Overview of PhD Work & Future Research Plans

Brendan Keith

Hooke Research Fellowship Presentation

January 8–9, 2018

Outline

Prelude: Background

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Act 1: Numerical Methods

- Discrete least-squares methods
- DPG methods
- DPG* methods
- Goal-oriented methods

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- Waves
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- ~~ESEAS~~
- ~~hp2D & hp3D~~
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Afterword: Future Acts

- NA Group
- OCIAM
- OxPDE

Prelude

About my work

PhD candidate at ICES

Supervisor: Dr Leszek Demkowicz

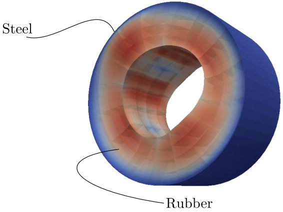
- Study discontinuous Petrov–Galerkin (DPG) methods

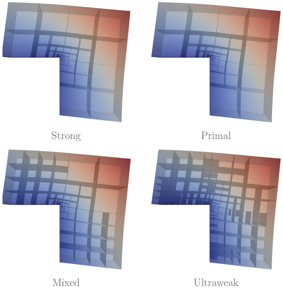
About my work

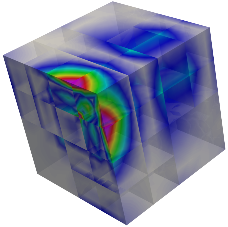
PhD candidate at ICES

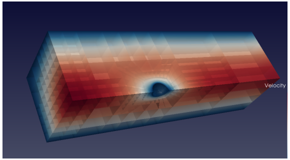
Supervisor: Dr Leszek Demkowicz

- Study discontinuous Petrov–Galerkin (DPG) methods
- Discovered DPG* methods
- Define discrete least-squares methods
- 3D simulations
- Adaptive mesh refinement
- Goal-oriented methods
- Applications!

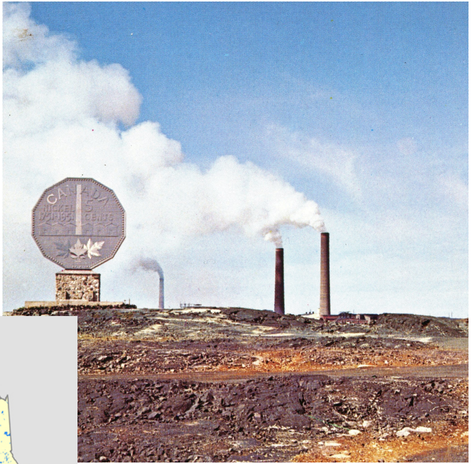




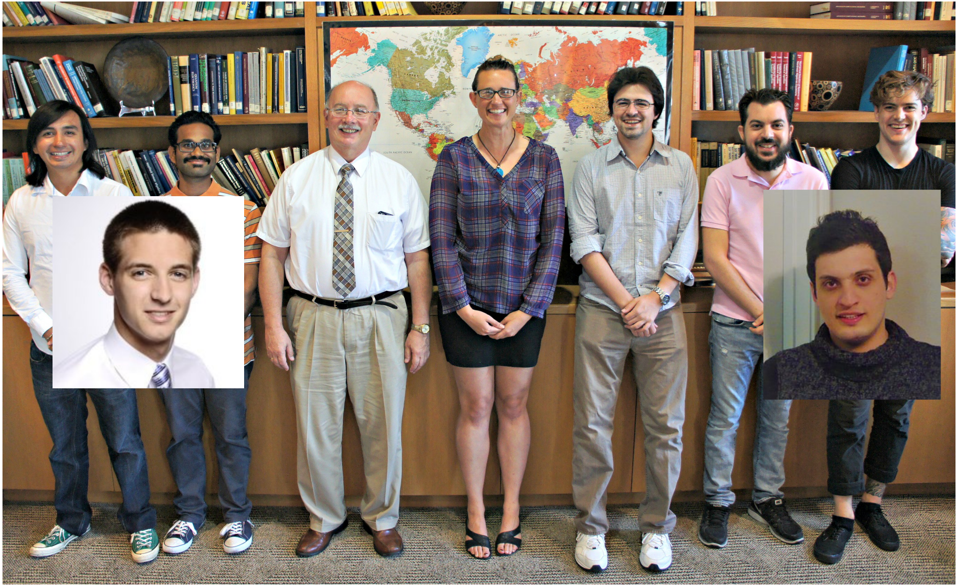




About me



About the DPG group



Act 1: Numerical Methods

Stability

Petrov–Galerkin methods

Let $b : U \times V \to \mathbb{R}$ be a continuous bilinear form.

