

Supplemental Material:
Greedy Stein Variational Gradient Descent: An
algorithmic approach for wave prospection problems
Supplemental Material

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1. The five points finite differences operator

The finite difference method is a numerical approach for solving differential equations by approximating the derivatives of the functions within the system. The numerical accuracy of this method, particularly when applied to wave and transport equations, has been well-documented and demonstrated by several authors [8, 9, 6, 5]. These studies highlight the effectiveness of the finite difference method in approximating numerical solutions to partial differential equations. This method is widely used in computational seismology, where it is often implemented as a *five-point operator* to approximate the spatial derivative.

Applying this numerical approach to solve the wave equation involves two key considerations. The first is the Courant number, also known as the Courant-Friedrichs-Lewy (CFL) condition. This number is used to establish the relationship between temporal and spatial resolutions to ensure numerical stability in the system's solution. Once the CFL condition is satisfied, it is crucial to determine the spatial resolution to ensure the accuracy of the approximation.

Traditional approaches in the finite difference method include the centered

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difference and backward difference methods. Both are third-order approximations of the derivative of a function based on Taylor's polynomial expansion.

Let

$$\boldsymbol{\alpha}_i = \begin{pmatrix} \alpha_1^i \\ \alpha_2^i \\ \alpha_3^i \\ \alpha_4^i \\ \alpha_5^i \end{pmatrix},$$

a column vector of real coefficients, and

$$\mathbf{T}_i = \begin{pmatrix} T_{i-2}^4 \\ T_{i-1}^4 \\ T_i^4 \\ T_{i+1}^4 \\ T_{i+2}^4 \end{pmatrix},$$

a column vector, where each component represents the 4th-degree Taylor polynomial center at x_i and evaluated in x_j . The n -order derivative and the coefficient values for the five-point operator are obtained from the Taylor polynomial using the following relation:

$$\frac{\partial^n f(x_i)}{\partial x^n} = \boldsymbol{\alpha}_i^\top \mathbf{T}_i + R_i(\boldsymbol{\alpha}, \Delta x, f^{(5)}), \quad (1)$$

where the error in the approximation, using the Lagrange version of the remainder, is given by:

$$\left| \frac{\partial^n f(x_i)}{\partial x^n} - \boldsymbol{\alpha}_i^\top \mathbf{T}_i \right| = \left| R(\boldsymbol{\alpha}, \Delta x, f^{(5)}) \right| \leq \frac{|f^{(5)}(c)| (2\Delta x)^5}{5!} (|\alpha_1| + |\alpha_2| + |\alpha_4| + |\alpha_5|) \quad (2)$$

where $c \in [x_{i-2}, x_{i+2}]$ is a point within the interval of approximation. If ε is the desired error in the approximation, then the spatial step size Δx must satisfy:

$$\Delta x \leq \frac{1}{2} \sqrt[5]{\frac{120\varepsilon}{|f^{(5)}(c)| (|\alpha_1| + |\alpha_2| + |\alpha_4| + |\alpha_5|)}}.$$

Consequently, the associated system of equations is given by:

$$\mathbf{A}(\phi_i) \boldsymbol{\alpha} = \mathbf{f}^{(n)} \approx \frac{\partial^n f(x_i)}{\partial x^n} \quad (3)$$

where the system matrix, \mathbf{A} , depends on the stencil ϕ_i used for the approximation, which in turn depends on the node's position within the discretized domain. The vector $\mathbf{f}^{(n)}$ represents the n -th derivative to be approximated. The maximum order of the derivative that can be approximated is equal to the stencil size, as determined by the formulation of the system of equations using the Taylor polynomial expansion on the selected stencil.

In our work, we identified five fundamental stencils and the associated systems of equations.

1. $\phi_0 = [x_0, x_1, x_2, x_3, x_4]$ This corresponds to the node x_0 located at the left boundary.

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 4 & 9 & 16 \\ 0 & 1 & 8 & 27 & 64 \\ 0 & 1 & 16 & 81 & 256 \end{pmatrix} \boldsymbol{\alpha}_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{dx} & 0 & 0 & 0 \\ 0 & \frac{2!}{dx^2} & 0 & 0 \\ 0 & 0 & \frac{3!}{dx^3} & 0 \\ 0 & 0 & 0 & \frac{4!}{dx^4} \end{pmatrix} \quad (4)$$

2. $\phi_1 = [x_0, x_1, x_2, x_3, x_4]$ This corresponds to the node x_1 .

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & 2 & 3 \\ 1 & 0 & 1 & 4 & 9 \\ -1 & 0 & 1 & 8 & 27 \\ 1 & 0 & 1 & 16 & 81 \end{pmatrix} \boldsymbol{\alpha}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{dx} & 0 & 0 & 0 \\ 0 & \frac{2!}{dx^2} & 0 & 0 \\ 0 & 0 & \frac{3!}{dx^3} & 0 \\ 0 & 0 & 0 & \frac{4!}{dx^4} \end{pmatrix} \quad (5)$$

3. $\phi_i = [x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}]$ This corresponds to the node x_i , associated with all central nodes.

