

Automating Fluid Simulations with Discontinuous Petrov-Galerkin Finite Elements

Truman Everett Ellis, PhD

Computational Science, Engineering, and Mathematics

Advisors: *Leszek Demkowicz, Robert Moser*

Collaborators: *Nathan Roberts (Sandia), Jesse Chan (Rice)*



Table of Contents

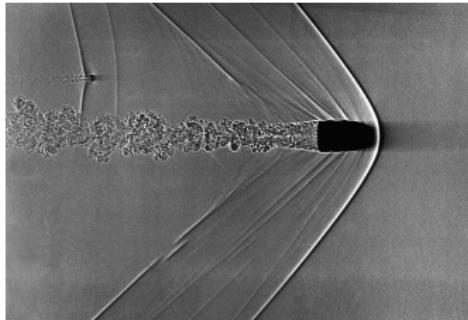
- 1 Motivation: Automating Scientific Computing
- 2 DPG: A Framework for Computational Mechanics
- 3 Space-Time Convection-Diffusion
- 4 Space-Time Compressible Navier-Stokes
- 5 Conclusions

Navier-Stokes Equations

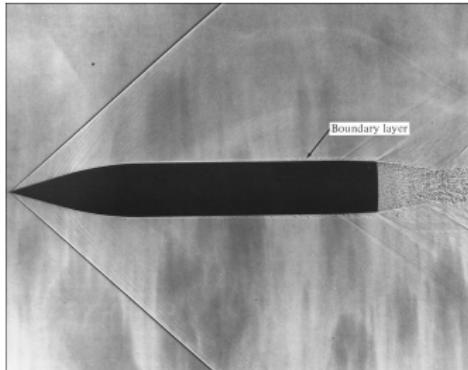
Numerical Challenges

Robust simulation of unsteady fluid dynamics remains a challenging issue.

- Resolving solution features (sharp, localized viscous-scale phenomena)
 - Shocks
 - Boundary layers - resolution needed for drag/load
 - Turbulence (non-localized)
- Stability of numerical schemes
 - Nonlinearity
 - Nature of PDE changes for different flow regimes
 - Coarse/adaptive grids
 - Higher order



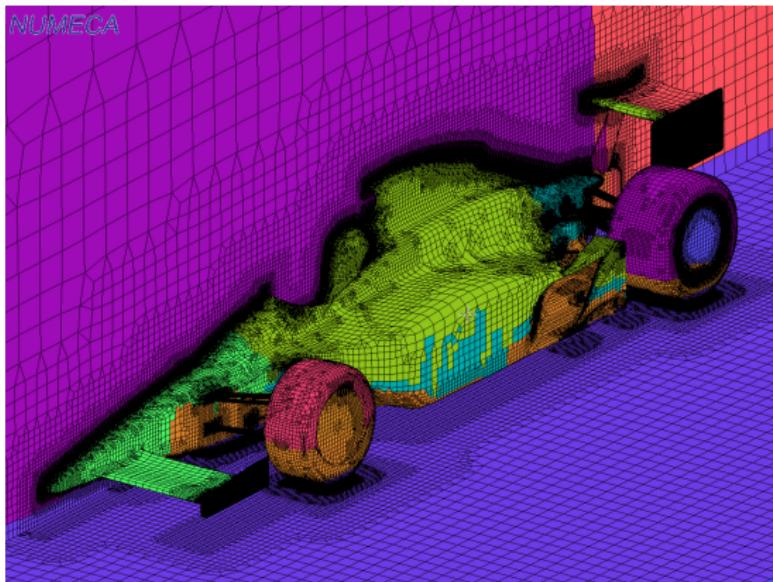
Shock



Motivation

Initial Mesh Design is Expensive and Time-Consuming

- Surface mesh must accurately represent geometry
- Volume mesh needs sufficient resolution for asymptotic regime
- Engineers often forced to work by trial and error
- Bad in the context of HPC

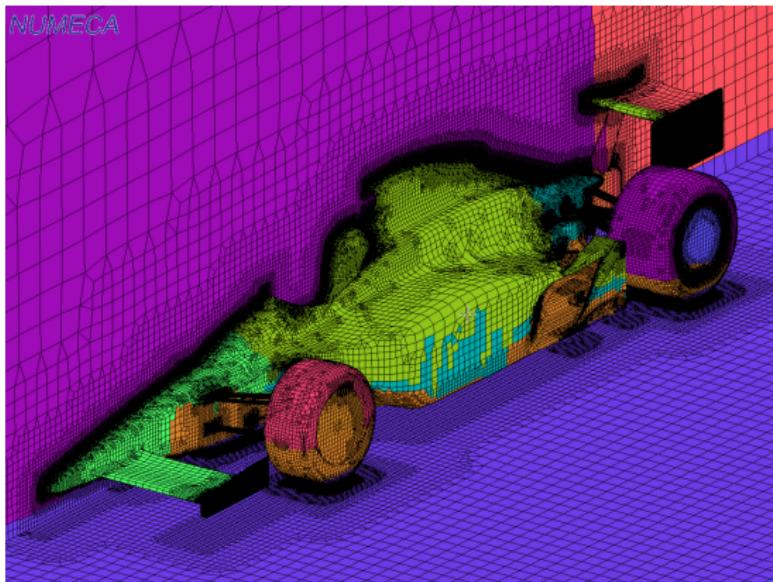


Formula 1 Mesh by Numeca

Motivation

Initial Mesh Design is Expensive and Time-Consuming

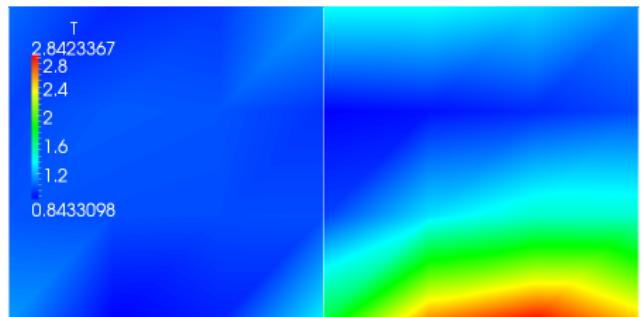
- Surface mesh must accurately represent geometry
- Volume mesh needs sufficient resolution for asymptotic regime
- Engineers often forced to work by trial and error
- Bad in the context of HPC
- We desire an automated computational technology



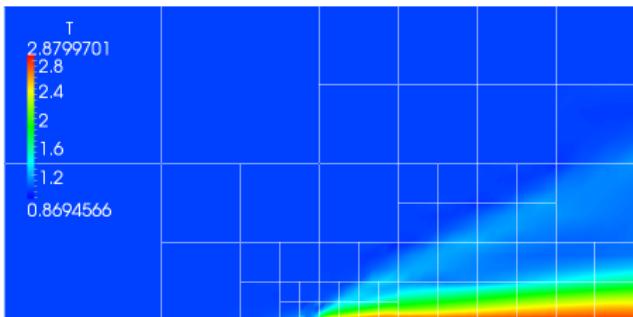
Formula 1 Mesh by Numeca

DPG on Coarse Meshes

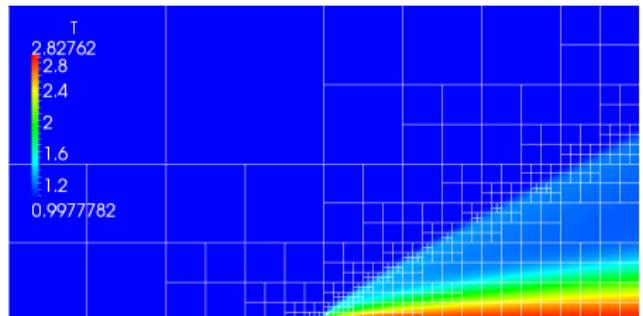
Adaptive Solve of the Carter Plate Problem¹ $Re = 1000$



