Automating Scientific Computing with Discontinuous Petrov-Galerkin Finite Elements

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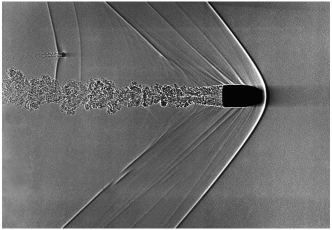
Navier-Stokes Equations

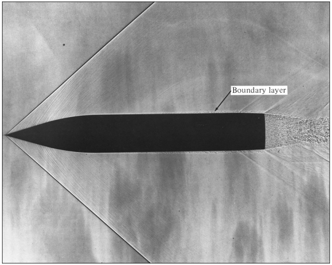
Numerical Challenges

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

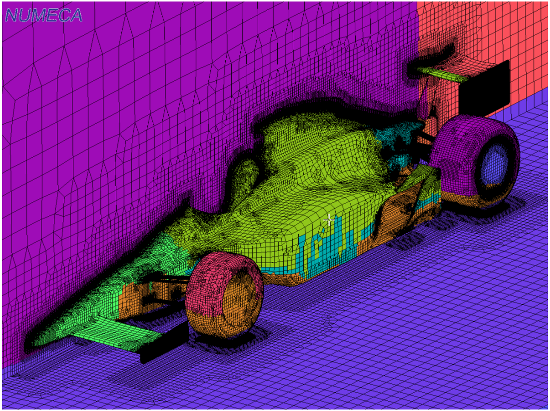


Boundary layer

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
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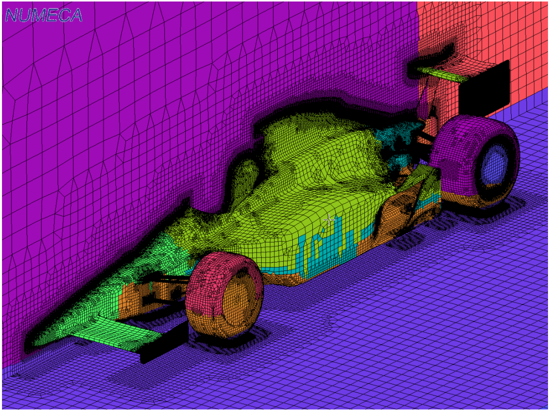
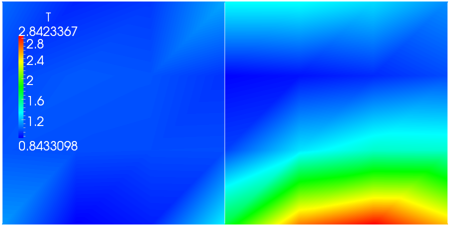
- Engineers often forced to work by trial and error
- Bad in the context of HPC
- We desire an automated computational technology



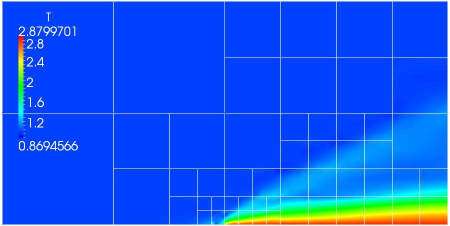
Formula 1 Mesh by Numeca

DPG on Coarse Meshes

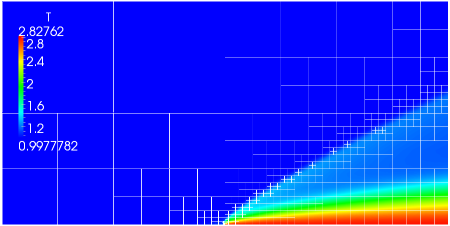
Adaptive Solve of the Carter Plate Problem[1] $Re = 1000$



