Space-Time Discontinuous Petrov-Galerkin Finite Elements for Transient Computational Fluid Dynamics

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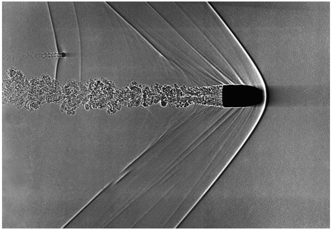
Navier-Stokes Equations

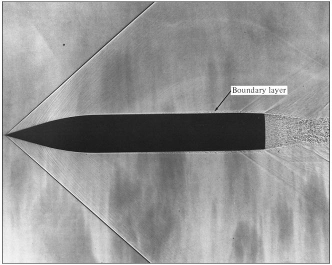
Numerical Challenges

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
  - Coarse/adaptive grids
  - Higher order



Shock

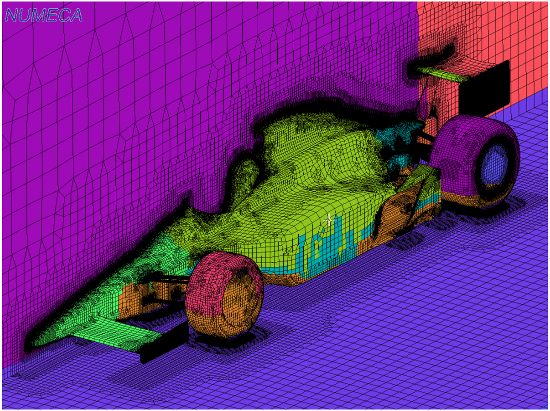


Boundary layer

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

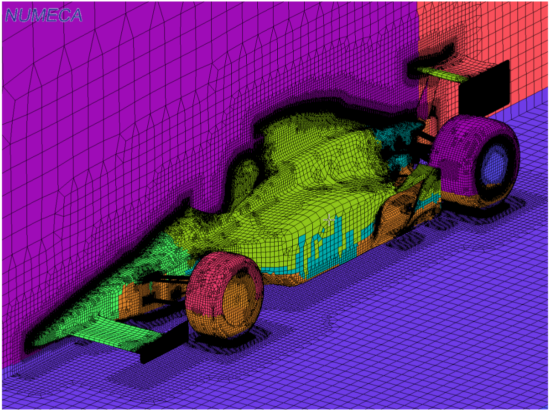


Formula 1 Mesh by Numeca

Motivation

Initial Mesh Design is Expensive and Time-Consuming

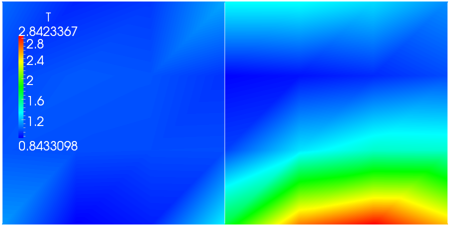
- Surface mesh must accurately represent geometry
- Volume mesh needs sufficient resolution for asymptotic regime
- Engineers often forced to work by trial and error
- Bad in the context of HPC
- We desire an automated computational technology



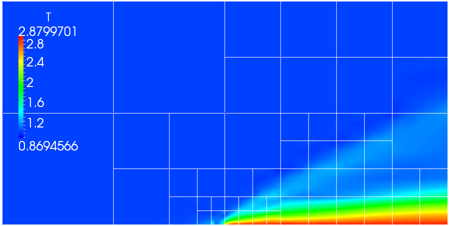
Formula 1 Mesh by Numeca

DPG on Coarse Meshes

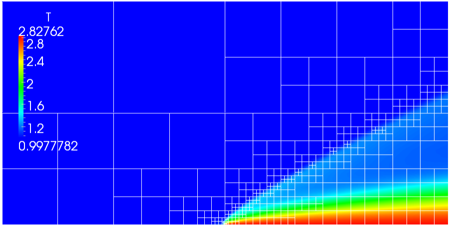
Adaptive Solve of the Carter Plate Problem[1] $Re = 1000$



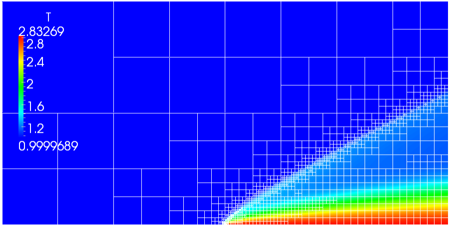
Temperature on Initial Mesh



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.