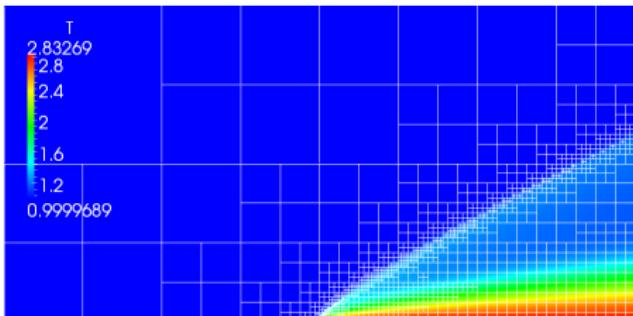
Temperature on Initial Mesh



Temperature after 4 Refinements



Temperature after 8 Refinements



Temperature after 11 Refinements

¹J.L. Chan. "A DPG Method for Convection-Diffusion Problems". PhD thesis. University of Texas at Austin, 2013.

Lessons from Other Methods

Streamline Upwind Petrov-Galerkin: Adaptively changing the test space can produce a method with better stability.

Discontinuous Galerkin: Discontinuous basis functions are a legitimate option for finite element methods.

Hybridized DG: Mesh interface unknowns can facilitate static condensation -- reducing the number of DOFs in the global solve.

Least-Squares FEM: The finite element method is most powerful in a minimum residual context (i.e. as a Ritz method).

Space-Time FEM: Highly adaptive methods should have adaptive time integration. Superior framework for problems with moving boundaries. Requires a method that is both temporally and spatially stable.

Motivation

DPG Summary

Overview of Features

- Stable for any well-posed variational problem
- Robust for singularly perturbed problems
- Works in the preasymptotic regime
- Designed for adaptive mesh refinement

DPG is a minimum residual method:

$$u_h = \arg \min_{w_h \in U_h} \frac{1}{2} \|Bw_h - l\|_{V'}^2$$



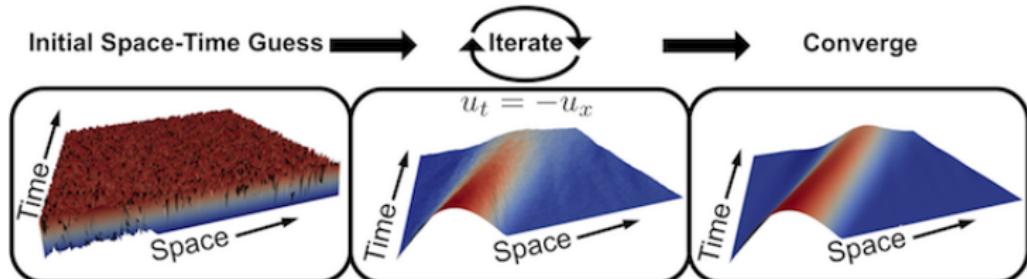
$$b(u_h, R_V^{-1} B \delta u_h) = l(R_V^{-1} B \delta u_h) \quad \forall \delta u_h \in U_h$$

where $v_{\delta u_h} := R_V^{-1} B \delta u_h$ are the **optimal test functions**.

Space-Time DPG

Extending DPG to Transient Problems

- Time stepping techniques are not ideally suited to highly adaptive grids
- Space-time FEM proposed as a solution
 - ✓ Unified treatment of space and time
 - ✓ Local space-time adaptivity (local time stepping)
 - ✓ Parallel-in-time integration (space-time multigrid)
 - ✗ Spatially stable FEM methods may not be stable in space-time
 - ✗ Need to support higher dimensional problems
- DPG provides necessary stability and adaptivity



Courtesy of XBraid by LLNL

Space-Time DPG for Convection-Diffusion

Space-Time Divergence Form

Equation is parabolic in space-time.

$$\frac{\partial u}{\partial t} + \beta \cdot \nabla u - \epsilon \Delta u = f$$

This is just a composition of a constitutive law and conservation of mass.

$$\sigma - \epsilon \nabla u = 0$$

$$\frac{\partial u}{\partial t} + \nabla \cdot (\beta u - \sigma) = f$$

We can rewrite this in terms of a space-time divergence.

$$\begin{aligned} \frac{1}{\epsilon} \sigma - \nabla u &= 0 \\ \nabla_{xt} \cdot \begin{pmatrix} \beta u - \sigma \\ u \end{pmatrix} &= f \end{aligned}$$

Space-Time DPG for Convection-Diffusion

Ultra-Weak Formulation with Discontinuous Test Functions

Multiply by test function and integrate by parts over space-time element K.

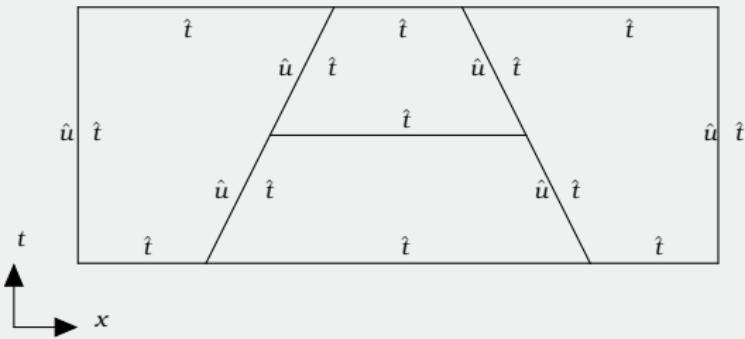
$$\begin{aligned} \left(\frac{1}{\epsilon} \boldsymbol{\sigma}, \boldsymbol{\tau} \right)_K + (u, \nabla \cdot \boldsymbol{\tau})_K - \langle \hat{u}, \boldsymbol{\tau} \cdot \mathbf{n}_x \rangle_{\partial K} &= 0 \\ - \left(\begin{pmatrix} \beta u - \boldsymbol{\sigma} \\ u \end{pmatrix}, \nabla_{xt} v \right)_K + \langle \hat{t}, v \rangle_{\partial K} &= f \end{aligned}$$

where

$$\hat{u} := \text{tr}(u)$$

$$\begin{aligned} \hat{t} &:= \text{tr}(\beta u - \boldsymbol{\sigma}) \cdot \mathbf{n}_x \\ &\quad + \text{tr}(u) \cdot n_t \end{aligned}$$

Support of Trace Variables



- Trace \hat{u} defined on spatial boundaries
- Flux \hat{t} defined on all boundaries