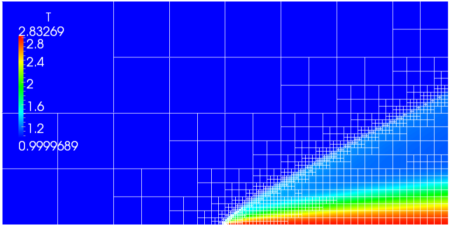
Temperature on Initial Mesh



Temperature after 4 Refinements



Temperature after 8 Refinements



Temperature after 11 Refinements

[1] J.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:

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

$$\Updownarrow$$

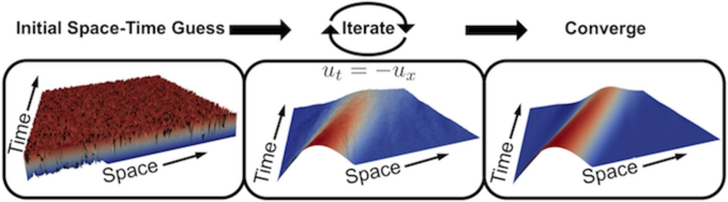
$$b(u_h, R_V^{-1} B\delta u_h) = l(R_V^{-1} B\delta u_h) \quad \forall \delta u_h \in U_h$$

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

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Equation is parabolic in space-time.

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

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

$$\begin{aligned} \boldsymbol{\sigma} - \epsilon \nabla u &= 0 \\ \frac{\partial u}{\partial t} + \nabla \cdot (\boldsymbol{\beta} u - \boldsymbol{\sigma}) &= f \end{aligned}$$

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

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

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.

$$\left(\frac{1}{\epsilon}\boldsymbol{\sigma},\boldsymbol{\tau}\right)_K + (u,\nabla\cdot\boldsymbol{\tau})_K - \langle\hat{u},\boldsymbol{\tau}\cdot\boldsymbol{n}_x\rangle_{\partial K} = 0$$

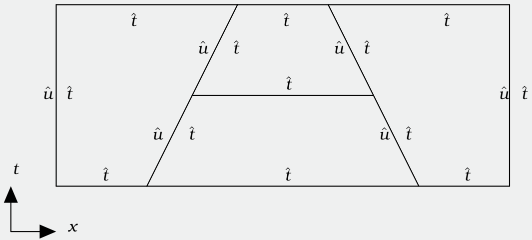
$$-\left(\begin{pmatrix}\beta u-\boldsymbol{\sigma}\\ u\end{pmatrix},\nabla_{xt}v\right)_K + \langle\hat{t},v\rangle_{\partial K} = f$$

where

$$\hat{u} := \mathrm{tr}(u)$$
$$\hat{t} := \mathrm{tr}(\beta u-\boldsymbol{\sigma})\cdot\boldsymbol{n}_x + \mathrm{tr}(u)\cdot n_t$$

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

Support of Trace Variables



Space-Time Compressible Navier-Stokes

First Order System with Primitive Variables

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

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

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

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

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

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

Compact Notation

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Conserved quantities

$$C_c := \rho$$
$$\boldsymbol{C}_m := \rho \boldsymbol{u}$$
$$C_e := \rho(C_v T + \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u})$$

Euler fluxes

$$\boldsymbol{F}_c := \rho \boldsymbol{u}$$
$$\mathbb{F}_m := \rho \boldsymbol{u} \otimes \boldsymbol{u} + \rho R T \mathbb{I}$$
$$\boldsymbol{F}_e := \rho \boldsymbol{u}\left(C_v T + \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u}\right) + \rho R T \boldsymbol{u}$$

Viscous fluxes

$$\boldsymbol{K}_c := \boldsymbol{0}$$
$$\mathbb{K}_m := \mathbb{D} + \mathbb{D}^T - \frac{2}{3}\operatorname{tr}(\mathbb{D})\mathbb{I}$$
$$\boldsymbol{K}_e := -\boldsymbol{q} + \boldsymbol{u}\cdot\left(\mathbb{D} + \mathbb{D}^T - \frac{2}{3}\operatorname{tr}(\mathbb{D})\mathbb{I}\right)$$

