Spectral Element Method in Elastodynamics

a Primer

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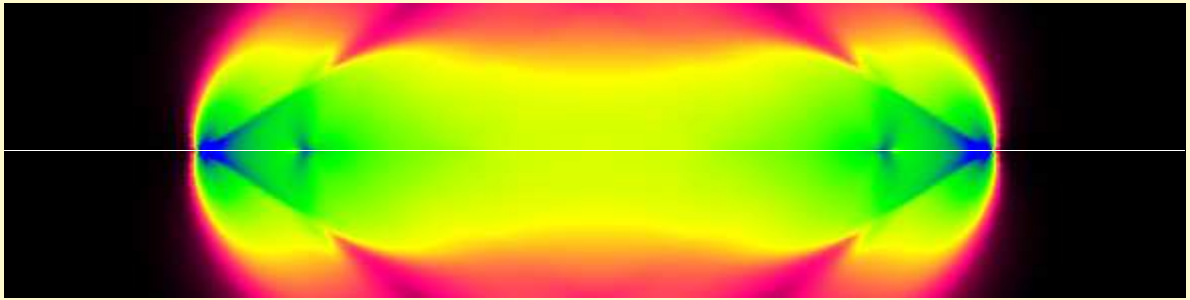
v.1.0



The Elastic System

Problem Geometry : Let consider an elastic medium $\boldsymbol{\Omega} \subset \mathbb{R}^{n_d}$,

$$\bar{\boldsymbol{\Omega}} = \boldsymbol{\Omega} \cup \bar{\boldsymbol{\Gamma}} \quad ; \quad \bar{\boldsymbol{\Gamma}} = \boldsymbol{\Gamma}^i \bar{\cup} \boldsymbol{\Gamma}^a \quad \text{with} \quad \boldsymbol{\Gamma}^i = \boldsymbol{\Gamma}^i_{\boldsymbol{u}} \cup \boldsymbol{\Gamma}^i_{\boldsymbol{T}}$$

Field Variables : Let $\boldsymbol{x} \in \boldsymbol{\Omega}$ and $t \in \mathbb{I} = [0, T]$,

$$\boldsymbol{u}(\boldsymbol{x}, t) : \boldsymbol{\Omega} \times \mathbb{I} \longrightarrow \mathbb{R}^{n_d} \; ; \; \boldsymbol{v}(\boldsymbol{x}, t) : \boldsymbol{\Omega} \times \mathbb{I} \longrightarrow \mathbb{R}^{n_d} \; ; \; \rho(\mathbf{x}) : \boldsymbol{\Omega} \longrightarrow \mathbb{R}^+$$

The Euler-Lagrange Equations (EL) : $\forall (\boldsymbol{x}, t) \in \boldsymbol{\Omega} \times \mathbb{I}$;

$$\rho \ddot{\boldsymbol{u}} = \operatorname{div} [\boldsymbol{\sigma}(\boldsymbol{\nabla} \boldsymbol{u})] + \boldsymbol{f}$$

with the initial conditions,

$$\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x}) \qquad \text{and} \qquad \boldsymbol{v}(\boldsymbol{x}, 0) = \boldsymbol{v}_0(\boldsymbol{x})$$

Notation *The symmetric* **Cauchy stress tensor** *is denoted by*

$$\boldsymbol{\sigma} : \boldsymbol{\Omega} \times \mathbb{I} \rightarrow \mathbb{S} \quad \textit{with} \qquad \boldsymbol{\sigma}(\boldsymbol{x}, t) := \sigma_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j$$

The **infinitesimal strain field** *is denoted by*

$$\boldsymbol{\epsilon}[\boldsymbol{u}] : \boldsymbol{\Omega} \times \mathbb{I} \rightarrow \mathbb{S} \textit{ with } \boldsymbol{\epsilon}[\boldsymbol{u}] \doteq \boldsymbol{\nabla}^s \boldsymbol{u} = \frac{1}{2}\left[\boldsymbol{\nabla} \boldsymbol{u} + (\boldsymbol{\nabla} \boldsymbol{u})^T\right]$$

where $\mathbb{S} \subset \mathbb{L}(\mathbb{R}^{n_d}, \mathbb{R}^{n_d})$ *is the subspace of symmetric second-order tensors of dimension* $d(d+1)/2$.

$\boldsymbol{f} : \boldsymbol{\Omega} \times \mathbb{I} \rightarrow \mathbb{R}^d$ *is a* **generalized body force**, *i.e.,*

$$\begin{aligned} \boldsymbol{f}(\boldsymbol{x}, t) &= \operatorname{div}[\boldsymbol{m}(\boldsymbol{x}, t)] \quad ; \quad \textit{with} \quad \boldsymbol{m}(\boldsymbol{x}, t) = m_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j \\ \boldsymbol{m}(\boldsymbol{x}, t) &= \boldsymbol{m}(t)\, \delta(\boldsymbol{x} - \boldsymbol{x}_s) \end{aligned}$$

and $\{\lambda_i\}_{i=1,3}$, *are* `eigenvalues` *of* $\boldsymbol{m}$, *i.e.,*

$\lambda_1 \neq 0$	$\lambda_2 = \lambda_3$	mode I source
$\lambda_1 = -\lambda_3$	$\lambda_2 = 0$	mode II source
$\lambda_1 = \lambda_2 = \lambda_3$		explosive source

Boundary conditions

Dirichlet boundary conditions

$$\boldsymbol{u}_{\boldsymbol{\Gamma}} = \bar{\boldsymbol{u}} \quad \text{or} \quad \boldsymbol{v}_{\boldsymbol{\Gamma}} = \bar{\boldsymbol{v}} \qquad \text{on} \qquad \boldsymbol{\Gamma}_{\boldsymbol{u}}^{i} \times \mathbb{I}$$

Neumann boundary conditions

$$\boldsymbol{\sigma}_{\boldsymbol{\Gamma}} \cdot \boldsymbol{n} = \bar{\boldsymbol{T}} \qquad \text{on} \qquad \boldsymbol{\Gamma}_{\boldsymbol{T}}^{i} \times \mathbb{I}$$

Remark *This conditions generates* `Rayleigh waves` *with celerity* c_R *given by*

$$\left(2 - \frac{c_R^2}{c_S^2}\right)^2 - 4\left(1 - \frac{c_R^2}{c_P^2}\right)^{1/2}\left(1 - \frac{c_R^2}{c_S^2}\right)^{1/2} = 0$$

Absorbing boundary conditions

$$\boldsymbol{\sigma}_{\boldsymbol{\Gamma}} \cdot \boldsymbol{n} = \boldsymbol{\mathcal{A}}_{\boldsymbol{\Gamma}}\left(\boldsymbol{u}_{\boldsymbol{\Gamma}}, \boldsymbol{v}_{\boldsymbol{\Gamma}}\right) \qquad \text{on} \qquad \boldsymbol{\Gamma}^{a} \times \mathbb{I}$$

$\boldsymbol{\mathcal{A}}_{\boldsymbol{\Gamma}}$ is a `DtN-surface operator` which is generally non local both in space and time.

