Overview of The Discontinuous Petrov-Galerkin Methodology

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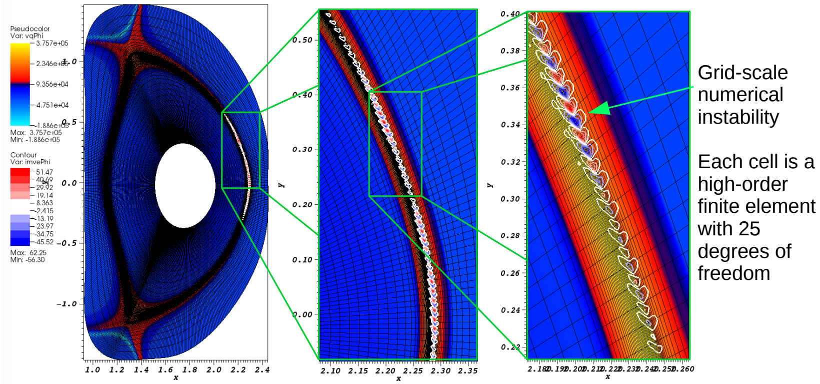
Outline

1. Motivation
2. Overview of The DPG Theory
3. Illustration using Poisson's Equation
4. Sound Wave Propagation with Flow
5. Shameless Advertisement
6. Conclusions

Advection challenges our Galerkin finite element formulation.



- Large $E \times B$ flows in the edge limit the time step in QH simulations [1]
- Advection is important in external kink and VDE simulations
- Petrov-Galkerin methods are designed to address advection

[1] Image from J. King 2018 Sherwood NIMROD Talk

Review of Galerkin Finite Element Formulation

- Consider Poisson's Equation:

$$\nabla^2\phi = -f \quad \in \Omega$$
$$\phi = 0 \quad \in \partial\Omega$$

- Expand ϕ onto trial basis functions:

$$\phi = \sum_i \phi_i \alpha_i \quad \alpha_i \in U^\delta$$

- Multiply by test functions and integrate over the domain:

$$\int_\Omega \phi_i \nabla\alpha_i \cdot \nabla\alpha_j d\Omega = \int_\Omega f \alpha_j d\Omega \quad \forall \alpha_j \in U^\delta$$
$$b\left(\phi_i\alpha_i, \alpha_j\right) = l\left(\alpha_j\right)$$

- Test and the trial functions belong to the same space.

The Galerkin formulation of Poisson's equation satisfies the continuity and coercivity conditions.

- Stability depends on the properties of the bilinear form: $b(\alpha_i, \alpha_j)$.
- Continuity ensures that the operator is bounded:

$$|b(\alpha_i, \alpha_j)| \leq \gamma \|\alpha_i\| \|\alpha_j\| \quad \forall \alpha_i, \alpha_j$$

- Coercivity ensures that the operator has no null space (the solution is unique):

$$b(\alpha_i, \alpha_i) \geq \beta \|\alpha_i\|^2 \quad \forall \alpha_i$$

- If $b(\alpha_i, \alpha_j)$ is both continuous and coercive then it is stable.

The standard Galerkin formulation of the advection operator is not coercive.

- Consider the case of 1D flow:

$$\vec{v} \cdot \nabla f \Rightarrow v_0 \frac{d}{dx} f$$

- Consider linear tent functions:

$$\alpha_i = \begin{cases} 1 - \frac{x - x_{i-1}}{x_i - x_{i-1}} & \text{for } x \in [x_{i-1}, x_i] \\ \frac{x - x_i}{x_{i+1} - x_i} & \text{for } x \in [x_i, x_{i+1}] \end{cases}$$

- The resulting bilinear form is not coercive if the mesh is equally spaced:

$$b(\alpha_i, \alpha_i) = \int_{x_{i-1}}^{x_i} v_0 \frac{d\alpha_i}{dx} \alpha_i dx + \int_{x_i}^{x_{i+1}} v_0 \frac{d\alpha_i}{dx} \alpha_i dx = -\frac{v_0}{2} + \frac{v_0}{2} = 0$$

- The existence of the null space permits spurious numerical modes

Petrov-Galerkin methods have been developed for problems with advection.

- The trail functions α_i and the test functions v^δ belong to different spaces.
- Stability relies on a generalized coercive condition:

$$\sup_{v^\delta \in V^\delta} \frac{\left| b\left(\alpha_i, v^\delta\right) \right|}{\left\| v^\delta \right\|_V} \geq \beta \left\| \alpha_i \right\|_U \quad \forall \alpha_i \in U$$

- Coercivity can be recovered by the choice of an good set of test functions.
  - Determining a suitable set of test functions is operator dependent
  - Difficult to generalize to arbitrary-order elements
- The DPG Methodology solves for the optimal set of test functions.

