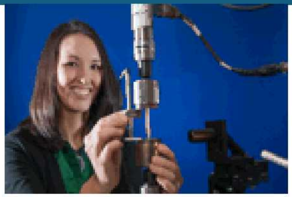
SAND2019-0210C

Validation Assessment of Hypersonic Double-Cone Flow Simulations using UQ, Sensitivity Analysis, and Validation Metrics



S. Kieweg, J. Ray, V.G. Weirs, B. Carnes, D. Dinzl, B. Freno, M. Howard, E. Phipps, W. Rider, and T. Smith

January 11, 2019. AIAA SciTech 2019.

Contact: skieweg@sandia.gov

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SAND2019-####C. UUR.

Hypersonic Simulations: Applications and QOIs

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

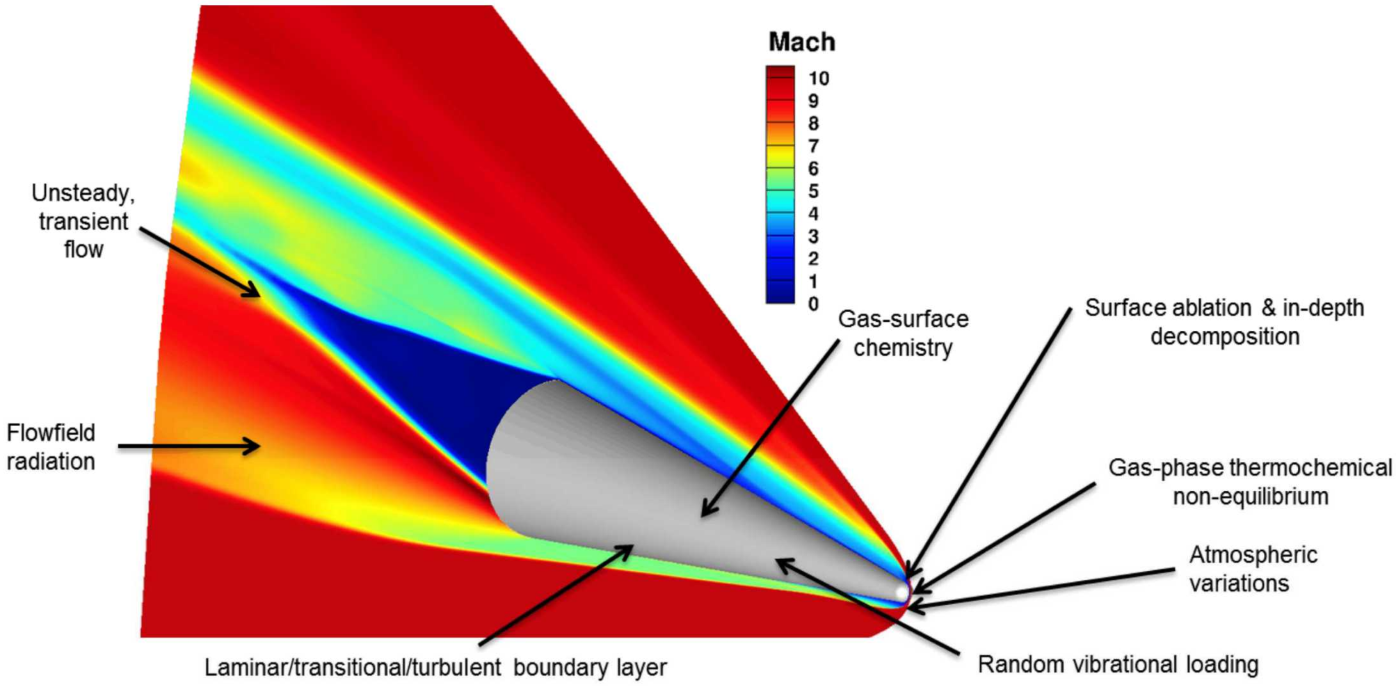
Atmospheric reentry of flight vehicles:

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

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

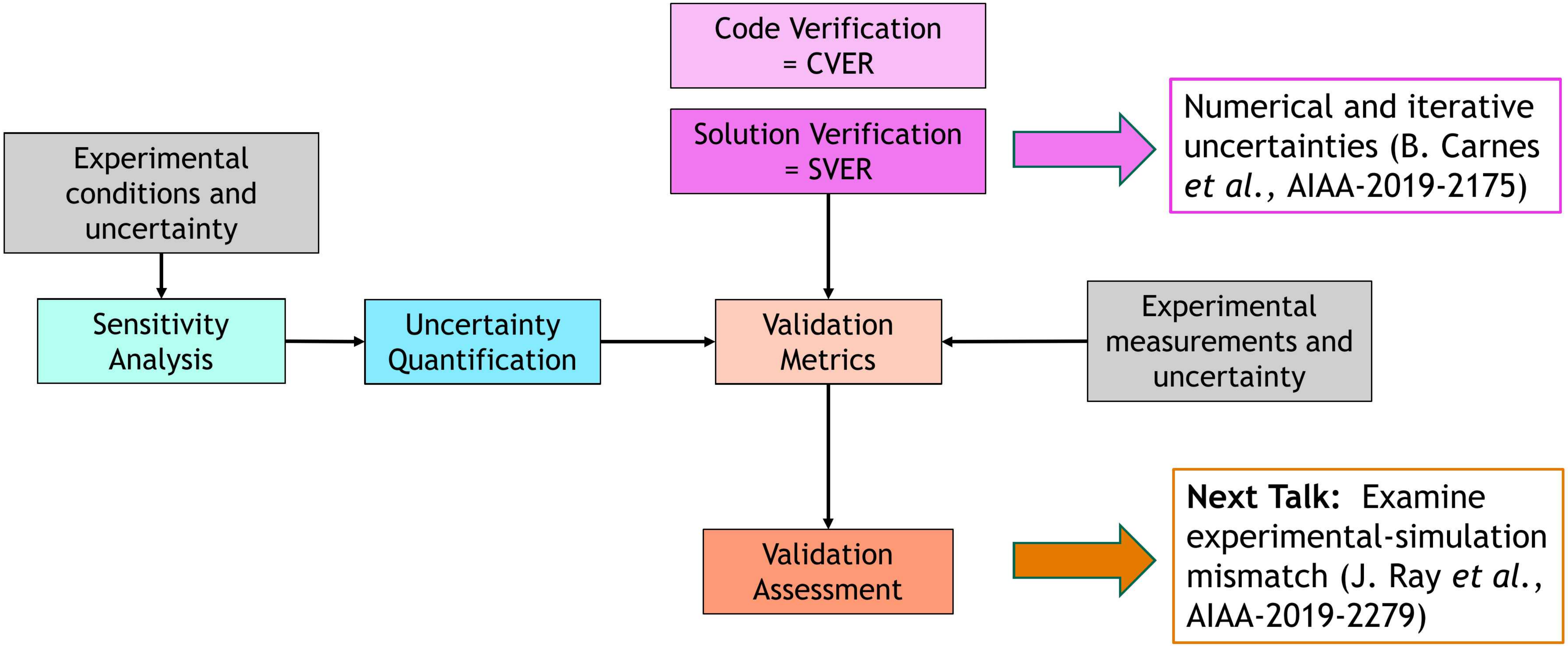
Quantities of Interest (QOIs) from experiments and simulations:

- Heat flux at surface
- Pressure on surface
- Separation length, separation point, and reattachment point



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

Approach: Verification & Validation / UQ Workflow



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

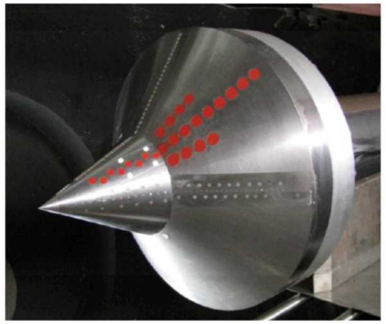
Validation Data: Double Cone (LENS XX)

LENS XX at CUBRC: Case 1 and Case 4

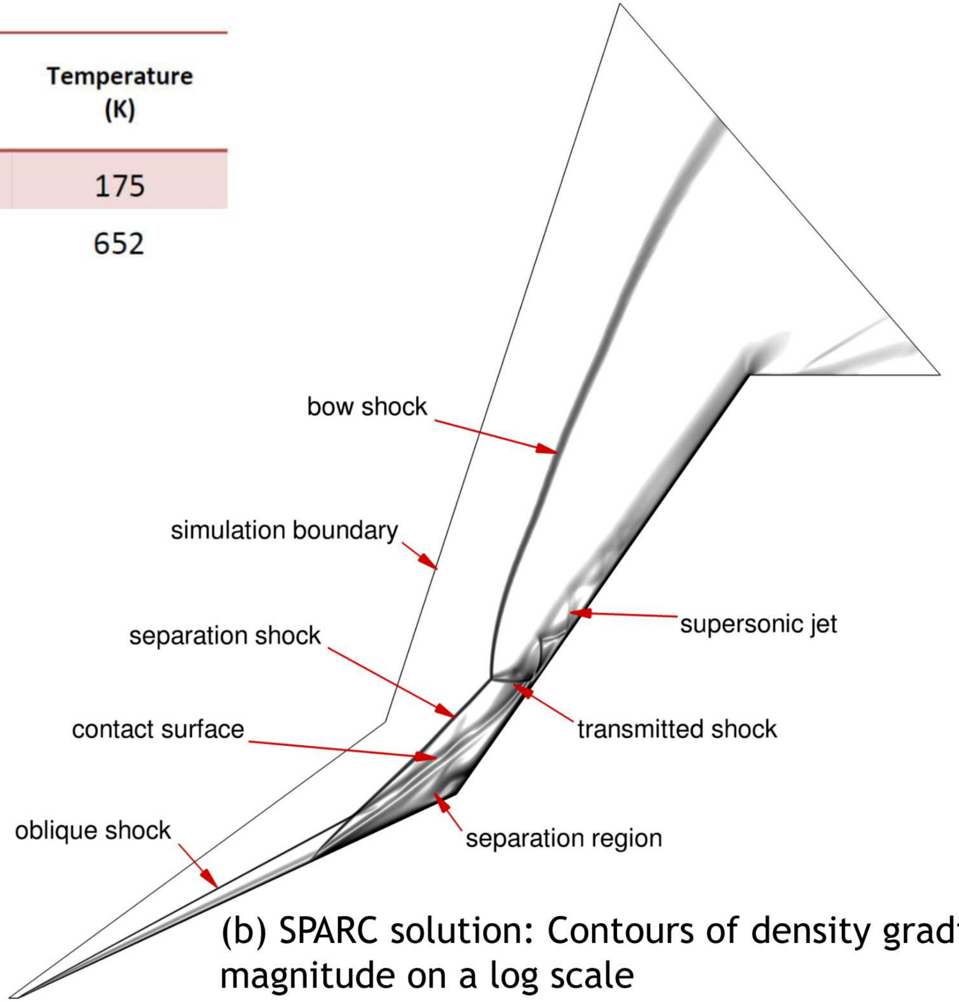
Run #	Total Enthalpy (MJ/kg)	Mach Number	Pitot Pressure (kPa)	Unit Reynolds Number /10⁶ (1/m)	Velocity (km/s)	Density (g/m³)	Temperature (K)
1	5.44	12.2	5.1	0.14	3.246	0.499	175
4	21.77	12.82	39.5	0.20	6.497	0.964	652

LENS XX data set provides a focus on **laminar flow** of an air mixture with **strong** thermochemical non-equilibrium.

The flow has interesting features in the shock – boundary layer interactions.



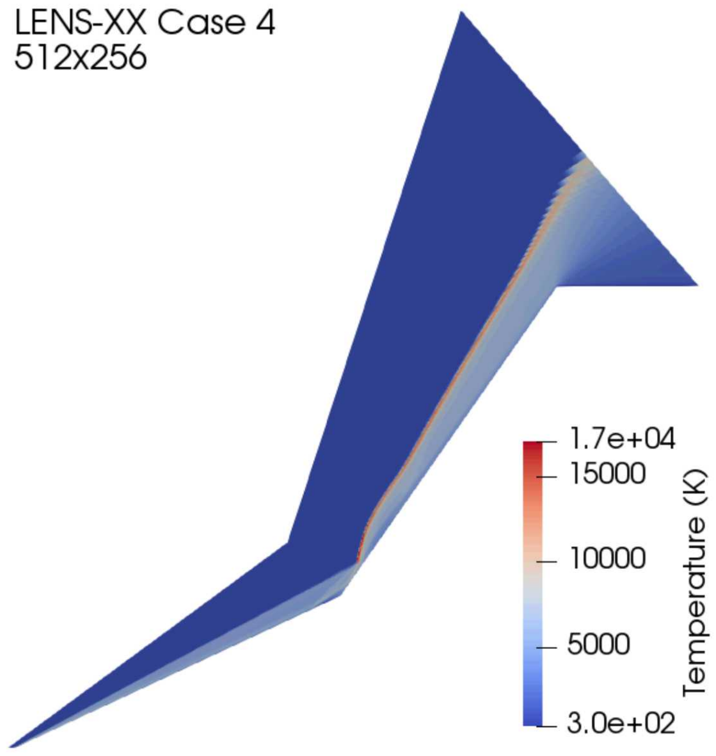
(a) Double cone photograph with sensor locations

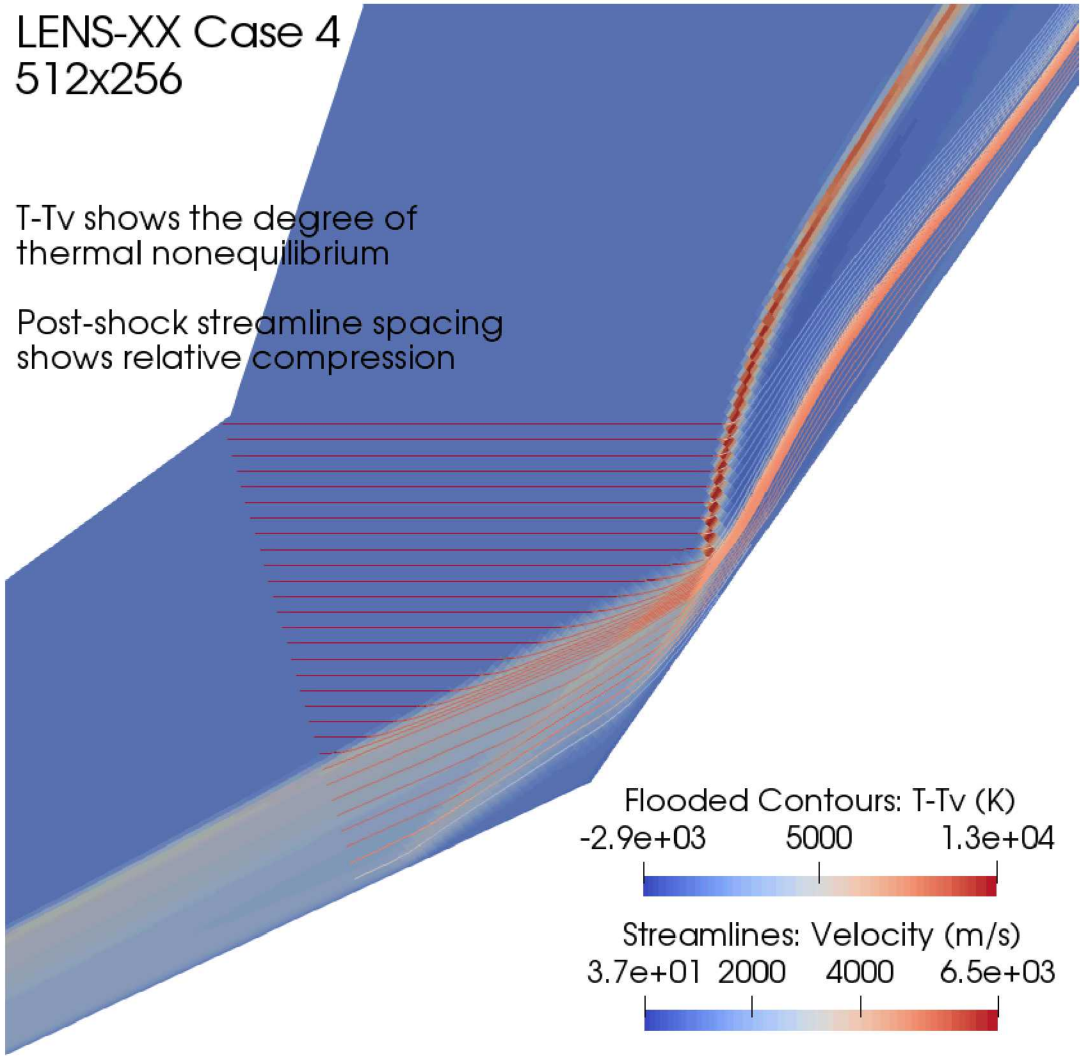


(b) SPARC solution: Contours of density gradient magnitude on a log scale

IMAGE (b) : SPARC solution of Run 35 (LENS I) by Derek Dinzl. Shown here to demonstrate phenomena. TABLE and image (a): MacLean *et al.*, 2014.

