

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

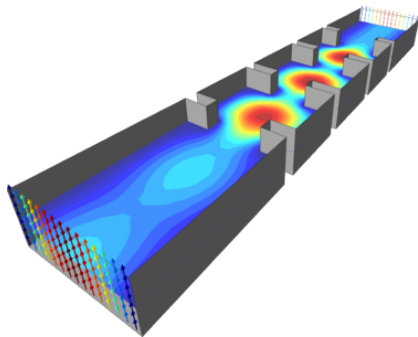
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Numerical simulation of wave propagation

Many procedures requires **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.

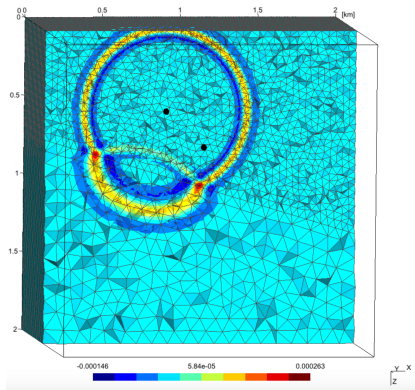
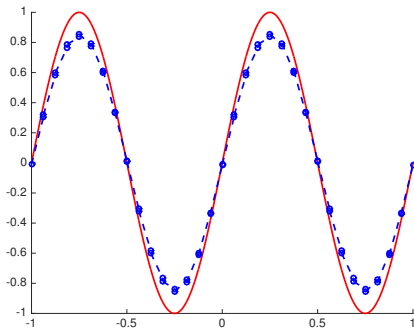


Figure courtesy of Axel Modave.

Discontinuous Galerkin (DG) methods for waves

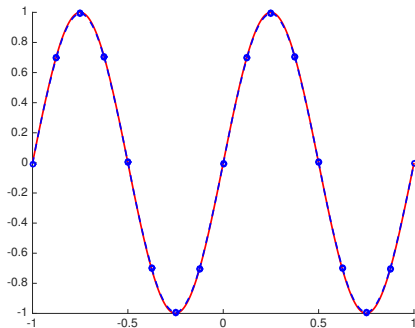
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Fine linear approximation.

Discontinuous Galerkin (DG) methods for waves

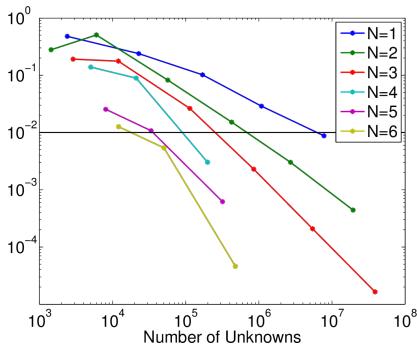
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Coarse quadratic approximation.

Discontinuous Galerkin (DG) methods for waves

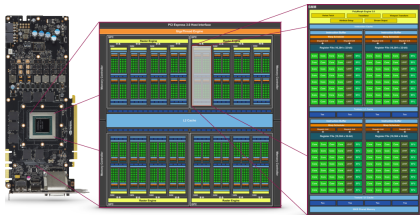
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Max errors vs. dofs.

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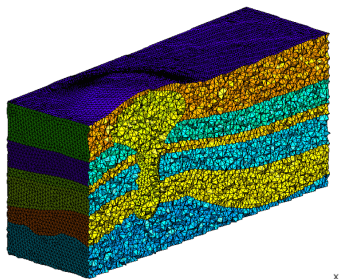


Graphics processing units (GPU).

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

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

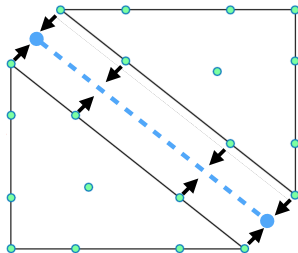
Example: advection equation.

$$\mathbf{M}_{ij} = \int_{D^k} \phi_j(\mathbf{x}) \phi_i(\mathbf{x})$$
$$\mathbf{L}_f = \mathbf{M}^{-1} \mathbf{M}_f.$$

