# Camellia: A Software Framework for a Discontinuous Petrov-Galerkin Methodology

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Trilinos User Group Meeting October 28, 2014



Office of Science



#### Collaborators

My collaborators in this work:

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- Paul Fischer (Argonne, UIUC)

#### Outline

#### Introduction to DPG

#### 2 Camellia

- Design Goals
- From Math to Code
- Feature List

#### 3 Camellia and Trilinos

#### DPG and HPC

#### DPG in Brief

DPG approach:

- Petrov-Galerkin: test and trial spaces differ
- discontinuous test and trial spaces
- · optimal test functions computed on the fly so that

$$(v_{e_i}^{\text{opt}}, v)_V = b(e_i, v) \,\forall v \in V$$

• key choice: which norm to use on the test space?

DPG features:

- automatic stability
- SPD stiffness matrix
- Error in  $u_h$  is minimized in the energy norm

$$||u_h||_E = \sup_{v \in V} \frac{b(u_h, v)}{||v||_V} = ||b(u_h, \cdot)||_{V'}$$

• Can measure the error in the energy norm to drive adaptivity.

#### DPG in Brief: Concept Map



\* Note: we approximate the infinite-dimensional test space by taking the polynomial order k for the trial and "enriching" it somewhat:  $k_{\text{test}} = k_{\text{trial}} + \Delta k$ —in all that follows,  $\Delta k = 1$  or  $\Delta k = 2$ .

# Building the ultraweak formulation

#### The DPG Solve

Computational steps for solving with DPG:

- **1** On each element, construct the Gram matrix  $G_{jk} \stackrel{\text{\tiny def}}{=} (v_j, v_k)_V$ .
- 2 On each element, solve:  $G_{jk}T_{ki} = B_{ji} \stackrel{\text{def}}{=} b(e_i, v_j)$  for the optimal test coefficients  $T_{ki}$ .
- 3 Since the stiffness matrix is given by

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

we can compute

$$(v_{e_i}, v_{e_j})_V = (G^{-1}B)^T G G^{-1}B = B^T G^{-1}B = B_{ki}^T T_{kj}.$$

That is, once we've determined the optimal test functions, just need a matrix-matrix multiply to determine the local stiffness matrix!

# DPG Applications to Date

DPG is a general framework, and has been successfully applied to a host of PDE problems, including:

- convection-dominated diffusion
- acoustics/wave propagation
- · linear elasticity
- Maxwell's equations (cloaking problem)
- Burgers' equations
- Euler equations
- compressible Navier-Stokes
- Stokes
- incompressible Navier-Stokes



flow past a cylinder, Re = 40

<sup>&</sup>lt;sup>1</sup>Bold items have Camellia-based implementations.

#### Classical Stokes Problem

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

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

where  $\mu$  is (constant) viscosity, p pressure, u velocity, and f a vector forcing function.

# DPG Applied to Stokes

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

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

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

$$egin{aligned} &oldsymbol{(\sigma-pI, 
abla v)}_{\Omega_h} - \left\langle \widehat{oldsymbol{t}}_n, oldsymbol{v} 
ight
angle_{\Gamma_h} = (oldsymbol{f}, oldsymbol{v})_{\Omega_h} \ &oldsymbol{(u, 
abla q)}_{\Omega_h} - \left\langle \widehat{oldsymbol{u}} \cdot oldsymbol{n}, q 
ight
angle_{\Gamma_h} = 0 \ &oldsymbol{(\sigma, \tau)}_{\Omega_h} + (\mu oldsymbol{u}, 
abla \cdot oldsymbol{\tau})_{\Omega_h} - \left\langle \widehat{oldsymbol{u}}, oldsymbol{\tau n} 
ight
angle_{\Gamma_h} = oldsymbol{0}, \end{aligned}$$

