

Space-Time DPG: Designing a Method for Massively Parallel CFD

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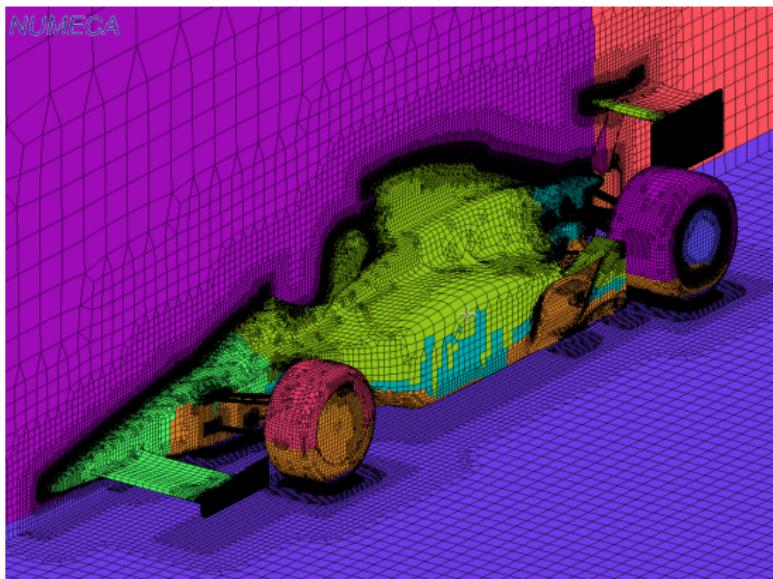
4 Conclusions

Motivation

Initial Mesh Design is Expensive and Time-Consuming

Stability requirements of numerical methods dictate that mesh must anticipate solution.

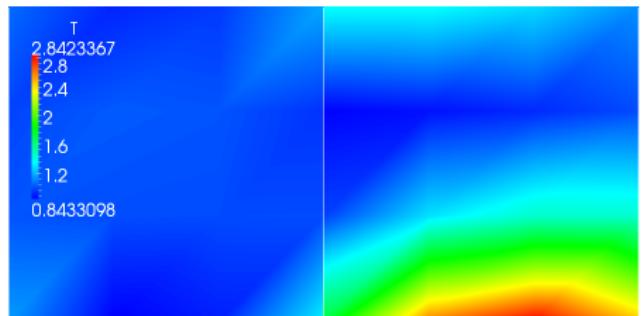
- Surface mesh must accurately represent geometry
- Volume mesh needs sufficient resolution for asymptotic regime
- Boundary layer meshes must respect y^+ guidelines
- Engineers often forced to work by trial and error
- Bad in the context of HPC



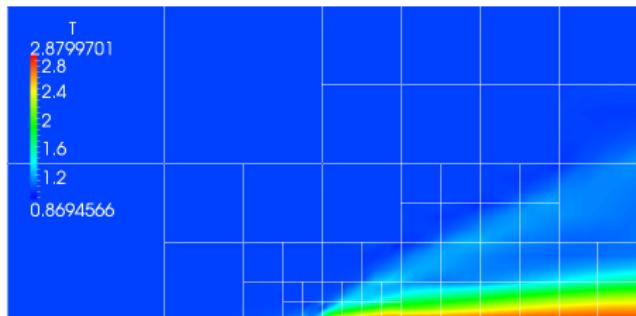
Formula 1 Mesh by Numeca

DPG on Coarse Meshes

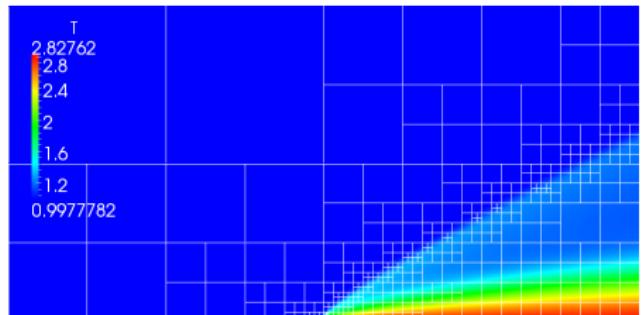
Adaptive Solve of the Carter Plate Problem¹ $Re = 1000$



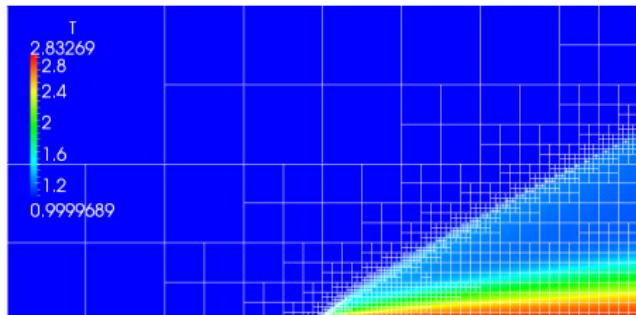
Temperature on Initial Mesh



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.

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Overview of DPG

DPG is a Minimum Residual Method

Find $u \in U$ such that

$$b(u, v) = l(v) \quad \forall v \in V$$

with operator $B : U \rightarrow V'$ defined by $b(u, v) = \langle Bu, v \rangle_{V' \times V}$.

This gives the operator equation

$$Bu = l \quad \in V'.$$

We wish to minimize the residual $Bu - l \in V'$:

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

Dual norms are not computationally tractable. Inverse Riesz map moves the residual to a more accessible space:

$$u_h = \arg \min_{w_h \in U_h} \frac{1}{2} \|R_V^{-1}(Bu - l)\|_V^2 .$$

Overview of DPG

DPG is a Minimum Residual Method

Taking the Gâteaux derivative to be zero in all directions $\delta u \in U_h$ gives,

$$(R_V^{-1}(Bu_h - l), R_V^{-1}B\delta u)_V = 0, \quad \forall \delta u \in U,$$

which by definition of the Riesz map is equivalent to

$$\langle Bu_h - l, R_V^{-1}B\delta u_h \rangle = 0 \quad \forall \delta u_h \in U_h,$$

with optimal test functions $v_{\delta u_h} := R_V^{-1}B\delta u_h$ for each trial function δu_h .