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \\ 4 & 1 & 0 & 1 & 4 \\ -8 & -1 & 0 & 1 & 8 \\ 16 & 1 & 0 & 1 & 16 \end{pmatrix} \boldsymbol{\alpha}_i = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{dx} & 0 & 0 & 0 \\ 0 & \frac{2!}{dx^2} & 0 & 0 \\ 0 & 0 & \frac{3!}{dx^3} & 0 \\ 0 & 0 & 0 & \frac{4!}{dx^4} \end{pmatrix} \quad (6)$$

4. $\phi_{N-1} = [x_{N-4}, x_{N-3}, x_{N-2}, x_{N-1}, x_N]$ This corresponds to the node x_{N-1} .

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -3 & -2 & -1 & 0 & 1 \\ 9 & 4 & 1 & 0 & 1 \\ -27 & -8 & -1 & 0 & 1 \\ 81 & 16 & 1 & 0 & 1 \end{pmatrix} \alpha_{N-1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{dx} & 0 & 0 & 0 \\ 0 & \frac{2!}{dx^2} & 0 & 0 \\ 0 & 0 & \frac{3!}{dx^3} & 0 \\ 0 & 0 & 0 & \frac{4!}{dx^4} \end{pmatrix} \quad (7)$$

5. $\phi_N = [x_{N-4}, x_{N-3}, x_{N-2}, x_{N-1}, x_N]$ This corresponds to the node x_N located at the right boundary.

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -4 & -3 & -2 & -1 & 0 \\ 16 & 9 & 4 & 1 & 0 \\ -64 & -27 & -8 & -1 & 0 \\ 256 & 81 & 16 & 1 & 0 \end{pmatrix} \alpha_N = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{dx} & 0 & 0 & 0 \\ 0 & \frac{2!}{dx^2} & 0 & 0 \\ 0 & 0 & \frac{3!}{dx^3} & 0 \\ 0 & 0 & 0 & \frac{4!}{dx^4} \end{pmatrix} \quad (8)$$

Each column of $\mathbf{f}^{(n)}$ corresponds to a different derivative order, from $n = 1$ to $n = 4$. The error shown in the equation (2), corresponds to the stencil ϕ_i . For the remaining stencils we have the following remainders.

$$\left| R_0(\alpha_0, \Delta x, f^{(5)}) \right| \leq \frac{|f^{(5)}(c)| (4\Delta x)^5}{5!} (|\alpha_1^0| + |\alpha_2^0| + |\alpha_3^0| + |\alpha_4^0|), \quad c \in [x_0, x_4] \quad (9)$$

$$\left| R_1(\alpha_1, \Delta x, f^{(5)}) \right| \leq \frac{|f^{(5)}(c)| (3\Delta x)^5}{5!} (|\alpha_0^1| + |\alpha_2^1| + |\alpha_3^1| + |\alpha_4^1|), \quad c \in [x_0, x_4] \quad (10)$$

$$\left| R_{N-1}(\alpha_{N-1}, \Delta x, f^{(5)}) \right| \leq \frac{|f^{(5)}(c)| (3\Delta x)^5}{5!} (|\alpha_0^{N-1}| + |\alpha_1^{N-1}| + |\alpha_2^{N-1}| + |\alpha_4^{N-1}|), \quad c \in [x_{N-4}, x_N] \quad (11)$$

$$\left| R_N(\alpha_N, \Delta x, f^{(5)}) \right| \leq \frac{|f^{(5)}(c)| (4\Delta x)^5}{5!} (|\alpha_0^N| + |\alpha_1^N| + |\alpha_2^N| + |\alpha_3^N|), \quad c \in [x_{N-4}, x_N] \quad (12)$$

and the relation with the spatial resolution given the desire error in the approx-

imation

$$\Delta x \leq \frac{1}{4} \sqrt[5]{\frac{120\varepsilon}{|f^{(5)}(c)| (|\alpha_1^0| + |\alpha_2^0| + |\alpha_3^0| + |\alpha_4^0|)}} \quad (13)$$

$$\Delta x \leq \frac{1}{3} \sqrt[5]{\frac{120\varepsilon}{|f^{(5)}(c)| (|\alpha_0^1| + |\alpha_2^1| + |\alpha_3^1| + |\alpha_4^1|)}} \quad (14)$$

$$\Delta x \leq \frac{1}{3} \sqrt[5]{\frac{120\varepsilon}{|f^{(5)}(c)| (|\alpha_0^{N-1}| + |\alpha_1^{N-1}| + |\alpha_2^{N-1}| + |\alpha_4^{N-1}|)}} \quad (15)$$

$$\Delta x \leq \frac{1}{4} \sqrt[5]{\frac{120\varepsilon}{|f^{(5)}(c)| (|\alpha_0^N| + |\alpha_1^N| + |\alpha_2^N| + |\alpha_3^N|)}} \quad (16)$$

The challenge in determining the accuracy of the approximation based on the spatial numerical resolution lies in the 5th-order derivative of the function. This challenge arises because, in most cases, the form of the 5th derivative, or even the function itself, is unknown.