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

#### Formulation for Navier-Stokes

To derive a corresponding Navier-Stokes formulation, recall that the Navier-Stokes equations may be written

$$-\nabla p + \nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}$$
$$\boldsymbol{\sigma} - \mu \nabla \boldsymbol{u} = 0$$
$$\nabla \cdot \boldsymbol{u} = 0$$

where  $\mu = rac{1}{ ext{Re}}$ . Since  $\pmb{\sigma} = \mu 
abla \pmb{u}$ , we can write

$$-\nabla p + \nabla \cdot \boldsymbol{\sigma} - \frac{1}{\mu} \boldsymbol{u} \cdot \boldsymbol{\sigma} = \boldsymbol{f}$$
$$\boldsymbol{\sigma} - \mu \nabla \boldsymbol{u} = 0$$
$$\nabla \cdot \boldsymbol{u} = 0$$

#### Formulation for Navier-Stokes

$$-\nabla p + \nabla \cdot \boldsymbol{\sigma} - \frac{1}{\mu} \boldsymbol{u} \cdot \boldsymbol{\sigma} = \boldsymbol{f}$$
$$\boldsymbol{\sigma} - \mu \nabla \boldsymbol{u} = 0$$
$$\nabla \cdot \boldsymbol{u} = 0$$

Linearizing about  $u + du = (u + du, \sigma + d\sigma, p + dp)$ , we have

$$egin{aligned} b_{ ext{Stokes}}(du,v) &- \left( oldsymbol{d}oldsymbol{u} \cdot oldsymbol{\sigma} + rac{1}{\mu}oldsymbol{u} \cdot oldsymbol{d}oldsymbol{\sigma},oldsymbol{v} 
ight)_{\Omega_h} \ &= (oldsymbol{f},oldsymbol{v})_{\Omega_h} - b_{ ext{Stokes}}(u,v) + \left( rac{1}{\mu}oldsymbol{u} \cdot oldsymbol{\sigma},oldsymbol{v} 
ight)_{\Omega_h}. \end{aligned}$$

For now, we use the graph norm for Navier-Stokes (for high Reynolds numbers, we should do something else).

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#### Kovasznay Flow

A common test case for Navier-Stokes is an analytic solution due to Kovasznay [3]:

$$u_1 = 1 - e^{\lambda x} \cos(2\pi y)$$
$$u_2 = \frac{\lambda}{2\pi} e^{\lambda x} \sin(2\pi y)$$
$$p = \frac{1}{2} e^{2\lambda x} + C$$

where  $\lambda = \frac{\text{Re}}{2} - \sqrt{\left(\frac{\text{Re}}{2}\right)^2 + (2\pi)^2}$ . We use  $\Omega = (-0.5, 1.5) \times (0, 2)$  as our domain, and choose the constant C so that p has zero average on  $\Omega$ .



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Figure : Re = 40 flow results for DPG Navier-Stokes:  $L^2$  error of all field variables.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 0.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 1.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 2.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 3.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 5.

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Starting with a  $2 \times 2 \times 2$  quadratic mesh, we refine 6 times. Refinement 6.

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#### Convecting Cone Problem

Beginning with 2D data in the range [0, 1] in the shape of a cone as initial condition, we convect it in a circle, and examine the range of the final solution. Want to assess the spatial method, so we use Crank-Nicolson with  $\Delta t = \frac{2\pi}{2000}$  where the time for one revolution is  $2\pi$ .



 $k = 1,64 \times 64$  mesh, initial value.



 $k = 1,64 \times 64$  mesh, final value. Range: [-0.050, 0.66].

#### Convecting Cone Problem

Beginning with 2D data (in the shape of a cone) as initial condition in the range [0, 1], we convect it in a circle, and examine the range of the final solution.



#### **Convecting Cone Problem**



#### Convecting cone solution for $k = 8, 8 \times 8$ mesh: one revolution.

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# Camellia<sup>1</sup>

Design Goal: make DPG research and experimentation as simple as possible, while maintaining computational efficiency and scalability.



<sup>&</sup>lt;sup>1</sup>Nathan V. Roberts. Camellia: A software framework for discontinuous Petrov-Galerkin methods. *Computers & Mathematics with Applications*, 2014.

