Upwind Summation By Parts Methods for Large Scale Elastic Wave Equation

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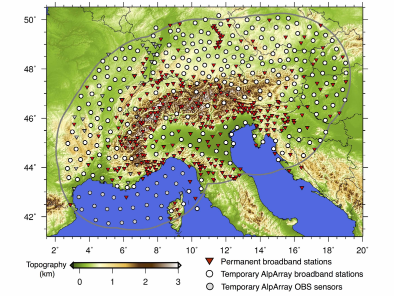
Seismological applications: AlpArray

Further understanding of mountain building processes from initial to final phases, including contemporary 3D-interactions of large plates with small plates and micro-ocean subduction.



- strong free-surface topography
- strong 3D media heterogeneity
- acoustic-elastic waves interaction

Scattering: Accurate modeling of surface waves and scattered waves.

Application Area

Physical Model

Let $t > 0$ be the time variable, $(v_x, v_y, v_z)^T$ be particle velocities, and $\sigma_{i,j}$ be the stresses. The first order time-dependent elastic wave equations in a source free, heterogeneous medium is

$$\begin{pmatrix} \rho\frac{\partial v_x}{\partial t} \\ \rho\frac{\partial v_y}{\partial t} \\ \rho\frac{\partial v_z}{\partial t} \\ \mathbf{S}\begin{pmatrix} \frac{\partial \sigma_{xx}}{\partial t} \\ \frac{\partial \sigma_{yy}}{\partial t} \\ \frac{\partial \sigma_{zz}}{\partial t} \\ \frac{\partial \sigma_{xy}}{\partial t} \\ \frac{\partial \sigma_{xz}}{\partial t} \\ \frac{\partial \sigma_{yz}}{\partial t} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \\ \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} \\ \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \\ \frac{\partial v_x}{\partial x} \\ \frac{\partial v_y}{\partial y} \\ \frac{\partial v_z}{\partial z} \\ \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \\ \frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \\ \frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \end{pmatrix} \tag{1}$$

WaveQLab 3D Upwind SBP Simulation

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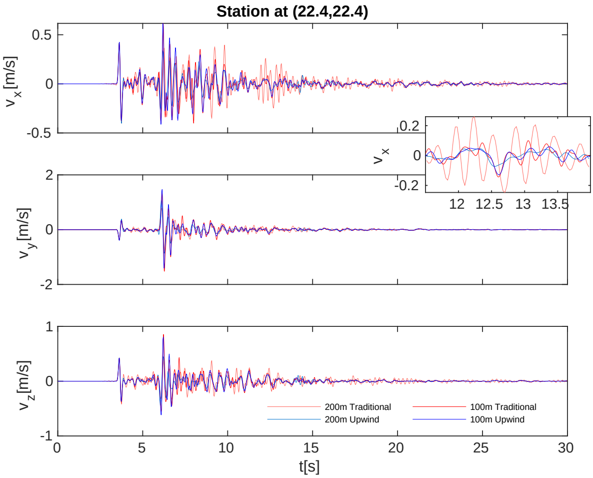

Figure: Seismograph from a station placed at $(22.4, 22.4)$ on the Earths surface.

Challenges for large scale simulations

1. Scalable code
2. Resolve high frequencies (0 - 20 Hz)
3. Mesh complex geometries
4. Computational efficiency

For efficiency, we use finite difference schemes to approximate the derivative in space.

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WaveQlab [K. Duru and E. M. Dunham. J. Comput. Phys., 305:185207, 2016.] is one of the few codes in the world that is both efficient and accurate enough to run these large scale computations.

Traditional SBP Operators

integration by parts formula:

$$\int_0^1 \frac{\partial}{\partial x}(f)g dx + \int_0^1 f\frac{\partial}{\partial x}(g)dx = f(1)g(1) - f(0)g(0). \tag{2}$$

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Definition

The tuple (H, D) is called a *summation-by-parts* approximate of order m if $H = H^T > 0$ and obeys Equation 3 (SBP property), and D is exact on polynomials of up to degree m.

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Example: 2nd order central finite difference operator

$$D(\mathbf{u})_i := \frac{u_{i+1} - u_{i-1}}{2\Delta x} \qquad D(\mathbf{u})_n := \frac{u_{n-1} - u_n}{\Delta x} \qquad D(\mathbf{u})_0 := \frac{u_0 - u_1}{\Delta x}$$

Upwind SBP Operators

Let $H >$ be a symmetric weight matrix that induces a discrete measure μ_n and inner product $\langle \cdot, \cdot \rangle_H$. Then we can find differential operators $D : \mathbb{R}^{n+1} \mapsto \mathbb{R}^{n+1}$, however D is not unique. In particular we can find the pair

$$(D_+ \boldsymbol{f})^T H \boldsymbol{g} + \boldsymbol{f}^T H (D_- \boldsymbol{g}) = f_n g_n - f_0 g_0, \tag{4}$$

We call (H, D_-, D_+) an upwind diagonal-norm dual-pair SBP operator of order m if the accuracy conditions

$$D_\eta(\boldsymbol{x}^i) = i \boldsymbol{x}^{i-1} \tag{5}$$

are satisfied for all $i \in \{0, \ldots, m\}$ and $\eta \in \{-, +\}$ where $\boldsymbol{x}^i := (x_0^i, \ldots, x_n^i)^T$.