Space-Time Compressible Navier-Stokes

First Order System with Primitive Variables

Assuming Stokes hypothesis, ideal gas law, and constant viscosity:

$$\frac{1}{\mu} \mathbb{D} - \nabla \mathbf{u} = 0$$

$$\frac{Pr}{C_p \mu} \mathbf{q} + \nabla T = 0$$

$$\nabla_{xt} \cdot \begin{pmatrix} \rho \mathbf{u} \\ \rho \end{pmatrix} = f_c$$

$$\nabla_{xt} \cdot \begin{pmatrix} \rho \mathbf{u} \otimes \mathbf{u} + \rho R T \mathbb{I} - (\mathbb{D} + \mathbb{D}^T - \frac{2}{3} \text{tr}(\mathbb{D}) \mathbb{I}) \\ \rho \mathbf{u} \end{pmatrix} = \mathbf{f}_m$$

$$\nabla_{xt} \cdot \begin{pmatrix} \rho \mathbf{u} (C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}) + \rho R T \mathbf{u} + \mathbf{q} - \mathbf{u} \cdot (\mathbb{D} + \mathbb{D}^T - \frac{2}{3} \text{tr}(\mathbb{D}) \mathbb{I}) \\ \rho (C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}) \end{pmatrix} = f_e$$

Space-Time Compressible Navier-Stokes

Compact Notation

Conserved quantities

$$C_c := \rho$$

$$\mathbf{C}_m := \rho \mathbf{u}$$

$$C_e := \rho(C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u})$$

Euler fluxes

$$\mathbf{F}_c := \rho \mathbf{u}$$

$$\mathbb{F}_m := \rho \mathbf{u} \otimes \mathbf{u} + \rho R T \mathbb{I}$$

$$\mathbf{F}_e := \rho \mathbf{u} \left(C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) + \rho R T \mathbf{u}$$

Viscous fluxes

$$\mathbf{K}_c := \mathbf{0}$$

$$\mathbb{K}_m := \mathbb{D} + \mathbb{D}^T - \frac{2}{3} \text{tr}(\mathbb{D}) \mathbb{I}$$

$$\mathbf{K}_e := -\mathbf{q} + \mathbf{u} \cdot \left(\mathbb{D} + \mathbb{D}^T - \frac{2}{3} \text{tr}(\mathbb{D}) \mathbb{I} \right)$$

Viscous variables

$$\mathbb{M}_{\mathbb{D}} := \mathbb{D}$$

$$\mathbf{M}_q := \frac{Pr}{C_p} \mathbf{q}$$

$$\mathbf{G}_{\mathbb{D}} := 2\mathbf{u}$$

$$G_q := -T$$

Space-Time Compressible Navier-Stokes

Define Group Variables

Group terms

$$C := \{C_c, \mathbf{C}_m, C_e\}$$

$$F := \{\mathbf{F}_c, \mathbb{F}_m, \mathbf{F}_e\}$$

$$K := \{\mathbf{K}_c, \mathbb{K}_m, \mathbf{K}_e\}$$

$$M := \{\mathbb{M}_{\mathbb{D}}, \mathbf{M}_{\mathbf{q}}\}$$

$$G := \{\mathbf{G}_{\mathbb{D}}, G_{\mathbf{q}}\}$$

$$f := \{f_c, \mathbf{f}_m, f_e\}$$

Group variables

$$W := \{\rho, \mathbf{u}, T\}$$

$$\hat{W} := \{2\hat{\mathbf{u}}, -\hat{T}\}$$

$$\Sigma := \{\mathbb{D}, \mathbf{q}\}$$

$$\hat{t} := \{\hat{t}_e, \hat{\mathbf{t}}_m, , \hat{t}_e\}$$

$$\Psi := \{\mathbb{S}, \tau\}$$

$$V := \{v_c, \mathbf{v}_m, , v_e\}$$

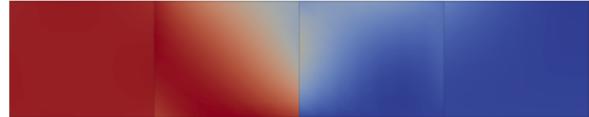
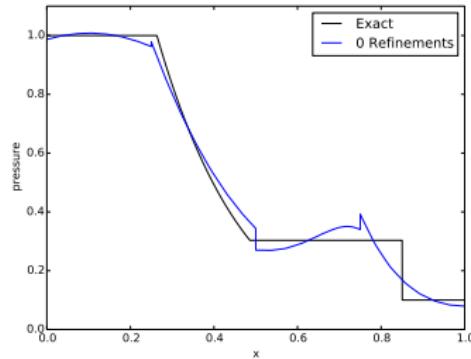
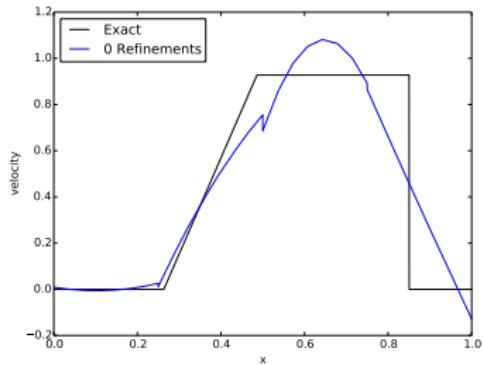
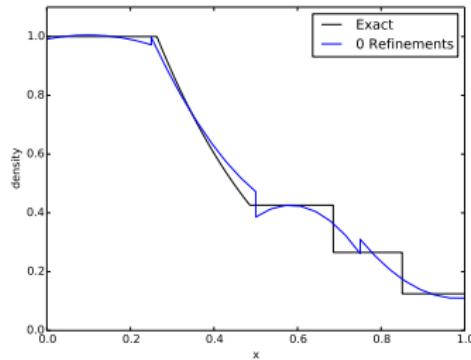
Navier-Stokes variational formulation is

$$\left(\frac{1}{\mu} M, \Psi \right) + (G, \nabla \cdot \Psi) - \langle \hat{W}, \Psi \cdot \mathbf{n}_x \rangle = 0$$

$$- \left(\begin{pmatrix} F - K \\ C \end{pmatrix}, \nabla_{xt} V \right) + \langle \hat{t}, V \rangle = (f, V)$$

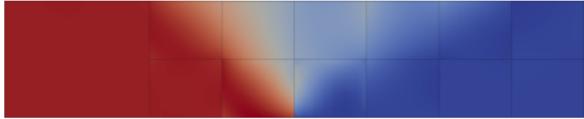
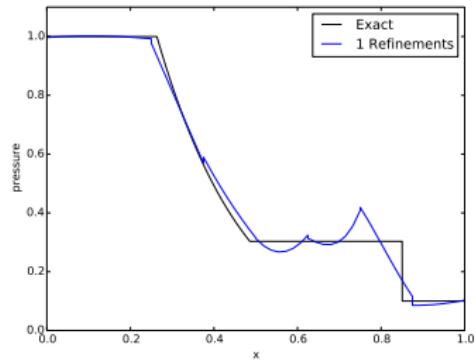
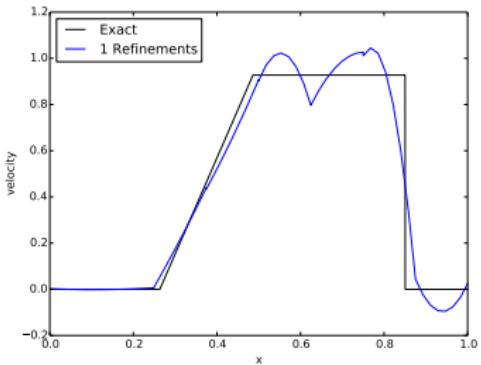
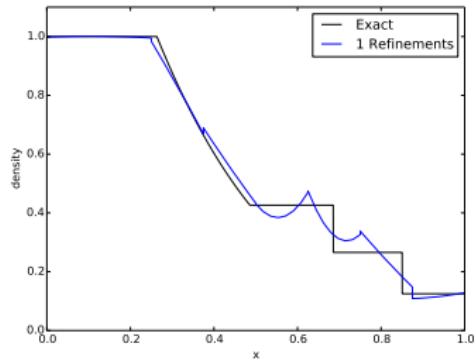
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