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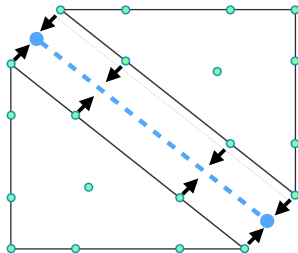
$$\frac{d\mathbf{u}}{dt} = \mathbf{D}_x \mathbf{u} + \sum_{\text{faces}} \mathbf{L}_f (\text{flux}).$$

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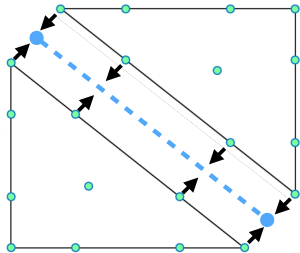
$$\frac{d\mathbf{u}}{dt} = \underbrace{\mathbf{D}_x \mathbf{u}}_{\text{Volume kernel}} + \underbrace{\sum_{\text{faces}} \mathbf{L}_f (\text{flux})}_{\text{Surface kernel}}.$$

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

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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)

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

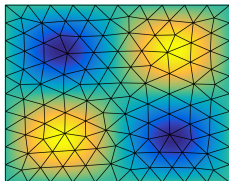
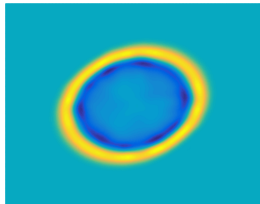
- Local formulation

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

- 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}

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

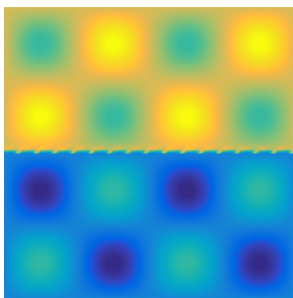
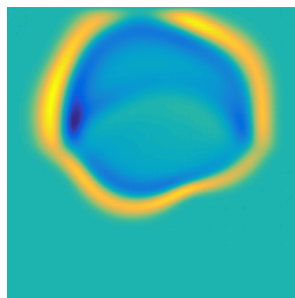
- New evaluation reuses implementation for constant wavespeed

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

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

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

WADG: nearly identical to DG w/weighted mass matrices

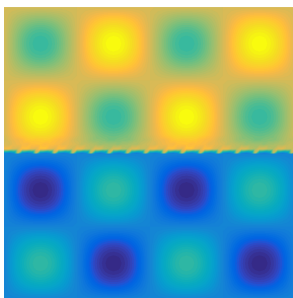
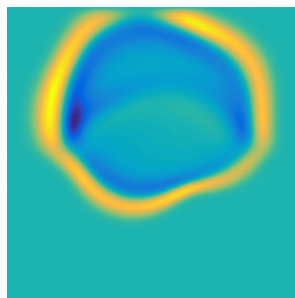
(a) $c^2(x, y)$ 

(b) Standard DG

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 $O(h^{N+2})$!

