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

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Table of Contents

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Table of Contents

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Navier-Stokes Equations

Numerical Challenges

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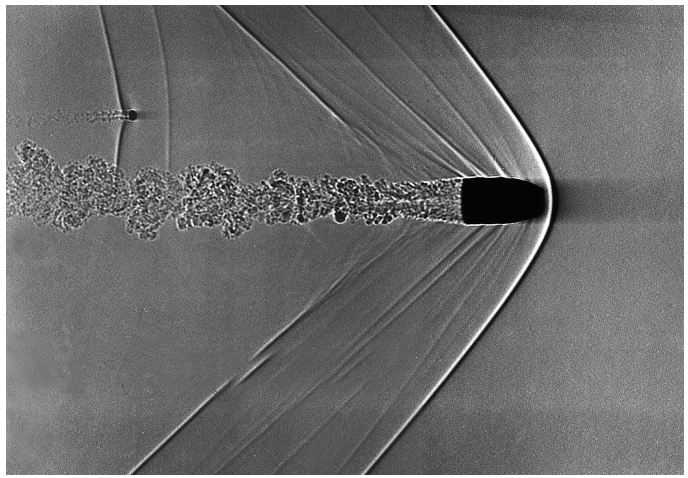
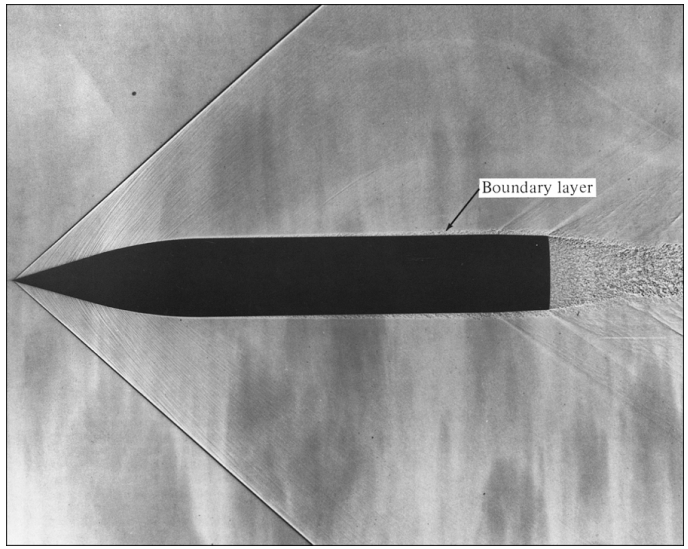
Robust simulation of unsteady fluid dynamics remains a challenging issue.

- Resolving solution features (sharp, localized viscous-scale phenomena)
  - Shocks
  - Boundary layers - resolution needed for drag/load
  - Turbulence (non-localized)
- Nonlinear convergence and uniqueness of solutions
- Stability of numerical schemes
  - Coarse/adaptive grids
  - Higher order



