

# Stable high order methods for time-domain wave propagation in complex geometries and heterogeneous media

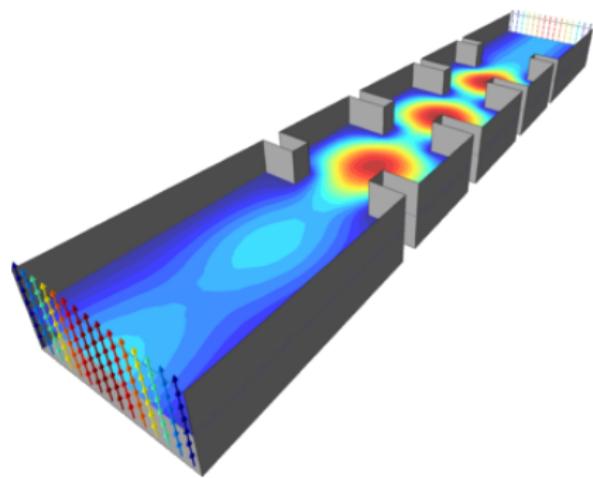
Kaihang Guo

Department of Computational and Applied Mathematics  
Rice University

# Numerical simulation of wave propagation

Many procedures require **accurately** and **efficiently** solving time-dependent wave equations in realistic settings.

- Imaging (seismic, medical)
- Engineering design  
(scattering, design)
- Computational physics  
(aeroacoustics, astrophysics)



# Discontinuous Galerkin (DG) methods for waves

- Unstructured (tetrahedral) meshes for geometric flexibility.
- High order: low numerical dissipation and dispersion.
- High order approximations: more accurate per unknown.
- Explicit time stepping: high performance on many-core.

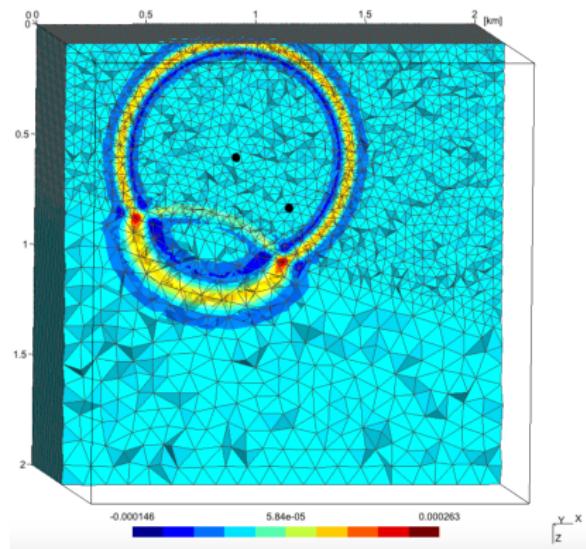
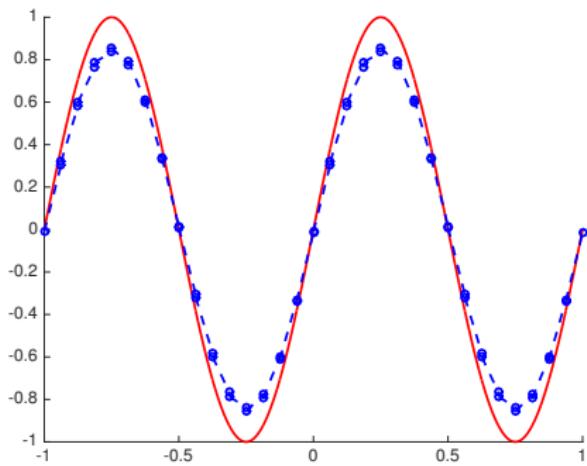


Figure courtesy of Axel Modave.

# Discontinuous Galerkin (DG) methods for waves

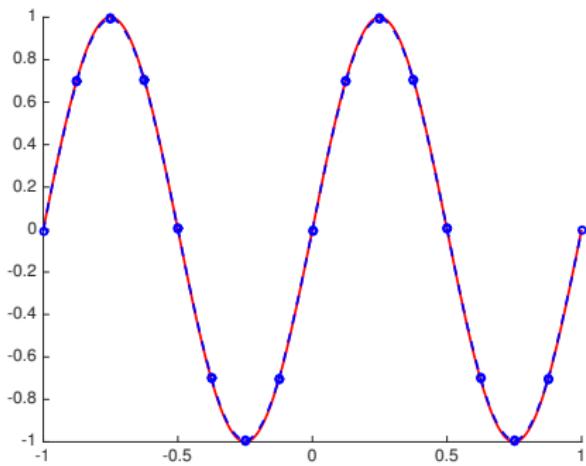
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**Fine** linear approximation.

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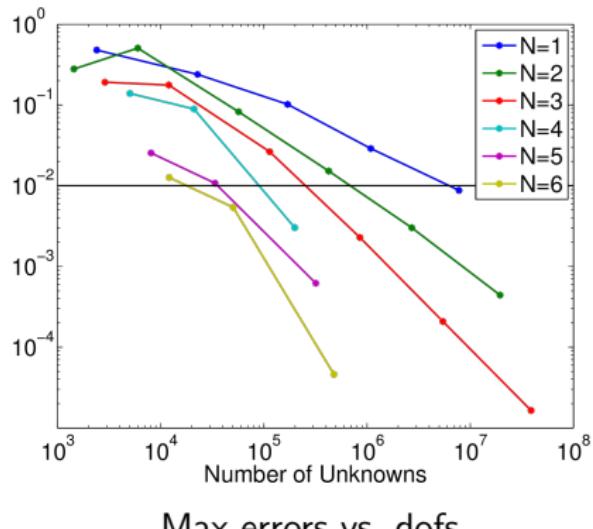
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**Coarse quadratic approximation.**

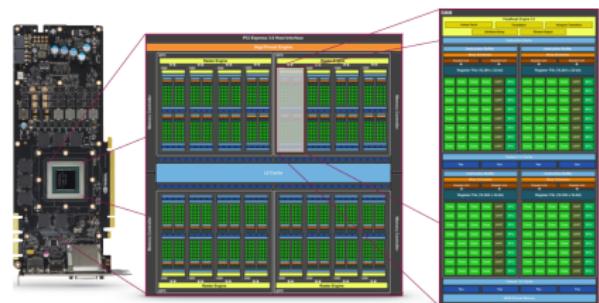
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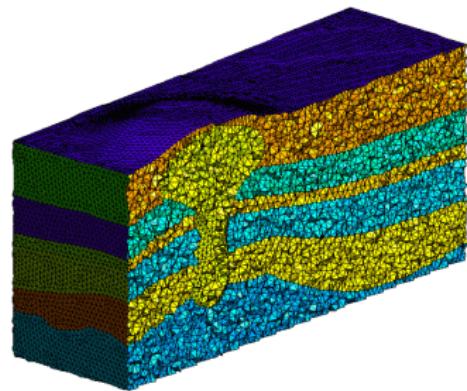


Graphics processing units (GPU).

# Time-domain nodal DG methods

Assume  $u(\mathbf{x}, t) = \sum \mathbf{u}_j \phi_j(\mathbf{x})$  on  $D^k$

- Compute numerical flux at face nodes (**non-local**).
- Compute RHS of (**local**) ODE.
- Evolve (**local**) solution using explicit time integration (RK, AB, etc).



Mesh courtesy of J.F. Remacle

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x}$$

Example: advection equation.