- Assume that the continuous problem is well-posed:

$$\sup_{v \in V} \frac{|b(\alpha_i, v)|}{\|v\|_V} \geq \beta \|\alpha_i\|_U \quad \forall \alpha_i \in U$$

- Introduce the operator $B : U \to V'$

$$\langle Bu, v \rangle_{V' \times V} = b(u, v)$$

- The Riesz operator transforms V to it's dual: $R_V : V \to V'$

$$\langle R_v v, \delta v \rangle_{V' \times V} = (v, \delta v)_V$$

The test functions are constructed using properties of the norm

- Property of the energy norm $\|B\alpha_i\|_{V'}$:

$$\sup_{v \in V} \frac{|b(\alpha_i, v)|}{\|v\|_V} = \|B\alpha_i\|_{V'}$$

- Apply the inverse Riesz operator:

$$\|B\alpha_i\|_{V'} = \left\| R_V^{-1} B\alpha_i \right\|_V = \frac{\left(R_V^{-1} B\alpha_i, R_V^{-1} B\alpha_i\right)_V}{\left\|R_V^{-1} B\alpha_i\right\|_V}$$

- Use the definition of B and R_V:

$$\frac{\left(R_V^{-1} B\alpha_i, R_V^{-1} B\alpha_i\right)_V}{\left\|R_V^{-1} B\alpha_i\right\|_V} = \frac{\left\langle B\alpha_i, R_V^{-1} B\alpha_i\right\rangle_{V' \times V}}{\left\|R_V^{-1} B\alpha_i\right\|_V} = \frac{b\left(\alpha_i, R_V^{-1} B\alpha_i\right)}{\left\|R_V^{-1} B\alpha_i\right\|_V}$$

Coercivity is assured with the appropriate choice of test functions

- Choosing the test functions $v_i^\delta = R_V^{-1} B\alpha_i$:

$$\sup_{v^\delta \in V^\delta} \frac{\left|b\left(\alpha_i, v^\delta\right)\right|}{\left\|v^\delta\right\|_V} \geq \frac{b\left(\alpha_i, v_i^\delta\right)}{\left\|v_i^\delta\right\|_V} = \sup_{v \in V} \frac{\left|b\left(\alpha_i, v\right)\right|}{\left\|v\right\|_V} \geq \beta \left\|\alpha_i\right\|_U \quad \forall \alpha_i \in U$$

- Discrete system is coercive if the continuous problem is coercive!
- The test functions are calculated by solving the equation

$$\left(v_i^\delta, \delta v\right)_V = b\left(\alpha_i, \delta v\right)$$

- The resulting finite element formulation has a **symmetric** matrix:

$$b\left(\alpha_i, v_j^\delta\right) = \left(v_i^\delta, v_j^\delta\right)_V$$

- One has to define the test inner product $(\cdot,\cdot)_V$ (or equivalent norm $\|\cdot\|_V$)

The test functions are calculated by solving a second set of equations

- Test functions are calculated by solving the equation:

$$\left(v_i^{\delta}, \delta v\right)_V = b\left(\alpha_i, \delta v\right)$$

- This global solve would be expensive.
- The system can be solved locally if the **test functions** are discontinuous.
  - Reduces the system size for each individual test function
  - Highly parallelizable and scales to large number of cores

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Poisson's equation is used to illustrate a typical DPG formulation in ultra-weak form[2]

- The ultra-weak from moves all differential operators to the test functions.
- Auxiliary variables are introduced to reduce Poisson's equation to a system of first order equations:

$$\nabla^2\phi = f \quad \Rightarrow \quad \begin{array}{l} \nabla\cdot\vec{\sigma} = f \\ \sigma - \nabla\phi = 0 \end{array}$$

- Multiply each equation by a test function and apply the chain rule:

$$\begin{array}{l} \nabla\cdot(\vec{\sigma}\tau_\phi) - \sigma\cdot\nabla\tau_\phi = f\tau_\phi \\ \vec{\sigma}\cdot\vec{\tau}_\sigma - \nabla\cdot(\phi\vec{\tau}_\sigma) + \phi\nabla\cdot\vec{\tau}_\sigma = 0 \end{array}$$

[2] Example is from the Camellia manual

Define separate variable for element interiors and element surfaces

- The system of equations is integrated over each element K:

$$\oint \hat{n} \cdot \vec{\sigma} \tau_\phi \partial K - \int \sigma \cdot \nabla \tau_\phi dK = \int f \tau_\phi dK$$
$$\int \vec{\sigma} \cdot \vec{\tau}_\sigma dK - \oint \phi \hat{n} \cdot \vec{\tau}_\sigma \partial K + \int \phi \nabla \cdot \vec{\tau}_\sigma dK = 0$$

