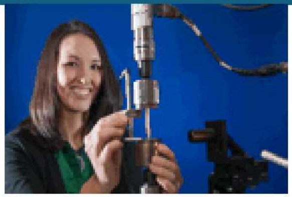
SAND2018-14342C

Code verification and numerical error estimation for use in model validation of laminar, hypersonic double-cone flows



PRESENTED BY

Brian Carnes

Brian Carnes, Greg Weirs, Tom Smith, Derek Dinzl

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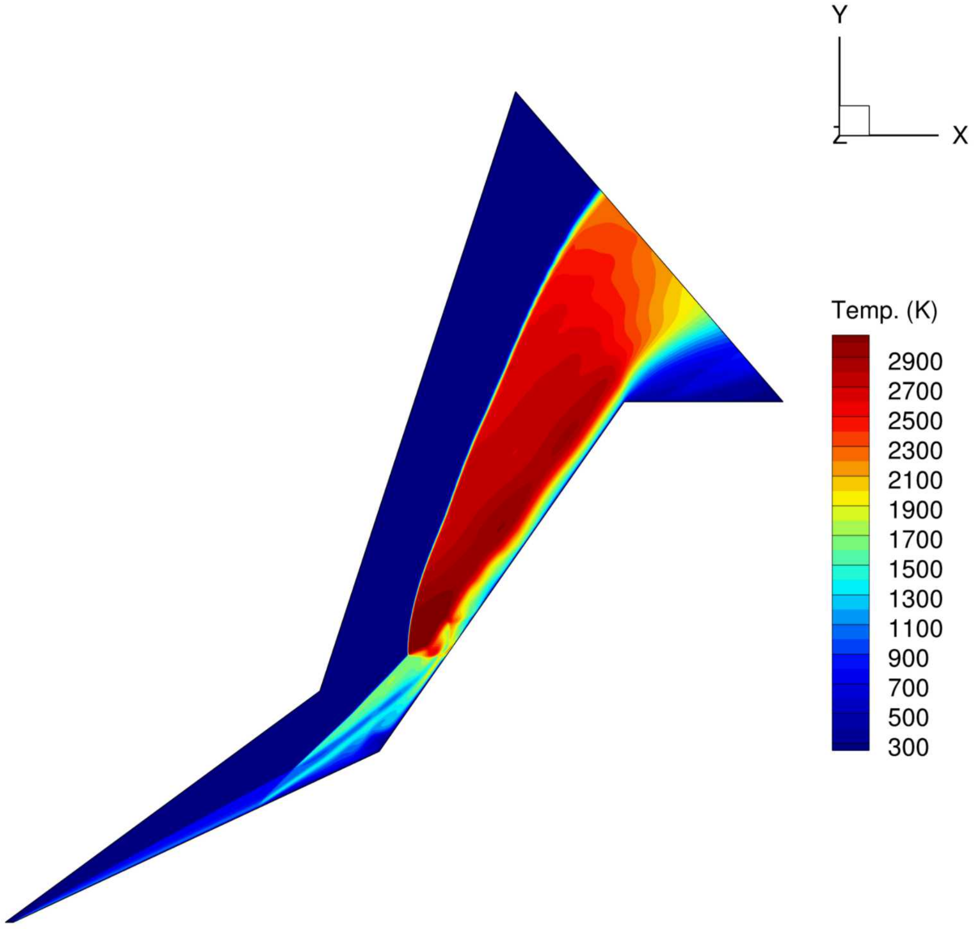
Plan of the Talk

Code verification
- Planning for test development
- Example tests
  - Prandtl-Meyer
  - Taylor-Maccol
  - Double ramp shock interaction

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

Conclusions



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

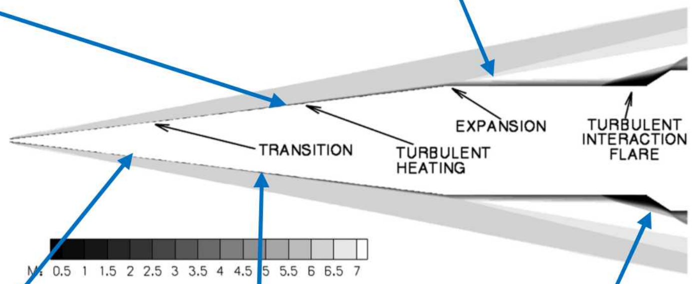
Choice of Exact Solutions is Driven by Validation Cases

Validation cases also drive test problem conditions

Turbulent (SA) compressible flat plate BL (MMS)

Prandtl-Meyer expansion

HIFiRE-1

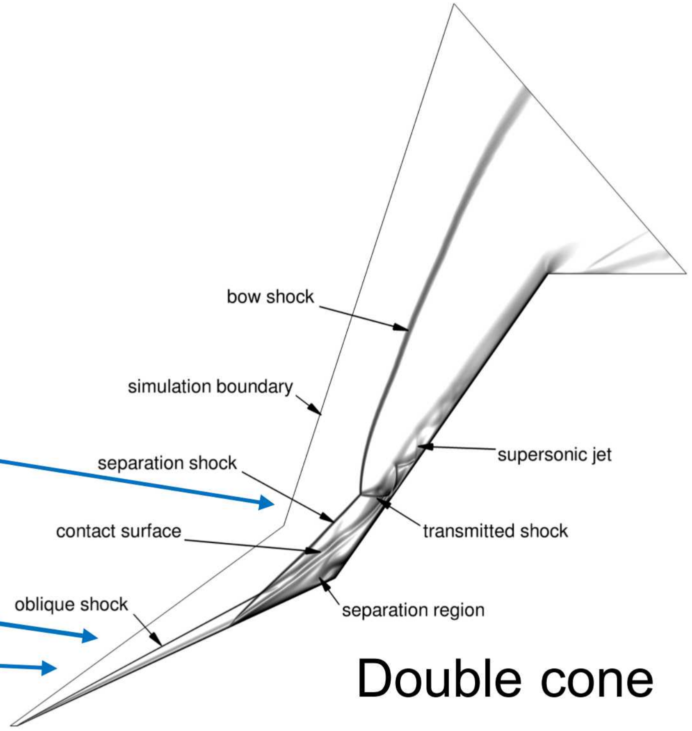


Oblique shock on ramp

Taylor-Maccoll (axisym)

Double ramp shock interaction

Laminar compressible flat plate BL (MMS)



Double cone

Double cone image computed using SPARC

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

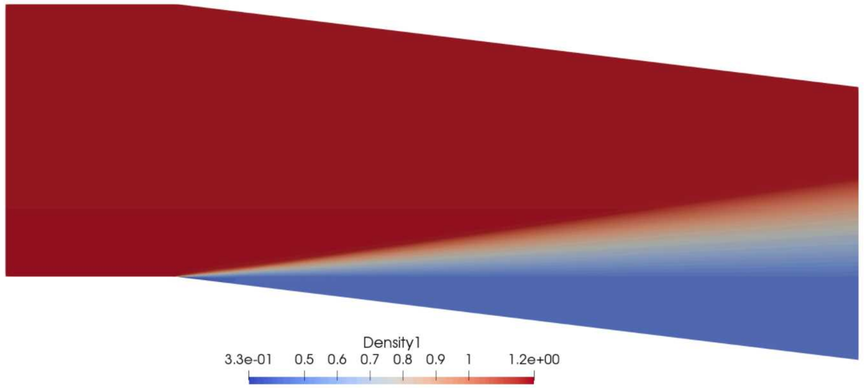
Code Verification Tests Are Organized by Physics and Solution Type

	Manufactured	Exact	Benchmark
Inviscid	• 2D trigonometric • 3D trigonometric	• Isentropic vortex annulus • Oblique shock • Double ramp • Prandtl-Meyer expansion • Taylor-Maccoll	
Laminar	• 2D exponential (interior) • Flat plate boundary layer		
Turbulent (RANS)	• Flat plate boundary layer		• NASA TMR Flat plate • NASA TMR bump in channel