WADG: nearly identical to DG w/weighted mass matrices

(a) $c^2(x, y)$ 

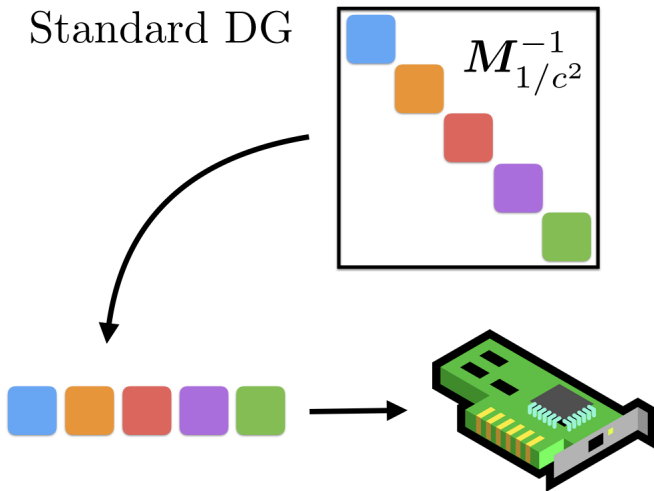
(b) Weighted-adjusted DG

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

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

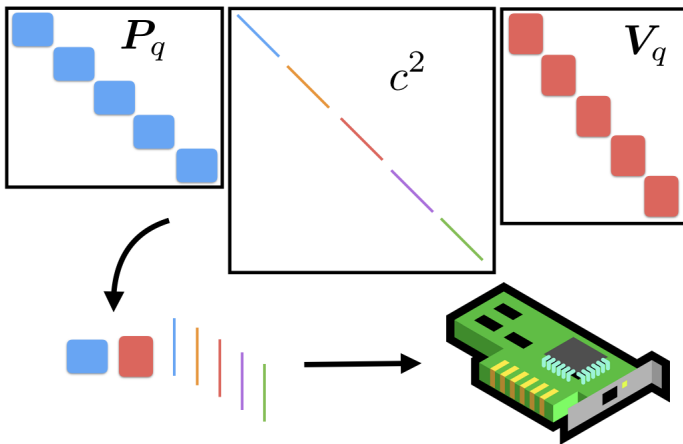
Standard DG



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 ± 1 or 0)

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

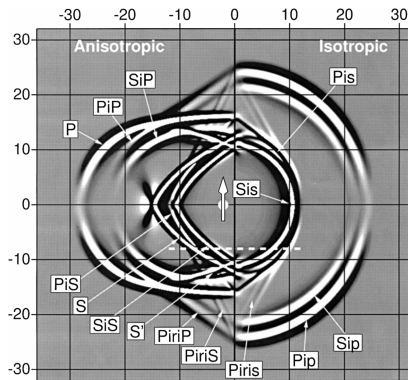
- DG formulation: *simple* penalty fluxes, matrix-weighted mass matrix

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

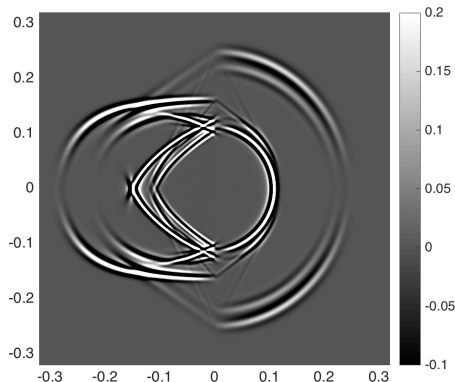
- Weight-adjusted approx. to $(\mathbf{M}_{\mathbf{C}^{-1}})^{-1}$ decouples each component

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

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

σ, 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

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

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

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

- 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

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

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

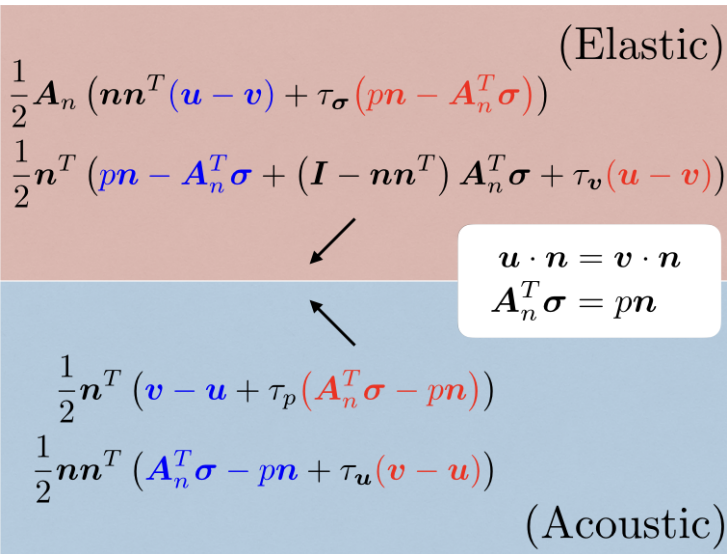
$$\frac{1}{2} \left(\mathbf{A}_n (\mathbf{v}^+ - \mathbf{v}) + \tau_\sigma \mathbf{A}_n \mathbf{A}_n^T (\boldsymbol{\sigma}^+ - \boldsymbol{\sigma}) \cdot \mathbf{n} \right) \mathbf{n}$$

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

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

(Acoustic)

Energy stable acoustic-elastic coupling



(Elastic)