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Continuous stability

Discrete stability

$$\inf_{u\in U}\sup_{v\in V}\frac{b(u,v)}{\|u\|_U\|v\|_V} = \gamma > 0 \quad \not\Rightarrow \quad \inf_{u_h\in U_h}\sup_{v_h\in V_h}\frac{b(u_h,v_h)}{\|u_h\|_U\|v_h\|_V} = \gamma_h > 0$$

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Q: How to satisfy the discrete inf-sup condition

$$\sup_{v_h \in V_h} \frac{b(u_h,v_h)}{\|v_h\|_V} \geq \gamma_h \|u_h\|_U \,, \quad \forall\, u_h \in U_h \quad ?$$

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$$\not\Rightarrow$$

Discrete stability

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Q: How to satisfy the discrete $\inf$-$\sup$ condition

$$\sup_{v_h \in V_h} \frac{b(u_h,v_h)}{\|v_h\|_V} \geq \gamma_h \|u_h\|_U \,, \quad \forall\, u_h \in U_h \quad ?$$

A: Fix U_h and increase the dimension of V_h until satisfied.

Discrete least-squares methods

Q: How to define a discrete solution when $\dim(V_h) > \dim(U_h)$?

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NB: For fixed U_h, the optimally stable FEM is always a minimum residual method!

Stiffness matrix:

$$\mathsf{B}_{ij} = b(u_j, v_i)$$

Load vector:

$$\mathsf{l}_i = \ell(v_i)$$

B. Keith, S. Petrides, F. Fuentes, and L. Demkowicz.
Discrete least-squares finite element methods.
Comput. Methods Appl. Mech. Engrg., 327:226–255, 2017.

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$$\mathrm{cond}(\mathsf{B}^\mathsf{T}\mathsf{B}) = \mathrm{cond}(\mathsf{B})^2$$

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$$\mathsf{B}^\mathsf{T}\mathsf{G}^{-1}\mathsf{B}\mathbf{u} = \mathsf{B}^\mathsf{T}\mathsf{G}^{-1}\mathsf{l}$$

where

$$\mathsf{G} \approx \mathsf{B}\mathsf{B}^\mathsf{T}$$

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DPG: G is block-diagonal

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In DPG, we solve

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In DPG*, we solve

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and then post-process **w**:

$$\mathsf{u} = \mathsf{G}^{-1}\mathsf{B}^\mathsf{T}\mathsf{w}$$

L. Demkowicz, J. Gopalakrishnan, and B. Keith.
Analysis of a DPG* method for the Poisson equation.
In preparation, 2018.

B. Keith, L. Demkowicz, and J. Gopalakrishnan.
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Highlights

- ⋆ DPG/DPG* always deliver SPD (HPD) stiffness matrices

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- ⋆ DPG/DPG* always deliver SPD (HPD) stiffness matrices
- ⋆ DPG/DPG* have built-in stability
- ⋆ DPG has a built-in error estimator
- ⋆ DPG* works for some problems without uniqueness

Goal-oriented methods

Consider the following abstract model:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathcal{F}(\mathbf{x}, \mathbf{u}; \mu)\,, \\ \mathbf{y} = \mathcal{G}(\mathbf{x})\,. \end{cases}$$

Solution variable: $\mathbf{x}$
Input: $\mathbf{u}$
Model parameter(s): μ
QoI (or output): $\mathbf{y}$.

Research interest:

- By designing numerical methods with only the given output $\mathbf{y}$ in mind, efficiency can sometimes be greatly improved.
- Example: goal-oriented adaptive mesh refinement.

