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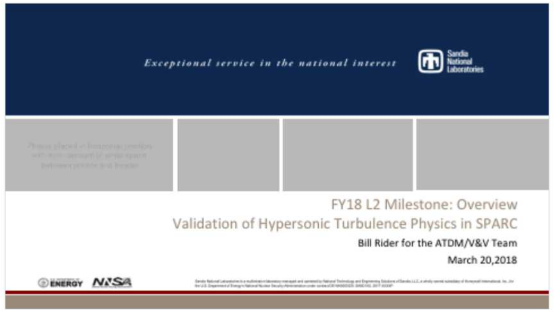

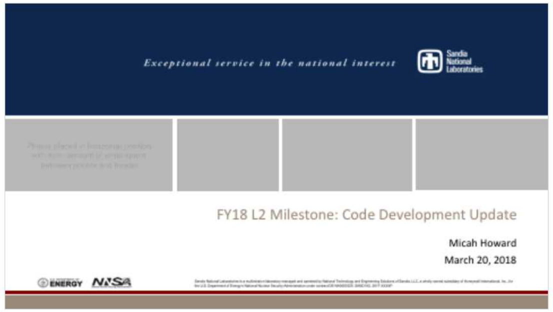

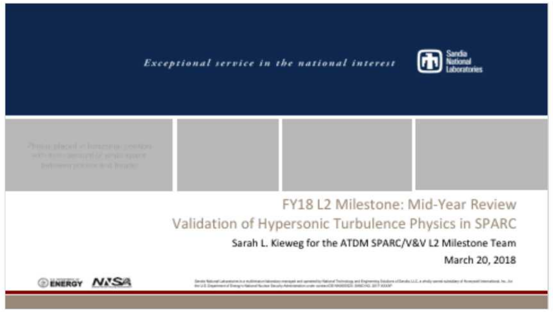

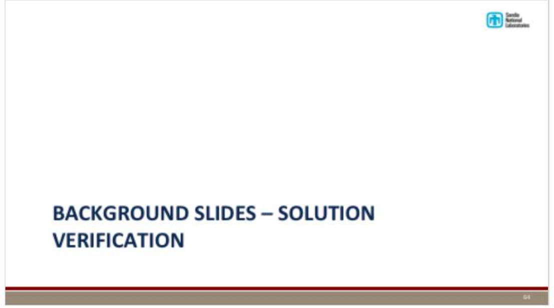

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FY18 L2 Milestone: Overview

Validation of Hypersonic Turbulence Physics in SPARC

Bill Rider for the ATDM/V&V Team

March 20,2018

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ATDM Vision

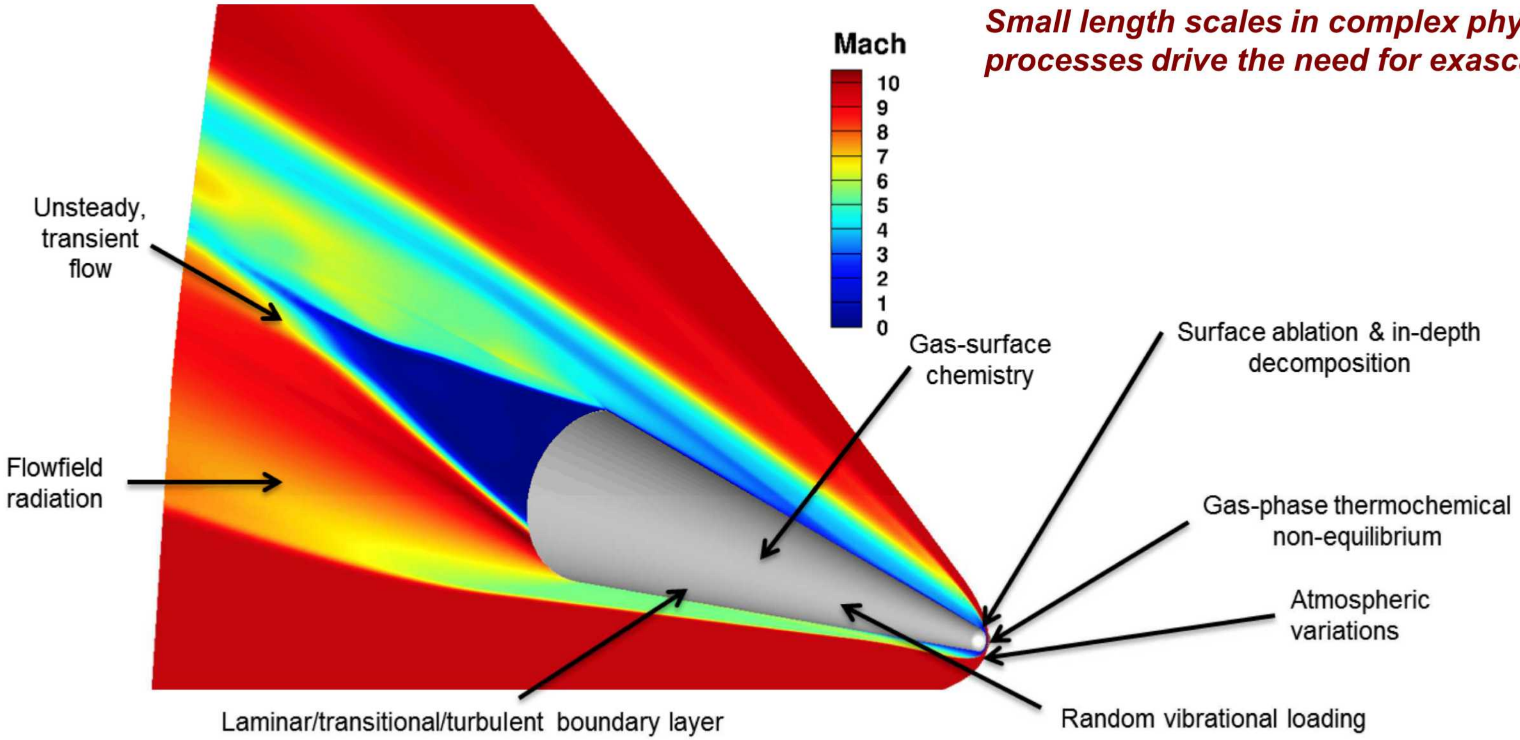
In partnership with Sandia's weapon engineers, the ATDM project will help usher in a new era of computational analysis for weapon life-cycle engineering by demonstrating embedded analysis and exceptional application performance on next-generation and exascale high-performance computing systems.

ATDM Mission

The Advanced Technology Development and Mitigation (ATDM) Project at Sandia is developing solutions to the problems posed by next-generation computing hardware and is mitigating the risk that Sandia weapons application codes will not be able to effectively utilize future high-performance computing systems.

- The project is developing two demonstrations of weapon engineering codes based on performance-portable mission-relevant agile software components. These application codes will demonstrate the use of the ATDM software components by each completing a weapons-relevant simulation with embedded analysis on more than half of each of the ATS-1, 2, and 3 systems.
- The software components will enable the rest of Sandia's broad suite of engineering codes to adapt to the ATS-3 system and beyond.
- The project will pursue high-risk, high-payoff approaches to target exceptional performance and a transformation in nuclear weapons analysis.

Reentry requires exascale simulation



Small length scales in complex physical processes drive the need for exascale

- Example problem: wall-resolved LES simulation of RV trajectory
  - *2 PB RAM, ~10^{11} cells, ~10^{7} time steps (per each high-fidelity simulation)*
- Ablation / structural / full-trajectory (6 Degree of Freedom) coupling
- On-the-fly mesh refinement, visualization, uncertainty quantification (UQ)
- Scalable solvers and verification and validation (V&V)

L2 Milestone Description & Overview

- **Description**: Demonstrate application physics capability to be used for the FY20 L1 Milestone for the hypersonic re-entry code SPARC through basic V&V. Demonstrations will include verification of the code's physics capability, physics modeling of fundamental validation experiments, and an application demonstration including error analysis and uncertainty quantification. Additional effort will explore the status of code performance and portability across available ATS and CTS platforms.
- The work will focus around one to three experiments chosen in conjunction with external experts (Candler U. Minn.). Validation will also be done with ASC V&V, ASC PEM, U. Minn. (US3D code) and DoD's CREATE Program (Kestrel code). The full V&V process will be exercised (including PIRT, PCMM, UQ, and credibility rollup)

Definitions

- Low bar: minimum for successful completion of L2 milestone requirement
- High bar: The work we want to accomplish for full assessment of the applied capability
- Stretch: If everything goes extremely well and time allows, additional work we will pursue

ATDM FY20 L1 Milestone - Reentry

A spectrum of capabilities for RV trajectory analysis

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 ▪ 2^{nd}-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 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, sensitivities, viz) ▪ V&V		▪ Scalable solvers ▪ Performance portability ▪ Embedded analysis ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V	▪ Performance portability ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V

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FY18 L2 Milestone: Code Development Update

Micah Howard

March 20, 2018

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Development Activities During FY18 Q1 & Q2

- Milestone Overview
- Validation Sets
- Code Verification
- Double Cone:
  - UQ: Experimental Challenges
  - UQ: Parametric Uncertainty
  - Calibration
  - Validation
  - Solution Verification
  - Sensitivity Analysis
- HI-FiRE -1
- HI-FiRE – 5B

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FY18 L2 Milestone: Mid-Year Review

Validation of Hypersonic Turbulence Physics in SPARC

Sarah L. Kieweg for the ATDM SPARC/V&V L2 Milestone Team

March 20, 2018

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Outline

- Milestone Overview
- Validation Sets
- Code Verification
- Double Cone:
  - UQ: Experimental Challenges
  - UQ: Parametric Uncertainty
  - Calibration
  - Validation
  - Solution Verification
  - Sensitivity Analysis
- HI-FiRE – 1
- HI-FiRE – 5B

Milestone Success Criteria

Progress Bar Key (~ % done): 80% 50%

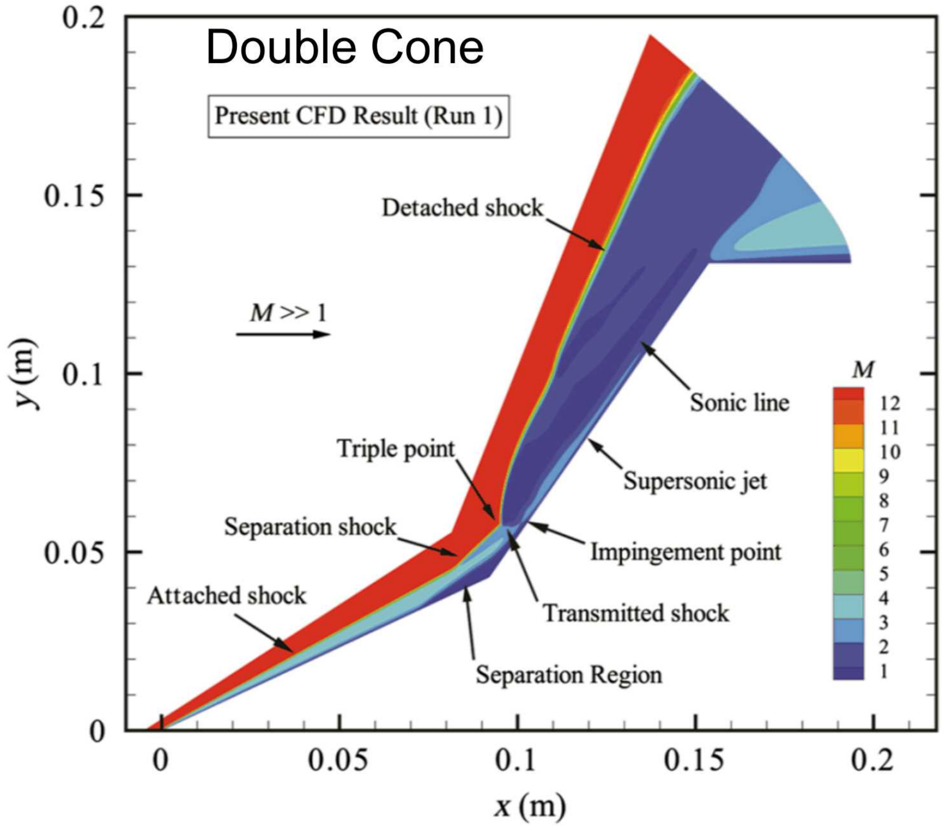
Sandia National Laboratories

Milestone Goal	Low-Bar Criteria	High-Bar Criteria
Validation Sets	- LENS XX - HI-FiRE-1	- Reentry flight experiment - Unsteady Separated flow experiment
Code Verification	- Individual separate physics - Identification of problems	- Combined physics - Correction of identified problems
Solution Verification	Grid convergence studies and estimates of numerical uncertainty	
Sensitivity Analysis	Perform local sensitivity analysis for validation sets using Sacado	Perform global sensitivity analysis for validation sets
UQ Studies	Use Dakota's sampling methods for forward propagation of uncertainties	- Use Dakota's gradient-enhanced sampling. - Use Bayesian methods for parameter estimation using statistical emulators
Calibration		- Perform single deterministic calibration
CTS/ATS Utilization	Use SRN CTS-1 systems	- Use Trinity - Replicate something on ATS-2
Subjective Factors	Use only Sandia analysis of V&V/UQ	- Compare with CREATE and U. of Minnesota - Multiple internal solutions with full V&V assessment

These have been paraphrased here – full description in Background slides.

Validation Sets

- Validation Set #1: Double cone *(Low-Bar)*
  - LENS I: ~2000-2007
    - laminar flows of **single species** (N2 or O2) in **mild** thermochemical nonequilibrium.
  - LENS XX: 2014-present
    - laminar flows of **air mixture** in **mild to strong** thermochemical nonequilibrium.
- Validation Set #2: *(Low-Bar)*
  - HIFiRE-1: turbulent, nonreacting flow
- Validation Set #3: *(High-Bar)*
  - HIFiRE-5B: reentry flight experiment



HIFiRE-1 ground test model (MacLean et al. 2008)

Full References in Slide Notes

Validation Hierarchy

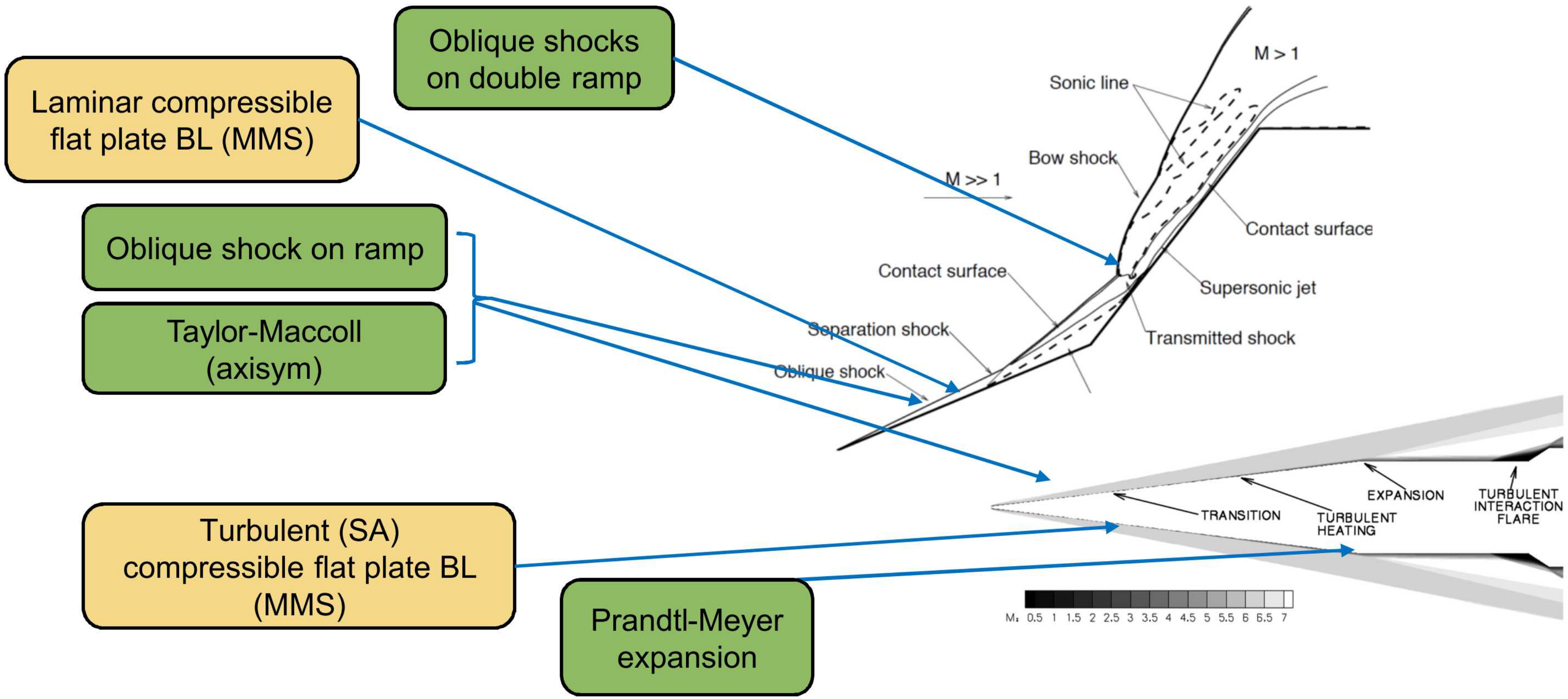
Sandia National Laboratories

Atmospheric reentry:
turbulent, thermochemical NEQ

- HIFiRE:
  Turbulent, single species
  (perfect gas RANS)
- Double Cone (LENS I):
  1-, 2-, or 5-species, vibrational NEQ
  Laminar reacting: <u>mild</u> non-eq
- Double Cone (LENS XX):
  5-species, vibrational NEQ
  Laminar reacting: <u>strong</u> non-eq

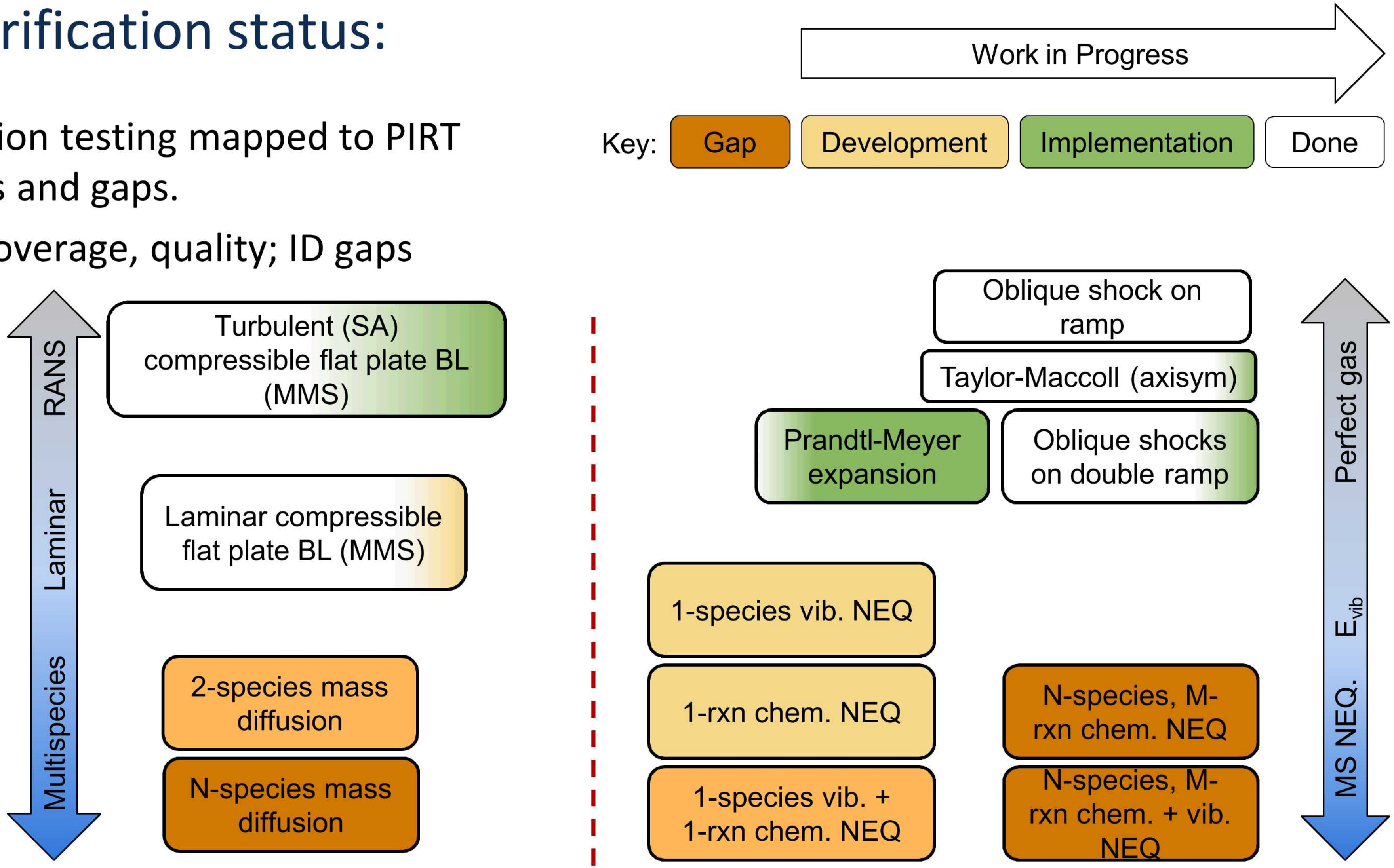
Code Verification: Identified Tests
Perfect gas verification tests are motivated by flow features

Reminder: Flow phenomena in validation sets drove our choices of code verification problems



Code verification status:

- Verification testing mapped to PIRT priorities and gaps.
- Assess coverage, quality; ID gaps

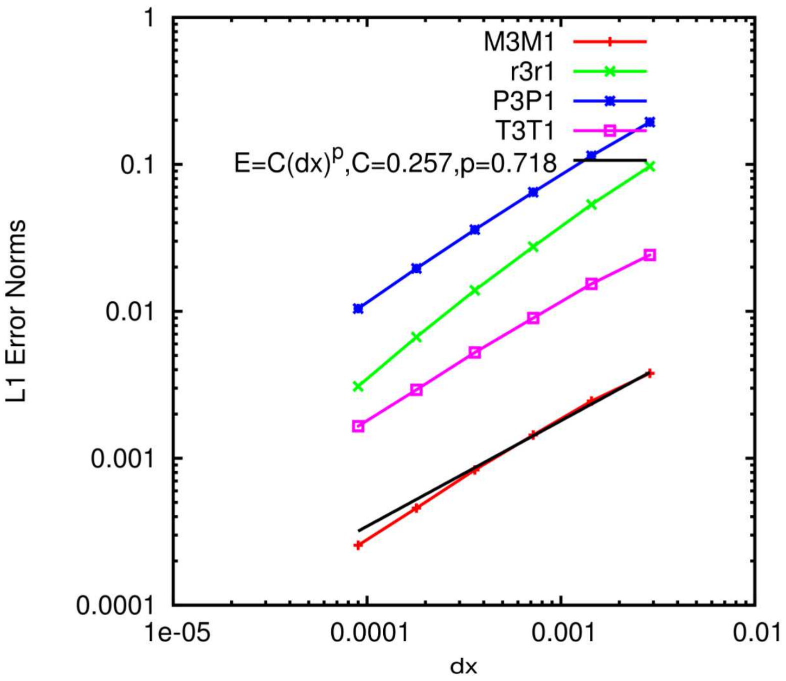


Code Verification: Taylor-Maccoll & Oblique Shocks Double Ramp

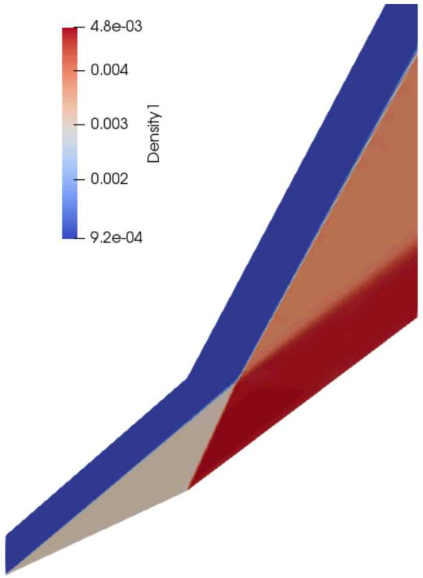
Taylor-Maccoll: inviscid axisymmetric cone flow

- Exact solution requires numerical solve of an ODE
- Demonstrated convergence of axisymmetric flow on a 3D mesh (narrow azimuthal slice, offset from axis)
- Established convergence across different mesh designs (inviscid vs. BL spacing, different topologies)

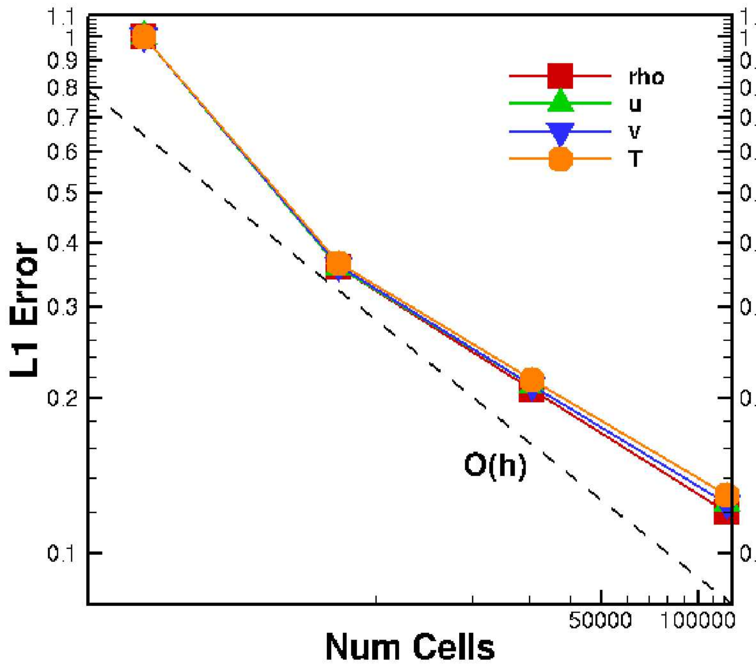
Single Cone 25 deg., M = 5, gamma=1.4, Rgas=287



25º-37º double ramp, M_∞=3.636



L1 Convergence



Double ramp: oblique shock interaction

- Exact solution requires iterative solution of some implicit equations
- Demonstrated convergence for oblique shock interaction in the interior of the flowfield

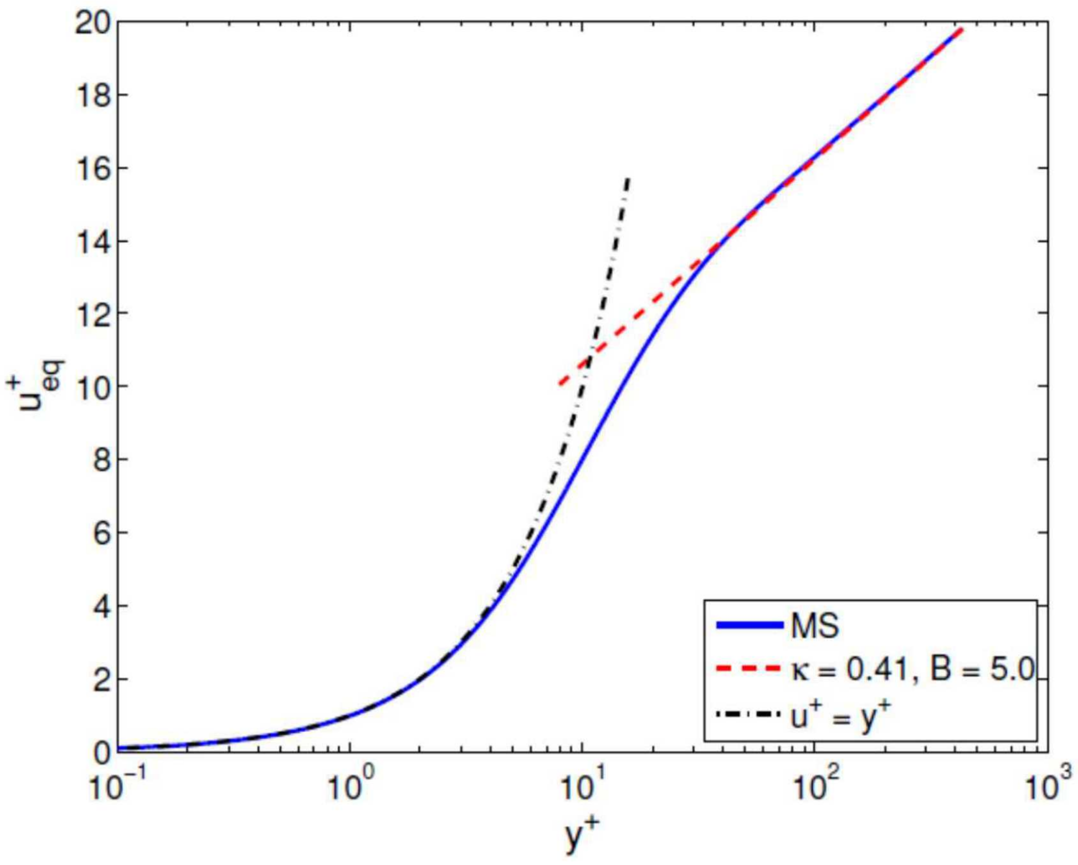
Code Verification: Turbulent (SA) compressible flat plate BL (MMS)

