Spectral Element Method applied to 1D wave equation

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December 27, 2020

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1 Setup

Consider the 1D wave equation, written in terms of the displacement field $u(z,t)$:

$$\rho(z)\,\frac{\partial^2 u}{\partial t^2}(z,t) \;-\; \frac{\partial}{\partial z}\left[\mu(z)\,\frac{\partial u}{\partial z}(z,t)\right] \;=\; f(z,t)\;, \tag{1}$$

with ρ the mass density, μ the shear modulus, and f the source term. The computational domain (referred to as Ω) is a 1D soil column: $\Omega = [0, -H]$, and time t goes from 0 to T. We assume that the surface is free, i.e. that the traction vector $\tau(z,t) = \mu(z)\,\frac{\partial u}{\partial z}(z,t)$ vanishes for $z = 0$ and for all times. At the bottom boundary, we assume that an absorbing condition holds:

$$\tau(z = -H, t) \;=\; \tau_{\text{abs}}(z = -H, t)\;. \tag{2}$$

We want to build an approximation $\tilde{u}$ to the solution of the wave equation on a grid of points $\{z_j\}$ for all discrete times t_n: $\tilde{u}(z_j, t_n) \simeq u(z_j, t_n)$. The way the grid of points $\{z_j\}$ is defined is not as straightforward as for example in the Finite Difference method, because the SEM (like the FEM) does not work directly on the wave equation (1), but on its weak form. The weak form (also referred to as the variational formulation) is obtained by dotting the wave equation with an arbitrary displacement field, w, then integrating over the computational domain Ω:

$$\int_\Omega \left(\rho(z)\,\frac{\partial^2 u}{\partial t^2}(z,t) \;-\; \frac{\partial}{\partial z}\left[\mu(z)\,\frac{\partial u}{\partial z}(z,t)\right] \;-\; f(z,t)\right) w(z)\;dz \;=\; 0\;. \tag{3}$$

This last equation has to hold for all admissible displacement fields w[1]. By admissible we mean in particular that the displacement field must be continuous[2] throughout the domain. Now, in eq. (3) we integrate by parts the term that contains a second derivative in space. We obtain:

$$\begin{aligned}\int_\Omega \rho(z)\,\frac{\partial^2 u}{\partial t^2}(z,t)\,w(z)\;dz \;&+\; \int_\Omega \mu(z)\,\frac{\partial u}{\partial z}(z,t)\,\frac{\partial w}{\partial z}(z)\;dz \\ &-\; \int_{\partial\Omega} \mu(z)\,\frac{\partial u}{\partial z}(z,t)\,w(z)\;dz \;=\; \int_\Omega f(z,t)\,w(z)\;dz\;.\end{aligned} \tag{4}$$

In eq. (4), the term on the boundary $\partial\Omega$ involves the traction vector $\tau(z,t)$:

$$\int_{\partial\Omega} \mu(z)\,\frac{\partial u}{\partial z}(z,t)\,w(z)\;dz \;=\; \tau(0,t)\,w(0) - \tau(-H,t)\,w(-H)\;. \tag{5}$$

We come to an important point of the SEM (which also applies to the FEM): in order to impose the free-surface condition, we simply cancel the surface traction term in eq. (5). The free surface condition is said to be a natural boundary condition in the FEM framework. We also replace the traction at the bottom boundary using the absorbing condition (2). We are thus left with the following weak form of the wave equation: Find $u(z,t)$ such that for any admissible displacement field $w(z)$:

$$\begin{aligned}\int_\Omega \rho(z)\,\frac{\partial^2 u}{\partial t^2}(z,t)\,w(z)\;dz \;&+\; \int_\Omega \mu(z)\,\frac{\partial u}{\partial z}(z,t)\,\frac{\partial w}{\partial z}(z)\;dz \\ &+\; \tau_{\text{abs}}(-H,t)\,w(-H) \;=\; \int_\Omega f(z,t)\,w(z)\;dz\;.\end{aligned} \tag{6}$$

[1] Mathematically, w belongs to the Sobolev space $H^1(\Omega)$.

[2] Continuity is understood in the weak sense, see the properties of the Sobolev $H^1(\Omega)$ space.

It is the weak form of the wave equation that we are now going to approximate. Before to proceed, let us recall that we are only working on the space domain here. The time approximation will be handled by a classical FD method as we will see later.

2 Spectral Element Discretization

There are three steps to build the Spectral Element approximation of the weak form (6):

1. Split the computational domain Ω into elements.
2. Define a polynomial basis on each element to approximate the elastic parameters and the solution of the wave equation.
3. Define a numerical rule to compute the integrals present in the weak form of the wave equation.

We are now going to detail these three steps.

2.1 Mesh generation

The mesh process is sometimes referred to in the finite element literature as the triangulation phase. We write this formally as:

$$\Omega = \bigcup_{e=1}^{E} \Omega_e \,, \tag{7}$$

where the Ω_e are the elements and Ω is the computational domain. In the classical SEM, the elements are restricted to quadrangles in 2D and hexahedra in 3D.

In 1D, the mesh generation consists in paving $\Omega = [0, -H]$ with contiguous, non-overlapping segments (the elements) $\Omega_e = [a_e, b_e]$. Each element is obtained from the reference element $\hat{\Omega} = [-1, 1]$ through a mapping, which we assume linear[3]:

$$z \;=\; \mathcal{F}_e(\xi) \;=\; \alpha_e\, \xi + \beta_e \,, \tag{8}$$

where ξ is the working coordinate on $\hat{\Omega}$ and

$$\left\{ \begin{array}{rcl} \alpha_e &=& (b_e - a_e)/2 \,, \\ \beta_e &=& (b_e + a_e)/2 \,. \end{array} \right. \tag{9}$$

2.2 Change of variables

Now that a mesh has been defined for our problem, we can split the weak form of the wave equation (6) onto the elements of the mesh using the linearity of the integral:

$$\begin{aligned} \sum_{e=1}^{E} \int_{\Omega_e} \rho(z)\, \frac{\partial^2 u}{\partial t^2}(z,t)\, w(z)\; dz \;\; &+ \;\; \sum_{e=1}^{E} \int_{\Omega_e} \mu(z)\, \frac{\partial u}{\partial z}(z,t)\, \frac{\partial w}{\partial z}(z)\; dz \\ &+ \;\; \tau_{\text{abs}}(-H,t)\, w(-H) \;\; = \;\; \sum_{e=1}^{E} \int_{\Omega_e} f(z,t)\, w(z)\; dz \;. \end{aligned} \tag{10}$$

[3] Any regular, invertible mapping could be used in theory, but in practice FEM mapping consist of polynomials of order 1 (linear) or 2 (quadratic).

