Spectral Element Methods (SEM) in 3D

March 31, 2021

1 SEM implementations in 3D

1.1 3-D Wave Equations: Strong and Weak form

1.1.1 Strong form

Elastodynamics PDEs

$$\rho \partial_t^2 \mathbf{s} = \nabla \cdot \mathbf{T} + \mathbf{f} \quad \text{in } \Omega \tag{1}$$

where the stress is related to strain based on the linear constitutive relation

$$\mathbf{T} = \mathbf{C} : \epsilon = \mathbf{C} : \nabla \mathbf{s} \tag{2}$$

and the wavefield satisifies the free surface boundary condition

$$\hat{n} \cdot \mathbf{T} = 0 \quad \text{on } \partial\Omega \tag{3}$$

and initial condition

$$\mathbf{s}(\mathbf{x}, t = 0) = 0, \quad \dot{\mathbf{s}}(\mathbf{x}, t = 0) = 0. \tag{4}$$

1.1.2 Weak form (Variational form)

Multiply a global test function $W(\mathbf{x})$ to both sides and integrate over Ω to obtain the weak form:

$$\int_\Omega \rho W \ddot{s}_i \, dV = \int_\Sigma W \hat{n}_j T_{ji} \, d\Sigma - \int_\Omega \partial_j W T_{ji} \, d\Omega + \int_\Omega W f_i \, d\Omega \tag{5}$$

1.2 Meshing

The computational domain Ω is discretized into quadrangles in 2D, or hexahedra in 3D *(iteration index $ispec$)*, defined with respect to a reference unit domain (also called reference element), square in 2D and cube in 3D by an invertible local mapping.

Each standard element (cube in 3D) has GLL grid points in 3 directions (index α,β,γ). Globally number all grid points (index I) and establish the projection

$$(\alpha, \beta, \gamma;\ ispec) \longrightarrow (I) \tag{6}$$

Notice this projection is one-to-one for grid points inside any element (valence $= 0$), and multiple-to-one for grid points on the boundaries that are shared by elements (valence ≥ 1).

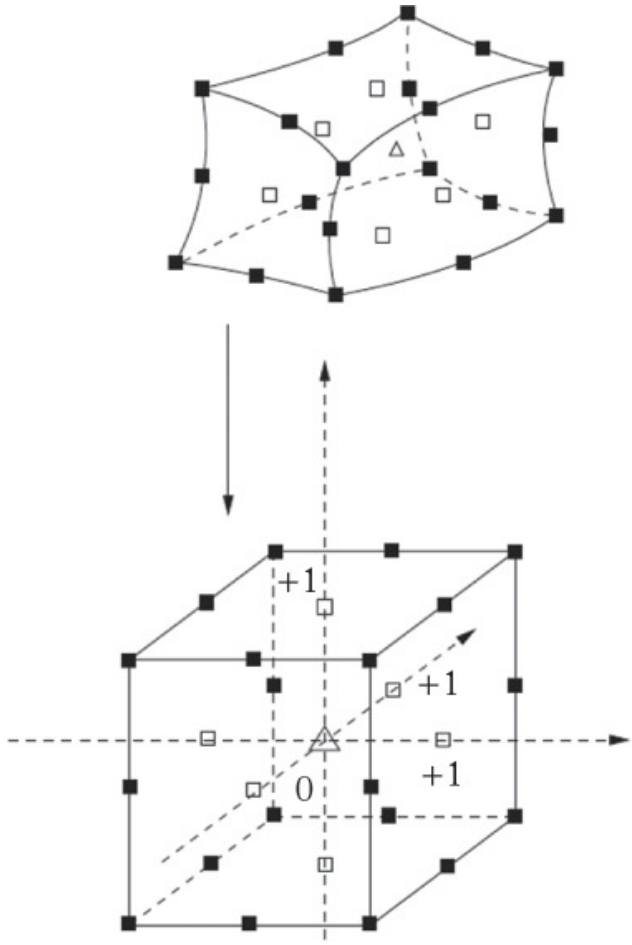

Figure 1: Shape functions in 3D

1.2.1 Interpolation of Shapes

For boundary and volumetric elements, we not only need to access location of grid points of the element, but also the location of any arbitrary point inside the element. We can interpolate the shape of the element by given 'anchors' $\mathbf{x}_a$.

