Camellia:

A Toolbox for a Class of Discontinuous Petrov-Galerkin Methods Using Trilinos

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Outline

From Strong-Form PDE to DPG Form

PDE

$$\triangle \phi = f$$

First-Order System

$$\nabla \cdot \psi = f$$
$$\psi - \nabla \phi = 0$$

Integration by Parts

$$(\psi \cdot n, v)_{\Gamma_h} - (\psi, \nabla v)_{\Omega_h} = (f, v)_{\Omega_h}$$
$$(\psi, q)_{\Omega_h} + (\phi, q \cdot n)_{\Gamma_h} - (\phi, \nabla \cdot q)_{\Omega_h} = 0$$

Ultraweak (DPG) Variational Formulation

$$(\widehat{\psi}_n, v)_{\Gamma_h} - (\psi, \nabla v)_{\Omega_h}$$
$$+(\psi, q)_{\Omega_h} + (\widehat{\phi}, q_n)_{\Gamma_h} - (\phi, \nabla \cdot q)_{\Omega_h} = (f, v)_{\Omega_h}$$

"$b(u,v) = l(v)$"

$$Au = f$$

$$(u, A^* v)_{\Omega_h} + \langle u, v \rangle_{\Gamma_h} = l(v)$$

$$(u, A^* v)_{\Omega_h} + \langle \widehat{u}, v \rangle_{\Gamma_h} = l(v)$$

Solving with DPG

Continuous Test Space

DPG Form

$$b(u_h, v) = l(v)$$

Optimal Test Functions

For each $u \in U_h$, find $v_u \in V : (v_u, w)_V = b(u, w) \forall w \in V$

Discrete Test Space

DPG Form

$$b(u_h, v_h) = l(v_h)$$

Optimal Test Functions

For each $u \in U_h$, find $v_u \in V_{p+\triangle p} : (v_u, w)_V = b(u, w)$ $\forall w \in V_{p+\triangle p}$

Stiffness Matrix

$$K_{ij} = b(e_i, v_{e_j}) = (v_{e_i}, v_{e_j})_V = (v_{e_j}, v_{e_i})_V = b(e_j, v_{e_i}) = K_{ji}$$

Error (for adaptivity)

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

Error (for adaptivity)

$$||u - u_h||_E \approx \left|\left|R_{V_{p+\Delta p}}^{-1}(Bu_h - l)\right|\right|_{V_{p+\Delta p}}$$

Graph Test Norm

For a strong operator A with formal adjoint A^*, the adjoint graph space is

$$H_{A^*} = \left\{ v \in L^2(\Omega) : A^* v \in L^2(\Omega) \right\}$$

and the (adjoint) graph norm on the test space V is given by

$$||v||_{\text{graph}} = ||v||_{H_{A^*}} = \left(||v||^2 + ||A^* v||^2 \right)^{1/2}.$$

E.g. if $A^* = \nabla$, then $H_{A^*} = H^1$, and $||v||_{H_{A^*}} = ||v||_{H^1}$.

Key Result: Well-posedness $\implies$ Optimal Convergence

Under modest technical assumptions (true for Stokes), we have[1]

$$||Au|| \geq \gamma \, ||u|| \implies \sup_{v \in H_{A^*}} \frac{b((u, \widehat{u}), v)}{||v||_{H_{A^*}}} \geq \gamma_{\mathrm{DPG}} \left(||u||^2 + ||\widehat{u}||^2_{\widehat{H}_A(\Gamma_h)} \right)^{1/2}$$

where $\gamma_{\mathrm{DPG}} = O(\gamma)$ is a mesh-independent constant, and $||\cdot||_{\widehat{H}_A(\Gamma_h)}$ is the minimum energy extension norm.