In every integral over Ω_e, we get back to the reference domain ($\hat{\Omega} = [-1, 1]$) by the change of variable: $z = \mathcal{F}^e(\xi)$.

For example, we get for the source term:

$$\int_{\Omega_e} f(z,t)\, w(z)\; dz \;=\; \int_{-1}^{1} f\big(\mathcal{F}^e(\xi), t\big)\, w\big(\mathcal{F}^e(\xi)\big)\, \mathcal{J}^e(\xi)\, d\xi \;, \tag{11}$$

where $\mathcal{J}^e$ is the so-called Jacobian of the mapping. $\mathcal{J}^e$ is the determinant of the Jacobian matrix $(\partial z/\partial \xi) = (\partial \mathcal{F}^e/\partial \xi)$. The Jacobian tells you how the length (resp. area in 2D or volume in 3D) of an element is changed by the mapping $\mathcal{F}^e$. In our simple 1D example, suppose that the length of element Ω_e is l_e. Then the Jacobian is $\alpha_e = l_e/2$ (because the length of the reference element $[-1, 1]$ is 2).

After this change of variables, all the integrals are formulated on the reference element. Now we need to say a word about the way we compute the integrals on the reference element.

2.3 Numerical Integration

All the integrals that we have to compute are of the form:

$$\int_{\hat{\Omega}} q(\xi)\, d\xi \;, \tag{12}$$

where $\hat{\Omega} = [-1, 1]$ is the reference interval and q is a scalar quantity.

A numerical integration rule is a formula like:

$$\int_{\hat{\Omega}} q(\xi)\, d\xi \;\simeq\; \sum_{i=0}^{N} \omega_i\, q(\xi_i) \;, \tag{13}$$

where the $N + 1$ points ξ_i are called the integration points and the $N + 1$ scalars ω_i are called the integration weights.

This kind of formula is in general not exact, but when q is a polynomial it is easy to find exact formulas. For example if q is a polynomial of order N, then any set of $N + 1$ distinct points provides an exact integration formula.

In the Legendre SEM, we use the Gauss-Lobatto-Legendre (GLL) integration rule [4]. When based upon $N + 1$ integration points, it provides a formula which is exact for polynomials of order up to $2N - 1$. The GLL points are defined as follows:

$$i = 0: \quad \xi_0 = -1 \tag{14}$$

$$i = 1 \ldots N-1: \quad L'_N(\xi_i) = 0, \text{where } L_N \text{ is the Legendre polynomial of order } N \tag{15}$$

$$i = N: \quad \xi_N = 1 \tag{16}$$

They are represented on fig. 1 for different polynomial orders. Note that the extremities of the reference segment (i.e. -1 and 1) are always part of the GLL points. Note also the clustering of the points near the edges as the polynomial order increases. It can be shown that the spacing between the points behaves like $1/N$ in the middle of the reference element, and like $1/N^2$ near the edges.

[4] The Chebychev SEM is based on the Gauss-Lobatto-Chebychev integration formula.