- Separate flux and trace variables are defined for the unknown quantities on the element boundaries:
  - Boundary flux: $\hat{f} = \hat{n} \cdot \sigma \quad \in \partial K$
  - Boundary potential: $\hat{\phi} = \phi \quad \in \partial K$
- Summing the two equations gives the finite element formulation

$$b(\cdot,\cdot) = l(\cdot)$$
$$b(\cdot,\cdot) = (-\vec{\sigma}, \nabla \tau_\phi)_K + \left\langle \hat{f}, \tau_\phi \right\rangle_{\partial K} + (\vec{\sigma}, \vec{\tau}_\sigma)_K + (\phi, \nabla \cdot \vec{\tau}_\sigma)_K - \left\langle \hat{\phi}, \hat{n} \cdot \tau_\sigma \right\rangle_{\partial K}$$
$$l(\cdot) = (f, \tau_\phi)_K$$

The finite element spaces and inner product are chosen based on the finite element formulation

$$b(\cdot,\cdot) = l(\cdot)$$
$$b(\cdot,\cdot) = (\vec{\sigma}, \vec{\tau}_\sigma - \nabla \tau_\phi)_K + \left\langle \hat{f}, \tau_\phi \right\rangle_{\partial K} + (\phi, \nabla \cdot \vec{\tau}_\sigma)_K - \left\langle \hat{\phi}, \hat{n} \cdot \tau_\sigma \right\rangle_{\partial K}$$
$$l(\cdot) = (f, \tau_\phi)_K$$

- The choice of test and trial spaces are informed by the differential operators that appear:

$$\tau_\phi \in H(K, \nabla)$$
$$\vec{\tau}_\sigma \in H(K, \nabla\cdot)$$
$$\vec{\sigma}, \phi \in L^2(K)$$

- The inner product is chosen to be the one that yields the graph norm:

$$\|(\tau_\sigma, \tau_\phi)\|_V = \|\tau_\sigma - \nabla \tau_\phi\|_{L^2} + \|\nabla \cdot \tau_\sigma\|_{L^2} + \|\tau_\phi\|_{L^2} + \|\tau_\sigma\|_{L^2}$$

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Sound wave propagation with flow is used as a surrogate model for NIMROD's semi-implicit advance.

- The model system has sound waves and advection

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = -\frac{1}{\gamma M^2} \nabla p + \frac{1}{Re} \nabla^2 \vec{v}$$
$$\frac{\partial p}{\partial t} + \vec{v} \cdot \nabla p = -\gamma p \nabla \cdot \vec{v}$$

- Sound waves are modeled by a self-adjoint operator

$$\frac{\partial^2 p}{\partial t^2} = \frac{1}{M^2} \nabla^2 p = L_p(p)$$

- A staggered time advance with the semi-implicit operator applied to the pressure equation is used

$$\frac{\Delta \vec{v}}{\Delta t} + \theta \Delta \vec{v} \cdot \nabla \vec{v}^j + \theta \vec{v}^j \cdot \nabla \Delta \vec{v} - \frac{\theta}{Re} \nabla^2 \Delta \vec{v} = -\vec{v}^j \cdot \nabla \vec{v}^j - \frac{\nabla p^{j+1/2}}{\gamma M^2} + \frac{1}{Re} \nabla^2 \vec{v}^j$$
$$\left(1 - \frac{C_0 \Delta t^2}{4M^2} \nabla^2\right) \frac{\Delta p}{\Delta t} + \theta \vec{v}^{j+1} \cdot \nabla \Delta p + \theta \gamma \Delta p \nabla \cdot \vec{v}^{j+1} =$$
$$- \vec{v}^{j+1} \cdot \nabla p^{j+1/2} - \gamma p^{j+1/2} \nabla \cdot \vec{v}^{j+1}$$

The linear sound wave system is solved in the ultra-weak form

- Introduce auxiliary variables for the gradients:

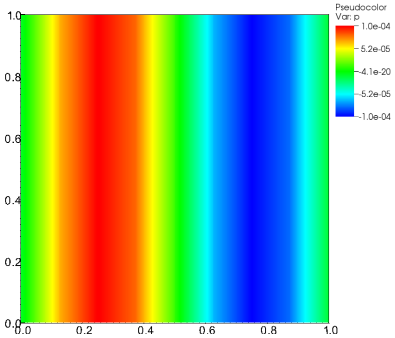
$$\vec{g}_p = \nabla p, \quad \vec{g}_{vx} = \nabla v_x, \quad \vec{g}_{vy} = \nabla v_y$$