Example Linearly Elastic Material

The stress response is characterized by a stored energy function $W : \boldsymbol{\Omega} \times \mathbb{S} \rightarrow \mathbb{R}$ *such that*

$$\boldsymbol{\sigma}(\boldsymbol{x}, t) = \frac{\partial W(\boldsymbol{x}, \boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}} \qquad i.e., \qquad \sigma_{ij}(\boldsymbol{x}, t) = \frac{\partial W}{\partial \epsilon_{ij}}$$

the linearized elasticity tensor *is defined as*

$$\boldsymbol{C}(\boldsymbol{x}, t) = \frac{\partial^2 W(\boldsymbol{x}, t)}{\partial \boldsymbol{\epsilon} \partial \boldsymbol{\epsilon}} \qquad i.e., \qquad C_{ijkl} = \frac{\partial^2 W}{\partial \epsilon_{ij} \partial \epsilon_{kl}}$$

which possesses `major and minor symmetries`

$$C_{ijkl} = C_{klij} = C_{ijlk} = C_{jikl}$$

which leads to 6 *coefficients for* $n_d = 2$ *and* 21 *for* $n_d = 3$.
`For infinitesimal theory,` $\boldsymbol{C}$ *is* positive definite *restricted to* $\mathbb{S}$,

$$\boldsymbol{\zeta} : \boldsymbol{C} : \boldsymbol{\zeta} = \zeta_{ij} C_{ijkl} \zeta_{kl} \geq \alpha(\boldsymbol{x}) |\boldsymbol{\zeta}|^2 \qquad \forall \boldsymbol{\zeta} \in \mathbb{S} \text{ and } \alpha > 0$$

Therefore W *is a* `convex function` *of* $\boldsymbol{\epsilon}$. *This implies the so-called Hadamard condition for real wave celerities.*

Remark *For the* **infinitesimal theory**,

$$W = \frac{1}{2}\boldsymbol{\epsilon} : \boldsymbol{C} : \boldsymbol{\epsilon} = \frac{1}{2}\boldsymbol{\nabla}\boldsymbol{u} : \boldsymbol{C} : \boldsymbol{\nabla}\boldsymbol{u}$$

and for a **free stress initial state**, *the stress perturbation is*

$$\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\epsilon} = \boldsymbol{C} : \boldsymbol{\nabla}\boldsymbol{u} \qquad i.e., \qquad \sigma_{ij} = C_{ijkl}\epsilon_{kl} = C_{ijkl}\frac{\partial u_k}{\partial x_l}$$

Remark *When* W *is rotationally invariant, and for a* **linearly isotropic elastic material**

$$\boldsymbol{C} = \lambda\, \mathbf{1} \otimes \mathbf{1} + 2\mu\, \boldsymbol{I} = \kappa\, \mathbf{1} \otimes \mathbf{1} + 2\mu \left[\boldsymbol{I} - \frac{1}{3}\boldsymbol{I} \otimes \boldsymbol{I} \right]$$

where λ, μ *are the* `Lamé parameters` *and* $\kappa = \lambda + \frac{2}{3}\mu$ *and*

$$\mathbf{1} = \delta_{ij}\boldsymbol{e_i} \otimes \boldsymbol{e_j} \quad \textit{and} \quad \boldsymbol{I} = \frac{1}{2}\left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right] \boldsymbol{e}_i \otimes \boldsymbol{e}_j \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l$$

with two real wave celerities : the `P-wave` *and* `S-wave` *celerities*

$$c_P = \sqrt{\frac{\lambda + \mu}{\rho}} \quad ; \quad c_S = \sqrt{\frac{\mu}{\rho}} \quad \textit{with} \quad c_P = \sqrt{\frac{2}{3\nu}}c_S \geq \sqrt{\frac{4}{3}}c_S$$

Note Lagrangian dynamics

The associated continuous Lagrangian system is defined by

$$\mathbb{L}\left(\boldsymbol{u}(\cdot,t),\boldsymbol{v}(\cdot,t),t\right) := \boldsymbol{\mathcal{I}}\left[\boldsymbol{v}\right] - \boldsymbol{\mathcal{V}}\left[\boldsymbol{u},t\right]$$

where $\boldsymbol{\mathcal{I}}$ *and* $\boldsymbol{\mathcal{V}} = \boldsymbol{\mathcal{V}}_{int} - \boldsymbol{\mathcal{V}}_{ext}$ *denotes the* `kinetic energy` *and the* `potential energy` *of the body, i.e.,*

$$\boldsymbol{\mathcal{I}}\left[\boldsymbol{v}(\cdot,t)\right] = \int_{\boldsymbol{\Omega}} \frac{1}{2}\rho_0 \boldsymbol{v}\cdot\boldsymbol{v}\, dV$$

$$\boldsymbol{\mathcal{V}}_{int}\left[\boldsymbol{u}(\cdot,t),t\right] = \int_{\boldsymbol{\Omega}} W\left(\boldsymbol{\nabla}\,\boldsymbol{u},\boldsymbol{x}\right)\, dV = \int_{\boldsymbol{\Omega}} \frac{1}{2}\boldsymbol{\epsilon}:\boldsymbol{C}:\boldsymbol{\epsilon}\, dV$$

$$\boldsymbol{\mathcal{V}}_{ext}\left[t\right] = \int_{\boldsymbol{\Omega}} \boldsymbol{f}(t)\cdot\boldsymbol{u}\, dV + \int_{\boldsymbol{\Gamma}^i_{\boldsymbol{T}}} \boldsymbol{T}(t)\cdot\boldsymbol{u}\, d\boldsymbol{\Gamma}$$

Considering the motion of the body during the time interval $\mathbb{I}$*, the* `action function` *is obtained by integration along a curve* $\boldsymbol{u}(\cdot,t)$*,*

$$\mathcal{S}\left[\boldsymbol{u}(\cdot,\cdot)\right] = \int_{\mathbb{I}} \mathbb{L}\left(\boldsymbol{u}(\cdot,t),\boldsymbol{v}(\cdot,t),t\right)\, dt$$

Note **Hamilton principle**

Hamilton's principle postulates that among all the admissible trajectories, i.e., satisfying the essential boundary condition on $\mathbf{\Gamma}_{\boldsymbol{u}}^{i}$*, the solution is the one that extremize the action function while holding the endpoints of the cure* $\boldsymbol{u}(\cdot, t)$ *fixed,*

$$\delta\mathcal{S}\left[\boldsymbol{u}(\cdot,\cdot)\right] = \delta\int_{\mathbb{I}} \mathcal{I} - \mathcal{V}\, dt = \int_{\mathcal{I}} \left[\frac{\partial \mathbb{I}}{\partial \boldsymbol{v}}\delta\boldsymbol{v} - \delta\mathcal{V}\right] dt$$

$$= \int_{\mathcal{I}} \left[-\frac{d}{dt}\left(\frac{\partial \mathbb{I}}{\partial \boldsymbol{v}}\right)\delta\boldsymbol{u} - \delta\mathcal{V}\right] dt + \left[\frac{\partial \mathcal{I}}{\partial \boldsymbol{v}}\delta\boldsymbol{u}\right]_0^{T_f}$$

with

$$\delta\mathcal{V} = \int_{\boldsymbol{\Omega}} \left[\frac{\partial W}{\partial \boldsymbol{\epsilon}} : \boldsymbol{\nabla}\,\delta\boldsymbol{u} - \boldsymbol{f}(t)\cdot\delta\boldsymbol{u}\right] dV - \int_{\mathbf{\Gamma}_{\boldsymbol{T}}^{int}} \boldsymbol{T}(t)\cdot\delta\boldsymbol{u}\, dx$$

Leading to

$$\int_{\boldsymbol{\Omega}} \rho\ddot{\boldsymbol{u}}\cdot\delta\boldsymbol{u} = -\int_{\boldsymbol{\Omega}} \left[\boldsymbol{\sigma} : \boldsymbol{\nabla}\,\delta\boldsymbol{u} + \boldsymbol{f}(t)\cdot\delta\boldsymbol{u}\right] dV + \int_{\mathbf{\Gamma}_{\boldsymbol{T}}^{int}} \boldsymbol{T}\cdot\delta\boldsymbol{u}\, dV$$