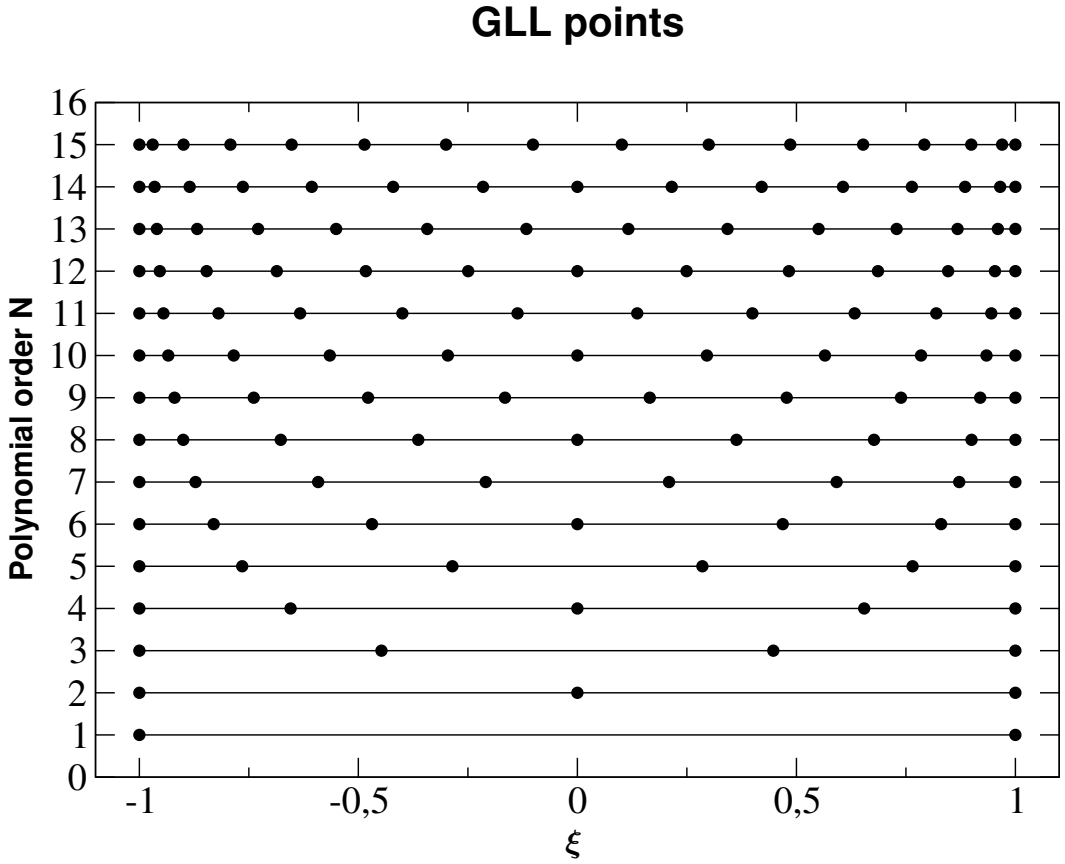

Figure 1: Gauss-Lobatto-Legendre integration points on $\hat{\Omega} = [-1, 1]$ as a function of the polynomial order N.

2.4 Polynomial approximation

Now that we know how to integrate, we still need to define the polynomial approximation of the elastic parameters and of the unknowns.

In the Legendre SEM, the GLL integration points are also used to define a polynomial basis on the reference element [5]. Let $(\xi_i)_{i=0,N}$ be the $N+1$ GLL integration points, we define their Lagrange interpolants as the $N+1$ polynomials h_j of degree N such that:

$$h_j(\xi_i) \;=\; \delta_{ij} \;=\; \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases} \tag{17}$$

The Lagrange interpolants h_j can be defined as follows:

$$h_j(\xi) \;=\; \frac{(\xi - \xi_0) \ldots (\xi - \xi_{j-1}) \, (\xi - \xi_{j+1}) \ldots (\xi - \xi_N)}{(\xi_j - \xi_0) \ldots (\xi_j - \xi_{j-1}) \, (\xi_j - \xi_{j+1}) \ldots (\xi_j - \xi_N)} \tag{18}$$

They are represented for $N = 4$ on fig. 2.

[5] The Chebychev SEM is based on Chebychev polynomials on the reference element (see e.g. Seriani & Priolo, 1994).

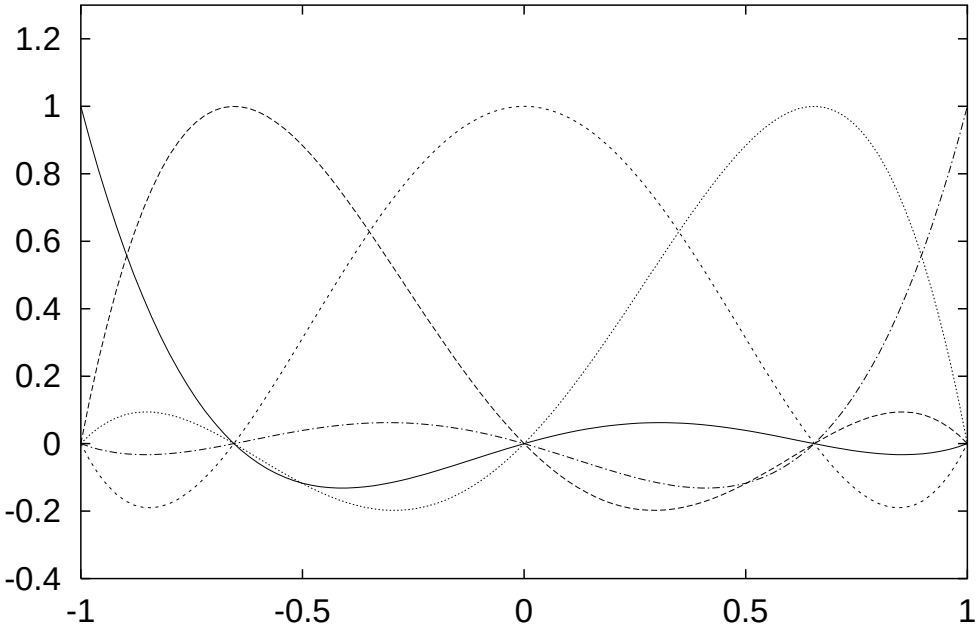

Figure 2: The five Lagrange interpolants of degree $N = 4$ on the reference interval $\hat{\Omega} = [-1, 1]$. The corresponding Gauss-Lobatto-Legendre points appear along the horizontal axis where the Lagrange polynomials vanish.

It is easy to use the Lagrange interpolants of the GLL points to define a polynomial basis on the reference element. Let indeed q be a polynomial of degree N on $\hat{\Omega}$, q can be expanded on the basis as:

$$q(\xi) \;=\; \sum_{i=0}^{N} q(\xi_i)\, h_i(\xi) \;. \tag{19}$$

You see that the expansion coefficients are the values of q at the GLL points.

Next, we use the basis of Lagrange interpolants and the mapping $\mathcal{F}_e$ to approximate any quantity on the computational domain; for example the solution of the wave equation at any $z \in \Omega_e$ is approximated by:

$$u(z,t) = u\big(\mathcal{F}^e(\xi), t\big) \;\simeq\; \sum_{i=0}^{N} u\big(\mathcal{F}^e(\xi_i), t\big)\, h_i(\xi) \;. \tag{20}$$

You see that the unknowns in the r.h.s. of eq. (20) are the values of u at the points $z_i^e = \mathcal{F}^e(\xi_i)$. These particular points are obtained by transporting the GLL integration points from the reference element $\hat{\Omega}$ to the elements of the mesh Ω_e. These points are sometimes referred to as the collocation points in the spectral element litterature. The set of all the points

$$\{z_i^e;\; e = 1 \ldots E,\; i = 0 \ldots N\}$$

forms the grid of SEM points. Note that the elements endpoints appear twice, which allows to define discontinuous quantities. This is a helpful property to define the parameters of the propagation medium (velocities, densities) but not the dynamic quantities, such as the displacement, which have to be continuous.