Viscous variables

$$\mathbb{M}_{\mathbb{D}} := \mathbb{D}$$
$$\boldsymbol{M}_{\boldsymbol{q}} := \frac{Pr}{C_p}\boldsymbol{q}$$
$$\boldsymbol{G}_{\mathbb{D}} := 2\boldsymbol{u}$$
$$G_{\boldsymbol{q}} := -T$$

Define Group Variables

Group terms

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

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

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

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

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

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

Group variables

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

$$\hat{W} := \left\{2\hat{\boldsymbol{u}}\,,\ -\hat{T}\right\}$$

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

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

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

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

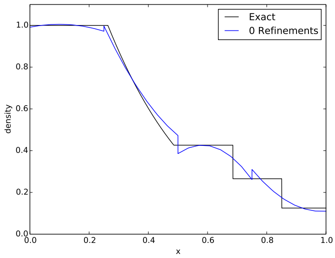
Navier-Stokes variational formulation is

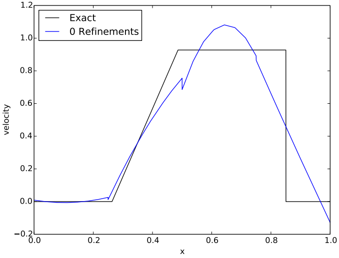
$$\left(\frac{1}{\mu}M, \Psi\right) + (G, \nabla\cdot\Psi) - \left\langle \hat{W}, \Psi\cdot\boldsymbol{n}_x\right\rangle = 0$$

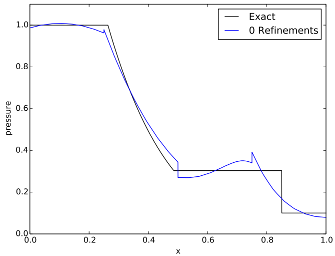
$$-\left(\begin{pmatrix} F-K \\ C \end{pmatrix}, \nabla_{xt} V\right) + \langle \hat{t}, V\rangle = (f, V)$$

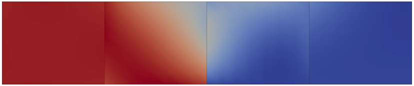
Compressible Navier-Stokes

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









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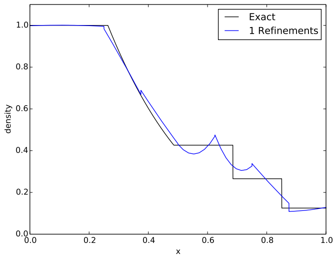

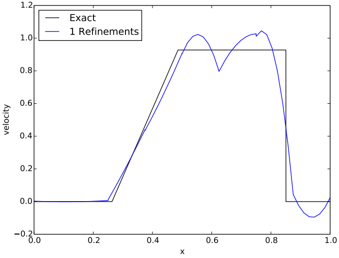

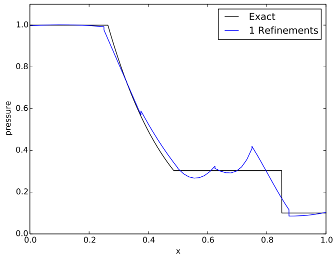

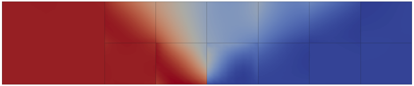

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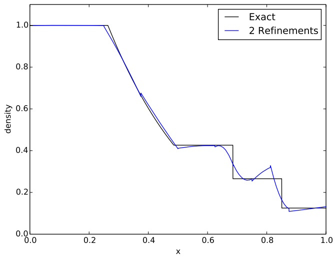