Example Flow Field: LENS XX Case 4





- Free stream BC: density (ρ), velocity (u), temperature (T), vibrational temperature (T_v)
- Outflow BC: Neumann
- Cone surface: Dirichlet (T, T_v), no slip

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 as a reference:

- Laminar, **single** species, **mild** thermochemical non-equilibrium.
- Nompelis *et al.* – used 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)

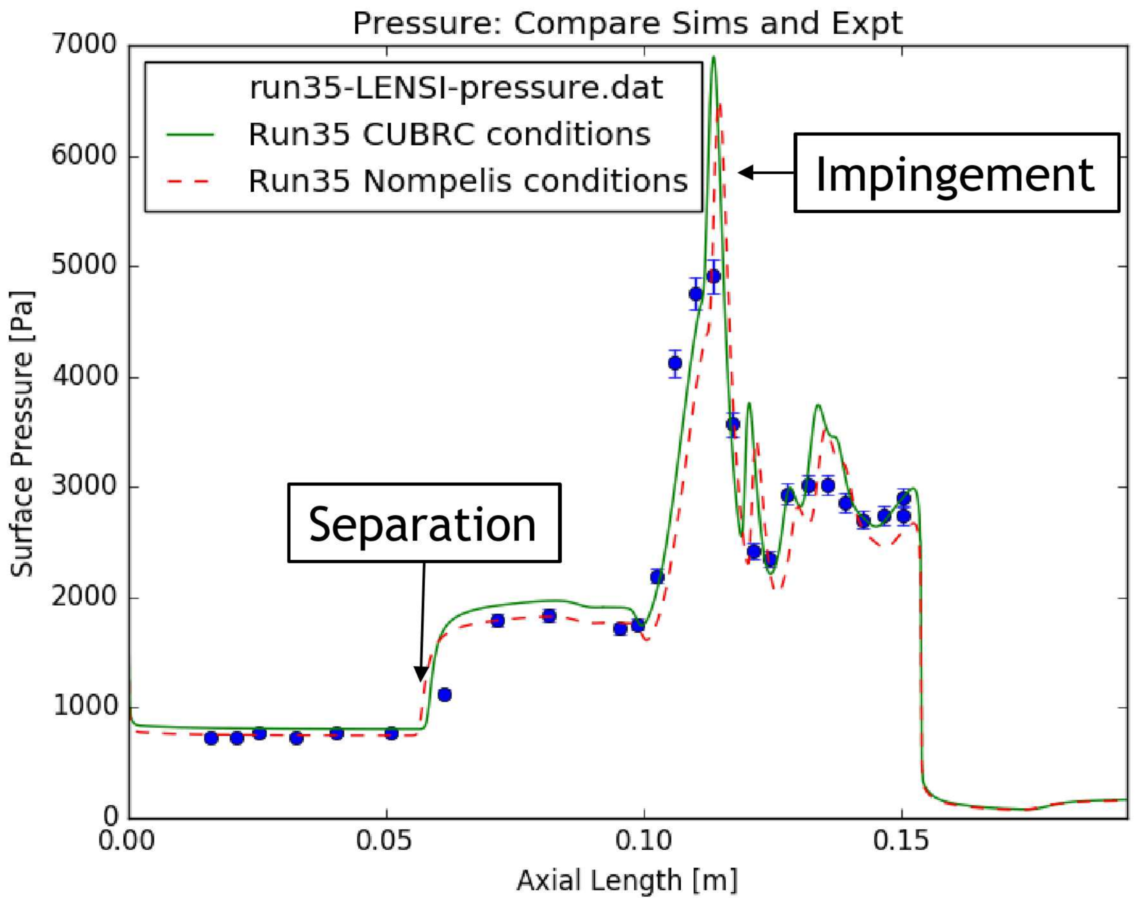
Table 1. Free-stream and wall conditions for Run 35 from Nompelis et al. 2003.

	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
$T_{\rm wall}$	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: Challenges with Freestream Conditions



Ioannis Nompelis *et al.*'s estimate of nonequilibrium freestream conditions improved predictions of heat flux in the attached region in Run 35.

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.

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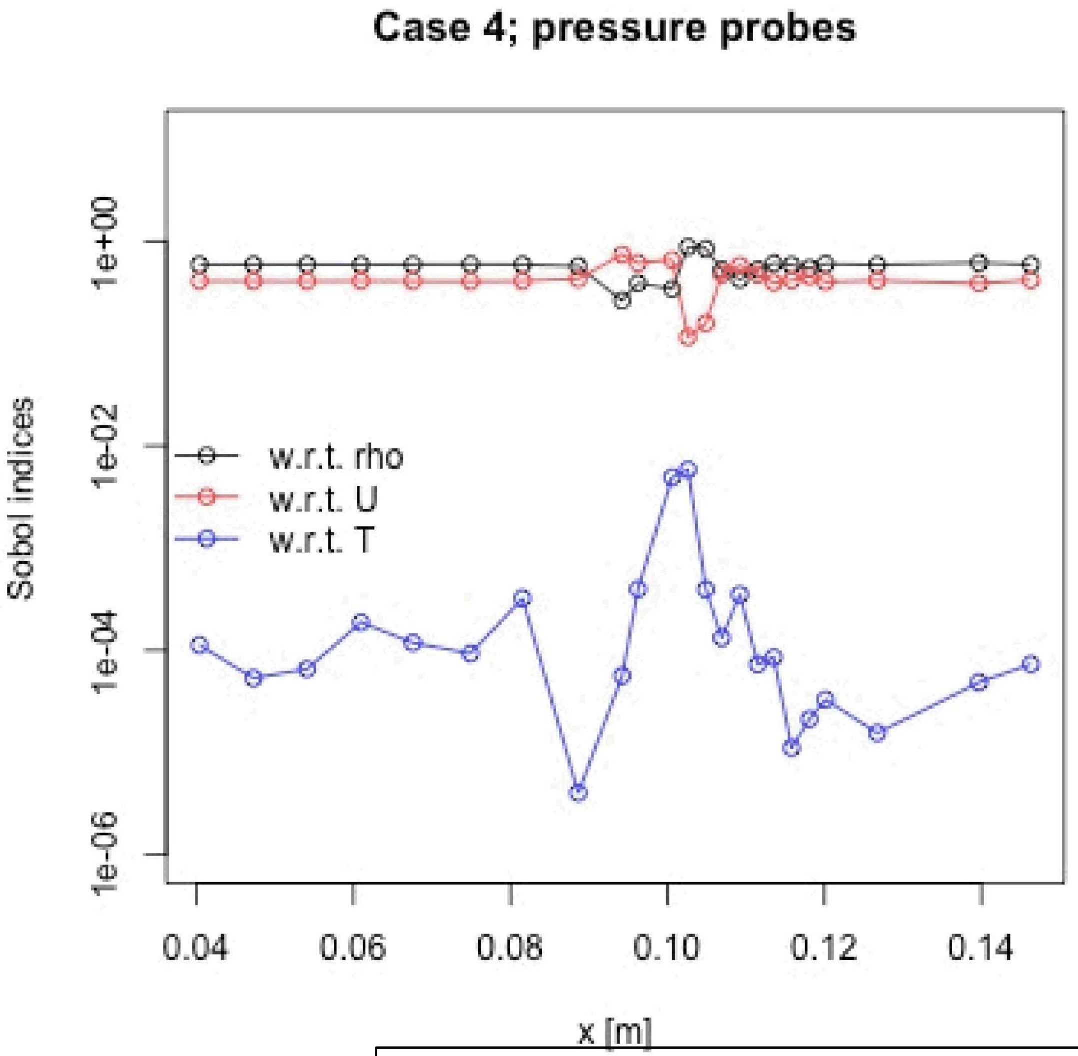
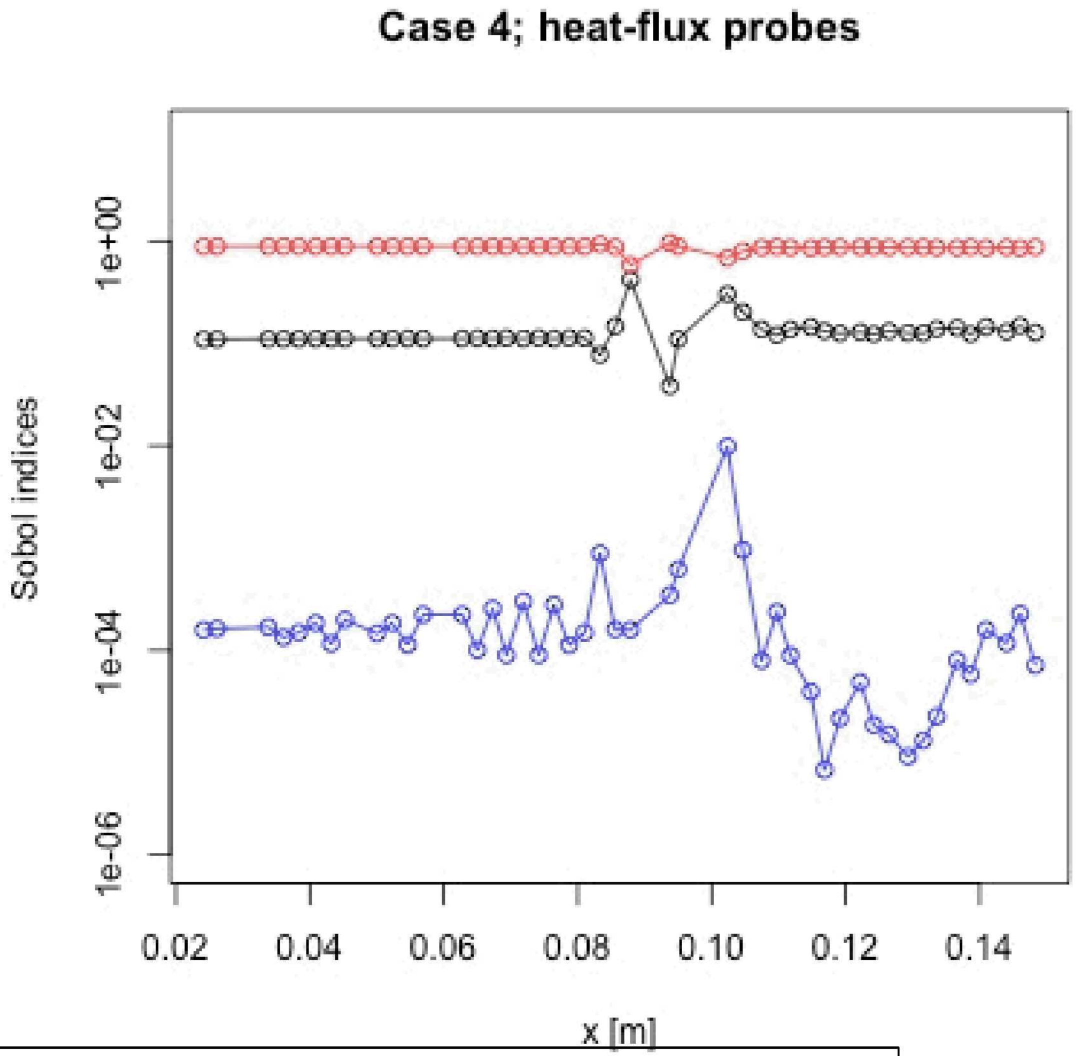
u_∞	2713	m/s	2545	m/s
T_{wall}	296.1	K	296.1	K
c_{N_2}	1.0		1.0	

NOTE: Experiment error bars, as provided by CUBRC: heat flux +/- 7 %, pressure +/- 5%.