Impact:

- This test is currently identifying faulty components and confirming their corrections, particularly non-uniform inflow and outflow BCs
- To run this test problem, manufactured solution infrastructure in SPARC has been extended to include laminar transport terms and the SA RANS model

Remarks:

- This test is based on work of Eca (Portugal) and Oliver (UT); we are not aware of any other exact RANS solutions
- The ultimate goal is to test low and high Reynolds number flows using both sinusoidal and realistic manufactured solutions



Realistic manufactured velocity profile containing both a viscous sublayer and logarithmic layer; the Spalart-Allmaras model assumes this structure exists and fails to converge when it doesn't

Code Credibility Activity: Supersonic Flat Plate

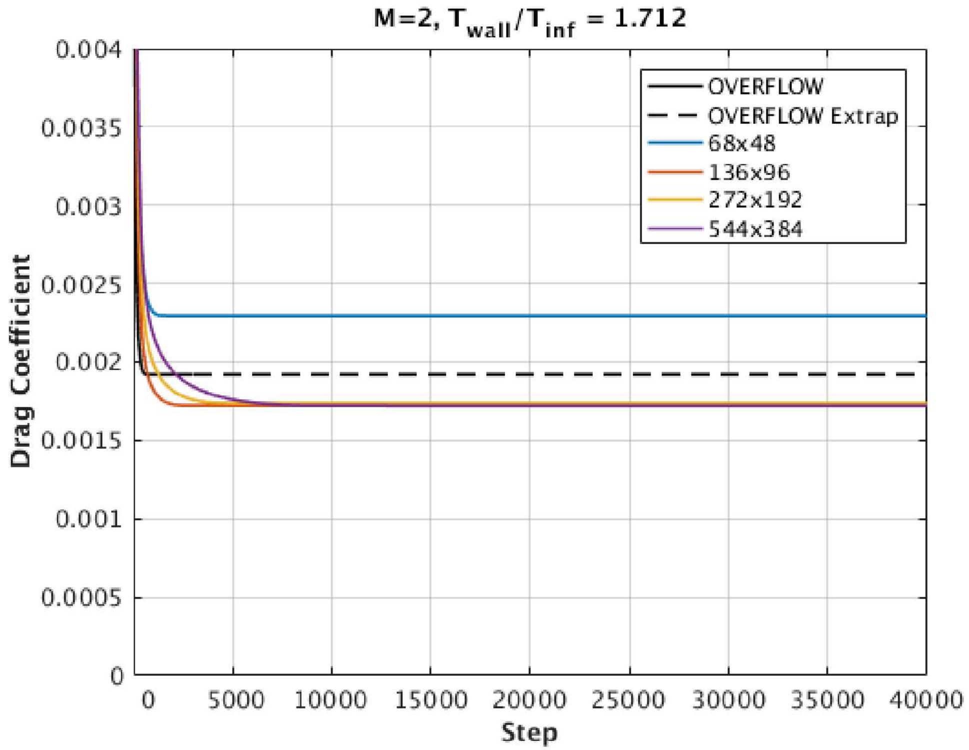
Objective: Code-to-code comparison for subsonic and supersonic cases with Spalart-Allmaras (SA) turbulence model

Impact:

- While not exact solutions, NASA benchmark solutions are well established, widely used and highly scrutinized tests of RANS model implementations
- Identified bug handling multiple BCs on a block boundary
- Additional tool development performed to output additional parameters needed for code-to-code comparisons (e.g. momentum thickness)

Status: Work in progress

- Four cases with varying Mach numbers (2,5) and wall temperatures run over series of four structured meshes
- Drag convergence behavior monitored and compared with OVERFLOW CFD code
- Upcoming: test SPARC against NASA CFD codes (CFL3D, FUN3D, WND, OVERFLOW) and Stanford (JOE) to analyze behavior near leading edge of plate



Drag convergence comparison with NASA Langley OVERFLOW code for M=2, T_{wall}/T_{inf} = 1.712. $Re_{L=1}$ = 15 million. OVERFLOW results are for 544x384 mesh.

Code Credibility Activity: Supersonic Bump in Channel

Objective: Code-to-code comparison for subsonic and supersonic cases with Spalart-Allmaras (SA) turbulence model

Impact:

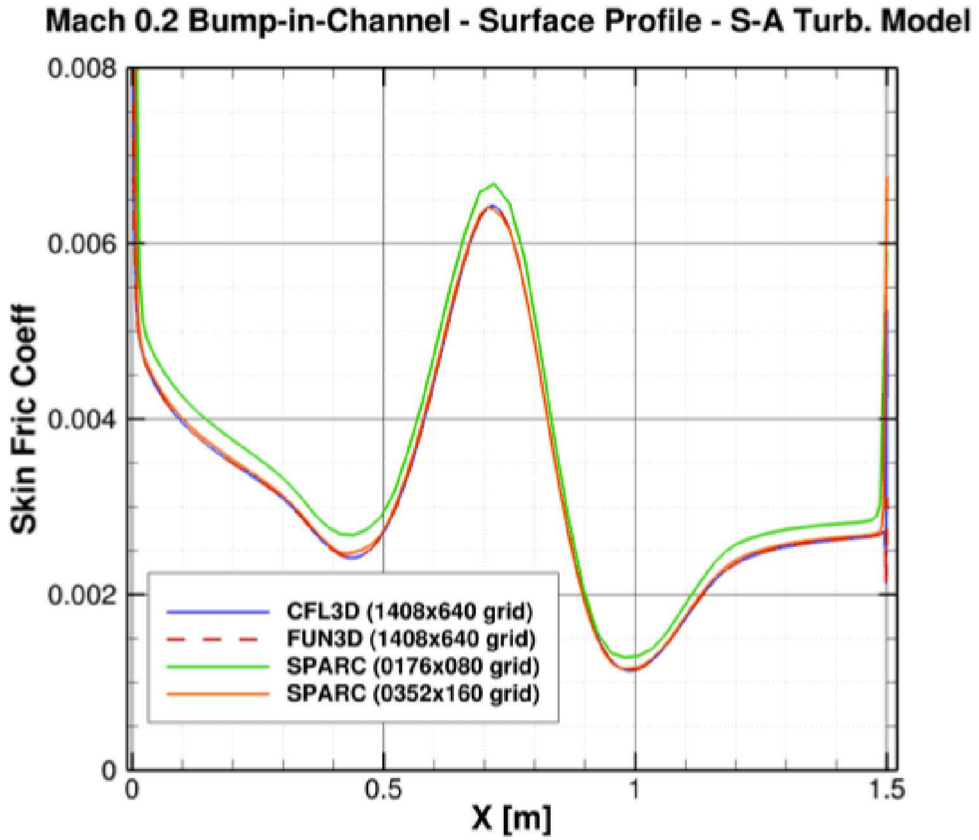
- Examine Steger-Warming entropy fix (numerics parameter) effect on turbulent boundary layers
  - the entropy fix has a strong effect on the solution (see figure)
  - the solution residuals flatten for sufficiently low values of entropy fix, hinting at convergence issues

Status: In-progress

- Two cases run over two structured meshes
- Testing SPARC with NASA compressible CFD codes (CFL3D and FUN3D) and monitoring convergence for flow characteristics (lift, drag, wall skin friction, pressure, eddy viscosity, velocity)
- Work is ongoing to add more diagnostics, i.e., additional automated post-processing of the data

Skin friction profile over bump

Entropy fix = 0.1



Validation Set #1: non-equilibrium reacting air, laminar, shock wave/boundary-layer interaction

DOUBLE CONE (LENS XX, LENS I)

Uncertainty Quantification: Experimental Data Challenges

- Free stream conditions provided with "% error":
  - Interpreted as bounds of uniform distribution
- Heat flux and pressure measurements have "% error"
  - Interpreted as bounds of a uniform distribution
- No replicate experiments
- LENS I: Nompelis *et al.* – nozzle simulations to obtain free stream conditions.
- LENS XX: unresolved questions about free stream conditions

LENS I, Run 35: Free stream and wall condition (I. Nompelis)

Table 1. Free-stream and wall conditions for Run 35 from Nompelis et al. 2003.

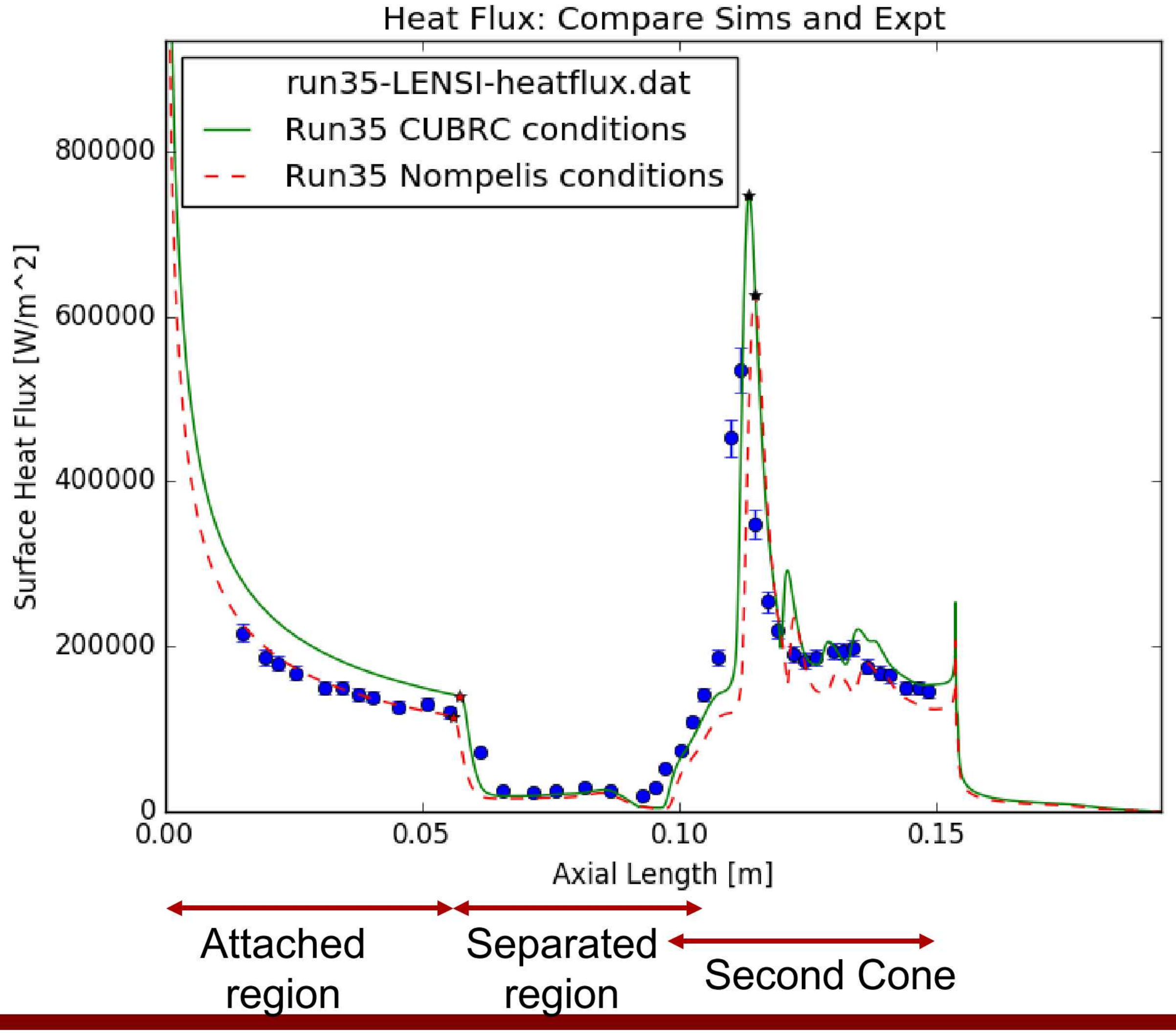
	Run 35 (nominal)		Run 35 (nonequilibrium)	
ρ_∞	5.515e-4	kg/m^3	5.848e-4	kg/m^3
T_∞	138.9	K	98.27	K
$T_{v\infty}$	138.9	K	2562	K
u_∞	2713	m/s	2545	m/s
T_{wall}	296.1	K	296.1	K
c_{N_2}	1.0		1.0	

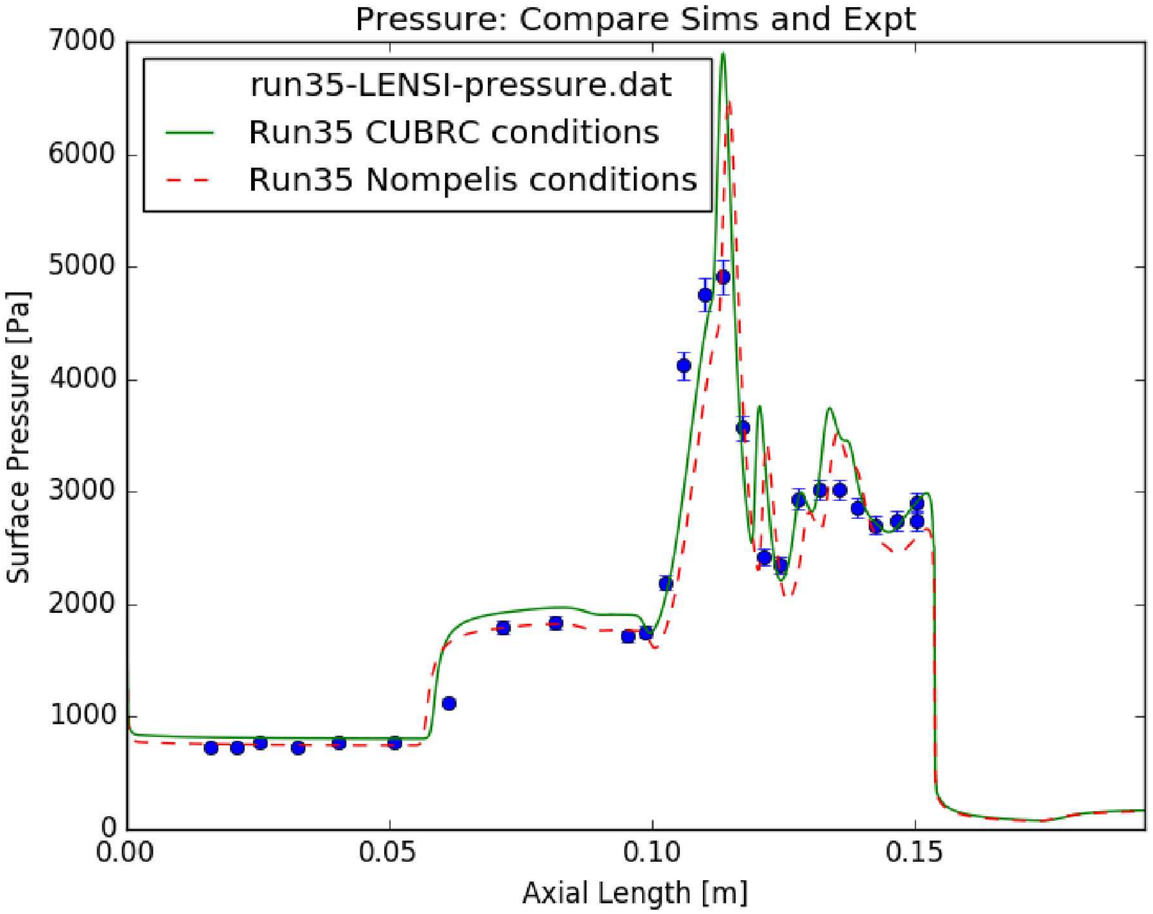
LENS XX: Case 1 and Case 4

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

LENS I (Run 35): Uncertainty Quantification

I. Nompelis *et al.:* Obtained free stream conditions from nozzle simulations

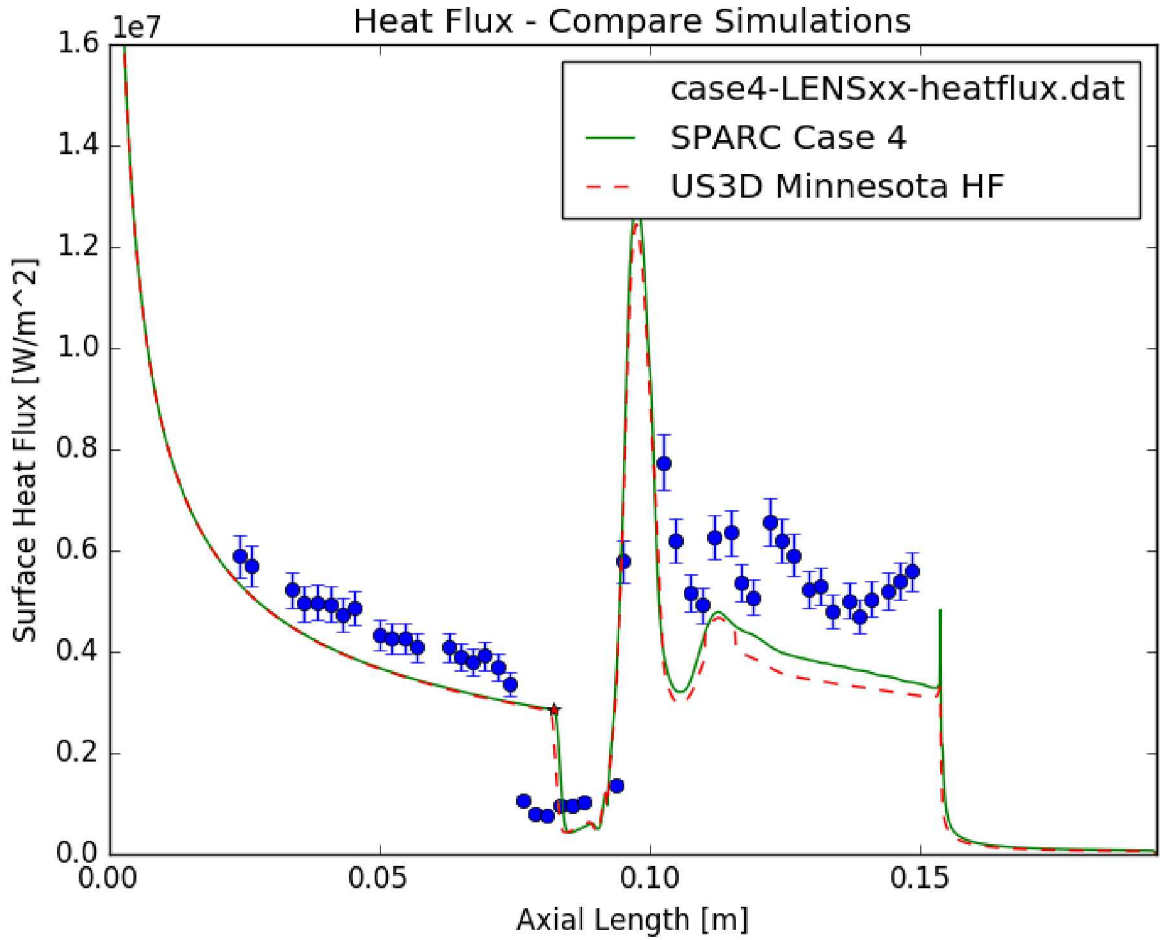


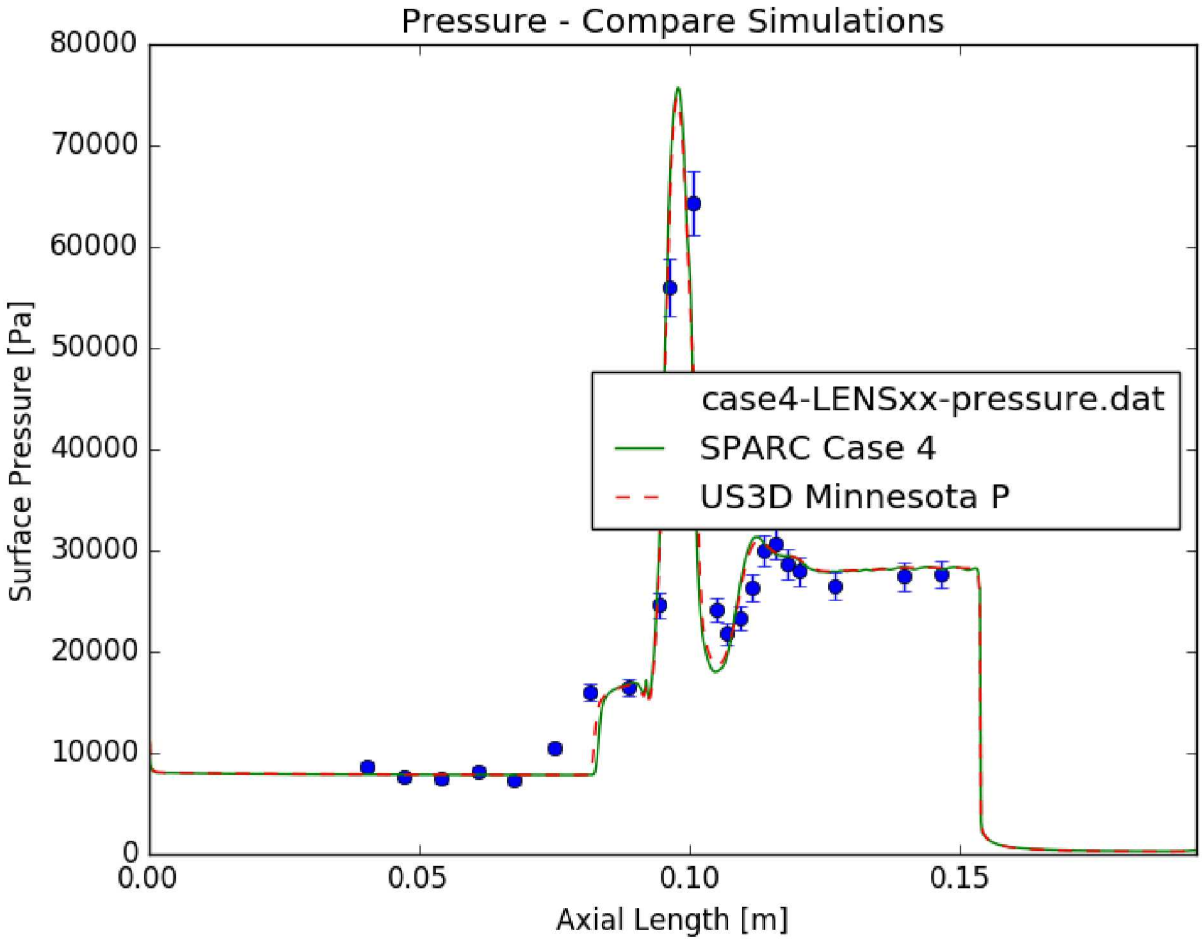


SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Expt error bars: hf +/- 5 %, p +/- 3% per CUBRC.

