# Overview of PhD Work & Future Research Plans

Brendan Keith

Hooke Research Fellowship Presentation
January 8, 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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- ~~ESEAS~~
- ~~$hp$2D & $hp$3D~~
- ~~Camellia~~

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Afterword: Future Acts

- NA Group
- OCIAM
- OxPDE

More information on my website:
`https://brendankeith.github.io`

# Prelude

# About My Work

PhD candidate at ICES

Supervisor: Dr Leszek Demkowicz

- Study discontinuous Petrov–Galerkin (DPG) methods

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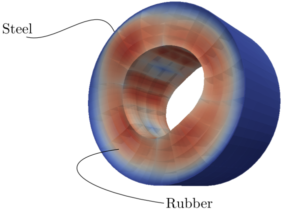
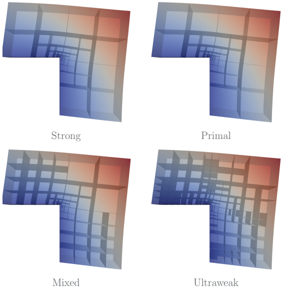
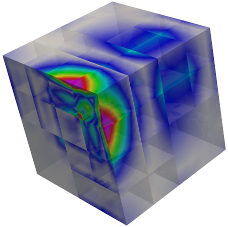
PhD candidate at ICES

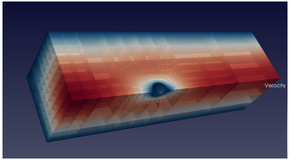
Supervisor: Dr Leszek Demkowicz

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

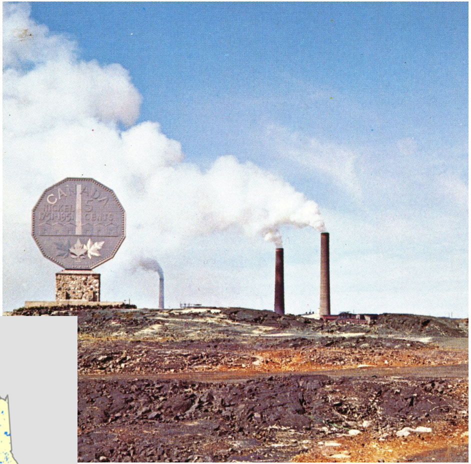


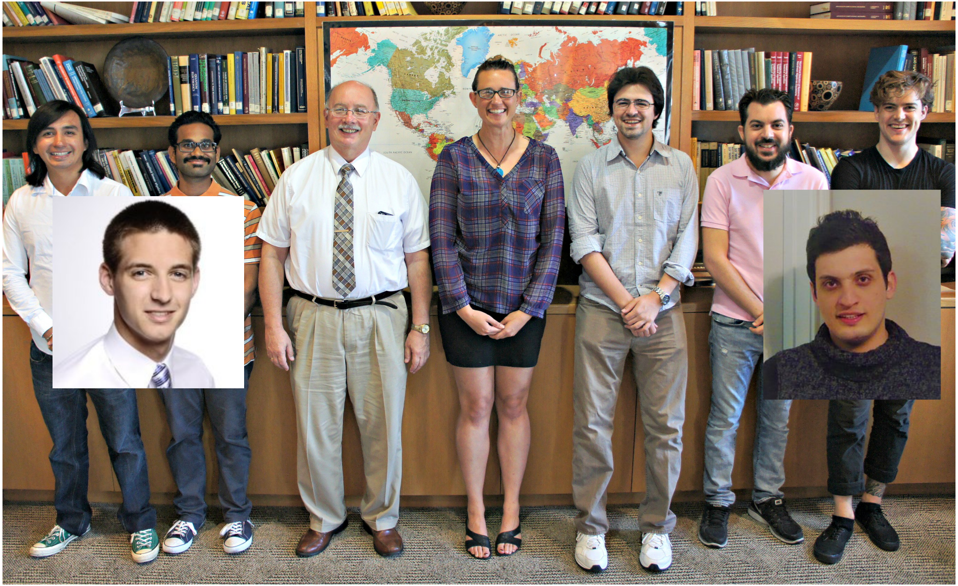





# About Me



# About the DPG Group



# About Life at UT

## The Texas Applied Mathematics and Engineering Symposium (`http://tames.io`)




# 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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$$\not\Rightarrow$$

### Discrete stability

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

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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 $\dim(V_h) > \dim(U_h)$?