2.5 Algebraic system

Let us now go back to the weak form of the wave equation. Remember that it must be valid for all admissible displacements. Since a displacement field is entirely known at the discrete level by its values at the collocation points, we will use the Lagrange interpolants (or shape functions) of the collocation points to define the basis of displacements.

Remember that the displacements of the basis must be continuous. To build a continuous basis, we need first to count the degrees of freedom (dof) in our grid of points: There are E elements with $N+1$ collocation points in each element. The total number of gridpoints is thus $E \times (N+1)$, but because of the choice of the GLL points we see that the points which belong to two elements are counted twice. The total number of degrees of freedom $\mathcal{N}$ is thus only $(E \times N + 1)$. The basis of admissible displacements is of size $\mathcal{N}$ because there can be only one value at the points pertaining to several elements for the sake of continuity.

Let α be one of the dof in $[1, \mathcal{N}]$. The correspondence between global numbering and local numbering can be written formally as $\alpha = \texttt{num}(e, i)$. Suppose that α is an interior point, i.e. such that $0 < i < N$. Using the one-to-one correspondence between α and (e, i) and the mapping between $\hat{\Omega}$ and Ω_e, we define the basis function w_α on Ω_e as:

$$w_\alpha(z) \;=\; w_\alpha\big(\mathcal{F}^e(\xi)\big) \;=\; h_i(\xi) \;,$$

where h_i is the Lagrange interpolant of the i-th GLL point on $\hat{\Omega}$. Outside of Ω_e, we extend w_α by zero. The resulting function is globally continuous on Ω.

Now, if α belongs to elements e and $e+1$ (i.e. $\alpha = \texttt{num}(e, N) = \texttt{num}(e+1, 0)$), then w_α is defined on Ω_e by:

$$w_\alpha(z) \;=\; w_\alpha\big(\mathcal{F}^e(\xi)\big) \;=\; h_N(\xi) \;,$$

and on Ω_{e+1} by:

$$w_\alpha(z) \;=\; w_\alpha\big(\mathcal{F}^{e+1}(\xi)\big) \;=\; h_0(\xi) \;.$$

And again, we extend w_α by zero outside Ω_e and Ω_{e+1}. By this process, we are sure that our basis will only generate continuous displacements.

The solution of the wave equation is thus expanded as:

$$u(z) \;=\; \sum_{\beta=1}^{\mathcal{N}} u(z_\beta)\, w_\beta(z) \;, \tag{21}$$

where the unknowns $u(z_\beta)$ are the values of the displacement at the collocation points.

Next, we write the weak form of the wave equation (6) for the particular basis function w_α and inject the expansion of the solution (21). We get:

$$\begin{aligned} \sum_{\beta=1}^{\mathcal{N}} \frac{\partial^2 u}{\partial t^2}(z_\beta, t) \int_\Omega \rho(z)\, w_\beta(z)\, w_\alpha(z)\; dz \;&+\; \sum_{\beta=1}^{\mathcal{N}} u(z_\beta, t) \int_\Omega \mu(z)\, \frac{\partial w_\beta}{\partial z}(z)\, \frac{\partial w_\alpha}{\partial z}(z)\; dz \\ &+\; \tau_{\text{abs}}(-H, t)\, w_\alpha(-H) \\ &=\; \int_\Omega f(z_\beta, t)\, w_\alpha(z)\; dz \;, \end{aligned} \tag{22}$$

which we rewrite:

$$\sum_{\beta=1}^{\mathcal{N}} M_{\alpha\beta}\, \ddot{u}(z_\beta, t) \;+\; \sum_{\beta=1}^{\mathcal{N}} K_{\alpha\beta}\, u(z_\beta, t) \;+\; \big[\mathbf{T}_{\text{abs}}\big]_\alpha(t) \;=\; [\mathbf{F}]_\alpha(t) \;, \tag{23}$$

where $[\mathbf{V}]_\alpha$ denotes the α component of vector $\mathbf{V}$ and where the dot over a symbol indicates time derivation. In eq. (23), the values $M_{\alpha\beta}$ are the components of the so-called mass matrix $\mathbf{M}$:

$$M_{\alpha\beta} \;=\; \int_\Omega \rho(z)\, w_\beta(z)\, w_\alpha(z)\; dz\,, \tag{24}$$

$K_{\alpha\beta}$ those of the stiffness matrix $\mathbf{K}$:

$$K_{\alpha\beta} \;=\; \int_\Omega \mu(z)\, \frac{\partial w_\beta}{\partial z}(z)\, \frac{\partial w_\alpha}{\partial z}(z)\; dz\,. \tag{25}$$

To form the global algebraic system, we introduce the vectors $\mathbf{U}(t)$ and $\ddot{\mathbf{U}}(t)$ that respectively store the values of displacement and acceleration on the grid at time t:

$$\mathbf{M}\,\ddot{\mathbf{U}}(t) \;+\; \mathbf{K}\,\mathbf{U}(t) \;+\; \mathbf{T}_{\text{abs}}(t) \;=\; \mathbf{F}(t)\;. \tag{26}$$

Any FEM would lead to the previous Ordinary Differential Equation in time (26). What makes each method unique is the way the matrices $\mathbf{M}$ and $\mathbf{K}$ and the vector $\mathbf{F}$ are computed, i.e., the choice of the polynomial basis and of the numerical integration formula. In the SEM, both the polynomial basis and the numerical integration formula are based on the GLL points. This choice yields a diagonal mass matrix, as demonstrated below.