LENS XX (Case 4): Example of Initial Validation Exercise without UQ

Compare SPARC to US3D and Experiment

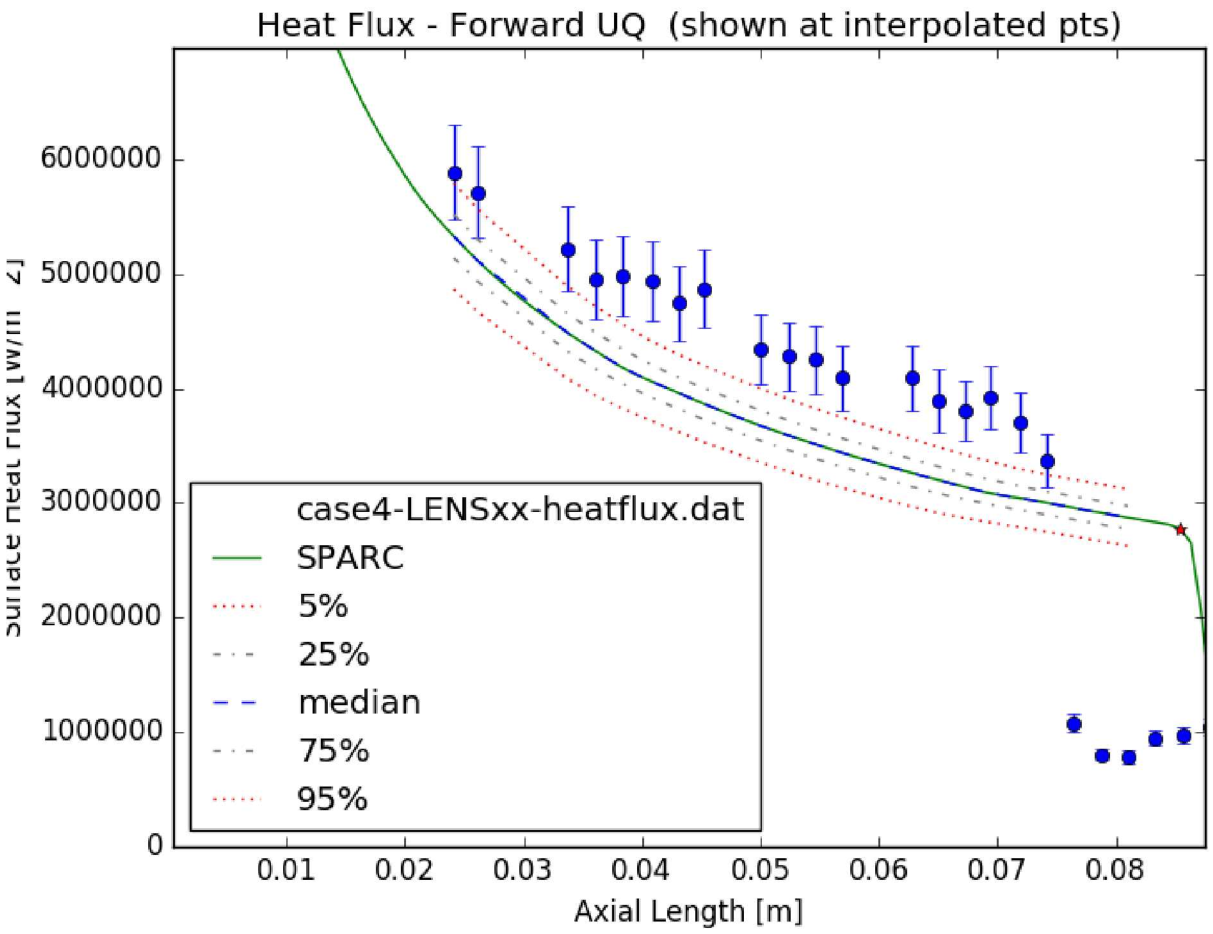


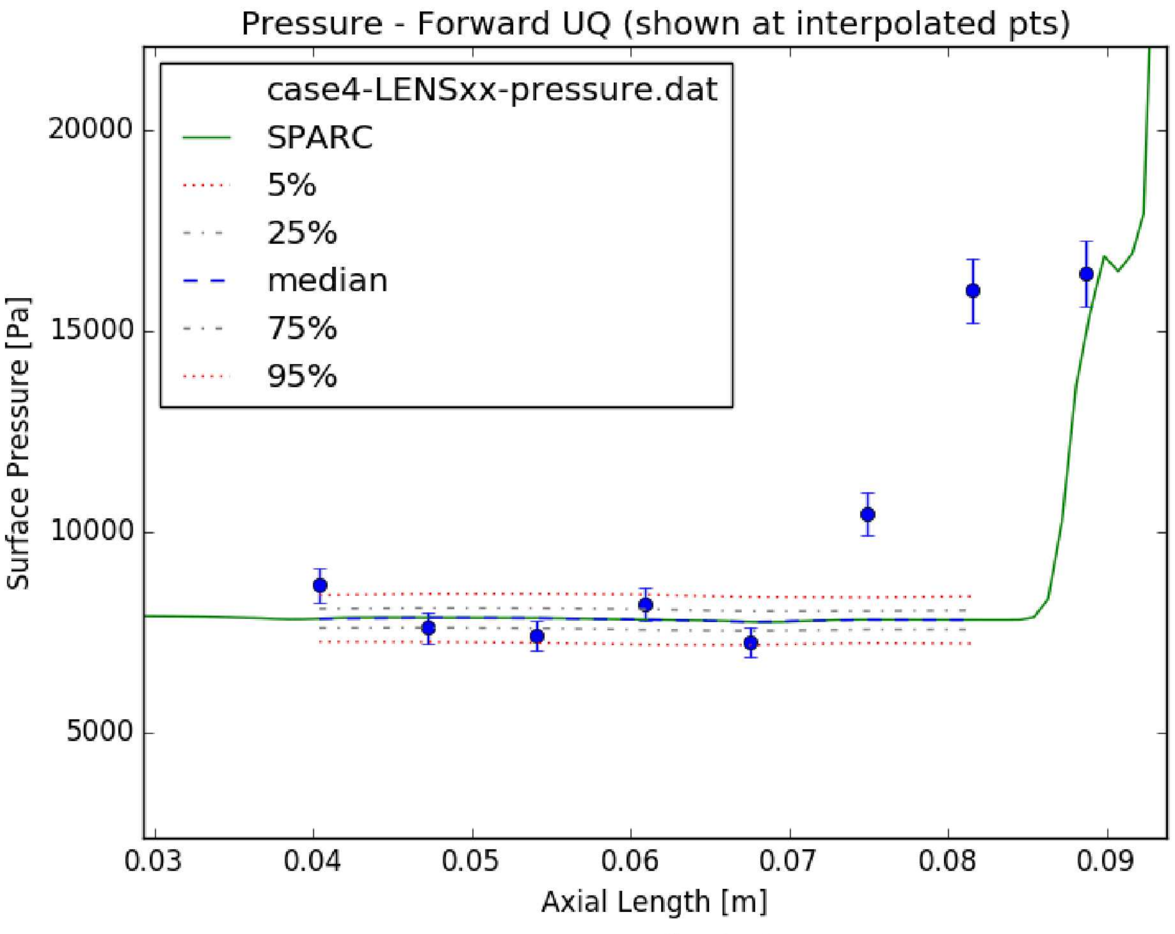


SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

LENS XX (Case 4): Uncertainty Quantification and Validation

Forward UQ on SPARC simulation → parametric uncertainty → need to calibrate





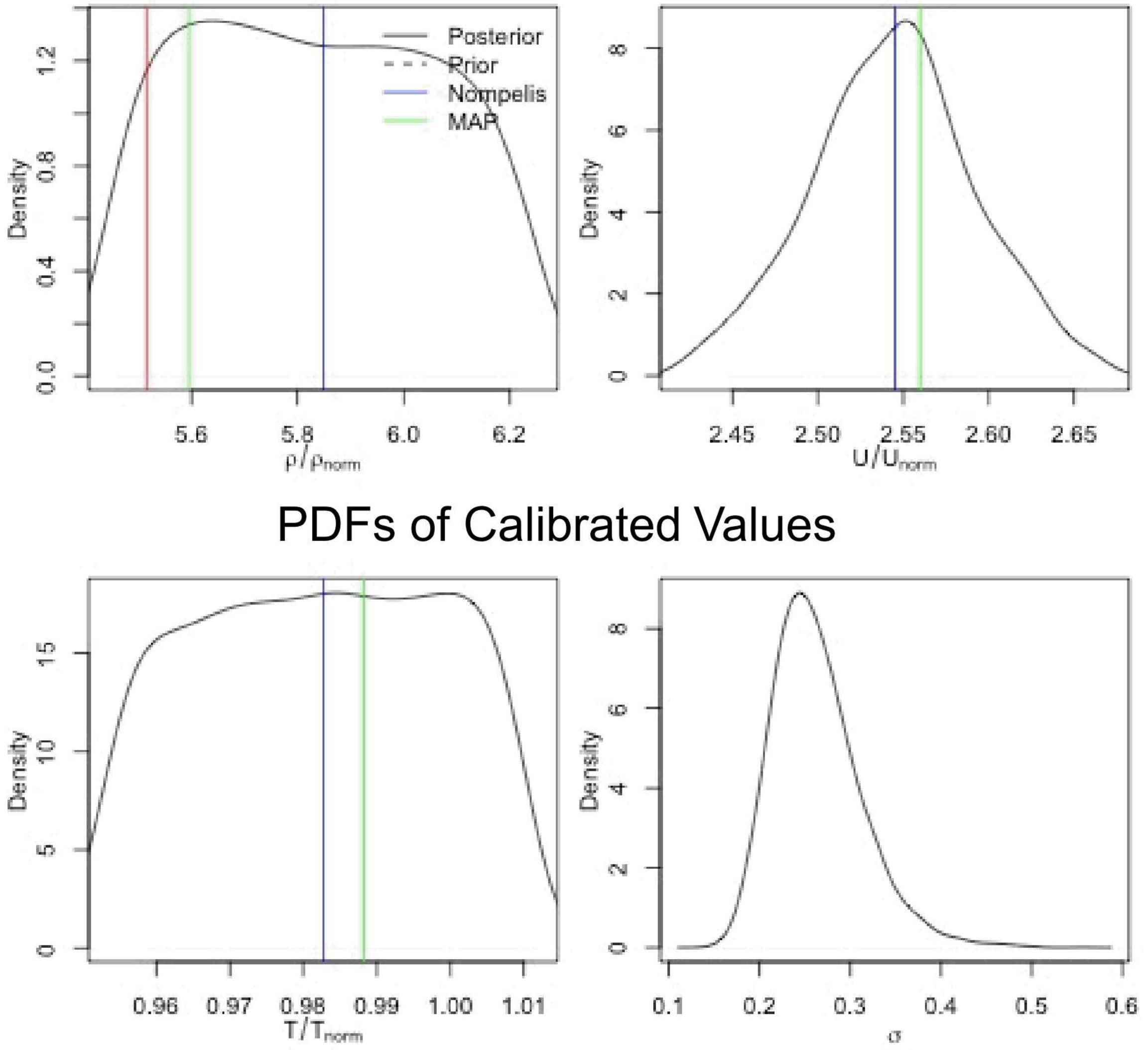
SPARC simulations use "coarse" v2_128x256 mesh, 100000 iterations. UQ ensemble from: 7, 3, and 3% rho, U, T per CUBRC; Tv = T.

Calibration and Validation

- Calibration Goals
  - Develop an inference technique to estimate $(\rho, U, T, T_v)_\infty$ and uncertainties from measurements of heat flux, pressure, total enthalpy and pitot pressure
    - Calibrate using attached region
    - Predict over entire flow regime
  - Demonstrated with LENS-I Run 35
  - Perform on LENS-XX Case 4, and possibly Case 1

- Validation Metrics
  - Demonstrated set of metrics
    - Use Forward UQ ensembles to estimate parametric uncertainty
    - Use experimental uncertainty
    - Include numerical uncertainty
  - Demonstrate for LENS-I Run 35 before and after calibration
  - Calculate for LENS-XX Case 4 before and after calibration

Calibration: LENS I (Run35) test case

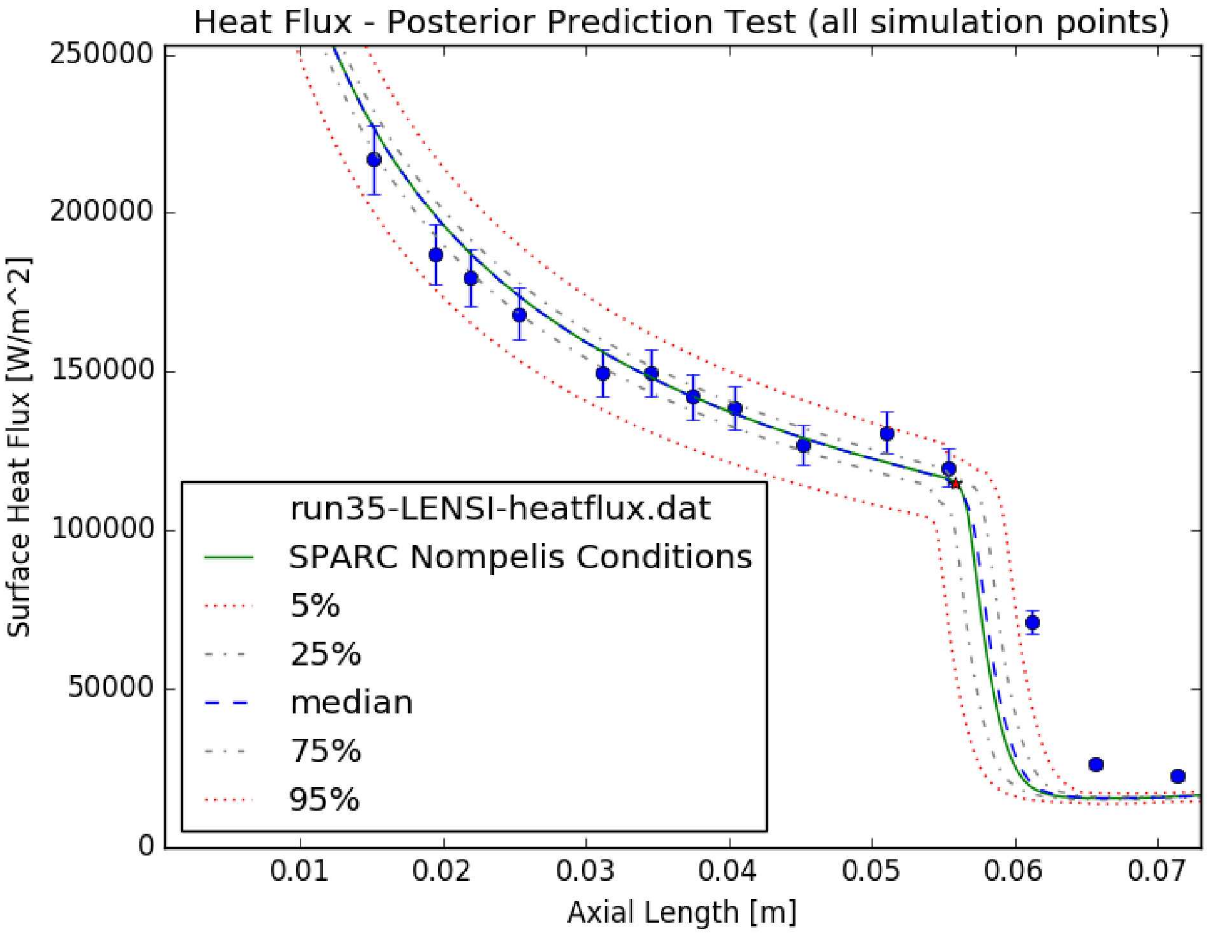


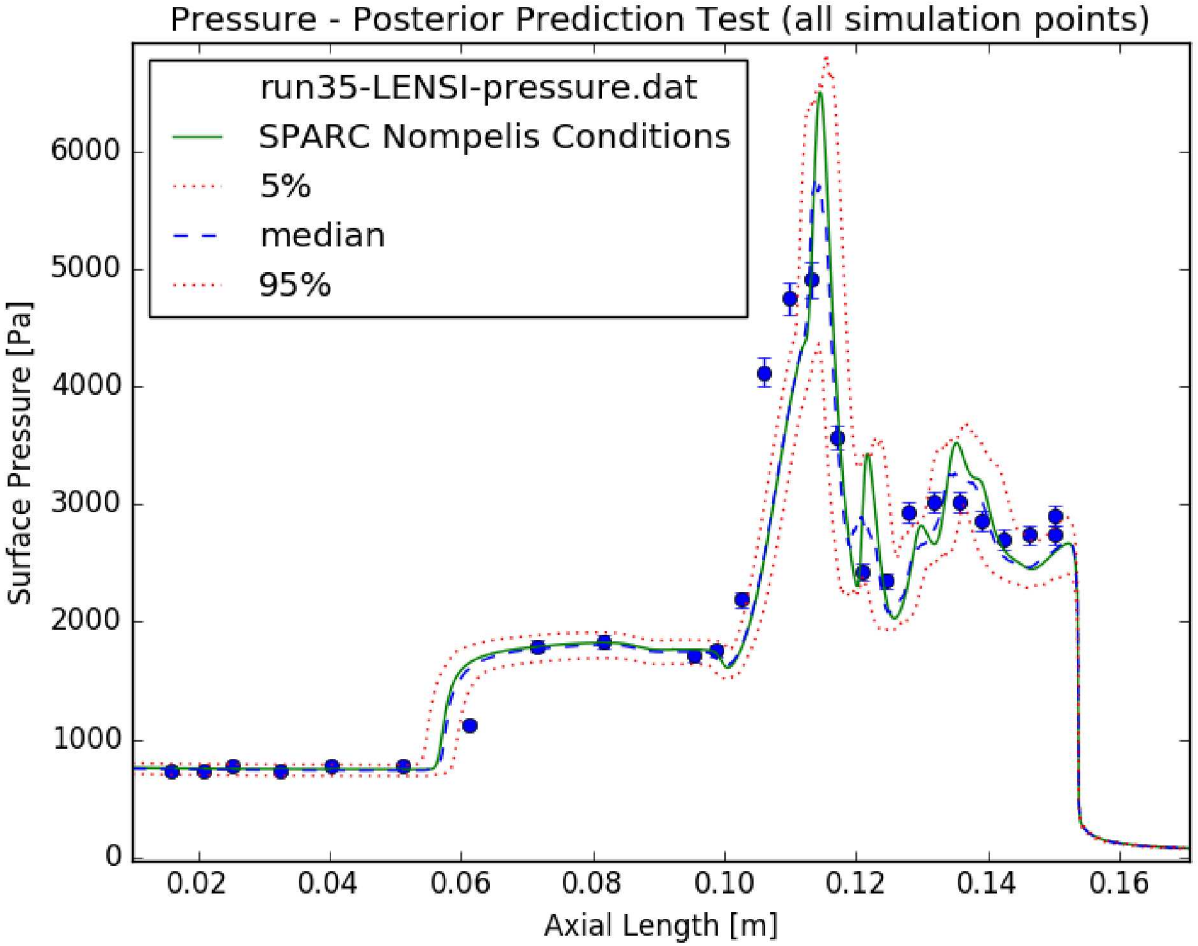
PDFs of Calibrated Values

- Compare:
  - CUBRC's original freestream conditions (not always in range of plots)
  - Nompelis' non-eq freestream conditions
  - Our calibrated freestream conditions (MAP)
- Our calibrated values have better agreement with Nompelis – and we reproduce observations

	Density (kg/m3)	U (m/s)	T (K)
CUBRC	5.515e-4	2713	138.9
Nompelis [non-eq]	5.845e-4	2545	98.27
MAP	5.595e-4	2560	98.82

Calibration: Calibrated LENS I (Run35) reproduces observations well

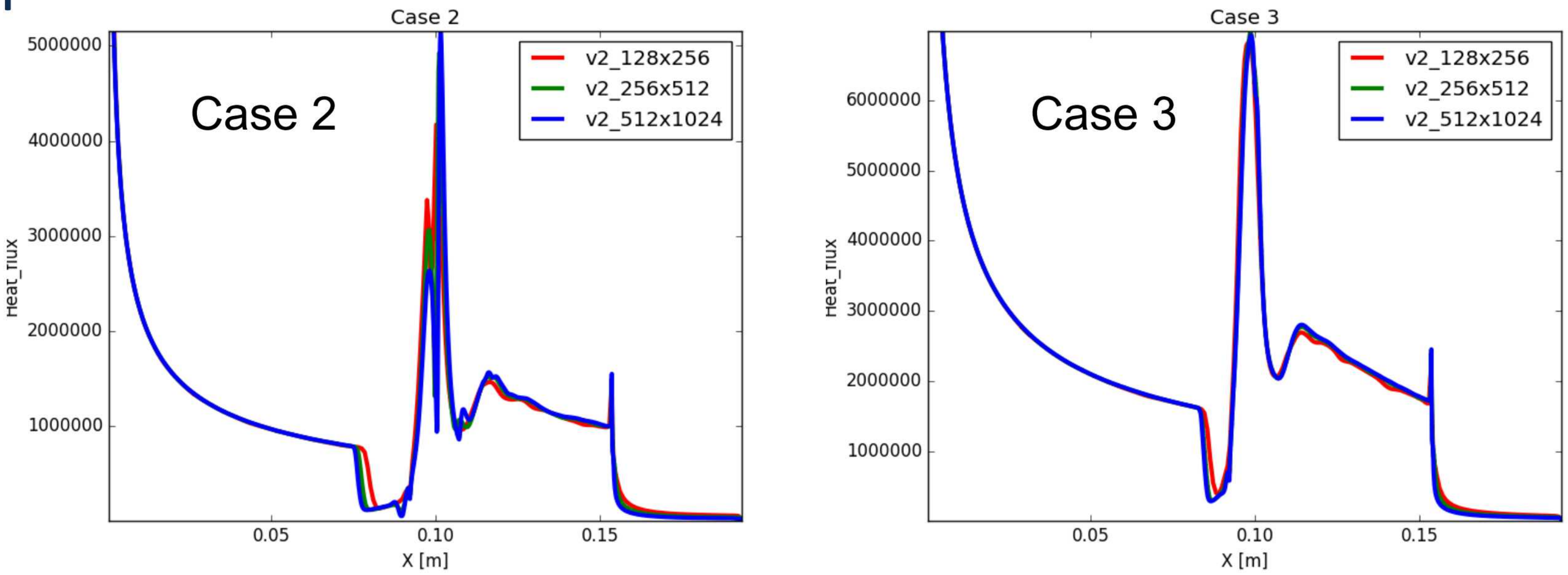


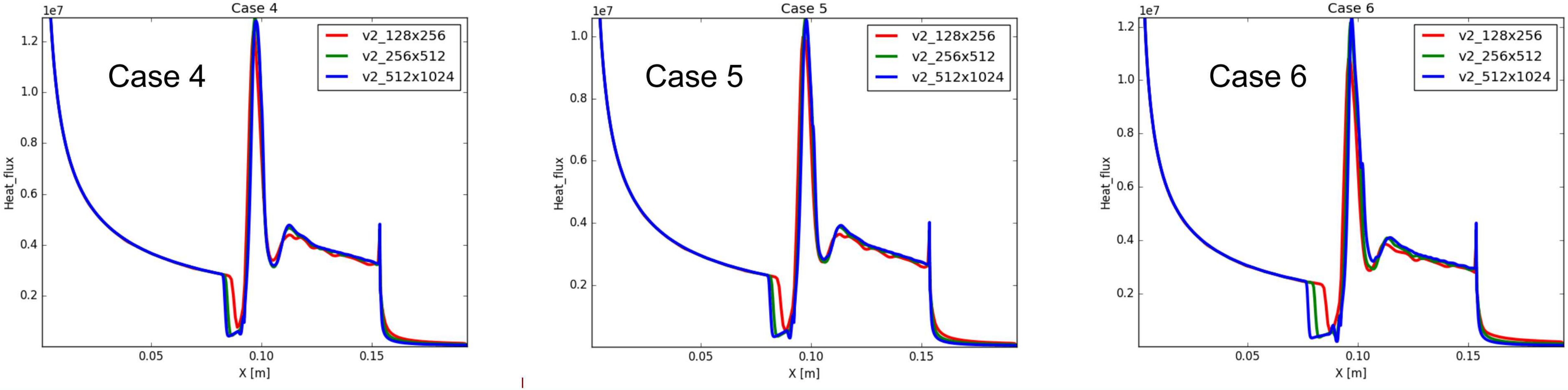


- Calibration used only attached region's experimental probe points. Prediction over the entire flow field using inferred conditions and uncertainties.
- 5th/95th percentiles contain measurements (attached region; 11 probes)
- SPARC simulations with "finer" grid (v2_512x1024, 50000 iterations)

LENS XX (5sp2T) Heat Flux: Qual. Solution Verification

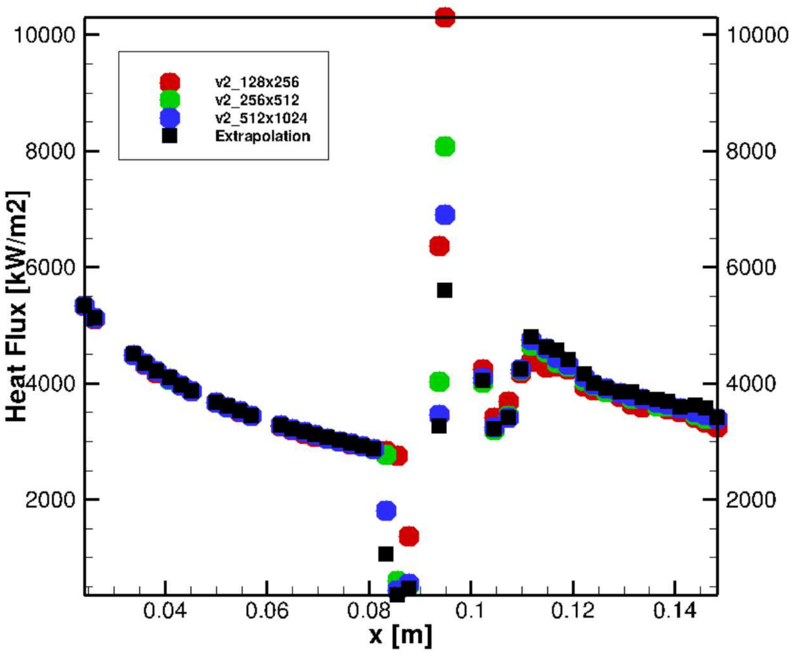
- Case 1: failed to run with 2T model
- Coarse grid oscillations on second cone go away on finer grids
- Case 6: largest error in detachment

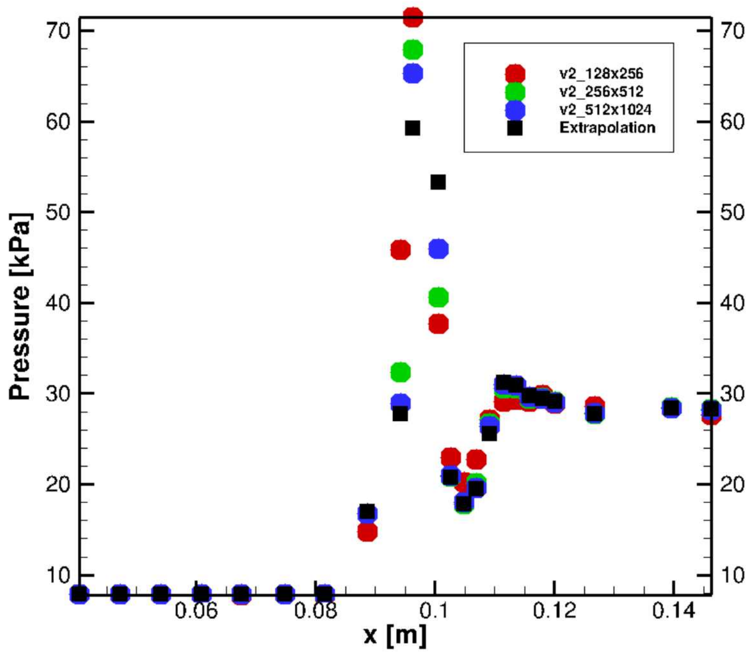




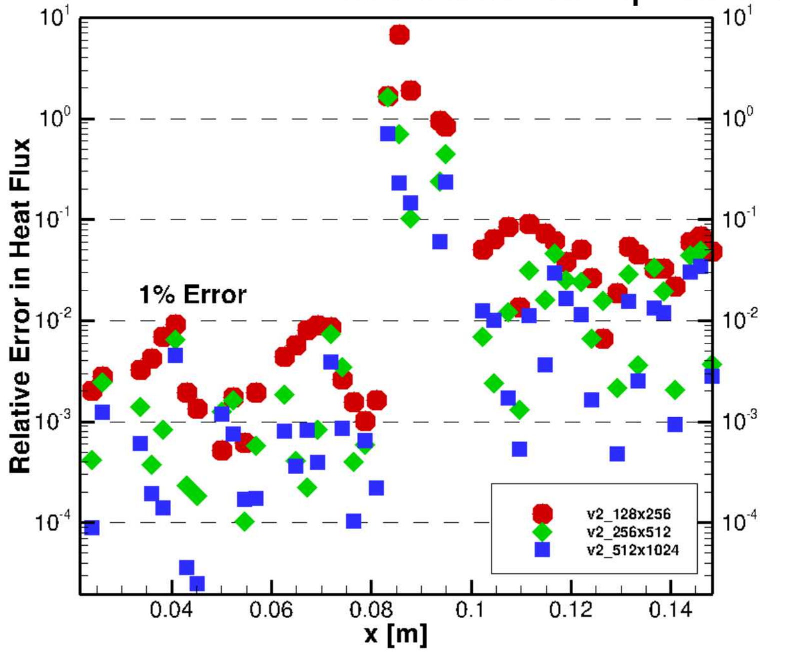
Quant. Solution Verification LENS XX Case 4 (5sp2T)

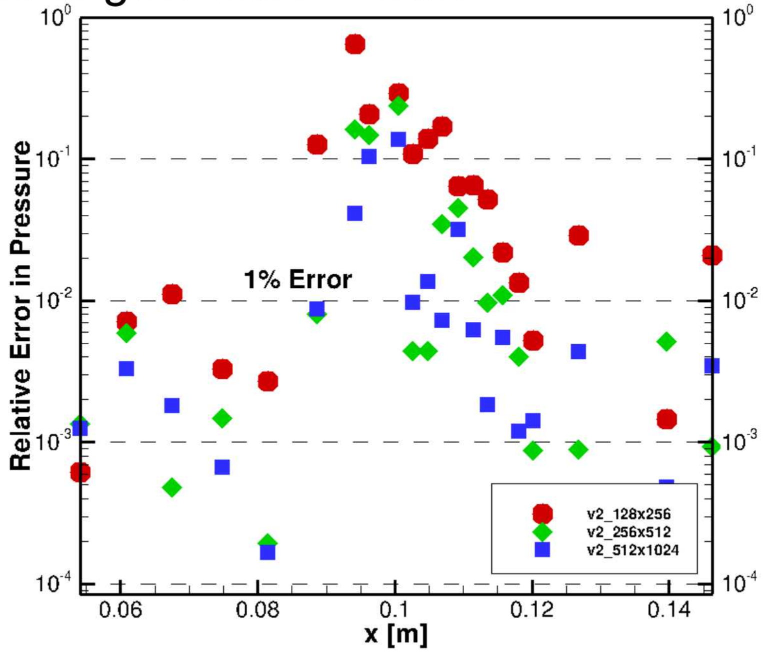
- Numerical error below some threshold can be ignored
- Largest errors in detached region and second cone
- Second cone error hard to resolve (espec. heat flux)
- Our plan will be to include (nominal) numerical error in validation as a bias
- Errors increase with increasing position
  - first cone attached: <1% error
  - second cone errors generally >10% even on 512x1024 grid





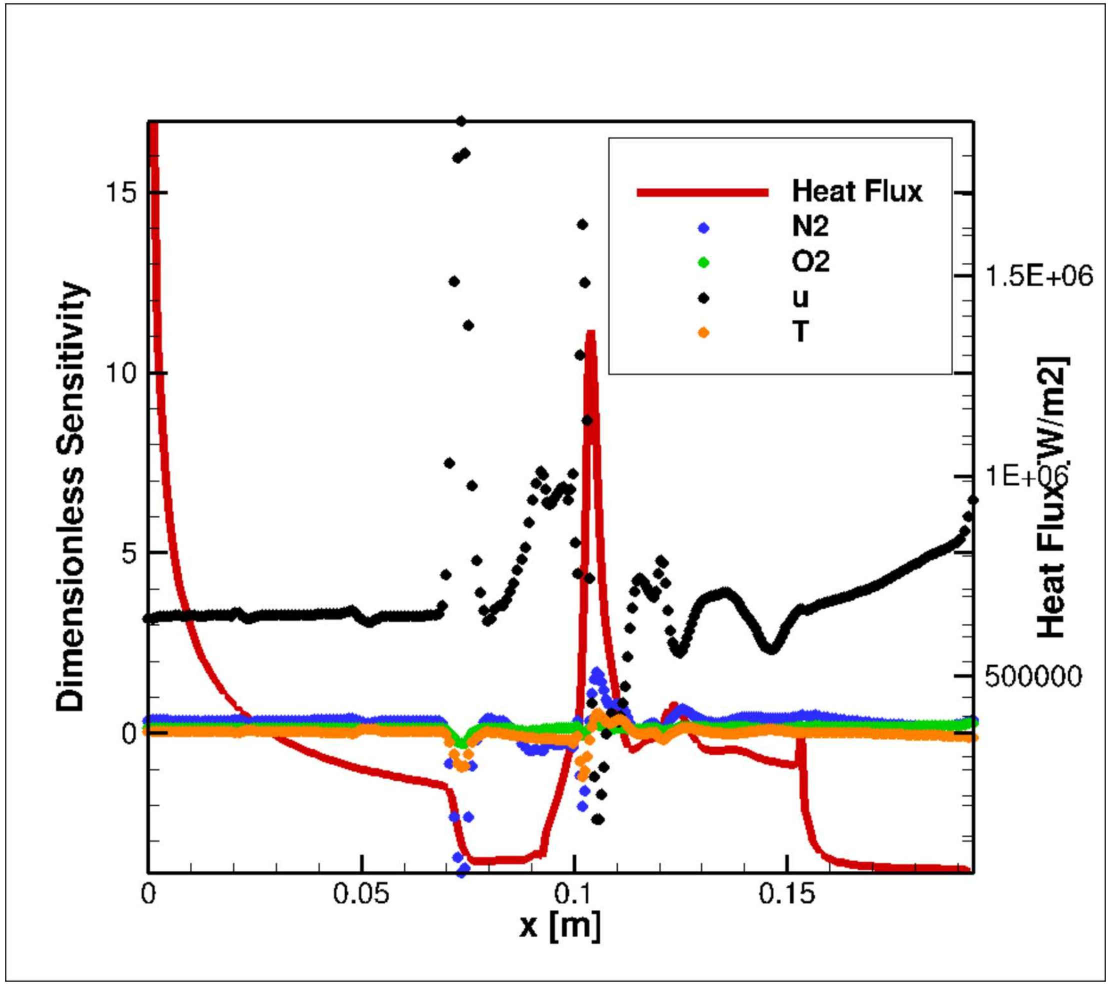
Subtract extrapolated value to get relative errors