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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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:

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

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DPG: G is block-diagonal

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

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With DPG, we solve

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

L. Demkowicz, J. Gopalakrishnan, and B. Keith.
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With DPG*, we solve

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

and then post-process $\mathbf{w}$:

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


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# Highlights

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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): $\mu$
QoI (or output): $\mathbf{y}$.

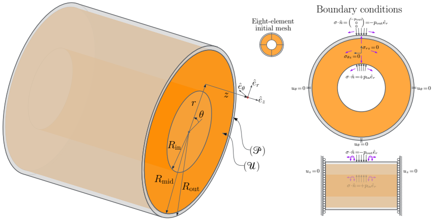
Research interest:

- 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.

# Act 2: Applications

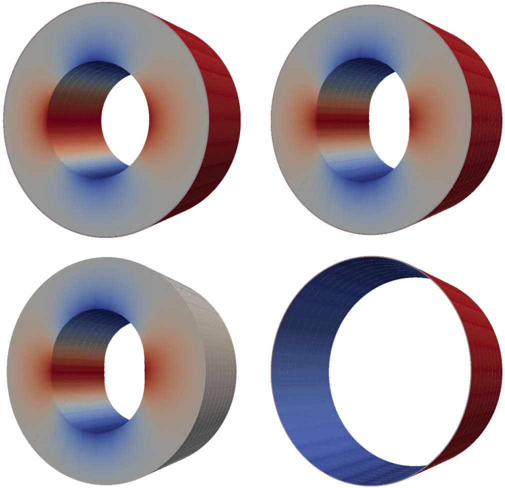
# Structural Mechanics

## Sheathed hose




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

## Circumferential stress: $\sigma_{\theta\theta}$



## Coupled formulations

- All coupled formulations are mutually compatible throughout the domain.


F. Fuentes, B. Keith, L. Demkowicz, and P. L. Tallec.
Coupled variational formulations of linear elasticity and the DPG methodology.
*J. Comput. Phys.*, 348:715--731, 2017.

B. Keith, F. Fuentes, and L. Demkowicz.
The DPG methodology applied to different variational formulations of linear elasticity.
*Comput. Methods Appl. Mech. Engrg.*, 309:579--609, 2016.

# Fluid Mechanics

## Oldroyd-B fluid

Conservation of mass and momentum:

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

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

Constitutive law:

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

where

$$\mathbf{T} + \lambda\,\mathfrak{L}_{\mathbf{u}}\mathbf{T} = 2\mu_P\,\varepsilon(\mathbf{u})\,.$$

Lie derivative:

$$\mathfrak{L}_{\mathbf{u}}\mathbf{T} = \frac{\partial\,\mathbf{T}}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{T} - \left(\boldsymbol{\nabla}\mathbf{u}\,\mathbf{T} - \mathbf{T}\,\boldsymbol{\nabla}^{\mathsf{T}}\mathbf{u}\right)\,.$$


B. Keith, P. Knechtges, N. V. Roberts, S. Elgeti, M. Behr, and L. Demkowicz.
An ultraweak DPG method for viscoelastic fluids.
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## Quantity of interest

Drag coefficient

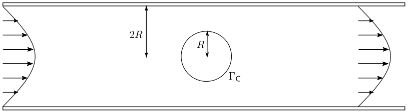
$$\mathfrak{K}(\hat{t}) = \frac{1}{\mu\bar{u}}\int_{\Gamma_C}\hat{t}\cdot\hat{\mathbf{e}}_x\,\mathrm{d}s\,.$$

$\Gamma_C$: boundary of cylinder

$\hat{t}$: traction

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

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




Confined cylinder domain.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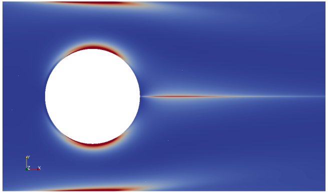
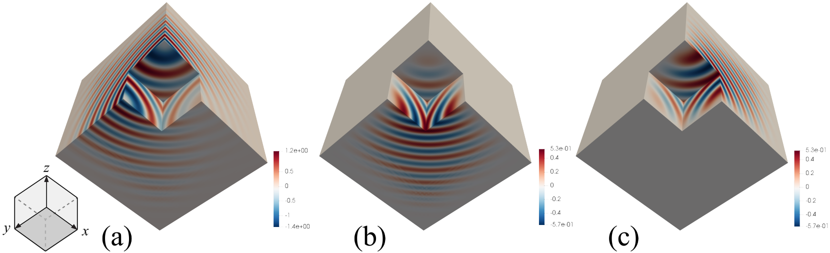


Close-up of rescaled $T_{11}$-component from $\lambda = 0.9$.