Resulting Petrov-Galerkin System

This gives a simple bilinear form

$$b(u_h, v_{\delta u_h}) = l(v_{\delta u_h}),$$

with $v_{\delta u_h} \in V$ that solves the auxiliary problem

$$(v_{\delta u_h}, \delta v)_V = \langle R_V v_{\delta u_h}, \delta v \rangle = \langle B\delta u_h, \delta v \rangle = b(\delta u_h, \delta v) \quad \forall \delta v \in V.$$

Overview of DPG²

Other Features

Discontinuous Petrov-Galerkin

- Continuous test space produces global solve for optimal test functions
- Discontinuous test space results in an embarrassingly parallel solve

Hermitian Positive Definite Stiffness Matrix

Property of all minimum residual methods

$$b(u_h, v_{\delta u_h}) = (v_{u_h}, v_{\delta u_h})_V = \overline{(v_{\delta u_h}, v_{u_h})_V} = \overline{b(\delta u_h, v_{u_h})}$$

Error Representation Function

Energy norm of Galerkin error (residual) can be computed without exact solution

$$\|u_h - u\|_E = \|B(u_h - u)\|_{V'} = \|Bu_h - l\|_{V'} = \|R_V^{-1}(Bu_h - l)\|_V$$

²L.F. Demkowicz and J. Gopalakrishnan. "Recent Developments in Discontinuous Galerkin Finite Element Methods for Partial Differential Equations (eds. X. Feng, O. Karakashian, Y. Xing)". In: vol. 157. IMA Volumes in Mathematics and its Applications, 2014. Chap. An Overview of the DPG Method, pp. 149–180.

Overview of DPG

High Performance Computing

Eliminates human intervention

- Stability
- Robustness
- Adaptivity
- Automaticity
- Compute intensive
- Embarrassingly parallel local solves
- Factorization recyclable
- Low communication
- SPD stiffness matrix
- Multiphysics



Stampede Supercomputer at TACC



Mira Supercomputer at Argonne

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Space-Time DPG

Motivation

Extends the capabilities of a DPG solver

- Preserves stability and robustness of DPG method
- Unified treatment of space and time
- Local space-time adaptivity (local time stepping)
 - Small solution features require small time step
 - Global time step not limited to smallest element
- Natural framework for moving meshes

More computationally difficult

- Solve requires $d + 1$ dimensions
- Mesh structure more difficult
- Need to differentiate between spatial and temporal boundaries
- Larger global solves than finite difference time stepping

Heat Equation

Simplest Nontrivial Space-Time Problem

Equation is parabolic in space-time.

$$\frac{\partial u}{\partial t} - \epsilon \Delta u = f$$

This is really just a composite of Fourier's law and conservation of energy.

$$\boldsymbol{\sigma} - \epsilon \nabla u = 0$$

$$\frac{\partial u}{\partial t} - \nabla \cdot \boldsymbol{\sigma} = f$$

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

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

Heat Equation

DPG Formulation

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

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

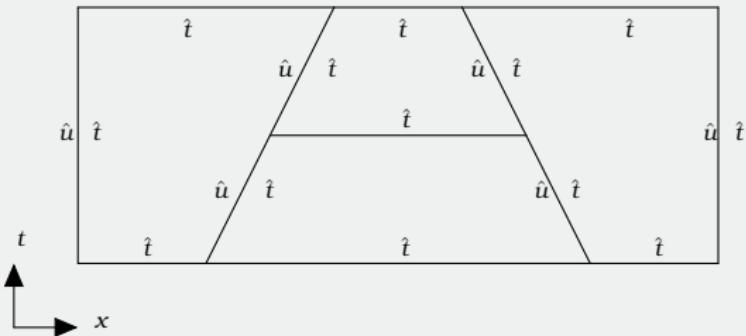
where

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

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

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

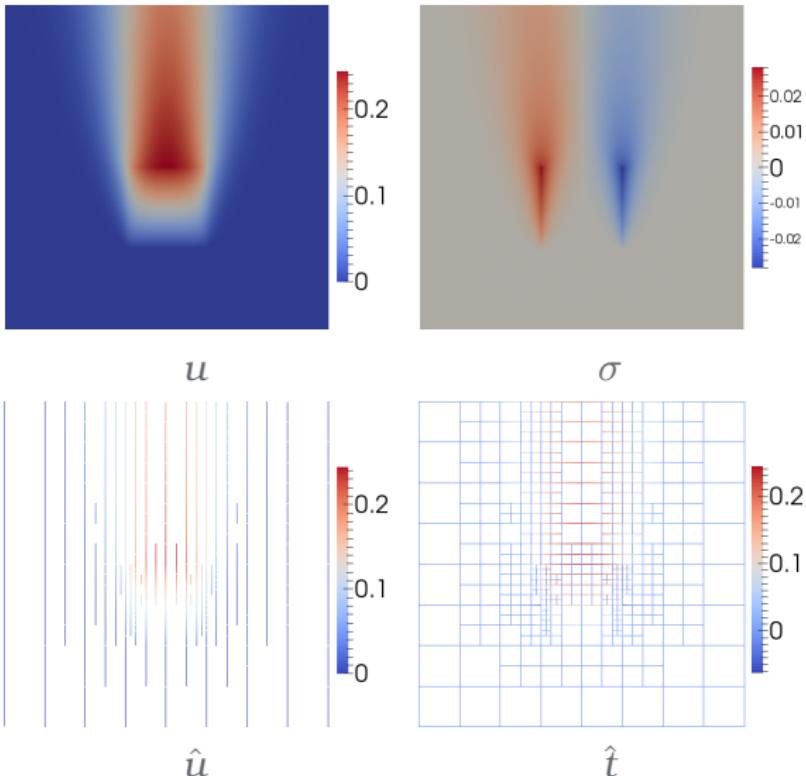
Support of Trace Variables



Heat equation

Pulsed Source Problem

- Initial condition
 $u = 0$.
- Apply unit source
 $x \in [3/8, 5/8]$,
 $t \in [1/4, 1/2]$.
- Should not violate causality
- Space-time adaptivity picks up areas of rapid change.