Goal-oriented adaptivity

Problem:

$$\begin{cases} \text{Find } u \in U \ : \\ b(u,v) = \ell(v)\,, \quad \forall\, v \in V \end{cases}$$

Dual Problem:

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DPG–DPG* orthogonality:

$$g(u - u_h) = b(u - u_h, v)$$

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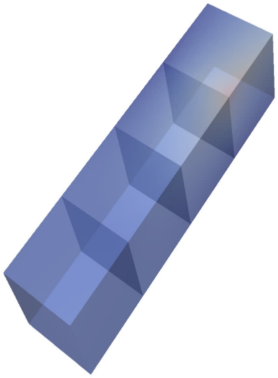
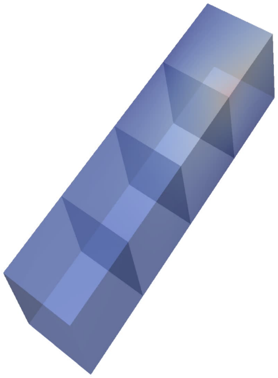
Goal-oriented adaptivity

Solution-oriented strategy



Goal-oriented strategy (1 of 3)



B. Keith and N. V. Roberts.
Goal-oriented adaptive mesh refinement with DPG methods for viscoelastic fluids.
In preparation, 2018.

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Goal-oriented adaptive mesh refinement for non-symmetric functional settings.
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Act 2: Applications

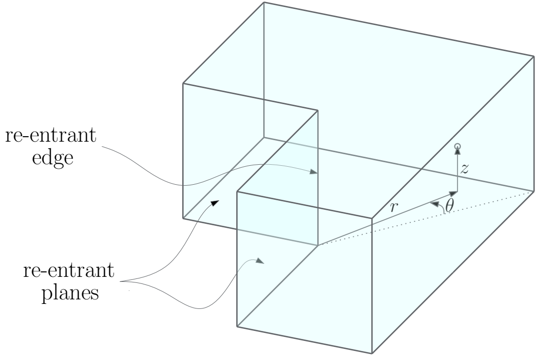
Structural Mechanics

The DPG methodology applied to different variational formulations of linear elasticity

Linear elasticity

$$\begin{cases} \sigma - \mathsf{C}:\varepsilon(u) = 0 & \text{in } \Omega\,, \\ -\operatorname{Div}\sigma = f & \text{in } \Omega\,, \\ u = u_0 & \text{on } \Gamma_u\,, \\ \sigma\cdot\hat{n} = g & \text{on } \Gamma_\sigma\,, \end{cases}$$

L-shaped domain



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Structural Mechanics

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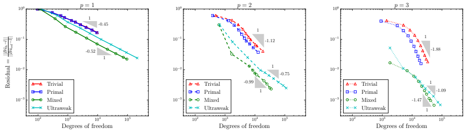
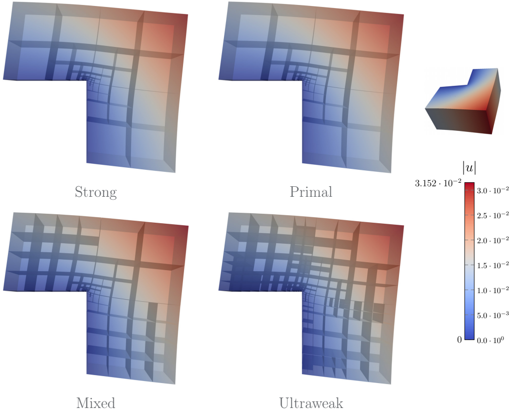
$$

Convergence rates



Residual in L-shaped domain with singular solution and adaptive refinements

L-shaped domain



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Structural Mechanics

Coupled variational formulations of linear elasticity and the DPG methodology

Linear elasticity

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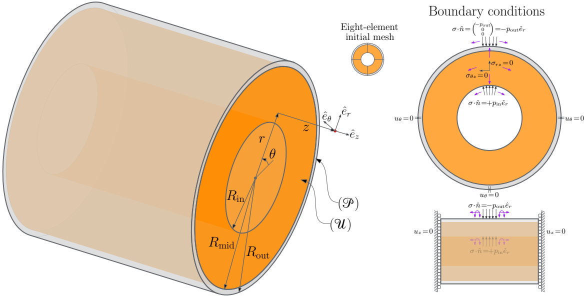
Sheathed hose ($E_{\text{steel}} = 200$GPA, $E_{\text{rubber}} = 0.01$GPA)



Coupled formulations

- All coupled formulations are mutually compatible in the same domain.