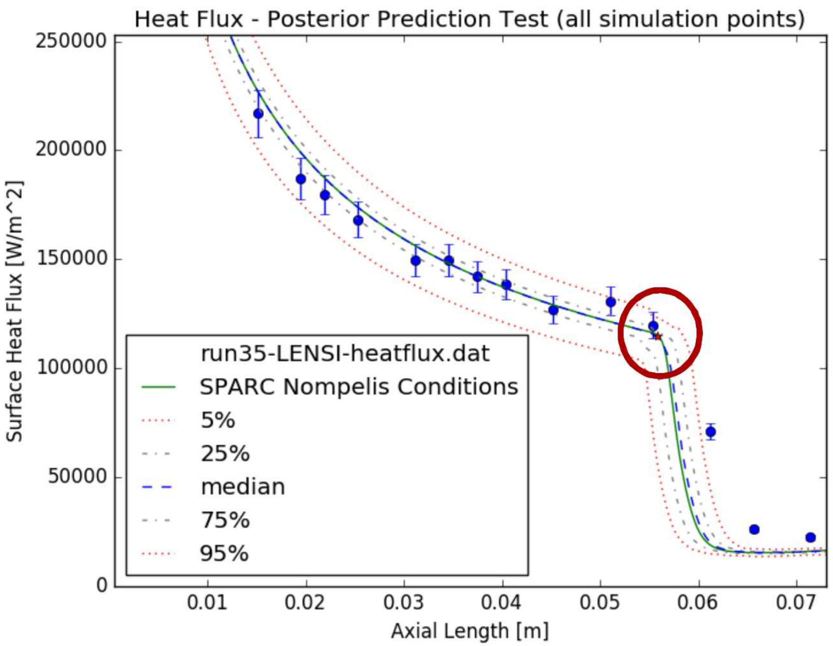
Sensitivity Analysis – Local

- SPARC can generate embedded sensitivity analysis
- Preliminary embedded local sensitivity analysis for LENS-XX Case 1 (using 5sp1T)
- Done using coarse mesh



Sensitivity Analysis - Global

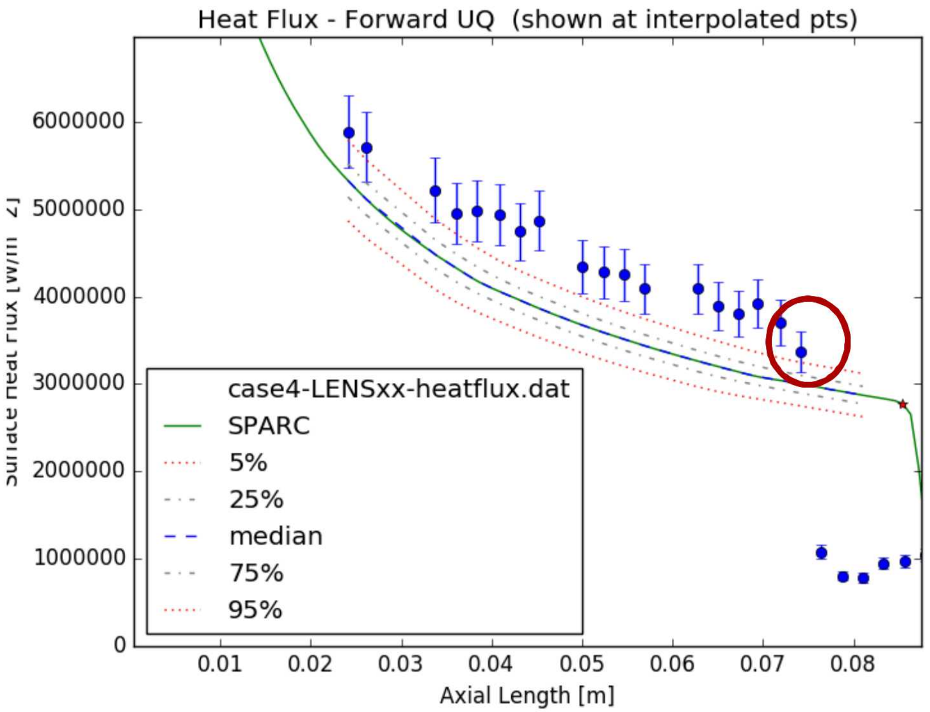
- Run 35 (LENS I) not sensitive to T:
  - Observed in posterior distributions after Bayesian calibration.
  - Sobol' indices for QOIs in attached region:
    - Heat flux point: least sensitive to T and most sensitive to u and – **see example in Table**.
    - Pressure: least sensitive to T, and most sensitive to u, but also to density.
    - From 100,000 samples on a level 3 PCE surrogate.



Sensitivity of 11th Heat Flux Value:	Main	Total
p (10% unc)	2.07e-2	2.18e-2
u (10% unc)	**9.78e-1**	**9.79e-1**
T (10% unc)	2.13e-4	2.87e-4
ρ , u	Interaction: 1.10e-3	(Other interactions smaller)

Sensitivity Analysis - Global

- Case 4 (LENS XX) not sensitive to T
  - Sobol' indices for QOIs in attached region:
    - Heat flux point: least sensitive to T and most sensitive to u – **see example Table**.
    - Pressure: least sensitive to T, and most sensitive to u, but also to density.
    - From 10000 samples on a level 2 PCE surrogate.
  - Challenge to calibrate T.



Sensitivity of 18th Heat Flux Value to:	Main	Total
P (7% unc)	1.06e-1	1.07e-1
u (3% unc)	**8.92e-1**	**8.93e-1**
T (3% unc) and Tv together	5.64e-4	7.16e-4
Interactions	All interactions are <= O(e-4)	

CTS/ATS Utilization

CTS-1 (SNL capacity computing)

- Exposed issues with random failures on long-running jobs
- Useful for smaller UQ/SVER runs
- Needed to use TLCC2 machines for reliability (previous generation hardware)

ATS-1 (Trinity at LANL)

- No significant usage yet
- Plan to use for large UQ runs (1000s of SPARC runs) on HIFIRE-1
- Also will use for 3D HIFIRE-5B

Subjective Factors

High-Bar Achieved:

- Compare meshes, solution, and V&V conclusion with U. of Minnesota
- Compare internal solutions of US3D with SPARC

Other Benefits:

- V&V/UQ activities expose issues for code development
  - Exercising and stressing SPARC with large ensemble runs.
  - LENS Case 1 at fine meshes
  - Heat flux post-processing
  - 2T model challenges

Validation Set #2: perfect air, laminar & turbulent

HIFIRE-1

Validation Set #2: HIFIRE-1

The objectives of HIFiRE-1 were to provide boundary layer transition, turbulent separation, and shock/boundary layer interaction data

- "Mildly" hypersonic: negligible thermochemical nonequilibrium
- However, velocities are significantly higher than those at which turbulence models are calibrated
- Transition is difficult to predict with RANS models, even at lower velocities; we don't expect to predict transition

- Free stream conditions:

CUBRC Run 30	
Mach	7.19
Velocity (m/s)	2168.7
Temperature (K)	226.7
Density (kg/m^3)	0.067014

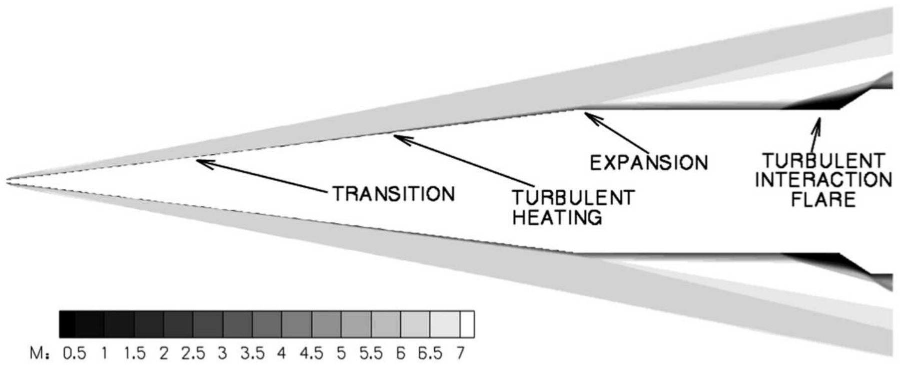


Image: Figure 5 of MacLean, Wadhams, Holden, and Johnson, "Ground Test Studies of the HIFiRE-1 Transition Experiment Part 2: Computational Analysis," JSR(45(6): 1149-1164 (2008).

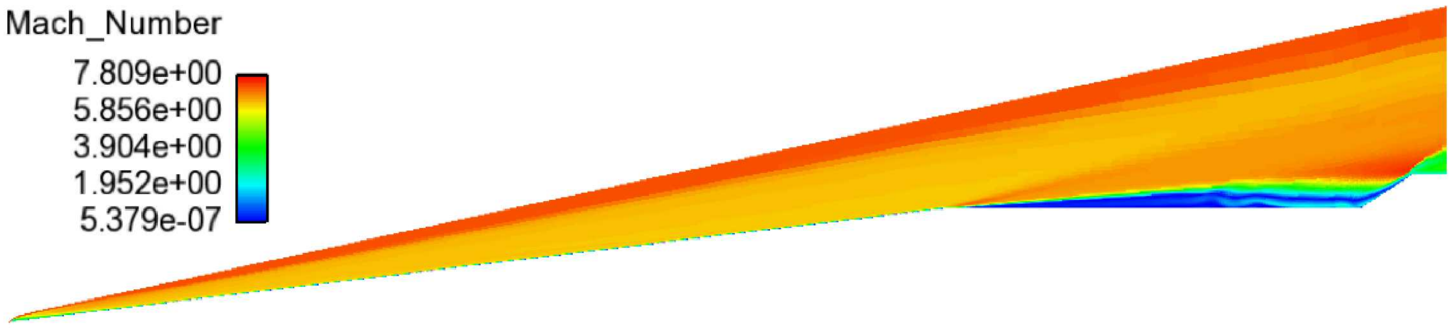
Validation Set #2: HIFIRE-1

Progress

- CUBRC condition B – Run 30 experiment
- Initial Scoping Study in progress
- Learned / Identified Obstacles:
  - Initial mesh geometry/domain too small - need bigger domain
  - CFL is limited with line solver vs. Jacobi solver when running SARANS
  - Unsteadiness in expansion region persists

Next Steps

- Construction of new meshes in progress
- Turbulence model (Spalart-Allmaras) – testing is continuing (e.g. NASA benchmarks)
- Only one data set
  - Forward UQ for parameter uncertainty
  - Solution Verification for numerical uncertainty



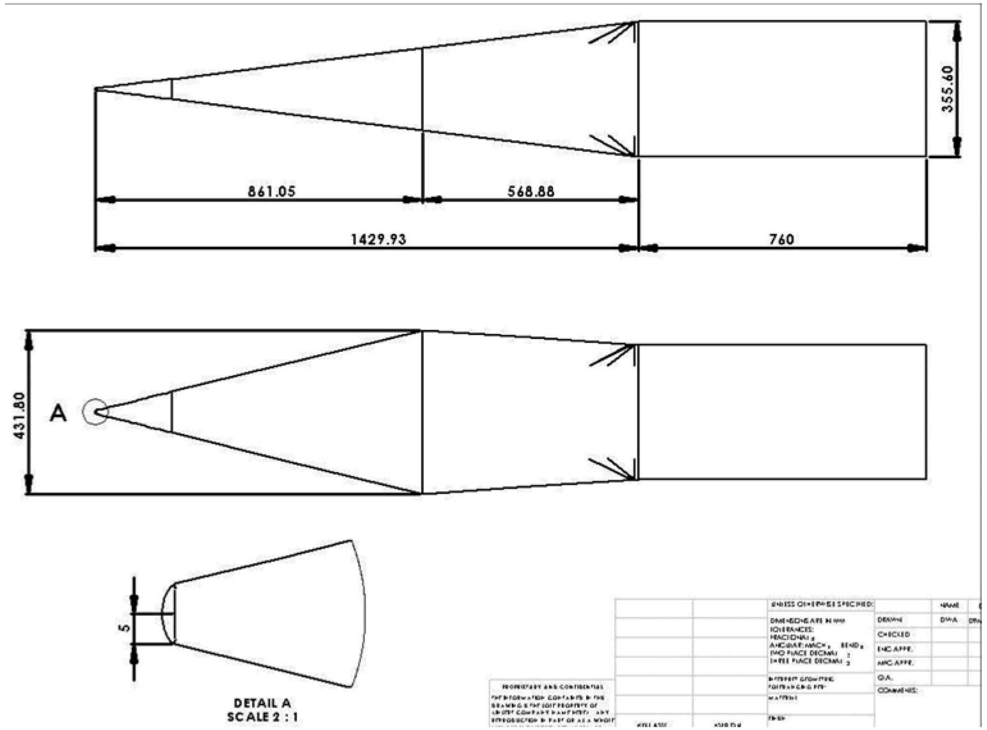
Validation Set #3: Reentry flight test

HIFIRE-5B

HIFIRE-5B

The objective of HIFiRE-5 is to provide boundary layer transition data on a 3D body

- Exhibits several transition mechanisms not relevant in HIFiRE-1 (i.e., leading edge transition, crossflow instabilities and their interactions with primary and secondary mode instabilities)



HIFiRE-1 (axisymmetric)

HIFiRE-5 (2:1 elliptic cross-section)

HIFiRE-5B as a validation target

- − Flight tests have larger uncertainties than ground tests
- − Flow regime does not stress thermochemical NEQ models
- − Flow regime is not well-suited to SPARC's existing methods
- + Multiple experimental ground test efforts
- + Relatively well-characterized data
- + Timely community visibility and collaboration

Image: Figure 1 of Kimmel, et al., "HIFiRE-1 and HIFiRE-5 Flight and Ground Tests," AIAA paper 2018-0056.

Acknowledgements

- V&V/UQ Team
  - PM: Veena Tikare
  - PI: William Rider
  - Brian Carnes, Derek Dinzl, Brian Freno, Micah Howard, Sarah Kieweg, Erin Mussoni, Eric Phipps, Jaideep Ray, William Rider, Denis Ridzal, Thomas Smith, Greg Weirs
- Re-Entry Development Team
  - PM: Paul Crozier
  - PI: Micah Howard
  - Dev Team: Steve Bova, Andrew Bradley, Brian Carnes, Derek Dinzl, Jeff Fike, Travis Fisher, Mark Hoemmen, Robert Knauss, James Overfelt, Eric Phipps, Tom Smith, Ross Wagnild, et al.
- Collaborators and Resources
  - DoD HPCMP/CREATE-AV
  - U of Minnesota
  - CUBRC

BACKGROUND SLIDES – FULL MILESTONES, PIRT, AND CVER

Milestone Success Criteria

Milestone Goal	Low-Bar Criteria	High-Bar Criteria
1.) Validation Sets	a.) HIFiRE-1 Experiment in LENS-1 (perfect gas, laminar and turbulent) b.) 25-55 Double Cone in LENS-XX (NEQ air, laminar)	c.) Reentry flight experiment (e.g., Reentry-F (NASA, UUR) or LBRV (Sandia, SRD) d.) Unsteady Separated flow experiment (e.g., Mach 6 capsule (CUBRC, UUR)
2.) Code Verification	a.) Relevant code verification activities of individual separate physics b.) Identification of problems	c.) Relevant code verification activities of combined physics d.) correction of identified problems
3.) Solution Verification	Grid convergence studies and estimates of numerical uncertainty	
4.) Sensitivity Analysis	Perform local sensitivity analysis for validation sets using Sacado	Perform global sensitivity analysis for validation sets
5.) UQ Studies	Use Dakota's sampling methods for forward propagation of uncertainties	Use Dakota's gradient-enhanced sampling methods for propagation of uncertainties. Use Bayesian methods for parameter estimation using statistical emulators
6.) Calibration		Perform single deterministic calibration
7.) CTS/ATS Utilization	a.) Validation set computations performed on SRN CTS-1 systems (serrano, ghost)	b.) Some portion of validation set computations performed on SCN ATS-1 system (Trinity) c.) Replicate some portion of a validation set computations on an ATS-2 early-access system
8.) Subjective Factors	a.) Use only Sandia analysis of V&V/UQ	b.) Compare meshes, solution, and V&V conclusions with CREATE and U. of Minnesota c.) Multiple internal solutions with full V&V assessment

PIRT

PIRT = Phenomena Identification Ranking Table

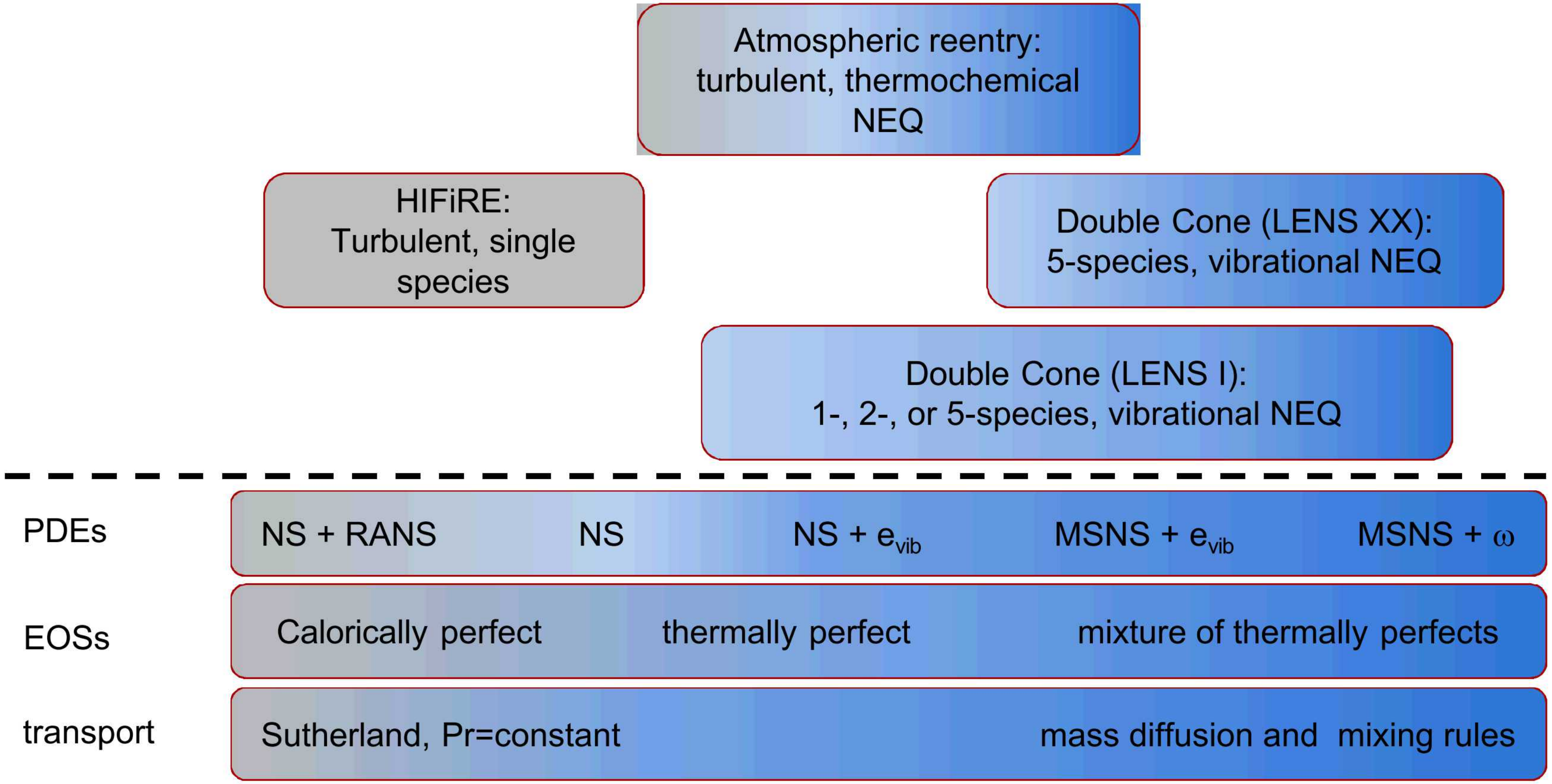
Double Cone (LENS XX)

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

HI-FiRE

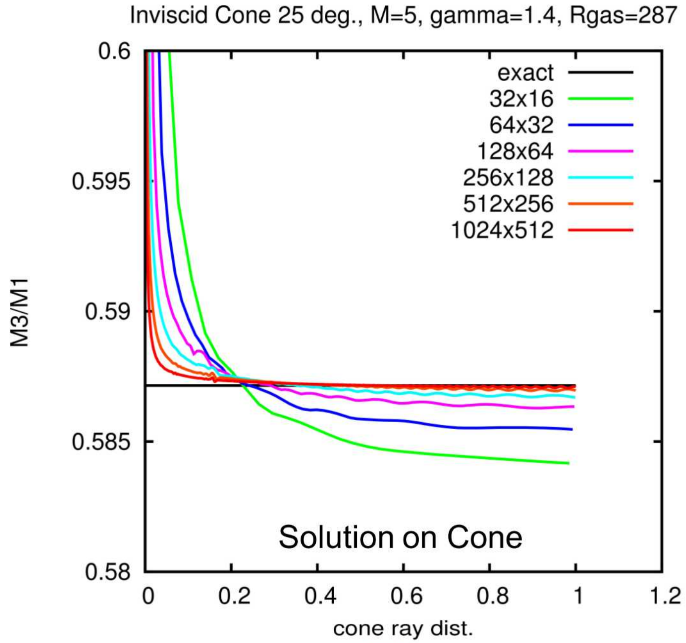
Application: HI-FiRE		
Quantity of Interest: heat flux, pressure		
Contact: Sarah Kieweg		
Assessment Team: SPARC team		
Date: 10/19/17		
ID	***Phenomena***	***Importance***
A	**Hypersonics**	
A1	shock structure	H/M
A2	flow expansion from cone to cylinder	L
A3	Nonequilibrium vibrational energy	M
A4	transient effects	L
A5	Molecular viscosity model for thermochem neq	L/?
B	**Laminar Boundary Layer + interactions**	
B1	Attached laminar BL	H
C	**Turbulence**	
C1	Transition	H
C2	Attached turbulent BL (RANS)	H
C3	Separation of Turbulent BL	H
C4	Reattachment of Turbulent BL	H
C5	Shock train downstream of flare	M
D	**Gas Models**	
D1	Real gas model	H

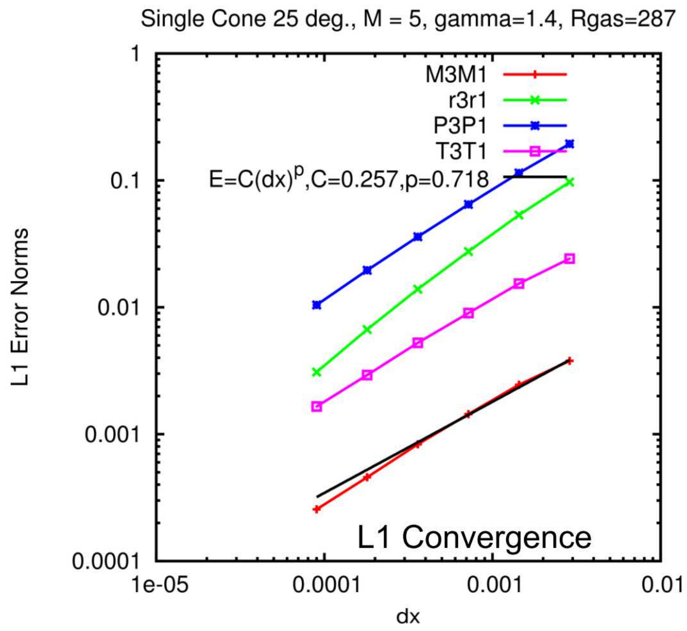
Validation Hierarchy

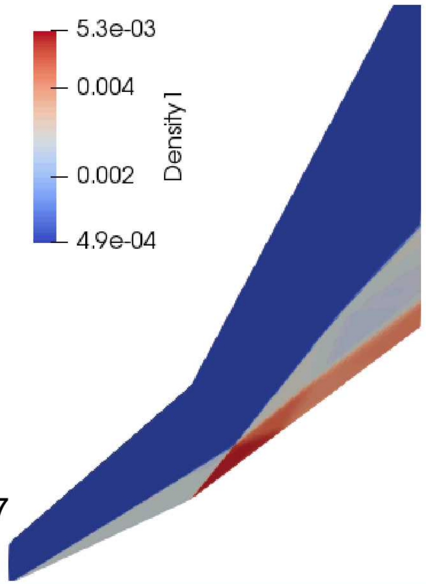


Code Verification: Taylor-Maccoll & Oblique Shocks Double Ramp

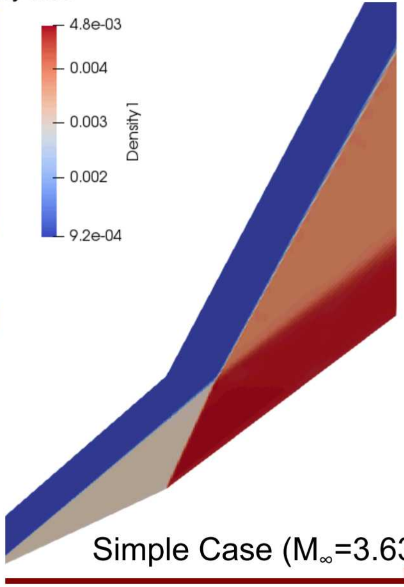
- Supersonic Inviscid Axisymmetric Cone Flow – Taylor-Maccoll Equation
  - **Status**-Done
  - **What was Studied** - Convergence of Solution variables using similar mesh design and assumptions as double-cone simulations
  - **Impact** - Mesh design used to simulate axisymmetric flows produces convergent cone solutions
- Oblique Shocks – Double Ramp
  - **Status**-Completed simple case, more work would be needed for more complex cases
  - **What was Studied** – 25º-37º double ramp with exact inviscid solution (M_∞=3.636)
  - **Impact** – Convergence of inviscid solution for simple case with shock interactions demonstrates correct shock handling



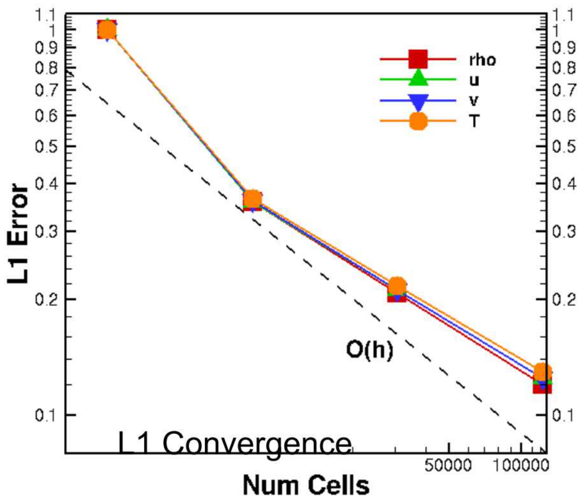




LENS-XX Case 4 with M_∞ =12.7



Simple Case (M_∞=3.636)