[1] Nathan V. Roberts, Tan Bui-Thanh, and Leszek F. Demkowicz. The DPG method for the Stokes problem. Technical Report 12-22, ICES, 2012

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By Babuška's Theorem,

$$\implies \left(||u - u_h||^2 + ||\widehat{u} - \widehat{u}_h||^2_{\widehat{H}_A(\Gamma_h)} \right)^{1/2} \leq \frac{M}{\gamma_{\mathrm{DPG}}} \, (\mathrm{B.A.E.}) \, .$$

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Suffices to show that $||Au|| \geq \gamma \, ||u||$ to prove optimal convergence rate!

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Classical Stokes Problem

The classical strong form of the Stokes problem in $\Omega \subset \mathbb{R}^2$ is given by

$$\begin{aligned} -\mu\Delta\boldsymbol{u} + \nabla p &= \boldsymbol{f} && \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} &= 0 && \text{in } \Omega, \\ \boldsymbol{u} &= \boldsymbol{u}_D && \text{on } \partial\Omega, \end{aligned}$$

where μ is viscosity, p pressure, $\boldsymbol{u}$ velocity, and $\boldsymbol{f}$ a vector forcing function. Since by appropriate non-dimensionalization we can eliminate the constant μ, we take $\mu = 1$ throughout.

DPG Applied to Stokes

To apply DPG, we need a first-order system. We introduce $\boldsymbol{\sigma} = \nabla \boldsymbol{u}$:

$$
\begin{aligned}
-\nabla \cdot \boldsymbol{\sigma} + \nabla p &= \boldsymbol{f} && \text{in } \Omega, \\
\nabla \cdot \boldsymbol{u} &= 0 && \text{in } \Omega, \\
\boldsymbol{\sigma} - \nabla \boldsymbol{u} &= 0 && \text{in } \Omega.
\end{aligned}
$$

Testing with $(\boldsymbol{v}, q, \boldsymbol{\tau})$, and integrating by parts, we have

$$
\begin{aligned}
(\boldsymbol{\sigma} - p\boldsymbol{I}, \nabla \boldsymbol{v})_{\Omega_h} - \left\langle \widehat{\boldsymbol{t}}_n, \boldsymbol{v} \right\rangle_{\Gamma_h} &= (\boldsymbol{f}, \boldsymbol{v})_{\Omega_h} \\
(\boldsymbol{u}, \nabla q)_{\Omega_h} - \langle \widehat{\boldsymbol{u}} \cdot \boldsymbol{n}, q \rangle_{\Gamma_h} &= 0 \\
(\boldsymbol{\sigma}, \boldsymbol{\tau})_{\Omega_h} + (\boldsymbol{u}, \nabla \cdot \boldsymbol{\tau})_{\Omega_h} - \langle \widehat{\boldsymbol{u}}, \boldsymbol{\tau}\boldsymbol{n} \rangle_{\Gamma_h} &= \boldsymbol{0},
\end{aligned}
$$

where traction $\boldsymbol{t}_n \stackrel{\text{def}}{=} (\boldsymbol{\sigma} - p\boldsymbol{I})\boldsymbol{n}$, and the hatted variables $\widehat{\boldsymbol{t}}_n$ and $\widehat{\boldsymbol{u}}$ are new unknowns representing the traces of the corresponding variables at the boundary.

DPG Applied to Stokes

DPG Formulation:

$$\begin{aligned} b(u,v) = &(\boldsymbol{\sigma} - p\boldsymbol{I}, \nabla \boldsymbol{v})_{\Omega_h} - \left\langle \widehat{\boldsymbol{t}}_n, \boldsymbol{v} \right\rangle_{\Gamma_h} \\ &+ (\boldsymbol{u}, \nabla q)_{\Omega_h} - \langle \widehat{\boldsymbol{u}} \cdot \boldsymbol{n}, q \rangle_{\Gamma_h} \\ &+ (\boldsymbol{\sigma}, \boldsymbol{\tau})_{\Omega_h} + (\boldsymbol{u}, \nabla \cdot \boldsymbol{\tau})_{\Omega_h} - \langle \widehat{\boldsymbol{u}}, \boldsymbol{\tau}\boldsymbol{n} \rangle_{\Gamma_h} = (\boldsymbol{f}, \boldsymbol{v})_{\Omega_h} = l(v). \end{aligned}$$