Remark **The Neumann boundary conditions are natural conditions.**

Definition Functional spaces

At that stage, we introduce the spaces of admissible displacement and admissible displacement variation,

$$\mathcal{S}_{\boldsymbol{u}} = \left\{ \boldsymbol{u}(\boldsymbol{x},t) : \boldsymbol{\Omega} \times \mathbb{I} \rightarrow \mathbb{R}^d \mid \boldsymbol{u}(\cdot,t) \in H^1(\boldsymbol{\Omega})^d \, ; \boldsymbol{u} = \bar{\boldsymbol{u}} \text{ on } \boldsymbol{\Gamma}_{\boldsymbol{u}}^{int} \right\}$$
$$\delta\mathcal{S} = \left\{ \boldsymbol{w}(\boldsymbol{x},t) : \boldsymbol{\Omega} \times \mathbb{I} \rightarrow \mathbb{R}^d \mid \boldsymbol{w}(\cdot,t) \in H^1(\boldsymbol{\Omega})^d \, ; \boldsymbol{w} = 0 \text{ on } \boldsymbol{\Gamma}_{\boldsymbol{u}}^{int} \right\}$$

Where

$$H^1(\boldsymbol{\Omega}) = \left\{ u \in L^2(\boldsymbol{\Omega}) \quad \text{such that} , \ \frac{\partial u}{\partial x_j} \in L^2(\boldsymbol{\Omega}) \right\}$$

and $L^2(\boldsymbol{\Omega})$ is the space of square integrable functions over $\boldsymbol{\Omega}$. Finally let denote the scalar product on $L^2(\boldsymbol{\Omega})^{n_d}$,

$$(\boldsymbol{u}, \boldsymbol{w}) = \int_{\boldsymbol{\Omega}} \boldsymbol{u} \cdot \mathbf{w} \, dV$$

Problem The Initial Boundary Value Problem (IBVP)

For all $\boldsymbol{w} \in \delta\mathcal{S}$ *and* $t \in \mathbb{I}$, *find* $(\boldsymbol{u}, \boldsymbol{v}) \in \mathcal{S}_{\boldsymbol{u}} \times \mathcal{S}_{\boldsymbol{v}}$, *such that*

$$(\boldsymbol{w}, \rho\dot{\boldsymbol{v}}) = -\mathcal{A}(\boldsymbol{w}, \boldsymbol{u}) + (\boldsymbol{w}, \boldsymbol{f}) + \langle \boldsymbol{w}, \boldsymbol{T} \rangle_{\boldsymbol{\Gamma}_{\boldsymbol{T}}^{int}}$$

$$(\boldsymbol{w}, \dot{\boldsymbol{u}}) = (\boldsymbol{w}, \boldsymbol{v})$$

with the initial conditions

$$(\boldsymbol{w}, \boldsymbol{u}(\cdot, 0)) = (\boldsymbol{w}, \boldsymbol{u}_0) \quad \textit{and} \quad (\boldsymbol{w}, \boldsymbol{v}(\cdot, 0)) = (\boldsymbol{w}, \boldsymbol{v}_0)$$

where $\boldsymbol{f} \in L_2(\boldsymbol{\Omega})^d$ *and* $\rho \in L^2(\boldsymbol{\Omega})$ *and*

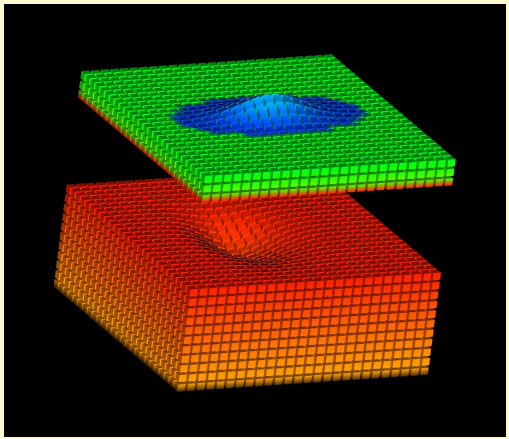
$$\mathcal{A}(\boldsymbol{w}, \boldsymbol{u}) = \int_{\boldsymbol{\Omega}} \boldsymbol{\nabla}\, \boldsymbol{w} : \boldsymbol{\sigma}(\boldsymbol{u})\, d\boldsymbol{\Omega} = \int_{\boldsymbol{\Omega}} \boldsymbol{\nabla}\, \boldsymbol{w} : \boldsymbol{C} : \boldsymbol{\nabla}\, \boldsymbol{u}\, d\boldsymbol{\Omega}$$

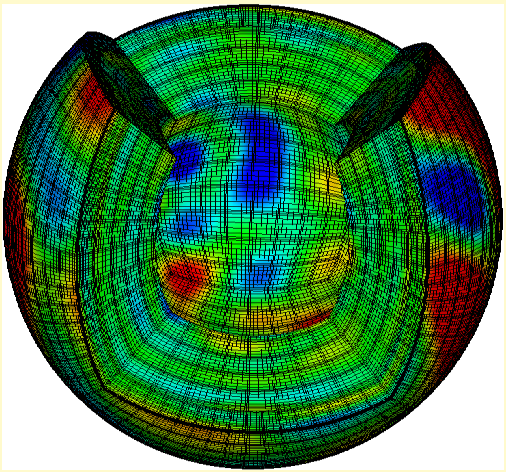
Geometrical Discretization

Like in FEM, the domain $\bar{\Omega}$ is approximated by a decomposition into n_e non-overlapping subdomains,e.g., elements,

$$\bar{\Omega} \approx \bar{\Omega}^h = \bigcup_{e=1}^{n_e} \bar{\Omega}_e \quad \text{and} \quad \Omega_e \cap \Omega_{e'} = \phi \text{ if } e \neq e'$$

This define a quadriangulation $\mathcal{I}^h$ of $\bar{\Omega}$. For classical SEM, each actual subdomain $\Omega_e \in \mathcal{I}^h(\bar{\Omega})$ is an `arbitrary convex quadrilateral`.





Geometric Mapping

Each subdomain $\bar{\Omega}_e \in \mathcal{I}^h(\bar{\Omega})$ is obtained as the image of a reference element $\square = [-1,1]^d$ using a `smooth locally compatible and invertible mapping` $\mathcal{F}_e : \square \to \bar{\Omega}_e$.

$$\mathcal{F}^e : \forall \boldsymbol{\xi} \in \square \to \boldsymbol{x} = \mathcal{F}^e(\boldsymbol{\xi}) \in \boldsymbol{\Omega}_e$$
$$\mathcal{F}^{e-1} : \forall \boldsymbol{x} \in \boldsymbol{\Omega}_e \to \boldsymbol{\xi} = \mathcal{F}^{e-1}(\boldsymbol{x}) \in \square$$