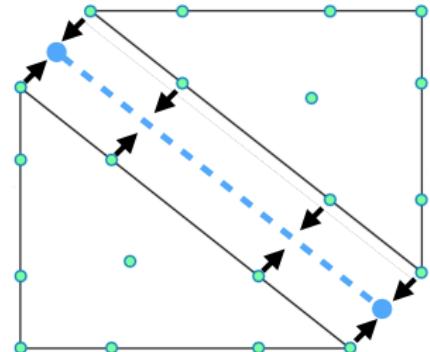
$$\mathbf{M}_{ij} = \int_{D^k} \phi_j(\mathbf{x}) \phi_i(\mathbf{x})$$

$$\mathbf{L}_f = \mathbf{M}^{-1} \mathbf{M}_f.$$

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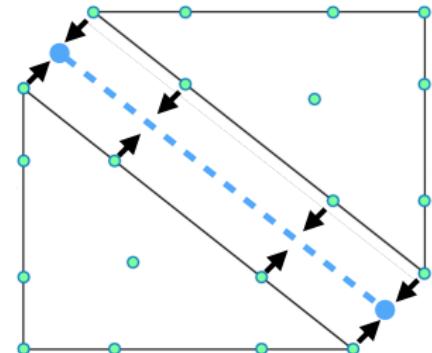
$$\frac{d\mathbf{u}}{dt} = \mathbf{D}_x \mathbf{u} + \sum_{\text{faces}} \mathbf{L}_f (\text{flux}).$$

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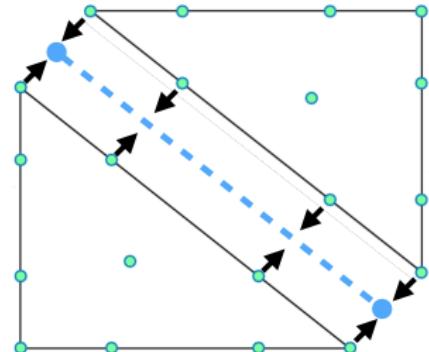
$$\frac{d\mathbf{u}}{dt} = \underbrace{\mathbf{D}_x \mathbf{u}}_{\text{Volume kernel}} + \underbrace{\sum_{\text{faces}} \mathbf{L}_f}_{\text{Surface kernel}} (\text{flux}).$$

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$$\underbrace{\frac{d\mathbf{u}}{dt}}_{\text{Update kernel}} = \underbrace{\mathbf{D}_x \mathbf{u}}_{\text{Volume kernel}} + \underbrace{\sum_{\text{faces}} \mathbf{L}_f (\text{flux})}_{\text{Surface kernel}}.$$

$$\mathbf{M}_{ij} = \int_{D^k} \phi_j(\mathbf{x}) \phi_i(\mathbf{x})$$
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# Outline

- 1 Weight-adjusted DG (WADG): high order heterogeneous media
- 2 Elastic-acoustic coupled media
- 3 Bernstein-Bezier WADG: high order efficiency

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# Energy stable discontinuous Galerkin formulations

- Model problem: acoustic wave equation (pressure-velocity system)

$$\frac{1}{c^2} \frac{\partial p}{\partial t} = \nabla \cdot \mathbf{u}, \quad \frac{\partial \mathbf{u}}{\partial t} = \nabla p$$

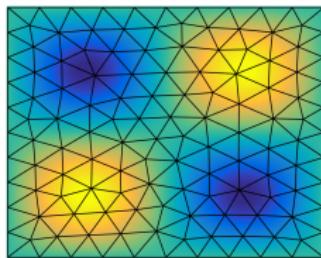
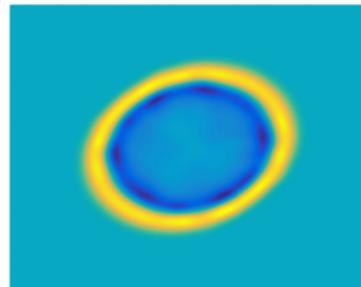
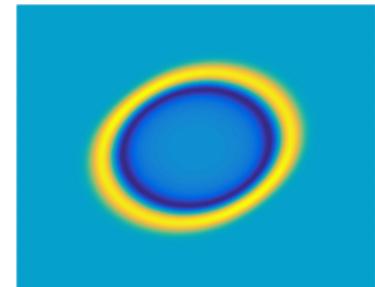
- Local formulation

$$\begin{aligned} \int_{D^k} \frac{1}{c^2} \frac{\partial p}{\partial t} q &= \int_{D^k} \nabla \cdot \mathbf{u} q + \frac{1}{2} \int_{\partial D^k} ([\![\mathbf{u}]\!] \cdot \mathbf{n} + \tau_p [\![p]\!]) q \\ \int_{D^k} \frac{\partial \mathbf{u}}{\partial t} \mathbf{v} &= \int_{D^k} \nabla p \cdot \mathbf{v} + \frac{1}{2} \int_{\partial D^k} ([\![p]\!] + \tau_u [\![\mathbf{u}]\!] \cdot \mathbf{n}) \mathbf{v} \end{aligned}$$

- High order accuracy, semi-discrete energy stability

$$\frac{\partial}{\partial t} \left( \sum_k \int_{D^k} \frac{p^2}{c^2} + |\mathbf{u}|^2 \right) = - \sum_k \int_{\partial D^k} \tau_p [\![p]\!]^2 + \tau_u [\![\mathbf{u} \cdot \mathbf{n}]\!]^2 \leq 0.$$

# High order approximation of smoothly varying media

(a) Mesh and exact  $c^2$ (b) Piecewise const.  $c^2$ (c) High order  $c^2$ 

- Piecewise const.  $c^2$ : energy stable and efficient, but inaccurate.

$$\frac{1}{c^2(\mathbf{x})} \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = 0, \quad \frac{\partial \mathbf{u}}{\partial t} + \nabla p = 0.$$

- High order wavespeeds: weighted mass matrices. Stable, but expensive (pre-computation + storage of matrix inverses)!

$$\mathbf{M}_{1/c^2} \frac{d\mathbf{p}}{dt} = \mathbf{A}_h \mathbf{U}, \quad (\mathbf{M}_{1/c^2})_{ij} = \int_{D^k} \frac{1}{c^2(\mathbf{x})} \phi_j(\mathbf{x}) \phi_i(\mathbf{x}).$$

# Weight-adjusted DG (WADG)

- Weight-adjusted DG: provably energy stable approx. of  $\mathbf{M}_{1/c^2}$

$$\mathbf{M}_{1/c^2} \frac{d\mathbf{p}}{dt} \approx \mathbf{M} (\mathbf{M}_{c^2})^{-1} \mathbf{M} \frac{d\mathbf{p}}{dt} = \mathbf{A}_h \mathbf{U}.$$

- New evaluation reuses implementation for constant wavespeed

$$\frac{d\mathbf{p}}{dt} = \underbrace{\mathbf{M}^{-1}(\mathbf{M}_{c^2})}_{\text{modified update}} \quad \underbrace{\mathbf{M}^{-1}\mathbf{A}_h\mathbf{U}}_{\text{constant wavespeed RHS}}$$

- Low storage matrix-free application of  $\mathbf{M}^{-1}\mathbf{M}_{c^2}$  using quadrature-based interpolation and  $L^2$  projection matrices  $\mathbf{V}_q, \mathbf{P}_q$ .

$$(\mathbf{M})^{-1} \mathbf{M}_{c^2} = \underbrace{\mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W} \text{diag}(c^2) \mathbf{V}_q}_{\mathbf{P}_q}.$$

## WADG: nearly identical to DG w/weighted mass matrices

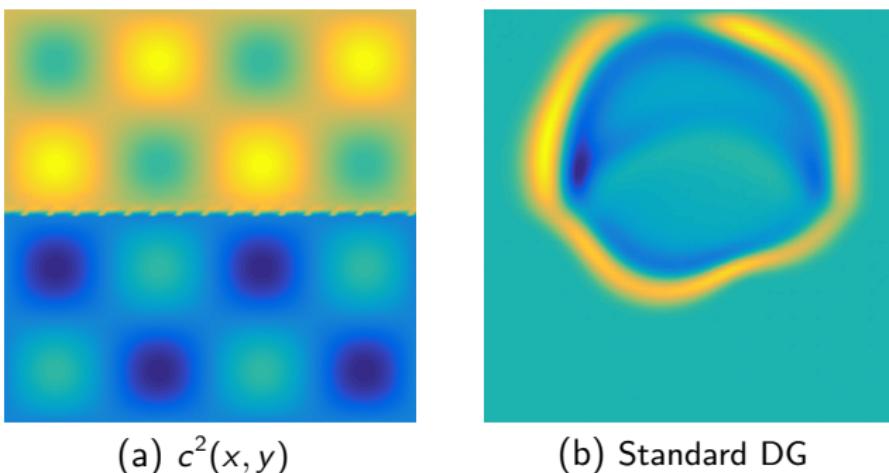


Figure: Standard vs. weight-adjusted DG with spatially varying  $c^2$ .