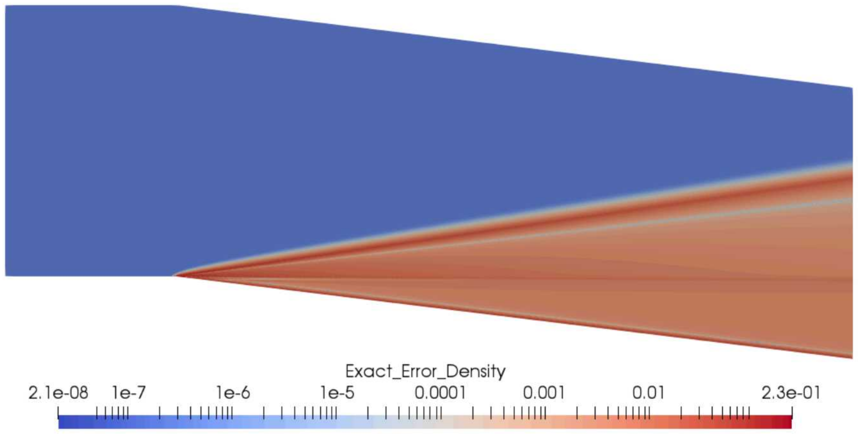
Prandtl-Meyer Expansion Fan Test

- Classic supersonic inviscid flow test near HIFiRE-1 conditions
- Three mesh topologies tested:
  - Flat top
  - Bent with vertical grid lines (shown)
  - Bent with normal grid lines
- Extensive set of discretization options tested
  - Only first order shows significantly lower rates

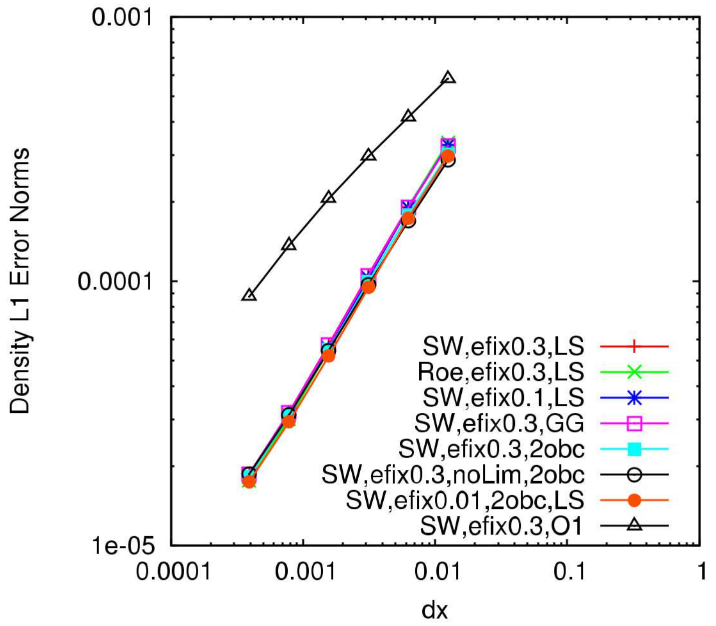
Mach=7, Ramp angle 7 degrees

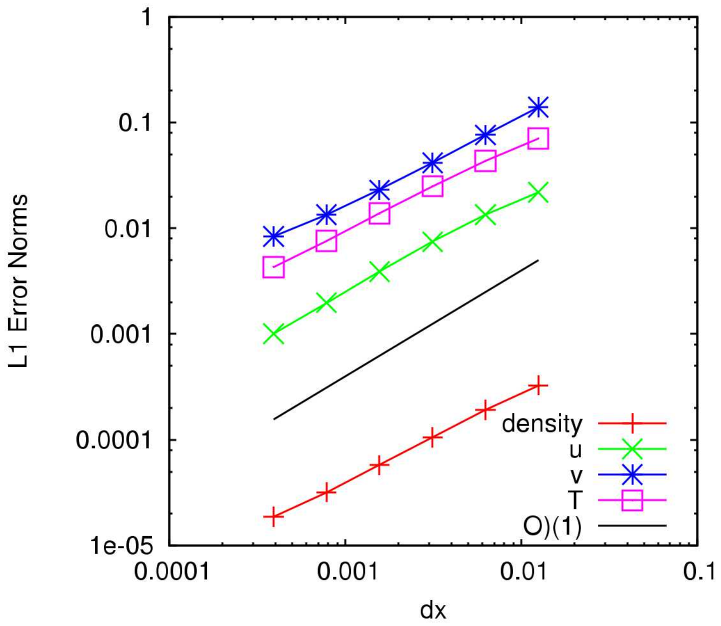


Density (mesh 6, 1600x512x1)



Density errors (mesh 6, 1600x512x1)





Additional Testing with Sod Shock Tube Test

- Results are convergent but less than expected first-order (L1)
- Run a simpler expansion fan test (1D spatial)
  - eliminate the boundary conditions
- Can run Sod test with only the expansion wave
- Clear first order convergence here
- Results suggest the boundary conditions are the issue

Meshes	ρ	u	v	T
1—2	0.77538	0.69308	0.87499	0.69969
2—3	0.85892	0.85933	0.88075	0.80001
3—4	0.87573	0.93849	0.84783	0.85515
4—5	0.84634	0.97250	0.78331	0.86182
5—6	0.77507	0.98007	0.67801	0.81667

Prandtl-Meyer: convergence rates (L1)

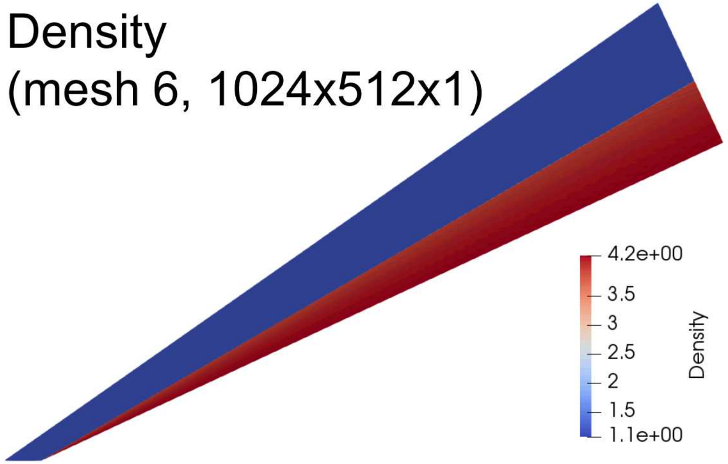
Meshes	ρ	u	T
1—2	1.0032	0.9941	0.9896
2—3	1.0078	1.0030	1.0119
3—4	1.0099	1.0032	1.0208
4—5	1.0096	1.0038	1.0207

Shock Tube: convergence rates (L1)

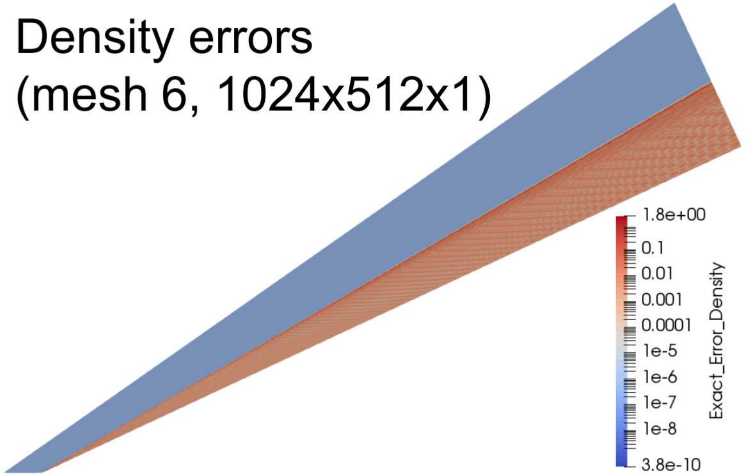
Taylor-Maccoll Conical Flow Test

Mach=5, Cone angle 25 degrees

Density
(mesh 6, 1024x512x1)



Density errors
(mesh 6, 1024x512x1)



- Axisymmetric supersonic inviscid flow over a cone near double cone conditions
- Requires numerical integration of ODE for flow behind shock; iterative solution of shock angle

- Four mesh topologies tested
- Extensive set of discretization options tested

$$
\begin{aligned}
\frac{dV_r}{d\theta} &= V_t \\
\frac{dV_t}{d\theta} &= \frac{1}{(k - V_t^2)} \left(V_t^2 V_r - k \left[2V_r + V_t \cot(\theta) \right] \right) \\
k &= \frac{\gamma - 1}{2} \left[V_{max}^2 - V_r^2 - V_t^2 \right],
\end{aligned}
$$