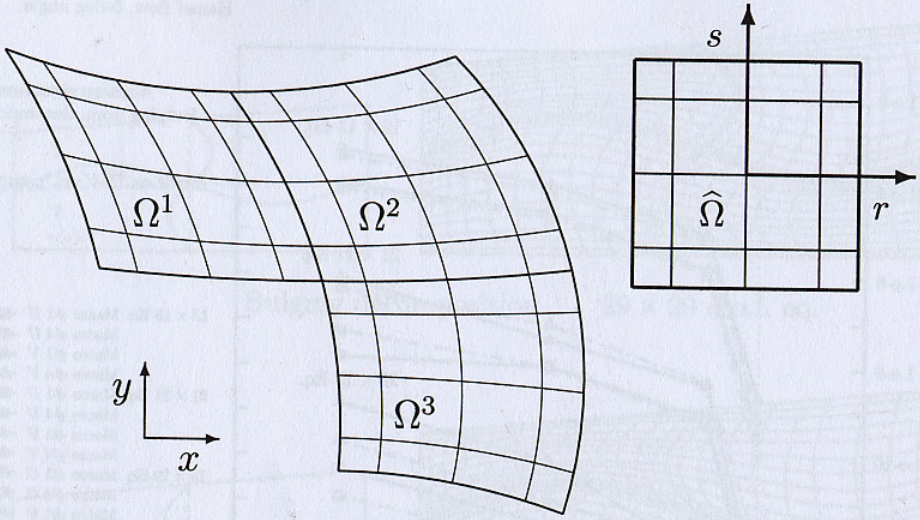
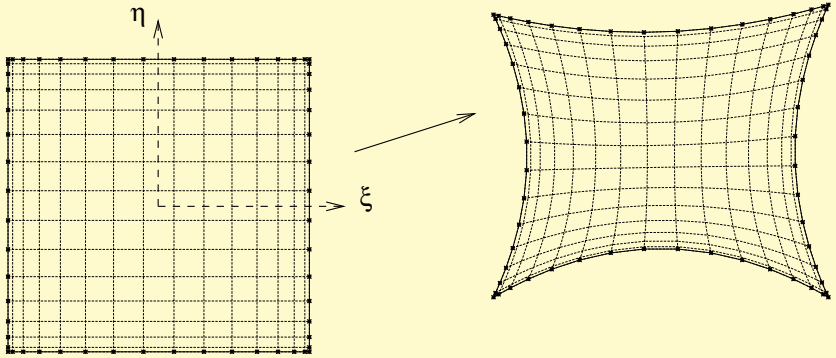


Figure 4.5.1. Example of spectral-element discretization in $\mathbb{R}^2$, showing GLL nodal lines for $(E, N) = (3, 4)$.

Note Parametric transformation



Let $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_{n_d})$, *the normalized Cartesian coordinate systems associated with the reference domain* $\square = [-1, +1]^2$, *and consider a subdomain* $\boldsymbol{\Omega}^e$ *with a geometry prescribed by a set of nodes on the boundary* $\tilde{\boldsymbol{x}}_a = \tilde{\boldsymbol{x}}(\boldsymbol{\xi}_a)$.

$$\boldsymbol{x} : \square \rightarrow \bar{\boldsymbol{\Omega}}_e \qquad ; \qquad \boldsymbol{x}(\boldsymbol{\xi}) = \sum_{a=1}^{n_g} \boldsymbol{N}_a(\boldsymbol{\xi}) \tilde{\boldsymbol{x}}_a$$

This interpolation functions needs to satisfy,

1. *Interpolation property :* $\boldsymbol{N}_a(\boldsymbol{\xi}_b) = \delta_{ab}$
2. *Constant sum property :* $\sum_a \boldsymbol{N}_a(\boldsymbol{\xi}) = 1$
3. *Conservation property :* $\sum_a \frac{\partial \boldsymbol{N}}{\partial \xi_k} = 0$

Note **2D-Subparametric transformation**

In 2D the geometrical nodes in the parent domain $\square$ *are either vertex or edge nodes.*

Example **Bilinear geometrical interpolation**

When only `vertex nodes` *are considered, a simple interpolation based on tensorized 1D Lagrangian interpolation is used,*

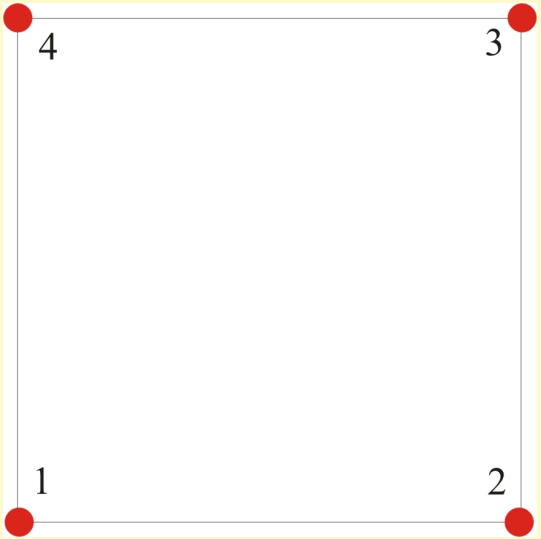
$$\textit{Vertex nodes} : N_a(\xi_1,\xi_2) = \frac{1}{4}\left(1+\xi_1\xi_{1,a}\right)\left(1+\xi_2\xi_{2,a}\right) \quad a \in [1,4]$$

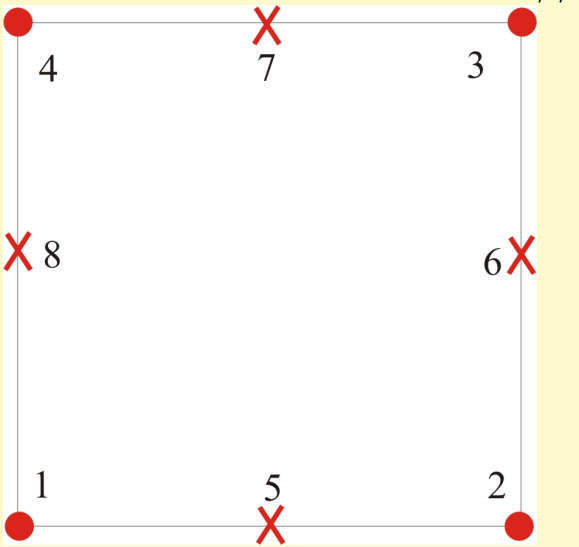
Example **Quadratic Interpolation**

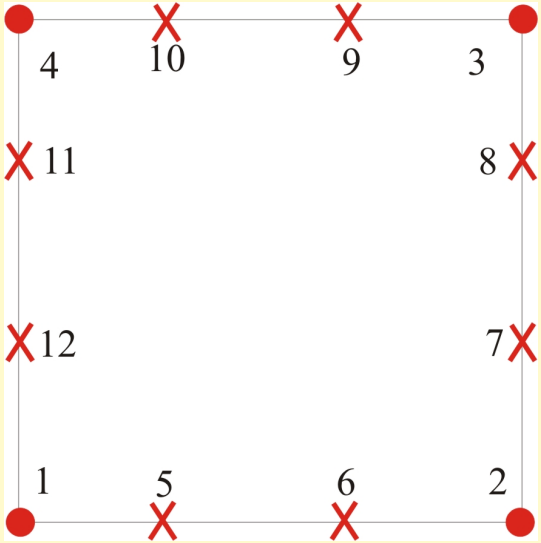
Geometrical nodes are now `vertex and midside nodes` *on each edge,*

$$\begin{aligned}
\textit{Vertex nodes} \quad & N_a(\xi_1,\xi_2) = \frac{1}{4}\left(1+\xi_1\xi_{1,a}\right)\left(1+\xi_2\xi_{2,a}\right) \quad a \in [1,4] \\
\textit{Midside nodes} \quad & N_a(\xi_1,\xi_2) = \frac{1}{2}\left(1-\xi_1^2\right)\left(1+\xi_2\xi_{2,a}\right) \quad a = 5,7 \\
& N_a(\xi_1,\xi_2) = \frac{1}{2}\left(1+\xi_1\xi_{1,a}\right)\left(1-\xi_2^2\right) \quad a = 6,8
\end{aligned}$$

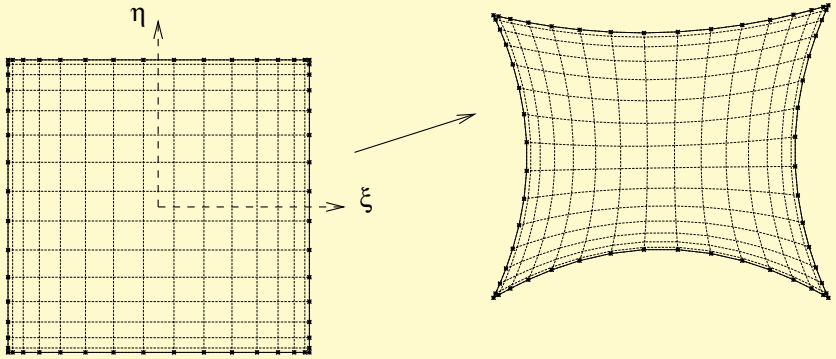
One can also alternatively use a blending technique derived from Gordon and Hall.