#### Camellia: Rapid Specification of Inner Products

Suppose we wish to specify a test space norm

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

To specify this in Camellia, simply do:

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

#### Camellia: Rapid Specification of Inner Products

What if you wanted a test norm that varied in space? Maybe something like:

$$||(v)||_{V}^{2} = ||v||^{2} + \left\| \nabla v \cdot \begin{pmatrix} 1-x \\ y \end{pmatrix} \right\|^{2}$$

We can handle that, too.

```
VarFactory varFactory;
VarPtr v = varFactory.testVar("v", HGRAD);
IPPtr ip = IP::ip();
ip->addTerm(v);
FunctionPtr x = Function::xn(1);
FunctionPtr y = Function::yn(1);
FunctionPtr weight = Function::vectorize(1-x, y);
ip->addTerm(weight * v->grad());
```

It is also simple to specify your own custom functions by subclassing  $\ensuremath{\mathsf{Function}}$  .

**Camellia Applications** 

## **Example Camellia Applications**



(a) Ramp Shock



(b) Sod Shock Tube (space-time)



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#### Camellia Features

Important features of Camellia:

- mechanisms for rapid specification of DPG variational forms, inner products, etc.
- distributed computation of stiffness matrix
- distributed representation of the solution
- 2D: curvilinear elements
- 2D: meshes of triangles and/or quads
- 3D: nonconforming hexahedra

Adaptivity features:

- *h* and *p*-refinements (anisotropic in *h* in 2D)
- arbitrarily irregular meshes
- modular interface: simple to implement new adaptive strategies

# Camellia Features (Coming Soon)

Features under development:

- robust iterative solver for the global solve (nearly there)
- space-time elements (partway there)
- distributed mesh representation (not yet there)



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#### Camellia and Trilinos

Camellia relies heavily on several Trilinos packages:

- Epetra—distributed matrices and vectors
- Intrepid—basis functions, pullbacks, FieldContainer
- Shards—cell topologies
- Teuchos—RCP, CLI options parsing, LAPACK interface
- Amesos—direct solver interface (MUMPS, SuperLUDist, KLU)
- AztecOO—CG and GMRES iterative solvers
- If Pack—additive Schwarz preconditioners
- Zoltan—mesh partitioning

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#### DPG and HPC

## Suitability of DPG for HPC

DPG has several attractive features for HPC:

- locality: optimal test functions embarrassingly parallel
- intensity: high-order computations take advantage of "free" flops
- automaticity: robust adaptivity means less human involvement

## DPG for HPC: Software Checklist

Feature	Camellia
parallel optimal test function determination	
distributed stiffness matrix	
high-order basis functions	
static condensation	
hp-adaptivity	
robust iterative solver (multigrid-preconditioned CG)	
distributed solution representation	
distributed mesh representation	
support for curvilinear geometry	
3D support	
time-domain support (space-time)	

## DPG for HPC: Software Checklist

Feature	Camellia
parallel optimal test function determination	$\checkmark$
distributed stiffness matrix	$\checkmark$
high-order basis functions	$\checkmark$
static condensation	$\checkmark$
hp-adaptivity	$\checkmark$
robust iterative solver (multigrid-preconditioned CG)	to-do
distributed solution representation	$\checkmark$
distributed mesh representation	to-do
support for curvilinear geometry	√ (2D)
3D support	$\checkmark$
time-domain support (space-time)	to-do

#### Thank you for your attention!

Questions?



#### For more info: nvroberts@alcf.anl.gov

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Questions

#### Flow Past a Cylinder: Initial Mesh



Starting with a minimal mesh on a domain  $30 \times 15$  cylinder diameters, we refine anisotropically to make the (cubic) mesh approximately isotropic and 1-irregular. The mesh on the right has 256 elements and 23,488 degrees of freedom.