Shock

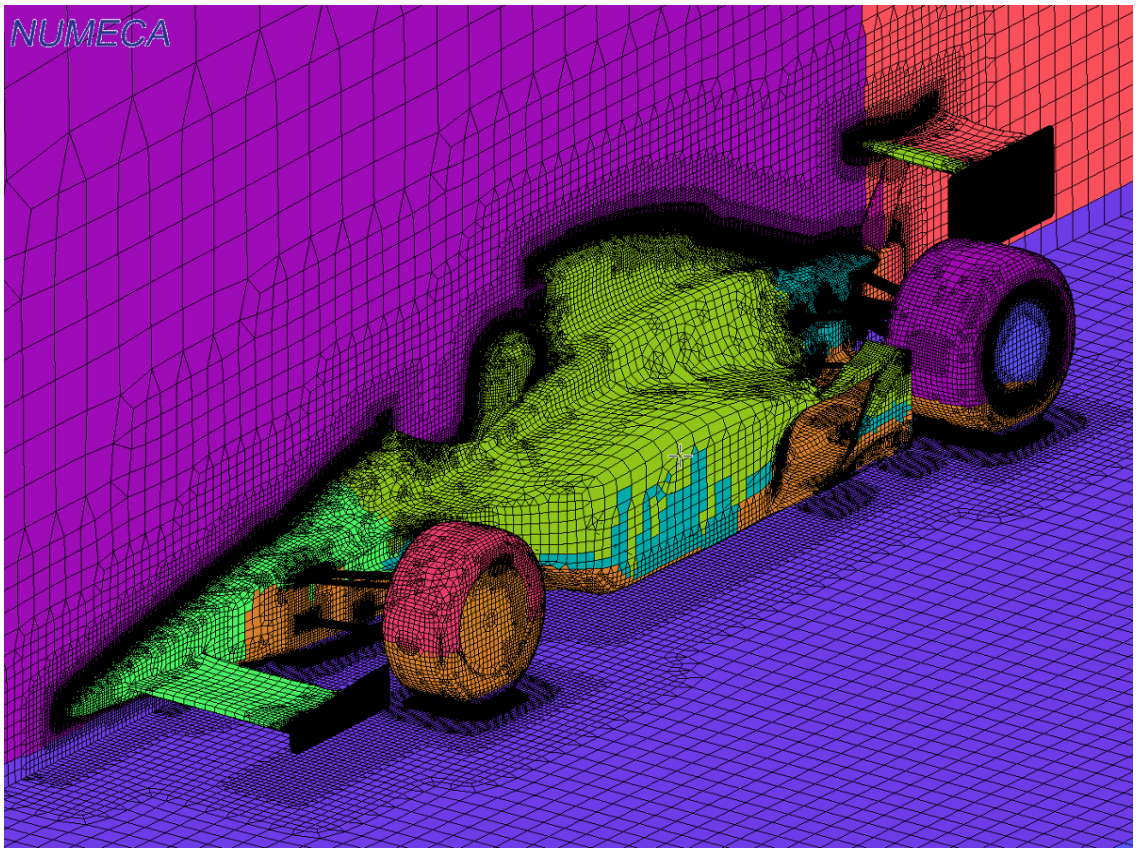


Boundary layer

Motivation

Initial Mesh Design is Expensive and Time-Consuming

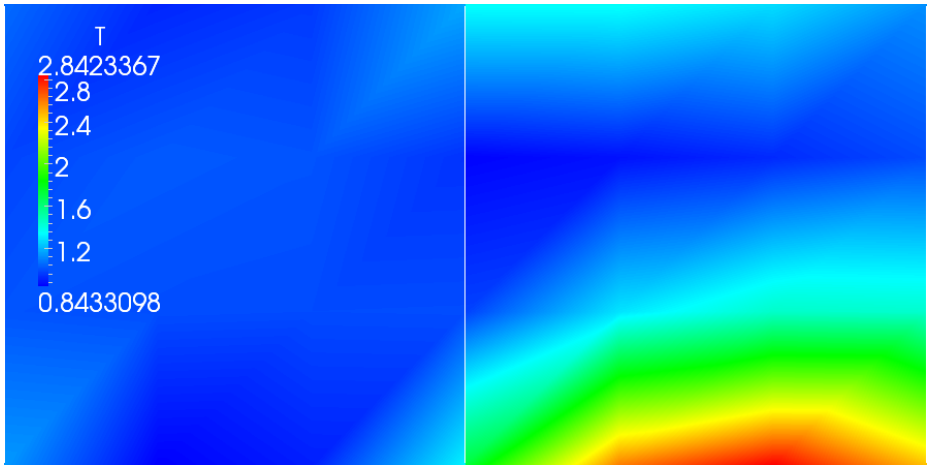
- Surface mesh must accurately represent geometry
- Volume mesh needs sufficient resolution for asymptotic regime
- Boundary layer meshes must respect y^+ guidelines
- Engineers often forced to work by trial and error
- Bad in the context of HPC