Proof. We start from the expression of the mass matrix (24) and choose α as an interior point: $\alpha = \texttt{num}(e,i)$ with $i \in [1, N-1]$. The mass matrix term $M_{\alpha\beta}$ involves the basis function w_α which vanishes outside Ω_e. It writes:

$$M_{\alpha\beta} \;=\; \int_{\Omega_e} \rho(z)\, w_\beta(z)\, w_\alpha(z)\; dz\,. \tag{27}$$

Assume that $\beta = \texttt{num}(e,j)$, then we use the change of variables and write:

$$M_{\alpha\beta} \;=\; \int_{\hat{\Omega}} \rho\big(\mathcal{F}_e(\xi)\big)\, h_i(\xi)\, h_j(\xi) \mathcal{J}_e(\xi) d\xi\,. \tag{28}$$

Next, we approximate the integral using the GLL integration formula and get:

$$M^{SEM}_{\alpha\beta} \;=\; \sum_{k=0}^{N} \omega_k\, \rho(z^e_k)\, h_i(\xi_k) h_j(\xi_k)\, \mathcal{J}_e(\xi_k)\;. \tag{29}$$

The values of the Lagrange polynomials at the integration points are either 0 or 1, which simplifies the above calculation to:

$$M^{SEM}_{\alpha\beta} = \sum_{k=0}^{N} \omega_k\, \rho(z^e_k)\, \delta_{ik}\delta_{jk}\, \mathcal{J}_e(\xi_k)\;, \tag{30}$$

$$M^{SEM}_{\alpha\beta} = \delta_{ij}\, \omega_i\, \rho(z^e_i) \mathcal{J}_e(\xi_i)\;, \tag{31}$$

$$M^{SEM}_{\alpha\beta} = \delta_{\alpha\beta}\, \omega_i\, \rho(z^e_i) \mathcal{J}_e(\xi_i)\;, \tag{32}$$

where δ is the Kronecker symbol.

Now, if α belongs to two elements, Ω_e and Ω_{e+1}, we have:

$$M_{\alpha\beta} \;=\; \int_{\Omega_e} \rho(z)\, w_\beta(z)\, w_\alpha(z)\; dz \;+\; \int_{\Omega_{e+1}} \rho(z)\, w_\beta(z)\, w_\alpha(z)\; dz. \tag{33}$$

The only case where $M_{\alpha\beta}$ is not zero is $\beta = \alpha$. Applying the change of variable on each element yields:

$$M_{\alpha\beta} \;=\; \int_{\hat{\Omega}} \rho\big(\mathcal{F}_e(\xi)\big)\, h_N(\xi)\, h_N(\xi) \mathcal{J}_e(\xi) d\xi \;+\; \int_{\hat{\Omega}} \rho\big(\mathcal{F}_e(\xi)\big)\, h_0(\xi)\, h_0(\xi) \mathcal{J}_e(\xi) d\xi \;. \tag{34}$$

And applying the numerical integration yields:

$$M^{SEM}_{\alpha\beta} \;=\; \delta_{\alpha\beta} \left(\omega_N\, \rho(z^e_N) \mathcal{J}_e(\xi_N) \;+\; \omega_0\, \rho(z^{e+1}_0) \mathcal{J}_{e+1}(\xi_0)\right). \tag{35}$$

The mass matrix is therefore diagonal. □

Note that in eq. (35), two values of the density corresponding to the same global point are summed to obtain the global mass matrix term. It illustrates that the SEM (or FEM) can account for discontinuous elastic parameters, provided that the discontinuity coincides with the element boundaries. Inside the elements, a physical interface will be approximated by a continuous, smooth contrast since the elastic parameters are expanded on the basis of the basis of Lagrange interpolants.

2.6 Assembly

The process of summing the local expressions of the mass matrix to get the global value, like in eq. (35), is called the assembly process in the Finite Element literature. Assembly is directly related to the continuity requirement for the basis functions.

2.6.1 Connectivity matrix

A simple way to express the assembly process, and to build the global mass and stiffness matrices, is to introduce the connectivity matrix $\mathbf{Q}$. Consider the vector $\mathbf{V}^G$ storing the values of an arbitrary quantity on the spectral element grid of points (i.e. the set of global degrees of freedom introduced earlier). The size of the vector $\mathbf{V}^G$ is $\mathcal{N}$. The same vector can be expressed in the local basis, i.e. by duplicating the values of $\mathbf{V}^G$ at the element boundaries. The local vector is denoted $\mathbf{V}^L$ and its size is $E \times (N+1)$. The connectivity matrix relates the local and global vectors through:

$$\mathbf{V}^L \;=\; \mathbf{Q}\, \mathbf{V}^G \,. \tag{36}$$

It is a rectangular matrix of size $\big(E \times (N+1)\,,\, \mathcal{N}\big)$ which is made of zeros and ones: the $n-th$ line of $\mathbf{Q}$ has only one non-zero term at position m, with n and m being the local and global numbers corresponding to the same dof.

Consider the simple example of a grid obtained from 3 elements and a polynomial order $N = 2$. The gridpoints can be are numbered globally from 1 to 7 as in Fig. 3, or locally from 1 to 9 as in Fig. 4.

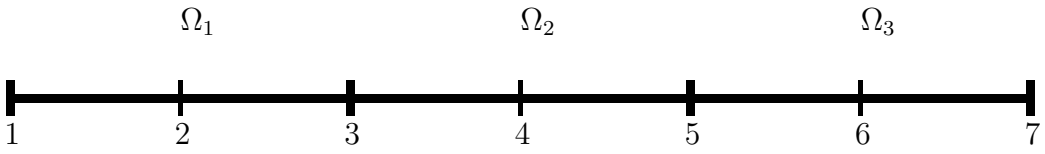

Figure 3: Example of global numbering of a FE or SE grid of points.

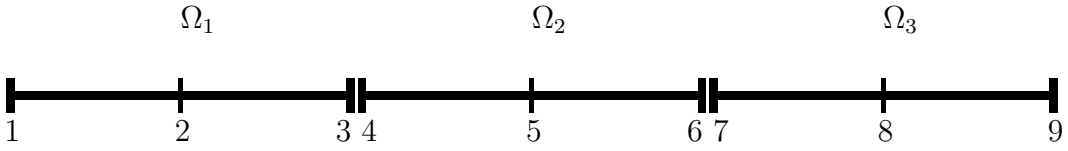

Figure 4: Example of local numbering of a FE or SE grid of points.