F. Fuentes, B. Keith, L. Demkowicz, and P. L. Tallec.
Coupled variational formulations of linear elasticity and the DPG methodology.
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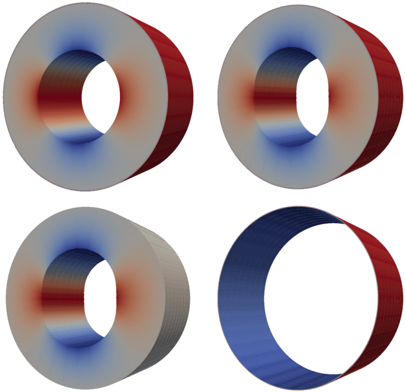

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Fluid Mechanics

An ultraweak DPG method for viscoelastic fluids

Oldroyd-B fluid

Conservation of mass and momentum

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \nabla\cdot\boldsymbol{\sigma} = \rho\,\mathbf{f} \quad \text{on } \Omega\times(0,T)\,.$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{on } \Omega\times(0,T)\,.$$

Constitutive law

$$\boldsymbol{\sigma} = -p\,\mathbf{I} + 2\mu_S\,\varepsilon(\mathbf{u}) + \mathbf{T}\,,$$

$$\mathbf{T} + \lambda\left(\frac{\partial \mathbf{T}}{\partial t} + \mathcal{L}_{\mathbf{u}}\mathbf{T}\right) = 2\mu_P\,\varepsilon(\mathbf{u})\,.$$

(Autonomous) Lie derivative

$$\mathcal{L}_{\mathbf{u}}\mathbf{T} = \mathbf{u}\cdot\nabla\mathbf{T} - \left(\nabla\mathbf{u}\,\mathbf{T} - \mathbf{T}\,\nabla^{\mathsf{T}}\mathbf{u}\right)\,.$$

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Conservation of mass and momentum

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \nabla\cdot\boldsymbol{\sigma} = \rho\,\mathbf{f} \quad \text{on } \Omega\times(0,T)\,.$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{on } \Omega\times(0,T)\,.$$

Constitutive law

$$\boldsymbol{\sigma} = -p\,\mathbf{I} + 2\mu_S\,\varepsilon(\mathbf{u}) + \mathbf{T}\,,$$

$$\mathbf{T} + \lambda\left(\frac{\partial \mathbf{T}}{\partial t} + \mathcal{L}_{\mathbf{u}}\mathbf{T}\right) = 2\mu_P\,\varepsilon(\mathbf{u})\,.$$

(Autonomous) Lie derivative

$$\mathcal{L}_{\mathbf{u}}\mathbf{T} = \mathbf{u}\cdot\nabla\mathbf{T} - \left(\nabla\mathbf{u}\,\mathbf{T} - \mathbf{T}\,\nabla^{\mathsf{T}}\mathbf{u}\right)\,.$$

Quantity of interest

Drag coefficient

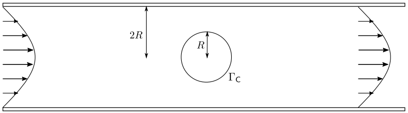
$$\mathfrak{K}(\hat{t}) = \frac{1}{\mu\bar{u}}\int_{\Gamma_C}\hat{t}\cdot\hat{\mathbf{e}}_x\,\mathrm{d}\,s\,.$$

Γ_C: boundary of cylinder

$\hat{t}$: traction

$\mu = \mu_S + \mu_P$: viscosity

$\bar{u}$: average inflow velocity.



Confined cylinder domain.

B. Keith, P. Knechtges, N. V. Roberts, S. Elgeti, M. Behr, and L. Demkowicz.
An ultraweak DPG method for viscoelastic fluids.
J. Non-Newton. Fluid Mech., 247:107--122, 2017.