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Definition

Let D_-, D_+ : $\mathbb{R}^n \mapsto \mathbb{R}^n$ be linear operators that solve Equation 4 for a diagonal weight matrix $H \in \mathbb{R}^{n \times n}$. If the matrix $S_+ := D_+ + D_+^T$ or $S_- := D_- + D_-^T$ is also negative semi-definite, then the 3-tuple (H, D_-, D_+) is called an upwind diagonal-norm dual-pair SBP operator.

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Some historical papers:

- Heinz-Otto Kreiss and Godela Scherer, Finite element and finite difference methods for hyperbolic partial differential equations. Mathematical Aspects of Finite Elements in Partial Differential Equations, New York: Academic Press , 1974, 195-212 p.
- Bo Strand, Summation by Parts for Finite Difference Approximations for d/d x. J. Comput. Phys., 110, 1994.
- Leonid Dovgilovich and Ivan Sofronov, High-accuracy finite-difference schemes for solving elastodynamic problems in curvilinear coordinates within multi-block approach, Appl. Numer. Math. 93(2015) 176–194.
- K. Mattsson,Diagonal-norm upwind sbp operators, J. Comput. Phys., 335 (2017), pp. 283–310.

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- The main benefit for these operators is that they can suppress poisonous spurious oscillations from unresolved wave-modes, which can destroy the accuracy of numerical simulations.
- However, these operators are asymmetric and dissipative, can potentially destroy symmetries that exist in the continuum problem.

Our overall goal is to carefully combine the upwind SBP operator pair so that we preserve the discrete anti-symmetric property and invariants of the underlying IBVP.

Traditional SBP Operator

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Upwind SBP Operators

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High Resolution Traditional SBP Operator

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General basis form

Let $\boldsymbol{e} := \{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ be a basis for $\mathbb{R}^3$.

$$\boldsymbol{P}^{-1}\frac{\partial \boldsymbol{Q}}{\partial t} = \nabla \cdot \boldsymbol{F}(\boldsymbol{Q}) + \sum_{\xi \in \{x,y,z\}} \boldsymbol{B}_\xi(\nabla \boldsymbol{Q}) \tag{6}$$

where $\boldsymbol{Q} := (\boldsymbol{v}, \boldsymbol{\sigma})^T$, $\boldsymbol{P} = \begin{pmatrix} \rho^{-1}\boldsymbol{1} & \boldsymbol{0} \\ \boldsymbol{0}^T & \boldsymbol{C} \end{pmatrix}$, $\quad \boldsymbol{C} = \boldsymbol{C}^T > 0$,

$$\boldsymbol{F}_\eta(\boldsymbol{Q}) := \begin{pmatrix} e_1\sigma_{xx} + e_2\sigma_{xy} + e_3\sigma_{xz} \\ e_1\sigma_{xy} + e_2\sigma_{yy} + e_3\sigma_{yz} \\ e_1\sigma_{xz} + e_2\sigma_{yz} + e_3\sigma_{zz} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \boldsymbol{B}_\xi(\nabla \boldsymbol{Q}) := \begin{pmatrix} 0 \\ 0 \\ 0 \\ e_1\frac{\partial v_x}{\partial \xi} \\ e_2\frac{\partial v_y}{\partial \xi} \\ e_3\frac{\partial v_z}{\partial \xi} \\ e_2\frac{\partial v_x}{\partial \xi} + e_1\frac{\partial v_y}{\partial \xi} \\ e_3\frac{\partial v_x}{\partial \xi} + e_1\frac{\partial v_z}{\partial \xi} \\ e_3\frac{\partial v_y}{\partial \xi} + e_2\frac{\partial v_z}{\partial \xi} \end{pmatrix} \tag{7}$$

with $\boldsymbol{F} := (\boldsymbol{F}_{\boldsymbol{e}_1}, \boldsymbol{F}_{\boldsymbol{e}_2}, \boldsymbol{F}_{\boldsymbol{e}_3})^T$.

Anti-symmetry

Lemma

Consider the anti-symmetric form given in Equation (6). For any basis $\mathbf{e}$ *that spans* Ω *we have*

$$\left(\left(\frac{\partial \boldsymbol{Q}}{\partial \xi}\right)^T \boldsymbol{F}_\xi\left(\boldsymbol{Q}\right) - \boldsymbol{Q}^T \boldsymbol{B}_\xi(\nabla \boldsymbol{Q})\right) = 0.$$

$$\langle \mathbf{Q}, \mathbf{F} \rangle := \int_\Omega \left(\mathbf{Q}^T \mathbf{F}\right) dxdydz, \tag{8}$$

and the corresponding energy-norm

$$\|\mathbf{Q}\left(\cdot,\cdot,\cdot,t\right)\|_P^2 = \left\langle \mathbf{Q}, \frac{1}{2}\mathbf{P}^{-1}\mathbf{Q}\right\rangle = \int_\Omega \left(\sum_{\eta \in \{x,y,z\}} \frac{\rho}{2} v_\eta^2 + \frac{1}{2}\boldsymbol{\sigma}^T S \boldsymbol{\sigma}\right) dxdydz. \tag{9}$$

The weighted L^2-norm $\|\mathbf{Q}\left(\cdot,\cdot,\cdot,t\right)\|_P^2$ is the mechanical energy, which is the sum of the kinetic energy and the strain energy.