Definition Jacobian of the geometrical transformation



Associated with the geometric transformation $\mathcal{F}_e$, one can define the Jacobian and the inverse metrics,

$$\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\xi}} = \boldsymbol{F}^e(\boldsymbol{\xi}) = \begin{pmatrix} \frac{\partial x_1(\boldsymbol{\xi})}{\partial \xi_1} & \frac{\partial x_1(\boldsymbol{\xi})}{\partial \xi_2} \\ \frac{\partial x_2(\boldsymbol{\xi})}{\partial \xi_1} & \frac{\partial x_2(\boldsymbol{\xi})}{\partial \xi_2} \end{pmatrix}$$

and

$$\frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{x}} = \boldsymbol{F}^{1e}(\boldsymbol{\xi}) = \begin{pmatrix} \frac{\partial \xi_1(\boldsymbol{x})}{\partial x_1} & \frac{\partial \xi_1(\boldsymbol{x})}{\partial x_2} \\ \frac{\partial \xi_2(\boldsymbol{x})}{\partial x_1} & \frac{\partial \xi_2(\boldsymbol{x})}{\partial x_2} \end{pmatrix}$$

as well the determinant $J^e(\boldsymbol{\xi})$ of F^e with

$$dV_{\boldsymbol{x}} = J^e \, dv_{\boldsymbol{\xi}}$$

Problem The Initial Boundary Value Problem revisited

Associated with the domain decomposition $\bar{\boldsymbol{\Omega}}^h = \bigcup_{e=1}^{n_e} \bar{\boldsymbol{\Omega}}_e$, *it is easy to note, noting* $\boldsymbol{u}^e = \boldsymbol{u}|_{\bar{\boldsymbol{\Omega}}_e}$, *that for example*

$$(\boldsymbol{w}, \rho \dot{\boldsymbol{v}}) = \sum_{e=1}^{n_e} (\boldsymbol{w}^e, \rho^e \dot{\boldsymbol{v}}^e)\,|_{\boldsymbol{\Omega}_e} \quad ; \quad \mathcal{A}(\boldsymbol{w}, \boldsymbol{u}) = \sum_{e=1}^{n_e} \mathcal{A}^e(\boldsymbol{w}^e, \boldsymbol{u}^e)$$

$$\begin{aligned}
(\boldsymbol{w}^e, \rho^e \dot{\boldsymbol{v}}^e)\,|_{\boldsymbol{\Omega}_e} &= \int_{\square} \boldsymbol{w}^e \cdot \rho^e \dot{\boldsymbol{v}}^e \; J^e dv_{\boldsymbol{\xi}} \\
\mathcal{A}^e(\boldsymbol{w}^e, \boldsymbol{u}^e) &= \int_{\bar{\boldsymbol{\Omega}}_e} \left[\boldsymbol{\nabla} \boldsymbol{w}^e : \boldsymbol{C} : \boldsymbol{\nabla} \boldsymbol{u}^e\right] \; dV \\
&= \int_{\square} \left[\boldsymbol{\nabla}_{\boldsymbol{\xi}} \boldsymbol{w}^e \boldsymbol{F}^{e-1} : \boldsymbol{C} : \boldsymbol{F}^{e-T} \boldsymbol{\nabla}_{\boldsymbol{\xi}} \boldsymbol{u}^{eT}\right] \; J^e dv_{\boldsymbol{\xi}}
\end{aligned}$$

Remark *At that stage, it should be noted that*

- Computation at element level → seek for piecewise polynomial approximation with strong orthogonality.
- Inner products = element integral computation → require efficient and accurate numerical integration

Functional Discretization

Associated with the domain decomposition $\mathcal{I}^h$, consider a `piece-wise polynomial approximation` of the admissible displacement $\boldsymbol{u}$ and of the admissible variations $\boldsymbol{w}$ fields.
Finite-dimensional subspaces $\mathcal{S}_{\boldsymbol{u}}^h \subset \mathcal{S}_{\boldsymbol{u}}$ and $\delta\mathcal{S}^h \subset \mathcal{S}$ are :

$$\mathcal{S}_{\boldsymbol{u}}^h = \left\{ \boldsymbol{u}^h \in \mathcal{S}_{\boldsymbol{u}} \quad \text{and} \quad \boldsymbol{u}^h|_{\bar{\boldsymbol{\Omega}}_e} \circ \mathcal{F}_e \in \text{span} \bigotimes_{i=1}^{d} [\mathbb{P}_N(\xi_i)] \right\}$$
$$\delta\mathcal{V}^h = \left\{ \boldsymbol{w}^h \in \delta\mathcal{V} \quad \text{and} \quad \boldsymbol{w}^h|_{\bar{\boldsymbol{\Omega}}_e} \circ \mathcal{F}_e \in \text{span} \bigotimes_{i=1}^{d} [\mathbb{P}_N(\xi_i)] \right\}$$

$\mathbb{P}_N(\xi_i)$: the space of polynomials of degree less or equal to N.

Remark *If* $\{p_k\}_{k=0}^N$ *is the base of* $\mathbb{P}_N$ *on* $[-1,1]$, *the tensorized base on* $\square = [-1,1]^2$ *is* $\{p_k, p_l\}_{k,l=0}^N$. *For each* $\bar{\boldsymbol{\Omega}}_e$, $\boldsymbol{w}^{eh}$ *is decomposed as*

$$P_N \boldsymbol{w}^{eh} = \sum_{k,l}^{N} \hat{u}_{kl}^{eh} \; p_k(\xi_1)\, p_l(\xi_2)$$

with $[\hat{w}_{00}^{eh}, \hat{w}_{10}^{eh}, \cdots, \hat{w}_{kl}^{eh}, \cdots, \hat{w}_{NN}^{eh}]^T$ *the components of* $\boldsymbol{w}^{eh}$.

Interpolation and Quadrature

Remark Polynomes are good for you ....!

- *Problems are not all periodics. Polynomial approximations are good approximations provided smoothness conditions.* **Piecewise polynomial approximations** *and* C^0 *continuity between elements : insured with* **Lagrangian interpolation**.
- **Orthogonality** *related to topology, e.g. local suport, and* `analytical` *nature of the basis functions. Not all polynomial approximations exhibit* **spectral accuracy**, *e.g., coefficients of expansion decay faster than algebraically in* k.

Remark Numerical quadratures

- *Inner products over* $\square$ *must be fast and accurate. Both end points* (± 1) *must be included in the quadrature knots. There is* `one and only one numerical quadrature` *method that use* $N+1$ *points, including* (± 1) *on* $[-1,1]$ *and which integrate* `exactly` *polynomes of degre* $N+1$,*i.e,* $\forall \phi \in \mathbb{P}_{2N-1}$:

$$\int_{-1}^{1} \phi d\xi = \sum_{i=0}^{N} \phi(\xi_i)\rho_i, \ \xi_0 = -1 < \xi_1 < \cdots < \xi_N = 1 \ \ \rho_i > 0$$

The Gauss-Lobatto-Jacobi method.