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

$$\frac{1}{2} \mathbf{n}^T \left(\mathbf{p} \mathbf{n} - \mathbf{A}_n^T \boldsymbol{\sigma} + (\mathbf{I} - \mathbf{n} \mathbf{n}^T) \mathbf{A}_n^T \boldsymbol{\sigma} + \tau_v (\mathbf{u} - \mathbf{v}) \right)$$

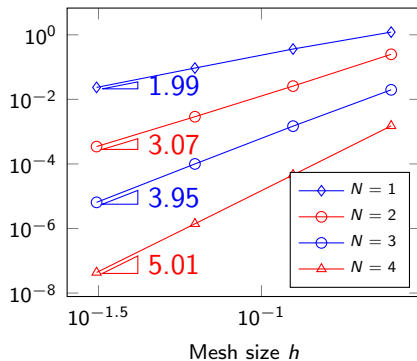
$\mathbf{u} \cdot \mathbf{n} = \mathbf{v} \cdot \mathbf{n}$
 $\mathbf{A}_n^T \boldsymbol{\sigma} = \mathbf{p} \mathbf{n}$

(Acoustic)

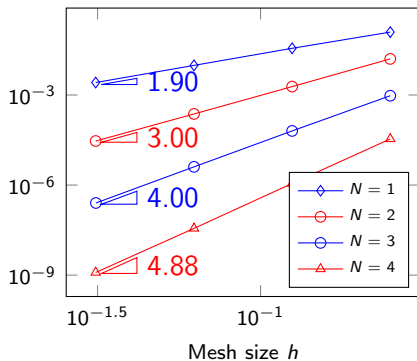
$$\frac{1}{2} \mathbf{n}^T \left(\mathbf{v} - \mathbf{u} + \tau_p (\mathbf{A}_n^T \boldsymbol{\sigma} - \mathbf{p} \mathbf{n}) \right)$$

$$\frac{1}{2} \mathbf{n} \mathbf{n}^T \left(\mathbf{A}_n^T \boldsymbol{\sigma} - \mathbf{p} \mathbf{n} + \tau_u (\mathbf{v} - \mathbf{u}) \right)$$

Numerical results: coupled acoustic-elastic media



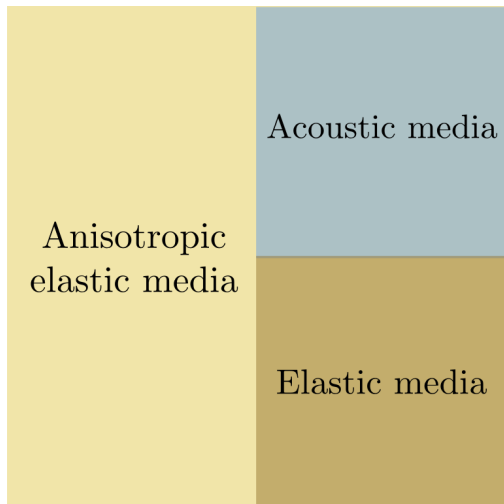
(a) Snell's law solution



(b) Scholte wave solution

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

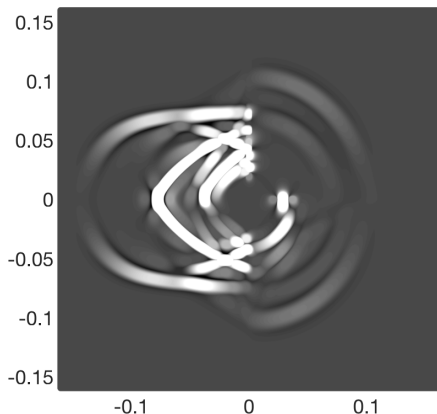
Example with isotropic-anisotropic acoustic-elastic media



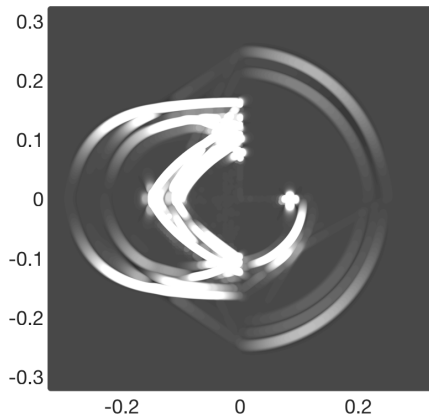
Komatitsch, Barnes, Tromp (2000). *Simulation of anisotropic wave propagation based upon a spectral element method*.