For Cauchy problem: $\|\mathbf{Q}\left(\cdot,\cdot,\cdot,t\right)\|_P^2 = \|\mathbf{Q}\left(\cdot,\cdot,\cdot,0\right)\|_P^2$

Curvilinear coordinates

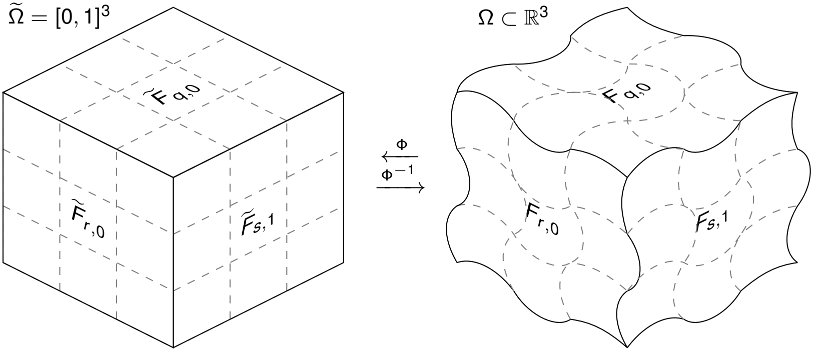


Figure: Curvilinear coordinate transform and boundary faces of the computational space $\widetilde{\Omega}$ and modelling space Ω.

Structure preserving curvilinear transformation

The curvilinear coordinates (q, r, s), with the gradient operator $\nabla := \left(\frac{\partial}{\partial q}, \frac{\partial}{\partial r}, \frac{\partial}{\partial s}\right)$ gives

$$\widetilde{\boldsymbol{P}}^{-1}\frac{\partial}{\partial t}\boldsymbol{Q} = \nabla \cdot \boldsymbol{F}(\boldsymbol{Q}) + \sum_{\xi \in \{q,r,s\}} \boldsymbol{B}_{\xi}(\nabla \boldsymbol{Q}), \tag{10}$$

where $\widetilde{\boldsymbol{P}} = J^{-1}\boldsymbol{P}$ and

$$\boldsymbol{F}_{\xi}(\boldsymbol{Q}) := \begin{pmatrix} J\left(\xi_x\sigma_{xx} + \xi_y\sigma_{xy} + \xi_z\sigma_{xz}\right) \\ J\left(\xi_x\sigma_{xx} + \xi_y\sigma_{xy} + \xi_z\sigma_{xz}\right) \\ J\left(\xi_x\sigma_{xx} + \xi_y\sigma_{xy} + \xi_z\sigma_{xz}\right) \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{B}_{\xi}(\nabla \boldsymbol{Q}) \begin{pmatrix} 0 \\ 0 \\ 0 \\ J\xi_x\frac{\partial v_x}{\partial \xi} \\ J\xi_y\frac{\partial v_y}{\partial \xi} \\ J\xi_z\frac{\partial v_z}{\partial \xi} \\ J\left(\xi_y\frac{\partial v_x}{\partial \xi} + \xi_x\frac{\partial v_y}{\partial \xi}\right) \\ J\left(\xi_z\frac{\partial v_x}{\partial \xi} + \xi_x\frac{\partial v_z}{\partial \xi}\right) \\ J\left(\xi_z\frac{\partial v_y}{\partial \xi} + \xi_y\frac{\partial v_z}{\partial \xi}\right) \end{pmatrix}. \tag{11}$$

Anti-symmetry

Remark

Equation (10) is structure preserving, that is Lemma 3 holds and we have

$$\left(\left(\frac{\partial \boldsymbol{Q}}{\partial \xi}\right)^{T} \boldsymbol{F}_{\xi}\left(\boldsymbol{Q}\right) - \boldsymbol{Q}^{T} \boldsymbol{B}_{\xi}\left(\nabla \boldsymbol{Q}\right)\right) = 0,$$

for all $\xi \in \{q, r, s\}$. This will be crucial in deriving high order accurate, structure preserving and provably energy stable scheme for the elastic wave equation in complex geometries.

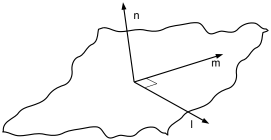
Theorem

The transformed elastic wave equation (10) in curvilinear coordinates satisfies the energy equation

$$\frac{d}{dt}\|\mathbf{Q}\left(\cdot, \cdot, \cdot, t\right)\|_{P}^{2} = BT(\boldsymbol{v}, \boldsymbol{T}).$$

$$BT(\boldsymbol{v}, \boldsymbol{T}) := \oint_{\Gamma} \boldsymbol{v}^{T} \boldsymbol{T} dS = \sum_{\substack{\xi \in \{q,r,s\} \\ i \in \{0,1\}}} (-1)^{i+1} \int_0^1 \int_0^1 J \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\, \boldsymbol{v}^{T} \boldsymbol{T} \frac{dqdrds}{d\xi}. \qquad (12)$$

Boundary surface



On the boundary surface, we extract the particle velocity vector and the traction vector, and the local rotation matrix

$$\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} T_x \\ T_y \\ T_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} \boldsymbol{n}^T \\ \boldsymbol{m}^T \\ \boldsymbol{l}^T \end{pmatrix}, \tag{13}$$

where $\det(\mathbf{R}) \neq 0$ and $\mathbf{R}^{-1} = \mathbf{R}^T$. Next, rotate the particle velocity and traction vectors into the local orthonormal basis, **l** , **m** and **n**, having

$$v_\eta = (\mathbf{Rv})_\eta, \quad T_\eta = (\mathbf{RT})_\eta, \quad \eta \in \{l, m, n\}. \tag{14}$$