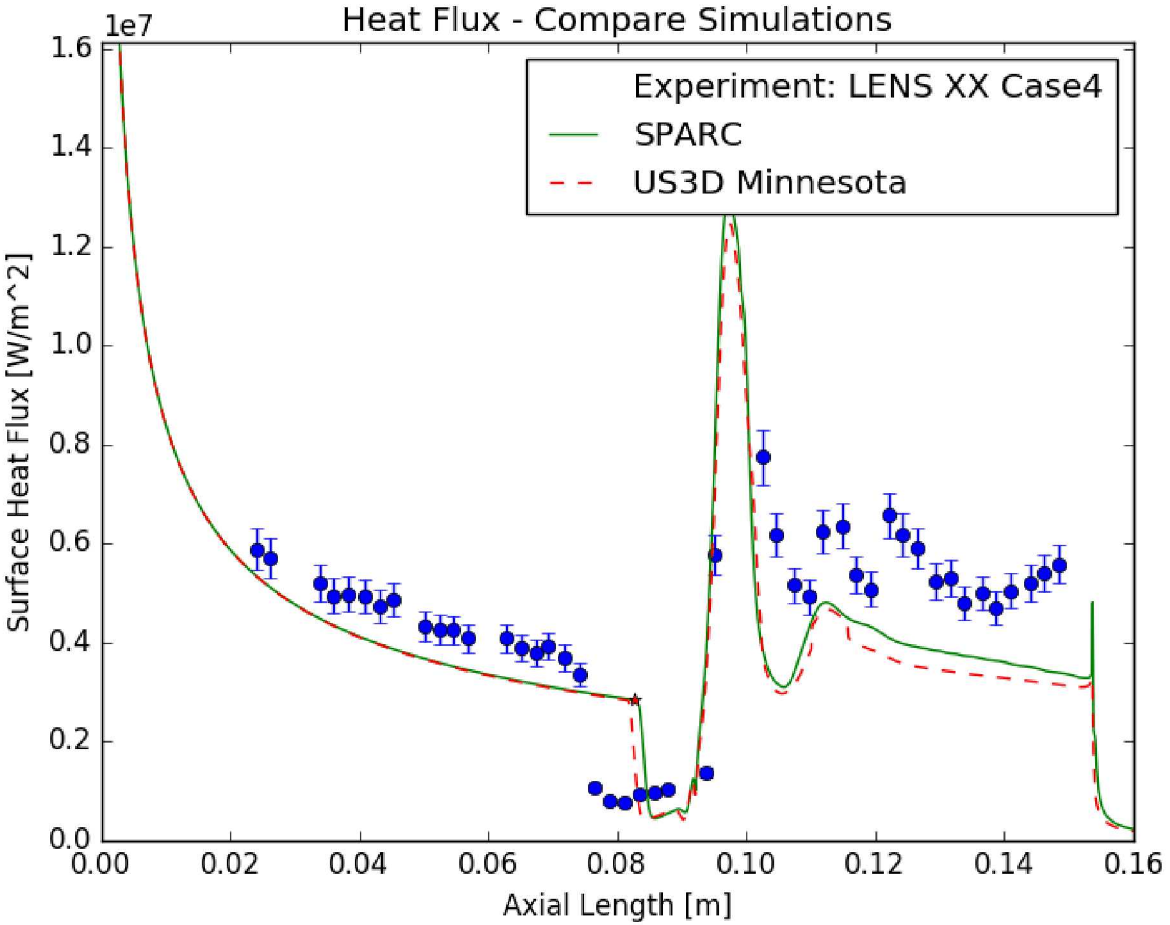
Global Sensitivity Analysis: Sobol' Indices from Propagation of CUBRC-provided Uncertainties

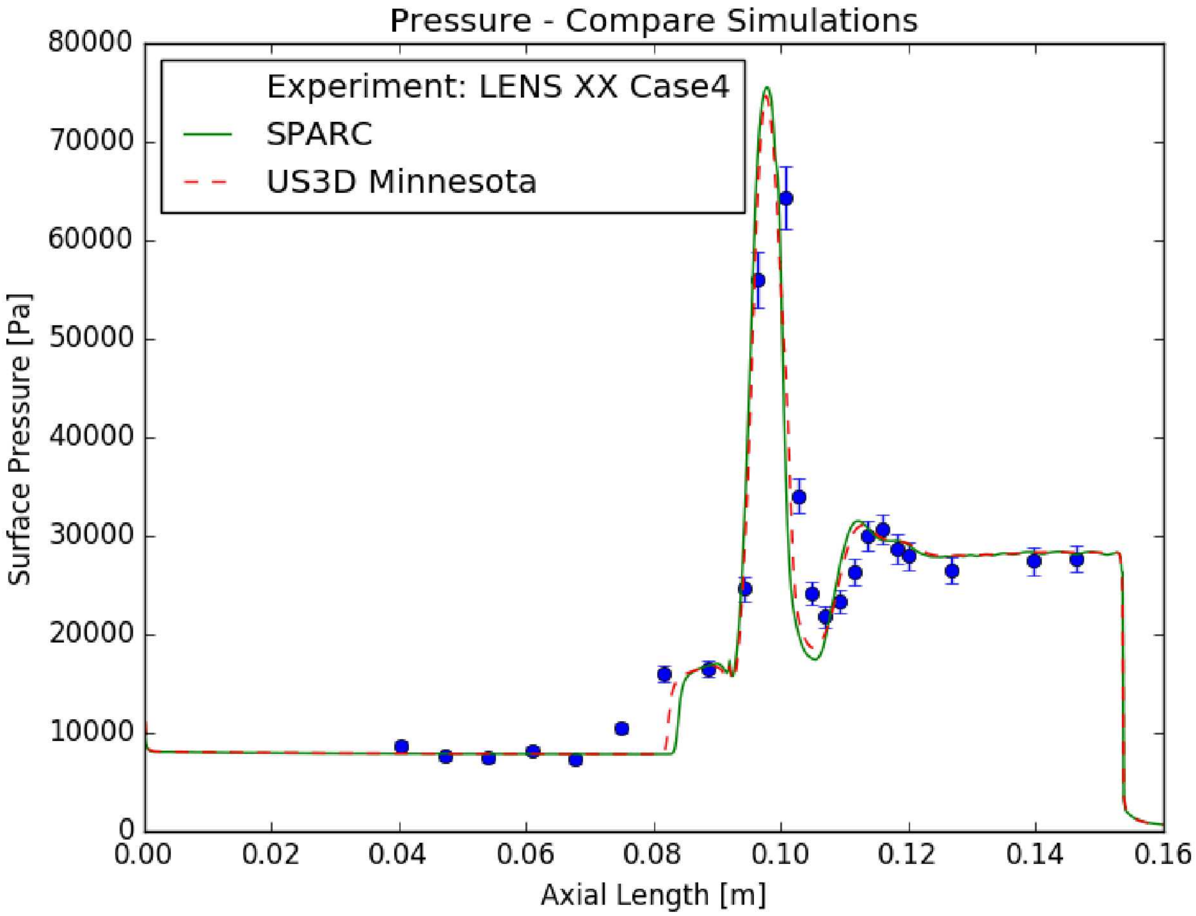




For heat flux: Freestream velocity (u) has the most influence; freestream temperature (T) has the least influence.

Validation Assessment
(Example with Double Cone LENS XX Case 4)





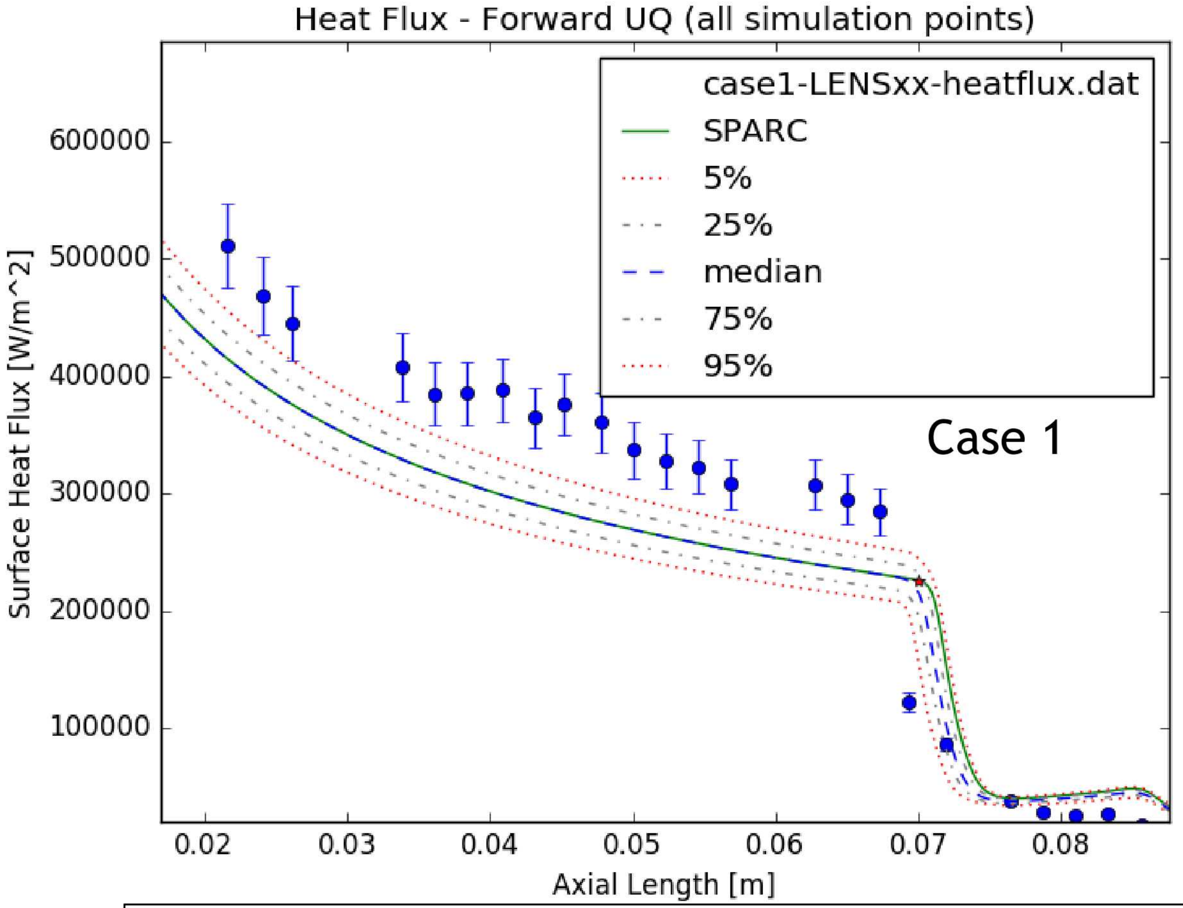
Compares to US3D. Next: does consideration of free stream uncertainty bracket experiments?

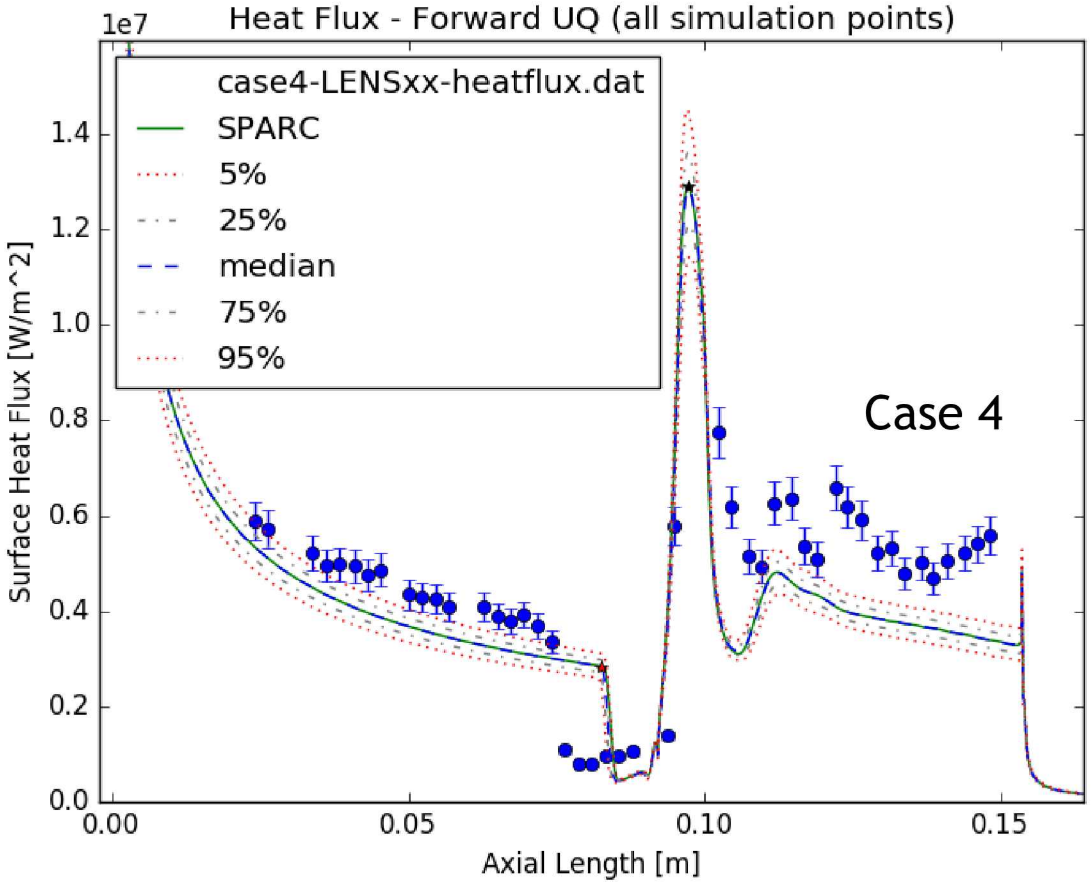
NOTE: SPARC simulations use "finer" v2_512x1024 mesh, 50000 iterations; US3D used same size mesh and similar iterative convergence. Expt error bars: heat flux +/- 7 %, pressure +/- 5% per CUBRC.

Validation Assessment **with** UQ

Forward Propagation of Uncertainty → parametric (input) uncertainty

(Forward propagation of uncertainty ensembles using Dakota w/ PCE surrogate built from SPARC runs.)

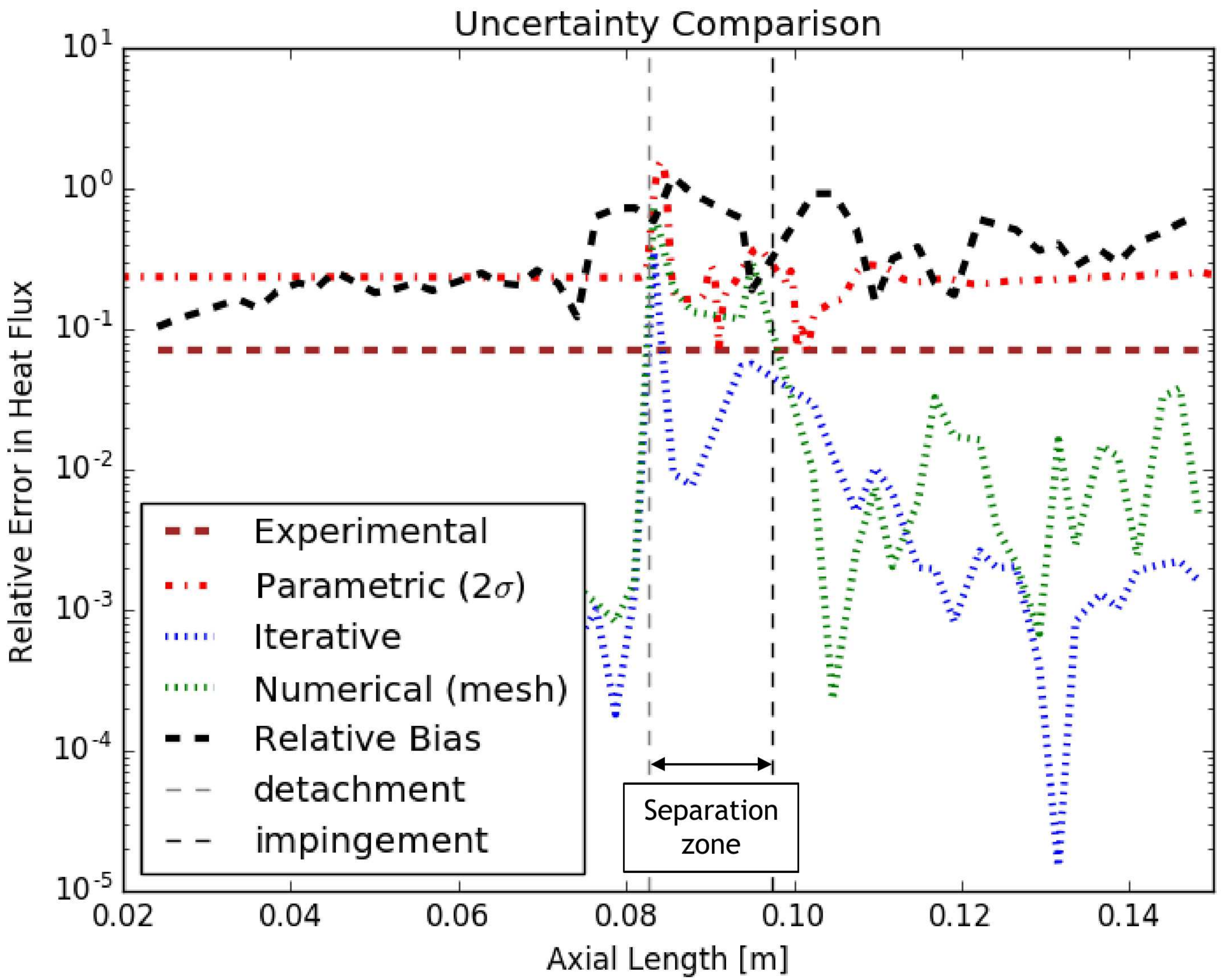




Using CUBRC-provided freestream uncertainties, we cannot bracket experiments.