- The  $L^2$  error is  $O(h^{N+1})$ , but the difference between the DG and WADG solutions is  $O(h^{N+2})$ !

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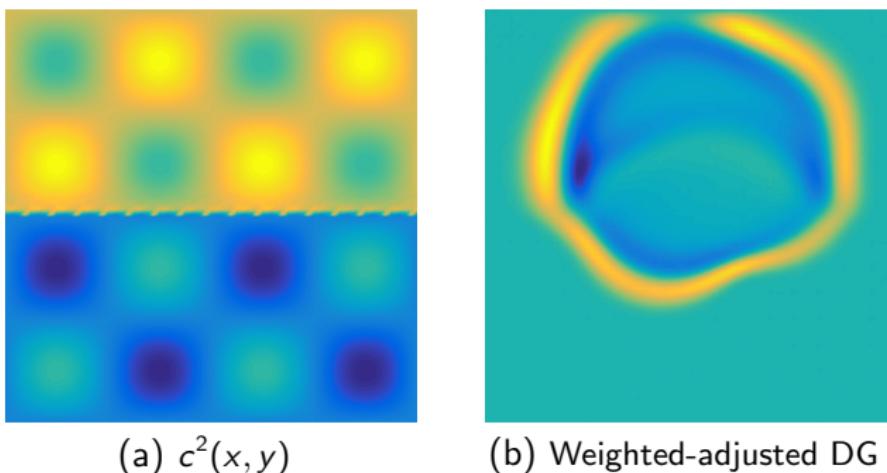
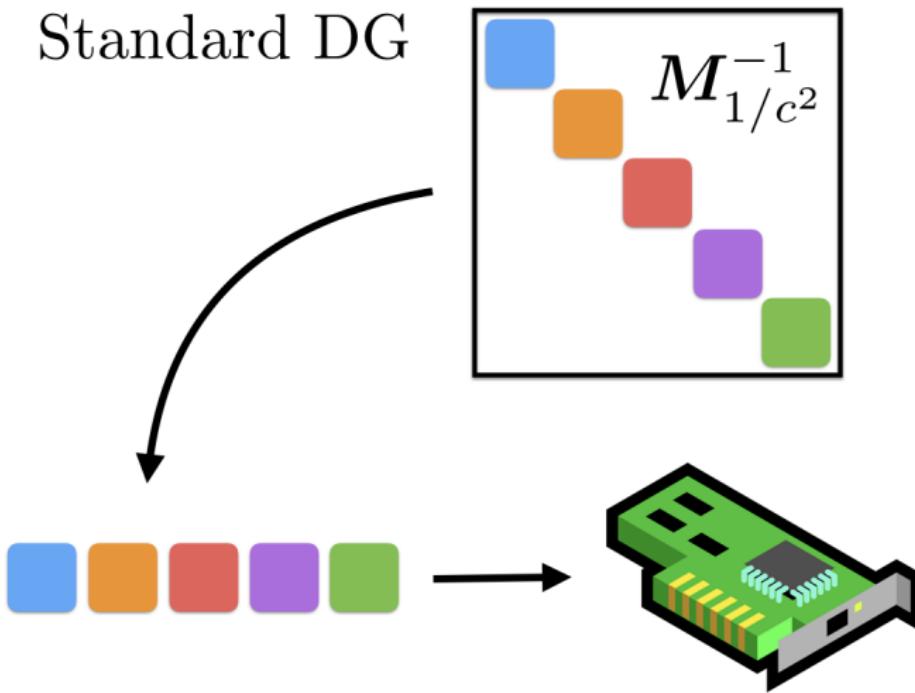


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WADG: more efficient than storing  $M_{1/c^2}^{-1}$  on GPUs

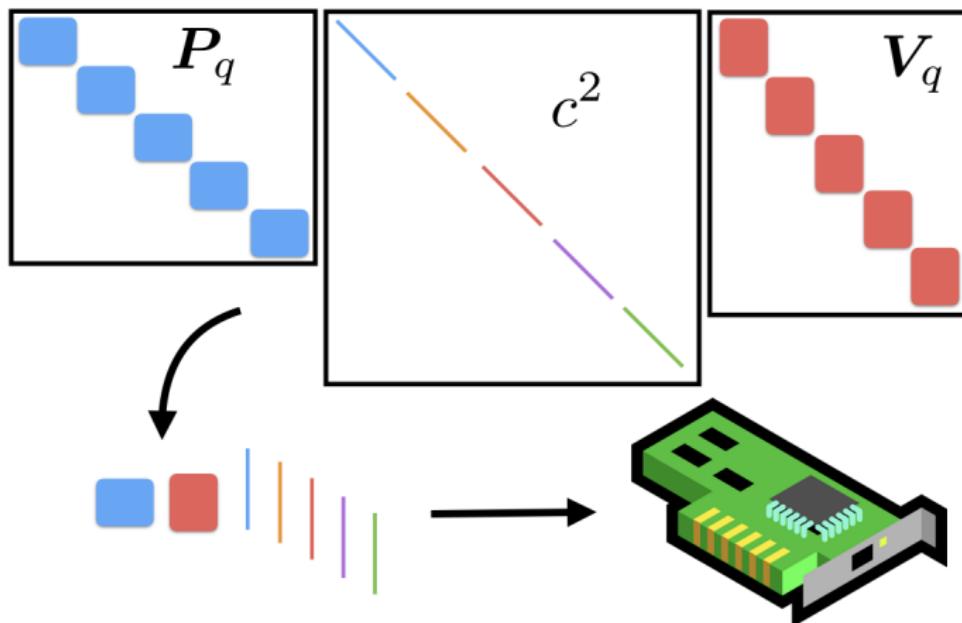
Standard DG



Efficiency on GPUs: reduce memory accesses and data movement!

WADG: more efficient than storing  $M_{1/c^2}^{-1}$  on GPUs

## Weight-adjusted DG



Efficiency on GPUs: reduce memory accesses and data movement!

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- 2 Elastic-acoustic coupled media
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# Matrix-valued weights and elastic wave propagation

- Symmetric velocity-stress formulation (entries of  $\mathbf{A}_i$  are  $\pm 1$  or 0)

$$\rho \frac{\partial \mathbf{v}}{\partial t} = \sum_{i=1}^d \mathbf{A}_i^T \frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{x}_i}, \quad \mathbf{C}^{-1} \frac{\partial \boldsymbol{\sigma}}{\partial t} = \sum_{i=1}^d \mathbf{A}_i \frac{\partial \mathbf{v}}{\partial \mathbf{x}_i}.$$

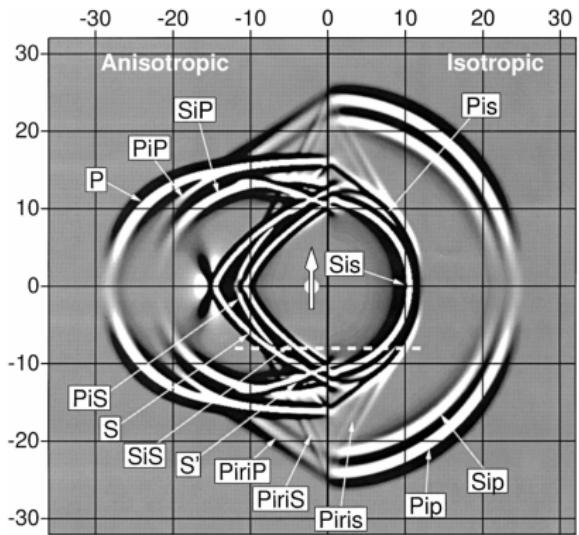
- DG formulation: *simple* penalty fluxes, matrix-weighted mass matrix

$$\mathbf{A}_1^T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{M}_{\mathbf{C}^{-1}} = \begin{pmatrix} \mathbf{M}_{C_{11}^{-1}} & \dots & \mathbf{M}_{C_{1d}^{-1}} \\ \vdots & \ddots & \vdots \\ \mathbf{M}_{C_{d1}^{-1}} & \dots & \mathbf{M}_{C_{dd}^{-1}} \end{pmatrix}$$