Boundary conditions

At the boundary faces $F_{\xi,i}$ we consider the linear boundary conditions,

$$
\begin{aligned}
\frac{Z_\eta}{2}\left(1-\gamma_\eta\right) v_\eta - \frac{1+\gamma_\eta}{2} T_\eta = 0, \quad (x,y,z) \in F_{\xi,0}, \\
\frac{Z_\eta}{2}\left(1-\gamma_\eta\right) v_\eta + \frac{1+\gamma_\eta}{2} T_\eta = 0, \quad (x,y,z) \in F_{\xi,1}.
\end{aligned}
\tag{15}
$$

Here γ_η are real parameters with $0 \le |\gamma_\eta| \le 1$.

$$
\begin{aligned}
v_\eta T_\eta > 0, \quad \forall |\gamma_\eta| < 1, \quad \text{and} \quad v_\eta T_\eta = 0, \quad \forall |\gamma_\eta| = 1, \quad \xi \equiv 0, \\
v_\eta T_\eta < 0, \quad \forall |\gamma_\eta| < 1, \quad \text{and} \quad v_\eta T_\eta = 0, \quad \forall |\gamma_\eta| = 1, \quad \xi \equiv 1.
\end{aligned}
\tag{16}
$$

$$
BTs(\mathbf{v}, \mathbf{T}) := \oint_\Gamma \mathbf{v}^T \mathbf{T} dS = \sum_{\substack{\xi \in \{q,r,s\} \\ i \in \{0,1\}}} (-1)^{i+1} \int_0^1 \int_0^1 J \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\, \mathbf{v}^T \mathbf{T} \frac{dqdrds}{d\xi}. \tag{17}
$$

Lemma

Consider the well-posed boundary conditions (15) with $|\gamma_\eta| \le 1$. The boundary term BTs defined in (17) is negative semi-definite, $\mathrm{BTs} \le 0$, for all $Z_\eta > 0$.

Energy estimate

Theorem

The transformed elastic wave equation (10) *in curvilinear coordinates subject to the boundary conditions* (15) *satisfies the energy equation*

$$\frac{d}{dt}\|\mathbf{Q}(\cdot,\cdot,\cdot,t)\|_P^2 = BT(\boldsymbol{v},\boldsymbol{T}) \le 0.$$

$$BT(\boldsymbol{v},\boldsymbol{T}) := \oint_\Gamma \boldsymbol{v}^T \boldsymbol{T} dS = \sum_{\substack{\xi\in\{q,r,s\}\\ i\in\{0,1\}}} (-1)^{i+1} \int_0^1 \int_0^1 J\sqrt{\xi_x^2+\xi_y^2+\xi_z^2}\,\boldsymbol{v}^T\boldsymbol{T}\frac{dqdrds}{d\xi}. \tag{18}$$

Spatial discretization

The 1D SBP operators can be extended to higher space dimensions using tensor products $\otimes$. Let $f(q, r, s)$ denote a 3D scalar function, and $f_{ijk} := f(q_i, r_j, s_k)$ denote the corresponding 3D grid function. The 3D scalar grid function f_{ijk} is rearranged row-wise as a vector $\boldsymbol{f}$ of length $n_q n_r n_s$. For $\xi \in \{q, r, s\}$ and $\eta \in \{-, +\}$ define:

$$\boldsymbol{D}_{\eta\xi} := \bigotimes_{k\in\{q,r,s\}} (\chi_{k=\xi} D_{\eta k} + \chi_{k\neq\xi} I_{n_k}), \qquad \boldsymbol{H} := \bigotimes_{k\in\{q,r,s\}} H_k, \tag{19}$$

where I_{n_ξ} is the identity matrix of size $n_\xi \times n_\xi$, and we take $\chi_{k=\xi} := \chi_{\{\xi\}}(k)$ and $\chi_{k\neq\xi} := 1 - \chi_{k=\xi}$. So $\boldsymbol{D}_{\xi\eta}$ approximates the partial derivative operator in the ξ direction. An inner product on $\mathbb{R}^{n_q+1} \times \mathbb{R}^{n_r+1} \times \mathbb{R}^{n_s+1}$ is induced by $\boldsymbol{H}$ through

$$\langle \boldsymbol{g}, \boldsymbol{f} \rangle_{\boldsymbol{H}} := \boldsymbol{g}^T \boldsymbol{H} \boldsymbol{f} = \sum_{i=0}^{n_q} \sum_{j=0}^{n_r} \sum_{k=0}^{n_s} f_{ijk} g_{ijk} h_i^{(q)} h_j^{(r)} h_k^{(s)} \tag{20}$$