1. For boundary element:

$$\mathbf{x}(\xi, \eta) = \sum_{a=1}^{N} N_a(\xi, \eta)\mathbf{x}_a \tag{7}$$

and the Jacobian matrix associated with this transformation

$$\mathbf{J}_b(\xi, \eta) = (\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}) \tag{8}$$

and the scalar Jacobian $J_b = \|\mathbf{J}_b\|$. The inverse transform is given by

$$(\frac{\partial \xi}{\partial \mathbf{x}} \times \frac{\partial \eta}{\partial \mathbf{x}}) = \mathbf{J}_b^{-1} \tag{9}$$

and the normal to the boundary is described by

$$\mathbf{n}(\xi, \eta) = \frac{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}}{\left|\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}\right|} \tag{10}$$

2. For volumetric element:

$$\mathbf{x}(\xi, \eta, \zeta) = \sum_{a=1}^{N} N_a(\xi, \eta, \zeta)\mathbf{x}_a \tag{11}$$

$$\mathbf{J}_a(\xi, \eta, \zeta) = (\frac{\partial \mathbf{x}(\xi, \eta, \zeta)}{\partial(\xi, \eta, \zeta)}) \tag{12}$$

$$J_a = \|\mathbf{J}_a\| \tag{13}$$

$$\frac{\partial(\xi, \eta, \zeta)}{\partial \mathbf{x}(\xi, \eta, \zeta)} = \mathbf{J}_a^{-1} \tag{14}$$

$N_a(\xi, \eta)$ and $N_a(\xi, \eta, \zeta)$ are the 2-D and 3-D shape functions. They are double or triple products of degree 1 or 2 Lagrangian polynomials. For example, degree 1 Lagrangian polynomials are $N_1(\xi) = \frac{1}{2}(1 + \xi)$ and $N_2(\xi) = \frac{1}{2}(1 - \xi)$ for given anchors at -1 and 1.

1.3 Interpolation of Function Field

Numerical integration is based on the tensor-product of a Gauss-Lobatto-Legendre (GLL) 1-D quadrature and the solution is expanded onto a discrete polynomial basis using Lagrange interpolants.

We interpolate function field on GLL points that satisfy:

$$(1 - \xi^2)\dot{P}_N(\xi) = 0 \tag{15}$$

and

$$\begin{aligned} f(\mathbf{x}(\xi, \eta))|_{\Sigma_e} &= \sum_{\alpha\beta} f^{\alpha\beta}\, l_\alpha(\xi) l_\beta(\eta) \\ f(\mathbf{x}(\xi, \eta, \zeta))|_{\Omega_e} &= \sum_{\alpha\beta\gamma} f^{\alpha\beta\gamma}\, l_\alpha(\xi) l_\beta(\eta) l_\gamma(\zeta) \end{aligned} \tag{16}$$

1.3.1 Derivatives

$$\partial_i f(\mathbf{x}(\xi,\eta,\zeta)) = \sum_{\alpha\beta\gamma} f^{\alpha\beta\gamma}\left[\dot{l}_\alpha(\xi)l_\beta(\eta)l_\gamma(\zeta)\frac{\partial\xi}{\partial x_i} + l_\alpha(\xi)\dot{l}_\beta(\eta)l_\gamma(\zeta)\frac{\partial\eta}{\partial x_i} + l_\alpha(\xi)l_\beta(\eta)\dot{l}_\gamma(\zeta)\frac{\partial\zeta}{\partial x_i}\right] \tag{17}$$

Notice $\frac{\partial\xi}{\partial x_i}$, $\frac{\partial\eta}{\partial x_i}$, $\frac{\partial\zeta}{\partial x_i}$ values can be calculated from the 2D and 3D shape functions. Specifically, to compute derivatives on GLL points:

$$\partial_i f|^{\alpha\beta\gamma} = \left[\sum_\sigma f^{\sigma\beta\gamma}\dot{l}_\sigma(\xi_\alpha)\right]\partial_i^{\alpha\beta\gamma}\xi + \left[\sum_\sigma f^{\alpha\sigma\gamma}\dot{l}_\sigma(\eta_\beta)\right]\partial_i\eta^{\alpha\beta\gamma} + \left[\sum_\sigma f^{\alpha\beta\sigma}\dot{l}_\sigma(\zeta_\gamma)\right]\partial_i\zeta^{\alpha\beta\gamma} \tag{18}$$