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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 $B : U \to V'$ 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 $Bu - l \in V'$:

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

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

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

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,

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

which by definition of the Riesz map is equivalent to

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

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

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

DPG is the Most Stable Petrov-Galerkin Method

Babuška's theorem guarantees that *discrete stability and approximability imply convergence*. If bilinear form $b(u,v)$, with $M := \|b\|$ satisfies the discrete inf-sup condition with constant γ_h,

$$\sup_{v_h \in V_h} \frac{|b(u,v)|}{\|v_h\|_V} \geq \gamma_h \|u_h\|_U \ ,$$

then the Galerkin error satisfies the bound

$$\|u_h - u\|_U \leq \frac{M}{\gamma_h} \inf_{w_h \in U_h} \|w_h - u\|_U \ .$$

Optimal test function realize the supremum guaranteeing that $\gamma_h \geq \gamma$.

Energy Norm

If we use the energy norm, $\|u\|_E := \|Bu\|_{V'}$ in the error estimate, then $M = \gamma = 1$. Babuška's theorem implies that the minimum residual method is the most stable Petrov-Galerkin method (assuming exact optimal test functions).

Overview of DPG

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

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

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

Extending DPG to Transient Problems

- Time stepping techniques are not ideally suited to highly adaptive grids
- Space-time FEM proposed as a solution
  - ✓ foo
  - ✗ bar

Space-Time DPG for Convection-Diffusion

Space-Time Divergence Form

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.

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

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

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

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

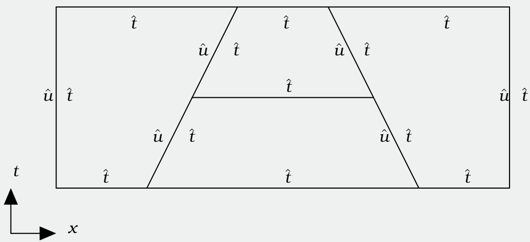
where

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

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

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

Support of Trace Variables



Space-Time Convection-Diffusion

Robust Norms

Bilinear form with group variables:

$$b\left(\left(u,\hat{u}\right),v\right)=\left(u,A_h^*v\right)_{L^2(\Omega_h)}+\langle\widehat{u},[\![v]\!]\rangle_{\Gamma_h}$$

For conforming v^* satisfying $A^*v^*=u$

$$\|u\|^2_{L^2(\Omega_h)}=b(u,v^*)=\frac{b(u,v^*)}{\|v^*\|_V}\|v^*\|_V$$

$$\leq\sup_{v^*\neq 0}\frac{|b(u,v^*)|}{\|v^*\|}=\|u\|_E\|v^*\|_V$$

Necessary robustness condition:

$$\|v^*\|_V\lesssim\|u\|_{L^2(\Omega_h)}$$

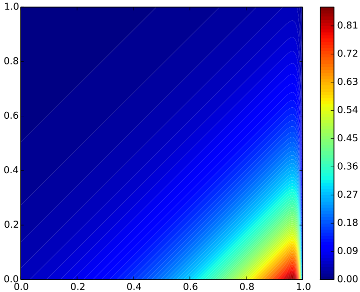
$$\Rightarrow\|u\|_{L^2(\Omega_h)}\lesssim\|u\|_E$$