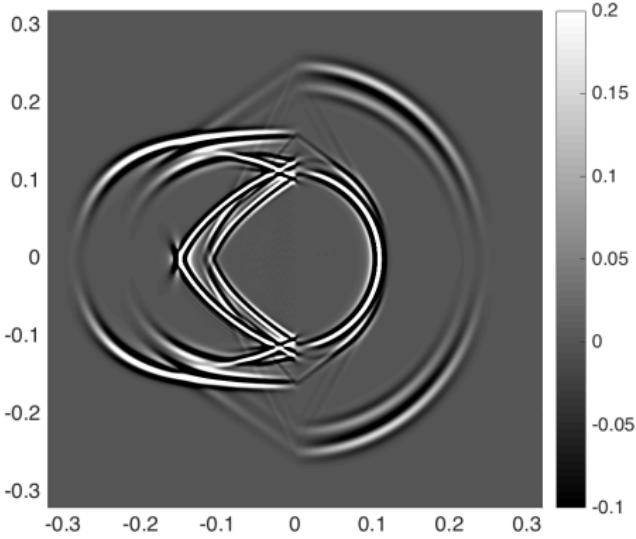
- Weight-adjusted approx. to  $(\mathbf{M}_{\mathbf{C}^{-1}})^{-1}$  decouples each component

$$\mathbf{M}_{\mathbf{C}^{-1}}^{-1} \approx (\mathbf{I} \otimes \mathbf{M}^{-1}) \mathbf{M}_{\mathbf{C}} (\mathbf{I} \otimes \mathbf{M}^{-1}).$$

# Simple to incorporate anisotropic media



(a) Reference solution



(b) WADG solution

Figure: Anisotropic media simply involves modifying the definition of  $\mathbf{C}$ .

Komatitsch, Barnes, Tromp (2000). *Simulation of anisotropic wave propagation based upon a spectral element method*.

Chan (2018). Weight-adjusted DG methods: matrix-valued weights and elastic wave prop. in heterogeneous media.

# Energy stable acoustic-elastic coupling

$\sigma, v$  (Elastic)

$$\begin{aligned} u \cdot n &= v \cdot n \\ A_n^T \sigma &= p n \end{aligned}$$

$p, u$  (Acoustic)

# Energy stable acoustic-elastic coupling

$$(\mathfrak{F}\mathbf{q})^* = \mathfrak{F}^- \mathbf{q}^- + \frac{\mathbf{n} \cdot [\![\mathbf{S}]\!] + \rho^+ c_p^+ [\![\mathbf{v}]\!]}{\rho^+ c_p^+ + \rho^- c_p^-} \begin{pmatrix} \mathbf{n} \otimes \mathbf{n} \\ \rho^- c_p^- \mathbf{n} \end{pmatrix}.$$

$$\begin{aligned} (\mathfrak{F}\mathbf{q})^* &= \mathfrak{F}^- \mathbf{q}^- + \frac{c_p^- c_p^+ \mathbf{n} \cdot [\![\mathbf{S}]\!] + c_p^- (\lambda^+ + 2\mu^+) [\![\mathbf{v}]\!]}{c_p^+ (\lambda^- + 2\mu^-) + c_p^- (\lambda^+ + 2\mu^+)} \begin{pmatrix} \mathbf{n} \otimes \mathbf{n} \\ \rho^- c_p^- \mathbf{n} \end{pmatrix} + \left( \frac{c_s^- c_s^+}{\mu^+ c_s^- + \mu^- c_s^+} \mathbf{s} \cdot [\![\mathbf{S}]\!] + \frac{c_s^- \mu^+}{\mu^+ c_s^- + \mu^- c_s^+} \mathbf{s} \cdot [\![\mathbf{v}]\!] \right) \begin{pmatrix} \text{sym}(\mathbf{s} \otimes \mathbf{n}) \\ \rho^- c_s^- \mathbf{s} \end{pmatrix} \\ &\quad + \left( \frac{c_s^- c_s^+}{\mu^+ c_s^- + \mu^- c_s^+} \mathbf{t} \cdot [\![\mathbf{S}]\!] + \frac{c_s^- \mu^+}{\mu^+ c_s^- + \mu^- c_s^+} \mathbf{t} \cdot [\![\mathbf{v}]\!] \right) \begin{pmatrix} \text{sym}(\mathbf{t} \otimes \mathbf{n}) \\ \rho^- c_s^- \mathbf{t} \end{pmatrix} = \mathfrak{F}^- \mathbf{q}^- + \frac{c_p^- c_p^+ \mathbf{n} \cdot [\![\mathbf{S}]\!] + c_p^- (\lambda^+ + 2\mu^+) [\![\mathbf{v}]\!]}{c_p^+ (\lambda^- + 2\mu^-) + c_p^- (\lambda^+ + 2\mu^+)} \begin{pmatrix} \mathbf{n} \otimes \mathbf{n} \\ \rho^- c_p^- \mathbf{n} \end{pmatrix} \\ &\quad - \frac{c_s^- c_s^+}{\mu^+ c_s^- + \mu^- c_s^+} \left( \text{sym}(\mathbf{n} \otimes (\mathbf{n} \times (\mathbf{n} \times [\![\mathbf{S}]\]))) \right) - \frac{c_s^- \mu^+}{\mu^+ c_s^- + \mu^- c_s^+} \left( \text{sym}(\mathbf{n} \otimes (\mathbf{n} \times (\mathbf{n} \times [\![\mathbf{v}]\]))) \right), \end{aligned}$$

$$(\mathfrak{F}\mathbf{q})^* = \mathfrak{F}^- \mathbf{q}^- + \frac{\mathbf{n} \cdot [\![\mathbf{S}]\!] + \rho^+ c_p^+ [\![\mathbf{v}]\!]}{\rho^+ c_p^+ + \rho^- c_p^-} \begin{pmatrix} \mathbf{n} \otimes \mathbf{n} \\ \rho^- c_p^- \mathbf{n} \end{pmatrix} - \frac{1}{\rho^- c_s^-} \left( \text{sym}(\mathbf{n} \otimes (\mathbf{n} \times (\mathbf{n} \times [\![\mathbf{S}]\]))) \right).$$

- Traditional upwind acoustic-elastic fluxes are complex to derive.
- Cannot prove energy stability in the case of heterogeneous media.

Wilcox, Stadler, Burstedde, Ghattas (2010). *A high-order discontinuous Galerkin method for wave propagation through coupled elastic-acoustic media.*

# Energy stable acoustic-elastic coupling

$$\mathbf{A}_n = \mathbf{A}_1 n_x + \mathbf{A}_2 n_y + \mathbf{A}_3 n_z \quad (\text{Elastic})$$

$$\frac{1}{2} (\mathbf{A}_n^T (\boldsymbol{\sigma}^+ - \boldsymbol{\sigma}) + \tau_{\mathbf{v}} \mathbf{A}_n^T \mathbf{A}_n (\mathbf{v}^+ - \mathbf{v}))$$

$$\frac{1}{2} (\mathbf{A}_n (\mathbf{v}^+ - \mathbf{v}) + \tau_{\boldsymbol{\sigma}} \mathbf{A}_n \mathbf{A}_n^T (\boldsymbol{\sigma}^+ - \boldsymbol{\sigma}) \cdot \mathbf{n}) \mathbf{n}$$

$$\frac{1}{2} ((\mathbf{u}^+ - \mathbf{u}) \cdot \mathbf{n} + \tau_p (p^+ - p))$$

$$\frac{1}{2} ((p^+ - p) + \tau_{\mathbf{u}} (\mathbf{u}^+ - \mathbf{u}) \cdot \mathbf{n}) \mathbf{n}$$

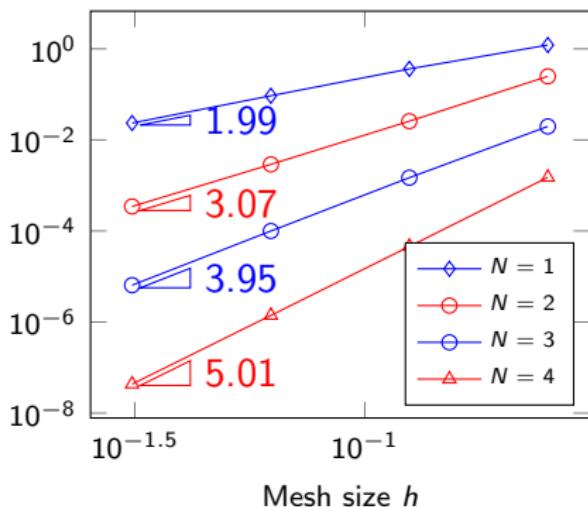
(Acoustic)