Compressible Navier-Stokes

Strong Form

The compressible Navier-Stokes equations are

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho e_0 \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} - \mathbb{D} \\ \rho \mathbf{u} e_0 + \mathbf{u} p + \mathbf{q} - \mathbf{u} \cdot \mathbb{D} \end{bmatrix} = \begin{bmatrix} f_c \\ \mathbf{f}_m \\ f_e \end{bmatrix},$$

where

$$\mathbb{D} = 2\mu \mathbf{S}^* = 2\mu \left[\frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{1}{3} \nabla \cdot \mathbf{u} \mathbf{I} \right],$$

$$\mathbf{q} = -C_p \frac{\mu}{Pr} \nabla T,$$

and (assuming an ideal gas EOS)

$$p = \rho R T.$$

Compressible Navier-Stokes

First Order Space-Time Form

Writing this in space-time in terms of ρ , \mathbf{u} , T , \mathbb{D} , and \mathbf{q} :

$$\mathbb{D} - \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \frac{2\mu}{3} \nabla \cdot \mathbf{u} \mathbf{I} = 0$$

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

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

$$\nabla_{xt} \cdot \begin{pmatrix} \rho \mathbf{u} \otimes \mathbf{u} + \rho R T \mathbf{I} - \mathbb{D} \\ \rho \mathbf{u} \end{pmatrix} = f_m$$

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

Compressible Navier-Stokes

DPG Formulation

Multiplying by test functions and integrating by parts:

$$\begin{aligned}
 (\mathbb{D}, \mathbb{S}) + (2\mu \mathbf{u}, \nabla \cdot \mathbb{S}) - \left(\frac{2\mu}{3} \mathbf{u}, \nabla \operatorname{tr} \mathbb{S} \right) - \langle 2\mu \hat{\mathbf{u}}, \mathbb{S} \mathbf{n}_x \rangle + \left\langle \frac{2\mu}{3} \hat{\mathbf{u}}, \mathbb{S} \mathbf{n}_x \right\rangle &= 0 \\
 (\mathbf{q}, \boldsymbol{\tau}) - \left(C_p \frac{\mu}{Pr} T, \nabla \cdot \boldsymbol{\tau} \right) + \left\langle C_p \frac{\mu}{Pr} \hat{T}, \boldsymbol{\tau}_n \right\rangle &= 0 \\
 - \left(\begin{pmatrix} \rho \mathbf{u} \\ \rho \end{pmatrix}, \nabla_{xt} \mathbf{v}_c \right) + \langle \hat{\mathbf{t}}_c, \mathbf{v}_c \rangle &= (f_c, \mathbf{v}_c) \\
 - \left(\begin{pmatrix} \rho \mathbf{u} \otimes \mathbf{u} + \rho R T \mathbf{I} - \mathbb{D} \\ \rho \mathbf{u} \end{pmatrix}, \nabla_{xt} \mathbf{v}_m \right) + \langle \hat{\mathbf{t}}_m, \mathbf{v}_m \rangle &= (\mathbf{f}_m, \mathbf{v}_m) \\
 - \left(\begin{pmatrix} \rho \mathbf{u} (C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}) + \mathbf{u} \rho R T + \mathbf{q} - \mathbf{u} \cdot \mathbb{D} \\ \rho (C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}) \end{pmatrix}, \nabla_{xt} \mathbf{v}_e \right) + \langle \hat{\mathbf{t}}_e, \mathbf{v}_e \rangle &= (f_e, \mathbf{v}_e),
 \end{aligned}$$

where $\hat{\mathbf{u}}$ and \hat{T} are spatial traces and $\hat{\mathbf{t}}_c$, $\hat{\mathbf{t}}_m$, and $\hat{\mathbf{t}}_e$ are fluxes.

Compressible Navier-Stokes

Flux and Trace Variables

Spatial traces and fluxes are defined as follows:

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

$$\hat{T} = \text{tr}(T)$$

$$\hat{t}_c = \text{tr}(\rho \mathbf{u}) \cdot \mathbf{n}_x + \text{tr}(\rho) n_t$$

$$\hat{\mathbf{t}}_m = \text{tr}(\rho \mathbf{u} \otimes \mathbf{u} + \rho R T \mathbf{I} - \mathbb{D}) \cdot \mathbf{n}_x + \text{tr}(\rho \mathbf{u}) n_t$$

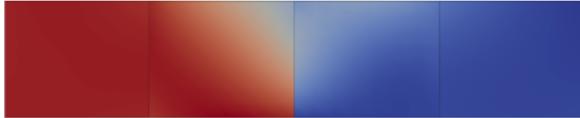
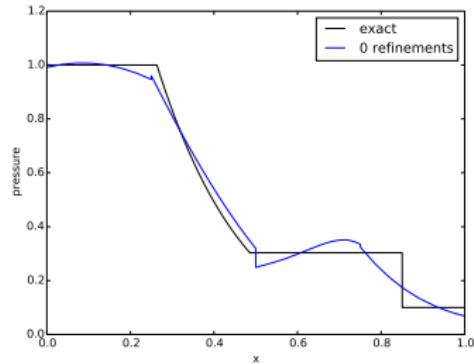
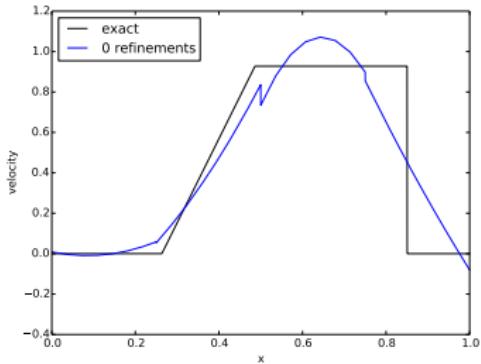
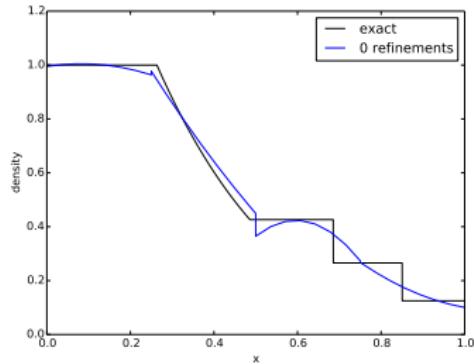
$$\begin{aligned} \hat{t}_e = & \text{tr} \left(\rho \mathbf{u} \left(C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) + \mathbf{u} \rho R T + \mathbf{q} - \mathbf{u} \cdot \mathbb{D} \right) \cdot \mathbf{n}_x \\ & + \text{tr} \left(\rho \left(C_v T + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) \right) n_t. \end{aligned}$$