Analytical Solution

$$u=e^{-lt}(e^{\lambda_1(x-1)}-e^{\lambda 2(x-1)})$$

$$\lambda_{1,2}=\frac{-1\pm\sqrt{1-4l\epsilon}}{-2\epsilon}$$

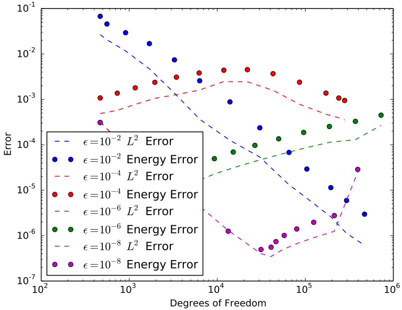
where $l=3,\quad\epsilon=10^{-2}$



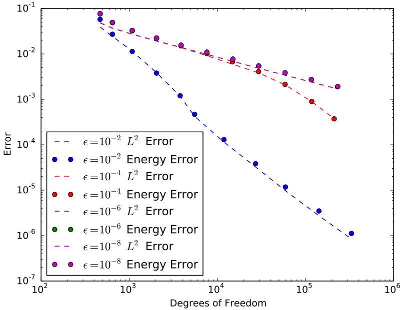
Space-Time Convection-Diffusion

Robust Norms

A norm should be: bounded by $\|u\|_{L^2(\Omega_h)}$, have good conditioning, not produce boundary layers in the optimal test function.



$$\|(v,\boldsymbol{\tau})\|^2 = \left\|\nabla\cdot\boldsymbol{\tau} - \tilde{\boldsymbol{\beta}}\cdot\nabla_{xt} v\right\|^2 + \left\|\frac{1}{\epsilon}\boldsymbol{\tau} + \nabla v\right\|^2 + \|v\|^2 + \|\boldsymbol{\tau}\|^2$$

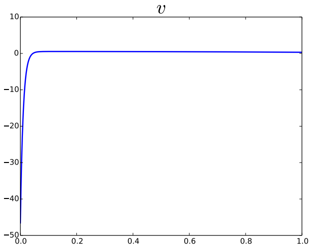


$$\|(v,\boldsymbol{\tau})\|^2 = \left\|\nabla\cdot\boldsymbol{\tau} - \tilde{\boldsymbol{\beta}}\cdot\nabla_{xt} v\right\|^2 + \min\left(\frac{1}{h^2},\frac{1}{\epsilon}\right)\|\boldsymbol{\tau}\|^2 + \epsilon\|\nabla v\|^2 + \|\boldsymbol{\beta}\cdot\nabla v\|^2 + \|v\|^2$$

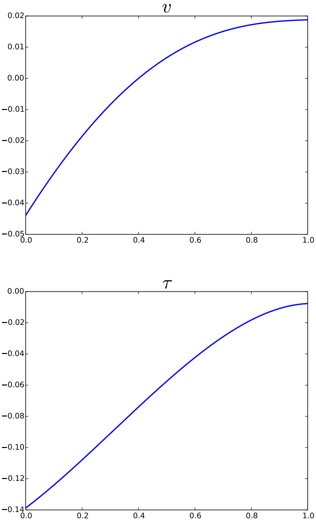
Space-Time Convection-Diffusion

Ideal Optimal Shape Functions

Graph Norm



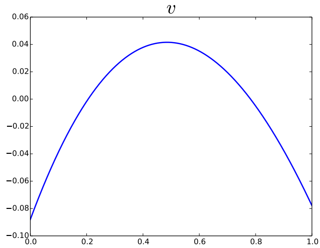
Robust Norm

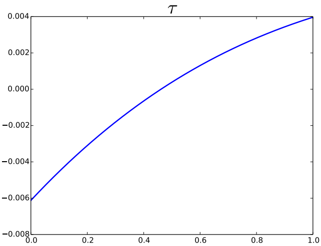


Space-Time Convection-Diffusion

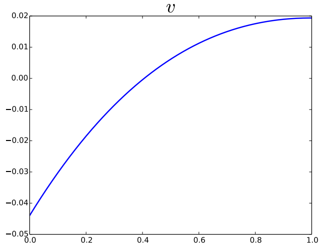
Approximated ($p = 3$) Optimal Shape Functions