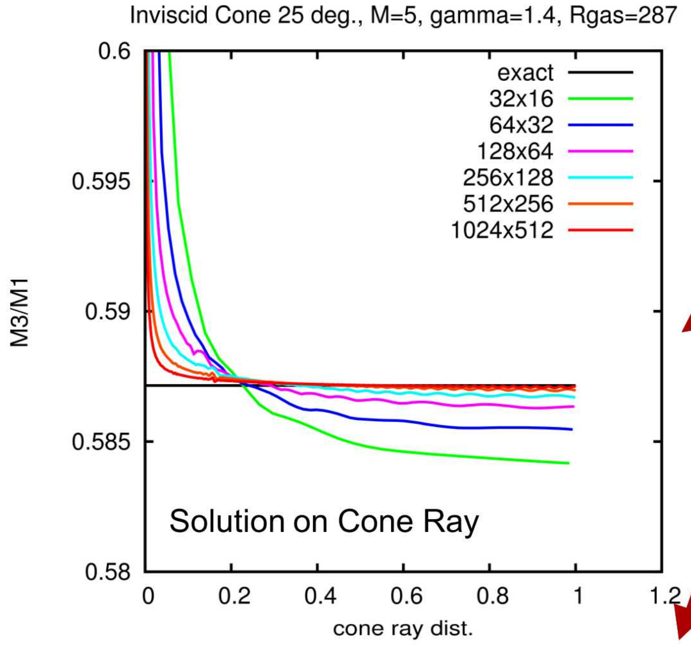
Code Verification: Taylor-Maccoll axisymmetric cone flow

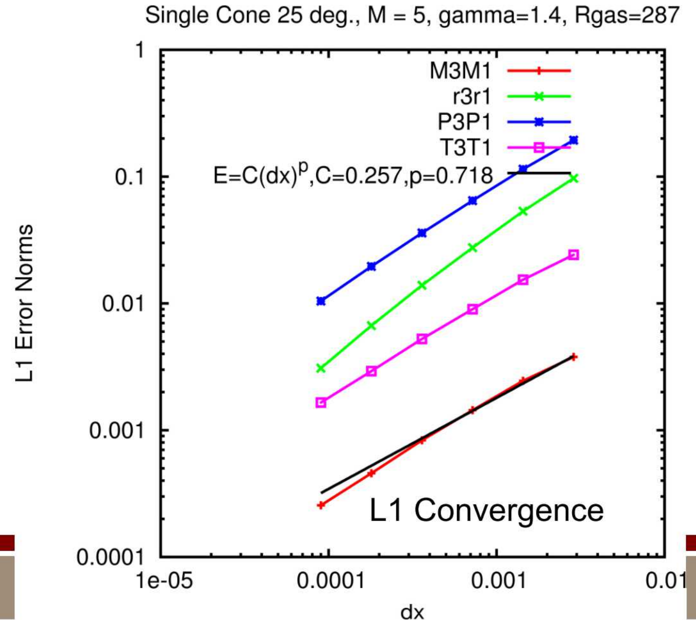
Background:

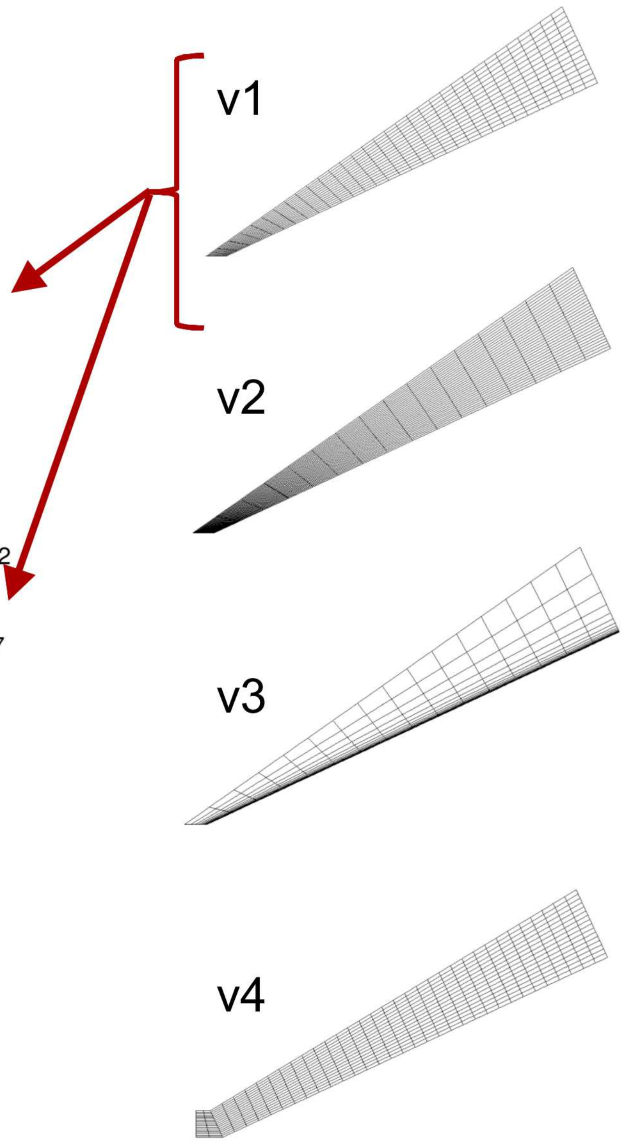
- The Taylor-Maccoll problem is a similarity solution for the supersonic inviscid axisymmetric flow over a sharp cone.
- The solution requires the numerical solution of a simple ODE (simple: well-behaved, not stiff)

Impact:

- Demonstrated convergence of SPARC's 3D approach to axisymmetric flow, i.e., convergence is not inhibited by
  - Simulating a narrow azimuthal wedge
  - Offsetting the mesh from the axis to avoid degenerate cell faces
  - Numerical error and convergence were examined across several mesh sequences with different spacing distributions and topologies







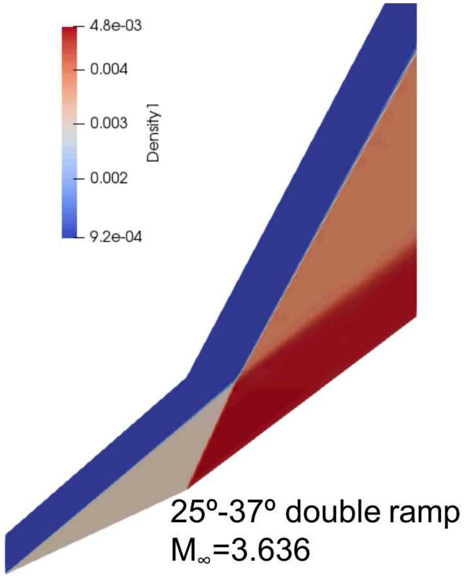
Code Verification: Double Ramp Oblique Shock Interaction

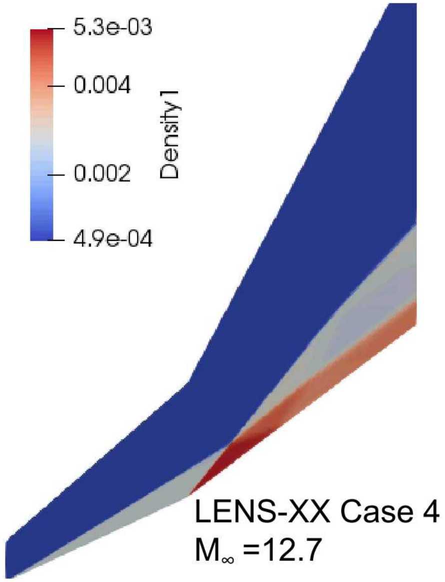
Background:

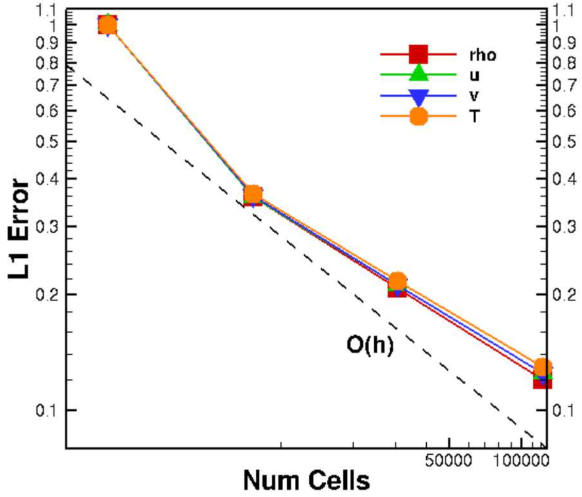
- Single ramp solution is captured by the well known θ-β-M implicit equation
- Exact solution requires iteration across three θ-β-M solutions to match states across several waves
- By design, the solution has three constant post-shock states with no reflected wave

Impact:

- Designed to test how well shock interactions are captured. (Note similarity of features to LENS-XX solution structure, right)
- Convergence results demonstrate SPARC's capability to correctly capture wave interactions in a complex flowfield

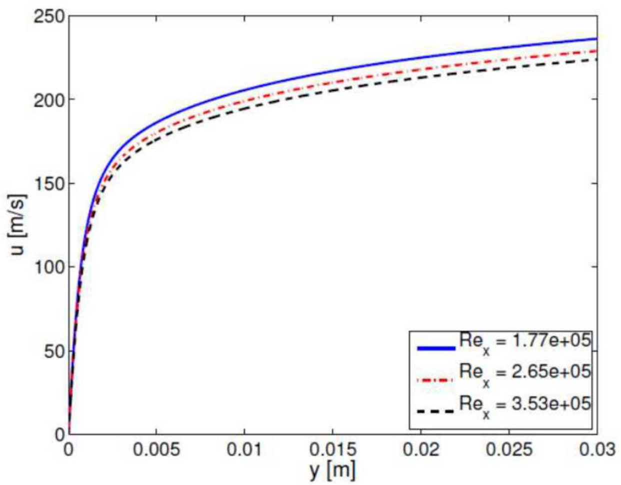


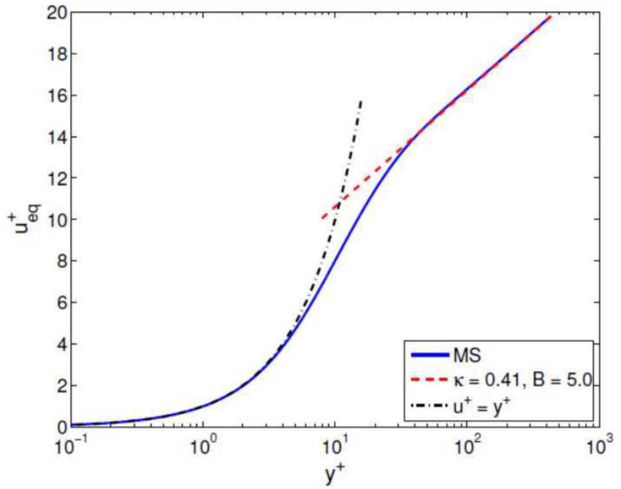




Code Verification: Turbulent (SA) compressible flat plate BL (MMS)

- Status
  - Basic infrastructure has been incorporated into SPARC to accommodate verification using manufactured solutions
    - Source term generation for laminar and turbulent term contributions
    - Manufactured solutions that include a turbulence variable
  - Spatial accuracy tests have begun
- Plan
  - The ultimate goal is to test low and high Reynolds number flows using both sinusoidal and realistic manufactured solutions
- Impact
  - Early tests resulted in truncation errors that did not reduce with mesh refinement
  - Faulty components are being isolated by testing intermediate options between a successfully second-order-accurate supersonic inviscid case and a turbulent (SA) case





Realistic manufactured velocity profile containing both a viscous sublayer and logarithmic layer

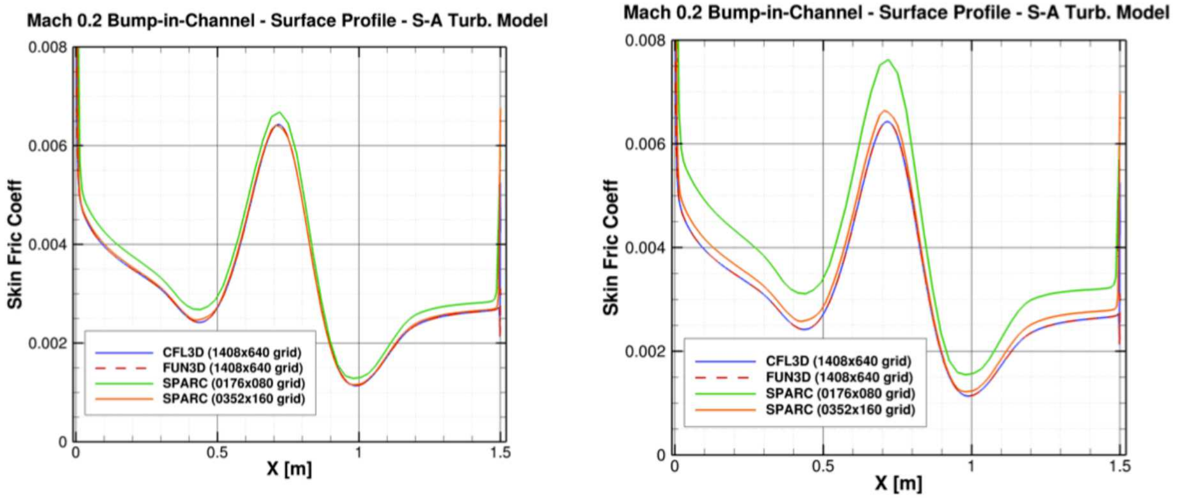
Code Credibility Activity: NASA Turbulence Modeling Resource

Objective: Code-to-code comparison for subsonic and supersonic cases with Spalart-Allmaras (SA) turbulence model

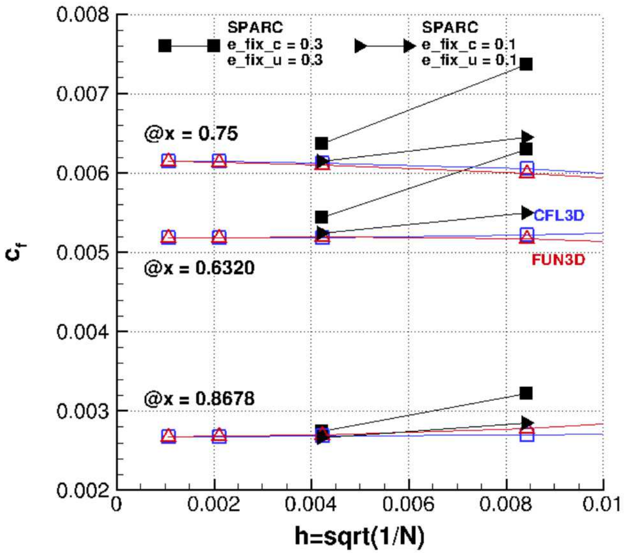
Subsonic Bump in Channel

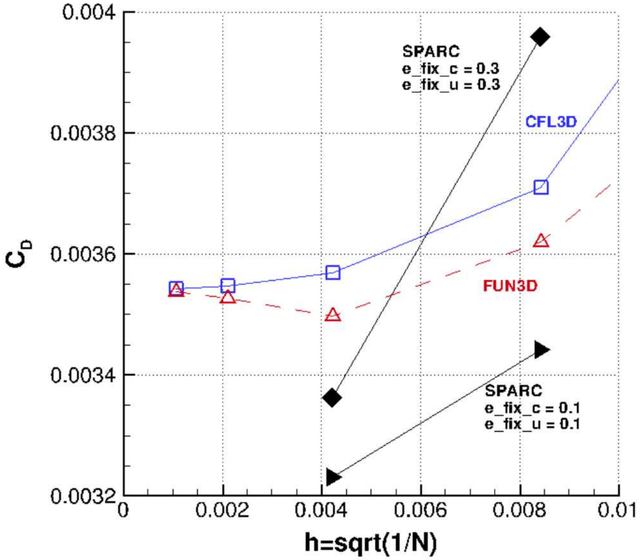
- Status
  - In-progress
  - Two cases run over two structured meshes
  - Testing SPARC with NASA compressible CFD codes (CFL3D and FUN3D) and monitoring convergence for flow characteristics (lift, drag, wall skin friction, pressure, eddy viscosity, velocity)
  - The solution residuals flatten for sufficiently low values of entropy fix, hinting at convergence issues.
- Plan
  - Work is ongoing to add more diagnostics, i.e., additional automated post-processing of the data
  - Will complete analysis and identify any opportunities for SPARC improvements by end of Q2
- Impact
  - Entropy fix has a strong effect on the solution and its convergence, making this an important test for SPARC

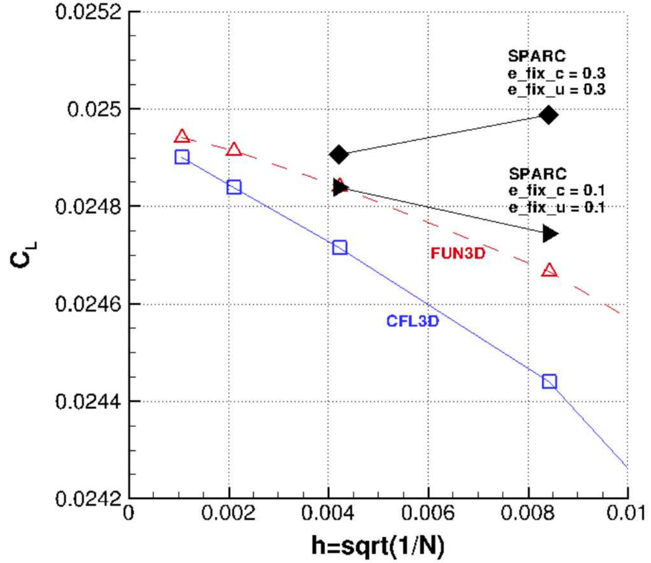
Skin friction profile over bump
Entropy fix = 0.1 (left)
Entropy fix = 0.3 (right)



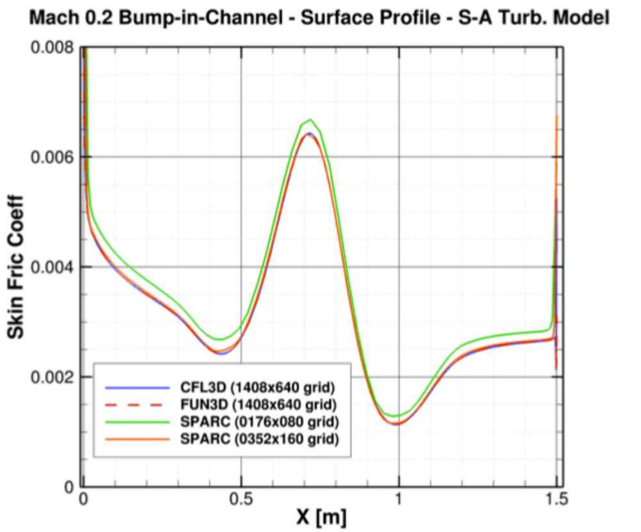
Subsonic Bump in Channel Preliminary Results

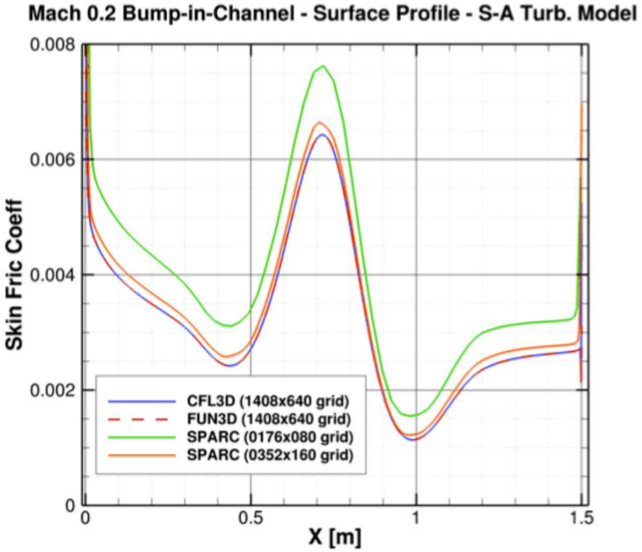






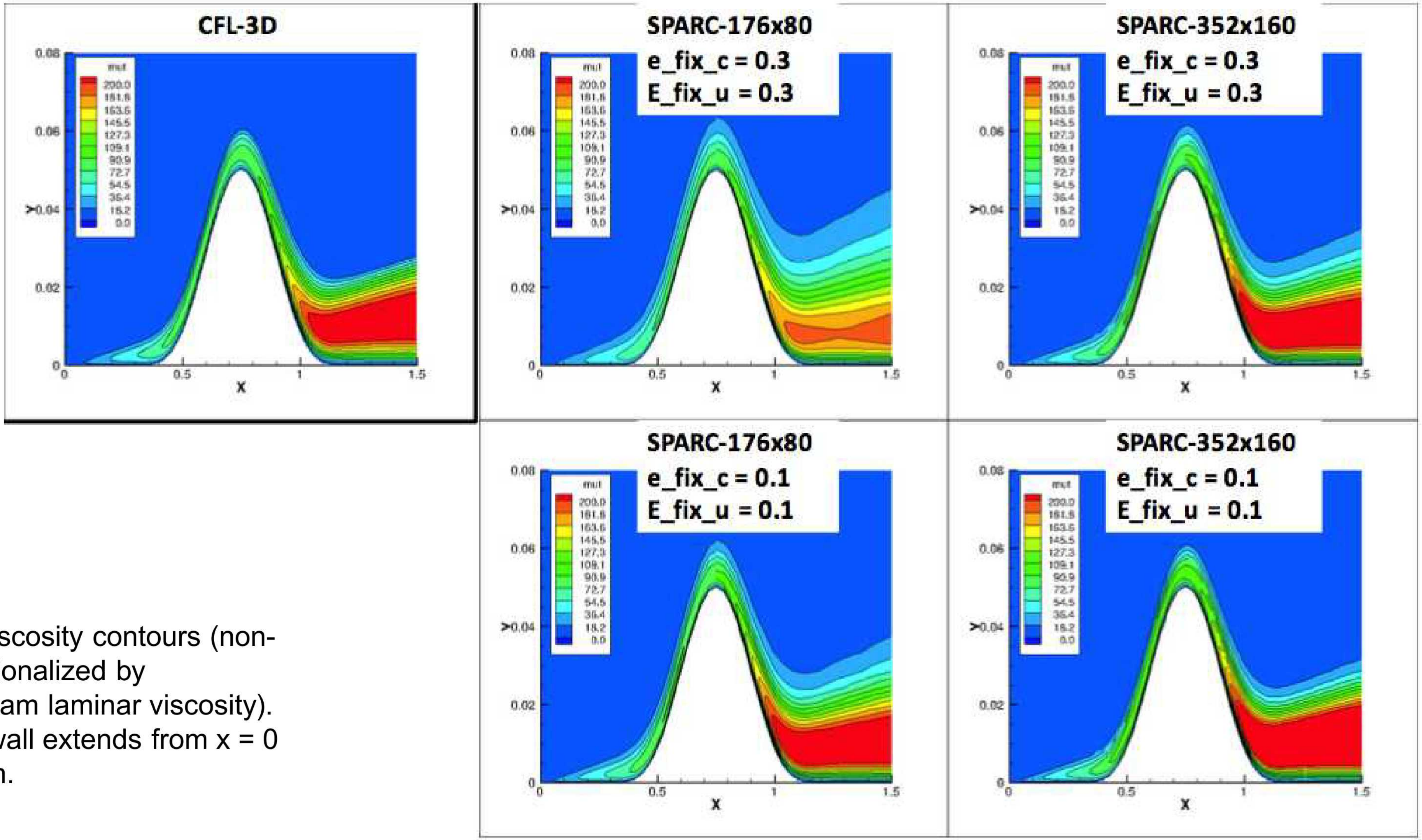
Skin friction coefficient, drag coefficient, and lift coefficient plots for varying mesh sizes. e_fix also varied between 0.1 and 0.3. (e_fix is entropy fix)





Skin friction profile over bump.
e_fix = 0.1 (top)
e_fix = 0.3 (bottom)

Subsonic Bump in Channel Preliminary Results



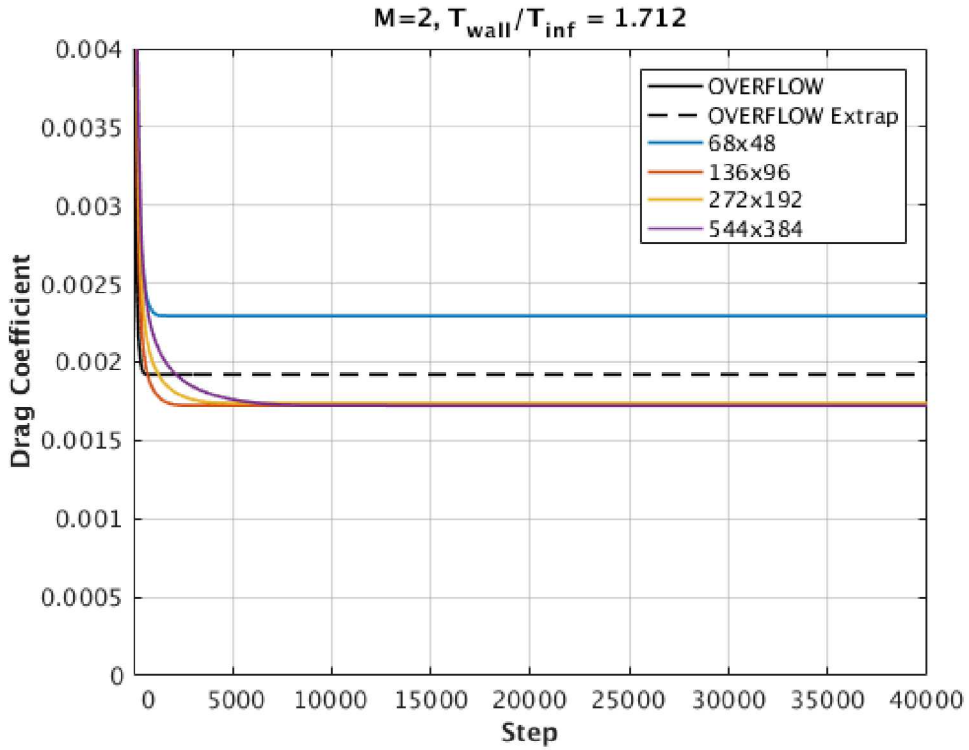
Eddy viscosity contours (non-dimensionalized by freestream laminar viscosity). Bump wall extends from x = 0 to 1.5 m.

Code Credibility Activity: NASA Turbulence Modeling Resource

Objective: Code-to-code comparison for subsonic and supersonic cases with Spalart-Allmaras (SA) turbulence model

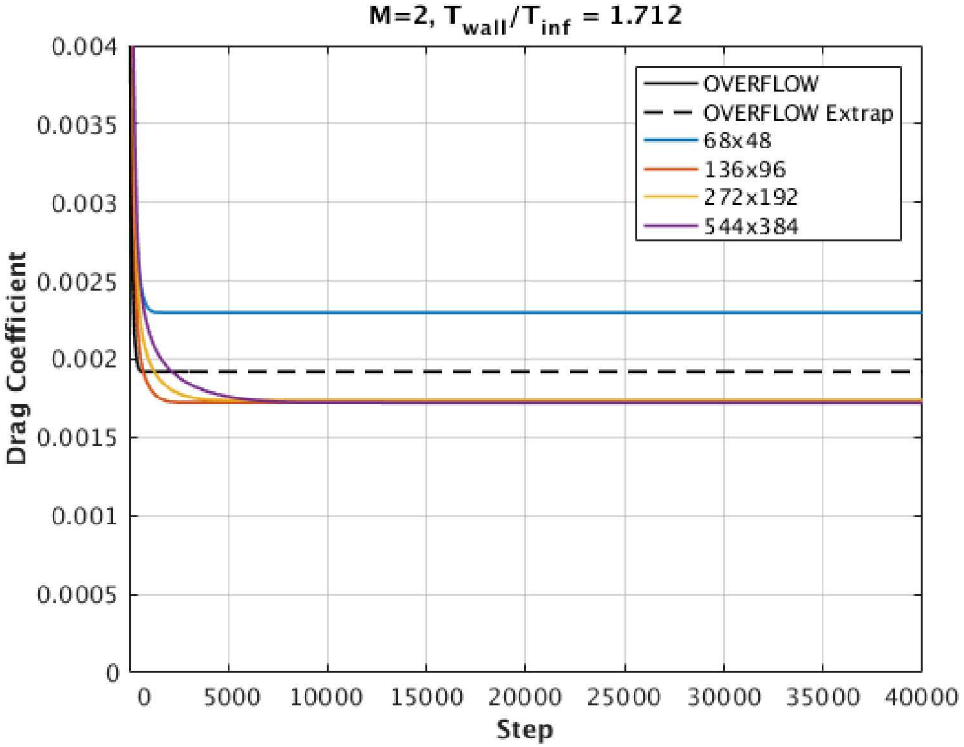
Supersonic Flat Plate

- Status
  - In-progress
  - Four cases with varying Mach numbers (2,5) and wall temperatures run over series of four structured meshes
  - Additional tool development performed to output additional parameters needed for code-to-code comparisons (e.g. momentum thickness)
  - Drag convergence behavior monitored and compared with OVERFLOW CFD code
- Plan
  - Test SPARC with compressible CFD codes from NASA (CFL3D, FUN3D, WND, OVERFLOW) and Stanford (JOE) to analyze behavior near leading edge of plate (first quarter of plate)
  - Will be completed by end of Q2
- Impact
  - Identified SPARC weakness being robust to grid (this was fixed by adjusting mesh but needs to be fixed in code)

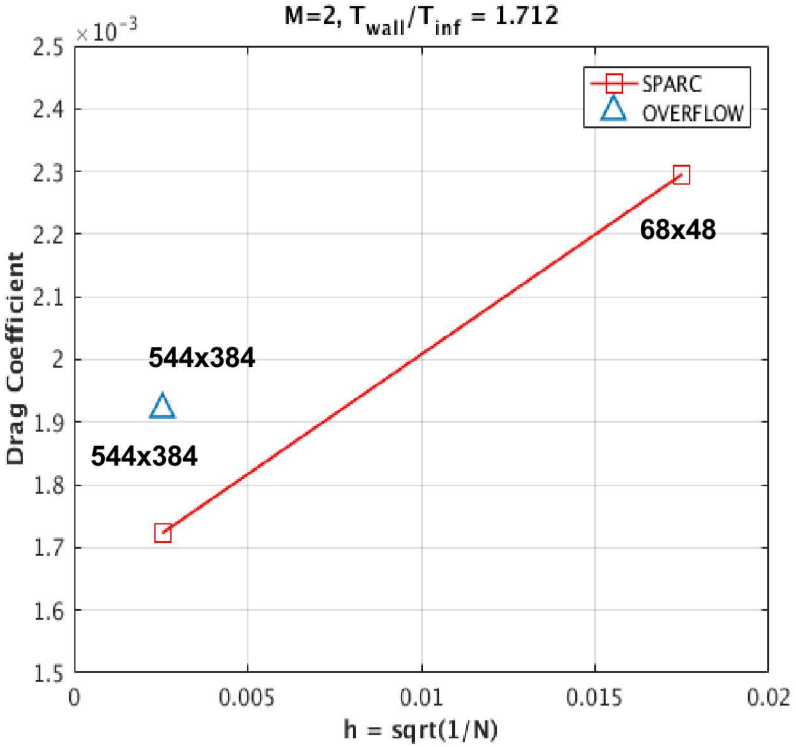


Drag convergence comparison with NASA Langley OVERFLOW code for M=2, T_{wall}/T_{inf} = 1.712. $Re_{L=1}$ = 15 million. OVERFLOW results are for 544x384 mesh.