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

Example with isotropic-anisotropic acoustic-elastic media



(a) $T = 30 \mu s$



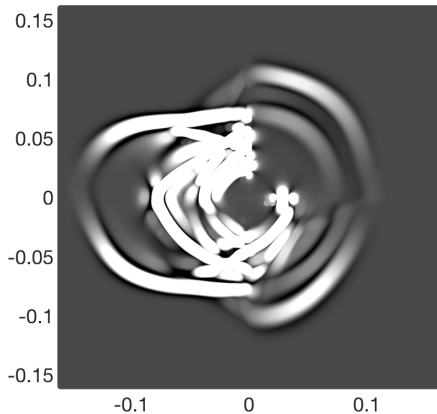
(b) $T = 60 \mu s$

Piecewise constant anisotropic-isotropic acoustic-elastic media.

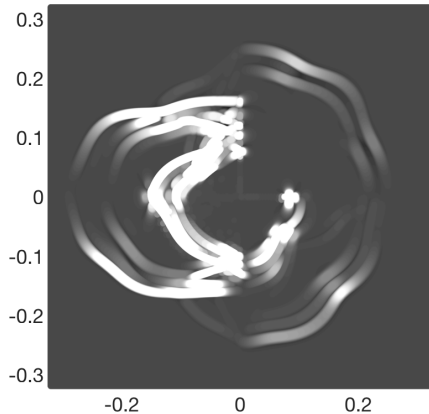
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Example with isotropic-anisotropic acoustic-elastic media



(a) $T = 30 \mu s$



(b) $T = 60 \mu s$

Piecewise smoothly varying 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.

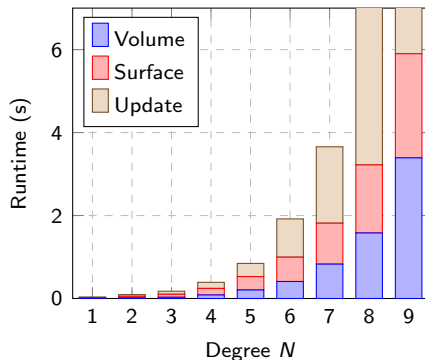
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Computational costs at high orders of approximation

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

WADG runtimes

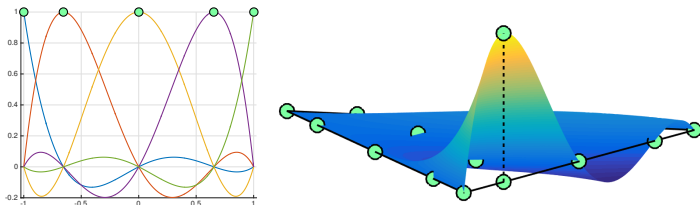


- Large **dense** matrices:
 $O(N^6)$ work per element.
- Idea: choose basis such that matrices are **sparse**.

WADG runtimes for 50 timesteps, 98304 elements.

BBDG: Bernstein-Bezier DG methods

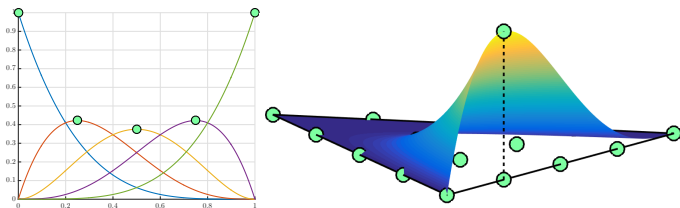
- Nodal DG: $O(N^6)$ cost in 3D vs $O(N^3)$ degrees of freedom.
- Switch to Bernstein basis: sparse and structured matrices.
- Optimal $O(N^3)$ application of differentiation and lifting matrices.



Nodal bases in one, two, and three dimensions.