Further, we have the multi-dimensional SBP property

$$\sum_{\xi \in \{q,r,s\}} \left(\left\langle \boldsymbol{D}_{-\xi}(\boldsymbol{f}), \boldsymbol{g} \right\rangle_{\boldsymbol{H}} + \left\langle \boldsymbol{f}, \boldsymbol{D}_{+\xi}(\boldsymbol{g}) \right\rangle_{\boldsymbol{H}} \right) = \sum_{\xi \in \{q,r,s\}} S_{\xi}\left(\boldsymbol{f}\boldsymbol{g}\right), \tag{21}$$

where $S_{\xi}\left(\boldsymbol{f}, \boldsymbol{g}\right)$ in the right hand side is the surface cubature, defined by

$$S_q\left(\boldsymbol{f}\boldsymbol{g}\right) = \sum_{i \in \{0, n_q\}} (-1)^{q_i+1} \sum_{j=0}^{n_r} \sum_{k=0}^{n_s} f_{ijk} g_{ijk} h_j^{(r)} h_k^{(s)}, \tag{22}$$

$$S_r\left(\boldsymbol{f}\boldsymbol{g}\right) = \sum_{j \in \{0, n_r\}} (-1)^{r_j+1} \sum_{i=0}^{n_q} \sum_{k=0}^{n_s} f_{ijk} g_{ijk} h_i^{(q)} h_k^{(s)}, \tag{23}$$

$$S_s\left(\boldsymbol{f}\boldsymbol{g}\right) = \sum_{k \in \{0, n_s\}} (-1)^{s_k+1} \sum_{i=0}^{n_q} \sum_{j=0}^{n_r} f_{ijk} g_{ijk} h_i^{(q)} h_j^{(r)}. \tag{24}$$

Note that $\xi_0 = 0$ and $\xi_{n_\xi} = 1$, for all $\xi \in \{q, r, s\}$.

Spatial discretization

The semi-discrete approximation reads

$$\widetilde{\mathbf{P}}^{-1} \frac{d}{dt}\mathbf{Q} = \boldsymbol{\nabla}_{D_-} \bullet \mathbf{F}\left(\mathbf{Q}\right) + \sum_{\xi \in \{q,r,s\}} \mathbf{B}_{\xi} \left(\boldsymbol{\nabla}_{D_+} \mathbf{Q}\right), \tag{25}$$

where the discrete operator $\boldsymbol{\nabla}_{D_\eta} = \left(\mathbf{D}_{\eta q}, \mathbf{D}_{\eta r}, \mathbf{D}_{\eta s}\right)^T$, with $\eta \in \{+, -\}$, is analogous to the continuous gradient operator $\boldsymbol{\nabla} = \left(\partial/\partial q, \partial/\partial r, \partial/\partial s\right)^T$. In $\boldsymbol{\nabla}_{D_\eta}$ we have replaced the continuous derivative operators in $\boldsymbol{\nabla}$ with their discrete counterparts.

Remark

The backward difference operator D_- is used to approximate the spatial derivative for the conservative flux term, whilst the forward difference operator D_+ is an approximant for the non-conservative product term. This combination of upwind operators and the specific choice of the anti-symmetric form (10) *is critical to deriving a conservative and energy stable scheme for the elastic wave equation in complex geometries.*

Spatial discretization

We will now prove the discrete equivalence of Lemma 3.

Lemma

Consider the semi-discrete approximation given in Equation 25. We have the discrete anti-symmetric form

$$\left(\left(\left(I_9 \otimes \boldsymbol{D}_{+\xi}\right) \boldsymbol{Q}\right)^T \boldsymbol{F}_\xi\left(\boldsymbol{Q}\right) - \boldsymbol{Q}^T \mathbf{B}_\xi\left(\boldsymbol{\nabla}_{D_+}\bar{\mathbf{Q}}\right)\right) = 0.$$

Further, for a 3D scalar field $f_{ijk} = f(x_i, y_j, z_k)$ we also introduce the surface cubature

$$\mathbb{I}_{q_i}\left(\mathbf{f}\right) = \sum_{j=0}^{n_r}\sum_{k=0}^{n_s}\left(J_{ijk}\sqrt{q_{xijk}^2 + q_{yijk}^2 + q_{zijk}^2} f_{ijk}\right) h_j^{(r)} h_k^{(s)}, \tag{26}$$

$$\mathbb{I}\left(\mathbf{f}\right) = \sum_{\xi\in\{q,r,s\}}\sum_{i\in\{0,n_\xi\}} (-1)^{\xi_i}\, \mathbb{I}_{\xi_i}\left(\mathbf{f}\right). \tag{27}$$

Therefore we have

$$\mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right) = \sum_{\xi\in\{q,r,s\}} S_\xi\left(\boldsymbol{J}\sqrt{\xi_x^2+\xi_y^2+\xi_z^2}, \boldsymbol{v}^T\boldsymbol{T}\right), \tag{28}$$

Spatial discretization

Theorem

Consider the semi-discrete approximation (25) of the elastic wave equation. We have

$$\frac{d}{dt}\|\mathbf{Q}(\cdot,\cdot,\cdot,t)\|_{HP}^2 = \mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right),$$

where $\mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right)$ is the surface term defined in (28).

Proof.