ODEs for velocity behind shock

Varying Azimuthal Angle of Meshes Improves Convergence Rates

- Original results were convergent but less than expected first-order (L1)
- Improved rates when azimuthal angle spanned by the domain is reduced as the mesh is refined

Meshes	ρ	u	v	T
1—2	0.93272	0.95219	0.94843	0.89824
2—3	0.93189	0.95012	0.94412	0.89997
3—4	0.90615	0.95072	0.92520	0.88353
4—5	0.89248	0.97059	0.95037	0.90861
5—6	**0.86166**	**0.95835**	**0.91305**	**0.88503**

Original convergence rates (L1)
One-cell thick meshes with constant azimuthal angle (0.1 degrees)

Meshes	ρ	u	v	T
1—2	0.96830	0.96921	0.96918	0.94044
2—3	0.97267	0.97790	0.97313	0.95844
3—4	0.95753	0.97423	0.96809	0.95279
4—5	0.94938	0.98100	0.96366	0.95158
5—6	**0.93923**	**0.99047**	**0.95781**	**0.95345**

Improved convergence rates (L1)
One-cell thick meshes with varying azimuthal angle (0.1 degrees on finest mesh)

Double Ramp Shock Test

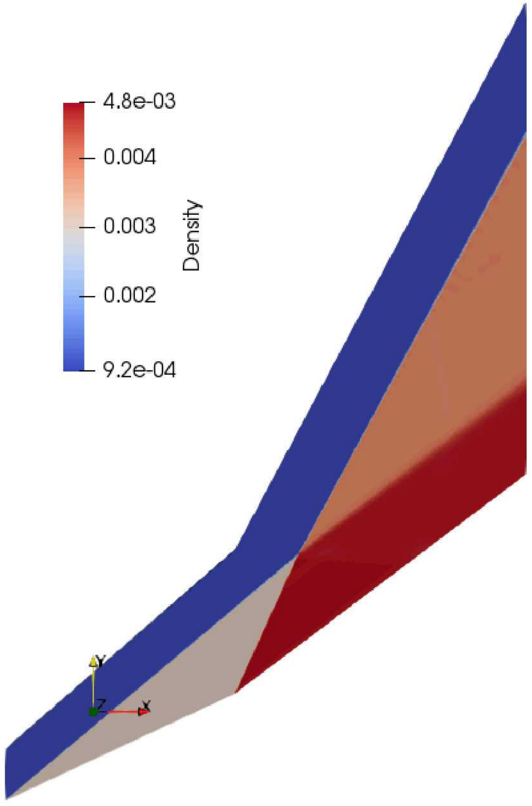
- Basic test case relevant to double cone
- Exact solution obtained by iteration, and consists of four constant states (inviscid, perfect gas)
- Convergence rates are less than first order (L1)
- Reduced rates also seen in shock tube tests that include contact discontinuities (rate = ½)

Local errors suggest the contact discontinuity is the source of reduced convergence rates

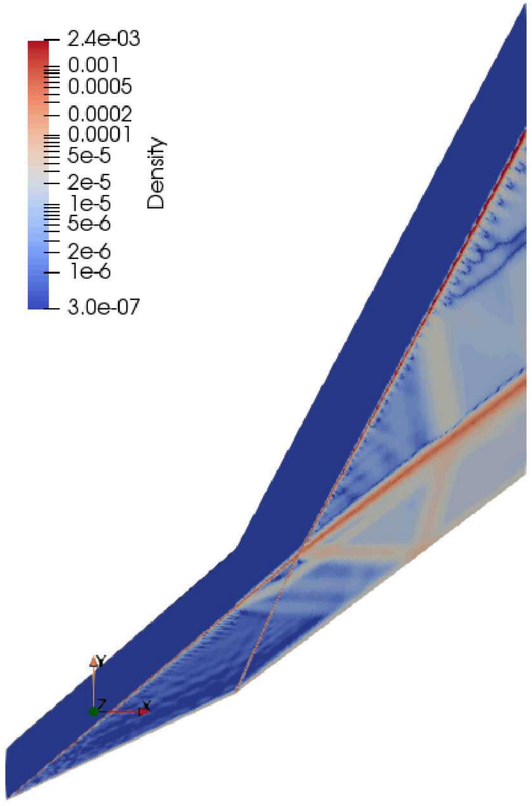
Meshes	ρ	u	v	T
0—1	0.8015	0.8089	0.7803	0.8294
1—2	0.7065	0.7525	0.7345	0.7495
2—3	0.7777	0.7632	0.7678	0.7550
3—4	0.7882	0.7627	0.7735	0.7516

Convergence rates (L1)

Mach=3.636, T=652, density=9.64e-4
Ramps at 25 and 37 degrees



Density (mesh 4)



Density errors (mesh 4)

Next Steps in Code Verification

Verification test suites:

- Manufactured solutions for laminar and turbulent boundary layers
- New test development in aero/thermal, thermal/ablation

Testing infrastructure:

- Enhance MMS capabilities in SPARC (reacting gas, thermal/ablation)
- Standardized tools for automated verification testing

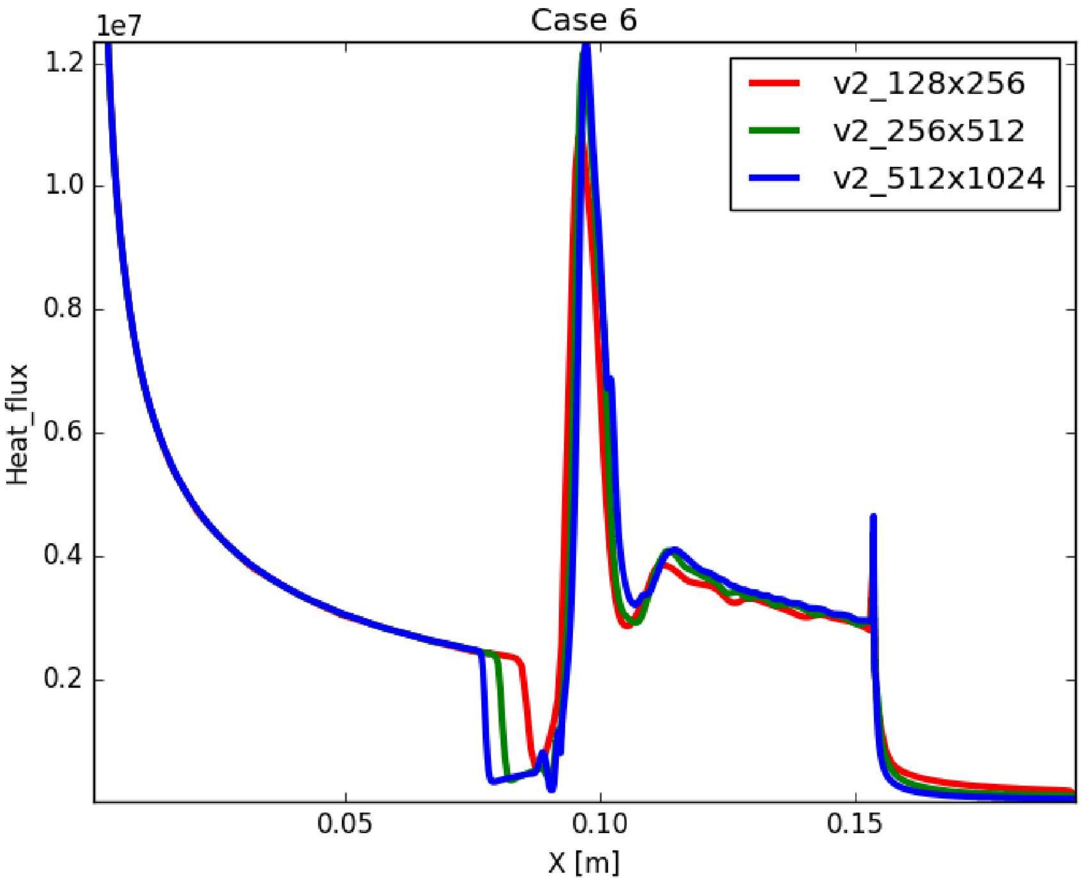
Solution Verification: Introduction

Goal: Provide quantitative estimates for discretization errors in QoIs

Dominant error sources (in this work):
1. iterative convergence to steady state
2. mesh resolution