SA Supersonic Flat Plate Preliminary Results



Drag convergence comparison with NASA Langley OVERFLOW code for M=2, T_{wall}/T_{inf} = 1.712. $Re_{L=1}$ = 15 million. OVERFLOW results are for 544x384 mesh.



Drag coefficient comparison with NASA Langley OVERFLOW code for M=2, T_{wall}/T_{inf} = 1.712. $Re_{L=1}$ = 15 million.

Initial Validation before UQ

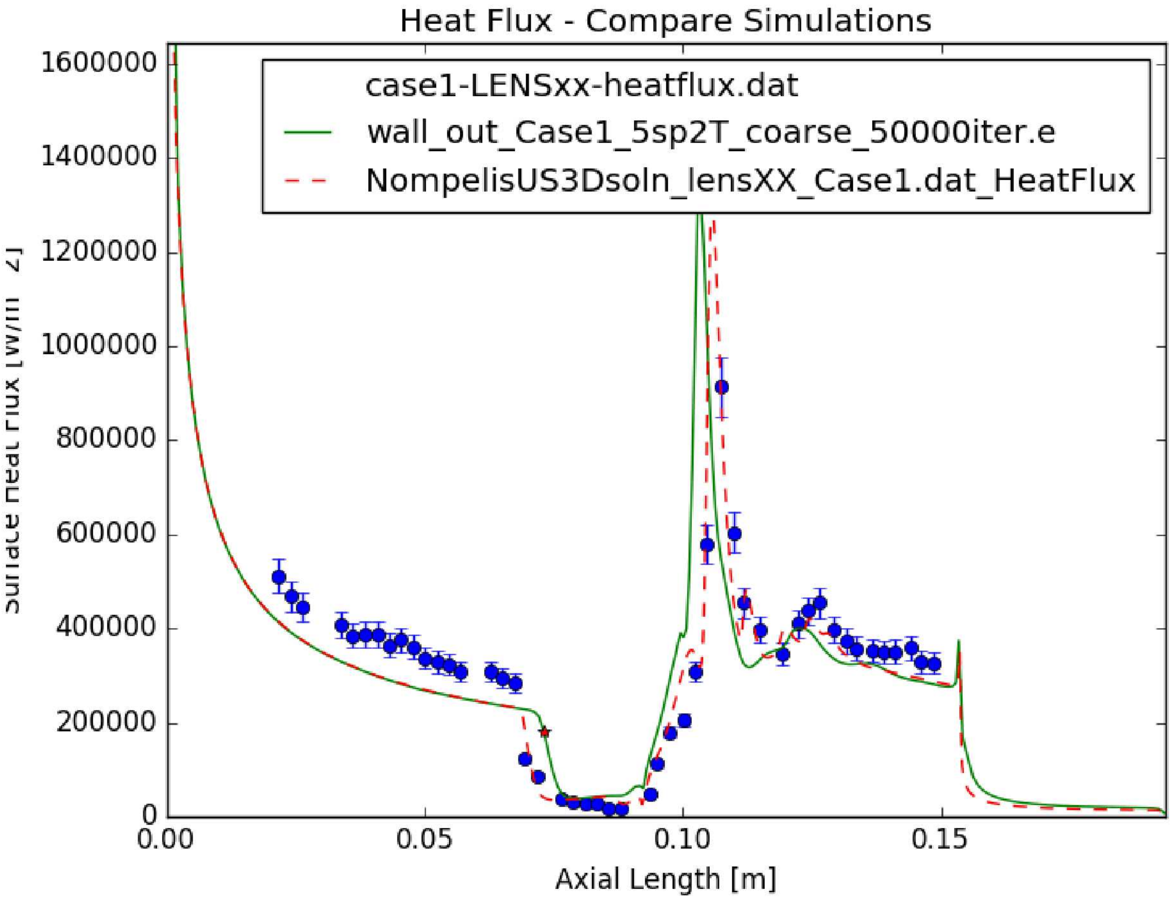
BACKGROUND SLIDES – ALL LENS XX CASE 1 – 6 PLOTS

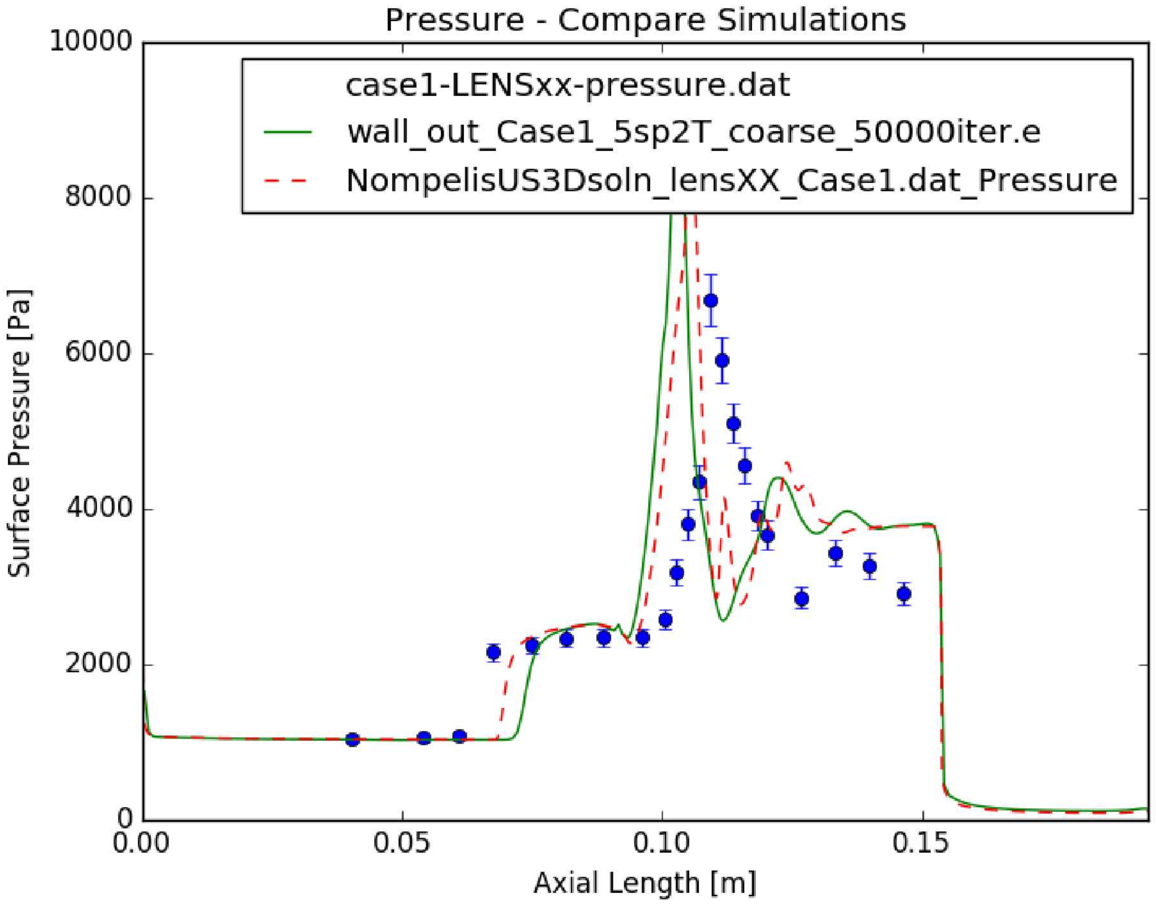
LENS XX Conditions

Table 1. Freestream Conditions for Double Cone Test Cases

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
2	9.65	10.90	17.5	0.19	4.303	0.984	389
3	18.70	13.23	18.0	0.11	6.028	0.510	521
4	21.77	12.82	39.5	0.20	6.497	0.964	652
5	18.51	13.14	36.8	0.23	5.996	1.057	523
6	15.23	11.46	59.0	0.39	5.466	2.045	573

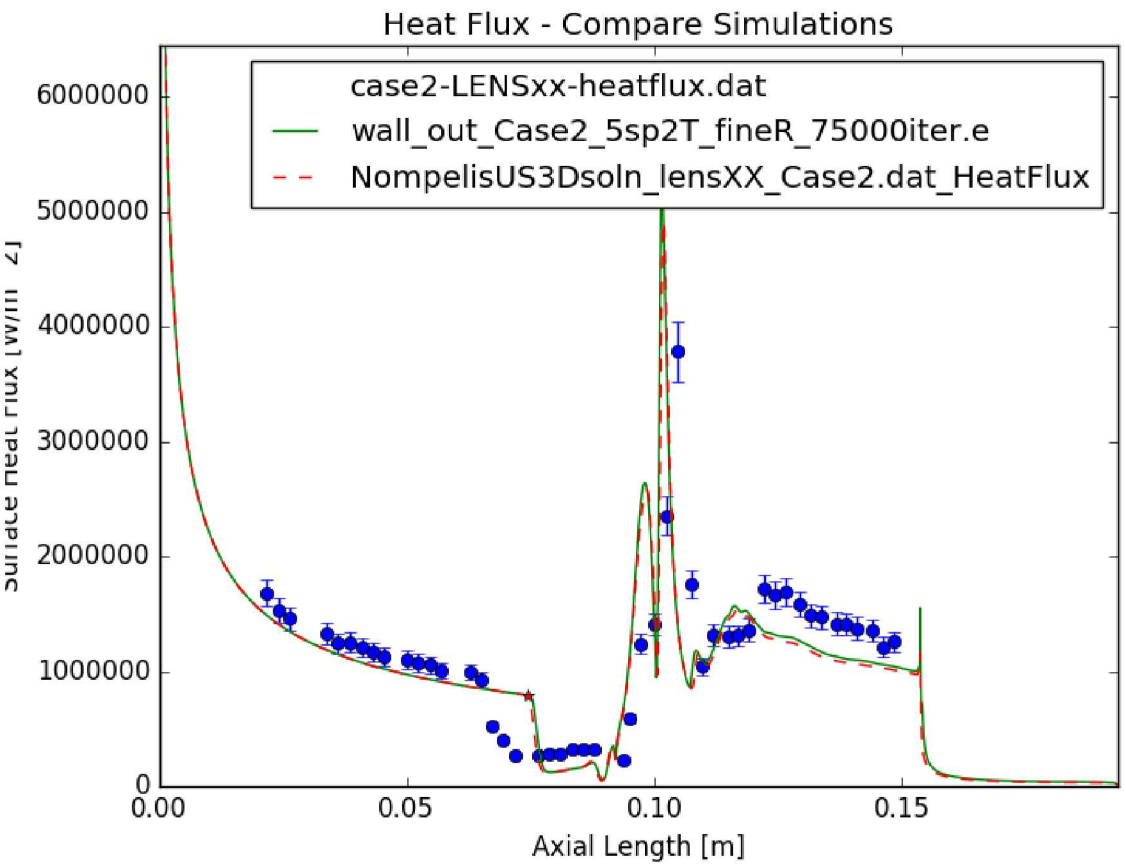
LENS XX: Case 1

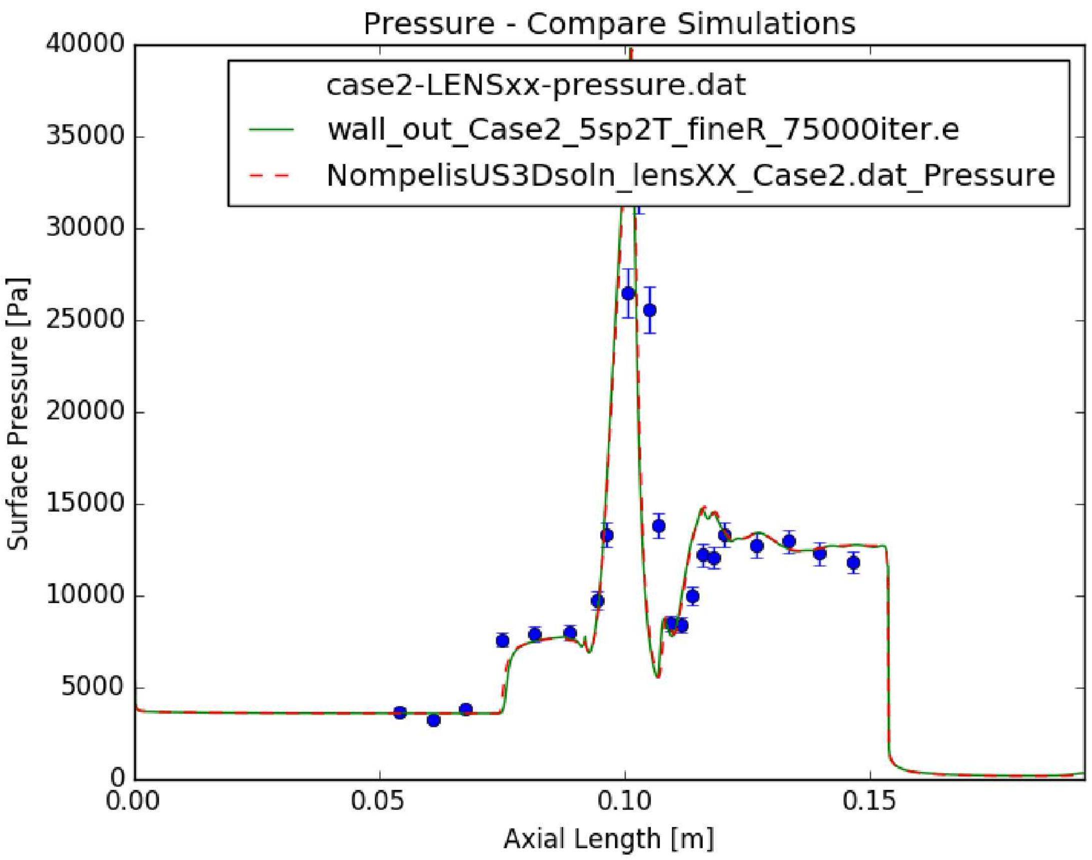




Case 1 SPARC is on a coarse mesh. Differences in separation region likely due to mesh differences.

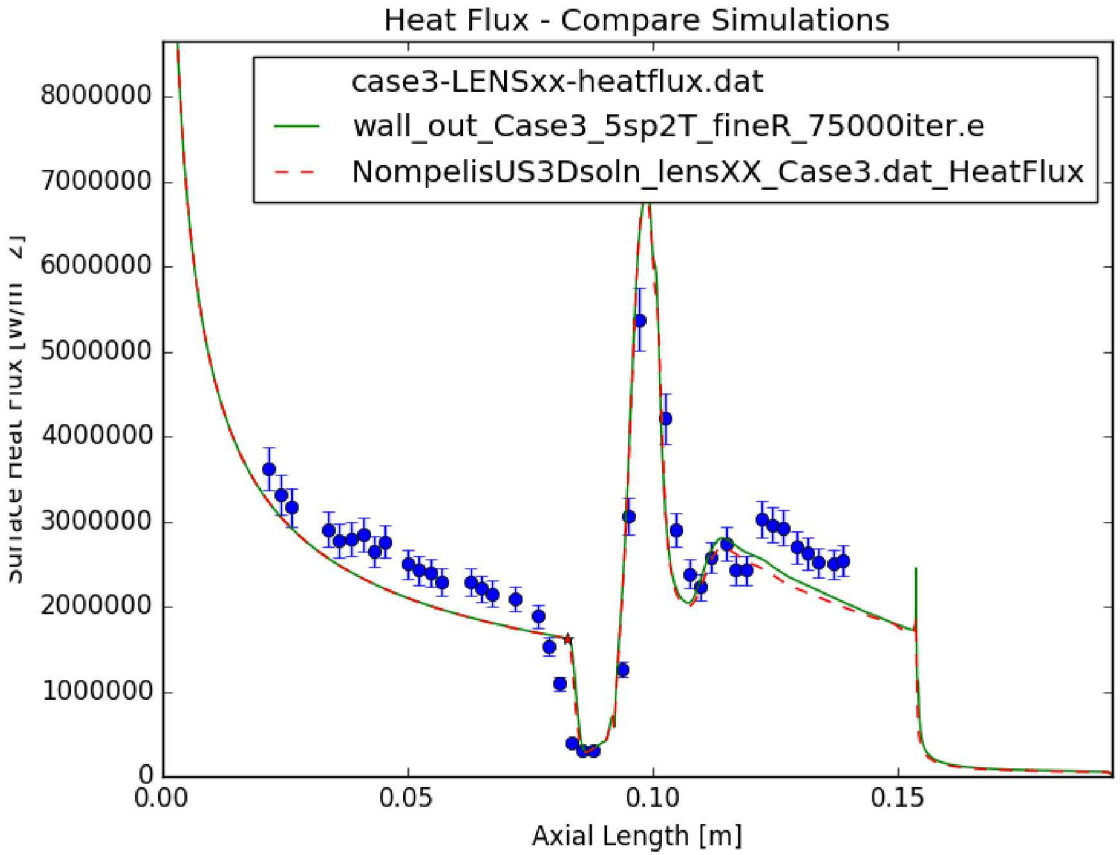
LENS XX: Case 2

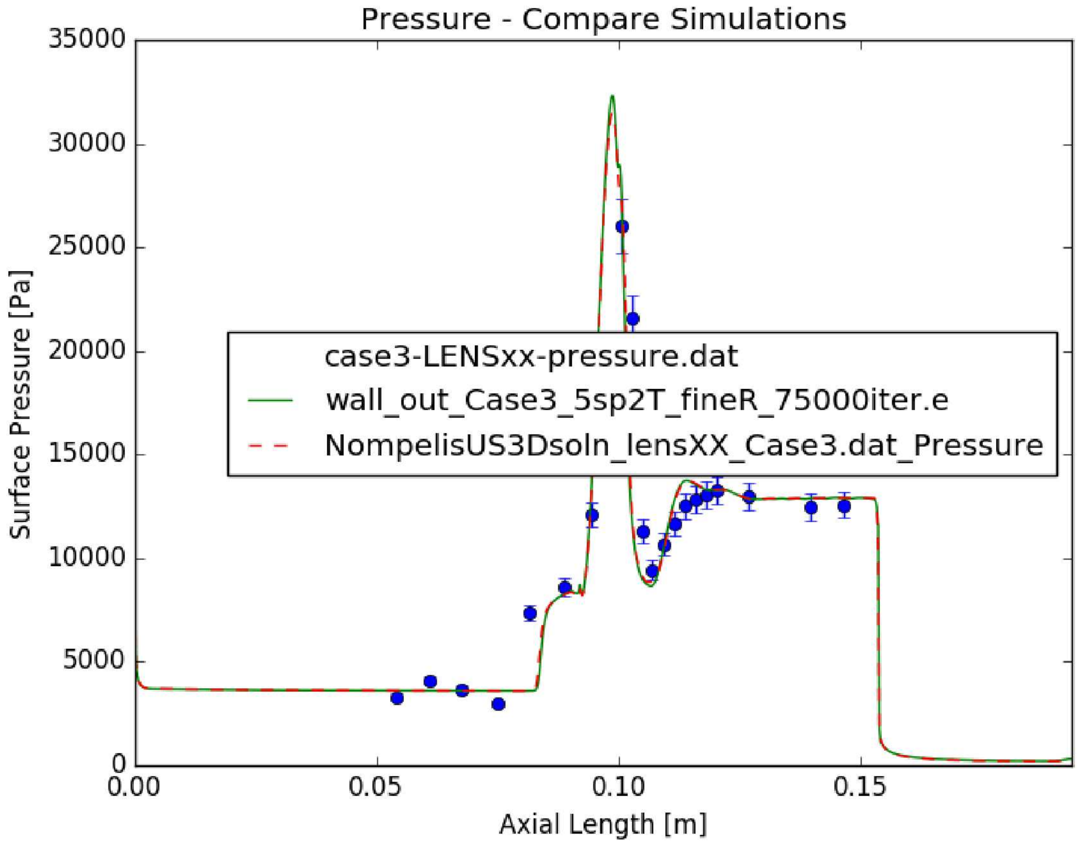




SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Nompelis’ mesh similar size. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

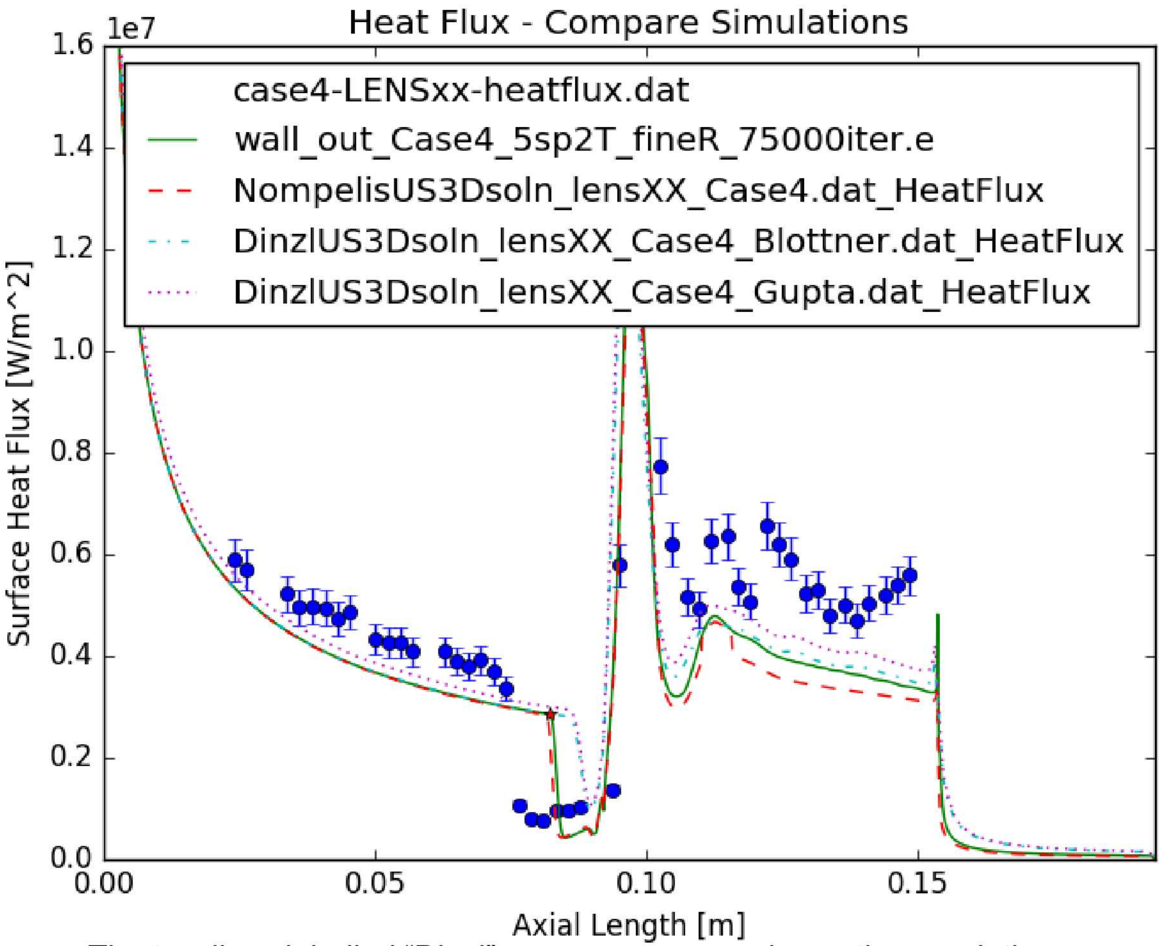
LENS XX: Case 3

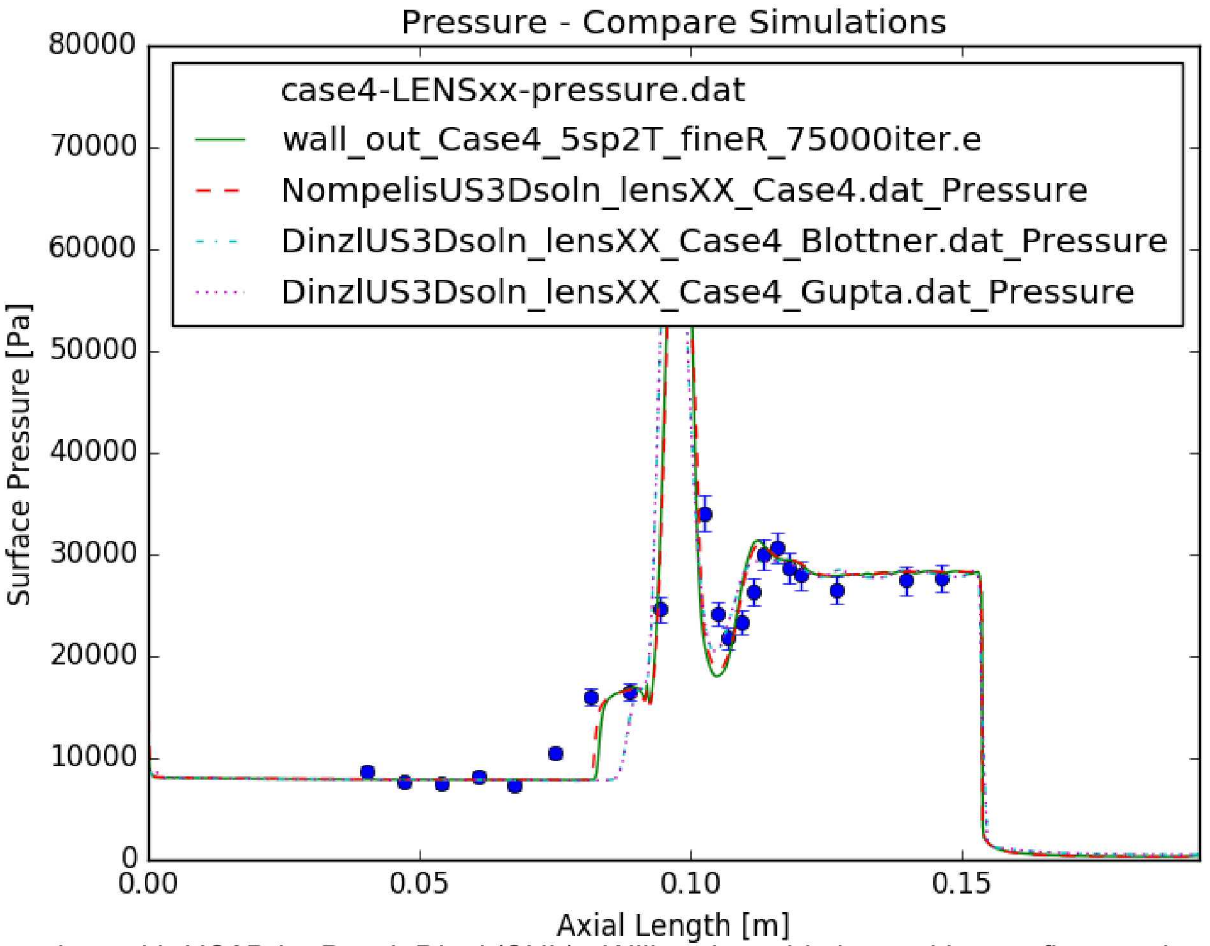




SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Nompelis’ mesh similar size. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