Linearization

Fluxes, traces, and \mathbf{q} are linear in the above bilinear form, but we need to linearize in ρ , \mathbf{u} , T , and \mathbb{D} (Jacobian and residual not shown here).

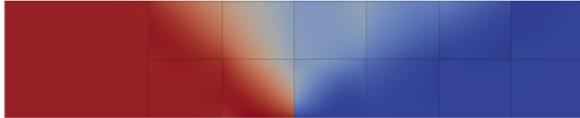
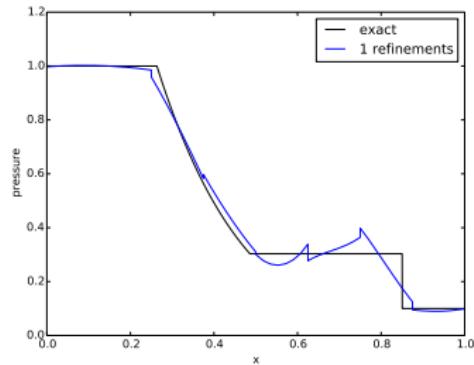
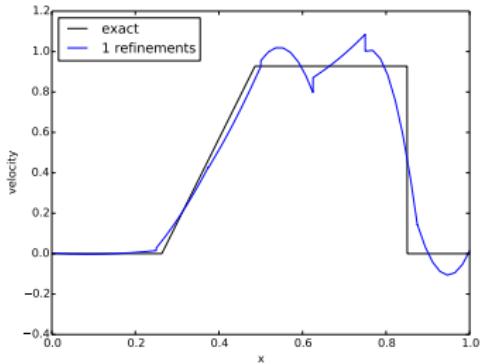
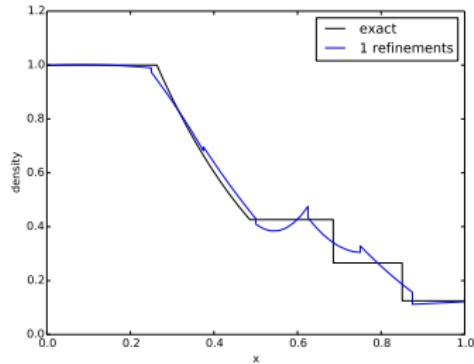
Compressible Navier-Stokes

