacting flow; thermal/ablation
  - Framework to translate verification and validation tests to a test suite
- **R&D for Validation and Sensitivity Analysis**
  - Sensitivity analysis strategies and visualization tools to down-select parameters
  - Isolation and examination of several sources of uncertainty and inclusion in quantitative validation metric



Predictive Capability Maturity Model (PCMM) facilitates planning and communication of credibility evidence.

Summary | **Benefits of Concurrent Code Development with V&V/UQ**

- **Benefits of battle-hardening SPARC and analysis workflow:**
  - Exercising and stressing SPARC with large ensemble runs on our HPC systems.
  - Develop robust analysis and V&V/UQ workflow
- **Exposes improvements for code development:**
  - Robustness; User guardrails and experiences
  - Ease of templatizing input safely for UQ processes
  - Demonstrates that V&V/UQ doesn't add to the development timeline – feedback to developers while capability development is the focus
- **Exposes improvements in V&V/UQ:**
  - Translations of V&V/UQ into a V&V Suite
  - Becomes one workflow: Analysis and V&V/UQ integrated
- **Co-develop V&V Test Suites**
- **Increases pedigree and exposure of SPARC to external community through V&V/UQ publications**
- **Comes with challenges as well. Benefits outweigh costs because we have very good collaboration amongst teams**



References

Code & solution verification:

- B. Carnes, V. G. Weirs, and T. Smith, “Code verification and numerical error estimation for use in model validation of laminar, hypersonic double-cone flows,” *2019 AIAA SciTech Forum*. https://doi.org/10.2514/6.2019-2175
- B. Freno, B. Carnes, and V. G. Weirs, “Code-verification techniques for hypersonic reacting flow in thermochemical nonequilibrium,” *Journal of Computational Physics,* 2021*,* https://doi.org/10.1016/j.jcp.2020.109752
- B. Freno, B. Carnes, and N. Matula, “Nonintrusive manufactured solutions for ablation”, 2021 AIAA SciTech Forum.

Validation:

- S. L. Kieweg et al, “Validation Assessment of Hypersonic Double-Cone Flow Simulations Using Uncertainty Quantification, Sensitivity Analysis, and Validation metrics,” *2019 AIAA SciTech Forum*. https://doi.org/10.2514/6.2019-2278
- J. Ray et al, “Estimation of Inflow Uncertainties in Laminar Hypersonic Double-Cone Experiments, *AIAA Journal 2020,58:10,* 4461-4474. https://doi.org/10.2514/1.J059033
- S. L. Kieweg et al, “ASC ATDM FY18 Level 2 Milestone Report: Validation of Hypersonic Turbulence Physics in SPARC,” *Sandia Technical Report*, SAND2018-10261, September 2018. (OUO/ECI/ITAR)
- V. Brunini et al, “ASC ATDM FY19 Level 2 Milestone Report: SPARC Credibility, Performance and Scaling,” *Sandia Technical Report*, SAND2019-10842, September 2019. (OUO/ECI/ITAR)