Consider

$$\frac{d}{dt}\|\mathbf{Q}(\cdot,\cdot,\cdot,t)\|_{HP}^2 = \left\langle \boldsymbol{Q}, P^{-1}\frac{\partial}{\partial t}\boldsymbol{Q}\right\rangle_H = \left\langle \boldsymbol{Q}, \boldsymbol{\nabla}_{D_-} \bullet \mathbf{F}(\mathbf{Q}) + \sum_{\xi\in\{q,r,s\}} \mathbf{B}_\xi\left(\boldsymbol{\nabla}_{D_+}\mathbf{Q}\right)\right\rangle_H. \tag{29}$$

Expanding the right hand side and applying the multi-dimensional SBP property (21) yields

$$\sum_{\xi\in\{q,r,s\}}\left(\left\langle \boldsymbol{Q}, \left(I_9\otimes \boldsymbol{D}_{-\xi}\right)\boldsymbol{F}_\xi\left(\boldsymbol{Q}\right)\right\rangle_H + \left\langle \boldsymbol{Q}, \mathbf{B}_\xi\left(\boldsymbol{\nabla}_{D_+}\bar{\mathbf{Q}}\right)\right\rangle_H\right)$$
$$= \mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right) + \sum_{\xi\in\{q,r,s\}}\left(\left\langle \boldsymbol{Q}, \boldsymbol{B}_\xi(\boldsymbol{\nabla}_{D_+}\boldsymbol{Q})\right\rangle_H - \left\langle \left(I_9\otimes \boldsymbol{D}_{+\xi}\right)\boldsymbol{Q}, \boldsymbol{F}_\xi(\boldsymbol{Q})\right\rangle_H\right).$$

Spatial discretization

The semi-discrete approximation with weak enforcement of boundary conditions is

$$\widetilde{\mathbf{P}}^{-1}\frac{d}{dt}\mathbf{Q} = \boldsymbol{\nabla}_{D_-} \bullet \mathbf{F}(\mathbf{Q}) + \sum_{\xi=q,r,s} \mathbf{B}_\xi \left(\boldsymbol{\nabla}_{D_+}\mathbf{Q}\right) + \sum_{\substack{\xi\in\{q,r,s\} \\ i\in\{0,n_\xi\}}} \mathbf{SAT}_{\xi,i}(\mathbf{Q}), \tag{30}$$

where $\mathbf{SAT}_{\xi,i}$ are penalty terms added to the discrete equation (25) at the boundaries to enforce the boundary conditions (15).

SAT terms

We consider specifically the free-surface boundary condition at all boundary surfaces, $F_{\xi,0},\ F_{\xi,1}$ for all $\xi \in \{q, r, s\}$. With the free-surface boundary condition, at $F_{\xi,0},\ F_{\xi,1}$, the traction vector vanishes $\left(\boldsymbol{T}_x, \boldsymbol{T}_y, \boldsymbol{T}_z\right) = 0$. We set the SAT terms

$$\begin{aligned}
\mathbf{SAT}_{\xi,0} &= \boldsymbol{H}_{\xi}^{-1}\mathbf{e}_{0_\xi}\boldsymbol{J}\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\left(\boldsymbol{T}_x, \boldsymbol{T}_y, \boldsymbol{T}_z, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}\right)^T, \\
\mathbf{SAT}_{\xi,n_\xi} &= -\boldsymbol{H}_{\xi}^{-1}\mathbf{e}_{n_\xi}\boldsymbol{J}\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\left(\boldsymbol{T}_x, \boldsymbol{T}_y, \boldsymbol{T}_z, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}\right)^T,
\end{aligned} \tag{31}$$

where

$$\boldsymbol{H}_q = \left(I_9 \otimes H_q \otimes I_{n_r} \otimes I_{n_s}\right), \quad \mathbf{e}_{0_q} = (I_9 \otimes e_{0_q} e_{0_q}^T \otimes I_{n_r} \otimes I_{n_s}), \quad \mathbf{e}_{n_q} = (I_9 \otimes e_{n_q} e_{n_q}^T \otimes I_{n_r} \otimes I_{n_s}),$$

$$e_{0_\xi} = (1, 0, 0, \cdots, 0)^T, \ e_{n_\xi} = (0, 0, 0, \cdots, 1)^T.$$

Here I_9 and I_{n_ξ} are identity matrices of size 9×9 and $n_\xi \times n_\xi$, respectively, and $\mathbf{e}_{0_\xi}$, $\mathbf{e}_{n_\xi}$ are boundary projection operators

A main result

Theorem

Consider the semi-discrete approximation (30) *of the elastic wave equation with the SAT terms* $\mathbf{SAT}_{\xi,i}$ *defined in* (31)*. We have*

$$\frac{d}{dt}\|\mathbf{Q}(\cdot,\cdot,\cdot,t)\|_{HP}^2 = 0.$$

Proof.

$$\frac{d}{dt}\|\mathbf{Q}(\cdot,\cdot,\cdot,t)\|_{HP}^2 = \left\langle \boldsymbol{Q}, P^{-1}\frac{\partial}{\partial t}\boldsymbol{Q}\right\rangle_H = \left\langle \boldsymbol{Q}, \boldsymbol{\nabla}_{D_-}\bullet \mathbf{F}(\mathbf{Q}) + \sum_{\xi\in\{q,r,s\}} \mathbf{B}_\xi\left(\boldsymbol{\nabla}_{D_+}\mathbf{Q}\right)\right\rangle_H$$

$$+\left\langle \boldsymbol{Q}, \sum_{\substack{\xi\in\{q,r,s\}\\ i\in\{0,1\}}} \mathbf{SAT}_{\xi,i}(\mathbf{Q})\right\rangle_H$$

$$= \mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right) + \sum_{\substack{\xi\in\{q,r,s\}\\ i\in\{0,n_\xi\}}} \left\langle \boldsymbol{Q}, \mathbf{SAT}_{\xi,i}(\mathbf{Q})\right\rangle_H$$

$$\sum_{\substack{\xi\in\{q,r,s\}\\ i\in\{0,n_\xi\}}} \left\langle \boldsymbol{Q}, \mathbf{SAT}_{\xi,i}(\mathbf{Q})\right\rangle_H = -\mathbb{I}\left(\boldsymbol{v}^T\boldsymbol{T}\right).$$