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



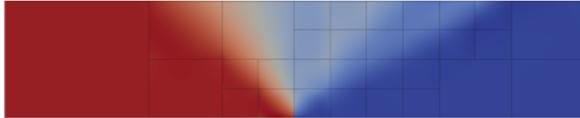
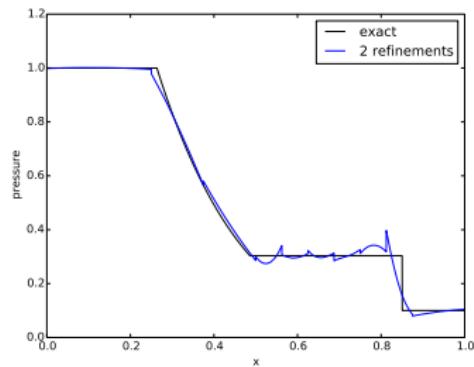
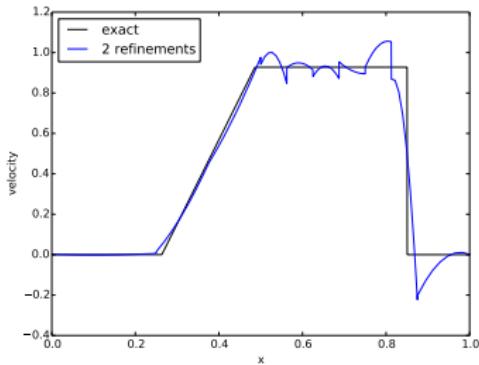
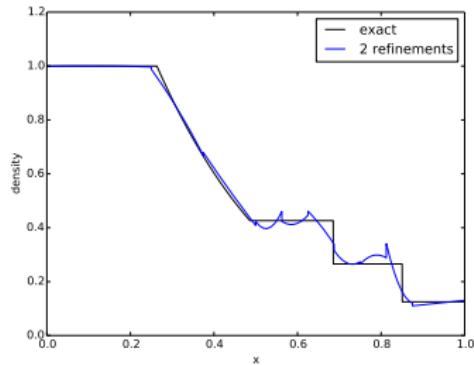
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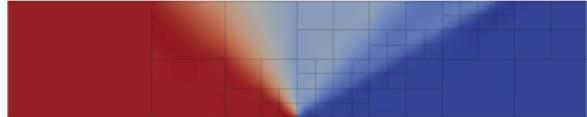
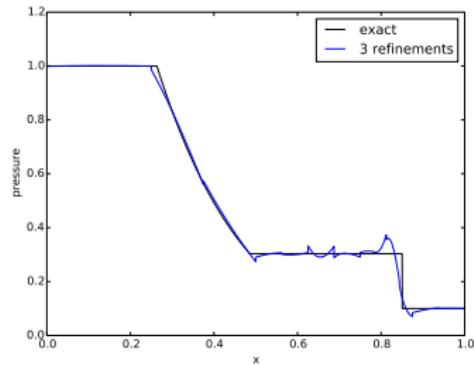
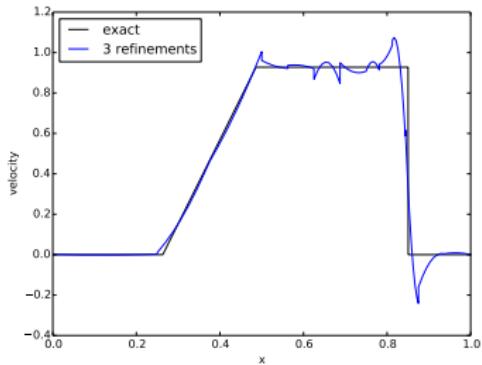
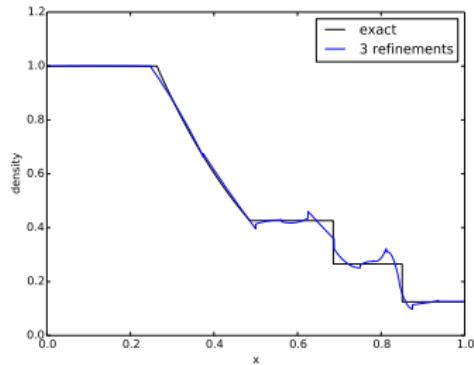
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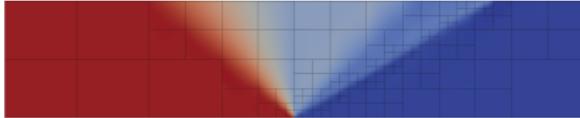
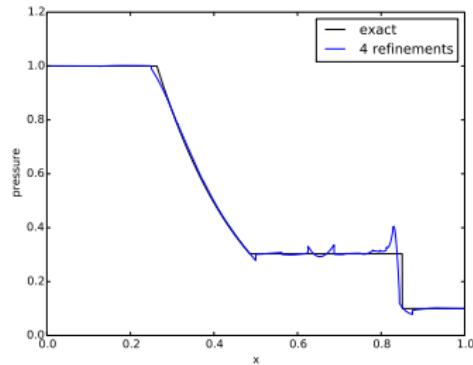
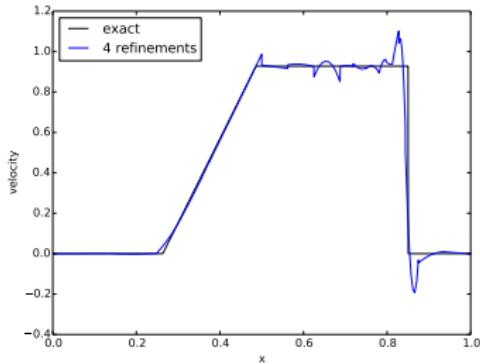
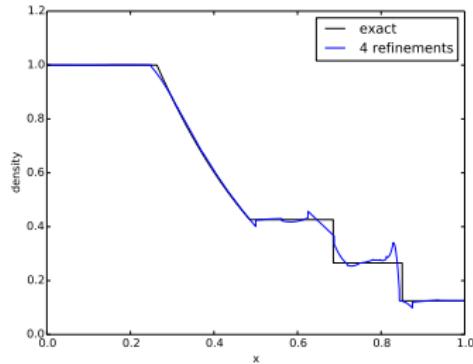
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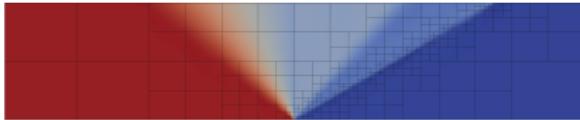
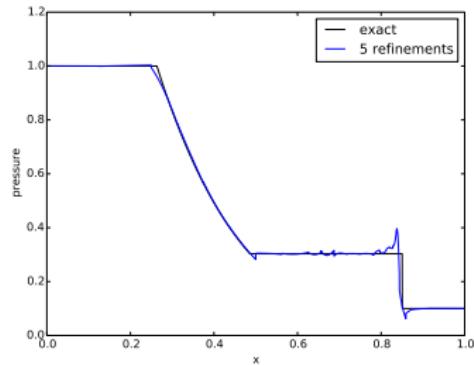
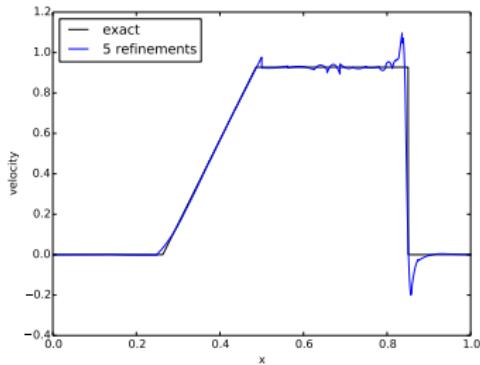
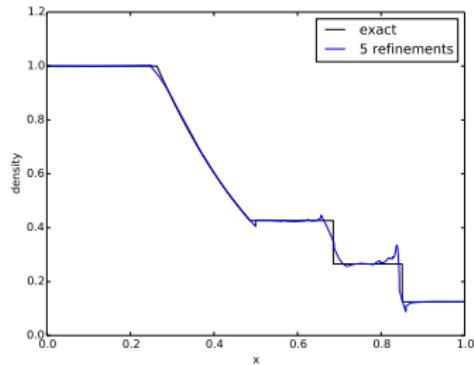