# Wave Mechanics

- Acoustics $$-\Delta p - \omega^2 p = f$$
- Electromagnetics $$\frac{1}{\mu}\nabla \times \nabla \times \mathbf{E} - \omega^2 \epsilon \mathbf{E} = i\omega \mathbf{J}^{\mathrm{imp}}$$
- Elastodynamics $$-\boldsymbol{\nabla} \cdot \left(\mathsf{C} : \boldsymbol{\nabla} \boldsymbol{u}\right) - \rho\omega^2 \boldsymbol{u} = \boldsymbol{f}$$




Electromagnetic wave scattering of the discrete electric field $\mathbf{E}$.

(a) The $x$-component; (b) the $y$-component; (c) the $z$-component. Only the real part of the solution is visualized.


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. Buliček, 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.

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$$\mathfrak{L}_{\mathbf{u}}\mathbf{T} = \frac{\partial \mathbf{T}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{T} - \left(\nabla\mathbf{u}\,\mathbf{T} - \mathbf{T}\,\nabla^{\mathsf{T}}\mathbf{u}\right)\,.$$

- 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.


M. Bulíček, J. Málek, V. Průša, and E. Süli.
PDE analysis of a class of thermodynamically compatible viscoelastic rate-type fluids with stress-diffusion.
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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.

# Other Possibilities

## The Numerical Analysis Group

| | |
|---|---|
| Prof. Patrick Farrell | Various things. |
| Prof. Andy Wathen | Preconditioners. |

## OCIAM

| | |
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| Prof. Andreas Münch | Liquid polymers. Phase-field models. |
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And anyone else with an interest in my work!

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*arXiv:1711.01996 (math.NA)*, 2017.

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

Thank you!

# Extra slides

# 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:

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

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### DPG–DPG$^*$ orthogonality:

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


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$$\begin{aligned} g(u-u_h) = b(u-u_h,v) = b(u-u_h,v-v_h) &= \ell(v-v_h) \\ &\leq \underbrace{\|\mathcal{B}u_h - \ell\|_{V'}}_{\lesssim \eta(u_h)} \underbrace{\|v-v_h\|_V}_{\lesssim \eta'(v_r)} \end{aligned}$$

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$$\boxed{g(u-u_h) \lesssim \eta(u_h)\,\eta'(v_r)}$$


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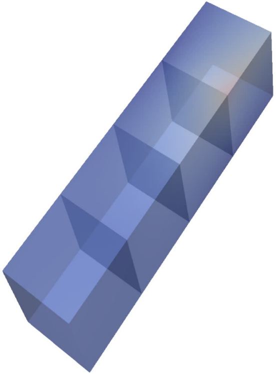
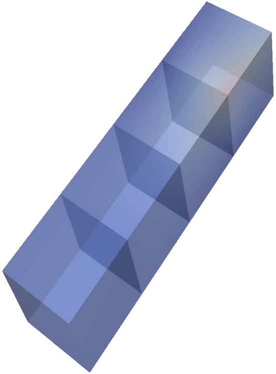
# Goal-Oriented Adaptivity

## Solution-oriented strategy



## Goal-oriented strategy (1 of 3)



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# Goal-Oriented Adaptivity

## Goal-oriented adaptive strategy

1. Solve the primal and dual DPG problems, for $u_h$ and $v_h$.
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 $\eta_K$ and $\eta'_K$ for each element $K$ in the mesh and mark those elements for refinement as dictated by a user-determined marking strategy.
4. Refine all marked elements and construct a new mesh with a user-determined refinement strategy.

# Discrete Least-Squares Methods

Factorization, etc.

We are solving the discrete least squares problem

$$\mathbf{u}^{\mathrm{opt}} = \operatorname*{arg\,min}_{\mathbf{u}\in\mathbb{R}^N} \left\| \mathsf{L}^{-1}(\mathsf{B}\mathbf{u} - \mathsf{l}) \right\|_2 .$$

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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