Define nominal discretization

Error estimates become part of validation assessment



LENS-XX Case 6 (5sp 2T): none of the meshes are “converged”

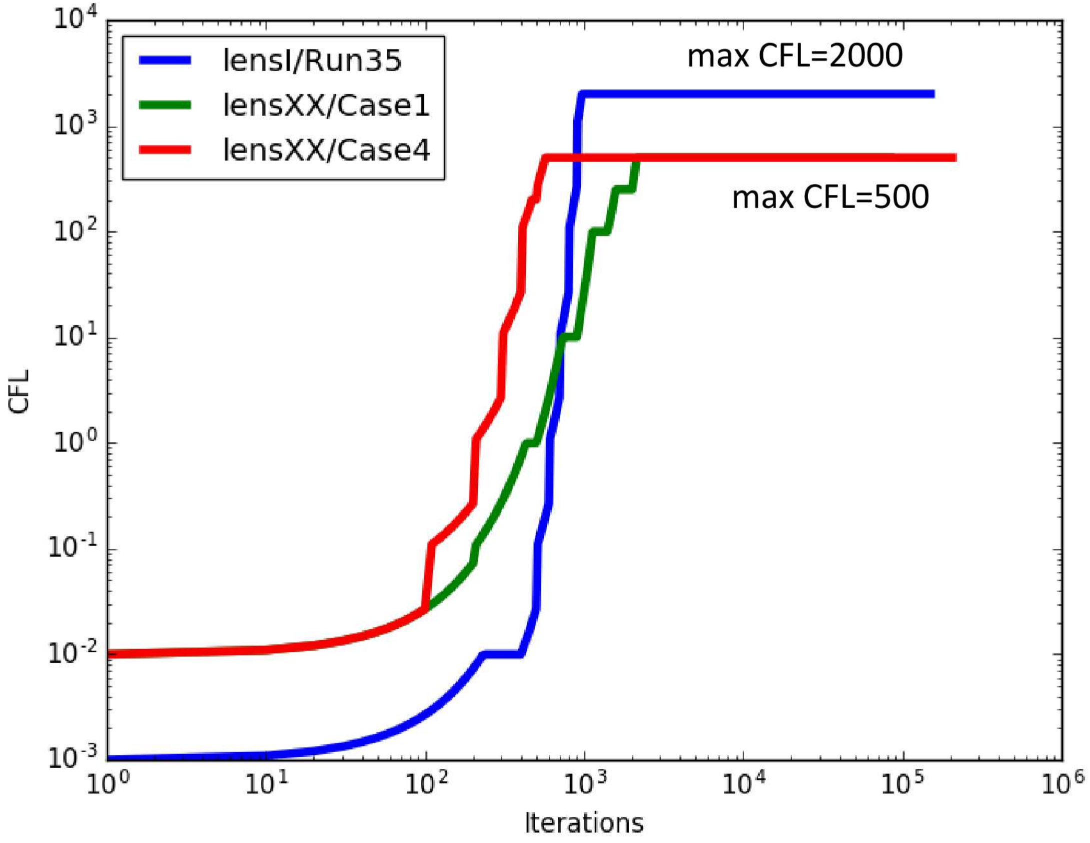
Nominal Discretization

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)

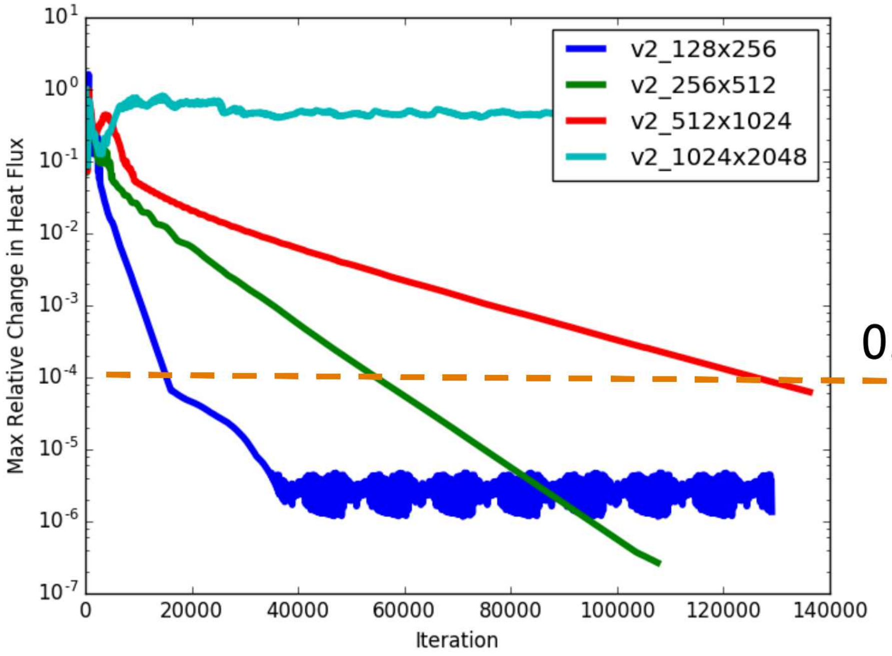
Feedback on run schedule benefited the code dev team



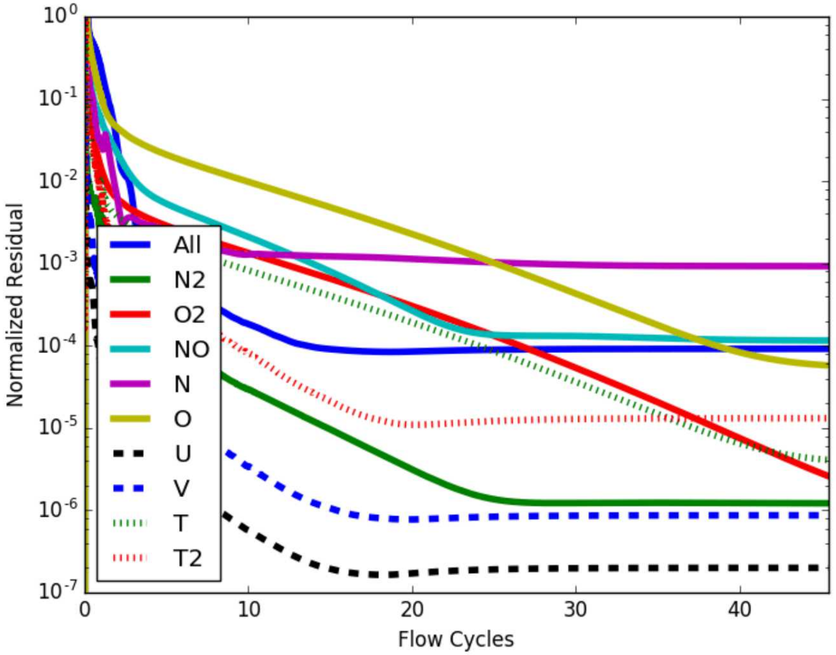
Double cone run schedules for nominal mesh: spend 99% of the time at max CFL

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:

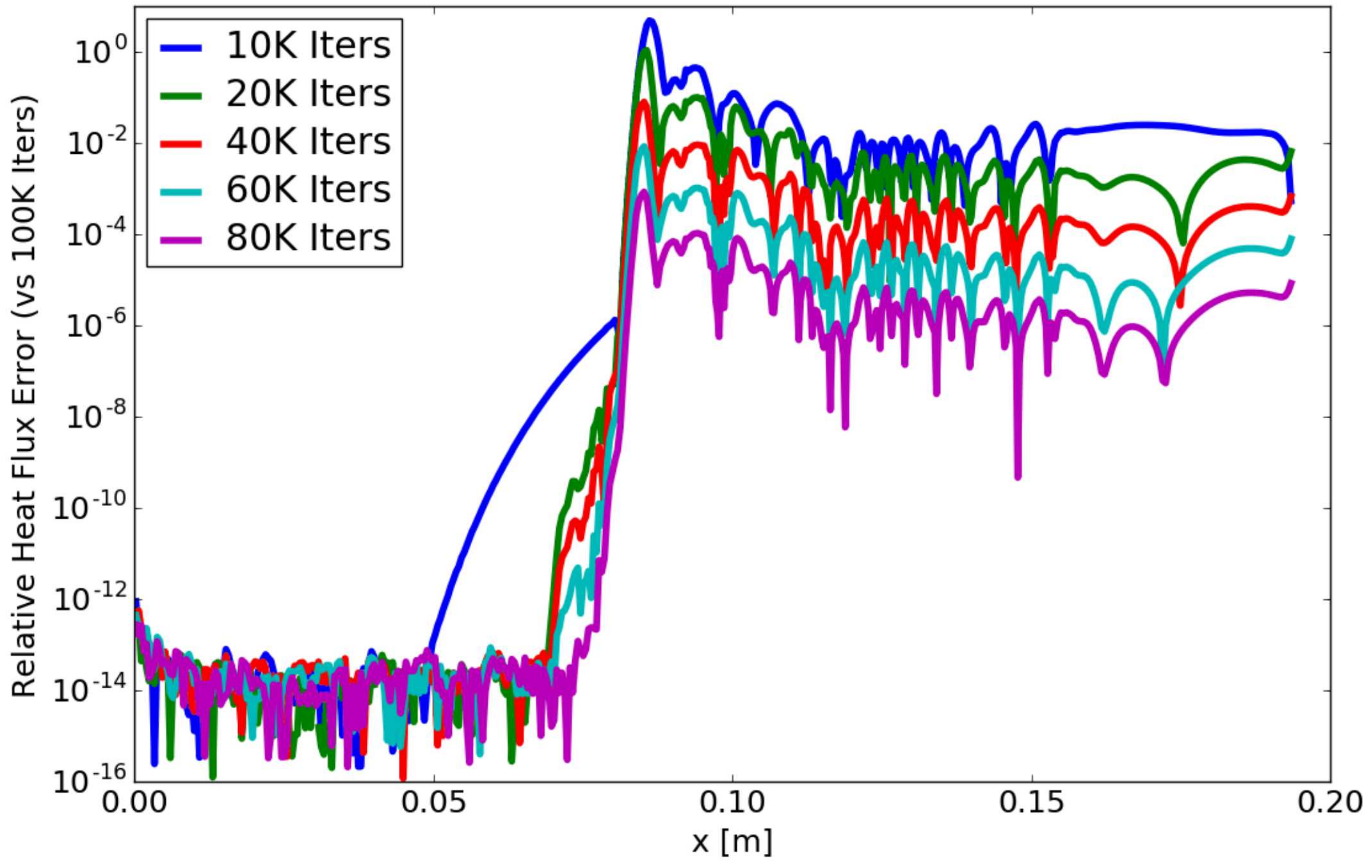
- •Monitor:
  - residuals (100 flow cycles)
  - heat flux change (0.01% goal)
  - residual reduction per time step
- •Control:
  - max CFL
  - run schedule to ramp CFL
  - iterations/tolerances (nonlinear, linear)

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)

Robust Extrapolation for Mesh Error Estimation

- Our extrapolation requirements:
  - robust, accurate, uncertainty estimates

$$Q(h) \approx Q + C\,h^p$$

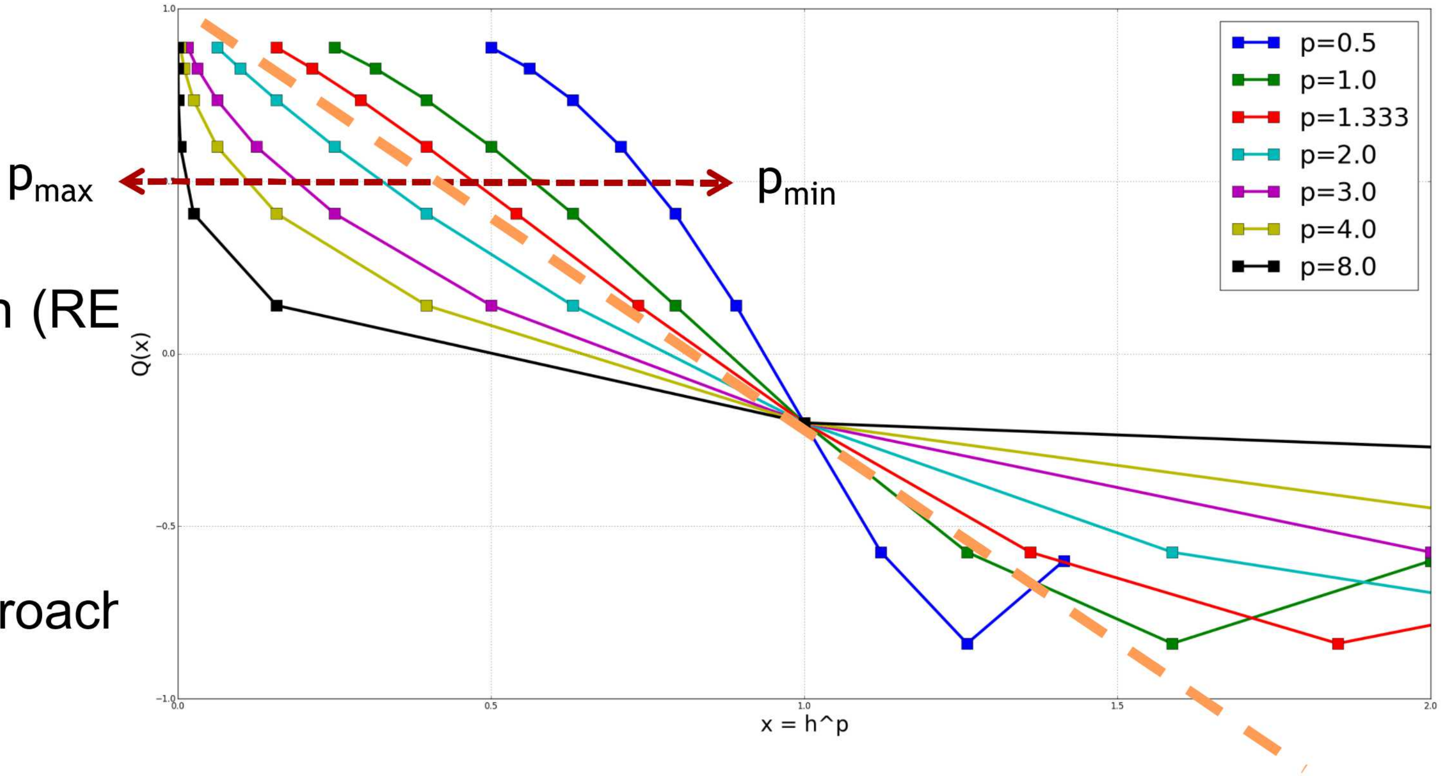
- Most common is Richardson extrapolation (RE
  - accurate but not robust

$$p = \frac{\log\left[(Q_3 - Q_2)/(Q_2 - Q_1)\right]}{\log r}$$

- We chose a constrained optimization approach based on inner least squares solve