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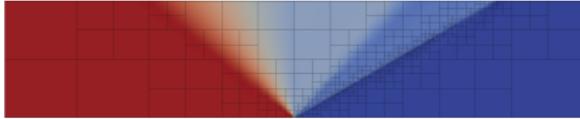
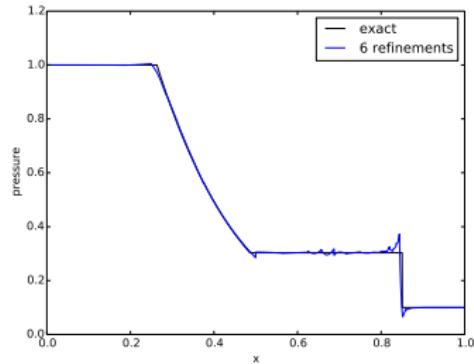
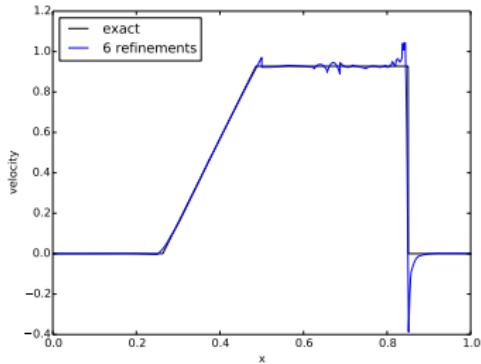
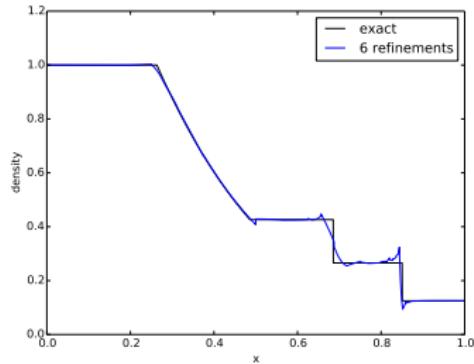
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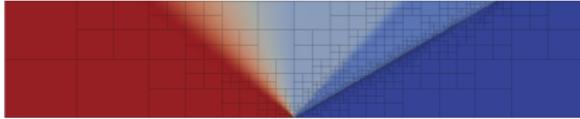
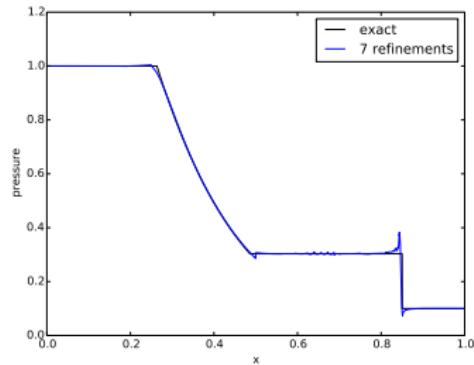
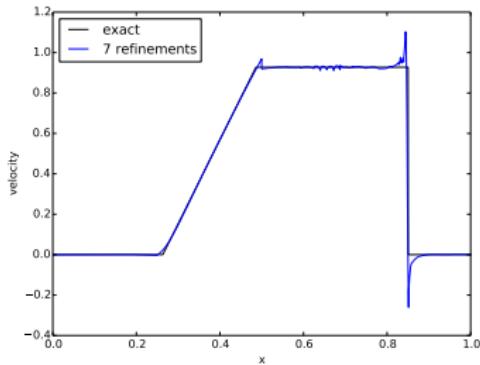
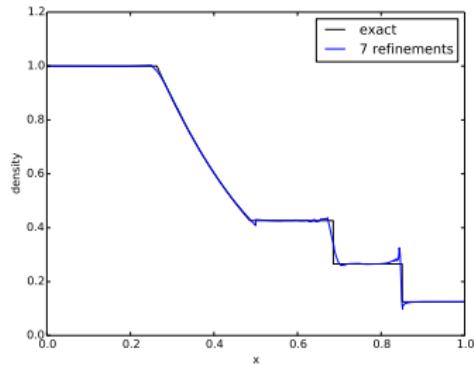
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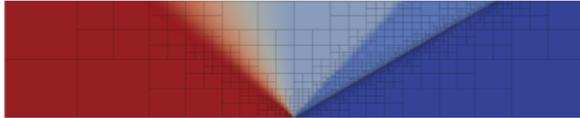
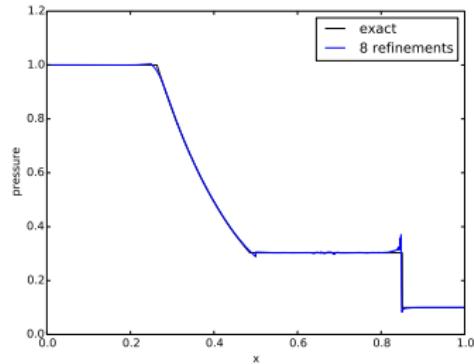
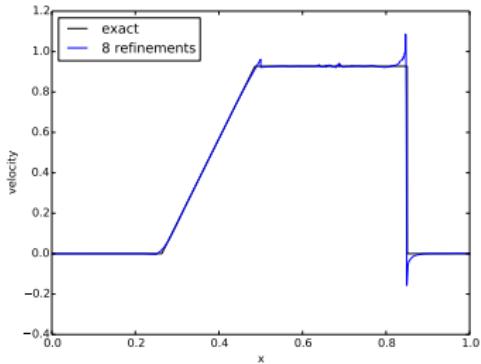
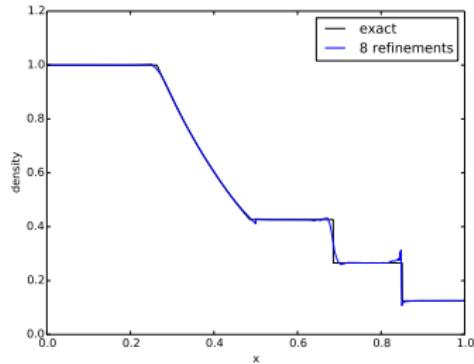
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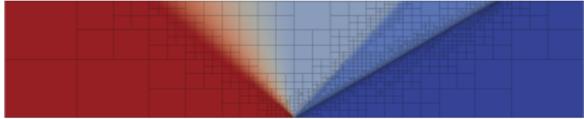
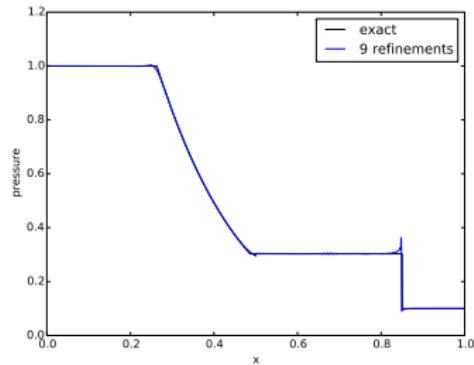
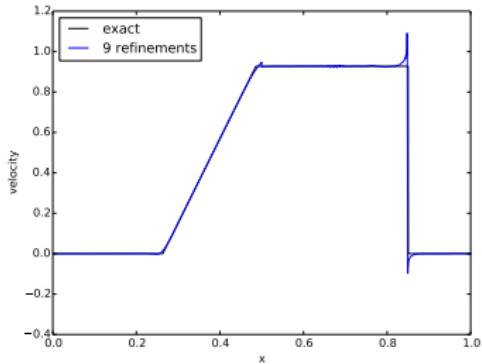
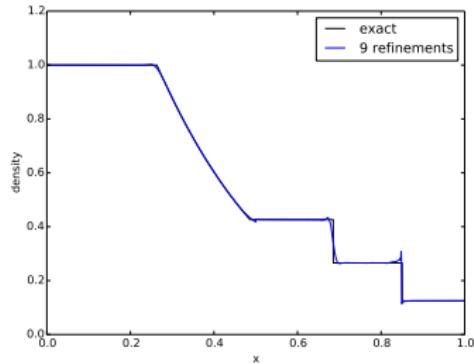
Compressible Navier-Stokes