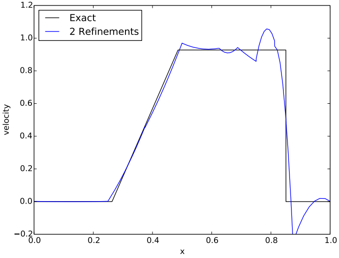

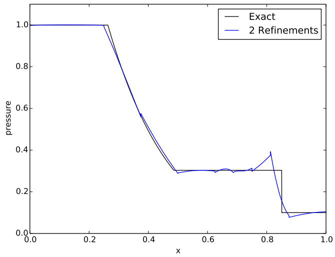

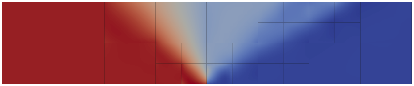

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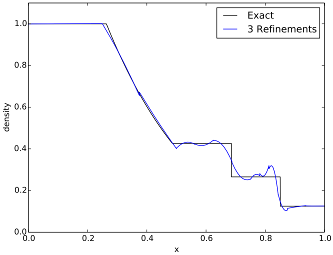

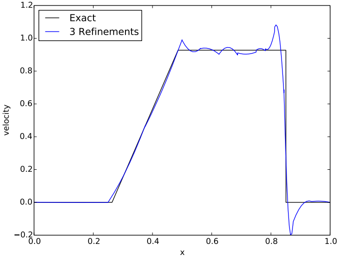

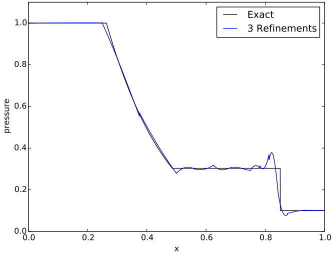

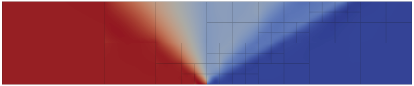

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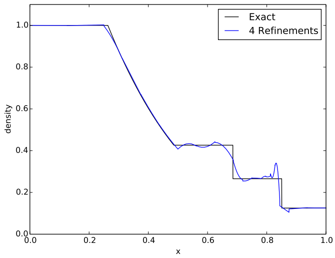

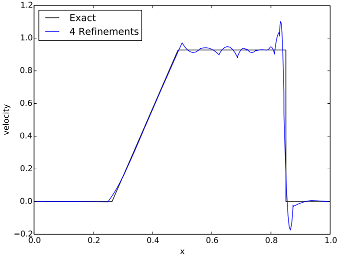

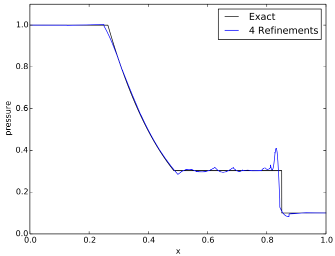

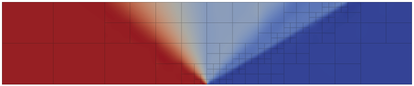

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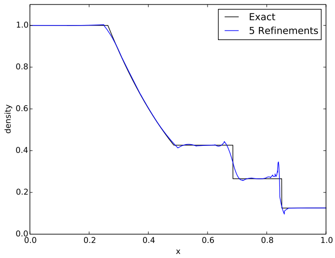

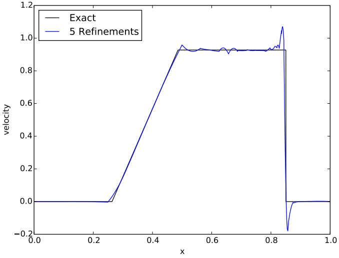

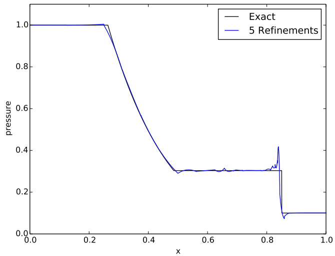

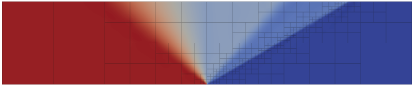

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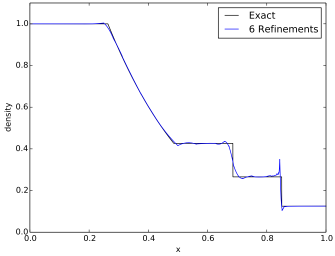