# Energy stable acoustic-elastic coupling

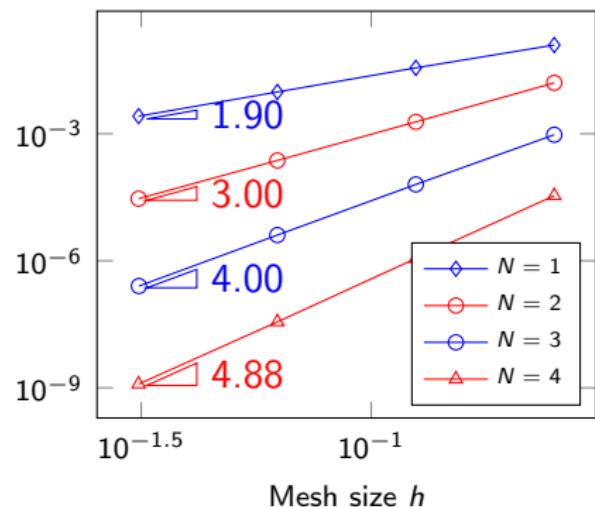
$$\begin{aligned}
 & \frac{1}{2} \mathbf{A}_n (\mathbf{n} \mathbf{n}^T (\mathbf{u} - \mathbf{v}) + \tau_{\boldsymbol{\sigma}} (p \mathbf{n} - \mathbf{A}_n^T \boldsymbol{\sigma})) \quad (\text{Elastic}) \\
 & \frac{1}{2} \mathbf{n}^T (p \mathbf{n} - \mathbf{A}_n^T \boldsymbol{\sigma} + (\mathbf{I} - \mathbf{n} \mathbf{n}^T) \mathbf{A}_n^T \boldsymbol{\sigma} + \tau_{\mathbf{v}} (\mathbf{u} - \mathbf{v})) \\
 & \qquad \qquad \qquad \downarrow \\
 & \frac{1}{2} \mathbf{n}^T (\mathbf{v} - \mathbf{u} + \tau_p (\mathbf{A}_n^T \boldsymbol{\sigma} - p \mathbf{n})) \\
 & \frac{1}{2} \mathbf{n} \mathbf{n}^T (\mathbf{A}_n^T \boldsymbol{\sigma} - p \mathbf{n} + \tau_{\mathbf{u}} (\mathbf{v} - \mathbf{u})) \quad (\text{Acoustic})
 \end{aligned}$$

$\mathbf{u} \cdot \mathbf{n} = \mathbf{v} \cdot \mathbf{n}$   
 $\mathbf{A}_n^T \boldsymbol{\sigma} = p \mathbf{n}$

# Numerical results: coupled acoustic-elastic media



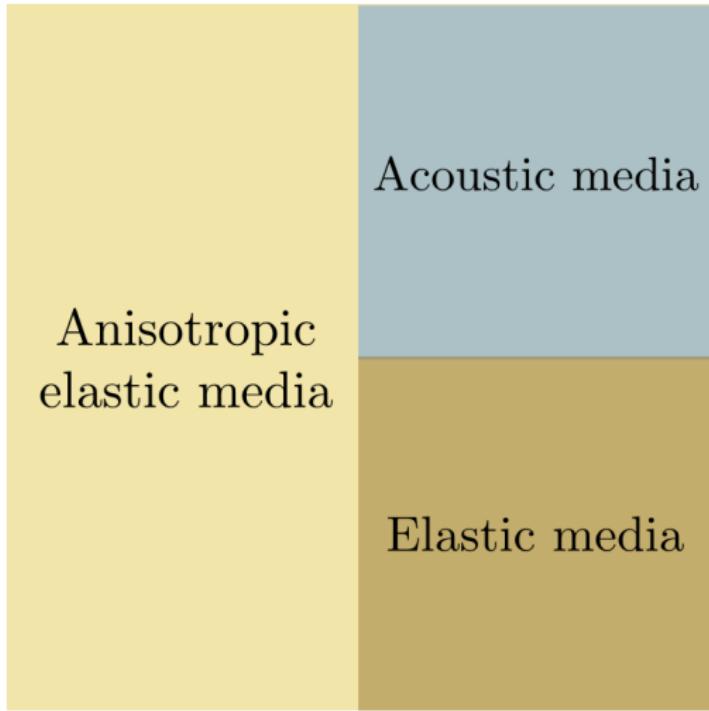
(a) Snell's law solution



(b) Scholte wave solution

High order convergence of  $L^2$  error for acoustic-elastic media.

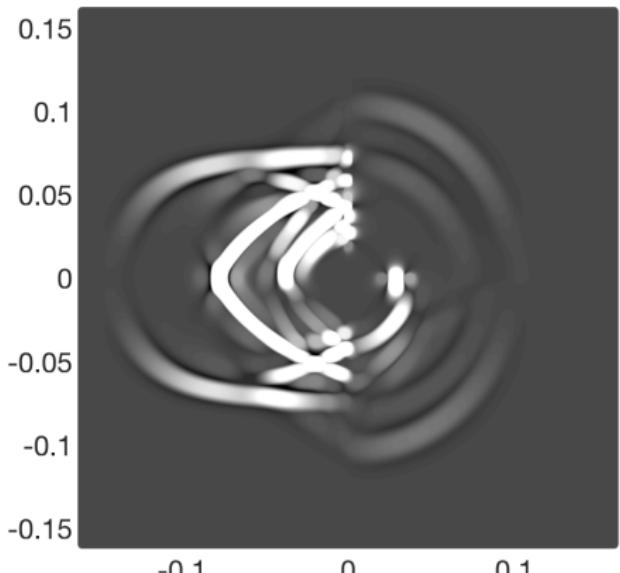
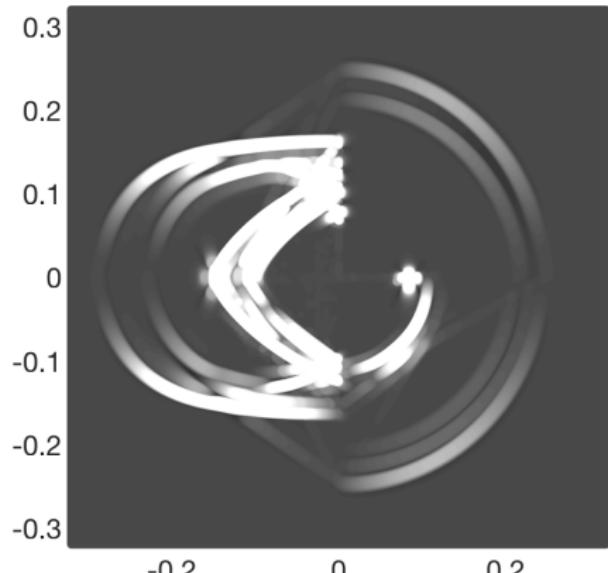
# Example with isotropic-anisotropic acoustic-elastic media



Komatitsch, Barnes, Tromp (2000). *Simulation of anisotropic wave propagation based upon a spectral element method*.

Guo, Acosta, Chan (2019). A weight-adjusted DG method for wave propagation in coupled elastic-acoustic media.