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



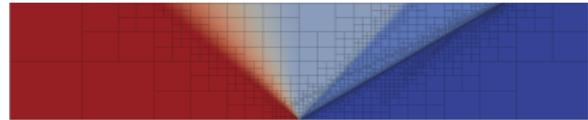
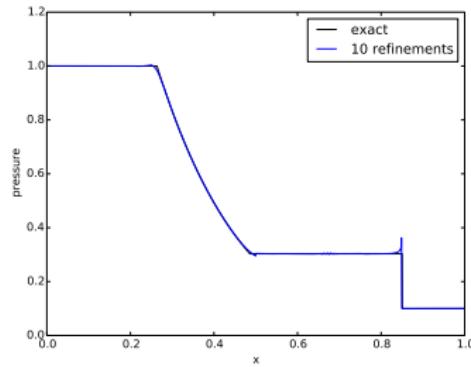
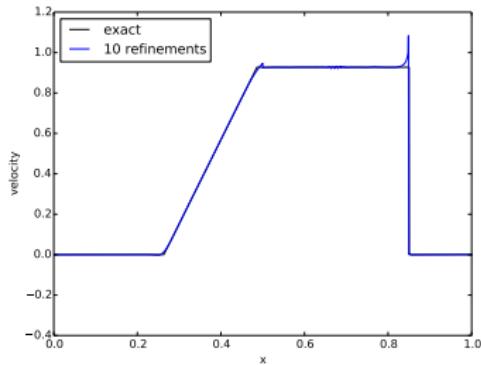
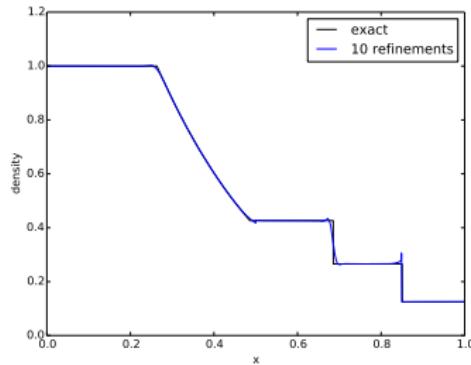
Compressible Navier-Stokes