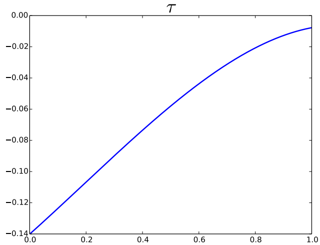
Graph Norm





Robust Norm





Space-Time Navier-Stokes

First Order System

Assuming Stokes hypothesis and ideal gas law:

$$\frac{1}{\mu}\mathbb{D} - \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right) + \frac{2}{3}\nabla \cdot \boldsymbol{u}\mathbb{I} = 0$$

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

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

$$\nabla_{xt} \cdot \begin{pmatrix} \rho\boldsymbol{u} \otimes \boldsymbol{u} + \rho RT\mathbb{I} - \mathbb{D} \\ \rho\boldsymbol{u} \end{pmatrix} = \boldsymbol{f}_m$$

$$\nabla_{xt} \cdot \begin{pmatrix} \rho\boldsymbol{u}\left(C_vT + \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u}\right) + \rho RT\boldsymbol{u} + \boldsymbol{q} - \boldsymbol{u}\cdot\mathbb{D} \\ \rho\left(C_vT + \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u}\right) \end{pmatrix} = f_e\,,$$

Space-Time Navier-Stokes

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

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

$$\mathbb{K}_m := \mathbb{D}$$

$$\boldsymbol{K}_e := -\boldsymbol{q} + \boldsymbol{u} \cdot \mathbb{D}$$

Viscous variables

$$\mathbb{M}_{\mathbb{D}} := \frac{1}{\mu}\mathbb{D}$$

$$\boldsymbol{M}_{\boldsymbol{q}} := \frac{Pr}{C_p \mu}\boldsymbol{q}$$

Viscous relations

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

$$G_{\boldsymbol{q}} := -T$$

Space-Time Navier-Stokes

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

$$(M, \Psi) + (G, \nabla \cdot \Psi) - \left\langle \hat{W}, \Psi \cdot \boldsymbol{n}_x \right\rangle = 0$$
$$-\left(\begin{pmatrix} F - K \\ C \end{pmatrix}, \nabla_{xt} V\right) + \langle \hat{t}, V \rangle = (f, V)\ .$$

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Design Goal

Make DPG research and experimentation as simple as possible, while maintaining computational efficiency and scalability.

Mature support for:

- Rapid specification of DPG variational forms, inner products, etc.
- Distributed computation of stiffness matrix
- 1D - 3D geometries
- Curvilinear elements
- h- and p-refinements (anisotropic in h)
- Arbitrarily irregular meshes
- Modular refinement strategy interface

Experimental support for:

- Space-time computations
- Iterative solvers (tested up to 32,768 cores)

Convection-Diffusion in Three Slides

Building the Bilinear Form

```
VarFactory vf;
//fields:
VarPtr u = vf.fieldVar("u", L2);
VarPtr sigma = vf.fieldVar("sigma", VECTOR_L2);

// traces:
VarPtr u_hat = vf.traceVar("u_hat");
VarPtr t_n = vf.fluxVar("t_n");

// test:
VarPtr v = vf.testVar("v", HGRAD);
VarPtr tau = vf.testVar("tau", HDIV);

double eps = .01;
FunctionPtr beta_x = Function::constant(1);
FunctionPtr beta_y = Function::constant(2);
FunctionPtr beta = Function::vectorize(beta_x, beta_y);

BFPtr bf = Teuchos::rcp( new BF(vf) );

bf->addTerm((1/eps) * sigma, tau);
bf->addTerm(u, tau->div());
bf->addTerm(-u_hat, tau->dot_normal());

bf->addTerm(sigma - beta * u, v->grad());
bf->addTerm(t_n, v);

RHSPtr rhs = RHS::rhs();
```