1.3.2 Integration

Integration quadrature

$$\int_{\Sigma_e} f(\mathbf{x})\,d\mathbf{x} = \sum_{\alpha\beta}\omega_\alpha\omega_\beta f^{\alpha\beta}J_b^{\alpha\beta} \tag{19}$$

$$\int_{\Omega_e} f(\mathbf{x})\,d\mathbf{x} = \sum_{\alpha\beta\gamma}\omega_\alpha\omega_\beta\omega_\gamma f^{\alpha\beta\gamma}J_a^{\alpha\beta\gamma} \tag{20}$$

1.4 Global Test Functions

Define global test functions $W^I(\mathbf{x})$, such that

$$W^I(\mathbf{x})|_{\Omega_e} = \begin{cases} l_\alpha(\xi)l_\beta(\eta)l_\gamma(\zeta) & \text{if } I\in\Omega_e\text{, and } I|_{\Omega_e} = (\alpha,\beta,\gamma) \\ 0 & \text{if } I\notin\Omega_e \end{cases} \tag{21}$$

If $I|_{\Omega_e} = (\alpha,\beta,\gamma)$ has zero valence, then $W^I(\mathbf{x})$ is simply a 3-D local Lagrangian function extended to the whole space; otherwise it consists several pieces (valence$+1$) of local lagrangian function (edge ones). Therefore, for integration, one needs to loop over spectral elements, then all the GLL points, and adds contributions to the corresponding global grid point.
Notice

$$W^I|_{\Omega_e}(\alpha',\beta',\zeta') = \delta_{\alpha\alpha'}\delta_{\beta\beta'}\delta_{\zeta\zeta'} \tag{22}$$

this simplifies the integration results.

1.5 Application to the Wave Equation

1.5.1 LHS

$$\int_\Omega \rho W^I \, \ddot{s}_i(t) \, d\mathbf{x} = \sum_e \int_{\Omega_e} \rho W^I|_{\Omega_e} \, \ddot{s}_i(t) \, d\mathbf{x} \tag{23}$$

$$= \sum_e \sum_{\alpha'\beta'\gamma'} \omega_{\alpha'}\omega_{\beta'}\omega_{\gamma'}\rho^{\alpha'\beta'\gamma'} J^{\alpha'\beta'\gamma'} \ddot{s}_i^{\alpha'\beta'\gamma'} \delta_{\alpha\alpha'}\delta_{\beta\beta'}\delta_{\zeta\zeta'} \tag{24}$$

$$= \sum_e \omega_\alpha\omega_\beta\omega_\gamma\rho^{\alpha\beta\gamma} J^{\alpha\beta\gamma} \ddot{s}_i^{\alpha\beta\gamma}(t) \tag{25}$$

1.5.2 Spatial Derivatives

For example,

$$\begin{aligned}
\partial_i s_j(\mathbf{x})|_{\Omega_e}^{\alpha\beta\gamma} &= \partial_i \left[\sum_{\alpha'\beta'\gamma'} s_j^{\alpha'\beta'\gamma'} l_{\alpha'}(\xi) l_{\beta'}(\eta) l_{\gamma'}(\zeta) \right] |_{\Omega_e}^{\alpha\beta\gamma} \\
&= [\sum_\sigma s_j^{\sigma\beta\gamma} \dot{l}_\sigma(\xi_\alpha)] \partial_i \xi(\xi_\alpha, \eta_\beta, \zeta_\gamma) \\
&+ [\sum_\sigma s_j^{\alpha\sigma\gamma} \dot{l}_\sigma(\eta_\beta)] \partial_i \eta(\xi_\alpha, \eta_\beta, \zeta_\gamma) \\
&+ [\sum_\sigma s_j^{\alpha\beta\sigma} \dot{l}_\sigma(\zeta_\gamma)] \partial_i \zeta(\xi_\alpha, \eta_\beta, \zeta_\gamma)
\end{aligned} \tag{26}$$

in the SEM code, $hprime(\alpha, \sigma) = \dot{l}_\sigma(\xi_\alpha)$. The stress tensor is given by:

$$T_{kl} = C_{klij}\partial_i s_j - R_{kl} \tag{27}$$

For isotropic and no pre-stress case,

$$T_{kl} = (\kappa - \frac{2}{3}\mu)\delta_{kl}\epsilon_{ii} + \mu(\epsilon_{kl} + \epsilon_{lk}) \tag{28}$$