#### **Deriving DPG**

Recall Babuška's Theorem:

Suppose we have a bilinear form b(u, v) defined on Hilbert spaces U and V, and suppose that

 $|b(u,v)| \leq M \left| |u| \right|_U \left| |v| \right|_V$ 

for continuity constant M,

#### **Deriving DPG**

Recall Babuška's Theorem:

Suppose we have a bilinear form b(u, v) defined on Hilbert spaces U and V, and suppose that

 $|b(u,v)| \leq M \left| |u| \right|_U \left| |v| \right|_V$ 

for continuity constant M, and suppose that the inf-sup condition holds:

$$\inf_{||u||_U=1} \sup_{||v||_V=1} b(u, v) \ge \gamma.$$

#### **Deriving DPG**

Now, consider a discretization  $U_h \subset U$ ,  $V_h \subset V$ , where  $\dim U_h = \dim V_h$ . If we have the discrete inf-sup condition

$$\inf_{||u||_{U_h}=1} \sup_{||v||_{V_h}=1} b(u,v) \ge \gamma_h > 0,$$

then Babuška's Theorem tells us that the continuous and discrete problems have unique solutions u and  $u_h$ , and that

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

#### **Originating Idea**

Can we choose our test space  $V_h$  so that the discrete inf-sup condition automatically holds?

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Can we choose our test space  $V_h$  so that the discrete inf-sup condition automatically holds?

For each basis function  $e_i \in U_h$ , find  $v_{e_i} \in V$  that realizes the supremum:

$$\sup_{||v||_V=1} b(e_i, v) = b(e_i, v_{e_i}).$$

We can find this by solving  $(v_{e_i}, v)_V = b(e_i, v) \ \forall v \in V.$ 

#### Originating Idea

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$$\sup_{||v||_V=1} b(e_i, v) = b(e_i, v_{e_i}).$$

We can find this by solving  $(v_{e_i}, v)_V = b(e_i, v) \ \forall v \in V$ . If we solve this exactly and use the  $v_{e_i}$  as our (optimal) test space, we can show that

Babuška's Theorem gives us

$$||u - u_h||_E = \inf_{w_h \in U_h} ||u - w_h||_E,$$

where

$$||u||_E \stackrel{\mathrm{\tiny def}}{=} \sup_{||v||_V = 1} b(u,v).$$

#### Questions

# 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 and l is linear in v. Writing in operator form

$$Bu = l,$$

and fixing discrete space  $U_h \subset U$ , we seek to minimize the residual

$$Bu_h - l$$
.

Specifically, we seek

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

#### Questions

#### The Abstract Problem and Minimization of the Residual

$$u_h = \operatorname*{arg\,min}_{w_h \in U_h} \; rac{1}{2} \, ||Bw_h - l||^2_{V'} \, .$$

Now, the dual space V' is not especially easy to work with; we would prefer to work with V itself. Recalling that the Riesz operator  $R_V: V \to V'$  defined by

$$R_V v = (v, \cdot)_V,$$

is an *isometry*— $||R_V v||_{V'} = ||v||_V$ —we can rewrite the term we want to minimize as a norm in V:

$$\frac{1}{2} ||Bw_h - l||_{V'}^2 = \frac{1}{2} ||R_V^{-1} (Bw_h - l)||_V^2$$
$$= \frac{1}{2} (R_V^{-1} (Bw_h - l), R_V^{-1} (Bw_h - l))_V.$$

#### The Abstract Problem and Minimization of the Residual

We seek to minimize

$$\frac{1}{2} \left( R_V^{-1} \left( Bw_h - l \right), R_V^{-1} \left( Bw_h - l \right) \right)_V.$$

The first-order optimality condition requires that the Gâteaux derivative be equal to zero for minimizer  $u_h$ ; since B is linear, we have

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

By the definition of  $R_V$ , this is equivalent to

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

## The Abstract Problem and Minimization of the Residual

We have:

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

Now, if we take  $e_i$  as a basis for  $U_h$  and identify  $v_{e_i} = R_V^{-1}Be_i$  as test functions, we can rewrite this as

$$b(u_h, v_{e_i}) = l(v_{e_i}).$$

Thus, the discrete solution that minimizes the residual is exactly attained by testing the original equation with appropriate test functions. We call these optimal test functions.<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov–Galerkin methods. Part II: Optimal test functions. *Numerical Methods for Partial Differential Equations*, 27(1):70–105, 2011.