Find $u \in L^2(\Omega_h)$, $\boldsymbol{\sigma} \in \boldsymbol{L}^2(\Omega_h)$, $\hat{u} \in H^{\frac{1}{2}}(\Gamma_h)$, $\hat{t}_n \in H^{-\frac{1}{2}}(\Gamma_h)$ such that

$$\frac{1}{\epsilon}(\boldsymbol{\sigma}, \boldsymbol{\tau}) + (u, \nabla \cdot \boldsymbol{\tau}) - \langle \hat{u}, \boldsymbol{\tau} \cdot \boldsymbol{n} \rangle - (\boldsymbol{\beta} u - \boldsymbol{\sigma}, \nabla v) + \langle \hat{t}_n, v \rangle = (f, v)$$

for all $v \in H^1(K)$, $\boldsymbol{\tau} \in \boldsymbol{H}(\text{div}, K)$,

where $\epsilon = 10^{-2}$, $\boldsymbol{\beta} = (1, 2)^T$ and

$f = 0$.

Convection-Diffusion in Three Slides

Boundary Conditions and Mesh

```
int k = 2;
int delta_k = 2;
MeshPtr mesh = MeshFactory::quadMesh(bf, k+1, delta_k);

BCPtr bc = BC::bc();

SpatialFilterPtr y_equals_one = SpatialFilter::matchingY(1.0);
SpatialFilterPtr y_equals_zero = SpatialFilter::matchingY(0);
SpatialFilterPtr x_equals_one = SpatialFilter::matchingX(1.0);
SpatialFilterPtr x_equals_zero = SpatialFilter::matchingX(0.0);

FunctionPtr zero = Function::zero();
FunctionPtr x = Function::xn(1);
FunctionPtr y = Function::yn(1);
bc->addDirichlet(t_n, y_equals_zero, -2 * (1-x));
bc->addDirichlet(t_n, x_equals_zero, -1 * (1-y));
bc->addDirichlet(u_hat, y_equals_one, zero);
bc->addDirichlet(u_hat, x_equals_one, zero);
```

Create a square mesh $[0,1] \times [0,1]$ with boundary conditions

- $\hat{t}_n = 2x - 2$ on $y = 0$
- $\hat{t}_n = x - 1$ on $x = 0$
- $\hat{u} = 0$ on $y = 1$
- $\hat{u} = 0$ on $x = 1$

Note

- Can subclass SpatialFilter to match any geometry
- Adding new mesh readers is straightforward

Convection-Diffusion in Three Slides

Test Norm, Solving, and Adaptivity

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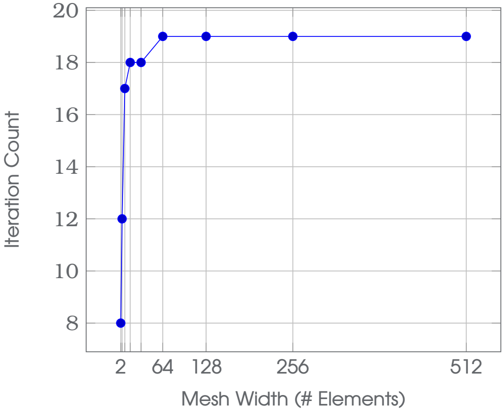
```
IPPtr ip = bf->graphNorm();

SolutionPtr soln = Solution::solution(mesh, bc, rhs, ip);

double threshold = 0.20;
RefinementStrategy refStrategy(soln, threshold);

int numRefs = 10;

ostringstream refName;
refName << "ConvectionDiffusion";
HDF5Exporter exporter(mesh,refName.str());

for (int refIndex=0; refIndex < numRefs; refIndex++) {
  soln->solve();

  double energyError = soln->energyErrorTotal();
  cout << "After " << refIndex << " refinements, energy error is " << energyError << endl;

  exporter.exportSolution(soln, vf, refIndex);

  if (refIndex != numRefs)
    refStrategy.refine();
}
```