1.5.3 Boundary terms

$$\begin{aligned}
\int_\Sigma W^I \hat{n}_j T_{ji} \, d\Sigma &= \sum_e \int_{\Sigma_e} W^I t_i \, d\Sigma_e \\
&= \sum_e \omega_\alpha\omega_\beta t_i^{\alpha\beta} J^{\alpha\beta}
\end{aligned} \tag{29}$$

Where Ith global grid point is on Σ_e elements, with local GLL index (α, β). Obviously, this term does not need to be computed for free surface boundary where the normal stress t_i vanishes. The normal stress is also continuous for any solid-solid internal boundaries. For fluid-solid coupling

problems, we may solve both side as independent domains, and the interchange of two fields will occur through this boundary condition. For regional problems, other boundaries are 'absorbing', where

$$\mathbf{t} = \hat{n} \cdot \mathbf{T} = -[\rho\alpha(\mathbf{v} \cdot \hat{n})\hat{n} + \rho\beta(\mathbf{v} - v_n\hat{n})], \quad t_i = -[\rho\alpha(\hat{n}_j\dot{s}_j)\hat{n}_i + \rho\beta(\delta_{ij} - \hat{n}_i\hat{n}_j)\dot{s}_j] \tag{30}$$

Note the $-$ sign seems to be missing from all Dimitri's papers. Clearly the $-$ sign should be there due to the paraxial approximation $u_t + \alpha\, u_z = 0$, which gurantees that the waves propagates in the positive z direction $u = u(t - z/\alpha)$. The traction boundary condition is a natural type of boundary condition for FEM type of methods. This is also known as *Neumann BC*.

Sometimes the boundary conditions may be given in terms of displacement (i.e. *Dirichlet BC*)

$$s(x,t)\big|_{\Sigma} = g(x,t) \tag{31}$$

Much less often seen is the *Robin BC*:

$$as(x,t) + b\frac{\partial s}{\partial n} = g \tag{32}$$

The initial condition is given as *Cauchy data*

$$s(x, t = 0) = a(x), \quad \dot{s}(x, t = 0) = b(x) \tag{33}$$

1.5.4 Volumetric integral terms

$$\begin{aligned}
\int_{\Omega} \partial_j W^I T_{ji}\, d\Omega &= \sum_e \int_{\Omega_e} \partial_j W^I|_{\Omega_e} T_{ji}\, d\Omega_e \\
&= \sum_e \int_{\Omega_e} [\dot{l}_\alpha \partial_j \xi l_\beta l_\gamma + l_\alpha \dot{l}_\beta \partial_j \eta l_\gamma + l_\alpha l_\beta \dot{l}_\gamma \partial_j \zeta] T_{ji}\, d\mathbf{x} \\
&= \sum_e \Bigg\{ \left[\sum_\sigma \omega_\sigma \dot{l}_\alpha(\xi_\sigma) \partial_j \xi(\xi_\sigma, \eta_\beta, \zeta_\gamma) T_{ji}^{\sigma\beta\gamma} J^{\sigma\beta\gamma} \right] \omega_\beta \omega_\gamma \\
&+ \left[\sum_\sigma \omega_\sigma \dot{l}_\beta(\eta_\sigma) \partial_j \eta(\xi_\alpha, \eta_\sigma, \zeta_\gamma) T_{ji}^{\alpha\sigma\gamma} J^{\alpha\sigma\gamma} \right] \omega_\alpha \omega_\gamma \\
&+ \left[\sum_\sigma \omega_\sigma \dot{l}_\gamma(\zeta_\sigma) \partial_j \zeta(\xi_\alpha, \eta_\beta, \zeta_\sigma) T_{ji}^{\alpha\beta\sigma} J^{\alpha\beta\sigma} \right] \omega_\alpha \omega_\beta \Bigg\}
\end{aligned} \tag{34}$$

in the SEM code, sums over σ are named as $temp[x|y|z][1|2|3]$.