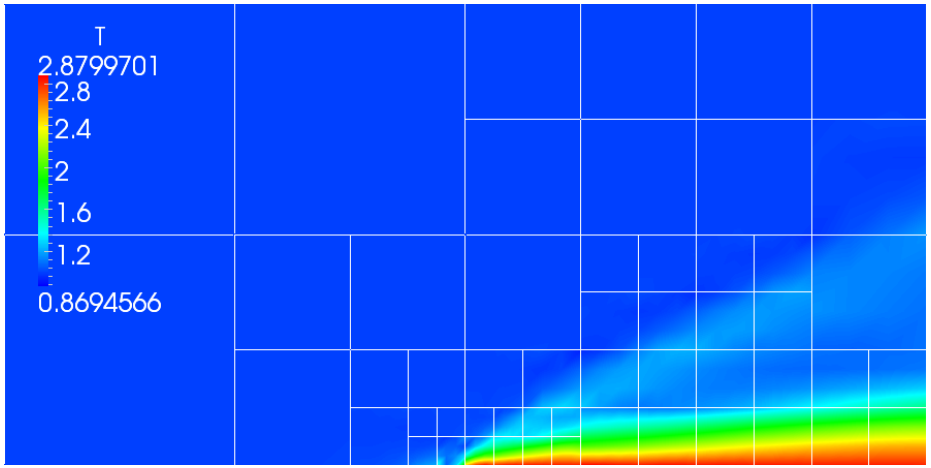
Formula 1 Mesh by Numeca

DPG on Coarse Meshes

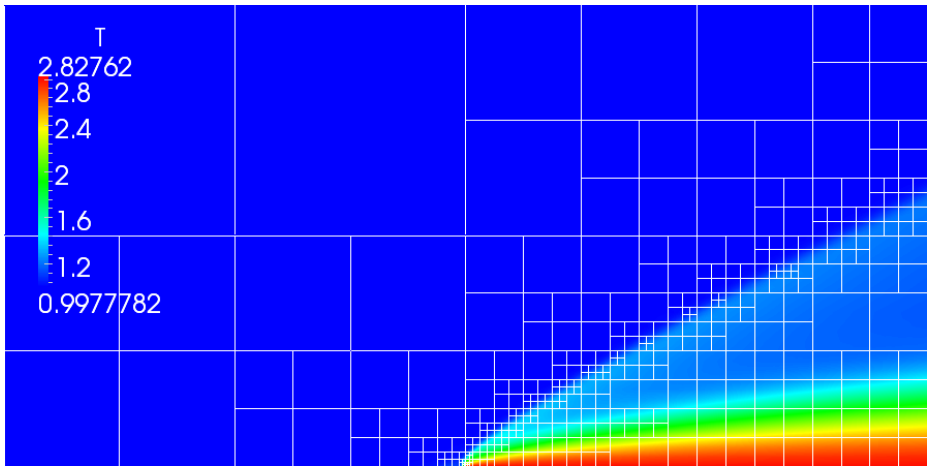
Adaptive Solve of the Carter Plate Problem[1] $Re = 1000$



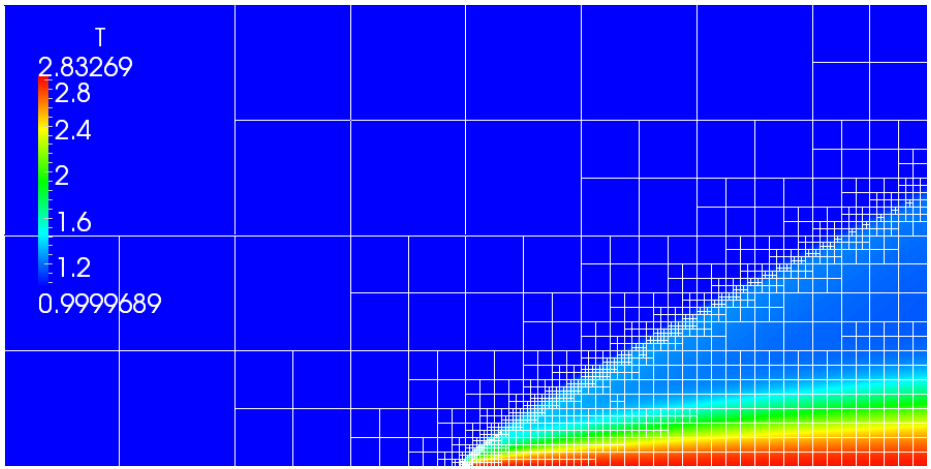
Temperature on Initial Mesh



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

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Streamline Upwind Petrov-Galerkin: Changing your 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 the a minimum residual context (i.e. as a Ritz method).