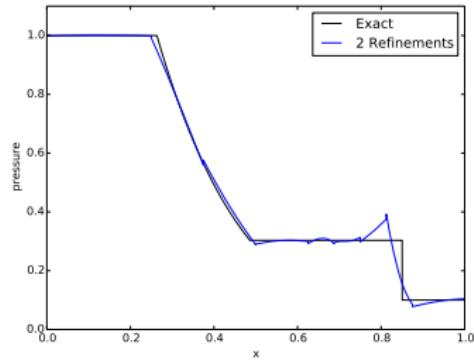
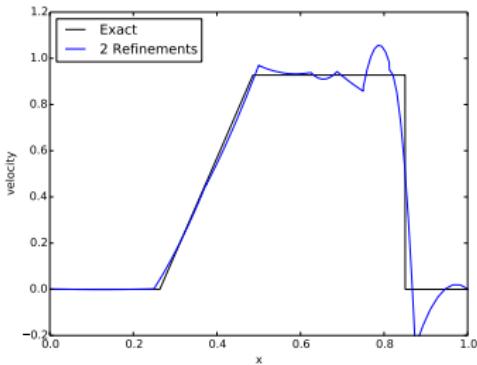
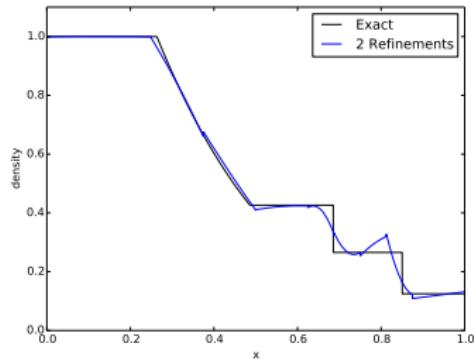
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



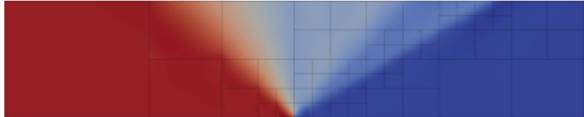
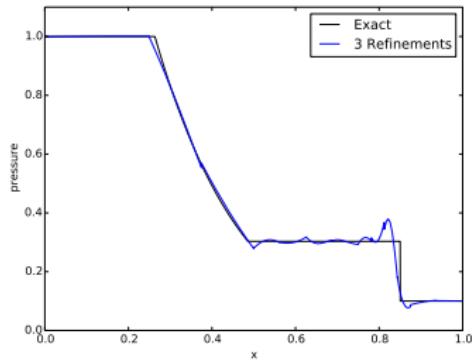
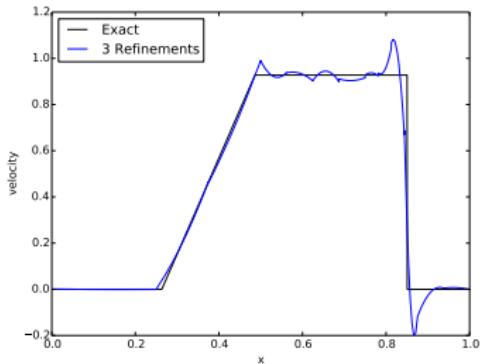
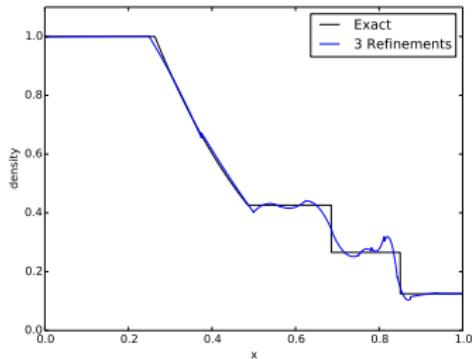
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



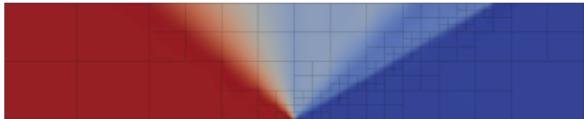
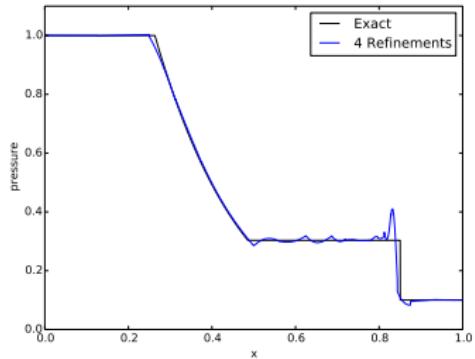
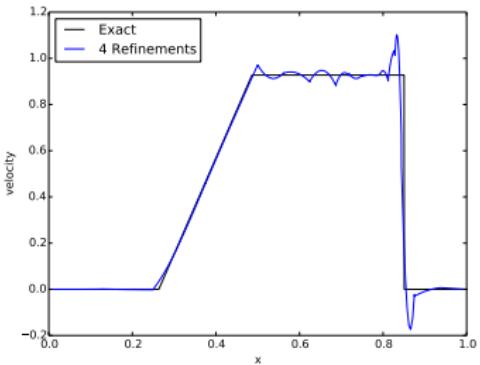
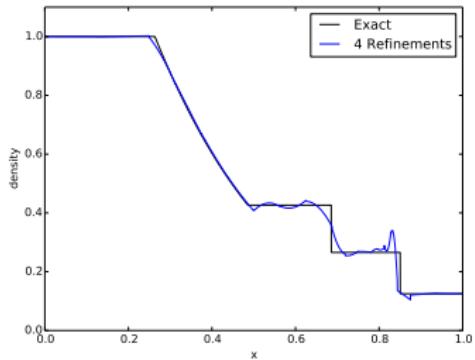
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