1.5.5 Forcing terms

The forcing term for a point force

$$f_i(\mathbf{x}, t) = f_i g(t)\delta(\mathbf{x} - \mathbf{x}_0) \tag{35}$$

and for a distributed moment tensor source (i.e., related to faulting)

$$f(\mathbf{x}, t) = -\nabla m(\mathbf{x}, t), \tag{36}$$

and for a point moment tensor it is reduced to

$$m(\mathbf{x}, t) = M_0\delta(\mathbf{x} - \mathbf{x}_0)g(t), \quad f(\mathbf{x}, t) = -M_0 g(t)\nabla\delta(\mathbf{x} - \mathbf{x}_0) \tag{37}$$

where $g(t)$ is the rise time function, and $\dot{g}(t)$ is the source time function for this moment tensor source.

1. For point force $f_i(\mathbf{x}, t) = f_i(t)\delta(\mathbf{x} - \mathbf{x}_0)$,

$$\begin{aligned}\int_\Omega W^I f_i \, d\Omega &= W^I(\mathbf{x}_0) f_i(t) \\ &= \begin{cases} f_i(t) & \text{if } \mathbf{x}_0 \to I \\ 0 & \text{if } \mathbf{x}_0 \to \text{other grid point} \\ l_\alpha(\xi(\mathbf{x}_0)) l_\beta(\xi(\mathbf{x}_0)) l_\gamma(\xi(\mathbf{x}_0)) f_i(t) & \text{else } \mathbf{x}_0 \in \Omega_e \end{cases}\end{aligned} \tag{38}$$

   if $\mathbf{x}_0$ has local parameter $\{ispec; \xi, \eta, \zeta\}$, then compute the Lagrange polynomial at the source location.

2. For Moment tensor point force $f_i(\mathbf{x}, t) = -M_{ij}\partial_j\delta(\mathbf{x} - \mathbf{x}_0)g(t)$,

$$\int_\Omega W^I f_i \, d\Omega = M_{ij}\partial_j W^I(\mathbf{x}_0) g(t) \tag{39}$$

   Since $\partial_j W = \frac{\partial W}{\partial \xi_k}\frac{\partial \xi_k}{\partial x_j}$ and define $G_{ik}(\xi, \eta, \zeta) = M_{ij}\frac{\partial \xi_k}{\partial x_j}$,

$$\begin{aligned} M_{ij}\partial_j W^I(\mathbf{x}_0) &= G_{ik}\frac{\partial W}{\partial \xi_k}(\xi_0) \\ &= \sum_{r,t,v} l_r(\xi_0) l_t(\eta_0) l_v(\zeta_0) G_{ik}(\xi_r, \eta_t, \zeta_v)\partial_{\xi_k}(l_\alpha(\xi_r) l_\beta(\eta_t) l_\gamma(\zeta_v)) \\ &= \sum_{r,t,v} l_r(\xi_0) l_t(\eta_0) l_v(\zeta_0) \left[G_{i1}(\xi_r, \eta_t, \zeta_v) l'_\alpha(\xi_r) l_\beta(\eta_t) l_\gamma(\zeta_v)) + \cdots\right] \end{aligned} \tag{40}$$

3. For body force field $f_i(\mathbf{x}, t)$,

$$\int_\Omega W^I f_i \, d\Omega = \sum_e \int_{\Omega_e} W^I|_{\Omega_e} F_i \, d\Omega_e$$
$$= \sum_e \omega_\alpha \omega_\beta \omega_\gamma F_i^{\alpha\beta\gamma}(t) J^{\alpha\beta\gamma} \tag{41}$$

4. For surface force field $f_i(\mathbf{x}, t) = \int_{\Sigma_0} \tau_i(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{x}_0) d\Sigma_0$, (monopoles on Σ_0)

$$\int_\Omega W^I f_i \, d\Omega = \int_\Omega W^I(\mathbf{x}) \left[\int_{\Sigma_0} \tau_i(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{x}_0) d\Sigma_0 \right] d\Omega \tag{42}$$
$$= \int_{\Sigma_0} \tau_i(\mathbf{x}_0, t) W^I(\mathbf{x}_0) \, d\Sigma_0 \tag{43}$$

to compute this in practice, loop over surface elements, and then for each surface GLL point $I = (\alpha, \beta)$,

$$\text{Contr. to I'th test function} + = \omega_\alpha \omega_\beta \tau_{\alpha\beta} J^{\alpha\beta} \tag{44}$$