Space-Time FEM: Highly adaptive methods should have adaptive time integration. Space-time is a very natural framework in which to do moving mesh simulations.

Table of Contents

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Overview of DPG

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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 $Bu - l \in V'$:

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

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

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

Overview of DPG

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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

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

Overview of DPG

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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[2]

Other Features

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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

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

[2] **DPGOverview2**.

Overview of DPG

High Performance Computing

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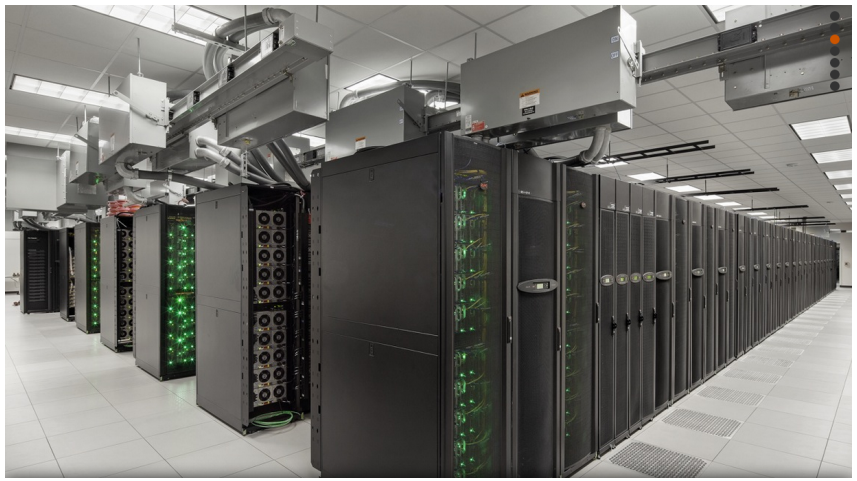
Eliminates human intervention

- 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

Table of Contents

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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

Table of Contents

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Camellia: DPG for the Masses