$$x \equiv h^p \qquad Q(x) \approx Q + C\,x$$

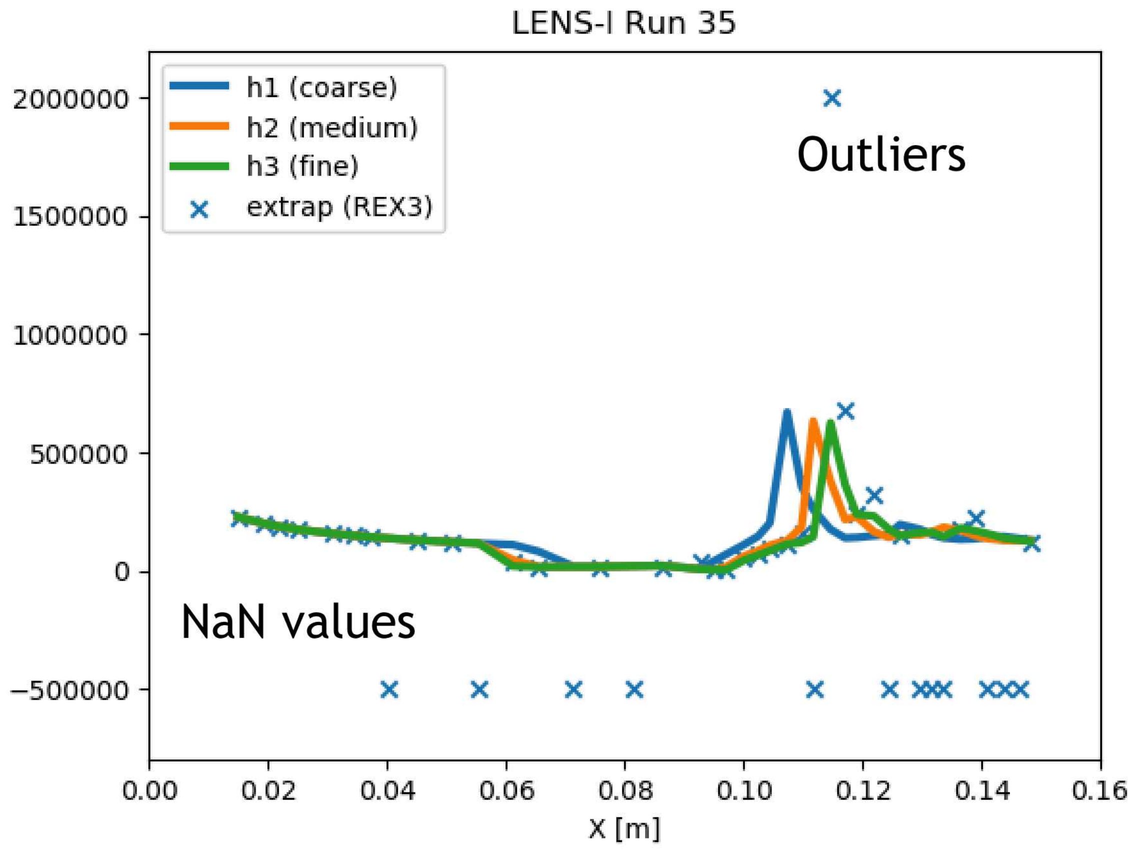
- Requires lower/upper bounds on the rate (p)

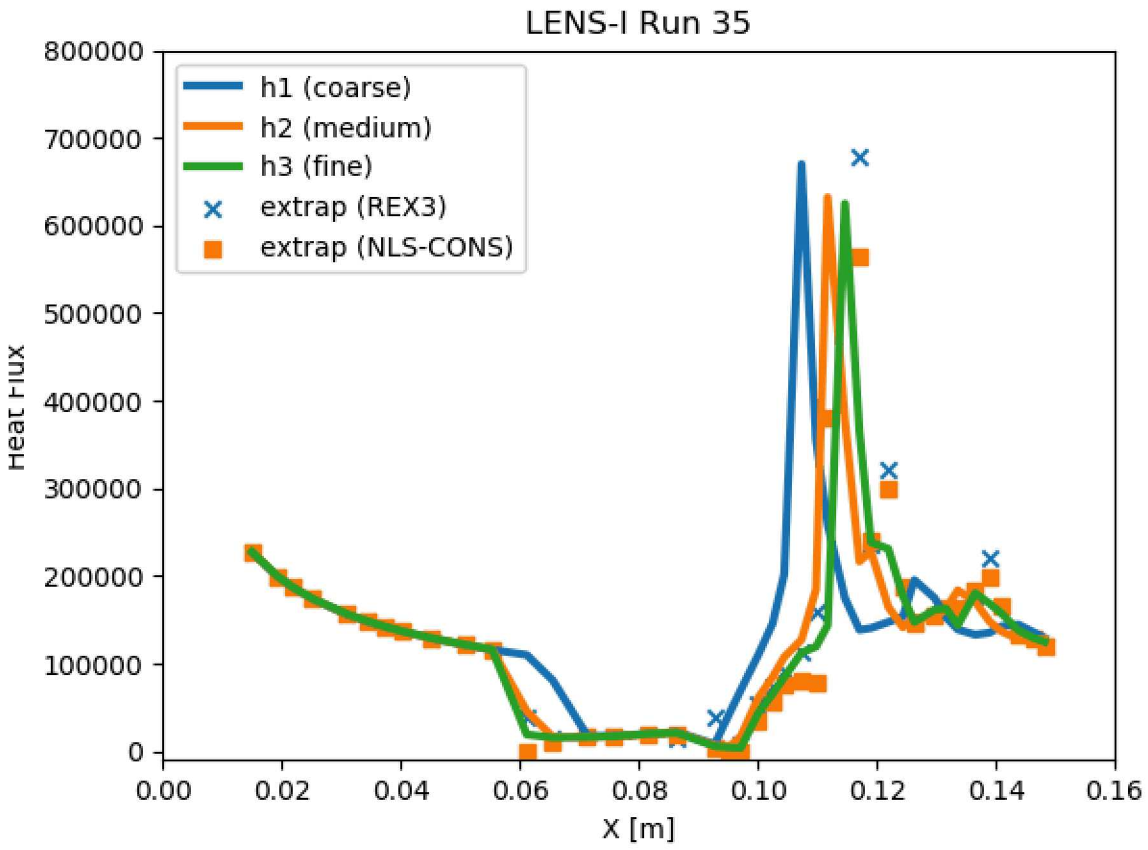


Changing p shifts the data on the horizontal axis

Example of Extrapolation

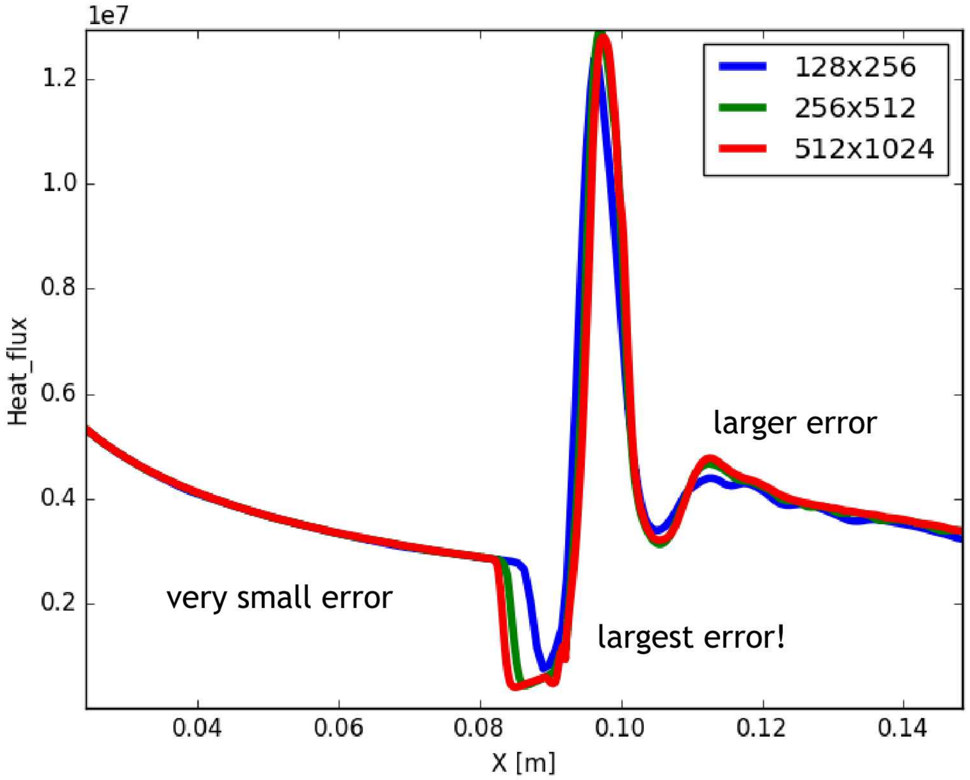
- Optimization approach more robust than RE
- Comparable accuracy on converging data