Towards a Robust Iterative Solver

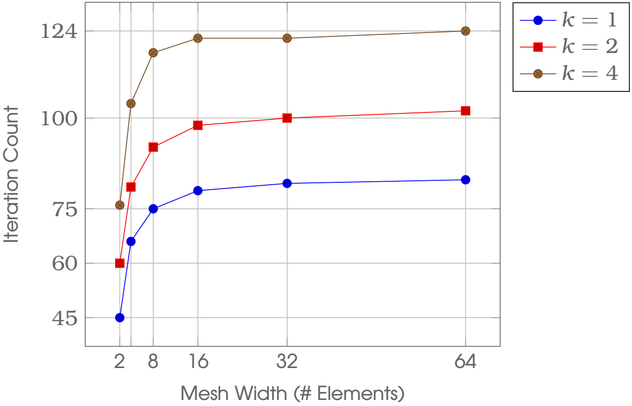
Poisson 1D, p-multigrid Preconditioners, $k = 16$



Poisson 1D: number of CG iterations to reduce error by a factor of 10^{10} using p-multigrid preconditioners with Schwarz smoother with 0 overlap for $k = 16$. The results for $k = 1, 2, 4$, and 8 are essentially identical.

Towards a Robust Iterative Solver

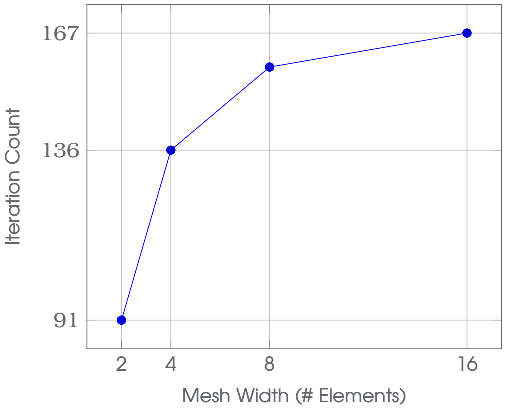
Stokes 2D, p-multigrid Preconditioners, Schwarz algebraic overlap 0



Stokes 2D: number of CG iterations to reduce error by a factor of 10^{10} using p-multigrid, algebraic Schwarz smoother with 0 overlap.

Towards a Robust Iterative Solver

Stokes 3D, p-multigrid Preconditioners, $k = 2$, Schwarz with Incomplete Cholesky



Stokes 3D: number of CG iterations to reduce error by a factor of 10^{10} using statically condensed system matrix with p-multigrid, algebraic Schwarz smoother, using Incomplete Cholesky factorization (fill ratio 5) for the Schwarz blocks.

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Other DPG Research

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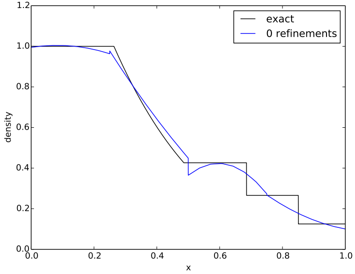
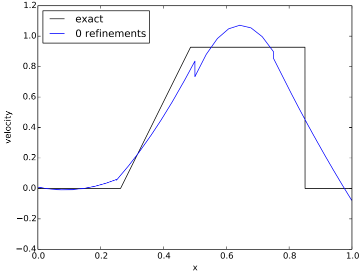
- Entropy scaling for physically meaningful test norms
- DPG for non-Hilbert L_p spaces

Thank You!


exact
0 refinements
density
x
0.0
0.2
0.4
0.6
0.8
1.0
1.2


exact
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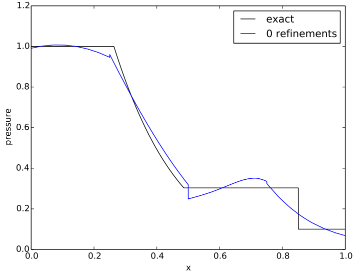
0.6
0.8
1.0
1.2


exact
0 refinements
pressure
x
0.0
0.2
0.4
0.6
0.8
1.0
1.2