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Overview

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

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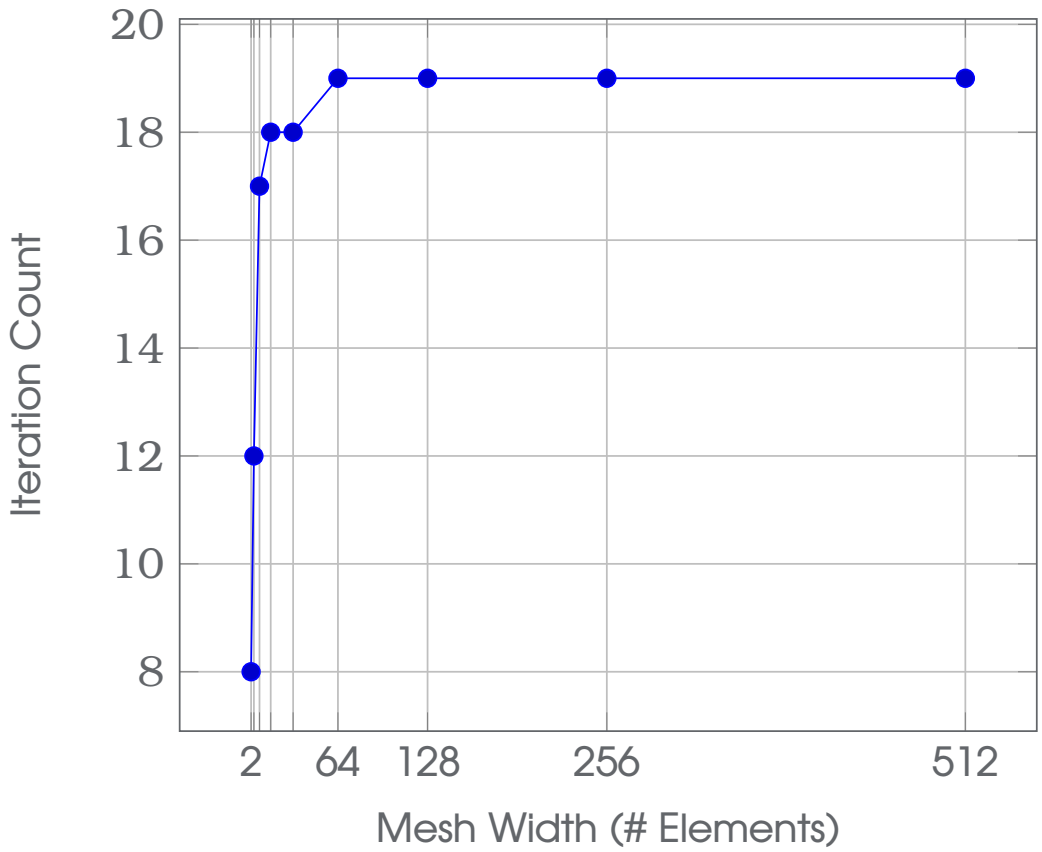
```
IPPtr ip = bf->graphNorm();

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 the indicated type of Schwarz smoother for $k = 16$. The results for $k = 1, 2, 4$, and 8 are essentially identical.

Towards a Robust Iterative Solver

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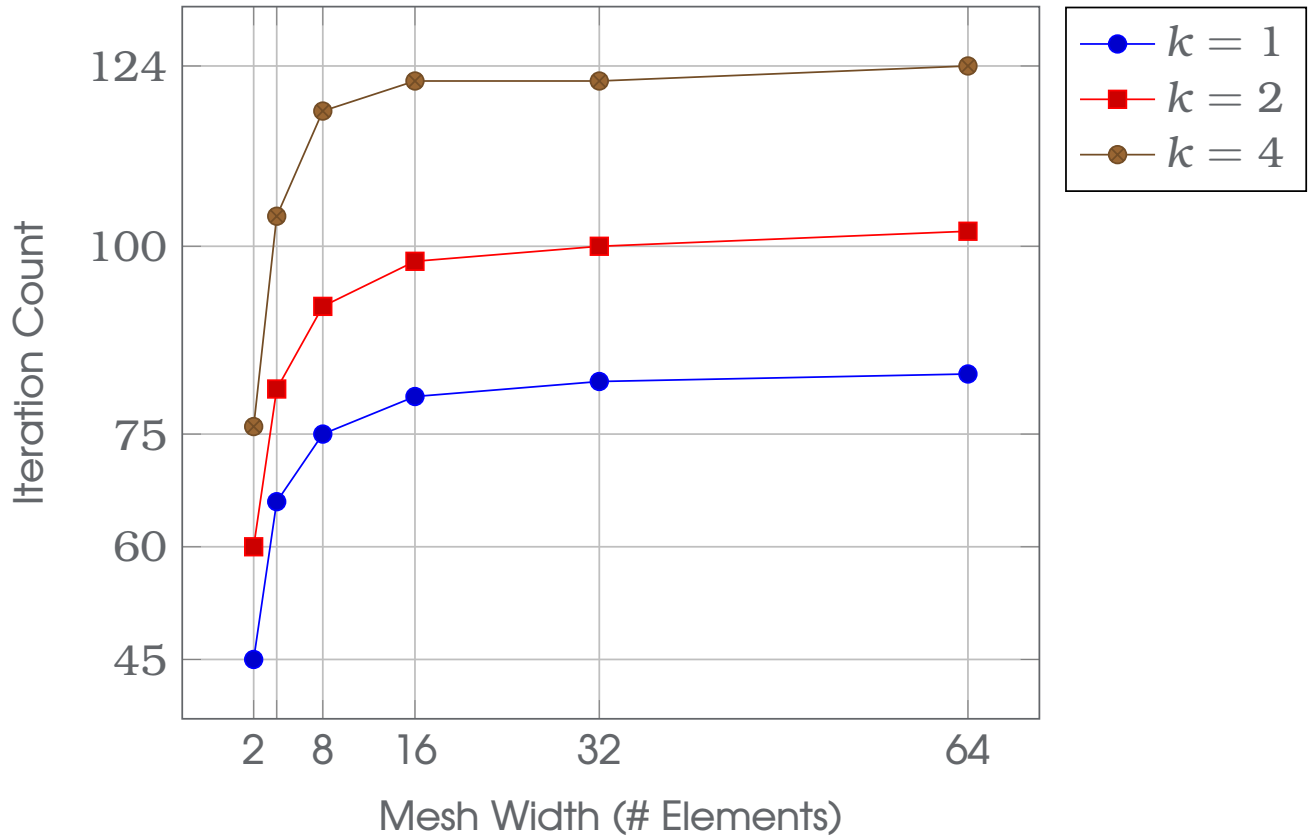