2. Wave equation

We use the wave equation to describe the velocity field of waves traveling within each of these layers. With the wave equation as our physical governing model, we construct two wave prospection models to describe the scenario of a static material perturbed by an external force. These external forces are modeled as waves entering the structure at each boundary and traveling uninterrupted out of it. By "uninterrupted," we mean that no additional forces or perturbations are present in the system other than those provided by the boundaries and the elastic tension of the materials.

For high-contrast scenarios, we assume that each homogeneous subregion is perturbed by two waves traveling in opposite directions, and the entire structure is treated as the continuous union of these subregions. This setup allows for the exploration of interactions between areas with differing compositions. Such exploration is essential to determine the reflection and transmission of waves traveling through the medium, as well as their propagation and amplitude. Similar approaches were developed by [2, 3], where the region of interest was modeled as a composition of homogeneous layers.

For low-contrast scenarios, we consider a single region perturbed by a wave entering from one boundary, while the wave travels uninterrupted out of the area of interest through the other boundary. This setup allows for the investigation

of the behavior of traveling waves in a non-homogeneous region. In this case, careful consideration is required for the discrete approximation of the differential model. We adopted the *Displacement* formulation of the 1D wave equation [7], excluding the damping term for simplicity.

2.0.1. One-Dimensional Wave Equation in a Homogeneous Layer

For a high-contrast stratified structure, we model a static layer perturbed by an external source, where the resulting disturbance propagates without interruption and exits through open boundaries. The displacement-based formulation for this scenario is:

$$\begin{aligned}
\partial_t 2u_r - v^2 \partial_x 2u_r &= 0, & x \in (0, L), \quad t \in (0, T] \\
u_r(x, 0) &= 0, & x \in [0, L] \\
\partial_t u_r(x, 0) &= 0, & x \in [0, L] \\
u_r(0, t) &= F_l(t), & t > 0 \\
\partial_t u_r(L, t) &= -v \partial_x u_r(L, t), & t > 0
\end{aligned} \tag{17}$$

$$\begin{aligned}
\partial_t 2u_l - v^2 \partial_x 2u_l &= 0, & x \in (0, L), \quad t \in (0, T] \\
u_l(x, 0) &= 0, & x \in [0, L] \\
\partial_t u_l(x, 0) &= 0, & x \in [0, L] \\
\partial_t u_l(0, t) &= v \partial_x u_l(0, t), & t > 0 \\
u_l(L, t) &= F_r(t), & t > 0
\end{aligned} \tag{18}$$

The equations (17) and (18) describe the same static structure perturbed by external forces F_l and F_r . This system models two waves propagating in opposite directions within a homogeneous layer with absorbing boundaries. The first-order open boundary conditions, $\partial_t u_r(L, t) + c \partial_x u_r(L, t) = 0$ and $\partial_t u_l(0, t) - c \partial_x u_l(0, t) = 0$, are derived from the equations proposed in [1]. To model the wave behavior, we apply the superposition principle.

Wave Superposition Principle. The principle of superposition states that when two or more waves propagate simultaneously through the same layer, the resulting displacement is the algebraic sum of the individual wave displacements [4, section 16-5: Interference of waves].

If u_l and u_r are the only waves present in the layer bounded by $[0, L]$, the resulting wave is:

$$u(x, t) = u_r(x, t) + u_l(x, t) \tag{19}$$

2.0.2. One-Dimensional Wave Equation in Non-Homogeneous Layer

Our modeling scenario in this case is similar to the previous section, but now we consider a non-homogeneous layer. This means that the transverse velocity of the wave depends on space, which introduces modifications to the wave equation system. The system describing a wave perturbing a non-homogeneous static medium, with one open boundary and the other acting as a source, is given by:

$$\begin{aligned}
\partial_t^2 u - \partial_x (v^2(x) \partial_x u) &= 0, & x \in (0, L), \quad t \in (0, T] \\
u(x, 0) &= 0, & x \in [0, L] \\
\partial_t u(x, 0) &= 0, & x \in [0, L] \\
\partial_t u(0, t) &= F_l(t), & t > 0 \\
u(L, t) &= -c_L \partial_x u(0, t), & t > 0
\end{aligned} \tag{20}$$

The wave equation is a hyperbolic partial differential equation that is sensitive to jumps on the velocity field. Meaning that the numerical solution for this system needs to be treated carefully.

To solve the wave equation within the homogeneous layers, we transform the second-order partial differential systems (17) and (18) into a first-order system.

Let

$$\mathbf{w} = \begin{bmatrix} u \\ \partial_t u \end{bmatrix}. \tag{21}$$

Then the system is given by:

$$\partial_t \mathbf{w} = \begin{pmatrix} 0 & 1 \\ v^2 \mathbf{L}_5(\cdot) & 0 \end{pmatrix} \mathbf{w} + \mathbf{F}, \tag{22}$$

where \mathbf{L}_5 is the five-point second-order operator, and \mathbf{F} is the source term associated with each system.

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