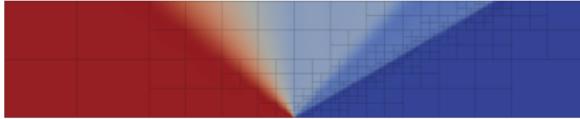
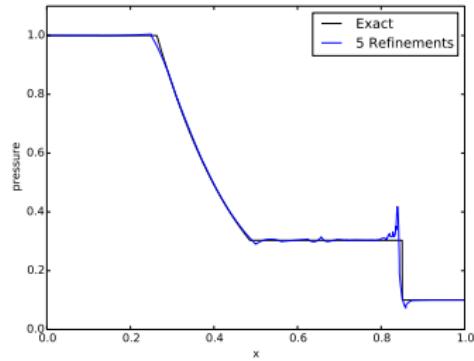
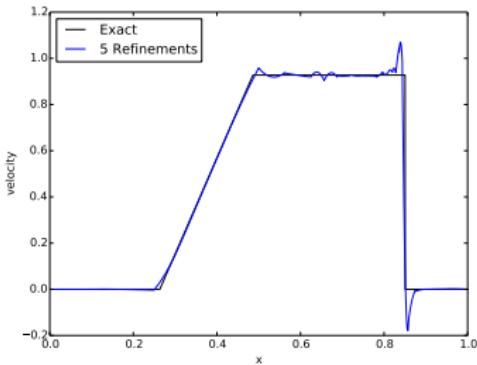
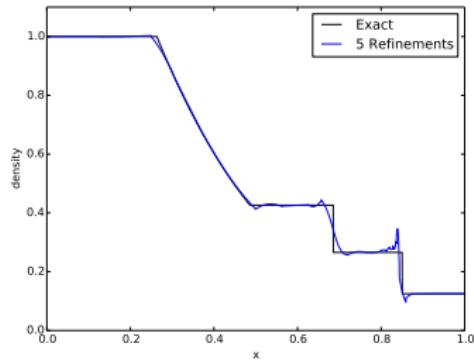
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



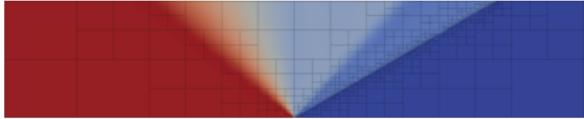
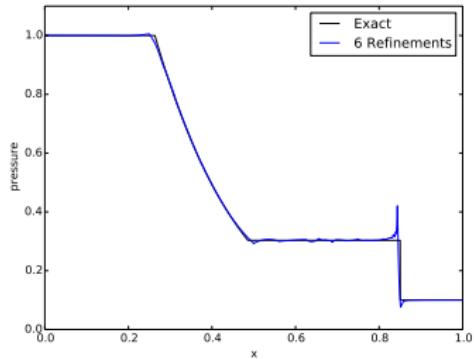
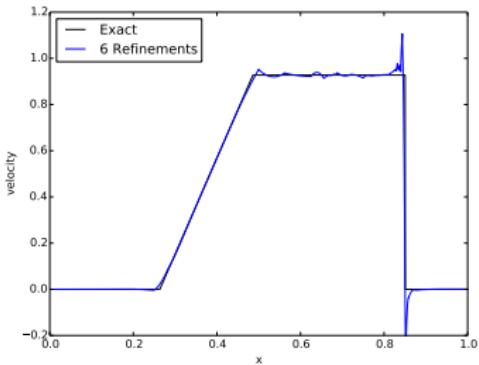
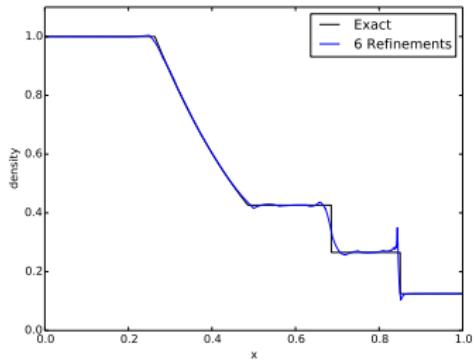
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



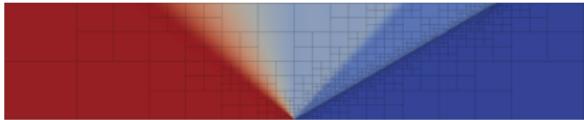
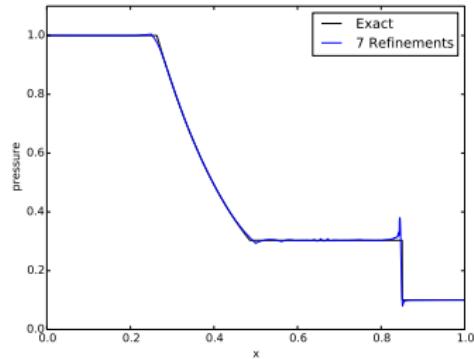
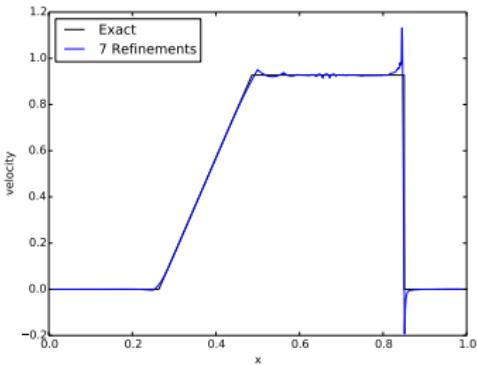
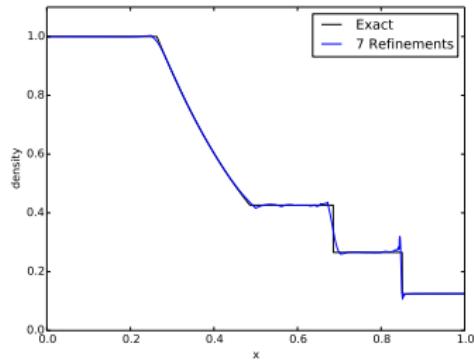
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



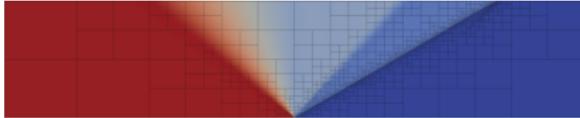
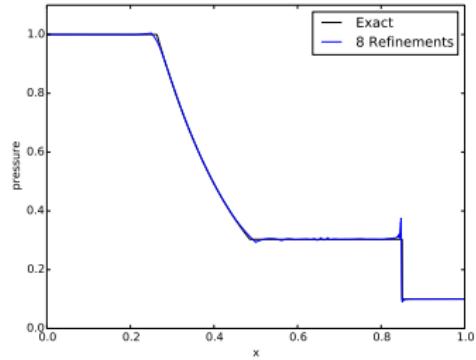
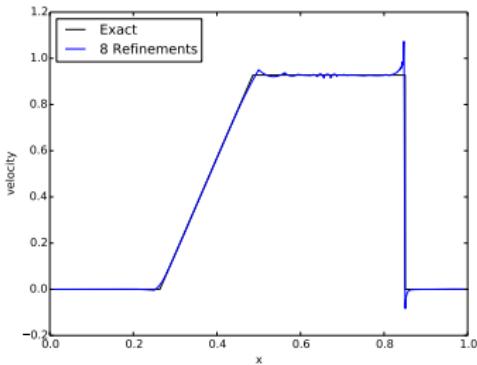
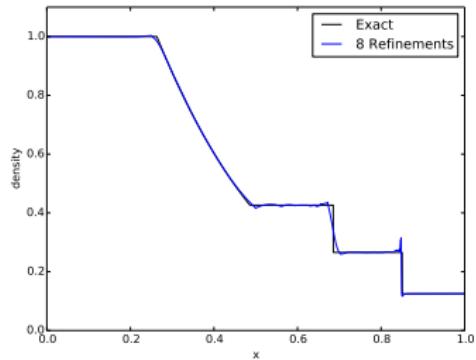
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