BBDG: Bernstein-Bezier DG methods

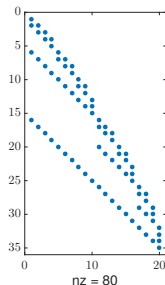
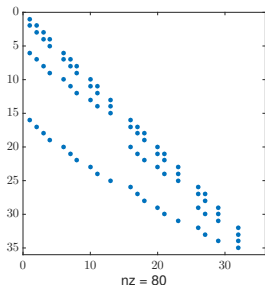
- Nodal DG: $O(N^6)$ cost in 3D vs $O(N^3)$ degrees of freedom.
- Switch to Bernstein basis: sparse and structured matrices.
- Optimal $O(N^3)$ application of differentiation and lifting matrices.



Bernstein bases in one, two, and three dimensions.

BBDG: Bernstein-Bezier DG methods

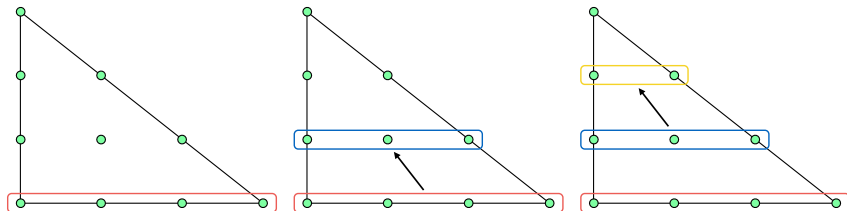
- Nodal DG: $O(N^6)$ cost in 3D vs $O(N^3)$ degrees of freedom.
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- Optimal $O(N^3)$ application of differentiation and lifting matrices.



Tetrahedral Bernstein differentiation and degree elevation matrices.

BBDG: Bernstein-Bezier DG methods

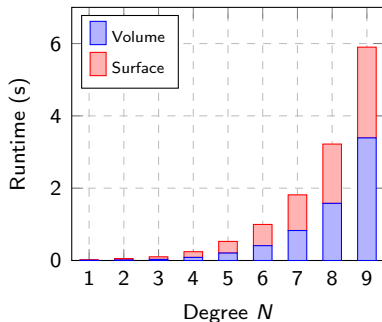
- Nodal DG: $O(N^6)$ cost in 3D vs $O(N^3)$ degrees of freedom.
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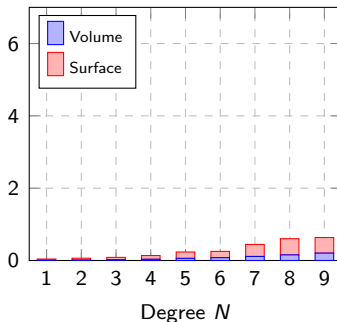
Optimal $O(N^3)$ complexity “slice-by-slice” application of Bernstein lift.

BBDG: efficient volume, surface kernels

Nodal DG

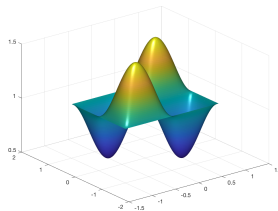
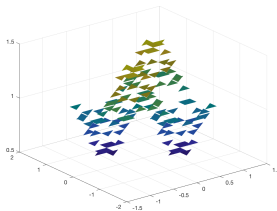
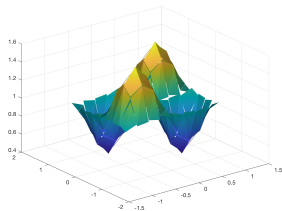