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

Relative Contributions of Uncertainty (Case 4)



- Define overall uncertainty (u_{val}) using the four uncertainty contributions:

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

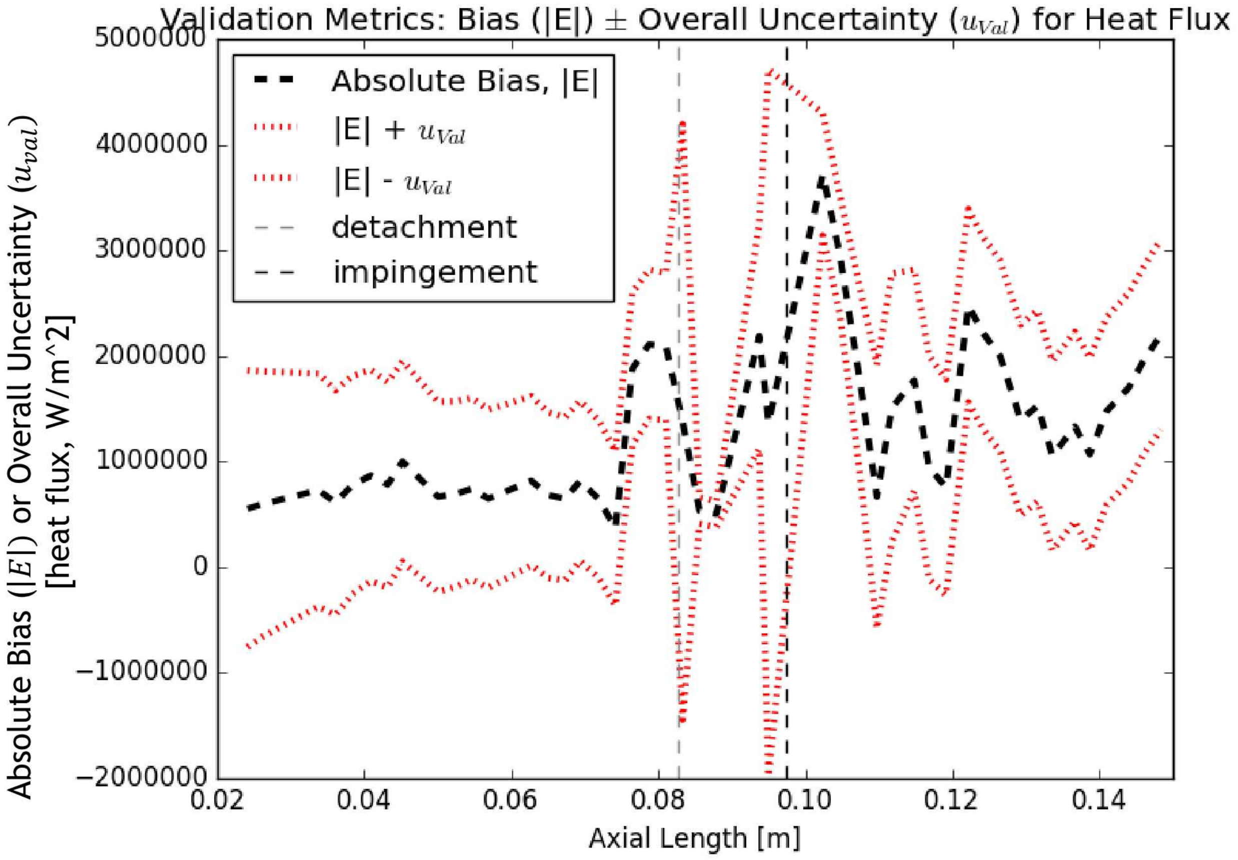
$$u_{\text{val}} = (u_{\text{val, rel}})(\text{median})$$

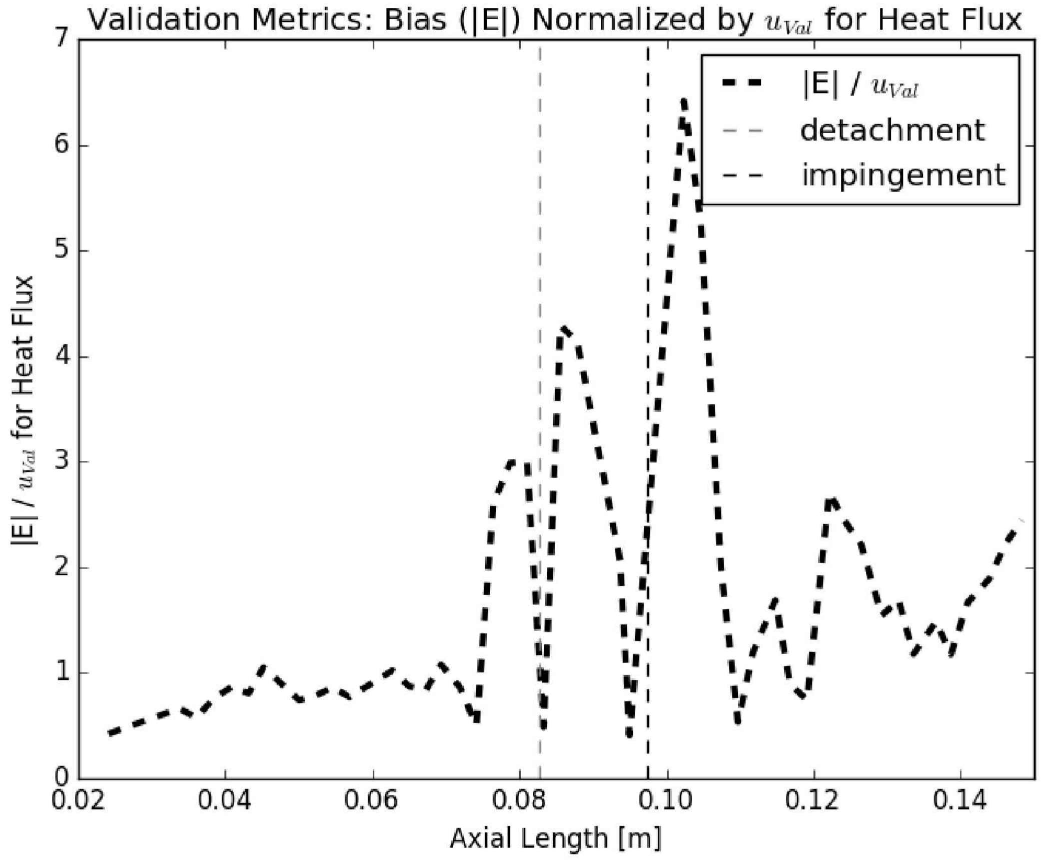
- **Numerical** and **iterative** uncertainties are much less than **parametric** uncertainty in most regions, except:
  - Detachment point
  - Separation zone

- The dominant contribution to the overall uncertainty (u_{val}) is from the **parametric** uncertainty due to freestream conditions.

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

Validation Metrics: Bias ($|E|$) and Overall Uncertainty (u_{val}) (Case 4)





In some regions, the overall uncertainty is large relative to the bias, i.e. (bias/unc)< 1.
How can we reduce uncertainties, and which ones?
Lack of information and larger uncertainties reduce our ability to discern source(s) of mismatch.

Validation Metrics

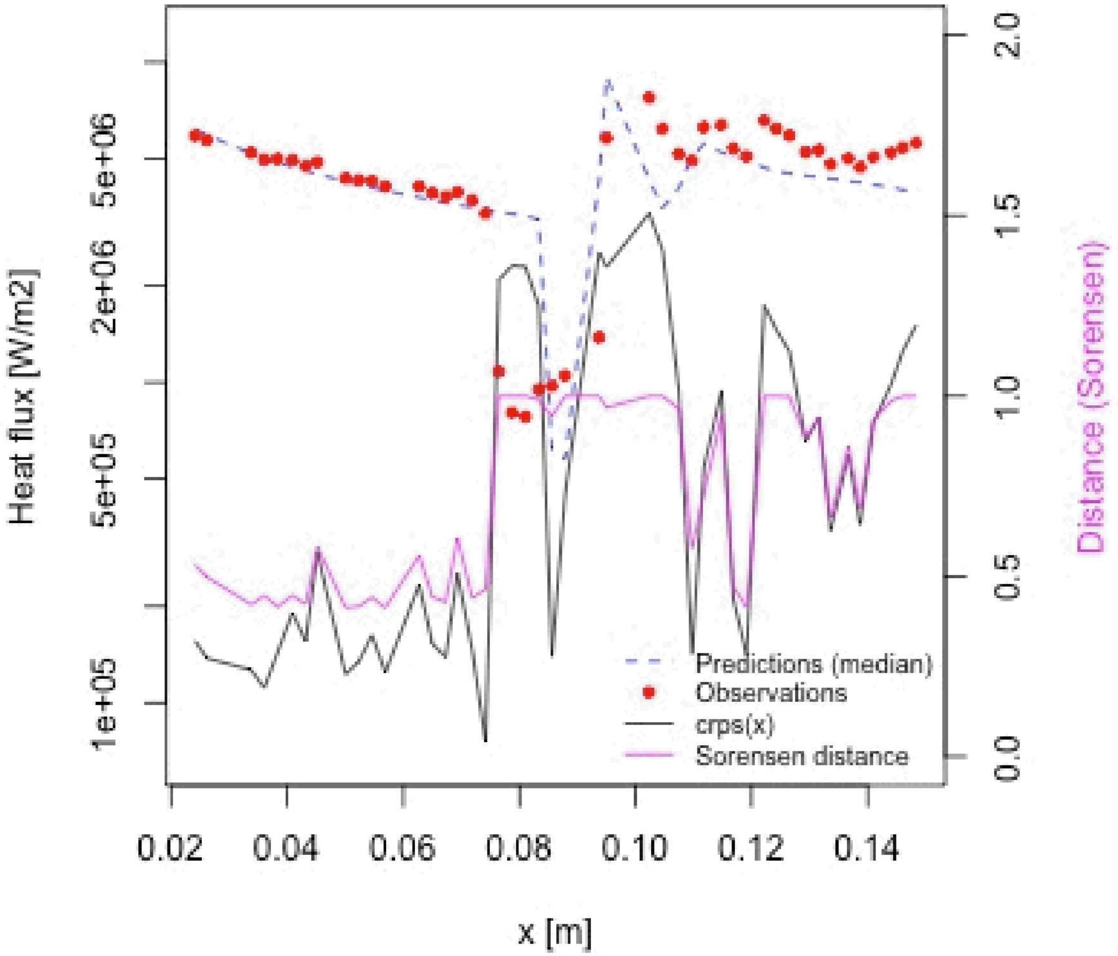
Consider “Certain” Experimental Observations:

- CRPS = Continuous Ranked Probability Score
- Represents distance between uncertain prediction and “certain” observation.
- Same units as the quantity of interest.
- Smaller values reflect closer match between simulation and experiment.

Consider Uncertainty of Experimental Observations:

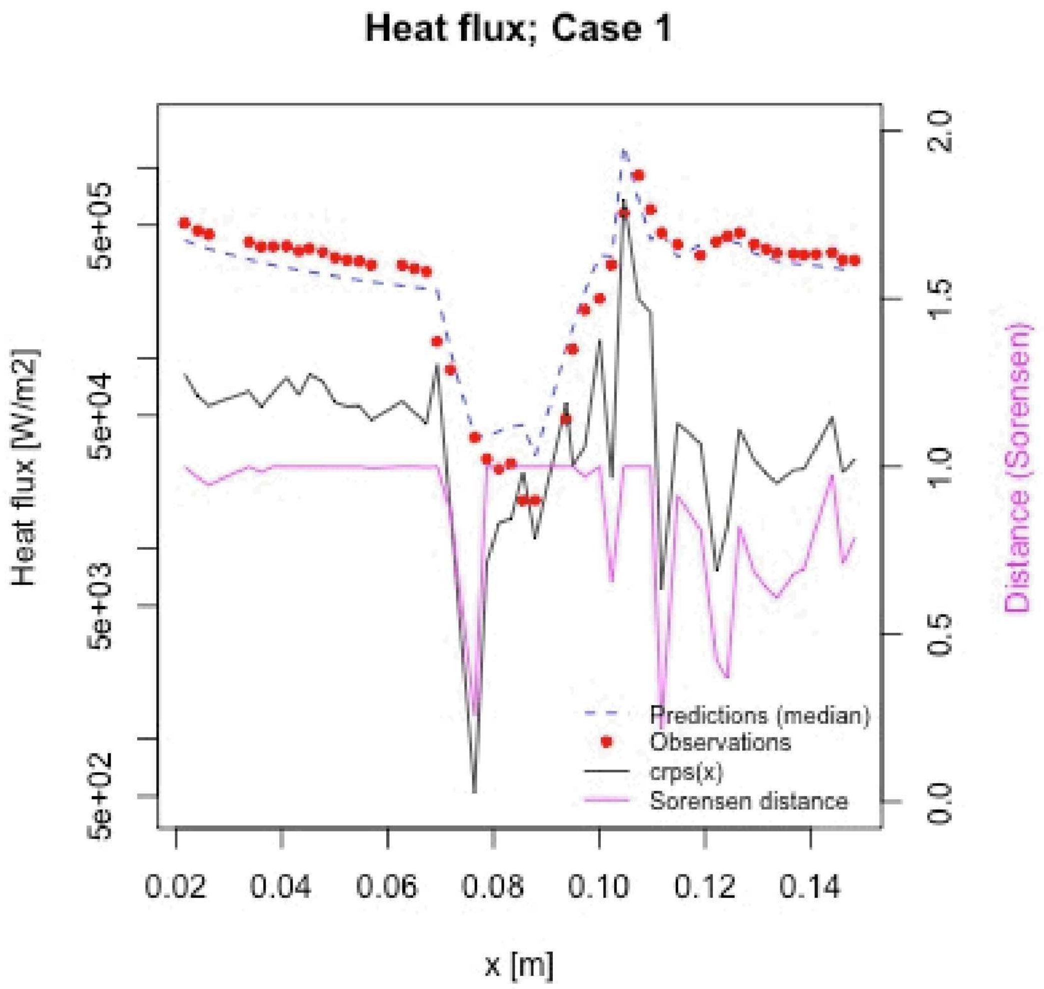
- Heat flux measurements have 7% error
  - Interpret as bounds of uniform distribution
- Simulation predictions with uncertainty propagation
- $d_S =$ Sorensen distance
- If predictions and observations are identical, $d_S = 0$
- If they do not overlap, $d_S = 1$

Example of CRPS and Sorensen Distance



Validation metrics provide a quantitative comparison of experiments and simulations. They will also be used in the next talk to examine possible causes in these observations for Cases 1 and 4.