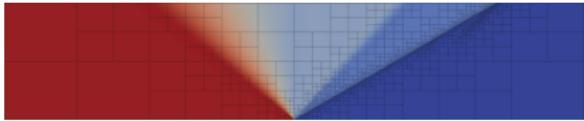
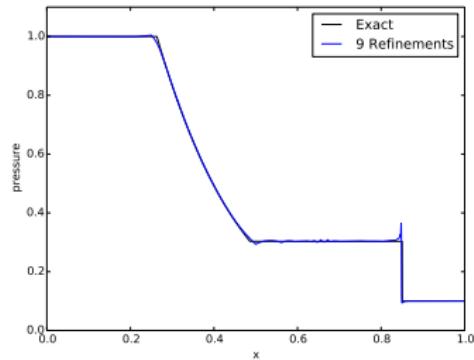
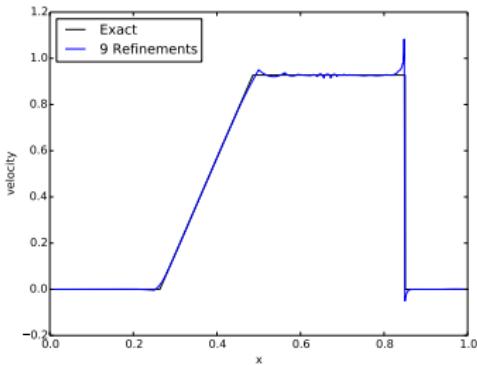
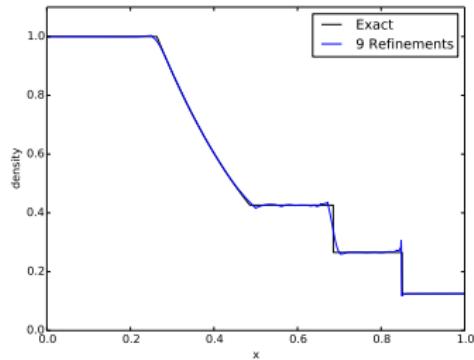
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



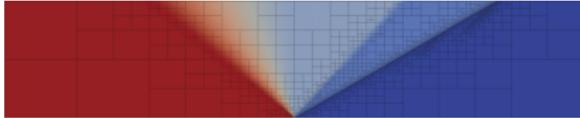
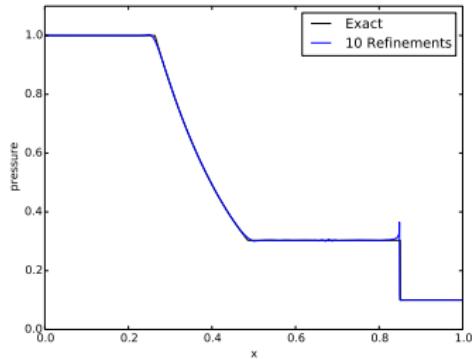
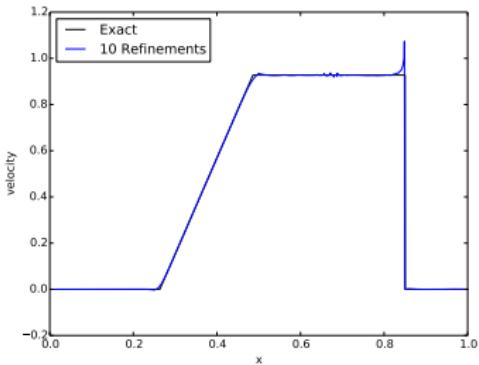
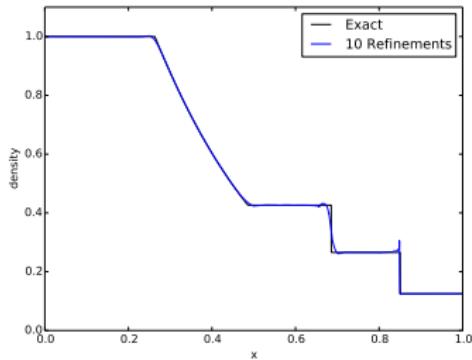
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



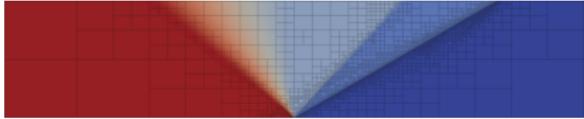
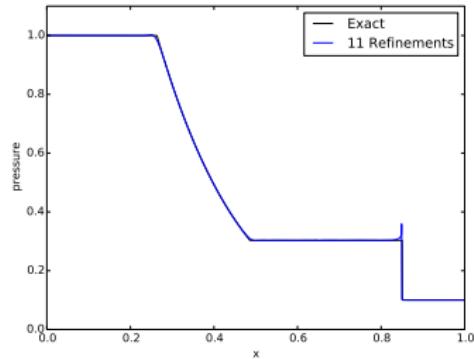
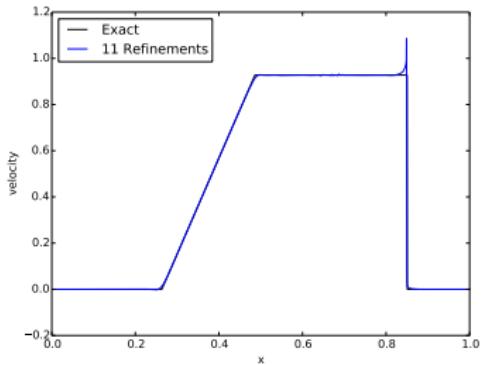
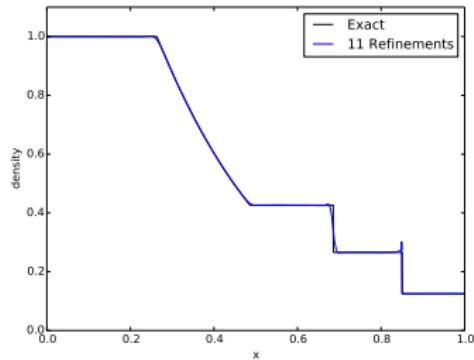
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