5. For surface double couple force field $f_p(\mathbf{x}, t) = -\int_{\Sigma_0} u_i(\mathbf{x}, t) n_j C_{ijpq} \partial_q \delta(\mathbf{x} - \mathbf{x}_0) \, d\Sigma_0$, assume that Σ_0 do not overlap with the surface Σ that encompasses Ω, then

$$\int_\Omega W^I f_p \, d\Omega = -\int_\Omega W^I(\mathbf{x}) \left[\int_{\Sigma_0} u_i(\mathbf{x}, t) n_j C_{ijpq} \partial_q \delta \, d\Sigma_0 \right] d\Omega$$
$$= -\int_{\Sigma_0} \left[\int_\Omega W^I(\mathbf{x}) u_i(\mathbf{x}, t) n_j C_{ijpq} \partial_q \delta(\mathbf{x} - \mathbf{x}_0) \, d\Omega \right] \int_\Omega W^I(\mathbf{x})$$
$$= \int_{\Sigma_0} \partial_q \left(u_i(t) n_j C_{ijpq} W^I \right) (\mathbf{x}_0) \, d\Sigma_0 \tag{45}$$

We define the corresponding moment density tensor $m_{pq}(t) = u_i(t) n_j C_{ijpq}$ on Σ_0. In the case of a fault in an isotropic medium where $\mathbf{u}$ is perpendicular to $\mathbf{n}$, $m_{pq} = \mu(u_p n_q + u_q n_p)$ is the standard moment density tensor that describes a seismic source. Now rewrite the above expression:

$$\int_\Omega W^I f_i \, d\Omega = \int_{\Sigma_0} \left[\partial_q m_{pq}(t) W^I + m_{pq(t)} \partial_q W^I \right] d\Sigma_0 \tag{46}$$

In practice, we store $f_p(t) = \partial_q m_{pq}$ and $m_{pq}(t)$ in advance for each grid point of the surface Σ_0, then the above two terms can be calculated with ease in runtime.

1.5.6 Assembling

$$\mathbf{M} \, \ddot{s}(t) = \mathbf{B} + \mathbf{T} + \mathbf{F}(t) \tag{47}$$

We can update the acceleration at time t by

$$\ddot{s}(t) = (\mathbf{M})^{-1}(\mathbf{B} + \mathbf{T} + \mathbf{F}(t)) \tag{48}$$

Notice that $\mathbf{M}$ is diagonal ($I \times I$), $\mathbf{B}, \mathbf{T}, \mathbf{F}, \ddot{s}(t)$ are all vectors ($I \times 1$). Try loop over $ispec$ and then (α, β, γ) to assemble the contribution of each grid point (in an element) into global matrices. This is true for all matrices, except the forcing term in which the contribution is added by looping over only elements that contain the forces and related GLL points.

1.6 Time Marching Schemes

Time marching based on explicit-implicit predictor-multicorrector format as in Newmark scheme
Predictor:

$$\begin{aligned} d^{n+1} &= d^n + v^n \Delta t + \frac{1}{2} a^n (\Delta t)^2 \\ v^{n+1} &= v^n + \frac{1}{2} a^n \Delta t \\ a^{n+1} &= 0 \end{aligned} \tag{49}$$

Corrector:

$$\begin{aligned} a^{n+1} &= (\mathbf{M})^{-1} (\mathbf{B} + \mathbf{T} + \mathbf{F}^{n+1}) \\ v^{n+1} &= v^{n+1} + \frac{1}{2} a^{n+1} \Delta t \\ d^{n+1} &= d^{n+1} \end{aligned} \tag{50}$$

1.7 Advantages and Disadvantages

Advantages: diagnoal mass matrix (δ operator), exponential convergence of spectral methods, accurate and fast.

Disadvantages: use hexhedral mesh, difficult to adapt to arbitrary interfaces. Currently a predictor-corrector Newmark scheme is used, after 40 minutes, dispersion may appear due to the inaccurate timing marching. A Runge-Kutta method may be more natural, requiring the storage of snapshots from 3-4 previous steps.

Another huge hinderance that makes it slow (or in other words cancels the benefit of the diagnonal matrix) is that fact that too many grid points requires too much storage to form the explicit stiffness matrix, therefore evaluation of stress is done in every step instead of a simple matrix-vector multiplication.