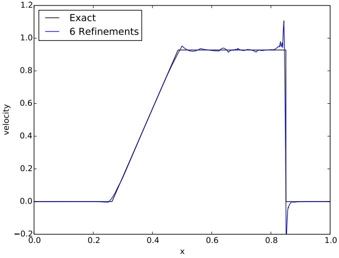

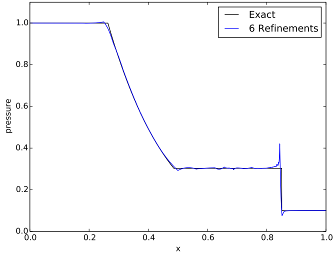

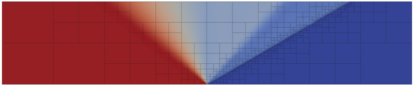

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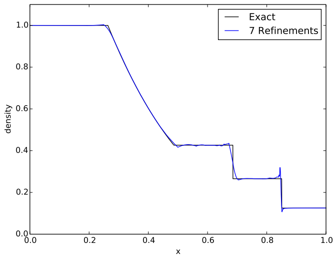

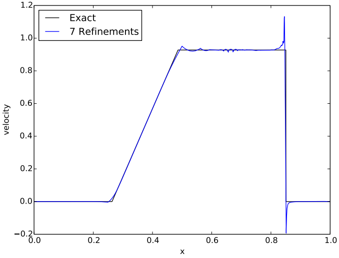

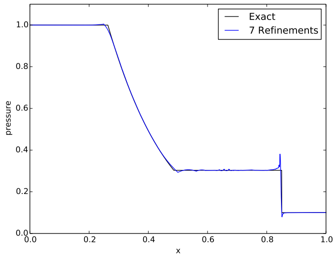

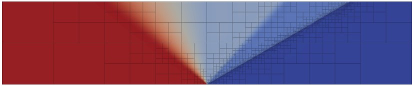

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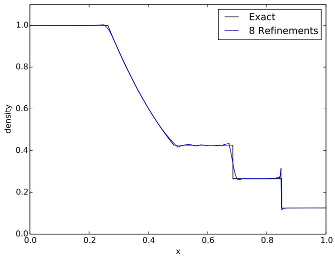

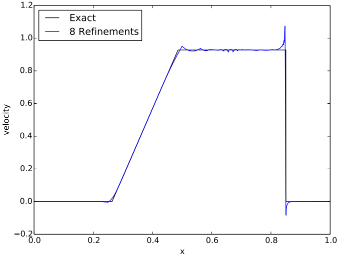

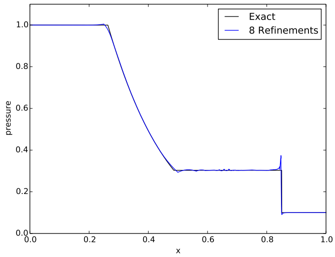

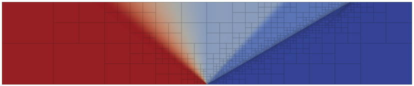

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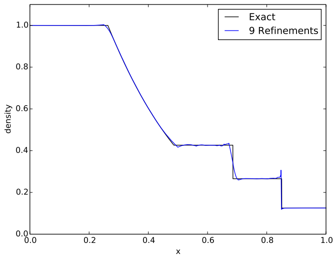