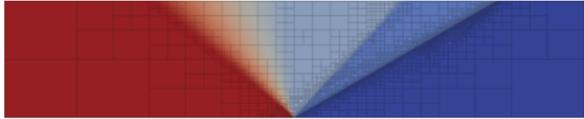
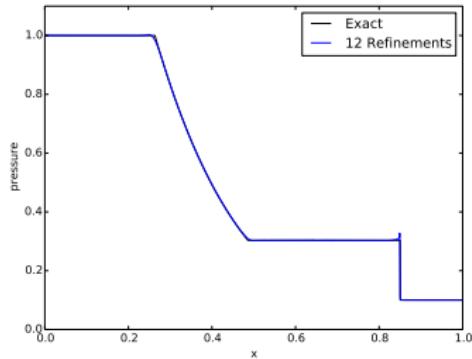
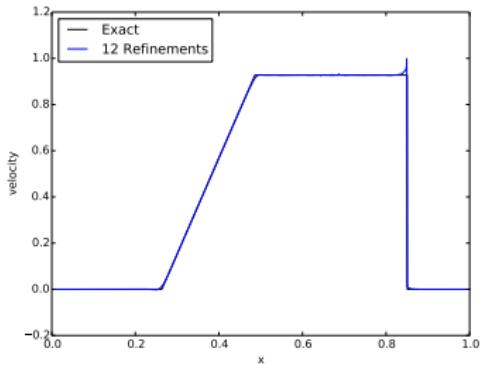
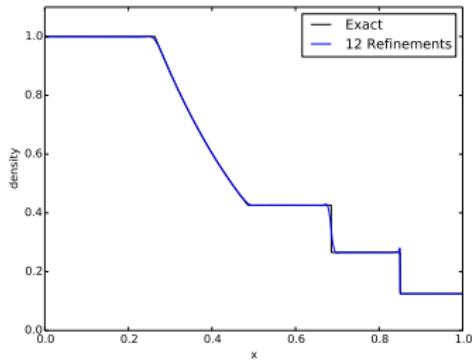
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



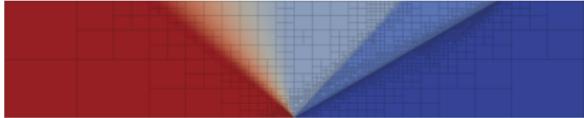
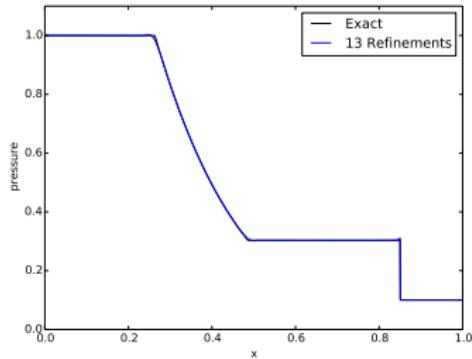
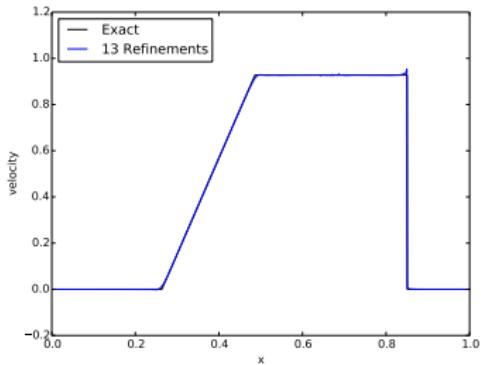
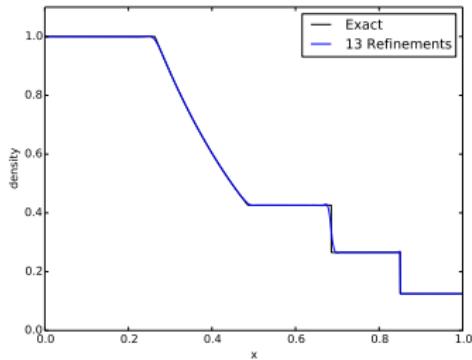
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



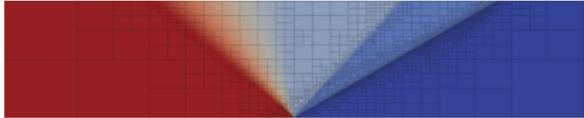
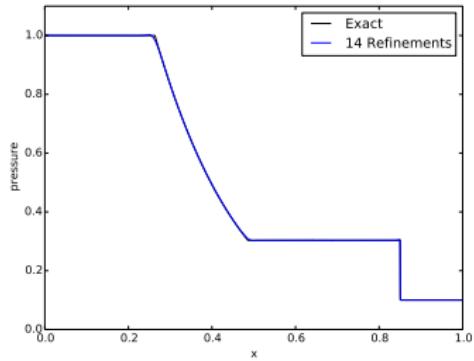
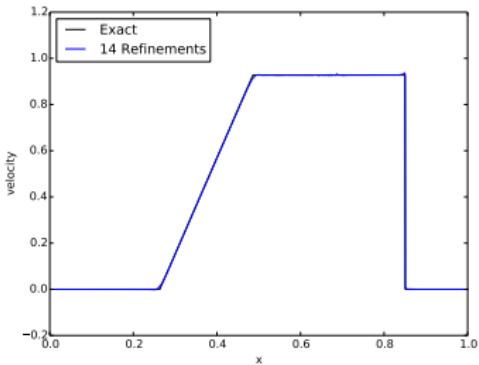
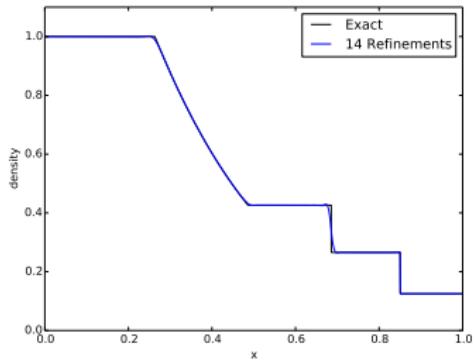
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$