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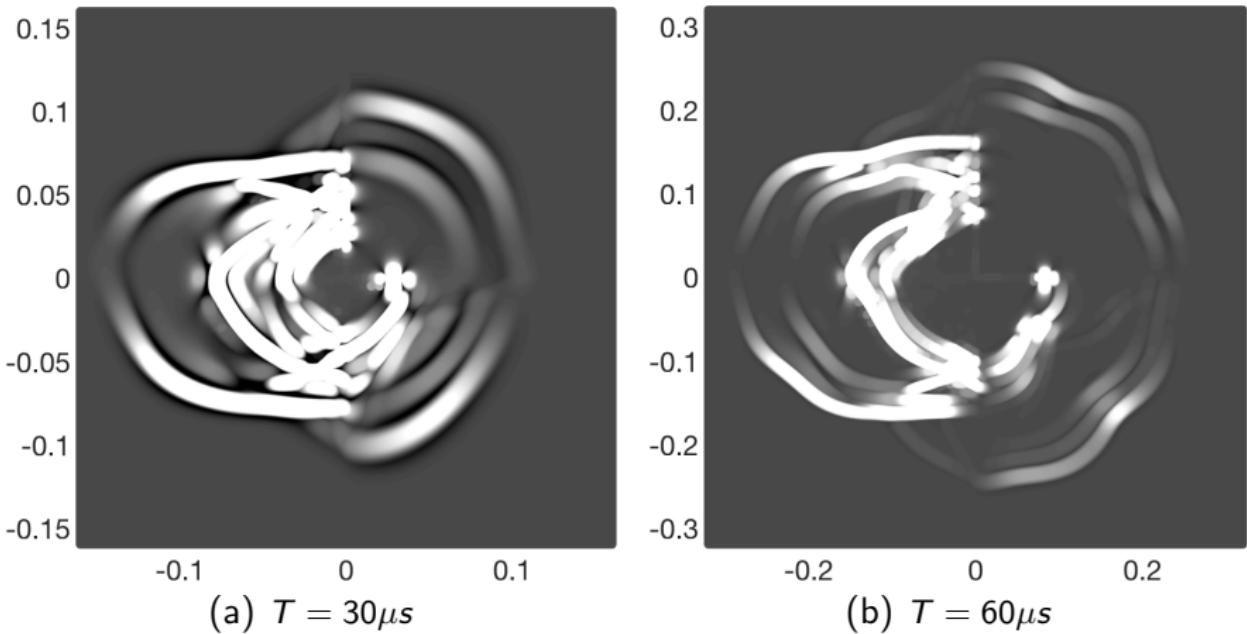
(a)  $T = 30\mu s$ (b)  $T = 60\mu s$ 

Piecewise constant anisotropic-isotropic acoustic-elastic media.

Komatitsch, Barnes, Tromp (2000). *Simulation of anisotropic wave propagation based upon a spectral element method*.

Guo, Acosta, Chan (2019). A weight-adjusted DG method for wave propagation in coupled elastic-acoustic media.

# Example with isotropic-anisotropic acoustic-elastic media



Piecewise smoothly varying anisotropic-isotropic acoustic-elastic media.

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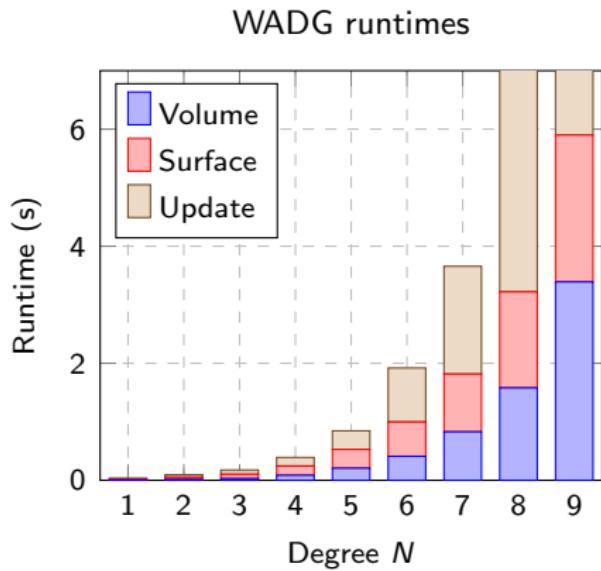
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# Computational costs at high orders of approximation

Problem: WADG at high orders becomes **expensive!**

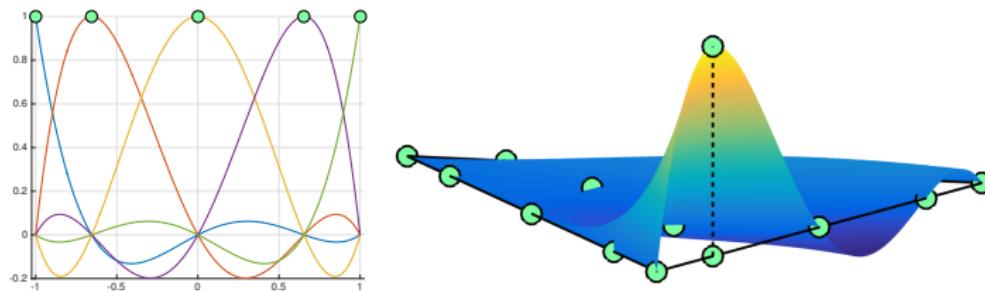


- Large **dense** matrices:  $O(N^6)$  work per element.
- Idea: choose basis such that matrices are **sparse**.

WADG runtimes for 50 timesteps, 98304 elements.

# BBDG: Bernstein-Bezier DG methods

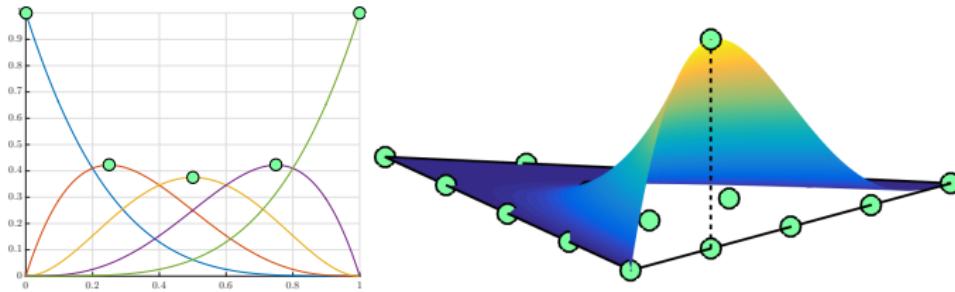
- Nodal DG:  $O(N^6)$  cost in 3D vs  $O(N^3)$  degrees of freedom.
- Switch to Bernstein basis: sparse and structured matrices.
- Optimal  $O(N^3)$  application of differentiation and lifting matrices.



Nodal bases in one, two, and three dimensions.

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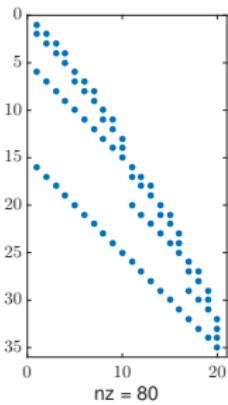
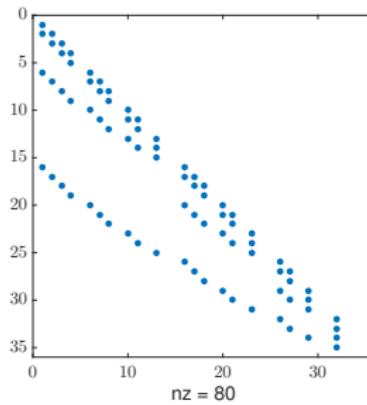
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Bernstein bases in one, two, and three dimensions.

# BBDG: Bernstein-Bezier DG methods

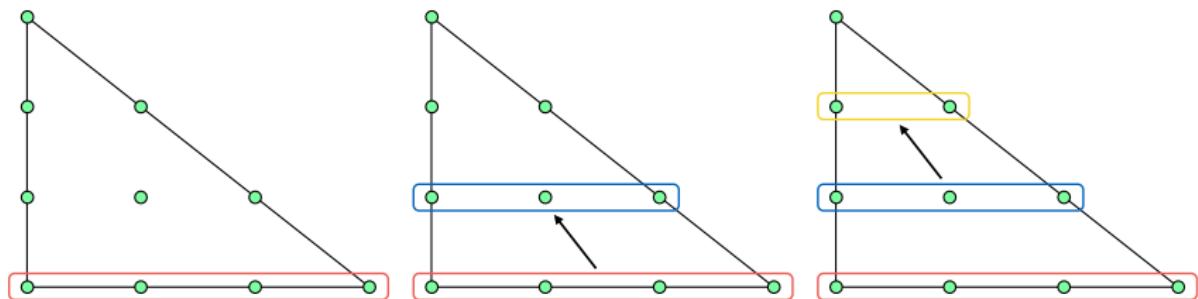
- Nodal DG:  $O(N^6)$  cost in 3D vs  $O(N^3)$  degrees of freedom.
- Switch to Bernstein basis: sparse and structured matrices.
- Optimal  $O(N^3)$  application of differentiation and lifting matrices.