Bernstein-Bezier DG



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

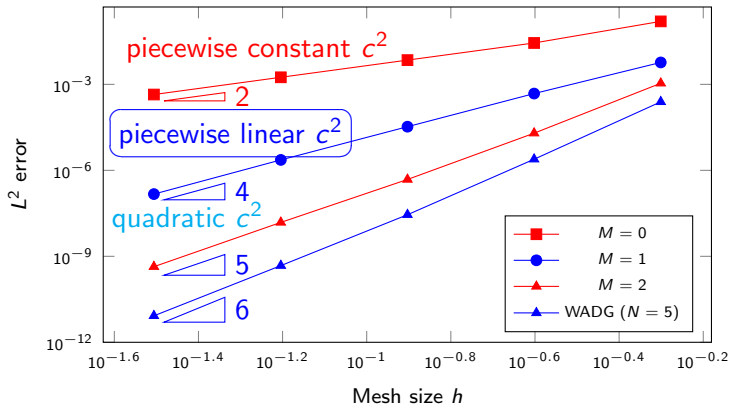
A faster BBWADG update kernel

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

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

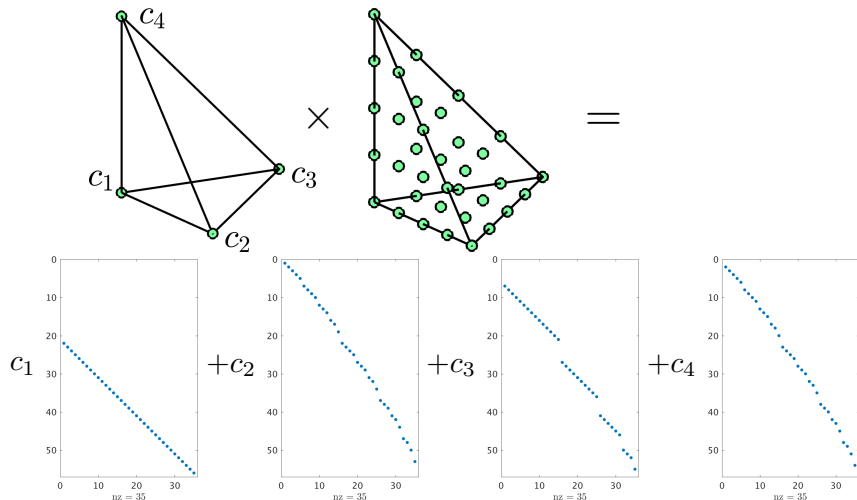
$$P_N(u(\mathbf{x})c^2(\mathbf{x})), \quad P_N = L^2 \text{ projection operator.}$$

- 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 $c^2(\mathbf{x})$ 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 .

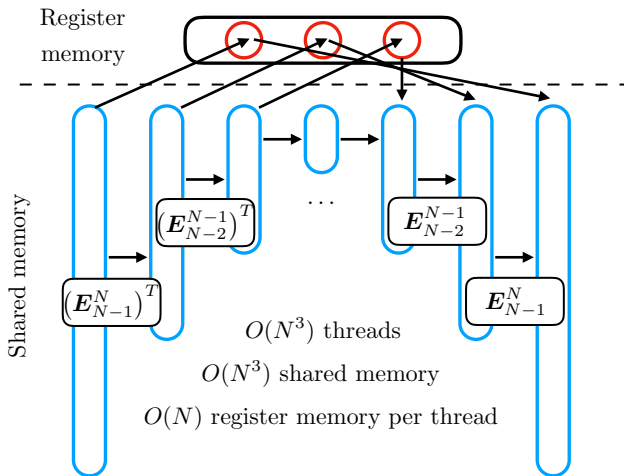
Fast Bernstein polynomial projection

- 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:

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

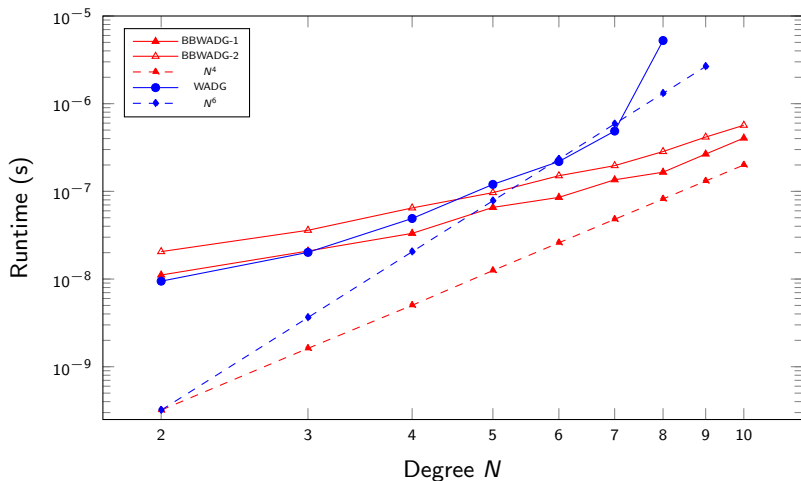
- “Telescoping” form of $\tilde{\mathbf{P}}_N$: $O(N^4)$ complexity, more GPU-friendly.

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

Sketch of GPU algorithm for \tilde{P}_N 

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

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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