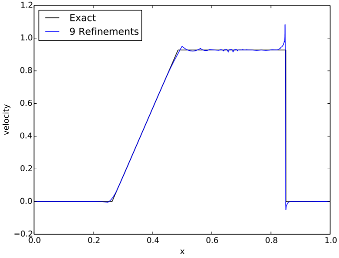

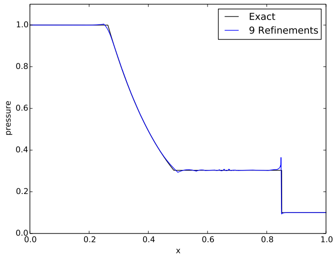

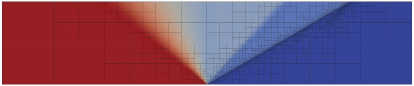

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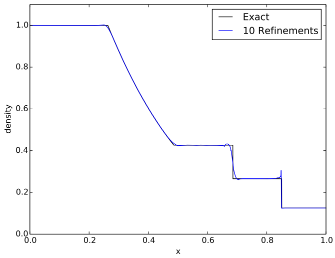
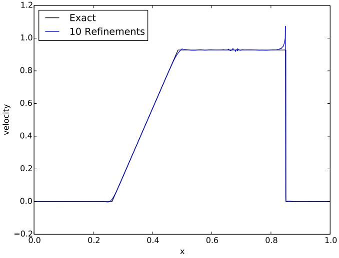
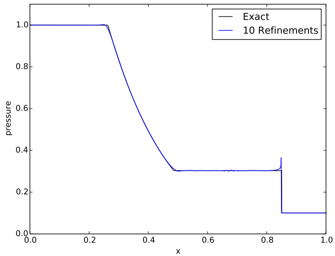
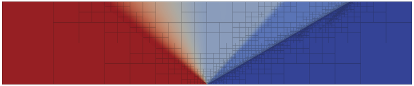
Sod Shock Tube with $\mu = 10^{-5}$