The connectivity matrix reads:

$$\mathbf{Q} = \begin{pmatrix} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{pmatrix} \tag{37}$$

The transpose of the connectivity matrix takes a vector in local coordinates to form a vector in global coordinates. In the above example, its reads:

$$\mathbf{Q}^t = \begin{pmatrix} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{\mathbf{1}} & \boxed{\mathbf{1}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \boxed{\mathbf{1}} & \boxed{\mathbf{1}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{pmatrix} \tag{38}$$

Note that the action of $\mathbf{Q}^t$ is to sum up the local contributions at the elements boundaries, i.e. $\mathbf{Q}^t$ does the assembly process. In parallel implementations of the SEM (or FEM) in 2D or 3D, the assembly process is implemented through communications between processors in order to exchange information about the nodes at the boundaries of the elements. But in 1D, one can simply store the connectivity matrix and use its transpose to make the assembly.

2.6.2 Elementary, local and global matrices

It is useful to write the global mass and stiffness matrices in term of the connectivity matrix and its transpose.

Elementary matrices We start from the definition of the elementary matrices M^e and K^e. For this, we consider two global numbers α and β which belong to the same element, for example $\alpha = \texttt{num}(e,i)$ and $\beta = \texttt{num}(e,j)$. The elementary matrix component M^e_{ij} is defined by:

$$M^e_{ij} \;=\; \int_{\Omega_e} \rho(z) w_\beta(z) w_\alpha(z)\, dz, \tag{39}$$

which, after changing variables from z to ξ, writes:

$$M^e_{ij} \;=\; \int_{\hat{\Omega}} \rho\big(\mathcal{F}_e(\xi)\big) h_i(\xi) h_j(\xi) \mathcal{J}_e(\xi)\, d\xi, \tag{40}$$

and applying the GLL numerical integration rule:

$$\boxed{M^e_{ij} \;=\; \omega_i\, \rho(z^e_i)\, \mathcal{J}_e(\xi_i)\; \delta_{ij}.} \tag{41}$$

Similarly, the elementary matrix component K^e_{ij} writes:

$$K^e_{ij} = \int_{\Omega_e} \mu(z)\, \frac{\partial w_\beta}{\partial z}(z)\, \frac{\partial w_\alpha}{\partial z}(z)\; dz\,, \tag{42}$$

Changing variables we have:

$$K^e_{ij} = \int_{\hat{\Omega}} \mu\big(\mathcal{F}^e(\xi)\big)\, \frac{\partial h_j}{\partial z}(\xi)\, \frac{\partial h_i}{\partial z}(\xi)\, \mathcal{J}_e(\xi)\, d\xi\,. \tag{43}$$

Here, we have to apply the chain rule to compute the spatial derivatives, for example:

$$\frac{\partial h_i}{\partial z}(\xi) \;=\; \frac{\partial h_i}{\partial \xi}(\xi)\, \frac{\partial \xi}{\partial z} \;=\; \frac{\partial h_i}{\partial \xi}(\xi)\, \mathcal{J}_e{}^{-1}(\xi) \tag{44}$$

Denoting $h' = \partial h/\partial \xi$, we obtain $\big(\text{since } \mathcal{J}_e{}^{-1}(\xi)\mathcal{J}_e(\xi) = 1\big)$:

$$K^e_{ij} \;=\; \int_{\hat{\Omega}} \mu\big(\mathcal{F}^e(\xi)\big)\, h'_j(\xi)\, h'_i(\xi) \mathcal{J}_e{}^{-1}(\xi)\, d\xi\,. \tag{45}$$

The SEM elementary stiffness matrix is finally obtained after applying the GLL quadrature to compute the integral:

$$\boxed{K^e_{ij} \;=\; \sum_{k=0}^{N} \omega_k\, \mu(z^e_k)\, h'_j(\xi_k)\, h'_i(\xi_k) \mathcal{J}_e{}^{-1}(\xi_k).} \tag{46}$$

Local matrices Combining all the elementary matrices we can form block-diagonal matrices, which we call the local matrices. Let A stand either for M or K, we define the local matrix $\mathbf{A}^L$ as:

$$\mathbf{A}^L \;=\; \begin{pmatrix} \boxed{A^1} & 0 & \cdots & 0 \\ 0 & \boxed{A^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \boxed{A^E} \end{pmatrix} \tag{47}$$

Global matrices Then, the global matrices, i.e. the one that are assembled, are obtained by:

$$\mathbf{A}^G \;=\; \mathbf{Q}^t\,\mathbf{A}^L\,\mathbf{Q}\;. \tag{48}$$

The action of the global matrix $\mathbf{A}^G$ on a global vector $\mathbf{F}^G$ can thus be decomposed into three steps:

1. form the local vector $\mathbf{F}^L \;=\; \mathbf{Q}\mathbf{F}^G$,
2. apply the local matrix to the local vector $\mathbf{A}^L\mathbf{F}^L$ (this can be computed independently on each element),
3. assemble the local results into a global vector by applying $\mathbf{Q}^t$.

3 Time marching

The Spectral Element discretization presented above applies to the spatial dimension. The way the SE solution is extrapolated in time is based on a Finite Difference scheme (or any method to integrate an Ordinary Differential Equation). For this purpose, we sample the time interval $[0, T]$ with discrete times $t_n = (n-1)\Delta t$, for $n = 1 \ldots N_t$ with $\Delta t = \frac{T}{N_t - 1}$, and we note with an upperscript n the value of a quantity at time t_n. For example, the displacement field vector at time t_n (containing the values of displacement at the grid points in the global numbering) is denoted $\mathbf{U}^n$.