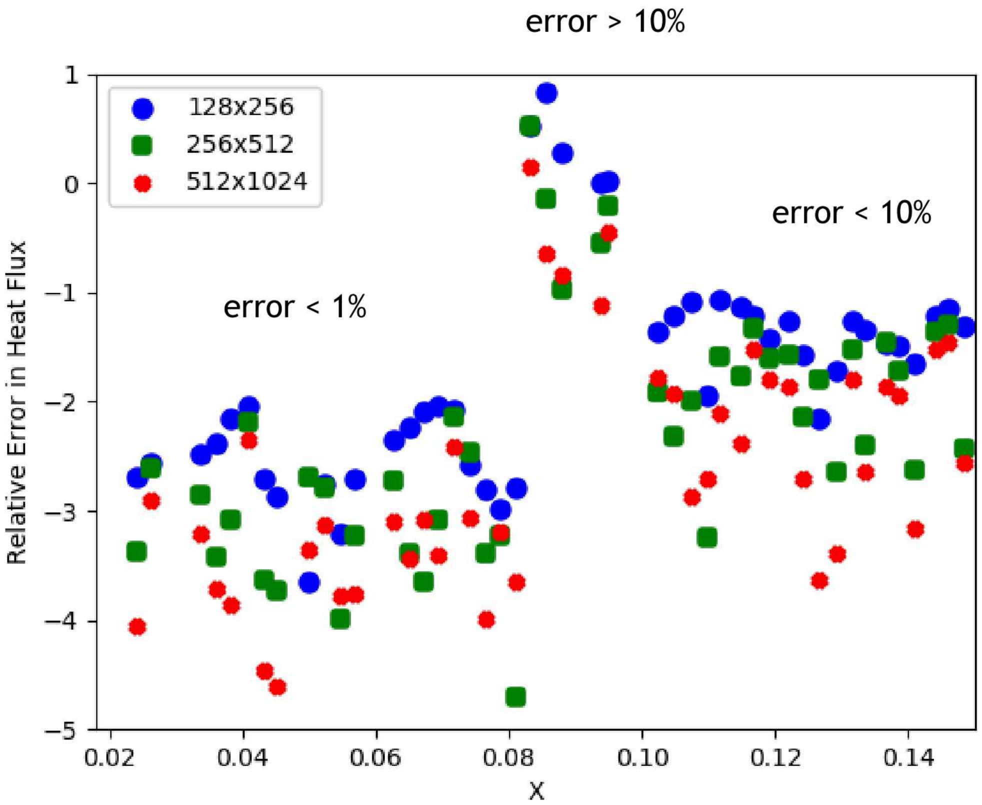




Estimation of Mesh Error: Qualitative or Quantitative?

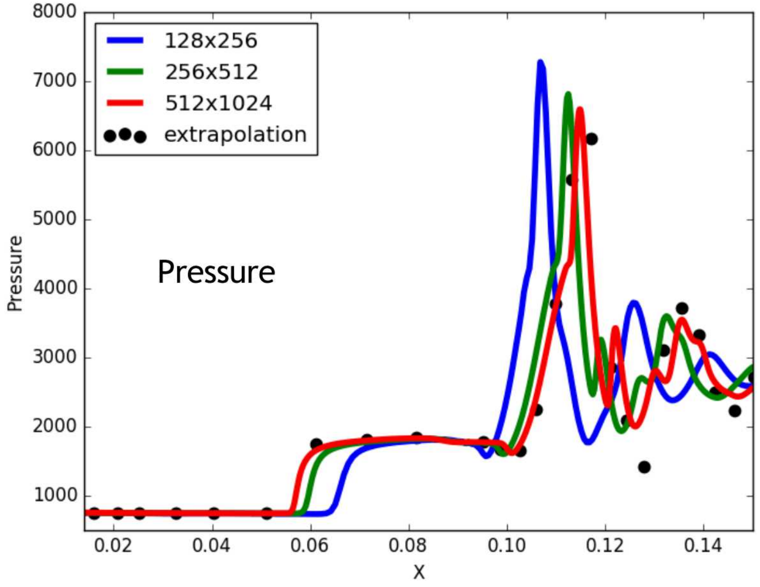
- Quantitative results better justify the nominal mesh (512x1024)
- Can also propagate into model validation
- Mesh converged? Should it be 10% or 1%?

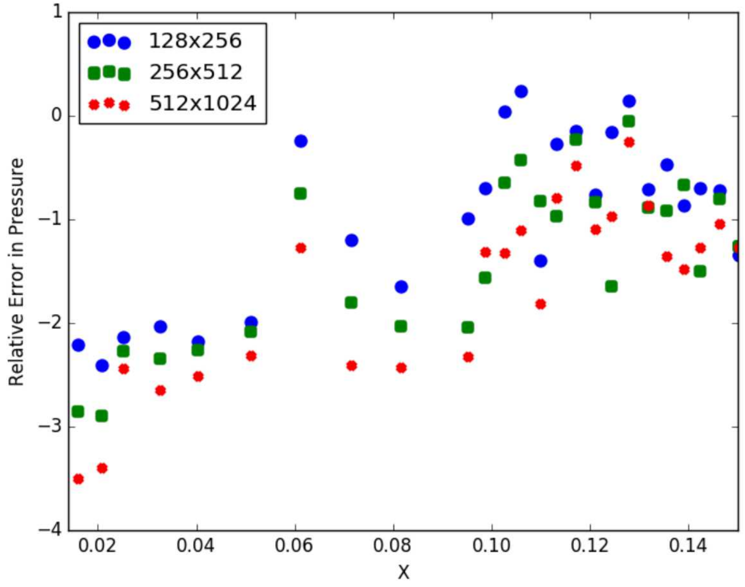


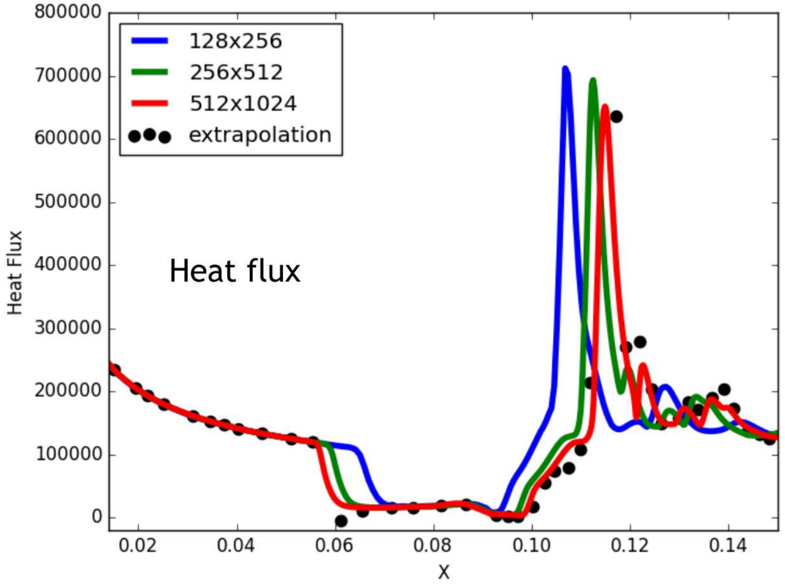


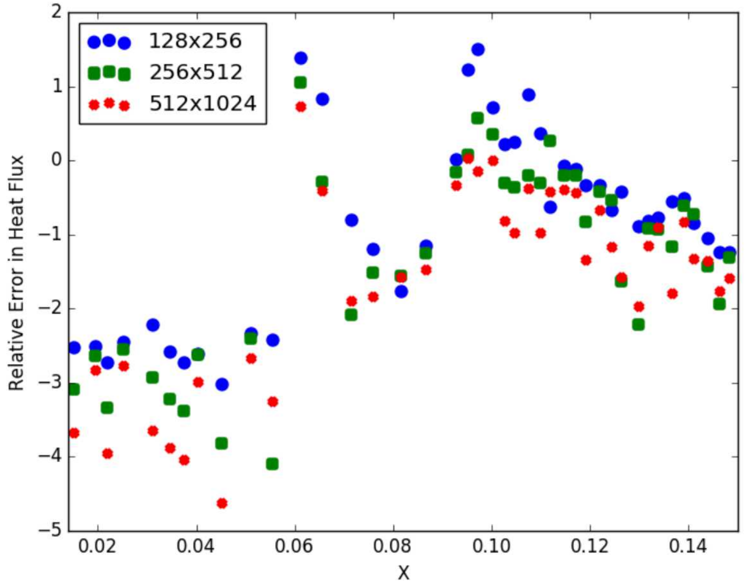
Result: Mesh Error for Double Cone (Low Enthalpy)

- LENS-I Run 35 (Perfect Gas)
- Errors on second cone not resolved even on finest mesh
- Large phase errors:
  - peak pressure / heat flux
  - detachment point
  - re-attachment point
- Should look at additional mesh (1024x2048)