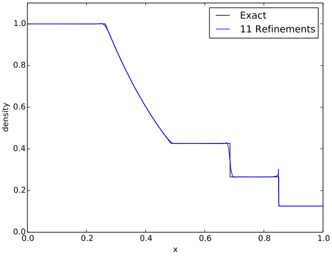


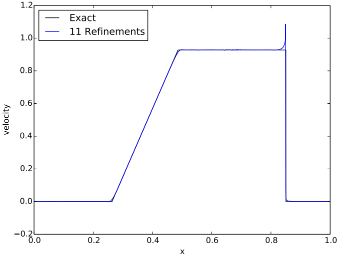


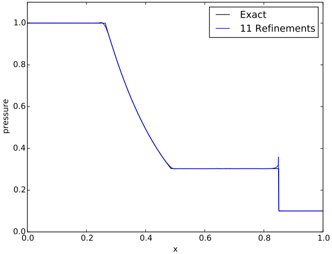


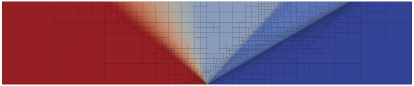
Compressible Navier-Stokes

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



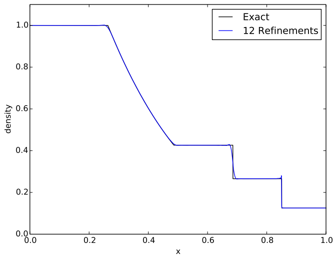


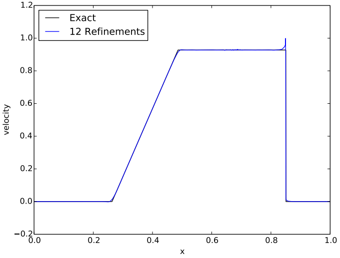


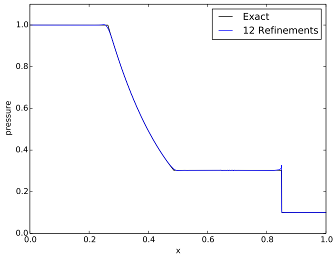


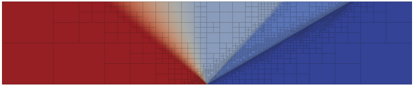
Compressible Navier-Stokes

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



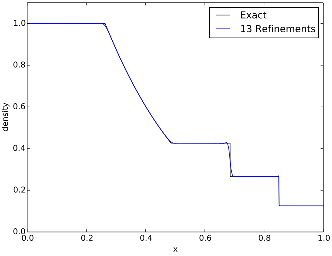


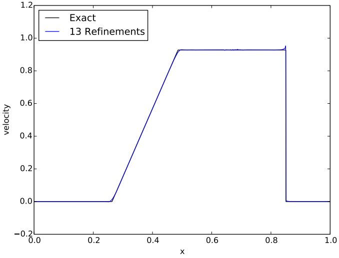


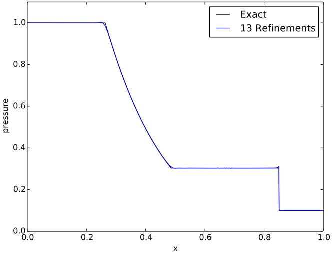


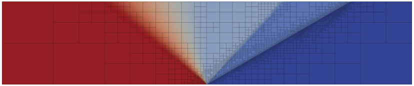
Compressible Navier-Stokes

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



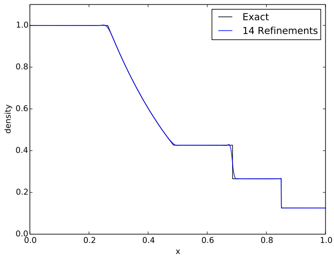


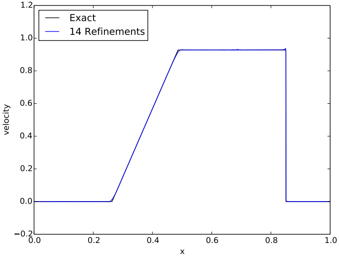


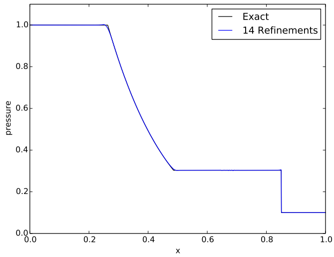


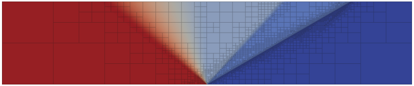
Compressible Navier-Stokes

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



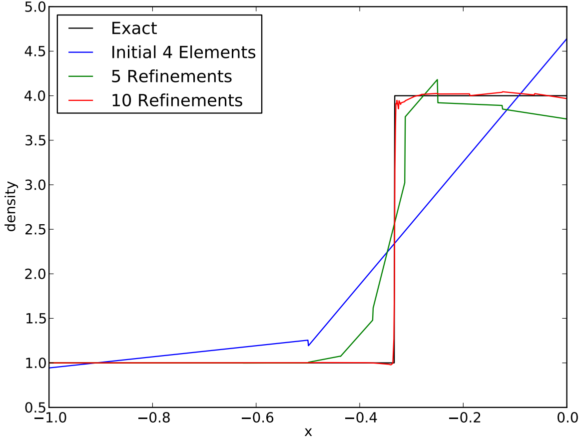




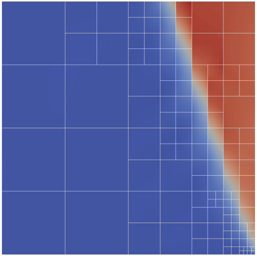


Space-Time Compressible Navier-Stokes

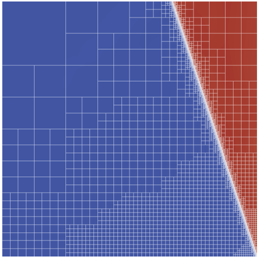