The natural spaces for the trial variables are then:

- fields: $p \in L^2(\Omega), \boldsymbol{u} \in \boldsymbol{L}^2(\Omega), \boldsymbol{\sigma} \in \boldsymbol{L}^2(\Omega)$,
- fluxes: $\widehat{\boldsymbol{t}}_n \in \boldsymbol{H}^{-1/2}(\Gamma_h)$,
- traces: $\widehat{\boldsymbol{u}} \in \boldsymbol{H}^{1/2}(\Gamma_h)$.

The natural norms for fluxes and traces are *minimum energy extension norms*.

Graph Test Norm

The adjoint graph norm for our Stokes formulation is:[2]

$$\begin{aligned}||(\boldsymbol{\tau}, \boldsymbol{v}, q)||^2_{\text{graph}} = &\left|\left|\nabla \cdot \boldsymbol{\tau} - \nabla q\right|\right|^2 + \left|\left|\nabla \cdot \boldsymbol{v}\right|\right|^2 + \left|\left|\boldsymbol{\tau} + \nabla \boldsymbol{v}\right|\right|^2 \\ &+ \left|\left|\boldsymbol{\tau}\right|\right|^2 + \left|\left|\boldsymbol{v}\right|\right|^2 + \left|\left|q\right|\right|^2.\end{aligned}$$

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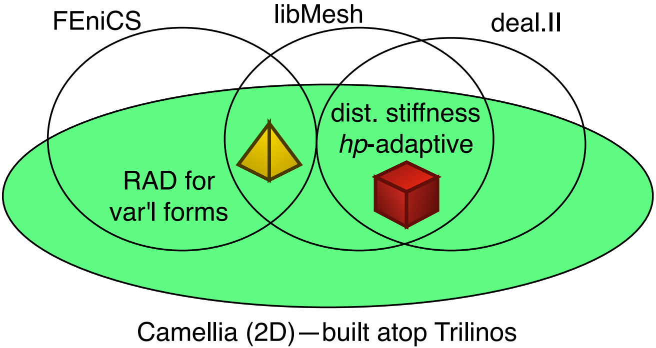
Camellia[4]

Design Goal: make DPG research and experimentation as simple as possible, without sacrificing too much by way of performance.



[3] Michael A. Heroux et al. An overview of the Trilinos project. *ACM Trans. Math. Softw.*, 31(3):397–423, 2005

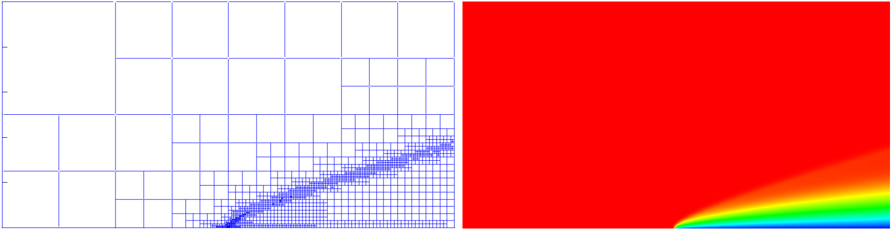
[4] Nathan V. Roberts, Denis Ridzal, Pavel B. Bochev, and Leszek F. Demkowicz. A Toolbox for a Class of Discontinuous Petrov-Galerkin Methods Using Trilinos. Technical Report SAND2011-6678, Sandia National Laboratories, 2011

Reliance on Trilinos

Feature	Trilinos Package
OO interface to MUMPS	Amesos
KLU solver	Amesos
conforming basis functions	Intrepid
pullbacks/Piola transforms	Intrepid
smart multidimensional arrays	Intrepid
distributed compressed row storage matrices	Epetra
cell topologies	Shards
reference-counted pointers	Teuchos
space-filling curves for spatially local mesh partitioning	Zoltan