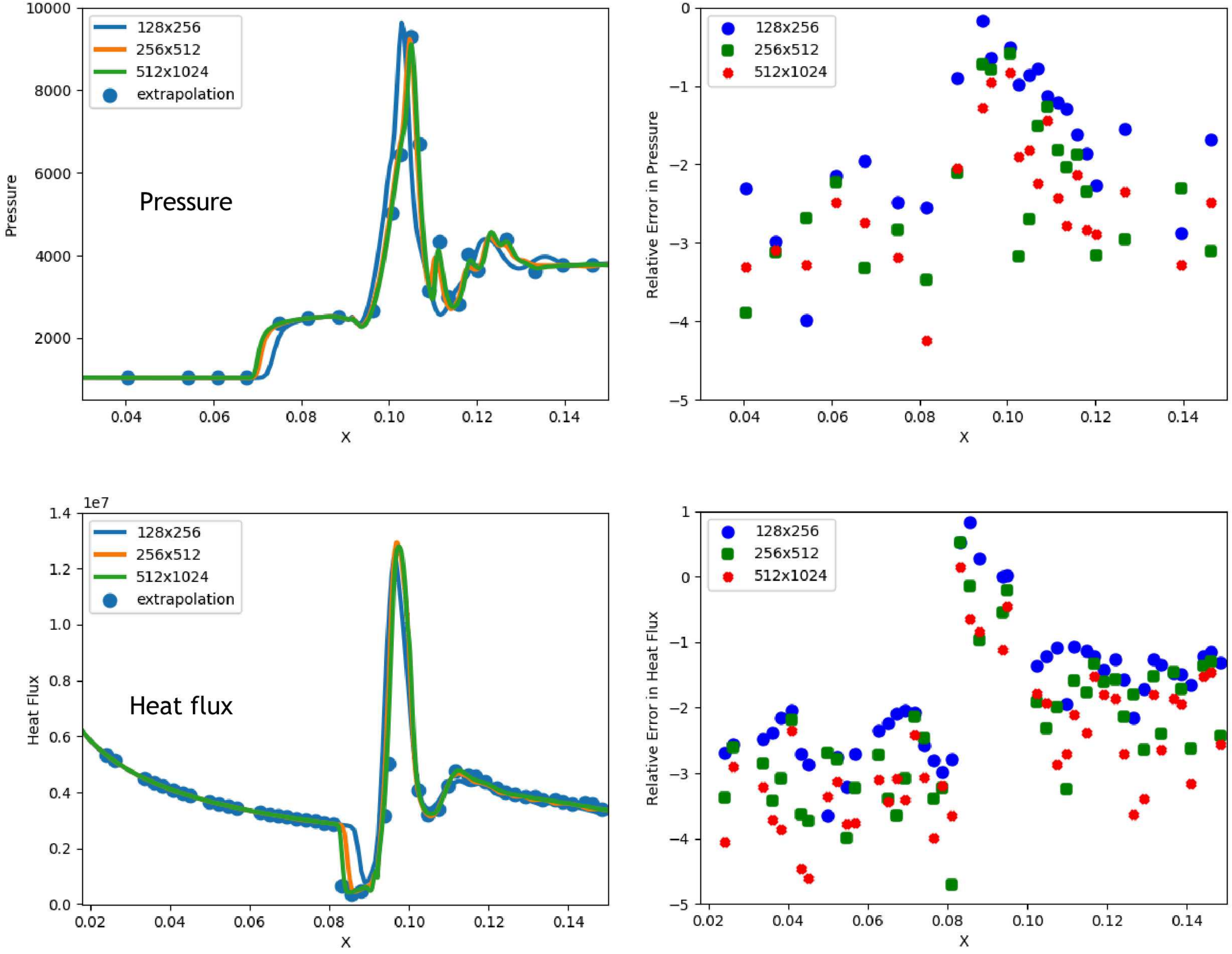




Result: Mesh Error for Double Cone (High Enthalpy)

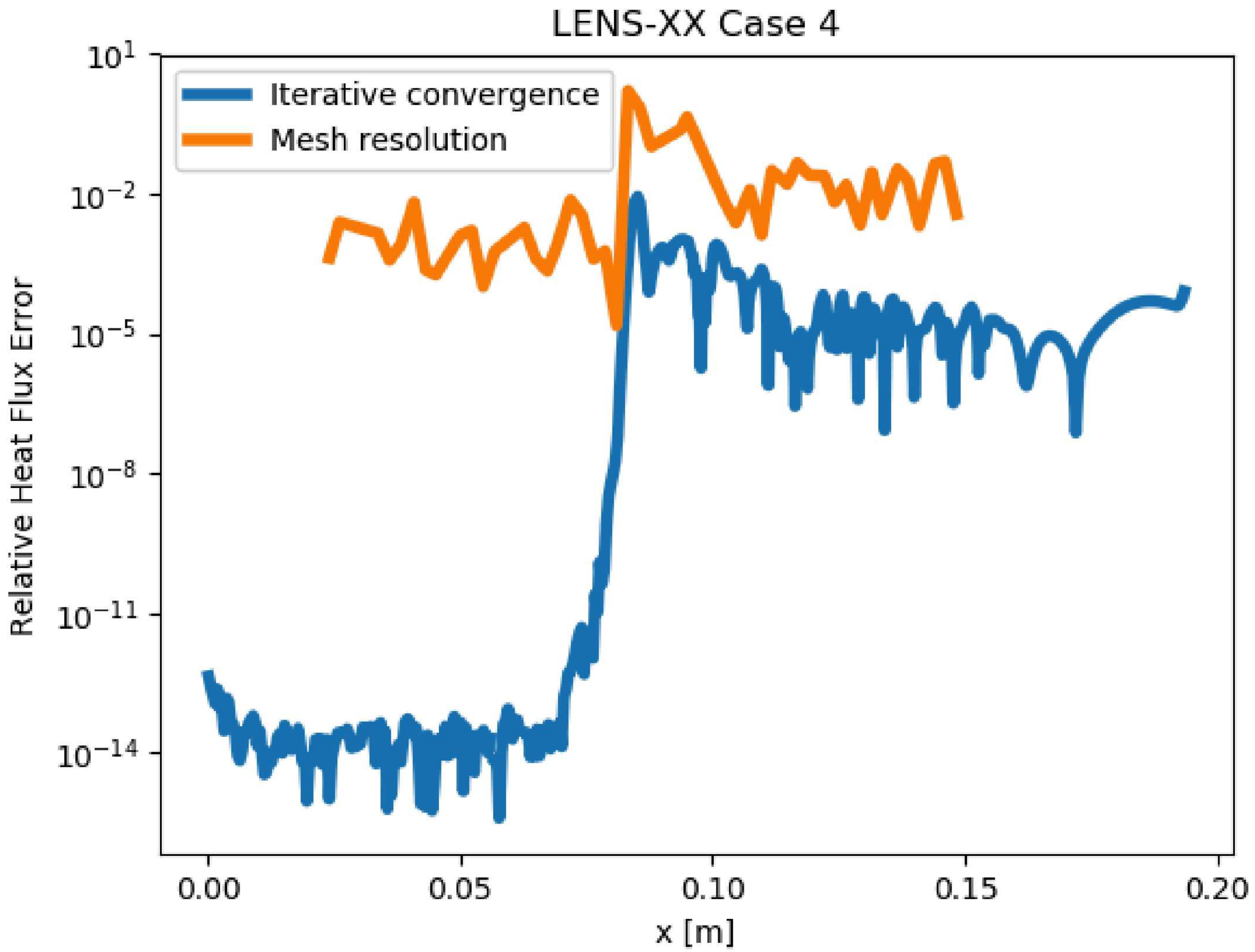
- LENS-XX Case 4 (5sp 2T)
- Compare to LENS-I Run 35:
  - less error with more physics
  - solution on second cone much more resolved

- Experimental locations and model predictions
  - align well with max pressure
  - not aligned with max heat flux



Combining Multiple Error Sources

- LENS-XX Case 4 (5sp 2T)
- Estimate errors in nominal
- Iterative convergence
  - Compare to 100K iterations
- Mesh resolution
  - Compare to 3-mesh extrapolation
- Dominated by mesh error
- Iterative convergence error less than 1% everywhere



Conclusions / Next Steps / Research

- We can provide a robust, quantitative error estimate useful for validation
- Iterative convergence of the flow field is an issue (reacting flow, turbulence) although QoIs may reach steady state

Next steps

- Iterative convergence of residuals should be improved (CFL controller)
- Investigate convergence rates of surface QoIs

Research

- Uncertainty estimates on extrapolation
- Better extrapolation of field data (not just pointwise)