Note Gauss-Lobatto-Legendre Quadratures

Let $\Xi_{N+1} := \{-1 = \xi_0 < \cdots < \xi_N = 1\}$, *denote* $N+1$ *quadrature nodes, generated as the solution of* $(1-x^2)\frac{d}{dx}L_N(x) = 0$, *then*

$$\int_{-1}^{1} \phi(\xi)\, dxi = \sum_{k=0}^{N} \omega_k \phi(\xi_k) \qquad \forall \phi(\xi) \in \mathbb{P}_{2N-1}$$

with $\omega_k = \frac{2}{N(N+1)} \frac{1}{(L_N(\xi_k))^2} > 0$

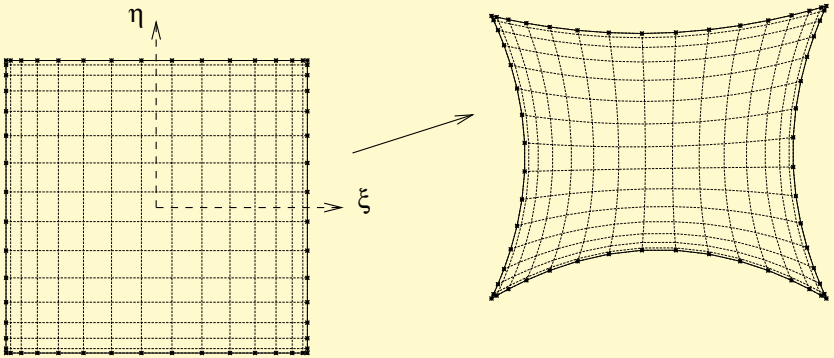
Remark *Locations of the zeros of* L'_N *can be estimated*

$$-1 \leq -\cos\left(\frac{k-1/2}{N-1/2}\right) \leq \xi_k \leq -\cos\left(\frac{k}{N-1/2}\right) \leq 1$$

The zeros of L'_N *tend to accumulate at the end points of* Λ, *a cosine expansion show that the node spacing* $\propto 1/N^2$ *near the end points and* $\propto N$ *in the middle.*

Remark *The inner products can be approximated as*

$$(w,u)_N := \sum_{k=0}^{N} \omega_k w(\xi_k) u(\xi_k) = (w,u)_{L^2(\Lambda)}\,; \forall u(x), w(x) \in \mathbb{P}_{N-1}$$



Remark *In the reference domain* $\square = [-1,1]^{n_d}$*, the quadrature is the tensor product of the 1D-GLL quadrature, defining a grid* $\bigotimes_{i=1}^{n_d} \Xi_{N+1}^{i}$ *of quadrature nodes.*

Note Discrete interpolation

$I_N u$ the Lagrange interpolation polynomial of u at $N+1$ GLL nodes,

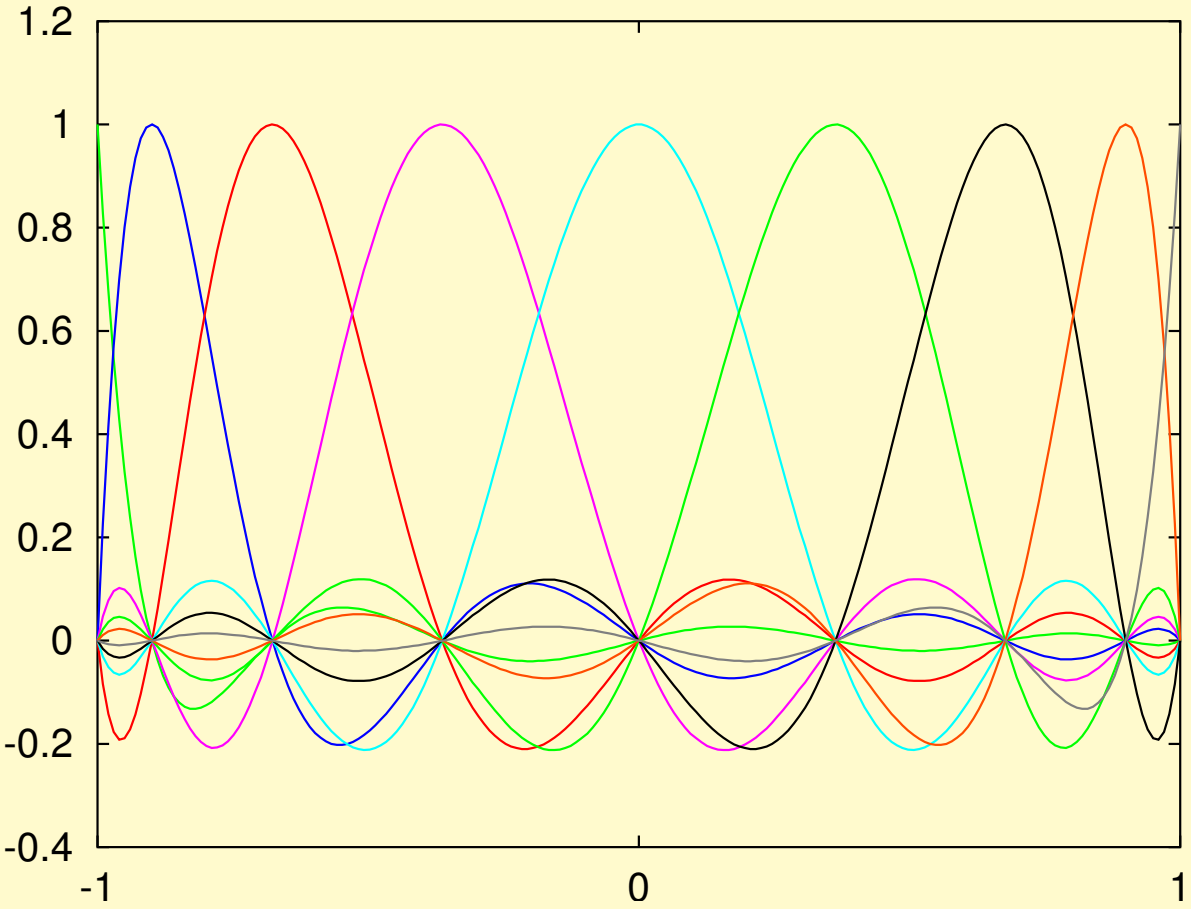
$$I_N u(\xi) = \sum_{j=0}^{N} u(\xi_j)\psi_j(\xi) \quad with \quad \psi_j(\xi) = \delta_{ij}$$

with Legendre polynomials

$$\psi_j(\xi) = -\frac{N}{N(N+1)} \frac{(1-\xi^2)L'_N(\xi)}{(\xi-\xi_j)L_N(\xi_j)}$$

Note that $(u,v)_N = (I_N u, v)_N, \forall v \in L^2(\Lambda)$

In SEM, $\mathbb{P}_N(\xi_i)$ is chosen as the space of Lagrange polynomials of degree less or equal to N associated with the $(N+1)$ Gauss-Lobatto-Legendre (GLL) quadrature nodes $\Xi_{N+1} := \{\xi_0, \xi_1, \cdots, \xi_N\} \in [-1,1]$.