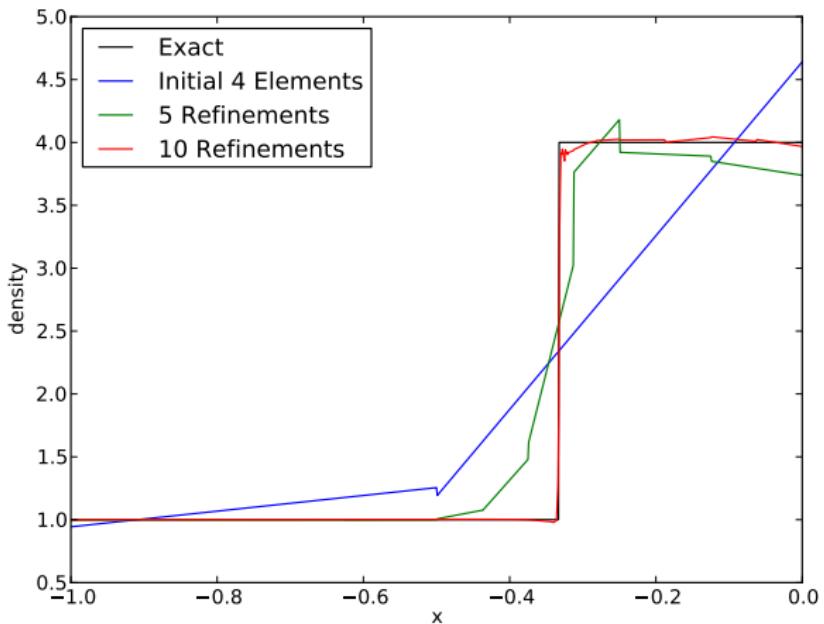
Compressible Navier-Stokes

Sod Shock Tube with $\mu = 10^{-5}$

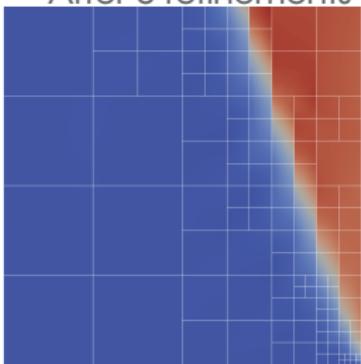


Space-Time Compressible Navier-Stokes

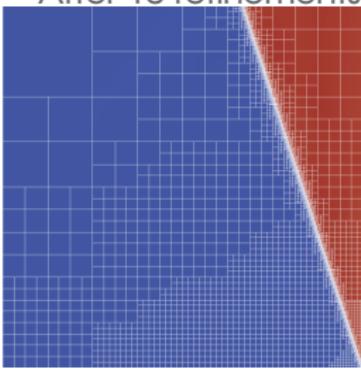
Noh Implosion with $\mu = 10^{-3}$



After 5 refinements



After 10 refinements



Space-Time Compressible Navier-Stokes

Piston with $\mu = 10^{-2}$

$$\hat{t}_c = \sqrt{2}(-\rho u + \rho)$$

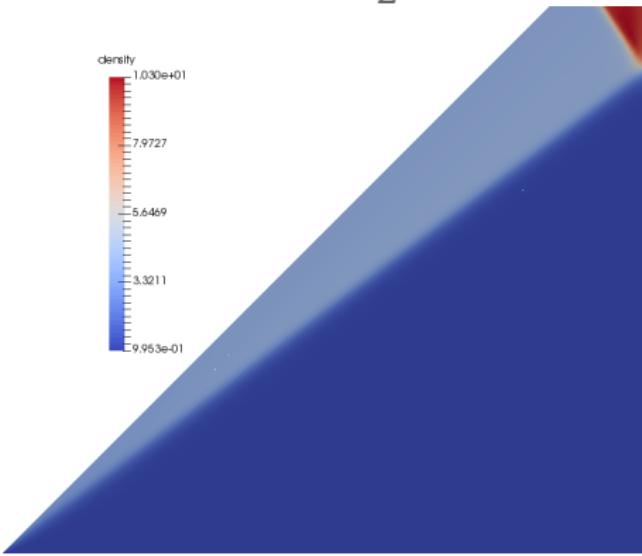
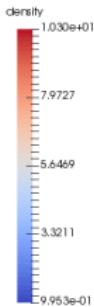
$$\hat{u} = 1$$

$$\hat{t}_m = \sqrt{2}(-\rho u^2 - \rho RT + \rho u)$$

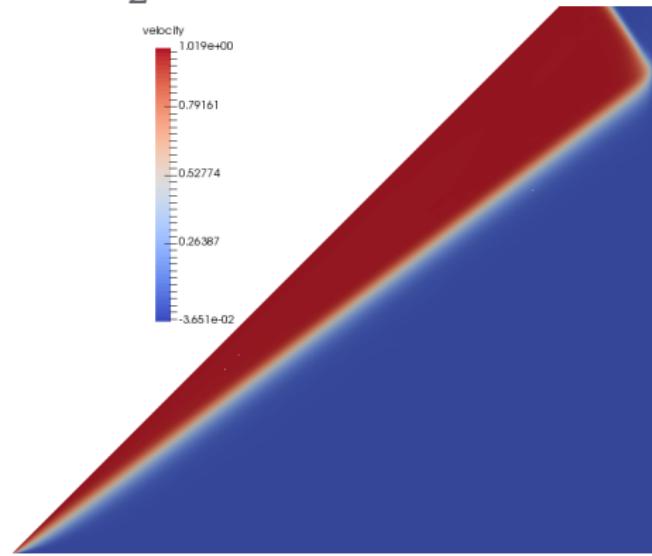
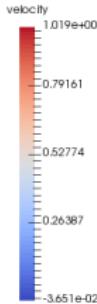
$$\hat{t}_c = 0$$

$$\hat{t}_e = \sqrt{2}(-\rho u(C_v T + \frac{1}{2}u^2) - u\rho RT + \rho(C_v T + \frac{1}{2}u^2))$$

$$\hat{t}_m - \hat{t}_e = 0$$



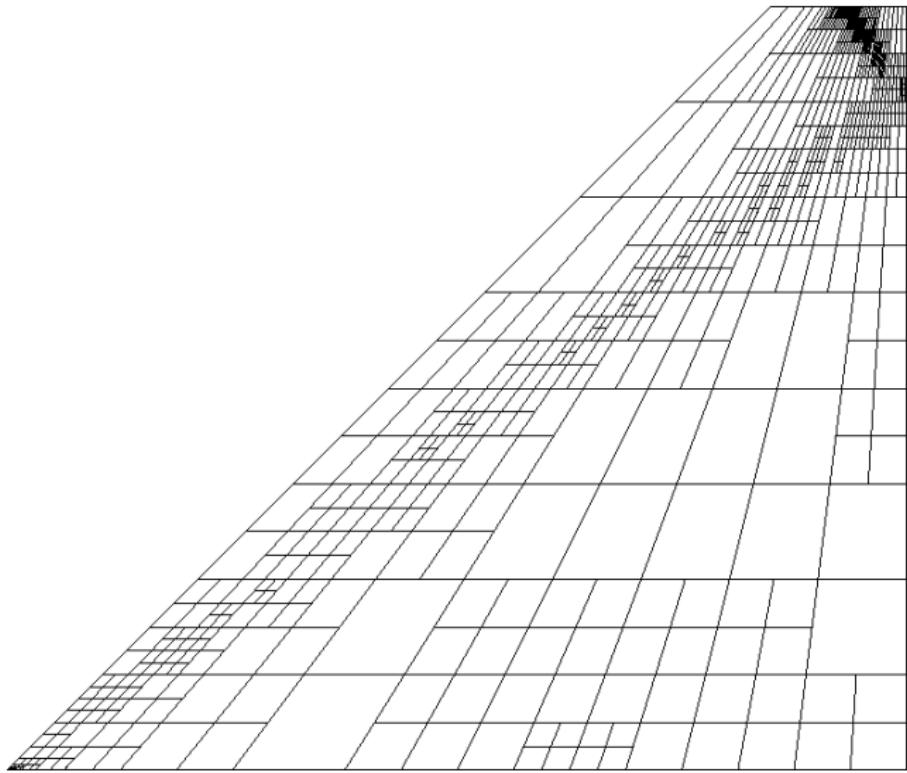
Density



Velocity

Space-Time Compressible Navier-Stokes

Piston with $\mu = 10^{-2}$



Mesh after 8 adaptive refinements

Conclusions and Epilogue

Research is fun: But my passion lies in solving real world engineering problems.

Current Work:

- **Plasma Physics:** Contributing to a highly scalable, production plasma physics code. Uses the Kokkos library to leverage parallelism of next generation HPC architectures.
- **Electromagnetics Simulations:** Running radar cross-section simulations using commercial and research codes as part of a verification study.
- **Stochastic Richardson Extrapolation:** Parallelized a Python code to do QOI prediction of stochastic simulations.
- **Particle Accelerator:** Jumped in on work with the HERMES III particle accelerator to study EMP effects on electrical components.
- **Project Management:** Learning agile development practices and taking responsibility for project management tasks within our group.

Myself in Four Thousand Words