Stokes 2D, p-multigrid Preconditioners, Schwarz algebraic overlap 0



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

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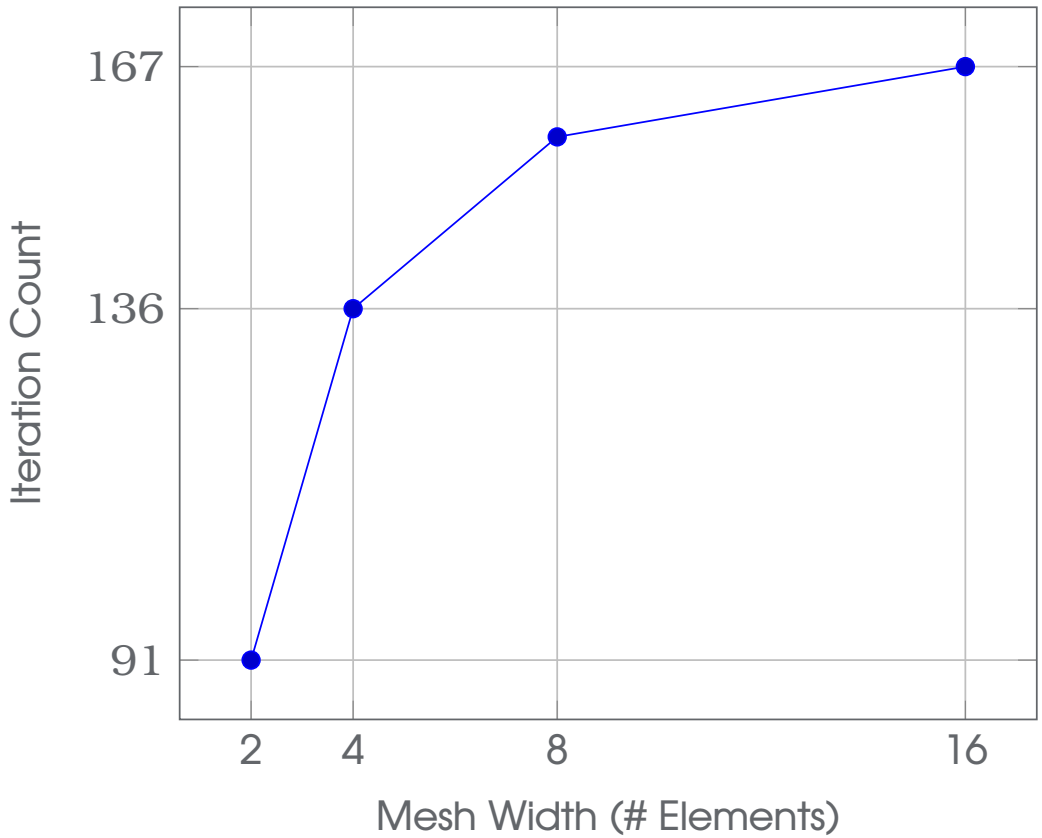
Stokes 3D, p-multigrid Preconditioners, $k = 2$, Schwarz with Incomplete Cholesky



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.

Table of Contents

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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!

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