LENS XX: Case 4

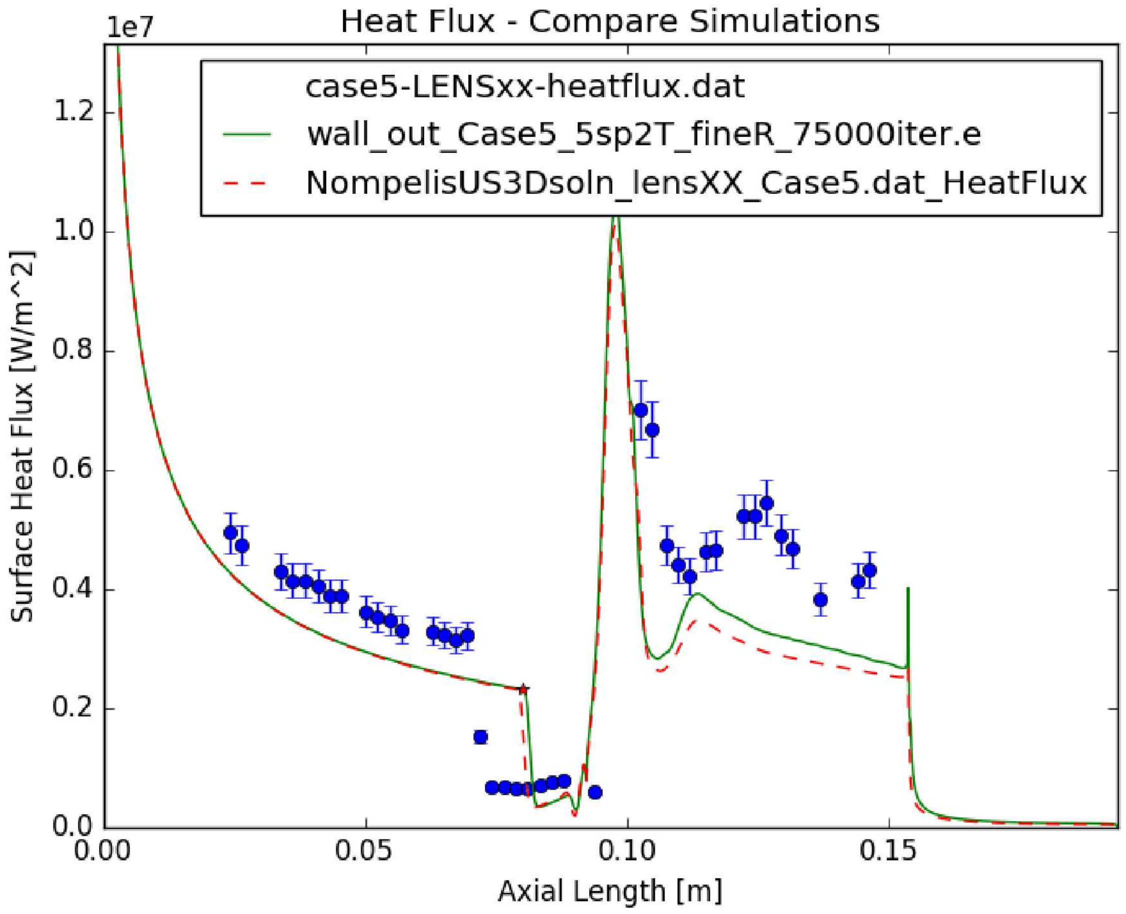


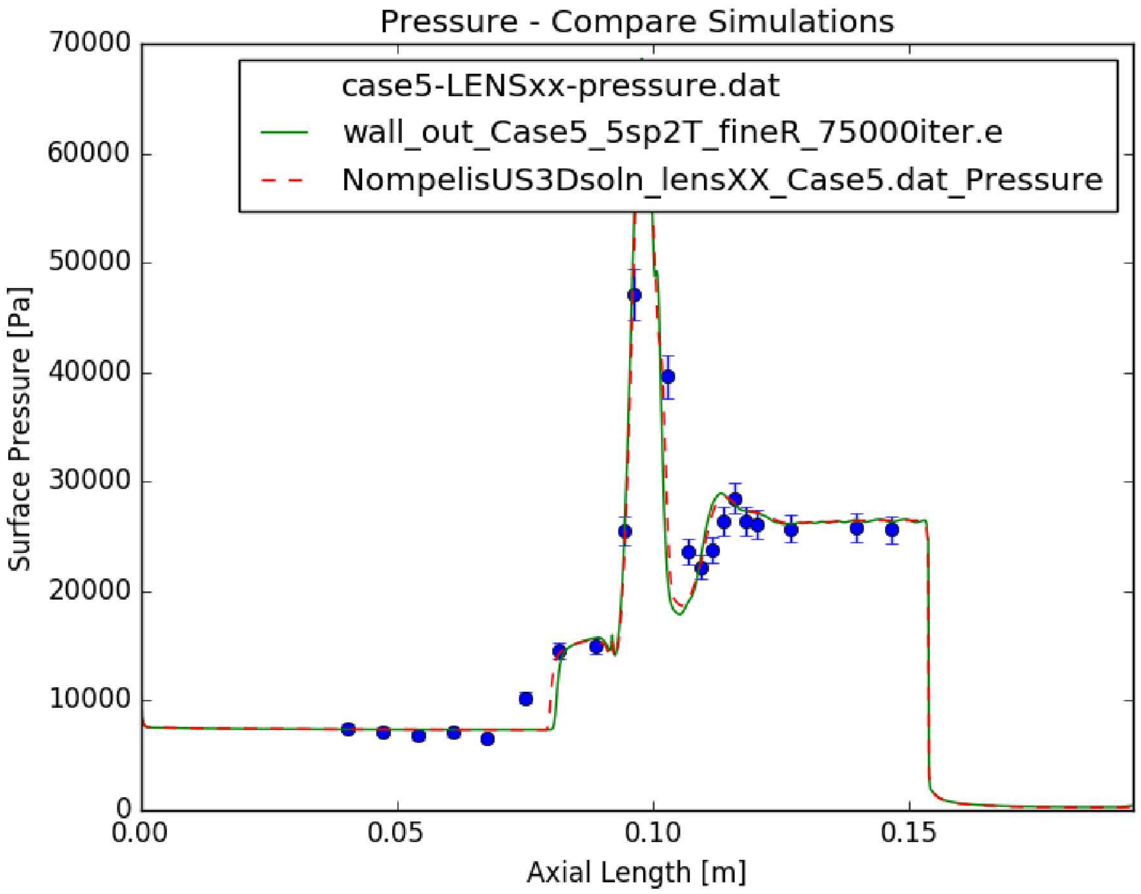


The two lines labelled “Dinzl” are on coarse meshes – these solutions use our meshes with US3D by Derek Dinzl (SNL). Will replace this later with very fine mesh solutions. Difference in separation region likely due to mesh. Notice our US3D Blottner solution matches I. Nompelis’s US3D solution and SPARC in the attached region (not mesh dependent there.)

SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Nompelis’ mesh similar size. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

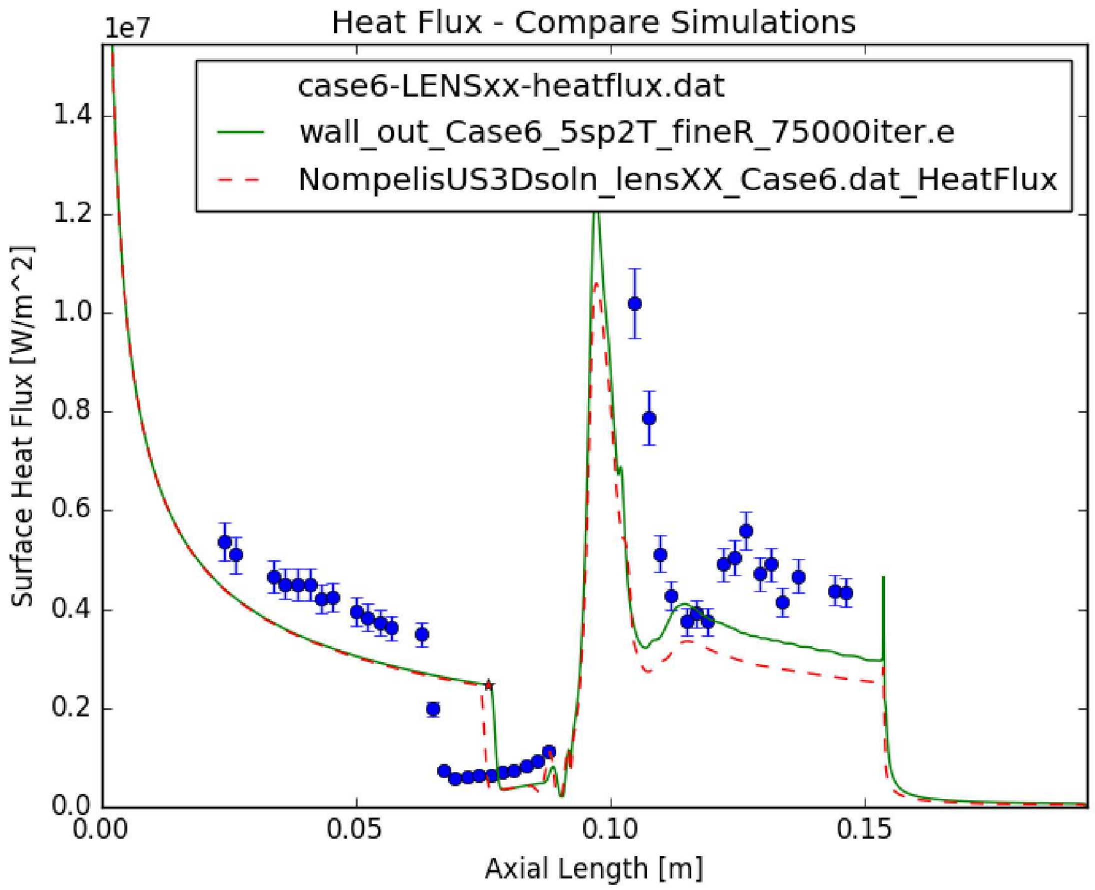
LENS XX: Case 5

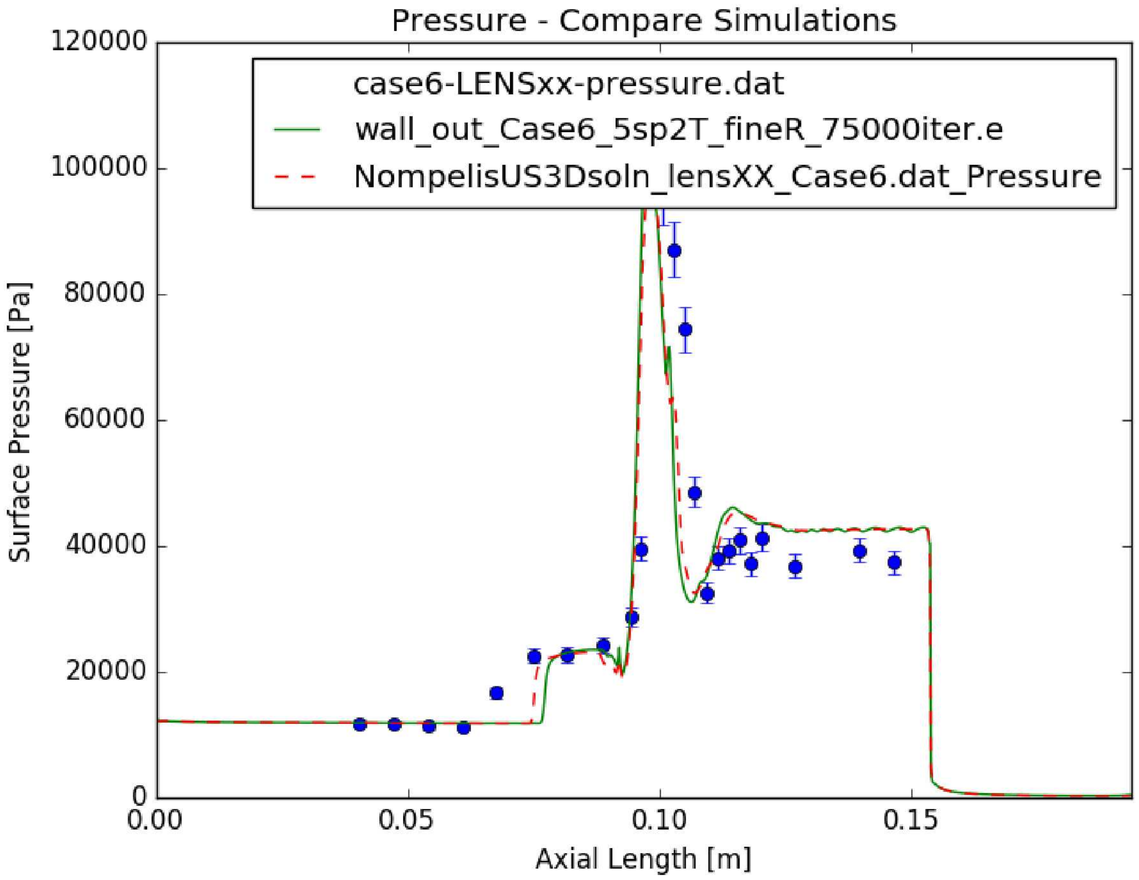




SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Nompelis’ mesh similar size. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

LENS XX: Case 6



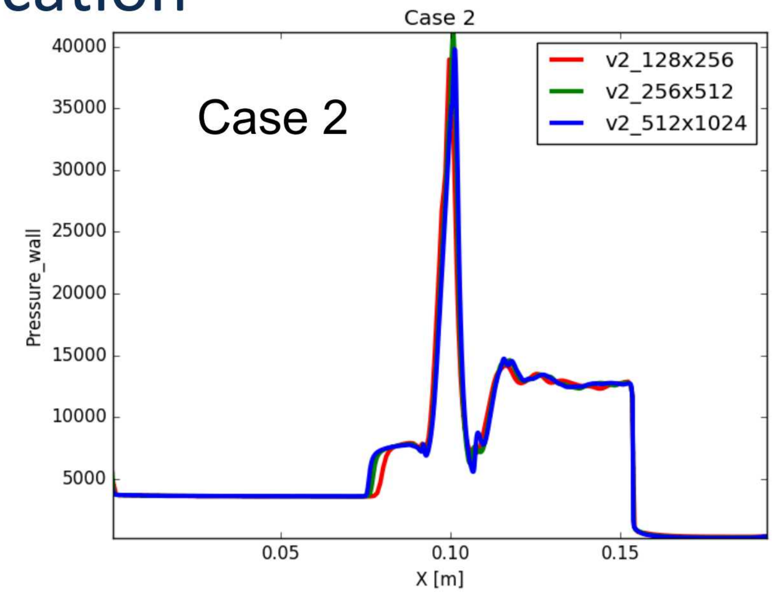


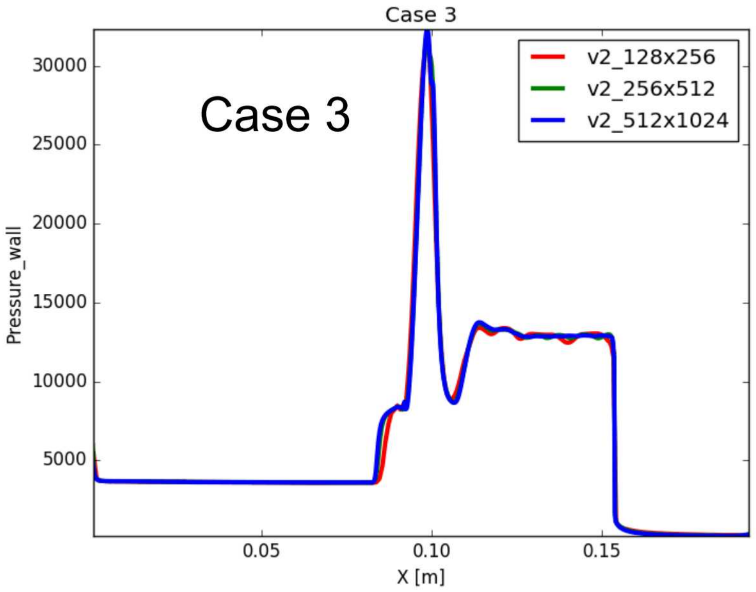
SPARC simulations use “finer” v2_512x1024 mesh, 50000 iterations. Nompelis’ mesh similar size. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

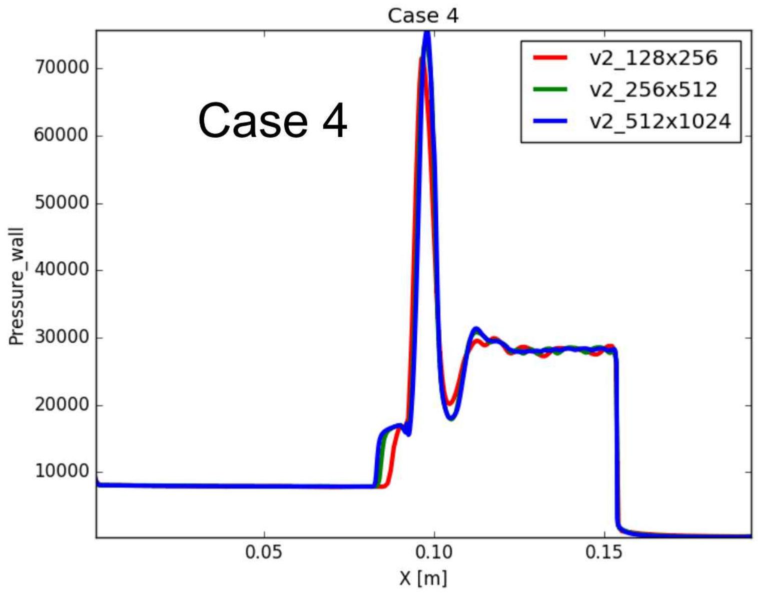
BACKGROUND SLIDES – SOLUTION VERIFICATION

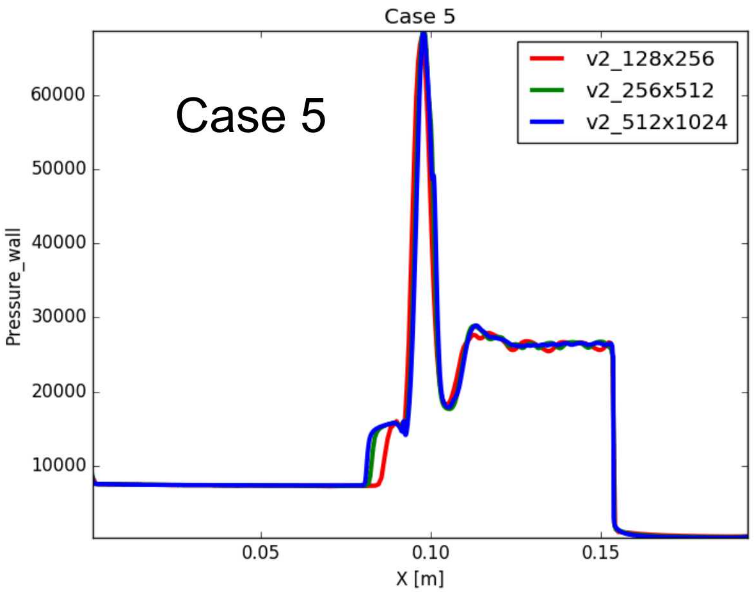
LENS XX (5sp2T) Pressure: Qualitative Solution Verification

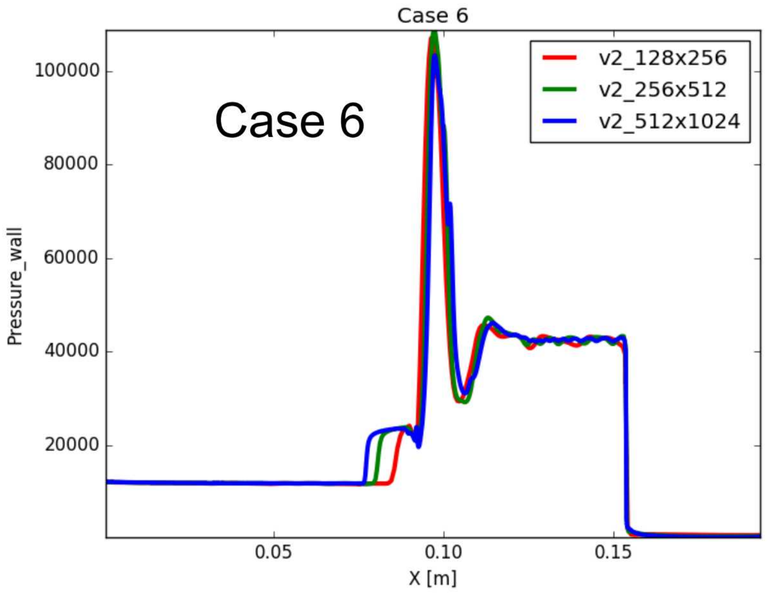
- Case 1 failed to run with 2T model
- Coarse grid oscillations on second cone go away on finer grids
- TODO use R/G/B coarse -> fine







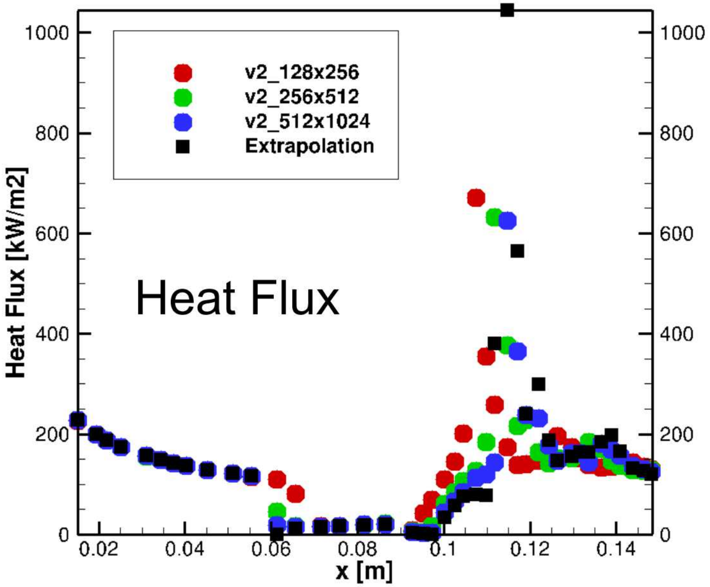


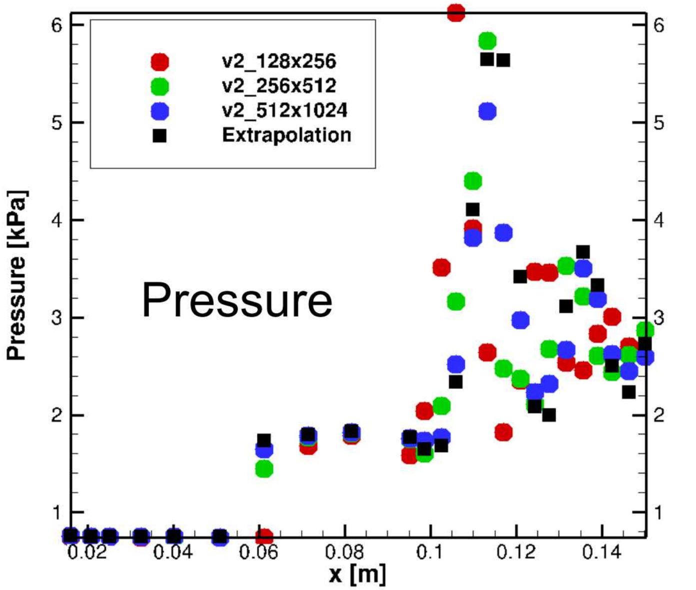


Solution Verification
LENS I Run 35 (5sp1T)

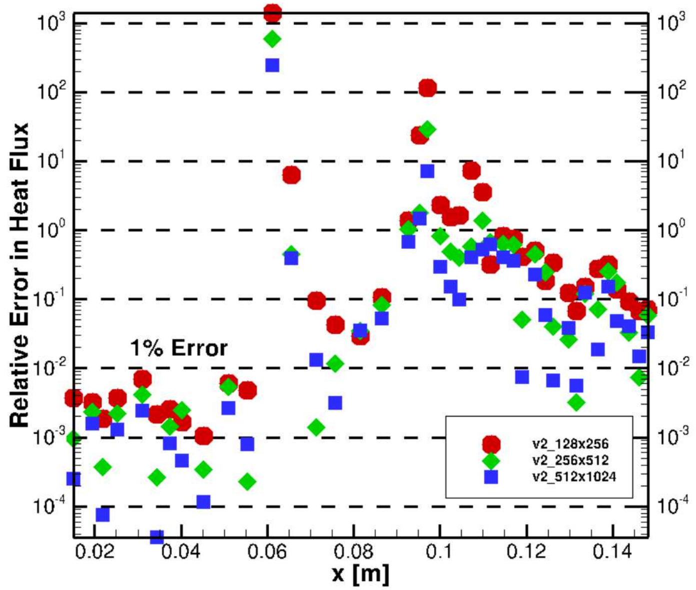
ies

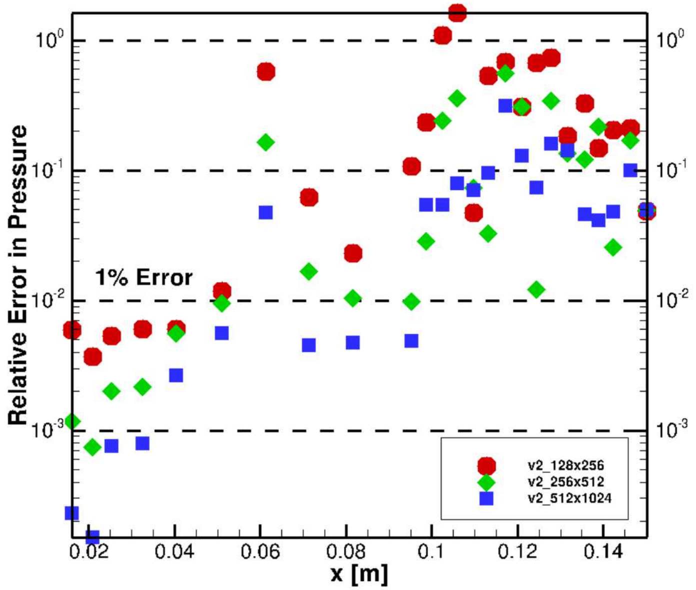
- Iterative convergence:
  - Ran 15-100 flow cycles
  - Residuals do not always converge near shocks
- Heat flux:
  - Monitor local change
  - Goal: 1e-5 tolerance
- Extrapolate QOIs using nonlinear LS extrapolation
  - bound rate of convergence within [0.5, 3]
- Errors increase with increasing position
  - first cone attached: <1% error
  - second cone errors generally >10% even on 512x1024 grid