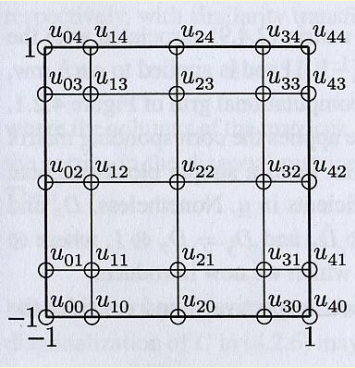

1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-1
0
1

Note Discrete element interpolation

In each $\bar{\mathbf{\Omega}}_e \in \mathcal{I}^h(\bar{\mathbf{\Omega}})$, *the tensor-product polynomial approximation :*

$$\boldsymbol{u}_i^h(\boldsymbol{x})|_{\mathbf{\Omega}_e} = u_i^{he} \circ \mathcal{F}^e(\boldsymbol{\xi}) = \sum_{r,s=0}^{N} u_{i|rs}^{he}\, h_r^N(\xi_1) h_s^N(\xi_2),$$

Useful vector representations are denoted



$$\begin{aligned}
\underline{u}_i^{eh} &:= \left(u_{i|1}^{eh}, \cdots, u_{i|\hat{l}}^{eh}, \cdots, u_{i|\mathcal{N}}^{eh}\right)^T \\
&:= \left(u_{i|00}^{eh}, u_{i|10}^{eh}, \cdots, u_{i|rs}^{eh}, \cdots, u_{i|NN}^{eh}\right)^T \\
\underline{\boldsymbol{u}}^{eh} &:= \left(\underline{u}_1^{eh}, \underline{u}_2^{eh}, \underline{u}_3^{eh}\right)^T \\
\underline{\boldsymbol{U}}_L^h &:= \left(\underline{\boldsymbol{u}}^{1h}, \underline{\boldsymbol{u}}^{2h}, \cdots, \underline{\boldsymbol{u}}^{n_e h}\right)^T
\end{aligned}$$

$\mathcal{N} = (N+1)^2$ *: total number of basis coefficients in an element,*
$\hat{l} = 1 + r + (N+1)\, s$

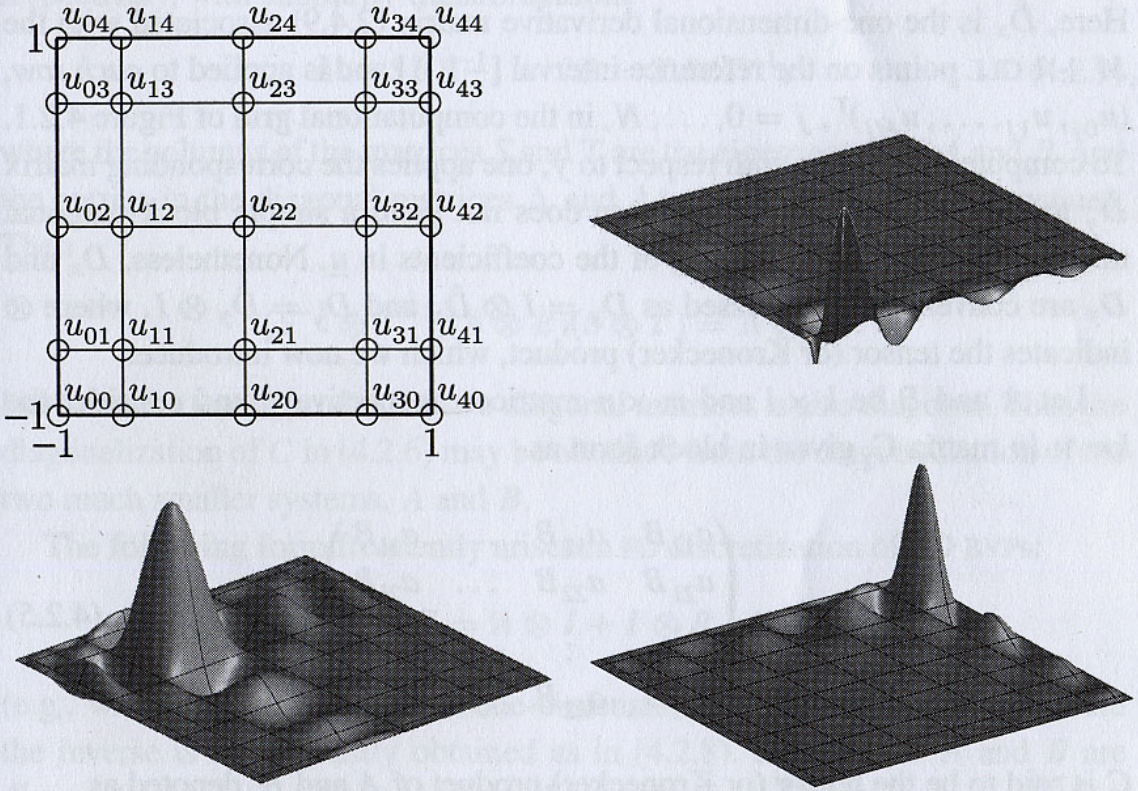


Figure 4.2.1. Clockwise from upper left: GLL nodal point distribution on $\hat{\Omega}$ for $M = N = 4$, and Lagrangian basis functions for $M = N = 10$: $\pi_{10}\pi_2$, $\pi_2\pi_9$, and $\pi_3\pi_4$.

Note Global and Local numbering

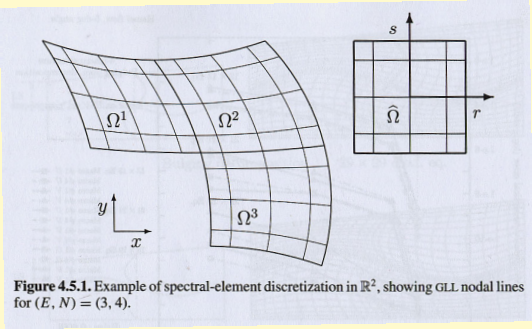


Figure 4.5.1. Example of spectral-element discretization in $\mathbb{R}^2$, showing GLL nodal lines for $(E, N) = (3, 4)$.

The construction of $\mathcal{S}_{\boldsymbol{u}}^h$ *and* $\delta\mathcal{V}^h$*, is achieved by piecing together the local polynomial interpolants and enforcing* C^0*-continuity of* $\boldsymbol{u}^{eh}$ *across the elements.*

Due to the Lagrangian basis, this simply achieved by equating coincident nodal values, e.g.

$$\boldsymbol{x}_{ij} = \boldsymbol{x}_{i'j'} \rightarrow u_l^{eh}(\boldsymbol{x}_{ij}) = u_l^{e'h}(\boldsymbol{x}_{i'j'})$$

If $\bar{\mathcal{N}}$ *is the number of distinct nodes of* $\mathcal{I}^h$*, and* $\underline{\boldsymbol{U}}^h \in \mathbb{R}^{\bar{\mathcal{N}}d}$*,the vector form associated with the global numbering. Continuity condition insures the existence of a Boolean connectivity matrix* $\boldsymbol{Q}$ *that maps* $\underline{\boldsymbol{U}}^h \rightarrow \underline{\boldsymbol{U}}_L^h$*, i.e.,*

$$\underline{\boldsymbol{U}}_L^h = \boldsymbol{Q}\underline{\boldsymbol{U}}^h.$$

Note Approximate evaluation of Derivatives

The ξ_i-derivative of $\boldsymbol{u}^{eh}$ at GLL-points (ξ_r, ξ_s),

$$u^{eh}_{i,\xi_1}(\xi_r,\xi_s) = \frac{\partial u^{eh}_i}{\partial \xi_1}(\xi_r,\xi_s) = \sum_{a,b=0}^{N} u^{eh}_{i|ab} \frac{dh^N_a}{d\xi}(\xi_r) h^N_b(\xi_s)$$

$$= \sum_{a=0}^{N} u^{eh}_{i|as} \frac{dh^N_a}{d\xi}(\xi_r) = \sum_{a=0}^{N} D^N_{ra} u^{eh}_{i|as}$$