3.1 Displacement-based scheme

A first example of a FD scheme to march the solution in time is the second-order displacement-based scheme:

$$\mathbf{U}^{n+1} \;=\; -\mathbf{U}^{n-1} \;+\; 2\,\mathbf{U}^n \;+\; \Delta t^2\,\ddot{\mathbf{U}}^n\;, \tag{49}$$

where the value of the acceleration is computed by solving the discrete wave equation (26):

$$\mathbf{U}^{n+1} \;=\; -\mathbf{U}^{n-1} \;+\; 2\,\mathbf{U}^n \;+\; \Delta t^2\,\left[\mathbf{M}^{-1}\,(\mathbf{F}^n \;-\; \mathbf{K}\mathbf{U}^n \;-\; \mathbf{T}^n_{\text{abs}})\right]\;. \tag{50}$$

The displacement based scheme needs to consecutive values of displacement to be initialized, for example $\mathbf{U}^0 = \mathbf{U}^1 = \mathbf{0}$.

You immediately see the benefit of dealing with a diagonal mass matrix: the time evolution scheme becomes costless. The main computational cost in the method is the evaluation of the matrix product with the stiffness matrix $\mathbf{K}$. Note that the Chebychev SEM does not have the

property of a diagonal mass matrix and therefore a matrix system has to be solved at each time step.

Finally, remember that the FD scheme applied here is conditionally stable, and therefore subject to a CFL stability condition when choosing the time step Δt. This will have important consequences for practical implementations as we will see next.

3.2 Newmark velocity-based scheme

The Newmark family of schemes is written as a map $(\mathbf{U}_n, \dot{\mathbf{U}}_n) \to (\mathbf{U}_{n+1}, \dot{\mathbf{U}}_{n+1})$ that is defined by enforcing the wave equation at time t_{n+1}:

$$\begin{cases} \ddot{\mathbf{U}}^{n+1} = \mathbf{M}^{-1} \left(\mathbf{F}^{n+1} - \mathbf{K}\mathbf{U}^{n+1} - \mathbf{T}_{\text{abs}}^{n+1} \right) \ , \\ \mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \, \dot{\mathbf{U}}^n + \Delta t^2 \left(\left(\frac{1}{2} - \beta \right) \ddot{\mathbf{U}}^n + \beta \ \ddot{\mathbf{U}}^{n+1} \right) \ , \\ \dot{\mathbf{U}}^{n+1} = \dot{\mathbf{U}}^n + \Delta t \, \left((1-\gamma) \, \ddot{\mathbf{U}}^n + \gamma \ \ddot{\mathbf{U}}^{n+1} \right) \ , \end{cases} \tag{51}$$

where one needs to select the two parameters $\gamma \in [0,1]$ and $\beta \in [0,1/2]$.

Second-order accuracy (instead of first-order) is obtained if and only if the velocity is updated based upon a centered scheme, i.e. if $\gamma = 1/2$. The particular choice of setting $\beta = 0$ and $\gamma = 1/2$ leads to the explicit central difference method, which is the most widely used in the context of spectral-element simulations of seismic wave propagation. It has the important property of conserving linear and angular momentum and having bounded energy errors. It writes:

$$\begin{cases} \ddot{\mathbf{U}}^{n+1} = \mathbf{M}^{-1} \left(\mathbf{F}^{n+1} - \mathbf{K}\mathbf{U}^{n+1} - \mathbf{T}_{\text{abs}}^{n+1} \right) \ , \\ \mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \, \dot{\mathbf{U}}^n + \dfrac{\Delta t^2}{2} \, \ddot{\mathbf{U}}^n, \\ \dot{\mathbf{U}}^{n+1} = \dot{\mathbf{U}}^n + \dfrac{\Delta t}{2} \, \left(\ddot{\mathbf{U}}^n + \ddot{\mathbf{U}}^{n+1} \right) \ . \end{cases} \tag{52}$$

4 Absorbing boundary condition

In the 1D case, the absorbing boundary condition can be easily implemented by enforcing the one-way wave equation at the bottom boundary ($z = -H$), i.e.:

$$\frac{\partial u}{\partial t}(-H,t) \ + \ c(-H) \, \frac{\partial u}{\partial z}(-H,t) \ = \ 0 \ , \tag{53}$$

where $c = \sqrt{\mu/\rho}$ is the wave speed. This indeed ensures that the solution u is of the form $u(z,t) = g(t + z/c)$ where g is an arbitrary function.

Multiplying by $\sqrt{\rho\mu}$ and identifying the traction vector, we obtain an explicit form of the traction to be applied at the absorbing boundary:

$$\tau_{\text{abs}}(z = -H, t) = \ -\sqrt{\rho(-H)\mu(-H)} \ \frac{\partial u}{\partial t}(-H,t) \ , \tag{54}$$

or

$$\tau_{\text{abs}}(z = -H, t) = \ -\rho(-H)c(-H) \ \frac{\partial u}{\partial t}(-H,t) \ . \tag{55}$$

Newmark scheme For example, this absorbing boundary condition can be imposed directly in the Newmark scheme by inserting

$$\mathbf{T}_{\text{abs}}^{n+1} \;=\; -\rho(-H)c(-H)\;\dot{\mathbf{U}}_{\text{abs}}^{n+1} \tag{56}$$

in the first line of equation (52), which in turns modifies slightly the third line of equation (52) to compute the velocity vector at the next time step. The modification only affects the global number corresponding to the bottom boundary, whence the "$_{\text{abs}}$" subscript on the velocity vector.

Displacement scheme In order to implement the absorbing boundary condition (55) in the displacement based scheme (50), we make use of the second order accurate velocity at time t_n:

$$\dot{\mathbf{U}}^n \;=\; \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n-1}}{2\,\Delta t}\;, \tag{57}$$

which gives the absorbing traction

$$\mathbf{T}_{\text{abs}}^{n} \;=\; -\rho(-H)c(-H)\;\dot{\mathbf{U}}_{\text{abs}}^{n}\;, \tag{58}$$

to be inserted in equation (50). Like in the Newmark case, this will only change the equation to be solved at the bottom boundary.