Tetrahedral Bernstein differentiation and degree elevation matrices.

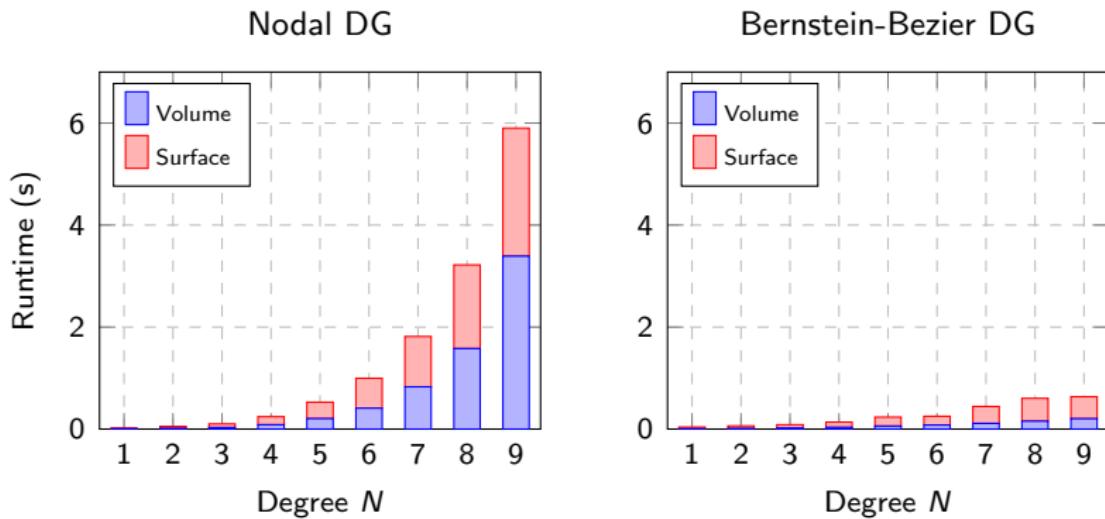
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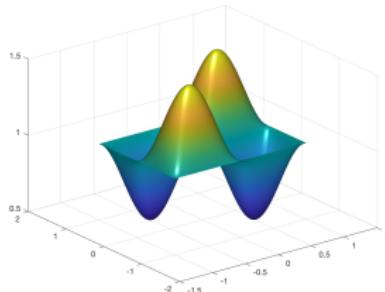
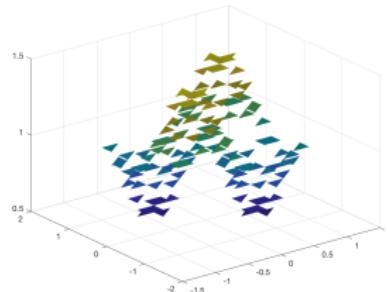
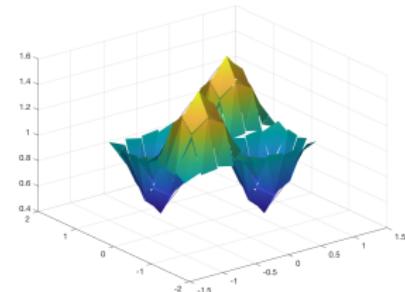
Optimal  $O(N^3)$  complexity “slice-by-slice” application of Bernstein lift.

# BBDG: efficient volume, surface kernels



$$\underbrace{\frac{d\mathbf{u}}{dt}}_{\text{Update kernel}} = \underbrace{\mathbf{D}_x \mathbf{u}}_{\text{Volume kernel}} + \underbrace{\sum_{\text{faces}} \mathbf{L}_f}_{\text{Surface kernel}} (\text{flux}), \quad \mathbf{L}_f = \mathbf{M}^{-1} \mathbf{M}_f.$$

# A faster BBWADG update kernel

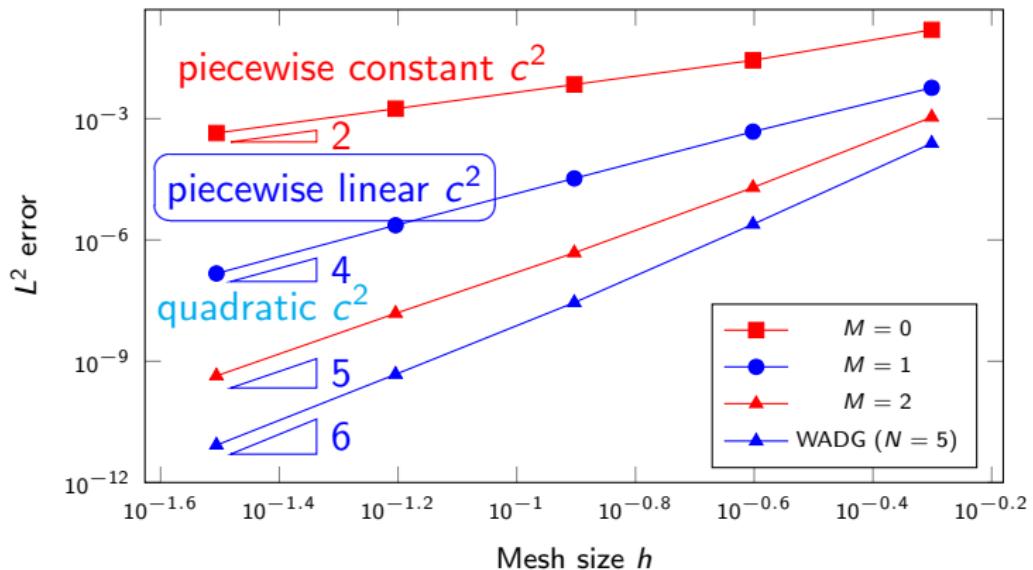
(a) Exact  $c^2$ (b)  $M = 0$  approximation(c)  $M = 1$  approximation

- Exploit continuous WADG steps: given  $u(\mathbf{x})$ , compute

$$P_N(u(\mathbf{x})c^2(\mathbf{x})), \quad P_N = L^2 \text{ projection operator.}$$

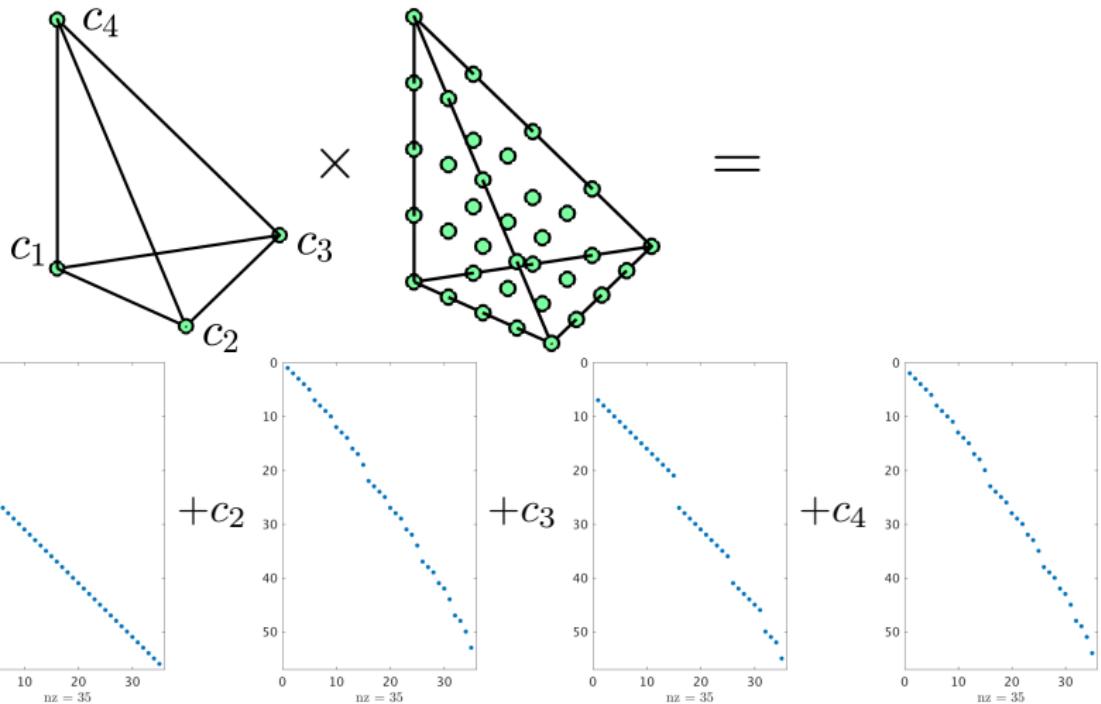
- Our approach: approx.  $c^2(\mathbf{x})$  with degree  $M$  polynomial, use fast Bernstein algorithms for polynomial multiplication and projection.
- Can reuse fast  $O(N^3)$  Bernstein-based volume and surface kernels.