Validation Metrics: Case 1



- CRPS : Continuous rank probability score
  - Units of quantity of interest
  - Smaller values reflect closer match

- Sorensen distance

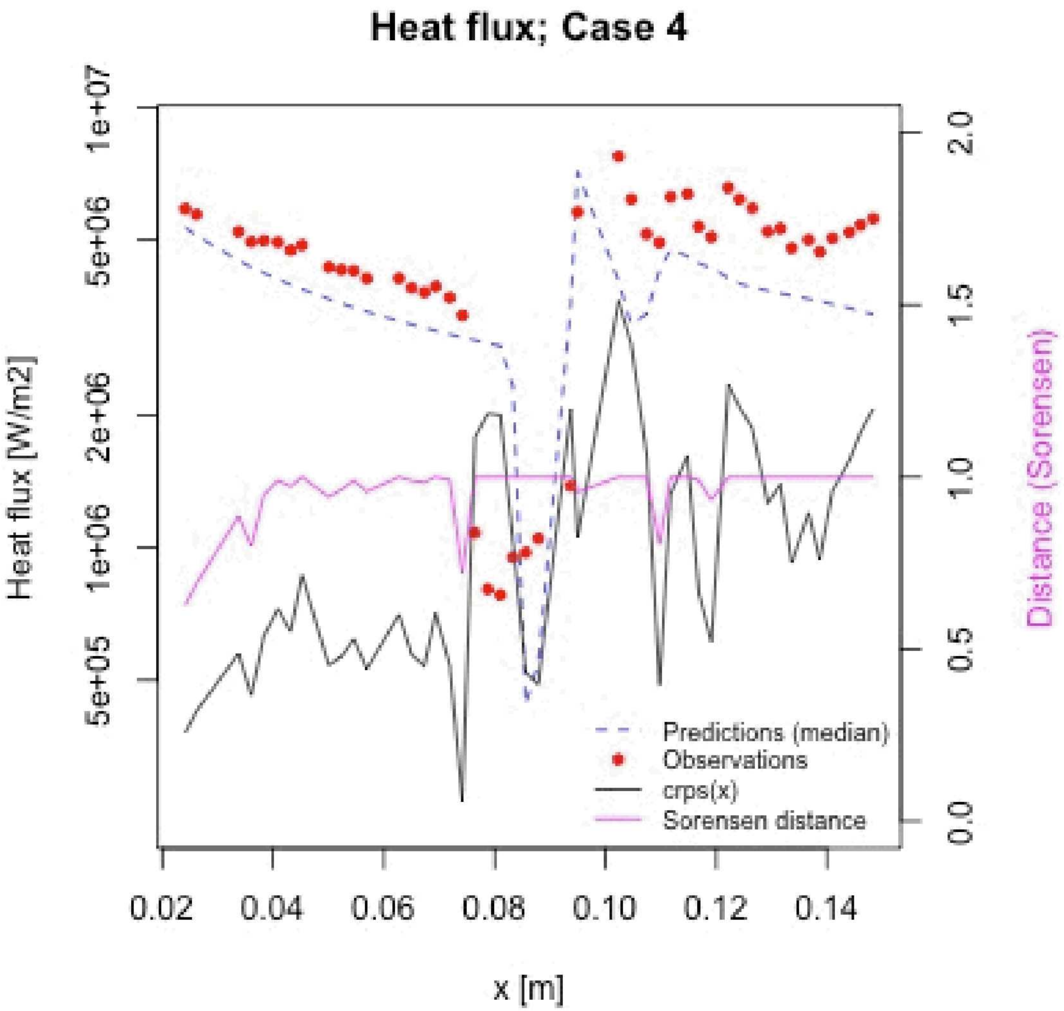
$$d_S = \frac{\sum_k |P_k(y) - Q_k(y)|}{\sum_k |P_k(y) + Q_k(y)|}$$

  - d_S = 1 (no overlap)
  - d_S = 0 (complete overlap)

The Sorensen distance indicates the observations and experiments do not overlap in **attached** region for **Case 1**.

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

Validation Metrics: Case 4



- CRPS : Continuous rank probability score
  - Units of quantity of interest
  - Smaller values reflect closer match

- Sorensen distance

$$d_S = \frac{\sum_k |P_k(y) - Q_k(y)|}{\sum_k |P_k(y) + Q_k(y)|}$$

  - d_S = 1 (no overlap)
  - d_S = 0 (complete overlap)

The Sorensen distance indicates the observations and experiments do not overlap in **attached** region and on the **aft-cone** for **Case 4**.

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

Conclusions and Motivation for Next Steps

- US3D and SPARC systematically under-predict measured data
  - Using CUBRC-provided uncertainties on freestream conditions, we cannot bracket the experimental LENS XX measurements in the laminar attached region (Cases 1 and 5), and the Aft-cone region of Case 4.
  - We cannot predict the separation point.
  - Code-to-code comparisons are consistent.
- Parametric uncertainty dominates numerical and iterative uncertainties:
  - If we want to reduce the overall uncertainty of simulation predictions, then we need to know more information about, and reduce the uncertainty of, the freestream conditions.
  - Lack of information decreases ability to discern source(s) of mismatch and identify model form error.
- Importance of a formal validation process that considers uncertainties. Allows for identification of improvements and opportunities for experiments.
- Next Steps: Possible causes of simulation-experiment mismatch will be explored in the next talk using the quantified validation metrics presented here.

Acknowledgments

- We thank Graham Candler and Ioannis Nompelis at the University of Minnesota for sharing their simulation results files for LENS-XX Cases 1-6 (*), so that we could plot them in comparison with SPARC simulations.
  - *Reference: Candler G. V., "Next-Generation CFD for Hypersonic and Aerothermal Flows (Invited)," 22nd AIAA Computational Fluid Dynamics Conference, AIAA AVIATION Forum, (AIAA 2015-3048), 2015. doi: 10.2514/6.2015-3048
- We thank Tim Wadhams and Matthew MacLean at CUBRC for their data set files.

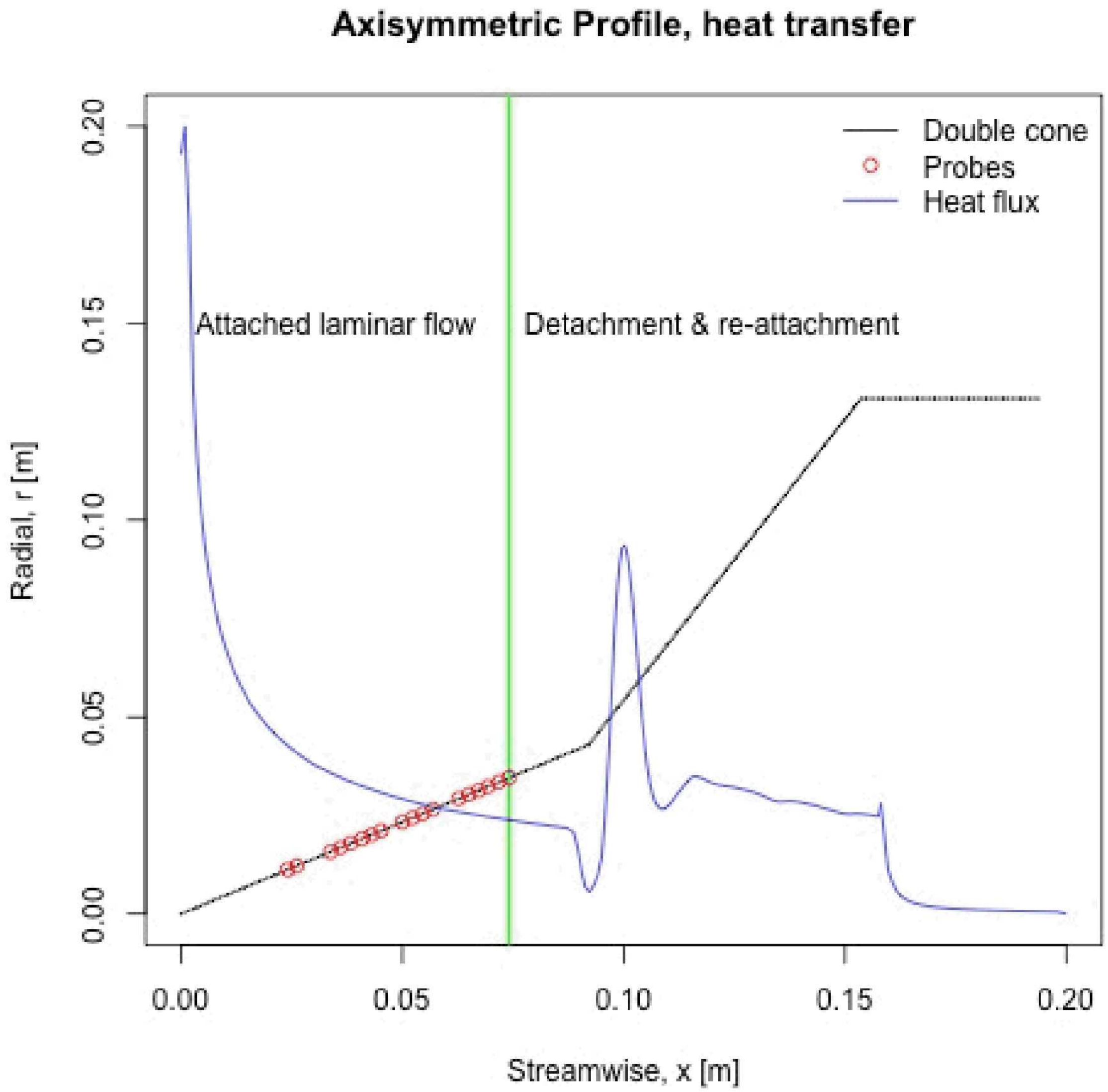
- Our companion papers:
  - **(10:30 am Gaslamp A)** Carnes, B., Weirs, V. G., Smith, T., and Dinzl, D., "Code verification and numerical error estimation with application to model validation of laminar, hypersonic flow over a double cone," AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2175**), 2019.

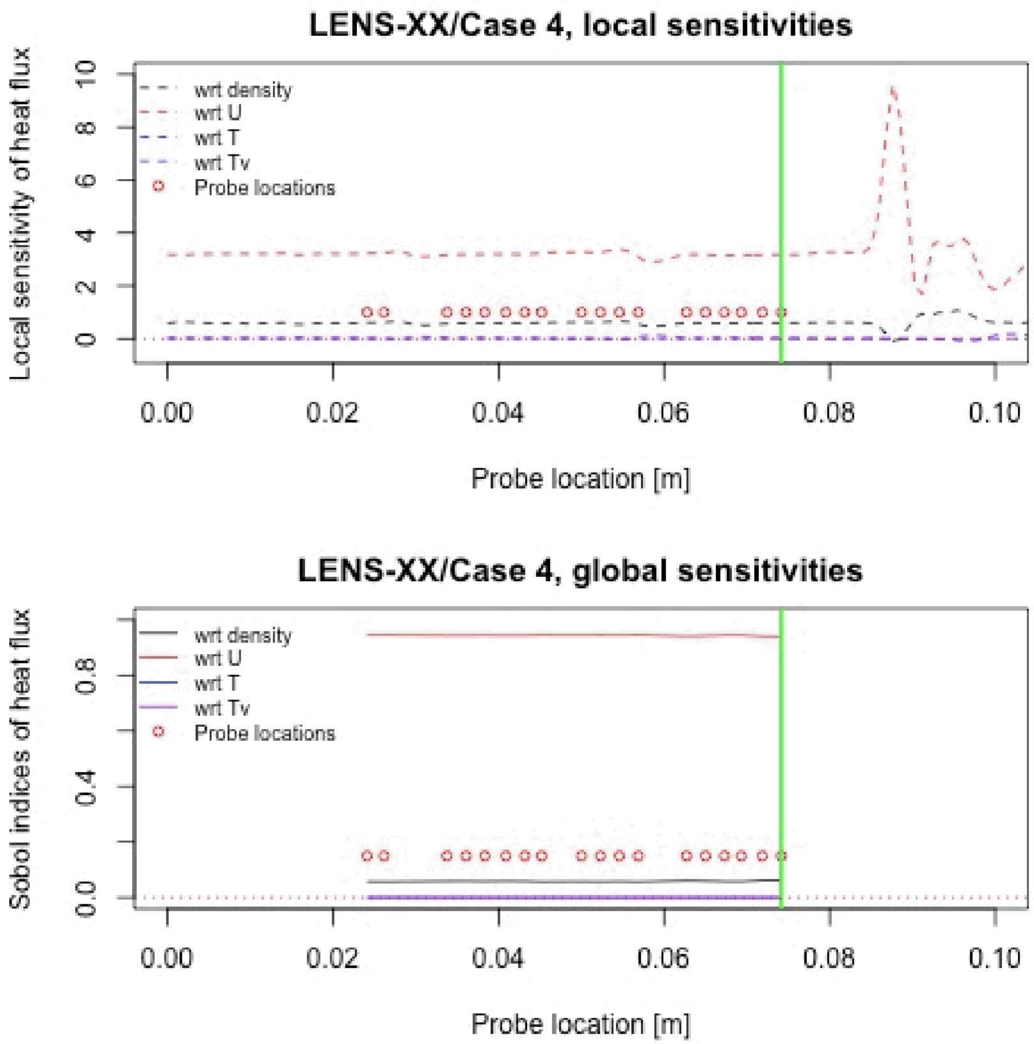
  - **(This Talk)** Kieweg, S., Ray, J., Weirs, V. G., Carnes, B., Dinzl, D., Freno, B., Howard, M., Phipps, E., Rider, W., and Smith, T. "Validation Assessment of Hypersonic Double-Cone Flow Simulations using Uncertainty Quantification, Sensitivity Analysis, and Validation Metrics,"AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2278**), 2019.