SAT terms

Similar to the DG framework[1], a weak boundary procedure can be derived by constructing boundary data, $\widehat{v}_\eta$, $\widehat{T}_\eta$, which are the solution of a Riemann-like problem constrained to satisfy the boundary condition (15) exactly. SAT penalty terms are constructed by penalizing data, that is $\widehat{v}_\eta$, $\widehat{T}_\eta$, against the in-going waves only.
Introduce the penalty terms

$$
\begin{aligned}
G_\eta &= \frac{1}{2} Z_\eta \left(v_\eta - \widehat{v}_\eta\right) - \frac{1}{2}\left(T_\eta - \widehat{T}_\eta\right)\Big|_{\xi=0}, \quad \widetilde{G}_\eta := \frac{1}{Z_\eta} G_\eta, \\
G_\eta &= \frac{1}{2} Z_\eta \left(v_\eta - \widehat{v}_\eta\right) + \frac{1}{2}\left(T_\eta - \widehat{T}_\eta\right)\Big|_{\xi=1}, \quad \widetilde{G}_\eta := \frac{1}{Z_\eta} G_\eta.
\end{aligned}
\tag{32}
$$

The penalty terms are computed in the transformed coordinates l, m, n. We will now rotate them to the physical coordinates x, y, z, we have

$$
\mathbf{G} := \begin{pmatrix} G_x \\ G_y \\ G_z \end{pmatrix} = \mathbf{R}^T \begin{pmatrix} G_n \\ G_m \\ G_l \end{pmatrix}, \quad \widetilde{\mathbf{G}} := \begin{pmatrix} \widetilde{G}_x \\ \widetilde{G}_y \\ \widetilde{G}_z \end{pmatrix} = \mathbf{R}^T \begin{pmatrix} \widetilde{G}_n \\ \widetilde{G}_m \\ \widetilde{G}_l \end{pmatrix}. \tag{33}
$$

SAT terms

We introduce the SAT vector that matches the eigen–structure of the elastic wave equation

$$\mathbf{SAT}_0 = \begin{pmatrix} G_x \\ G_y \\ G_z \\ -n_x\widetilde{G}_x, \\ -n_y\widetilde{G}_y \\ -n_z\widetilde{G}_z, \\ -\left(n_y\widetilde{G}_x + n_x\widetilde{G}_y\right) \\ -\left(n_z\widetilde{G}_x + n_x\widetilde{G}_z\right) \\ -\left(n_z\widetilde{G}_y + n_y\widetilde{G}_z\right) \end{pmatrix}, \quad \mathbf{SAT}_{n_\xi} = \begin{pmatrix} G_x \\ G_y \\ G_z \\ n_x\widetilde{G}_x, \\ n_y\widetilde{G}_y \\ n_z\widetilde{G}_z, \\ \left(n_y\widetilde{G}_x + n_x\widetilde{G}_y\right) \\ \left(n_z\widetilde{G}_x + n_x\widetilde{G}_z\right) \\ \left(n_z\widetilde{G}_y + n_y\widetilde{G}_z\right) \end{pmatrix}. \tag{34}$$

Here, $\mathbf{n} = (n_x, n_y, n_z)^T$ is the unit normal vector on the boundary defined in (**??**). Finally, the SAT terms for the general boundary conditions are defined as follows

$$\mathbf{SAT}_{\xi,i} = -\boldsymbol{H}_\xi^{-1}\mathbf{e}_{\xi,i}\boldsymbol{J}\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}\mathbf{SAT}_i. \tag{35}$$

Stability

Introduce the fluctuation term

$$F_{luc}\left(\boldsymbol{G}, \mathbf{Z}\right) := -\sum_{\xi \in \{q,r,s\}} \sum_{i \in \{0, n_\xi\}} \mathbb{I}_{\xi_i} \left(\sum_{\eta = l,m,n} \frac{1}{Z_\eta} |G_\eta|^2 \right) \le 0, \tag{36}$$

and discrete boundary surface terms $\mathbb{I}\left(\widehat{\mathbf{v}}^T \widehat{\mathbf{T}}\right)$. Note that

$$\mathbb{I}\left(\widehat{\mathbf{v}}^T \widehat{\mathbf{T}}\right) = \sum_{\xi \in \{q,r,s\}} S_\xi \left(\boldsymbol{J}\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}, \widehat{\mathbf{v}}^T \widehat{\mathbf{T}} \right). \tag{37}$$

Note also that the boundary term is never positive, $\mathbb{I}\left(\widehat{\mathbf{v}}^T \widehat{\mathbf{T}}\right) \le 0$ for all $|\gamma_\eta| \le 1$.
Also the fluctuation term is never positive, $F_{luc}\left(\boldsymbol{G}, \mathbf{Z}\right) \le 0$.