Noh Implosion with $\mu = 10^{-3}$



After 5 refinements



After 10 refinements



Space-Time Compressible Navier-Stokes

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

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

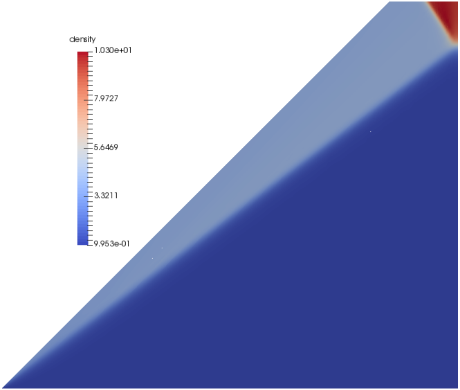
$$\hat{t}_m = \sqrt{2}(-\rho u^2 - \rho RT + \rho u)$$

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

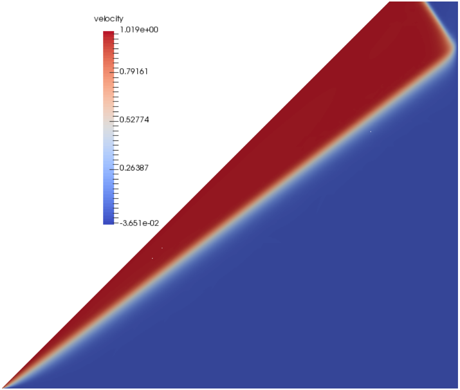
$$\hat{u} = 1$$

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

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



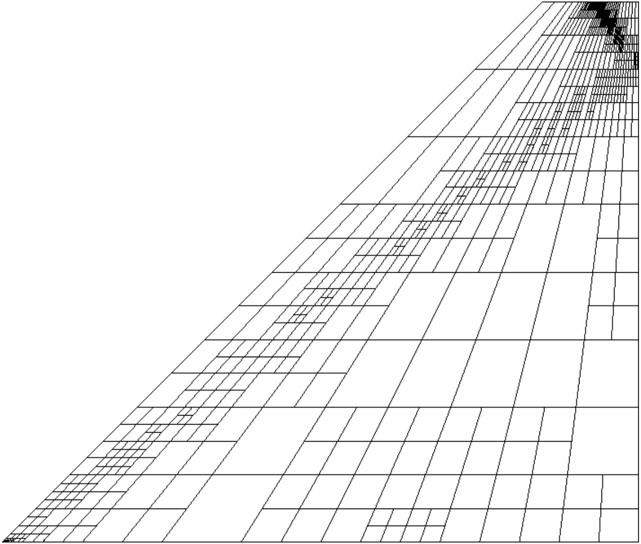
Density



Velocity

Space-Time Compressible Navier-Stokes

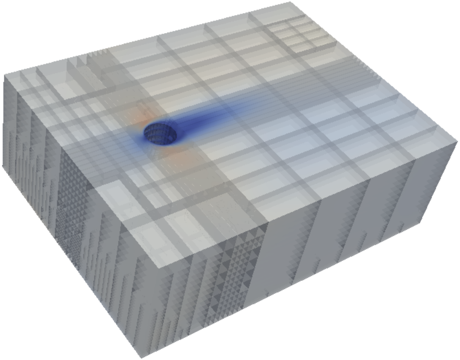
Piston with $\mu = 10^{-2}$



Mesh after 8 adaptive refinements

Future Directions

- **Improve performance:** line smoothing for multigrid
- **Shock capturing:** DPG makes no promises when it comes to Gibbs phenomenon
- **Non-Hilbert DPG:** L^1 is known to limit oscillations
- **Anisotropic refinements:** necessary for time slabs
- **More extensive 2D results:** shedding vortex problems, 2D shock problems
- **3D results:** will not be cheap



Incompressible Flow Over a Cylinder

Myself in Four Thousand Words