## Technical Assumptions (true for VGP Stokes)

Under modest technical assumptions (true for Stokes), we have<sup>3</sup>

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

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

In the next slides, we detail the assumptions.

<sup>&</sup>lt;sup>3</sup>Nathan V. Roberts, Tan Bui-Thanh, and Leszek F. Demkowicz. The DPG method for the Stokes problem. *Computers and Mathematics with Applications*, 2014.

Technical Assumptions (true for VGP Stokes)

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

Define C as the operator arising from integration by parts:

$$(Au, v)_{\Omega} = (u, A^*v)_{\Omega} + \langle Cu, v \rangle.$$

We split C into  $C_1$  and  $C_2$  such that

where  $C_1 u = f_D$  corresponds to the Dirichlet BCs imposed.

### Technical Assumptions (true for VGP Stokes)

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

Assumptions:

- Theorem Hypothesis: with homogeneous boundary condition  $C_1 u = 0$  in place, operator A is bounded below in the  $L^2$ -orthogonal component of its null space.
- $C_1$  and  $C_2$  are defined in such a way that

$$(\langle u, C'_2 v \rangle = 0 \quad \forall u : C_1 u = 0) \implies C'_2 v = 0.$$

- A and  $A^*$  are surjective.
- Both graph spaces  $H_A(\Omega)$  and  $H_{A^*}(\Omega)$  admit corresponding trace spaces  $\hat{H}_A(\partial \Omega)$  and  $\hat{H}_{A^*}(\partial \Omega)$ .
- The boundary term  $\langle Cu,v\rangle$  arising from integration by parts is definite.

## Naive Test Norm<sup>4</sup>

What if we don't use the graph norm, but a naive choice instead?

$$||(\boldsymbol{\tau}, \boldsymbol{v}, q)||_{\text{naive}}^2 = ||\boldsymbol{\tau}||^2 + ||\nabla \cdot \boldsymbol{\tau}||^2 + ||\boldsymbol{v}||^2 + ||\nabla \boldsymbol{v}||^2 + ||q||^2 + ||\nabla q||^2$$

<sup>&</sup>lt;sup>4</sup>N.V. Roberts, D. Ridzal, P.N. Bochev, L. Demkowicz, K.J. Peterson, and C. M. Siefert. Application of a discontinuous Petrov-Galerkin method to the Stokes equations. In *CSRI Summer Proceedings 2010*. Sandia National Laboratories, 2010.

Questions

#### Naive Test Norm: $u_1$ convergence



Figure : h-convergence with the naive norm:  $u_1$ . Dashed lines: best approximation error.

Questions

#### Naive Test Norm: $u_2$ convergence



Figure : h-convergence with the naive norm:  $u_2$ . Dashed lines: best approximation error.

#### Naive Test Norm: *p* convergence



Figure : h-convergence with the naive norm: p. Dashed lines: best approximation error.

#### Graph vs. Naive Test Norm

What's the difference between the two norms? Why are the results better with the graph norm?

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

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The naive norm is stronger—e.g. it requires  $\nabla \cdot \boldsymbol{\tau} \in L^2$  and  $\nabla q \in L^2$ , whereas the graph norm merely requires that  $\nabla \cdot \boldsymbol{\tau} - \nabla q \in L^2$ .

# Camellia<sup>5</sup>

Design Goal: make DPG research and experimentation as simple as possible, while maintaining computational efficiency and scalability.



<sup>&</sup>lt;sup>5</sup>Nathan V. Roberts. Camellia: A software framework for discontinuous Petrov-Galerkin methods. *Computers & Mathematics with Applications*, 2014.

#### Questions



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