  - **(Next Talk)** Ray, J., Kieweg, S., Dinzl, D., Carnes, B., Weirs, V. G., Freno, B., Dinzl, D., Howard, M., Smith, T., Nompelis, I., and Candler, G., "Estimation of Inflow Uncertainties in Laminar Hypersonic Double-Cone Experiments," AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2279**), 2019.

EXTRA SLIDES FOR QUESTIONS

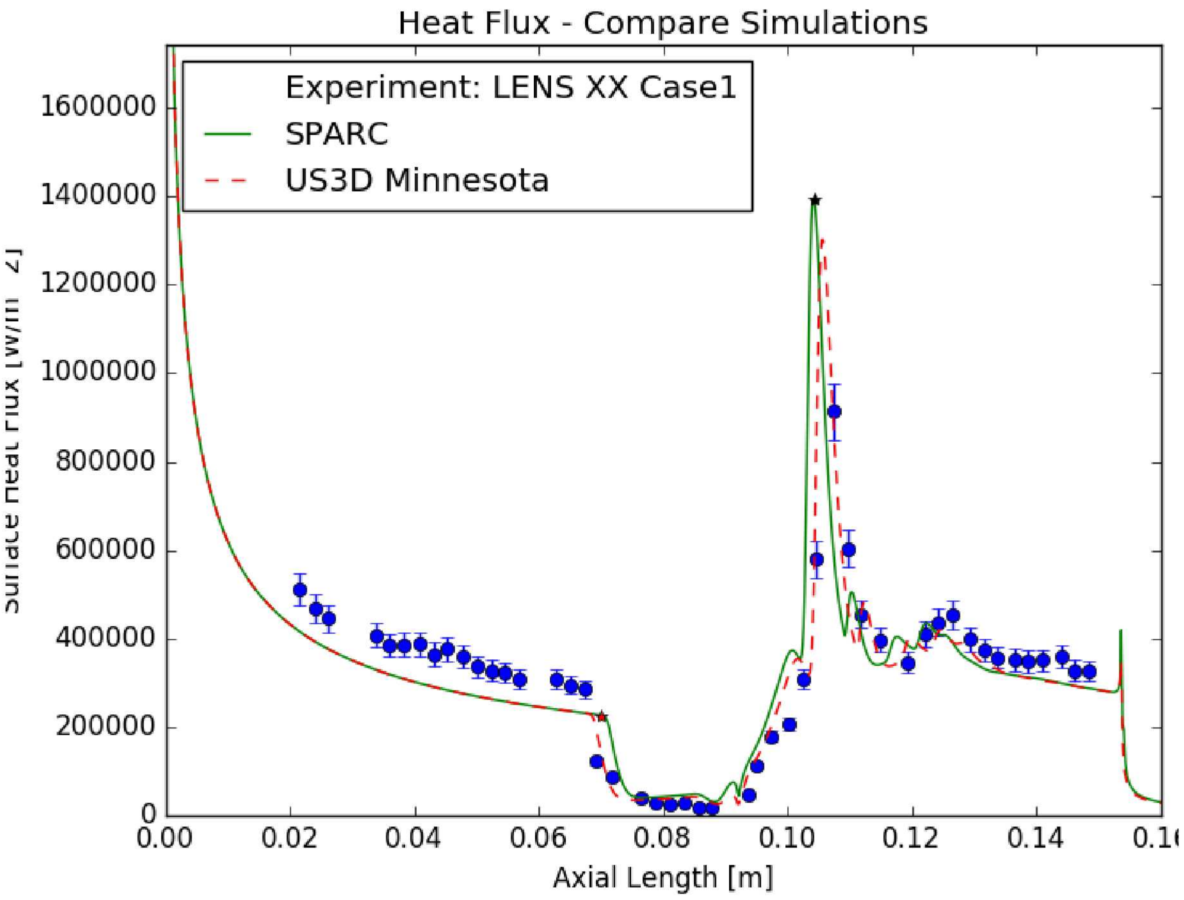
Sensitivity Analysis
(Example with Double Cone LENS XX Case 4)

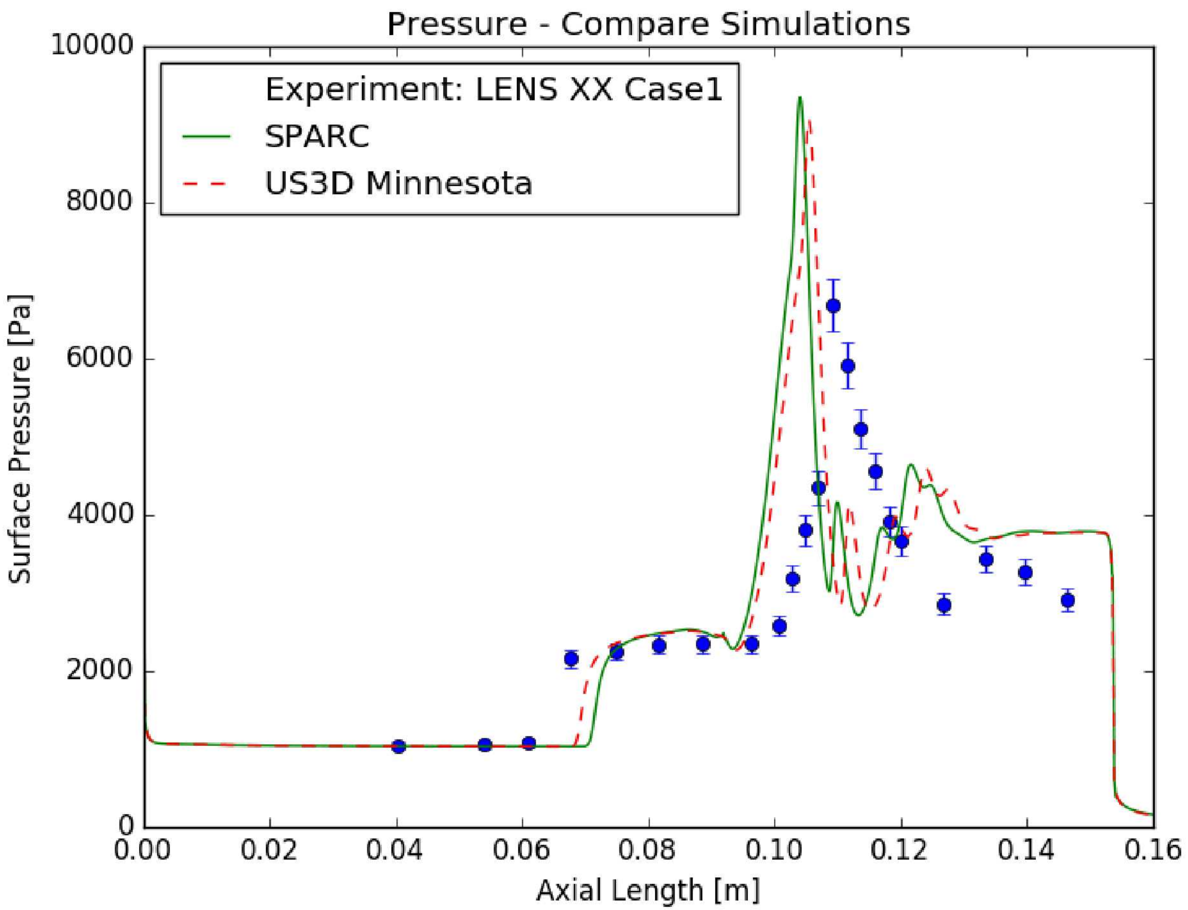




Freestream velocity has the most influence on heat flux; temperature has the least influence.

Validation Exercise
(Example with Double Cone LENS XX Case 1)

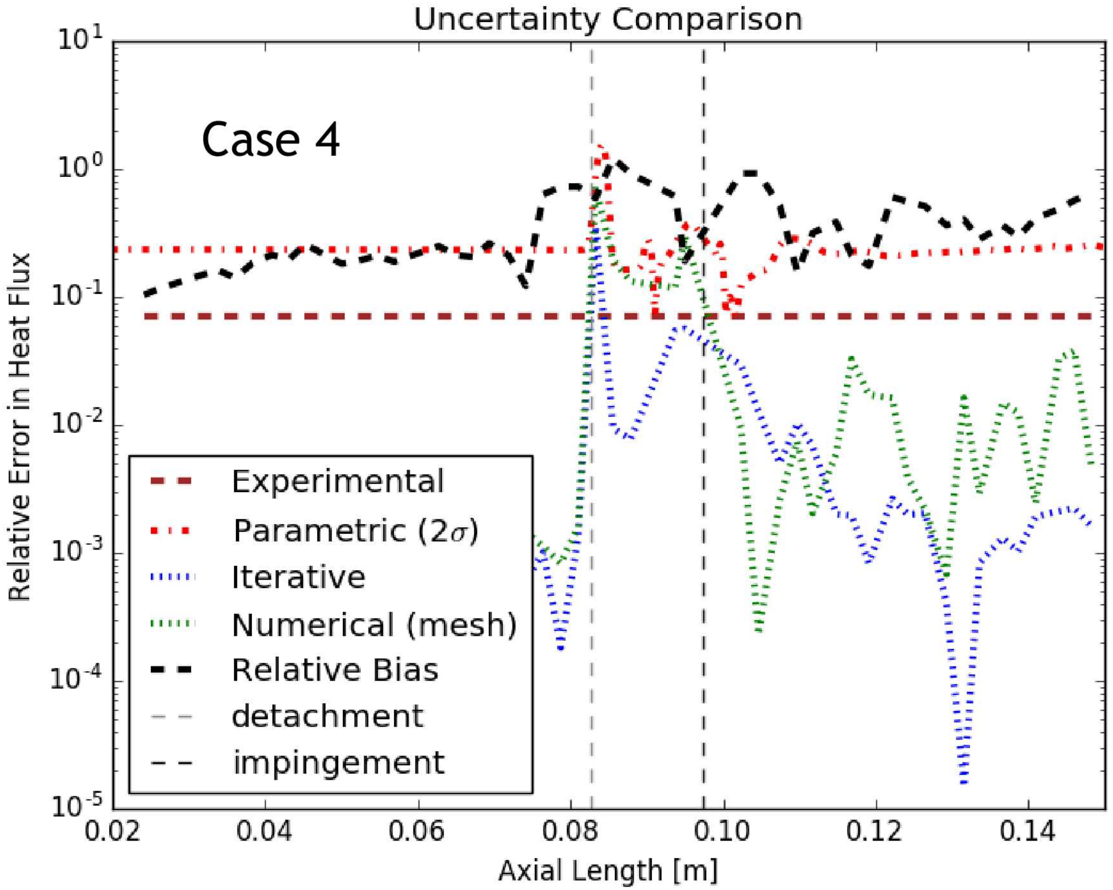


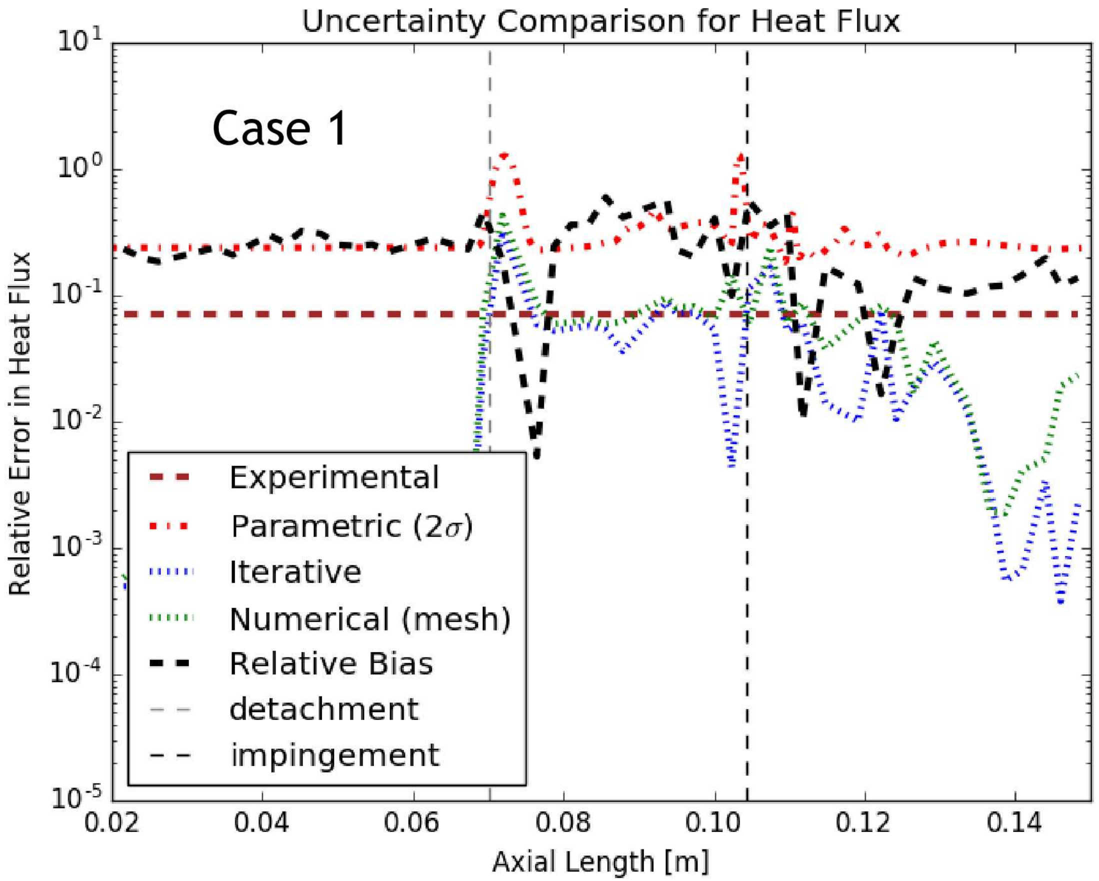


Compare to US3D. Next: does consideration of free stream uncertainty bracket experiments?

SPARC simulations use "finer" v2_512x1024 mesh, 50000 iterations; US3D used same size mesh and similar iterative convergence. Expt error bars: hf +/- 7 %, p +/- 5% per CUBRC.