# BBWADG: effect of approximating $c^2$ on accuracy



Approximating smooth  $c^2(x)$  using  $L^2$  projection:  
 $O(h^2)$  for  $M = 0$ ,  $O(h^4)$  for  $M = 1$ ,  $O(h^{M+3})$  for  $0 < M \leq N - 2$ .

# Fast Bernstein polynomial multiplication



Bernstein polynomial multiplication ( $M = 1$  shown),  $O(N^3)$  cost for fixed  $M$ .

# Fast Bernstein polynomial projection

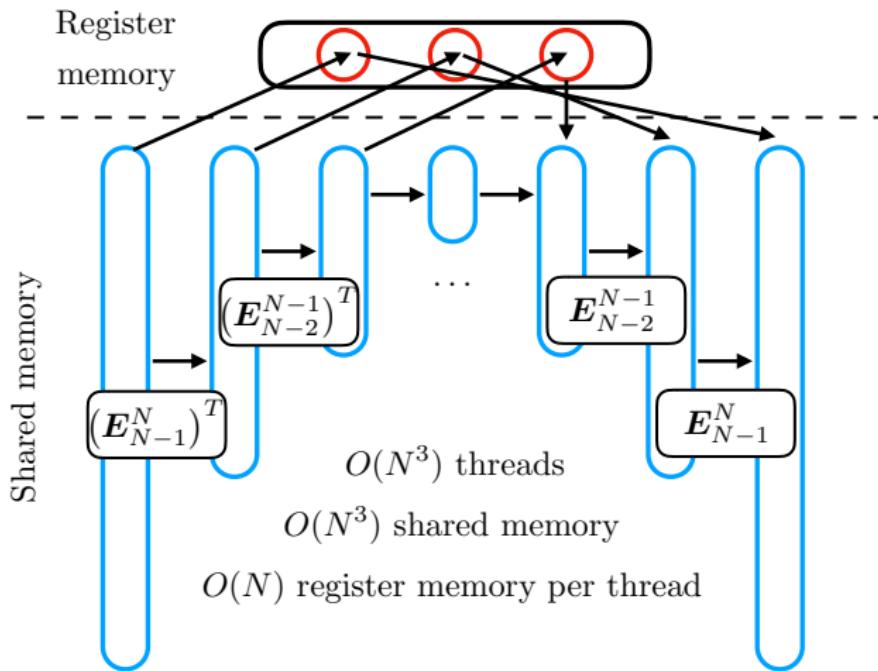
- Given  $c^2(\mathbf{x})u(\mathbf{x})$  as a degree  $(N + M)$  polynomial, apply  $L^2$  projection matrix  $\mathbf{P}_N^{N+M}$  to reduce to degree  $N$ .
- Polynomial  $L^2$  projection matrix  $\mathbf{P}_N^{N+M}$  under Bernstein basis:

$$\mathbf{P}_N^{N+M} = \underbrace{\sum_{j=0}^N c_j \mathbf{E}_{N-j}^N \left( \mathbf{E}_{N-j}^N \right)^T \left( \mathbf{E}_N^{N+M} \right)^T}_{\tilde{\mathbf{P}}_N}$$

- “Telescoping” form of  $\tilde{\mathbf{P}}_N$ :  $O(N^4)$  complexity, more GPU-friendly.

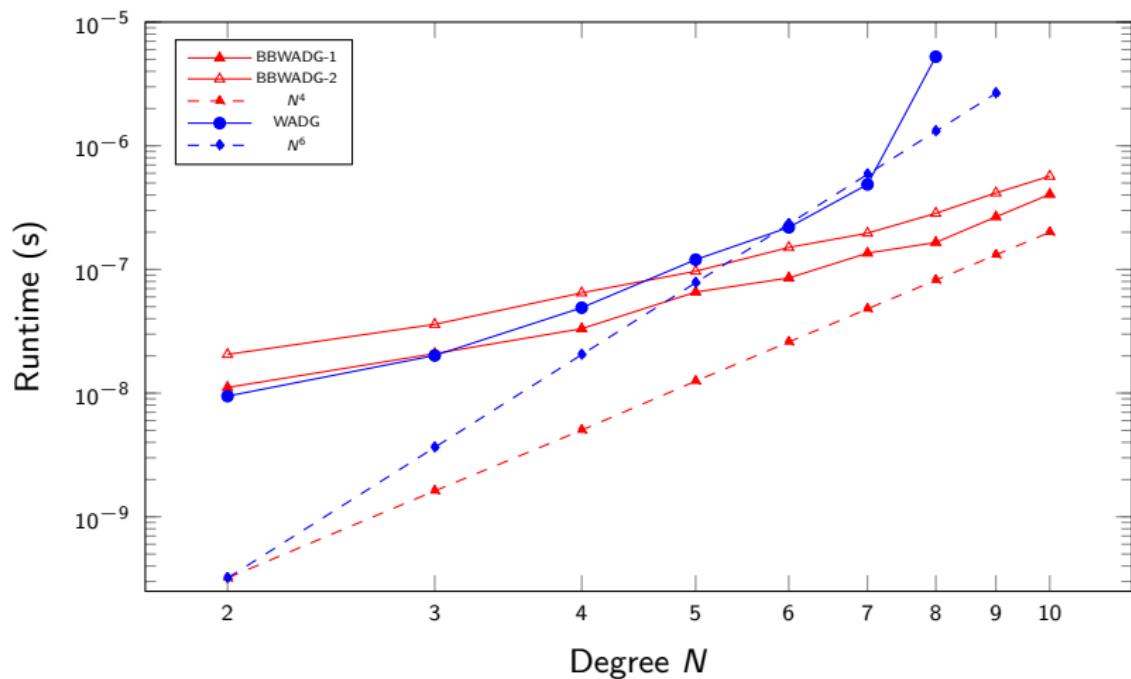
$$\left( c_0 \mathbf{I} + \mathbf{E}_{N-1}^N \left( c_1 \mathbf{I} + \mathbf{E}_{N-2}^{N-1} \left( c_2 \mathbf{I} + \cdots \right) \left( \mathbf{E}_{N-2}^{N-1} \right)^T \right) \left( \mathbf{E}_{N-1}^N \right)^T \right)$$

# Sketch of GPU algorithm for $\tilde{P}_N$



$$\left( c_0 \mathbf{I} + \mathbf{E}_{N-1}^N \left( c_1 \mathbf{I} + \mathbf{E}_{N-2}^{N-1} \left( c_2 \mathbf{I} + \cdots \right) \left( \mathbf{E}_{N-2}^{N-1} \right)^T \right) \left( \mathbf{E}_{N-1}^N \right)^T \right)$$

# BBWADG: computational runtime (3D acoustics)



Per-element runtimes of update kernels for BBWADG vs WADG (acoustic). We observe an asymptotic complexity of  $O(N^4)$  per element for  $N \gg 1$ .

# Summary and future work

- Weight-adjusted DG: high order accuracy, provable stability, and efficiency in heterogeneous acoustic-elastic media.
- Current work: stable WADG for moving curved meshes ( $r$ -adaptivity) and extension to nonlinear conservation laws.
- This work has been supported by TOTAL E&P Research and Technology USA and the National Science Foundation under DMS-1712639 and DMS-1719818.



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