PECOS

Predictive Engineering and Computational Sciences

Camellia:

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

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The Abstract Problem and Minimization of the Residual

Take U, V Hilbert. We seek $u \in U$ such that

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

where b is bilinear and l is linear in v. Define B by $Bu = b(u,\cdot) \in V'$.

We seek to minimize the residual in the discrete space $U_h \subset U$:

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

If we use test functions $v_{\delta u_h} = R_V^{-1} B \delta u_h$, then the discrete solution to

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

minimizes the residual. We call the $v_{\delta u_h}$ optimal test functions.[1]

[1] L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions. *Numer. Meth. Part. D. E.*, 2010. in print

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

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

$$b((\phi, \psi, \widehat{\phi}, \widehat{\psi}_n), (v, q)) = (f, v)_{\Omega_h}$$
$$\text{“}b(u, v) = l(v)\text{”}$$

$$Au = f$$

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

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

$$b((u, \widehat{u}), v) = l(v)$$
$$\text{“}b(u, v) = l(v)\text{”}$$

Solving with DPG

- We drive adaptivity using an energy norm in which we can precisely determine the error:

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

- In practice, must approximate R_V^{-1}. We do this by using "enriched" test space $V_{p+\Delta p}$. ($\Delta p =$ 1 or 2, usually.)
- Test functions belong to a broken (element-wise conforming) space.
- Discontinuous test space $\implies$ optimal test functions can be determined element-locally.
- The system matrix is symmetric-positive definite:

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

Key Features of DPG

- guarantees minimum residual in a norm that depends on the test space, a free choice
- for non-singularly-perturbed, well-posed linear problems, provably optimal convergence rates when the “adjoint graph norm” is used for the test space
- nonlinear problems: so far, apply the linear method to the linearized problem
- have also derived a method that instead minimizes the nonlinear residual

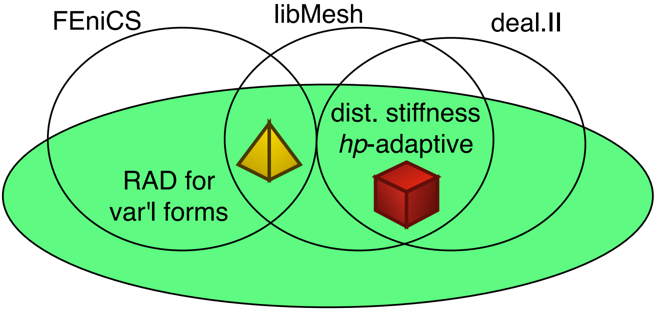
Adjoint Graph Norm

For a strong operator A with formal adjoint A^*, the adjoint graph norm on the test space V is given by

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

Camellia[3]

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



Camellia (2D)—built atop Trilinos[2]

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

[3]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

Camellia: 2011 Design

- Camellia defines abstract classes for bilinear form, inner product, right-hand side, boundary conditions.
- User implements problem-specific code through subclassing.
- Allows automatic definition of adjoint graph norm.

Implementation	Lines of Code
Stokes bilinear form	341
Stokes RHS and BCs	251
Automatic graph norm	198

Camellia: 2012 Design

- Key observation: bilinear form, inner product, and RHS can all be defined using linear terms involving the trial and test space variables.
- We can define a linear term as `lt = f * v` where `f` is a function and `v` is a variable.
- Functions can depend on spatial coordinates, and may be scalar-, vector-, or tensor-valued.
- Variables might be operated on by a linear differential operator.
- Using these as primitives, Camellia allows declarative specification of bilinear form, inner product, and RHS.

Camellia: 2012 Design, Poisson implementation

Recall our Poisson formulation:

$$\text{“}b(u,v)\text{”} = (\widehat{\psi}_n, v)_{\Gamma_h} - (\boldsymbol{\psi}, \nabla v)_{\Omega_h}$$
$$+(\boldsymbol{\psi}, \boldsymbol{q})_{\Omega_h} + (\widehat{\phi}, \boldsymbol{q}\cdot\boldsymbol{n})_{\Gamma_h} - (\phi, \nabla\cdot\boldsymbol{q})_{\Omega_h} = (f, v)_{\Omega_h}.$$

```
VarFactory varFactory;
VarPtr v = varFactory.testVar("v", HGRAD);
VarPtr q = varFactory.testVar("q", HDIV);

VarPtr psi_hat_n = varFactory.fluxVar("\\widehat{\\psi}_n");
VarPtr phi_hat = varFactory.traceVar("\\widehat{\\phi}");
VarPtr psi = varFactory.fieldVar("\\psi", VECTOR_L2);
VarPtr phi = varFactory.fieldVar("\\phi", L2);
```

Camellia: 2012 Design, Poisson implementation

Recall our Poisson formulation:

$$\text{“}b(u,v)\text{”} = (\widehat{\psi}_n, v)_{\Gamma_h} - (\boldsymbol{\psi}, \nabla v)_{\Omega_h}$$
$$+(\boldsymbol{\psi}, \boldsymbol{q})_{\Omega_h} + (\widehat{\phi}, \boldsymbol{q}\cdot\boldsymbol{n})_{\Gamma_h} - (\phi, \nabla\cdot\boldsymbol{q})_{\Omega_h} = (f, v)_{\Omega_h}.$$

```
BFPtr bf = Teuchos::rcp( new BF(varFactory) );

bf->addTerm(psi_hat_n, v);
bf->addTerm(-psi, v->grad());

bf->addTerm(psi, q);
bf->addTerm(phi_hat, q->dot_normal());
bf->addTerm(-phi, q->div());
```

RHS, BCs, and test space norms can be specified in a similar fashion.

Camellia: 2012 vs. 2011 Design, Lines of Code

Implementation	Lines of Code, Old	Lines of Code, New
Stokes bilinear form	341	50
Stokes RHS and BCs	251	90
Automatic graph norm	198	36

Camellia: Future Work

- support for curved geometry.
- minimize the *nonlinear* residual (adds a hessian term).
- in further future: 1D and 3D mesh support, distributed mesh and solution storage.

Thank you!

Questions?

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L. Demkowicz and J. Gopalakrishnan.
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