Relative Contributions of Uncertainty (Case 4 and Case1)

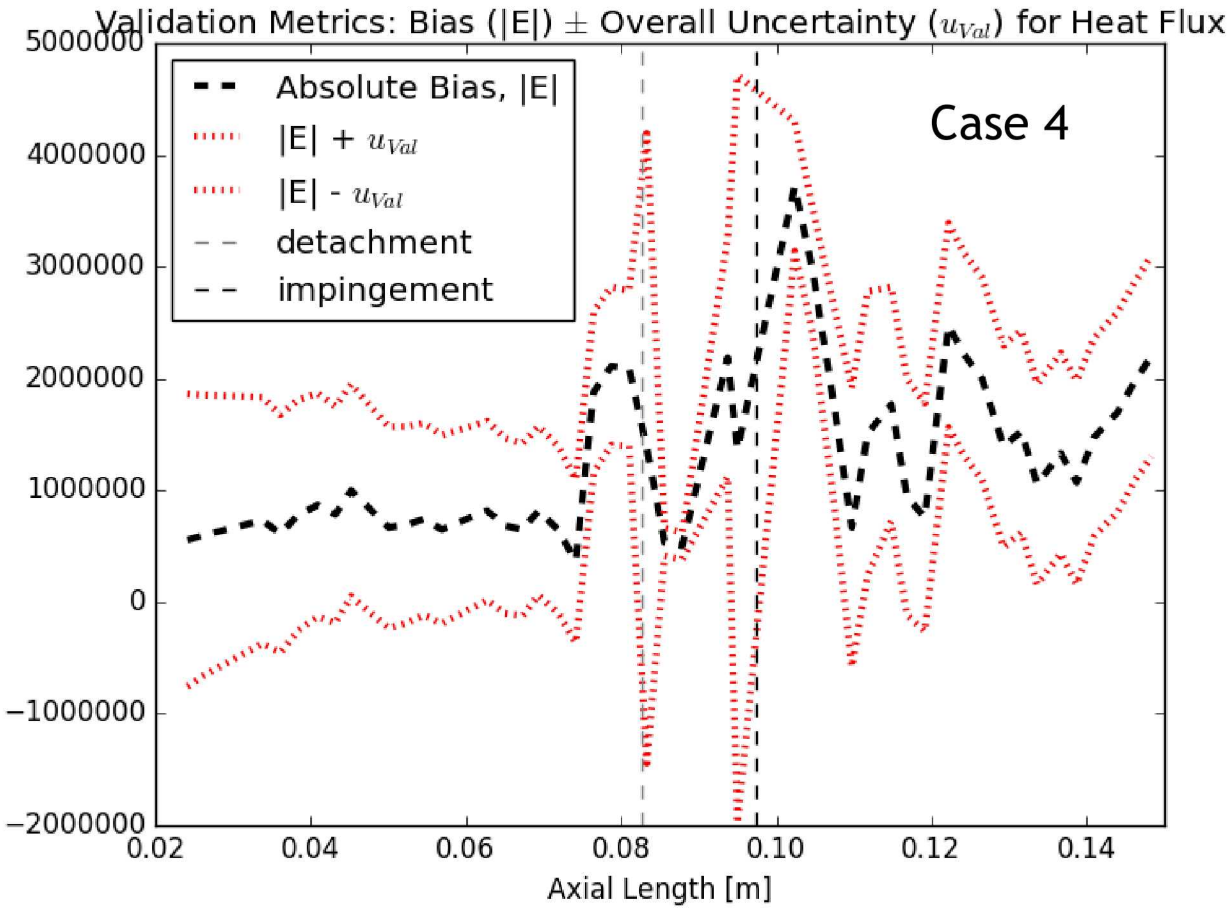


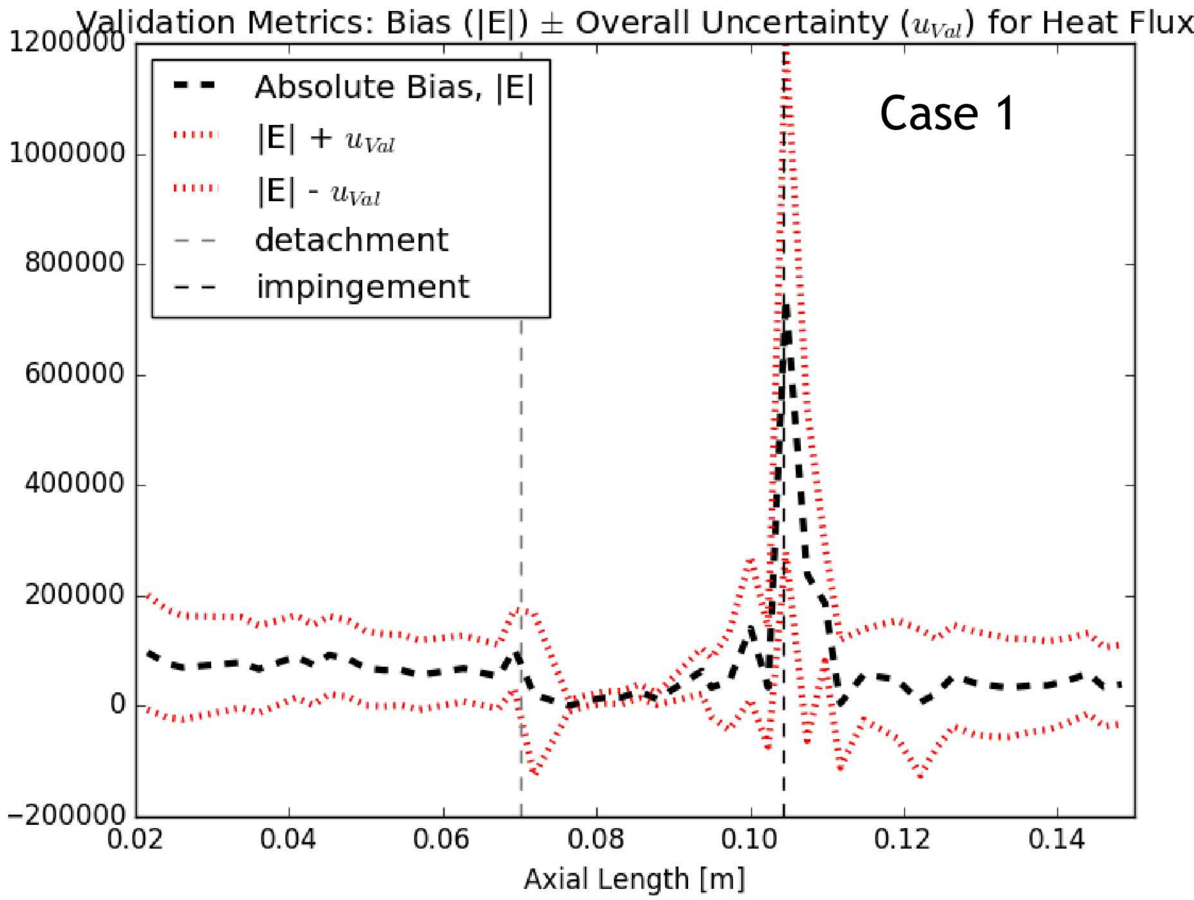


The dominant contribution to uncertainty in predictions is the uncertainty in the freestream conditions.

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

Validation Metrics: Bias and Overall Uncertainty (Case 4 and Case 1)





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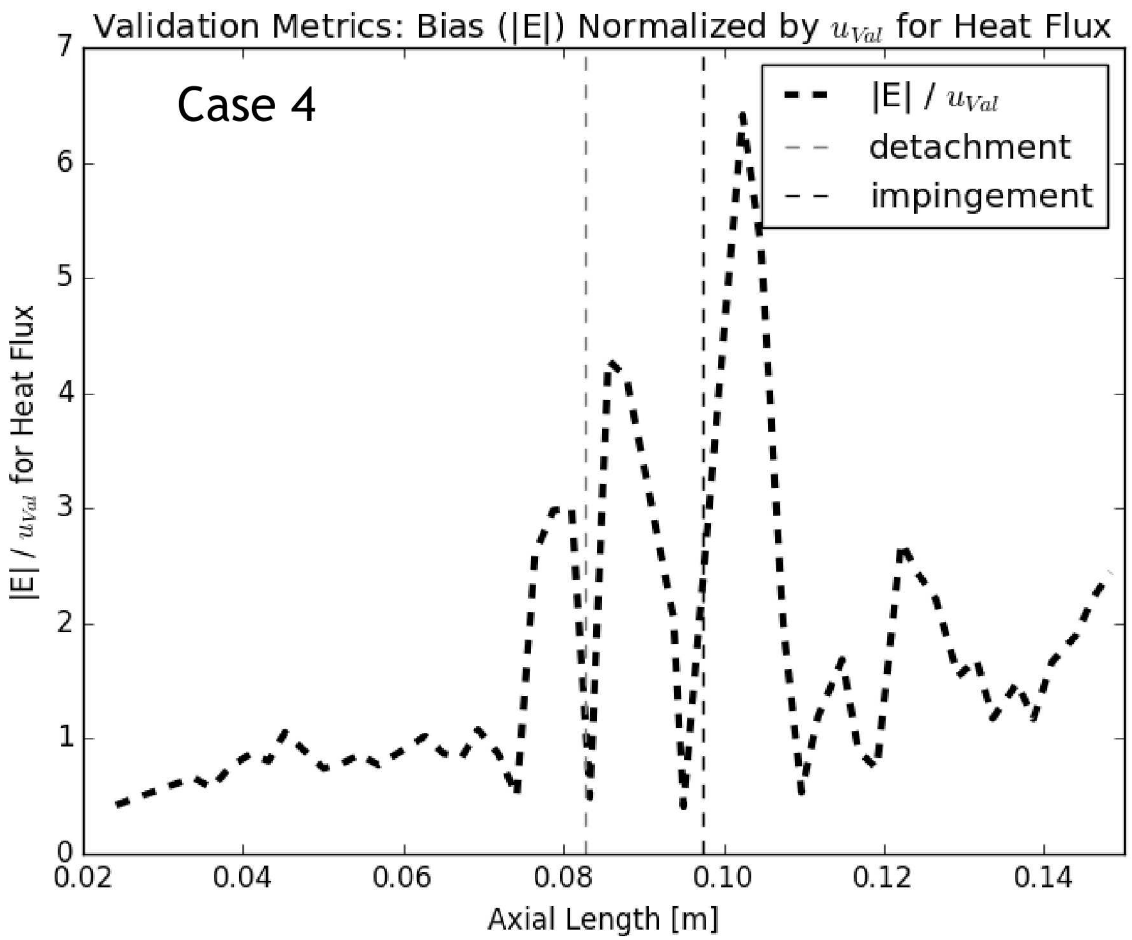
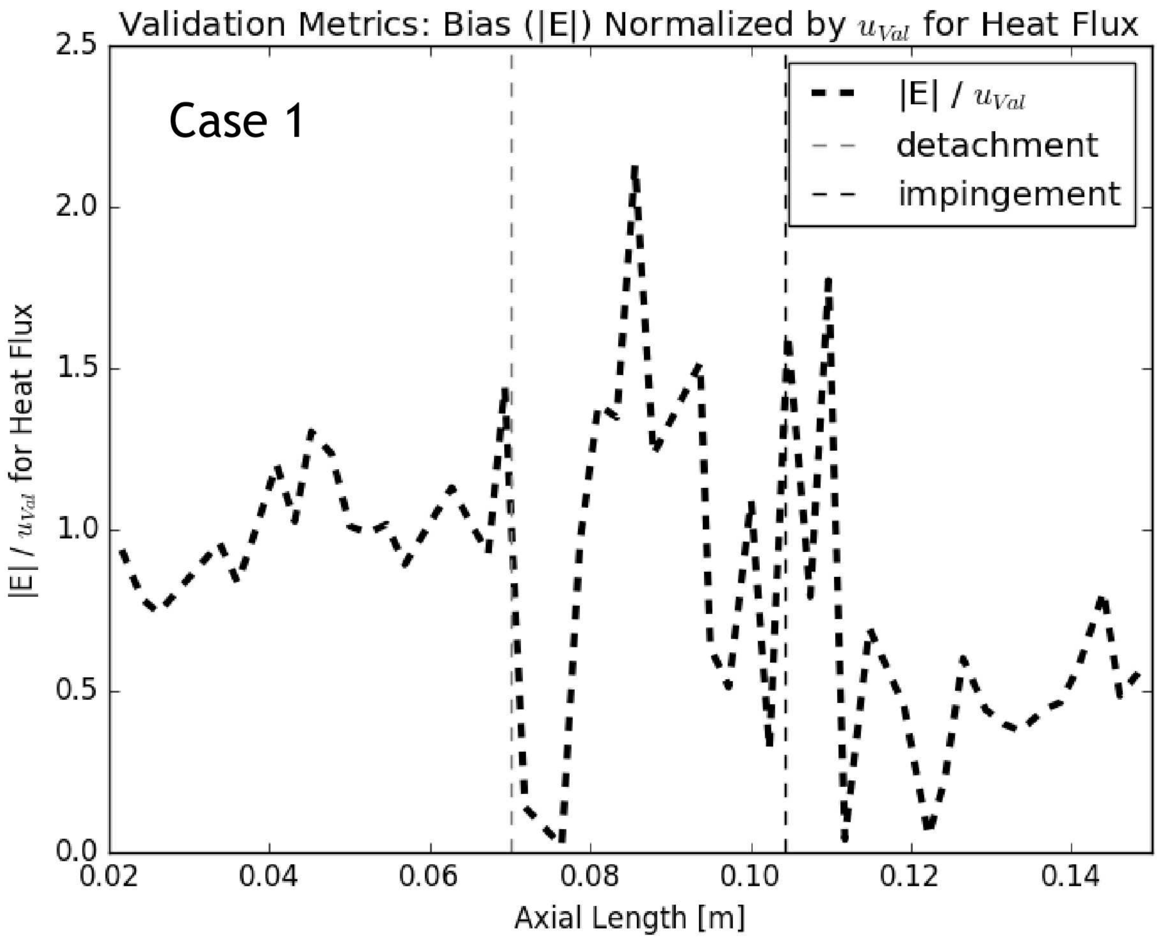
Validation Metrics: Bias and Overall Uncertainty (Case 4 and Case 1)





In some regions, the overall uncertainty is large relative to the bias, i.e. (bias/unc)< 1.