Subtract extrapolated value to get relative errors





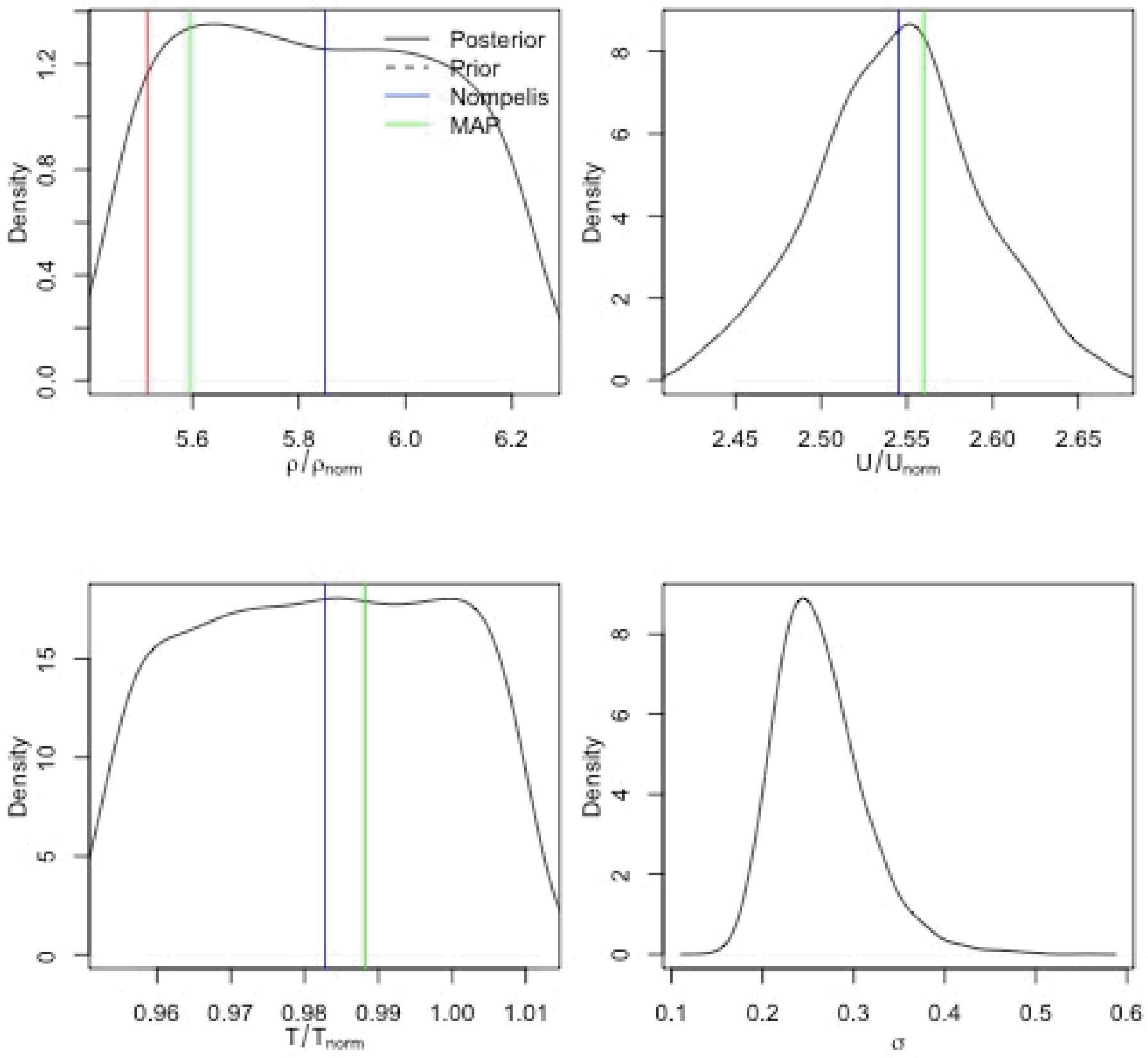
BACKGROUND SLIDES – CALIBRATION AND VALIDATION METRICS

Reproducing LENS-xx experiments

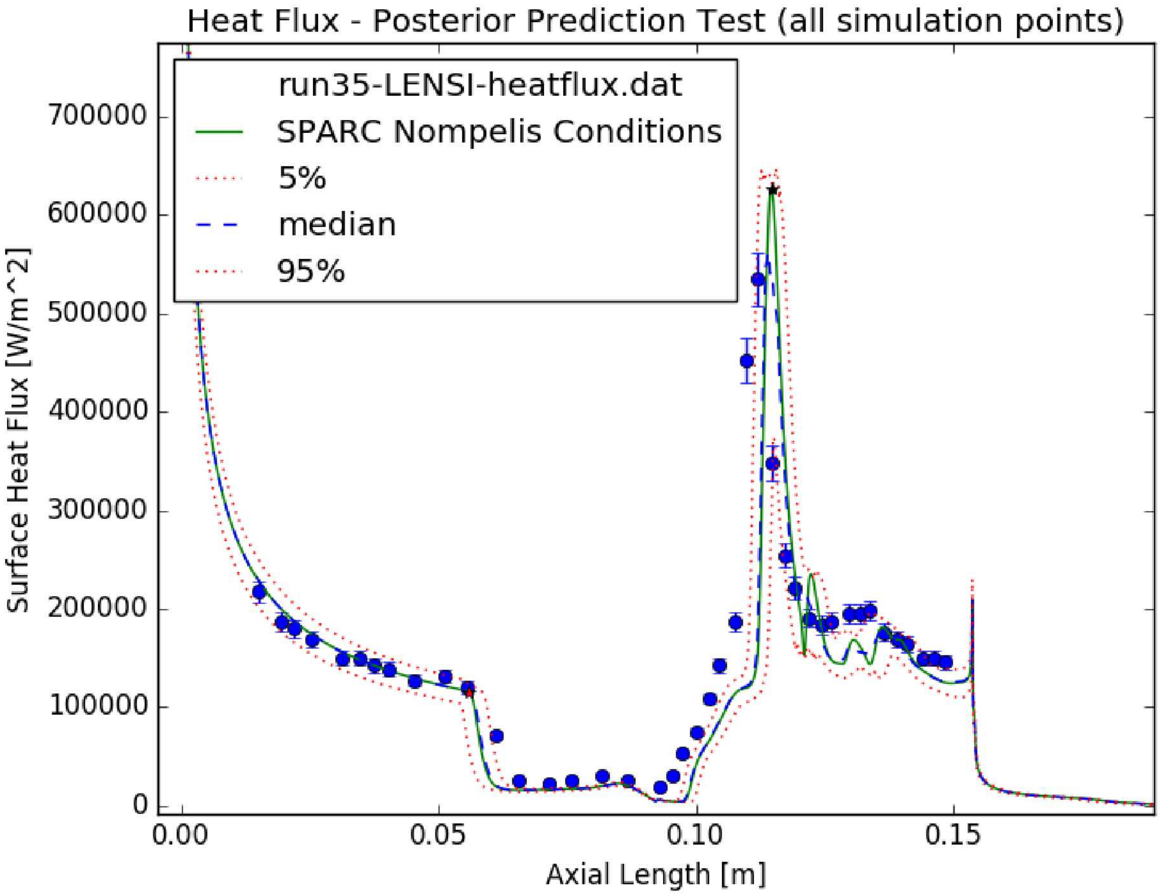
- Aim: Using (known) uncertainties in experimental freestream conditions, try to reproduce experimental measurements of pressure and heat-flux on double cone
- Result: Failed, under-predicted even when accounting for freestream uncertainties. Two possible reasons:
  - Sparc has a bug
  - Specified freestream conditions are wrong. The particular experimental group has been wrong before
- Solution: Develop an inference technique to estimate $(\rho, U, T, T_v)_\infty$ from measurements of heat flux, pressure, total enthalpy and pitot pressure
  - As a test, do so for LENS-I/run35 where we know the correct answer (Nompelis et al, 2003, AIAAJ)
  - Use measurements from the attached flow at front part of the double cone (easy to simulate)
  - Not enough measurements, so do Bayesian estimation (develop a joint PDF over the freestream conditions)
  - Test by predicting flow over the entire double cone. Do the calibrated freestream conditions bracket data?

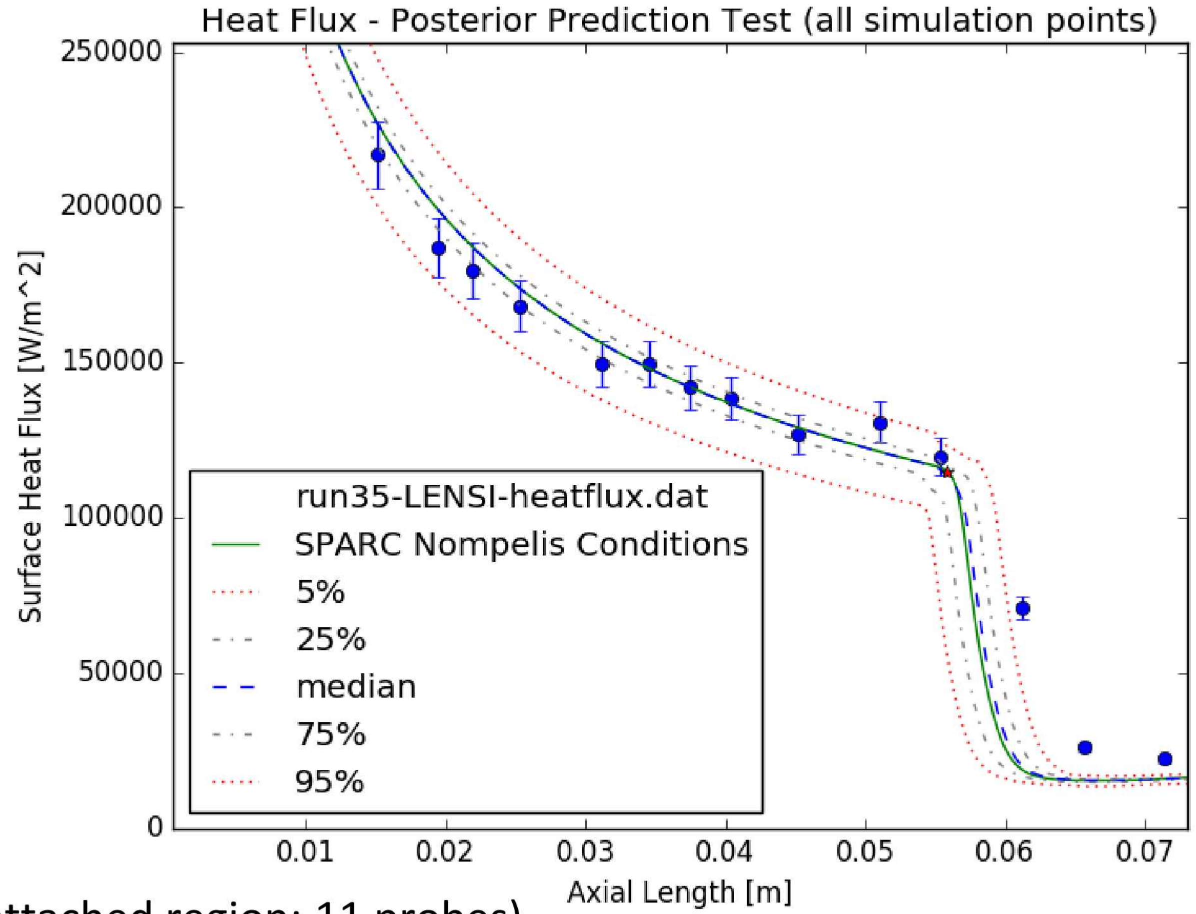
Run35 test case

- Low enthalpy case, frozen vibrational models
  - Freestream conditions: (ρ, U, T)
- Inference done with a polynomial chaos expansion surrogate of sparc
  - Needed ~ 100 sparc runs to construct
- Bayesian inference using Markov chain Monte Carlo sampling to construct a 3D posterior PDF over (ρ, U, T)
  - Also estimated a mismatch between observations and predictions, modeled as N(0, σ^2)
  - Needed ~50,000 invocations of sparc surrogate
- Test:
  - Sample 100 (ρ, U, T) from posterior, recreate pressure and heat flux measurements. Do we bracket observations?



Heat flux predictions

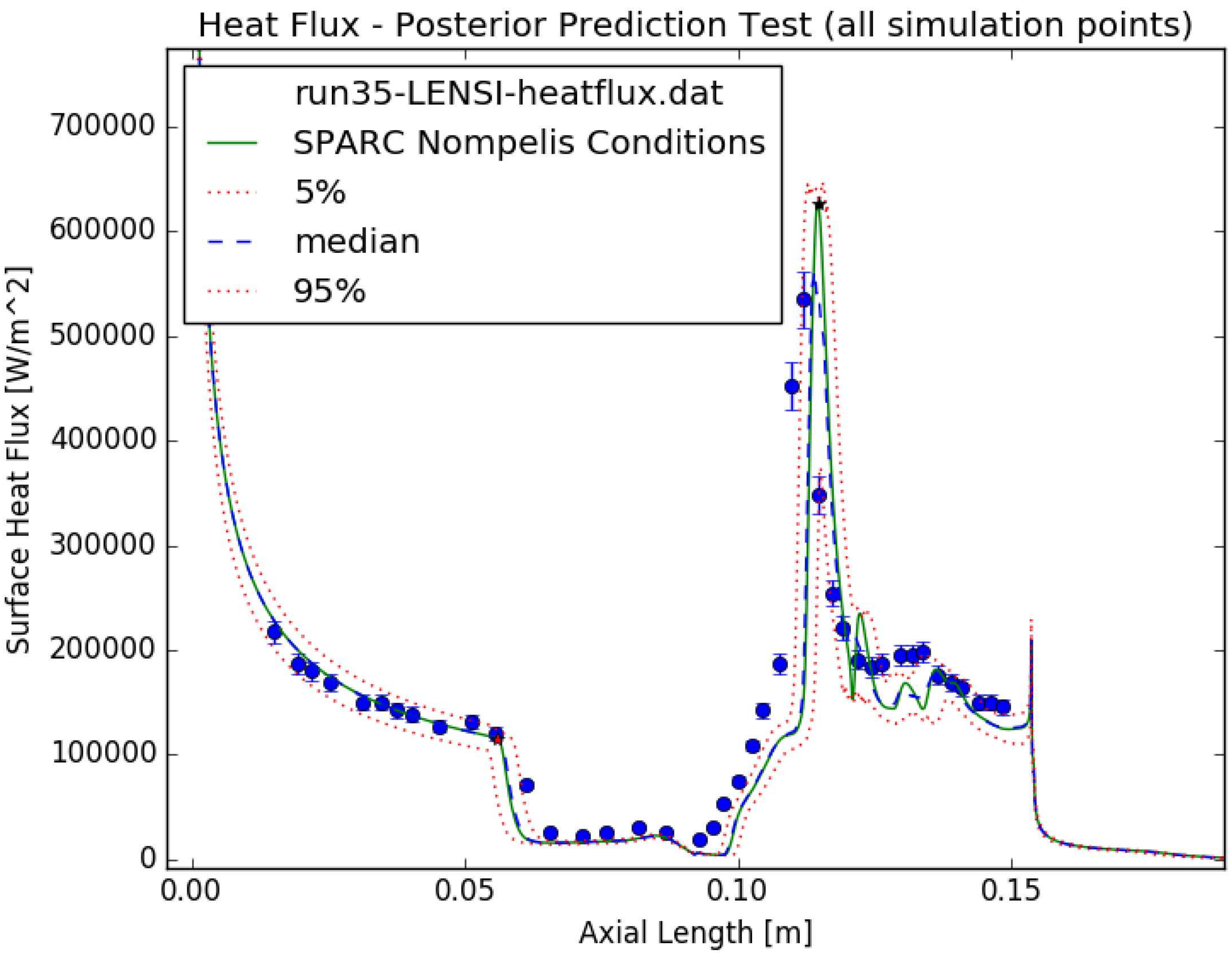




- $5^{th}/95^{th}$ percentiles contain measurements (attached region; 11 probes)
- But we don't do well after detachment
- SPARC simulations all with "finer" mesh v2_512x1024

Pressure

- Very good results for attached region
  - Matched Nompelis et al, AIAAJ 2003 everywhere
  - Also, uncertainty bounds much better if you use SPARC, not its emulator
- Not so good post re-attachment
  - Mesh: 512x1024
  - Flow-through times:
    - Body = 0.15 meters
    - Velocity = 2545m/s
    - Flow over time = 0.15/2545 = 5.6e-5 sec
    - Time run = 1.1e-2 sec
    - Flow-through times = 0.196e+3 = ~196 flow-through times
  - So, bad match post re-attachment is NOT due to lack of temporal convergence



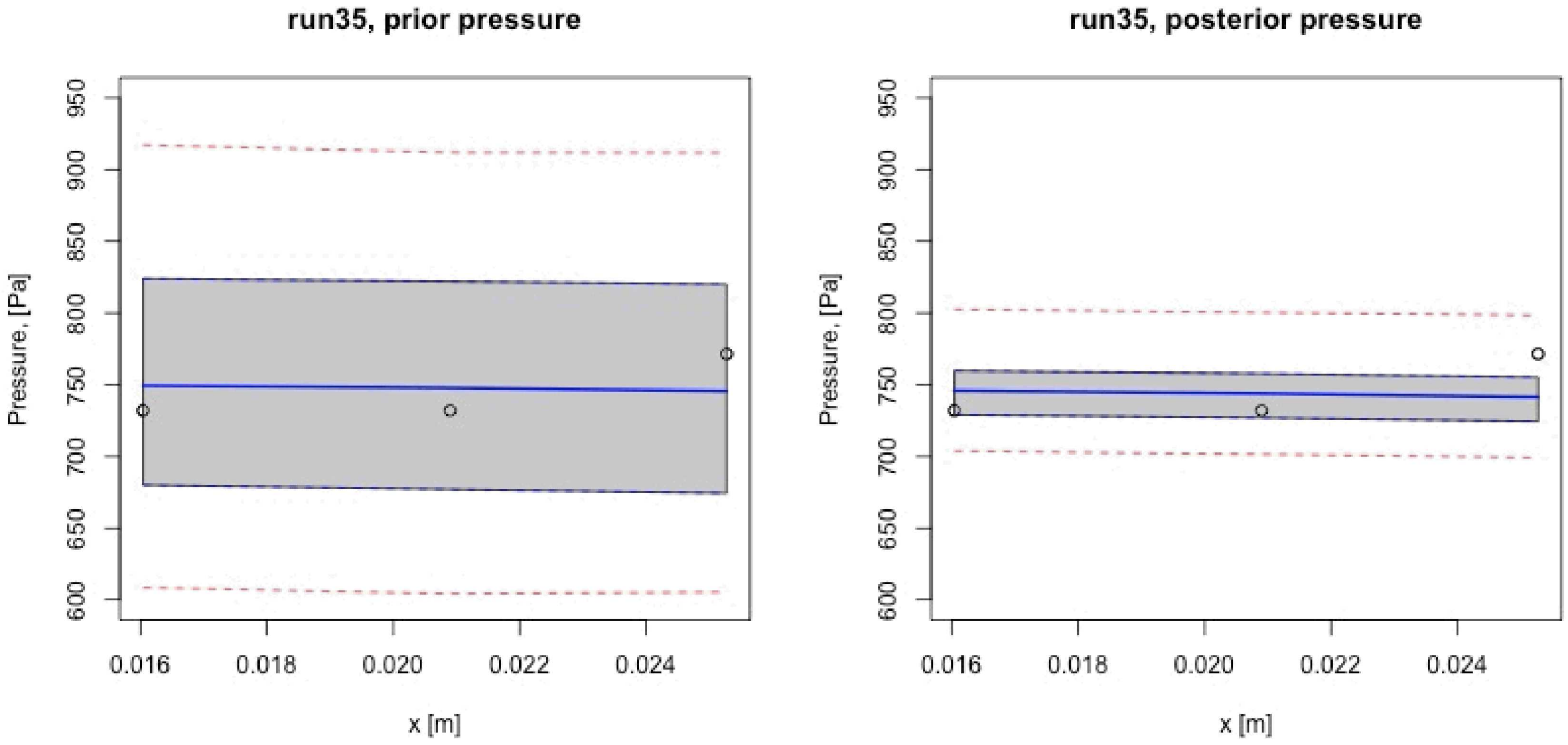
SPARC simulations all with “finer” mesh v2_512x1024

Comparison and what next?

- Compare our predictions (MAP value) to CUBRC's freestream conditions, and Nompelis's.
  - Better agreement with Nompelis – and we reproduce observations
- Next steps
  - Redo inference using gradient-based optimization; use sparc, not its surrogate
    - Uses gradients & sensitivities encoded in sparc, not finite-differences
    - Still, very computationally expensive
  - Perform Bayesian inference of freestream conditions for medium- and high-enthalpy experiments from LENS-xx
  - Assess: Do we need freestream inference at all? Is CUBRC correct?

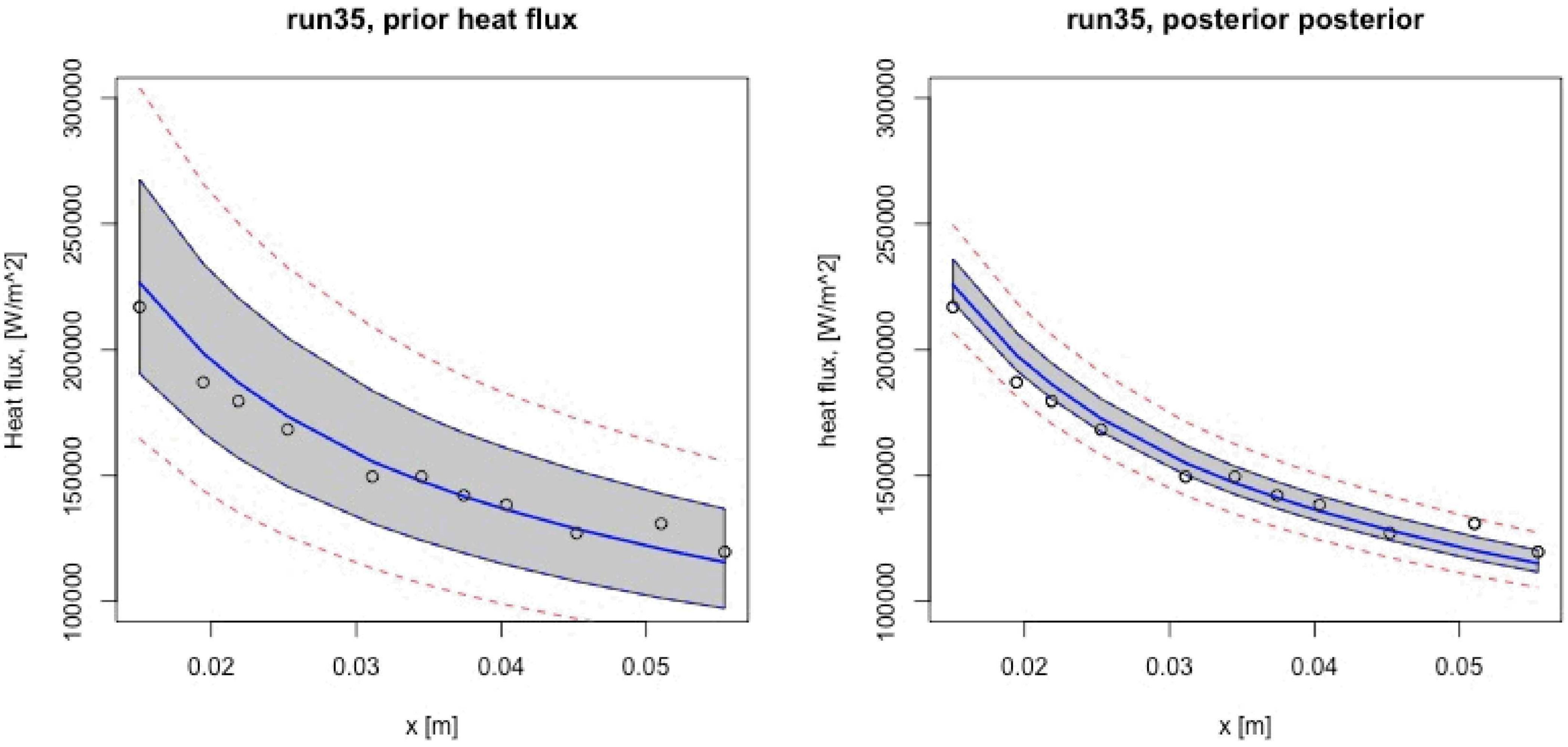
	Density (kg/m3)	U (m/s)	T (K)
CUBRC	5.515e-4	2713	138.9
MAP	5.595e-4	2.56e+3	98.82
Nompelis [non-eq]	5.845e-4	2.545e+3	98.27

Comparing prior and posterior predictions - pressure



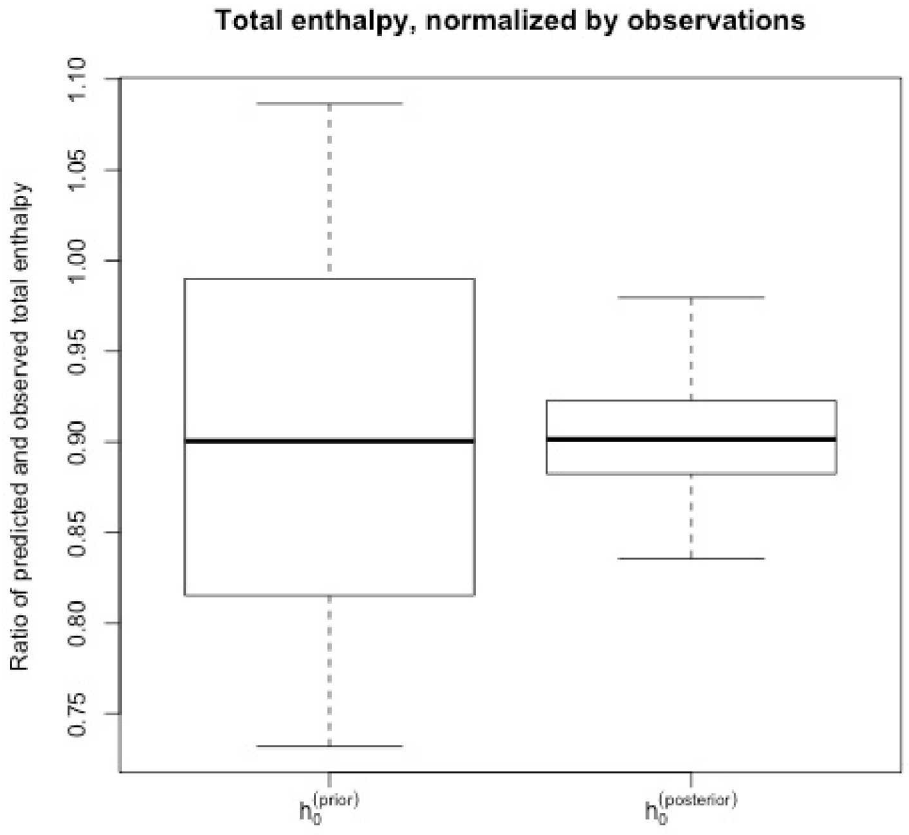
- Tightens up pressure prediction – assimilating experimental data helps

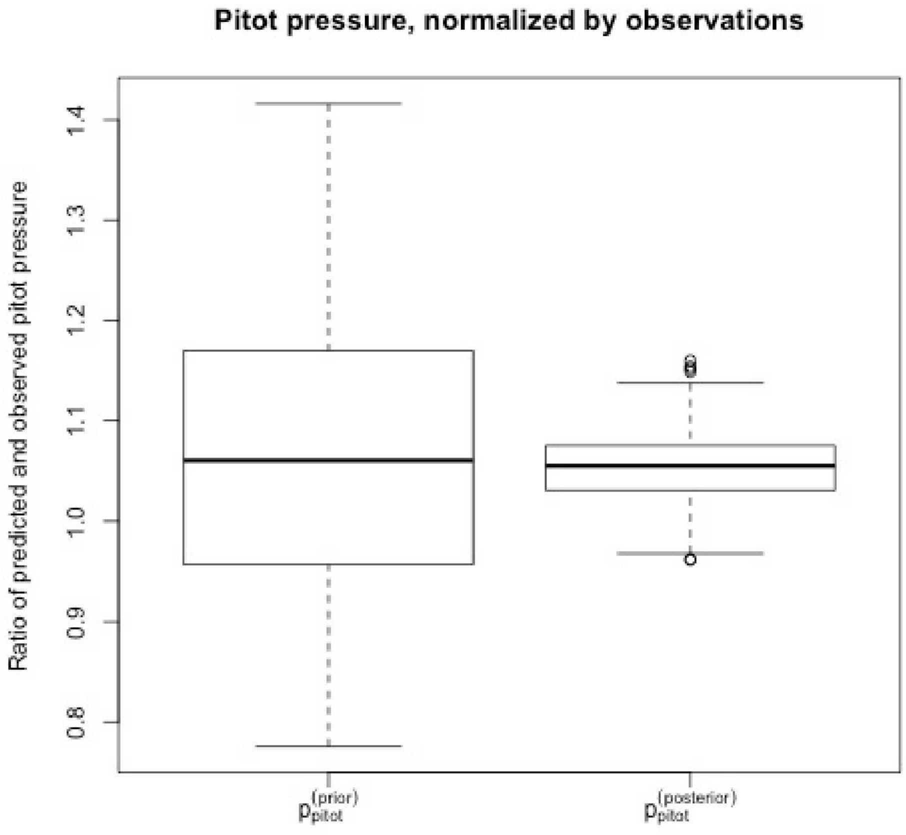
Comparing prior and posterior predictions – heat flux



- Tightens up q prediction – assimilating experimental data helps

Comparing prior and posterior predictions – h_0 & P_{pitot}





- Under-predicting h_0
- Over-predicting P_{pitot} slightly

Validation Metrics and Assessment

- Preliminary results: Four metrics to compare uncertain predictions with observations.
- For "certain" observations:
  - Verification Rank Histogram
  - Continuous Ranked Probability Score- crps(x)
  - Function of spatial location
  - Summarize with scalars:
    - RMS deviation (VRH)
    - CRPS = mean crps(x)
- For uncertain observations:
  - Hellinger distance
  - Sorensen distance

CRPS = mean(crps(x))
Uniform : 72.77e+3 W/m^2
Normal : 76.83e+3 W/m^2