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



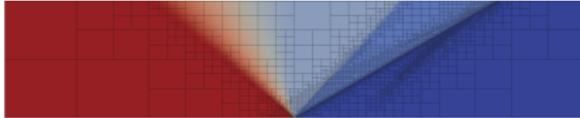
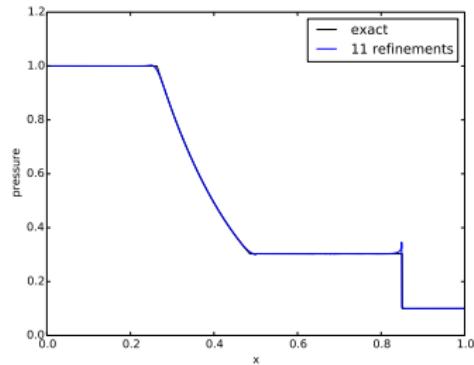
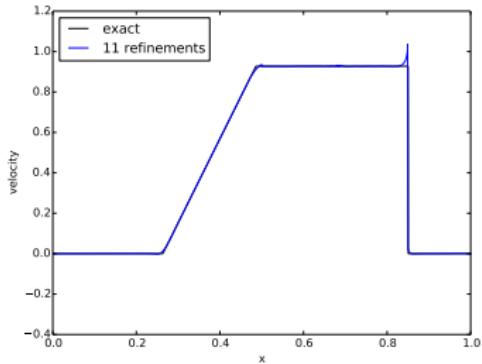
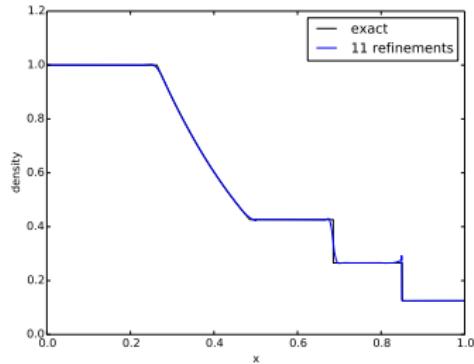
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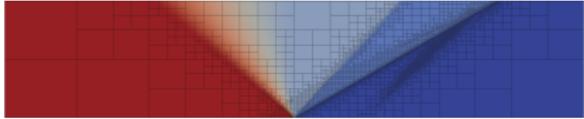
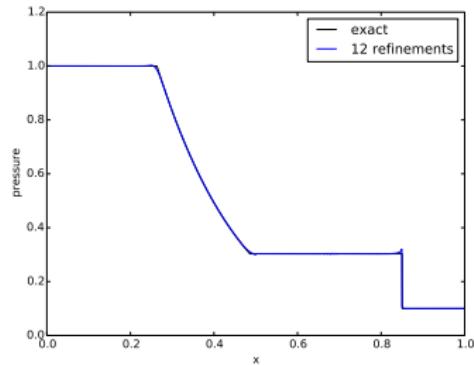
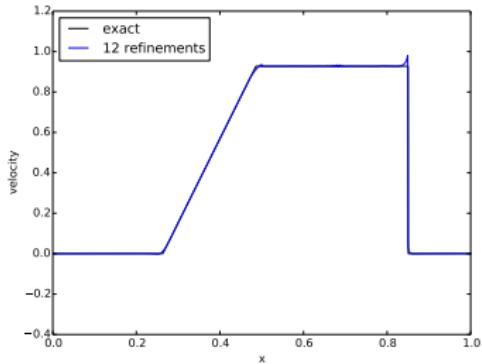
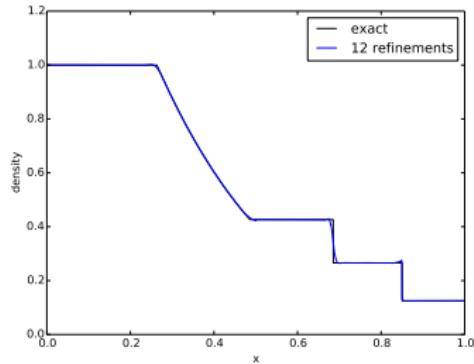
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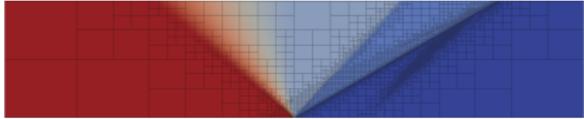
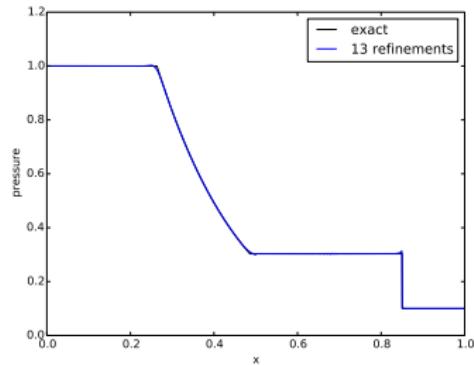
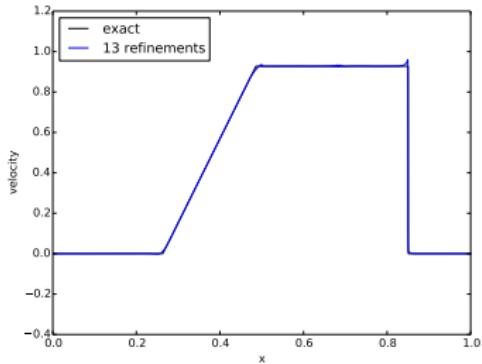
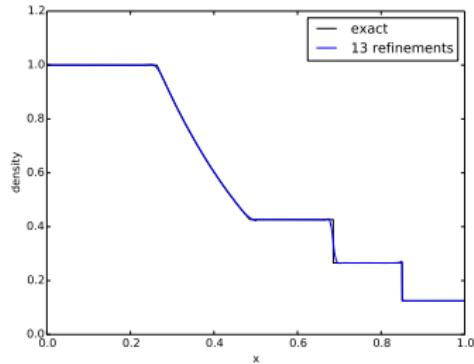
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Compressible Navier-Stokes

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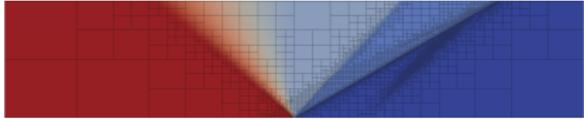
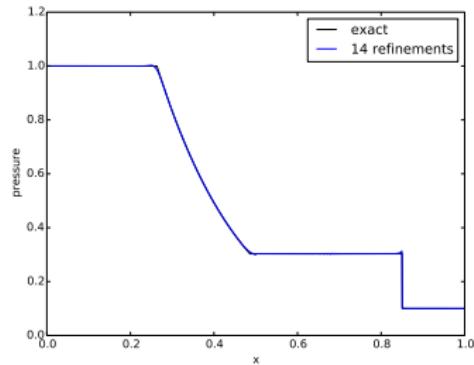
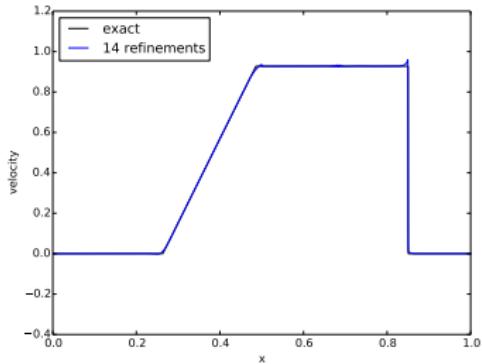
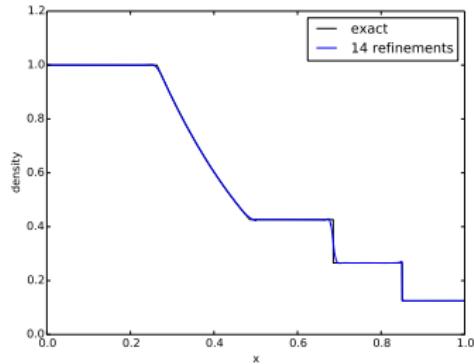


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2 DPG Overview

3 Space-Time DPG

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Conclusions and Future Work

Conclusions

- A problem in conservation form can be transformed to a space-time divergence.
- Fluxes change character from spatial to temporal boundaries.
- Traces are only defined on spatial boundaries.

Future Work

- Proof of robustness for convection-diffusion.
- Analysis of robust test norms.
- Time slabs will reduce the simulation cost.
- Two and three dimensions for more realistic problems.
- Incompressible Navier-Stokes.
- Iterative solvers for parallel scalability.

Thank You!