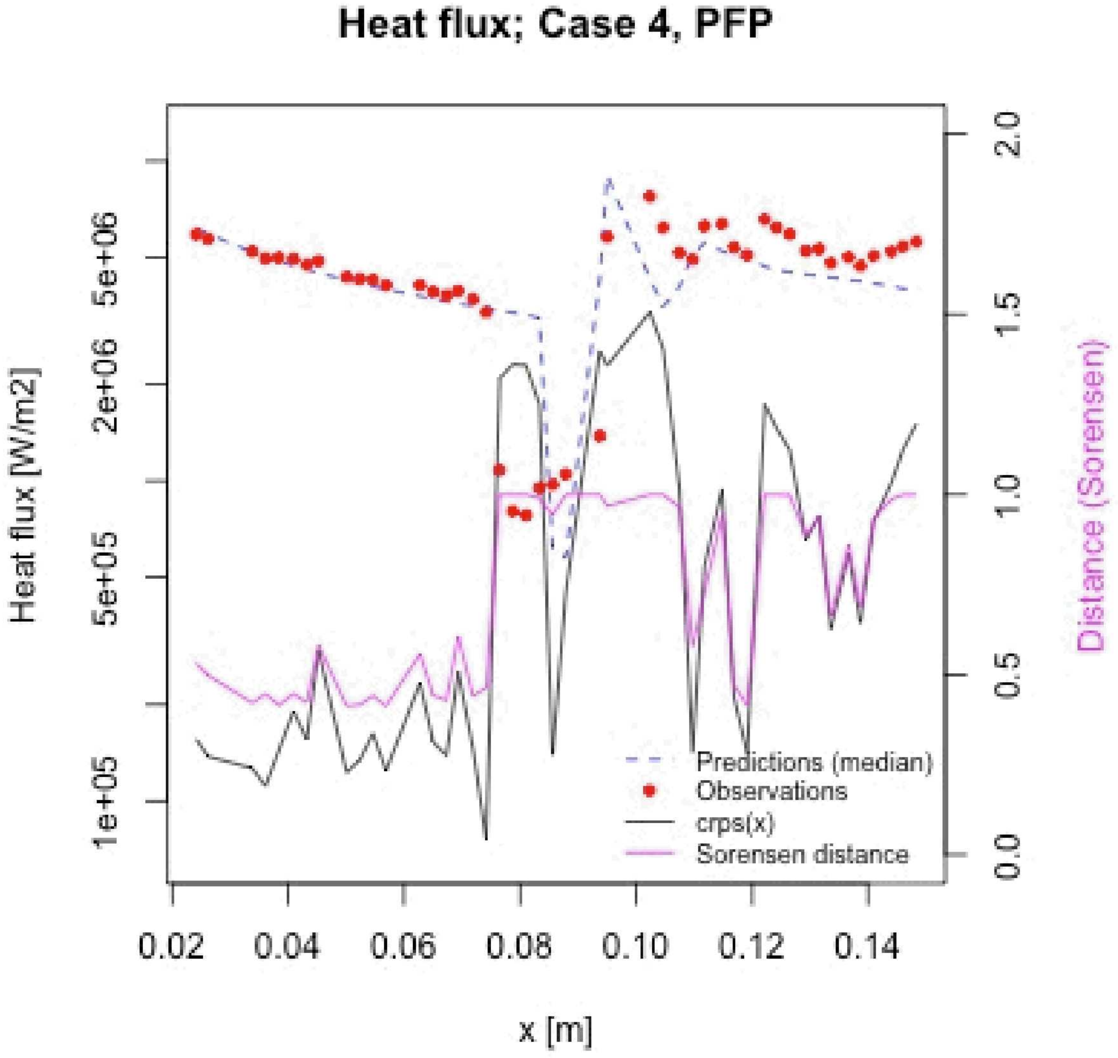
Validation Metrics

Consider Uncertain Observations:

- Heat flux measurements have 7% error
  - Interpret as bounds of uniform distribution
- At each probe we have 2 distributions:
  - P(q), from SPARC, binned into histogram
  - O(q), the uniform distribution around the observation
- Define
  - $d_S = \frac{\sum |P_i(q) - O_i(q)|}{\sum (P_i(q) + O_i(q))}$, Sorensen distance
  - If P(q) and O(q) are identical, $d_S = 0$
  - If they do not overlap, $d_S = 1$

CRPS (Continuous Ranked Probability Score):

- Distance between:
  - CDF of formed by 10,000 predictions at each probe location and the CDF (step function) of error-free observations
- Small values show less difference
- Units of variable being compared
- Scalar summary value: mean of the CRPS overall all spatial locations



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

Following Slides from Brian Carnes' Talk

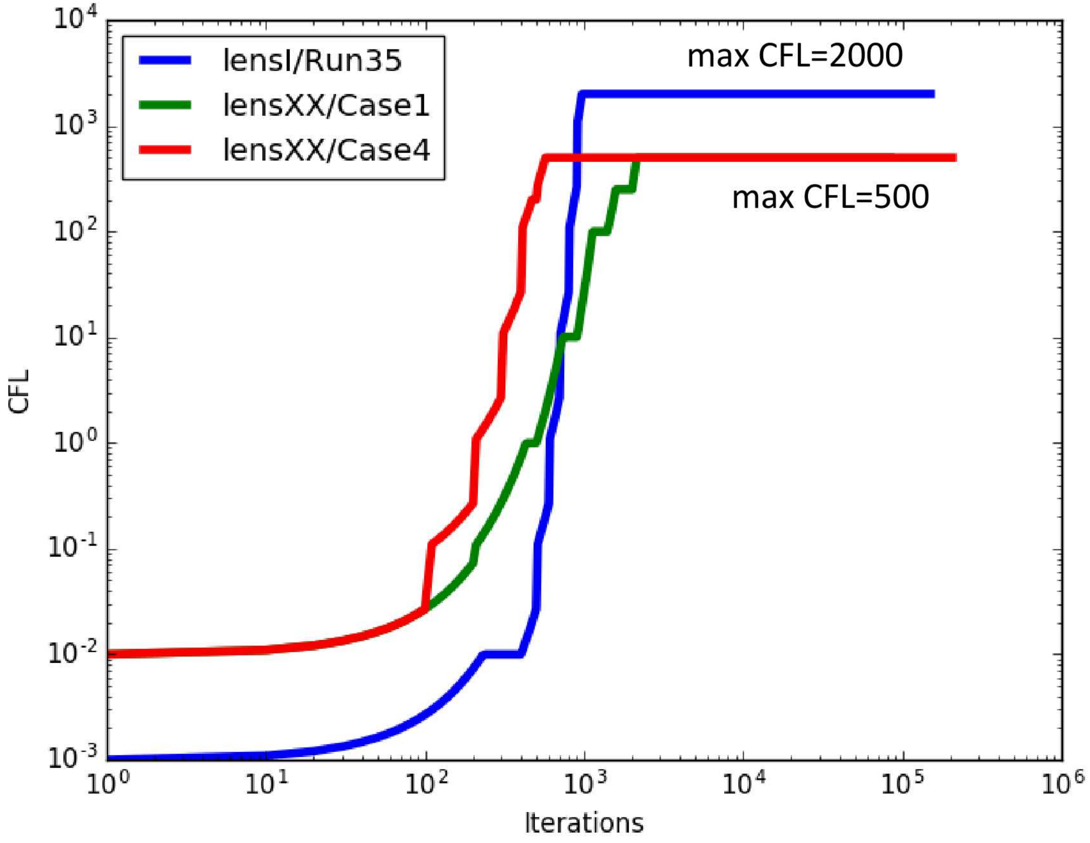
Nominal Discretization

Nominal is the discretization that we use in validation, calibration and uncertainty quantification

- •Choose (uniform) mesh from available
- •Determine a run schedule (how to ramp time step)
- •Set all the solver options (fluxes, limiters, entropy fix)
- •Define nominal parameter values (free stream conditions)

Determining the nominal discretization requires solution verification analysis (at nominal parameter values)

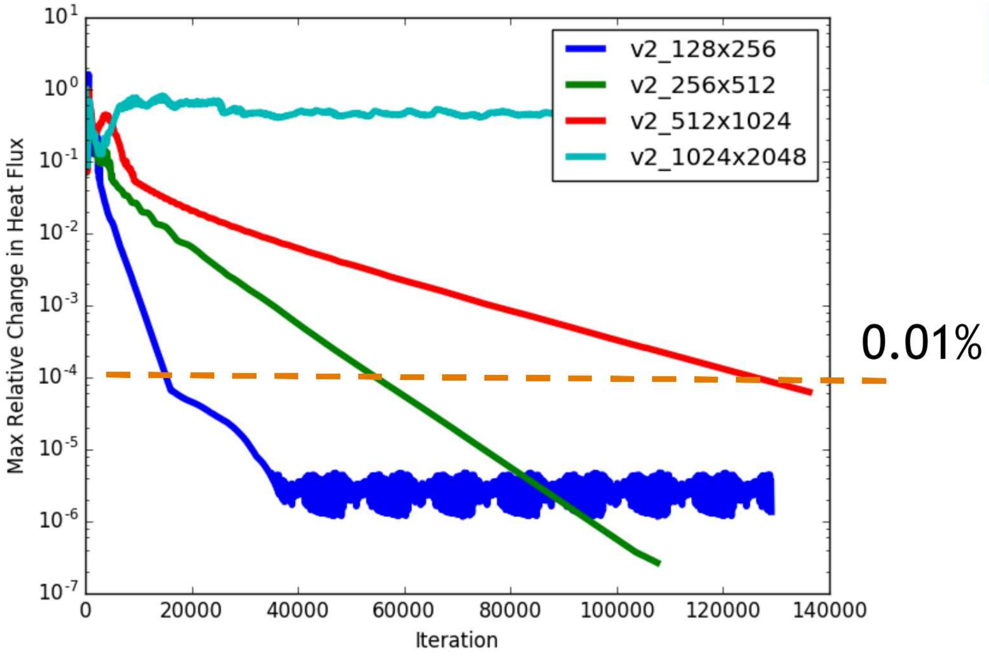
Feedback on run schedule benefited the code dev team



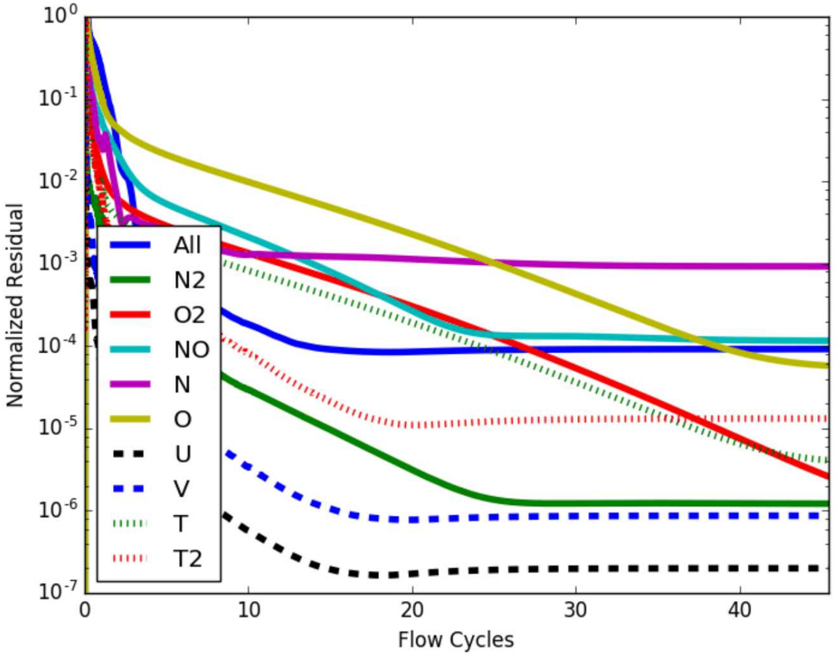
Double cone run schedules for nominal mesh: spend 99% of the time at max CFL

Iterative Convergence

- Residuals are most commonly used
- Not robust – can often fail to converge (local stall)
- Change in QoI more robust
- We monitored max relative change in local heat flux



Finest mesh cannot be used



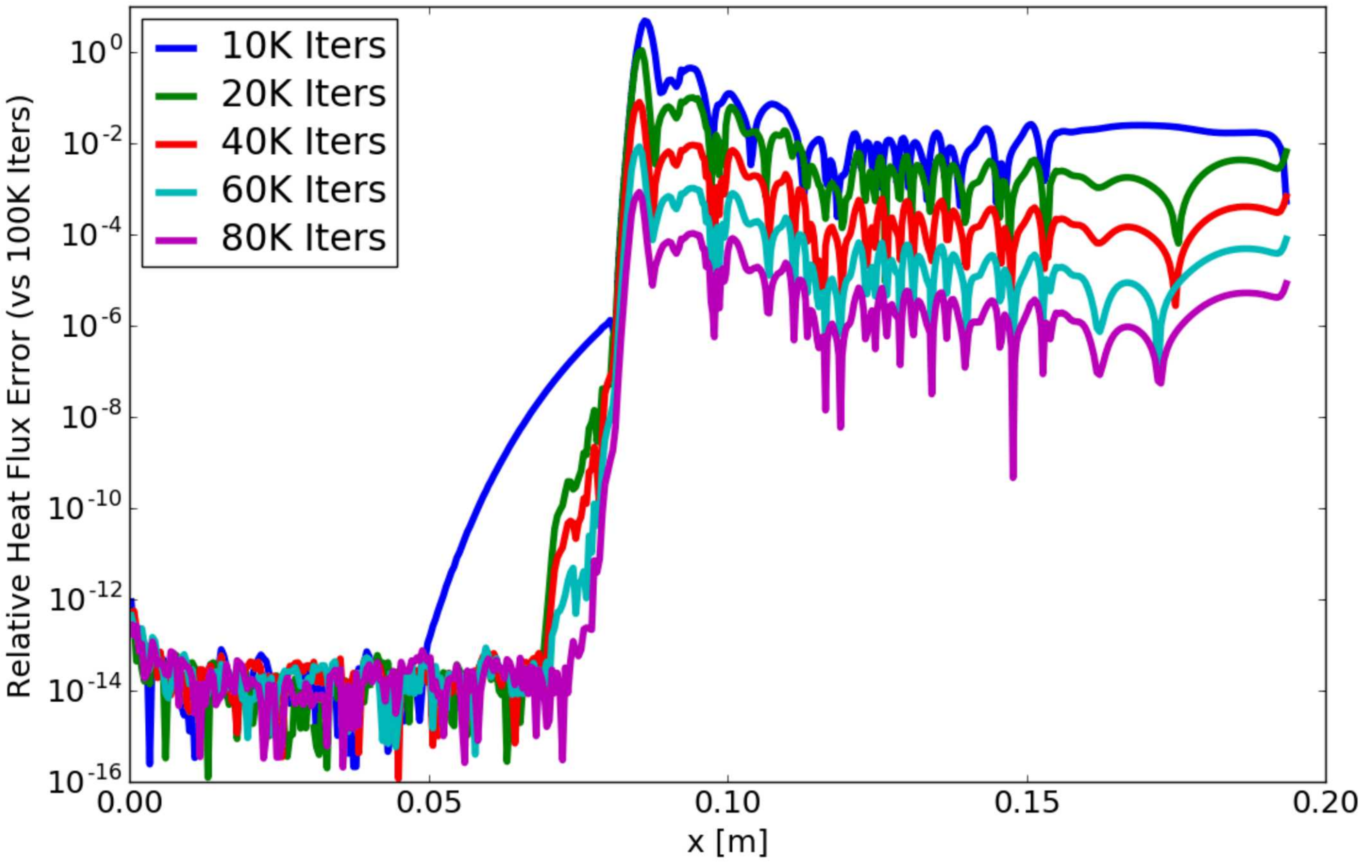
Inadequate residual convergence for reacting DC flow with thermal non-equilibrium

Methodology:

- Monitor:
  - residuals (100 flow cycles)
  - heat flux change (0.01% goal)
  - residual reduction per time step
- Control:
  - max CFL
  - run schedule to ramp CFL
  - iterations/tolerances (nonlinear, linear)

Result: Iterative Convergence of Heat Flux for Double Cone

- Reference case is 100K iterations
- Suggested nominal iterations: 50K
  - goal: keep iteration error < 1%
- Performed on 256x512 mesh
- Some regions converge faster (first cone) than others (shock interaction on second cone)



LENS-XX Case 4 (5sp 2T)

Example of Extrapolation

- Optimization approach more robust than RE
- Comparable accuracy on converging data