5 Accuracy and practical considerations

For smooth problems, the numerical solution computed with any spectral method is expected to converge exponentially (when increasing the polynomial order) to the exact solution of the problem. For wave propagation problems the property still holds for the SEM in space but, because we deal with a space-time problem we are more concerned with more physical properties of the numerical solution such as numerical dispersion. There are basic questions for which we need an answer: how does numerical dispersion behaves in the SEM when the polynomial order or the number of elements is increased? How many gridpoints per wavelength are needed to reach a given accuracy?

Note that dispersion analysis are not easy to derive analytically in the SEM (contrary to the FDM) because the gridpoints are not regularly spaced, and for a long time, the answers to the questions mentioned above were only based on numerical experiments. It is only in the mid 2000 that a complete answer has been provided (Seriani & Oliveira, 2007; Basabe & Sen, 2007). Fig. 5 shows the phase velocity error as a function of the normalized wavenumber H ($H = 1/q$ where q is the average number of gridpoints per wavelength). As seen in the figure, the numerical dispersion in the SEM can be maintained at a very low level with 4 to 5 gridpoints per wavelength ($H \in [0.2, 0.25]$), provided that the polynomial order is larger than about 4. Note that increasing N beyond 8 does not decrease considerably the number of gridpoints per wavelength needed for a given level of phase error (theoretical arguments suggest that this number is always greater than π).

The polynomial order needed to reach such accuracy must always be greater than 4, so the SEM can be considered as a high-order FEM (generally restricted to $N \leq 2$). On the other hand, there is a upper limitation in the polynomial order that can be used in time dependent

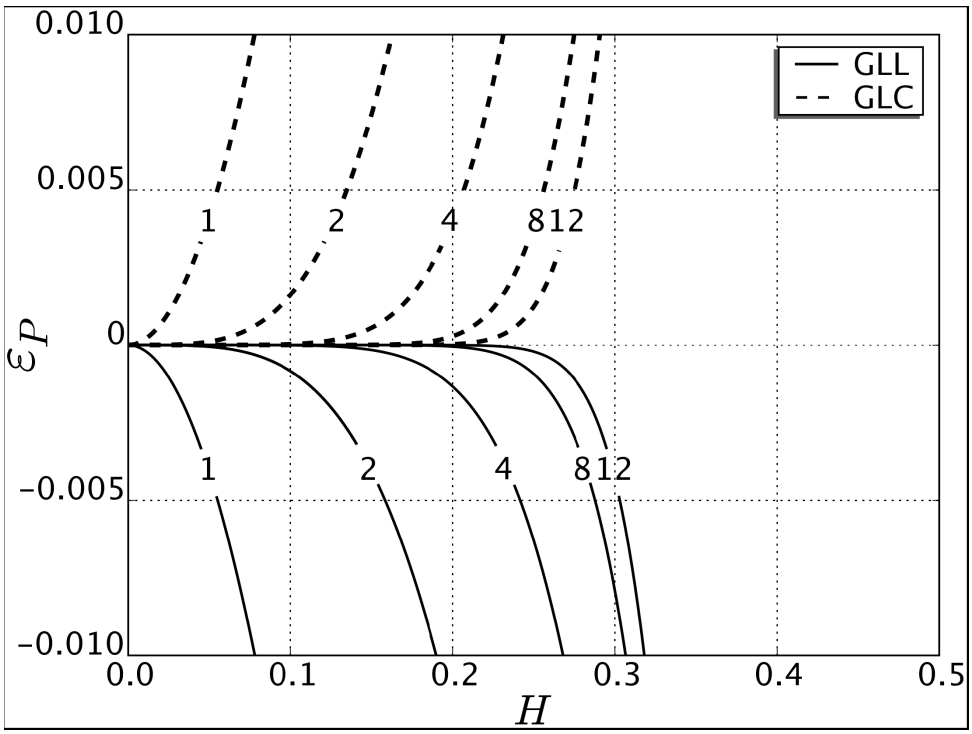

Figure 5: Relative error on phase velocity $\epsilon_P = 1 - c/c_0$ plotted as a function of the inverse of the discretization parameter for Chebychev (dashed lines) and Legendre (solid lines) SEM using different polynomial order $N = 1, 2, 4, 8, 12$. The analysis does not include errors due to low-order time schemes. *After Oliveira & Seriani (2007).*

problems, especially when an explicit FD scheme is used to march the solution in time. In that case indeed, the time step is constrained by the CFL condition:

$$\Delta t \ \leq \ \mathcal{C} \left(\frac{\Delta z}{c} \right)_{\min} , \tag{59}$$

where $\mathcal{C}$ is a constant. We have seen that the grid step Δz decreases like $1/N^2$ near the edges of the elements, so there is a clear tradeoff between the accuracy of the numerical solution, enhanced by increasing the polynomial order, and the computational time, limited by the value of the timestep.

In practical applications of the SEM, polynomial orders between 4 and 8 are used: $N > 4$ is required to have a minimal numerical dispersion, whereas $N \leq 8$ yields a timestep larger than 0.4 that of a regular grid (the smallest distance between two GLL points for $N = 8$ is about 2.5 smaller than the distance obtained in a regular grid).

6 Implementation

In order to implement the above 1D SEM in a computer code, one needs to follow the recipe:

0. Define the geometry of the problem and the physical parameters.
1. Choose the position of the elements by defining the values of a_e and b_e.
2. Compute the jacobians (α_e) and their inverses.
3. Choose the polynomial order.
4. Compute the connectivity matrix and its transpose.
5. Compute the elementary mass and stiffness matrices.
6. Compute the global mass and stiffness matrices by matrix multiplications with the connectivy matrix and its transpose.
7. Solve the system in time.

The only input needed, to compute the elementary matrices, are:

- The values of the GLL integration points and weights for any polynomial order.
- The values of the derivatives of the Lagrange interpolants at the GLL points.

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