- The pressure advance has the following form:

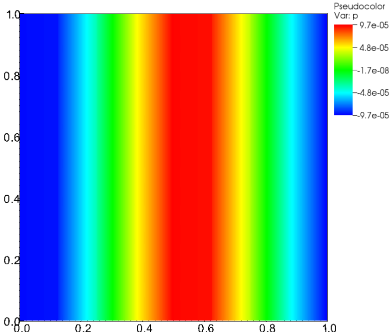
$$\left(\frac{1}{\Delta t}\Delta p, \tau_p\right) + \left(\frac{C_0 \Delta t}{4M^2} g_p, \nabla \Delta \tau_p\right) + \left\langle -\widehat{\Delta F}_p, \tau_p \right\rangle + \left(\theta \vec{v}_0 \cdot \Delta \vec{g}_p, \tau_p\right)$$
$$+ \left(\theta \Delta g_p, \vec{\tau}_{gp}\right) + \left\langle -\theta \widehat{\Delta p}, \hat{n} \cdot \vec{\tau}_{gp} \right\rangle + \left(\theta \Delta p, \nabla \cdot \vec{\tau}_{gp}\right)$$
$$= \left(-\vec{v}_0 \cdot g_p^{j+1/2}, \tau_p\right) + \left(-\gamma \left[\hat{e}_x \cdot \vec{g}_{vx}^{j} + \hat{e}_y \cdot \vec{g}_{vy}^{j}\right], \tau_p\right)$$
$$+ \left(-g_p^{j+1/2}, \vec{\tau}_{gp}\right) + \left\langle \widehat{p^{j+1/2}}, \hat{n} \cdot \vec{\tau}_{gp} \right\rangle + \left(-p^{j+1/2}, \nabla \cdot \vec{\tau}_{gp}\right)$$

- Blue terms are due to the auxiliary equation: $\nabla p = \vec{g}_p$
- The inner product is chosen to produce the norm:

$$\left\|(\tau_p . \vec{\tau}_{gp})\right\|_p = \left\|\frac{\tau_p}{\Delta t}\right\| + \|\nabla \tau_p\| + \|\vec{v}_0 \cdot \nabla \tau_p\| + \|\vec{\tau}_{gp}\| + \|\nabla \cdot \vec{\tau}_{gp}\|$$



$t = 50\ \tau_{Cs}$



$t = 100,050\ \tau_{Cs}$

- The simulation is stable at large Δt
- Example shows $v_0 \Delta t = 100 \Rightarrow \quad CFL \approx\ 1000$

Shameless Advertisement: Apollo is framework for quickly testing discretization schemes across a wide range of physical test cases

- Built around the Camellia tool-kit
  - Designed as a research tool for investigating DPG
  - Supports scalar and vector variables
  - $H(\nabla)$, $H(\cdot)$, $H(\times)$, and L^2 basis functions
  - Support for standard Galerkin, DG, FOSLS, and hybridizable DG methods
  - Built on Trillinos
- Apollo Framework: https://github.com/ApolloFramework/
- Camellia Main Trunk: https://bitbucket.org/nateroberts/camellia
- SemiImplicit Test Case: /ApolloFramework/theaceae/tree/master/fluid_dynamics

Conclusions: The Discontinuous Petrov-Galerkin methodology is new finite element methodology designed for systems with advection.

- Solve for the optimal test functions that guarantee stability
  - Calculation is local to each element
  - User defines test space inner product
- Modeling shows stable sound wave propagation at large CFLs
- References:
  - Demkowicz and Gopalakrishnah, ICES Report 15-20, 2015, https://www.ices.utexas.edu/media/reports/2015/1520.pdf
  - Roberts, ANL/ALCF-16/3, 2016, http://www.ipd.anl.gov/anlpubs/2016/11/130782.pdf

The DPG Method is a Minimum Residual Method

- Choosing the trial norm to be the energy norm:

$$\|u\|_E = \|Bu\|_{V'} = \left\| R_V^{-1} Bu \right\|_V$$

- The coercivity coefficient is > 1:

$$\sup_{v^\delta \in V^\delta} \frac{\left| b\left(\alpha_i, v^\delta\right) \right|}{\left\| v^\delta \right\|_V} \geq \sup_{v \in V} \frac{\left| b\left(\alpha_i, v\right) \right|}{\left\| v \right\|_V} = \|\alpha_i\|_U \quad \forall \alpha_i \in E$$

- Babuska theorem shows that the DPG error is orthogonal to the trail space

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

- The error in the energy norm is equal to the residual

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

- If the test norm is the L^2 norm, then the DPG method reduces to the least squares method.