Fluid Mechanics

An ultraweak DPG method for viscoelastic fluids

Oldroyd-B fluid

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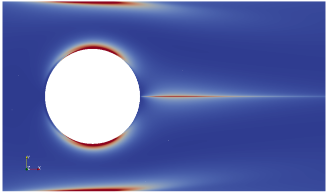

Close-up of rescaled T_{11}-component from $\lambda = 0.9$.

Wave Mechanics

On perfectly matched layers and non-symmetric variational formulations

Add figures

A. Vaziri Astaneh, B. Keith, and L. Demkowicz.
On perfectly matched layers and non-symmetric variational formulations.
Submitted, 2017.

Afterword: Future Acts

Viscoelastic rate-type fluids with stress diffusion

Potential collaboration with Prof. Endre Süli

Oldroyd-B fluid with stress diffusion

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M. Bulíček, J. Málek, V. Průša, and E. Süli.
PDE analysis of a class of thermodynamically compatible viscoelastic rate-type fluids with stress-diffusion.
arXiv:1707.02350 (math.AP), 2017.

J. Málek, V. Průša, T. Skřivan, and E. Süli.
Thermodynamics of viscoelastic rate-type fluids with stress diffusion.
arXiv:1706.06277 (physics.flu-dyn), 2017.

Viscoelastic rate-type fluids with stress diffusion

Potential collaboration with Prof. Endre Süli

Oldroyd-B fluid with stress diffusion

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- No systematic derivation of such fluid models with a stress diffusion term until now.
- Analyze such models with adaptive DG-type methods.
- Possible applications include polymer melts and die extrusion in 3D.

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Other possibilities

The Numerical Analysis Group

Prof. Coralia Cartis	Optimization techniques for DLS methods.
Prof. Mike Giles	Adjoint methods.
Prof. Patrick Farrell	Various things.
Prof. Andy Wathen	Preconditioners.

OCIAM/The Wolfson Centre

Prof. Andreas Münch	Polymer liquids. Phase-field models.
Prof. Sarah Waters	Fluid flows.
Prof. Dominic Vella	Various applications.

OxPDE

Prof. John Ball	Nonlinear minimum residual theory; applications to elasticity.

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And anyone else with an interest in my work!

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A. Vaziri Astaneh, B. Keith, and L. Demkowicz.
On perfectly matched layers and non-symmetric variational formulations.
Submitted, 2017.

Thank you!

Extra slides

A new hat. An old hat.

We are solving the discrete least squares problem

$$\mathbf{u}^{\text{opt}} = \arg\min_{\mathbf{u}\in\mathbb{R}^N} \|\mathsf{L}^{-1}(\mathsf{B}\mathbf{u} - \mathsf{l})\|_2 \,.$$

or

$$(\mathsf{L}^{-1}\mathsf{B})^{\mathsf{T}}(\mathsf{L}^{-1}\mathsf{B})\,\mathbf{u} \;=\; (\mathsf{L}^{-1}\mathsf{B})^{\mathsf{T}}(\mathsf{L}^{-1}\mathsf{l})\,. \tag{$\star\star$}$$

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- Note that $(\star\star)$ suggests an efficient way to locally construct $\mathsf{B}^{\mathsf{T}}\mathsf{G}^{-1}\mathsf{B}$.
- It hints at solution strategies based on least squares solvers.

  Trefethen and Bau (SIAM, 1997) belabour least squares problems and there is a untapped literature on sparse least squares solvers.
- There are many stable solution techniques for SPD linear systems, however the matrix $\mathsf{B}^{\mathsf{T}}\mathsf{G}^{-1}\mathsf{B}$ has a squared condition number.
- This opportunity does not exist with FOSLS because it does not discretize the Riesz map, $\mathcal{R}_V : V \to V'$.

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Goal-oriented error estimation and adaptivity

Goal-oriented adaptive strategy

1. Solve the primal and dual DPG problems, for u_h and $\boldsymbol{\omega}_h$.
2. Estimate the global error in the quantity of interest and cease further computations if the estimate is sufficiently small.
3. Estimate local errors in the quantity of interest by computing η_K^{Q} for each element in the mesh and mark those elements for refinement as dictated by a user-determined marking strategy.
4. Choose whether to refine isotropically in either h or p.
5. Refine all marked elements and construct a new mesh with a user-determined refinement strategy.