Camellia: Users

- Jesse Chan: compressible Navier-Stokes
- Truman Ellis: compressible Navier-Stokes with turbulence
- Nate Roberts: incompressible Navier-Stokes



(a) Mesh (b) u_1

Figure: Compressible Navier-Stokes for Carter flat plate problem, $\mathrm{Re} = 1000, \mathrm{Ma} = 3.$

Implementation with Camellia

1. Identify variables involved: fields, traces, fluxes, and test functions.
2. Define the bilinear form.
3. Define right-hand side.
4. Define inner product.
5. Define boundary conditions.
6. Create initial mesh.
7. Create solution object (and solve).
8. Adaptively refine the mesh.

Identify variables involved.

For Stokes, we have trial variables:

- fields: scalar $p \in L^2(\Omega)$, vector $\boldsymbol{u} \in \boldsymbol{L}^2(\Omega)$, tensor $\boldsymbol{\sigma} \in \boldsymbol{L}^2(\Omega)$,
- fluxes: vector $\widehat{\boldsymbol{t}}_n \in \boldsymbol{H}^{-1/2}(\Gamma_h)$,
- traces: vector $\widehat{\boldsymbol{u}} \in \boldsymbol{H}^{1/2}(\Gamma_h)$.

```
VarFactory varFactory;
VarPtr p = varFactory.fieldVar("p");
VarPtr u1 = varFactory.fieldVar("u_1");
VarPtr u2 = varFactory.fieldVar("u_2");
VarPtr sigma11 = varFactory.fieldVar("\\sigma_11");
VarPtr sigma12 = varFactory.fieldVar("\\sigma_12");
VarPtr sigma21 = varFactory.fieldVar("\\sigma_21");
VarPtr sigma22 = varFactory.fieldVar("\\sigma_22");
VarPtr t1n = varFactory.fluxVar("\\hat{t}_1n");
VarPtr t2n = varFactory.fluxVar("\\hat{t}_2n");
VarPtr u1 = varFactory.traceVar("\\hat{u}_1");
VarPtr u2 = varFactory.traceVar("\\hat{u}_2");
```

Camellia: Rapid Specification of Inner Products

Suppose we have a problem whose graph norm is

$$||(v, \boldsymbol{q})||_{\text{graph}}^2 = ||v||^2 + ||\boldsymbol{q}||^2 + \left|\left|\frac{\partial v}{\partial x} - \frac{\partial v}{\partial y} + \nabla \cdot \boldsymbol{q}\right|\right|^2.$$

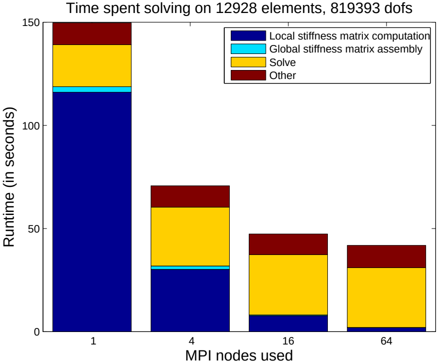
To specify this in Camellia, simply do:

```
VarFactory varFactory;
VarPtr v = varFactory.testVar("v", HGRAD);
VarPtr q = varFactory.testVar("q", HDIV);
IPPtr ip = Teuchos::rcp( new IP);
ip->addTerm(v);
ip->addTerm(q);
ip->addTerm(v->dx() - v->dy() + q->div());
```

The bilinear form can be specified similarly.

Camellia: Stiffness Matrix Timing Test

- local stiffness matrix computation is embarrassingly parallel
- minimize assembly costs: spatially local mesh partitioning
- timing tests on Lonestar: solve convection-dominated diffusion



- collaborators working on parallel solvers: Kyungjoo Kim (shared memory architecture), Maciej Paszynski (distributed memory)

Thank you!

Questions?

For more info:
nroberts@ices.utexas.edu

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