Theorem

Consider the semi-discrete approximation (30) of the elastic wave equation with the SAT-terms $\mathbf{SAT}_{\xi,i}$ defined in (35). We have

$$\frac{d}{dt}\|\mathbf{Q}\left(\cdot,\cdot,\cdot,t\right)\|_{HP}^2 = F_{luc}\left(\boldsymbol{G}, \mathbf{Z}\right) + \mathbb{I}\left(\widehat{\mathbf{v}}^T \widehat{\mathbf{T}}\right) \le 0.$$

LOH1 SCEC Benchmark problem

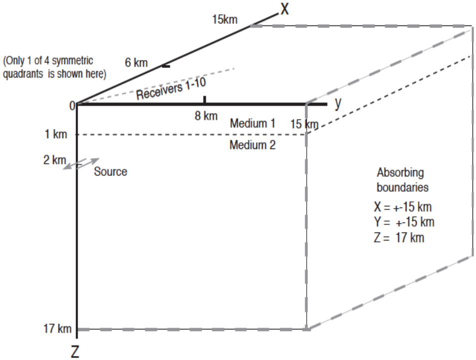
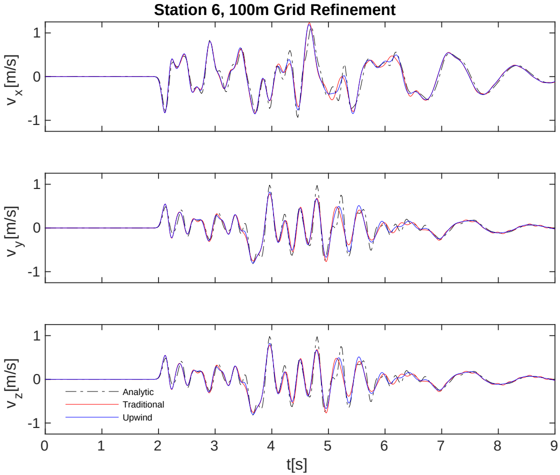


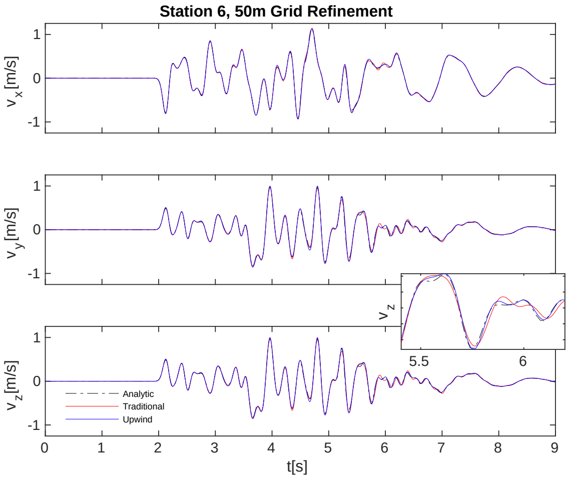
Figure: LOH1 Benchmark set-up.

A discontinuous medium with soft top layer and hard bedrock

LOH1 Benchmark 100 m



LOH1 Benchmark 50 m



WaveQLab 3D Upwind SBP Simulation

(Loading movie...)

WaveQLab 3D Upwind SBP Simulation

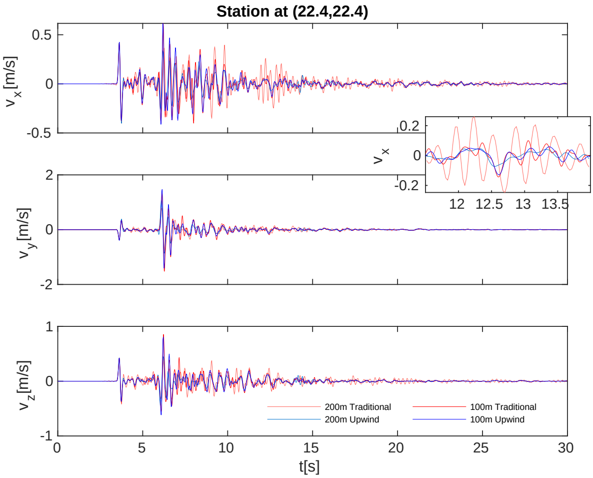
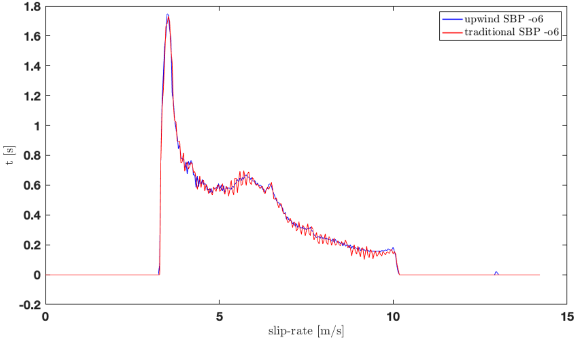


Figure: Seismograph from a station placed at (22.4, 22.4) on the Earths surface.

Summary

- Upwind SBP are implemented efficiently for the simulation of large-scale 3D elastic wave equation.
- We have shown through the energy method that our implementation is numerically stable.
- When compared to traditional central stencil operators, the upwind counterparts are more efficient for resolving high-frequencies.
- Preliminary dynamic rupture simulations show promise in increasing efficiency through using upwind SBPoperators



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