$\boldsymbol{D}^N$ the 1-D $(N+1)^2$ derivative matrix associated with the $N+1$ GLL points

$$D^N_{ij} := \frac{dh^N_j}{d\xi}(\xi_i) = \begin{cases} \frac{L_N(\xi_i)}{L_N(\xi_j)} \frac{1}{\xi_i - \xi_j} & \text{for } i \neq j, \\ -\frac{(N+1)N}{4} & \text{if } i = j = 0, \\ \frac{(N+1)N}{4} & \text{if } i = j = N, \\ 0 & \text{otherwise.} \end{cases}$$

and in vector form

$$\underline{u}^{eh}_{i,\xi_j} = \boldsymbol{D}_j \underline{u}^{eh}_i \quad \text{with} \quad \boldsymbol{D}_1 := \boldsymbol{I}_{N+1} \otimes \boldsymbol{D}^N \; ; \; \boldsymbol{D}_2 := \boldsymbol{D}^N \otimes \boldsymbol{I}_{N+1}$$

$\boldsymbol{I}_{N+1}$ is $(N+1)^2$ identity matrix and $\otimes$ the tensor product.

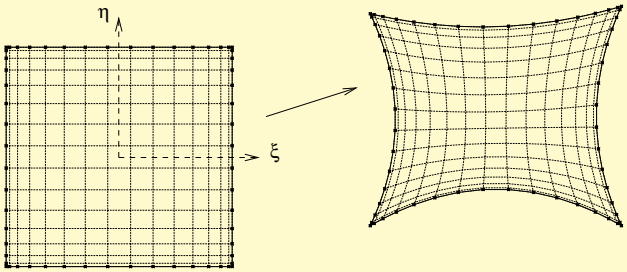
Remark *Analogously, the gradient operator in the physical domain is*

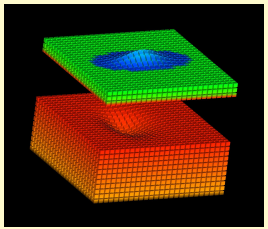
$$\underline{u}^{eh}_{i,j} := \frac{\partial \underline{u}^{eh}_i}{\partial x_j} = \sum_{p=1}^{d} \frac{\partial \underline{u}^{eh}_i}{\partial \xi_p} \underline{F}^{-1e}_{pj} = \sum_{p=1}^{d} \boldsymbol{D}_p \underline{u}^{eh}_i \underline{F}^{-1e}_{pj}$$

$$= \underline{u}^{ehT}_i \sum_{p=1}^{d} \boldsymbol{D}^T_p \underline{F}^{-1e}_{pj} = \underline{u}^{ehT}_i \tilde{\boldsymbol{D}}^T_j = \tilde{\boldsymbol{D}}_j \underline{u}^{eh}_i$$

where $F^{-1e}_{pj} = \partial \xi_p / \partial x_j$ *is the* (pj) *component of the the Jacobian associated with* $\mathcal{F}^{-1e}$.

A digest of the space discretization





- Discretization into n_e non-overlapping elements : $\bar{\mathbf{\Omega}} = \cup_{e=1}^{n_e} \bar{\mathbf{\Omega}}_e$
- mapped to a reference unit element, $\square = \Lambda^d$, $\Lambda = [-1, 1]$:

$$\mathcal{F}^e : \square \to \bar{\mathbf{\Omega}}_e \quad ; \quad \forall \boldsymbol{x} \in \bar{\mathbf{\Omega}}_e : \boldsymbol{x}(\boldsymbol{\xi}) = \mathcal{F}^e(\boldsymbol{\xi})$$

Gauss-Lobatto-Legendre Quadrature

- Gauss-Lobatto-Legendre (GLL) defined as roots of $(1 - \xi^2) L'_N(\xi)$;
- provides $(N + 1)$ points that integrate excatly polynomial of order $\leq (2N - 1)$
- defines on $\square$ a non uniform grid $\mathbf{\Xi}^N$
- polynomial approximation $\boldsymbol{w}_e^h$ chose as the Lagrange approximation on the grid $\mathbf{\Xi}^N$
- unique polynomial of $[\mathbb{P}_{\mathbb{N}}(\Lambda)]^d$ which coincides with $\boldsymbol{w}_e$ at the $N+1$-GLL points.

Semi-discrete Problem

Inserting polynomial interpolations into the variational formulation, leads to a **coupled system of ordinary differential equations**, governing the evolution at the global nodal positions,

$$\mathbb{M}\underline{\dot{\boldsymbol{V}}}^h = \mathbb{F}^{ext} - \mathbb{F}^{int}\left(\underline{\boldsymbol{U}}^h\right)$$

$$\underline{\dot{\boldsymbol{U}}}^h = \underline{\boldsymbol{V}}^h$$

where $\mathbb{M}$ is the $\left(d \cdot \bar{\mathcal{N}}\right) \times \left(d \cdot \bar{\mathcal{N}}\right)$ mass matrix.
$\mathbb{F}^{ext}$ and $\mathbb{F}^{int}\left(\underline{\boldsymbol{U}}\right)$ denote the vectors containing the external and internal forces respectively at the global nodes.

Note Assembled Matrices and Forces

The global matrices and vector forces are assembled, i.e.,

$$\mathbb{M} = \mathbf{A}_{e=1}^{n_e} \left\{ \mathbb{M}^e \right\} \; ; \; \mathbb{F}^{ext} = \mathbf{A}_{e=1}^{n_e} \left\{ \underline{\boldsymbol{F}}^{ext,e} \right\} \; ; \; \mathbb{F}^{int} = \mathbf{A}_{e=1}^{n_e} \left\{ \underline{\boldsymbol{F}}^{int,e} \right\}$$

where $\mathbf{A}_{e=1}^{n_e}$ *is the classical assembling operation, the action of which is the summation of the entries of coincident nodal values.*

Note Element Matrices

The element matrices and vector-forces are given by

$$\mathbb{M}^e = \boldsymbol{I}_d \otimes \hat{\boldsymbol{M}}^e$$
$$\underline{\boldsymbol{F}}^{e,ext} = \left(\underline{F}_1^{e,ext}, \cdots, \underline{F}_d^{e,ext}\right)^T$$
$$\underline{\boldsymbol{F}}^{e,int} = \left(\underline{F}_1^{e,int}, \cdots, \underline{F}_d^{e,int}\right)^T$$

$\boldsymbol{I}_d$ *is the* $d \times d$*-identity matrix;* $\hat{\boldsymbol{M}}^e$*, a* $\mathcal{N} \times \mathcal{N}$ *matrix and* $\underline{F}_i^{e,ext}$ *and* $\underline{F}_i^{e,int}$*,* $\mathcal{N}$*-vectors. and making use of the GLL-quadrature with* $\alpha\beta \in \bigotimes_{i=1}^{n_d=2} \Xi_{N+1}^i$

$$\hat{\boldsymbol{M}}^e_{\hat{k}\hat{k}} = \rho\left(\xi_\alpha, \xi_\beta\right) J^e\left(\xi_\alpha, \xi_\beta\right) \omega_{\alpha\beta}, \;\; \hat{k} := 1 + \alpha + (N+1)\beta$$
$$\underline{F}_i^{ext,e} = \begin{cases} \underline{f}_i^{ext,e}\, \underline{J}^e \underline{\omega} \\ \tilde{\boldsymbol{D}}_j^T \underline{m}_{ij}^e \underline{J}^e \underline{\omega} \end{cases}$$

with $\underline{J}^e_{\hat{k}} = J^e(\xi_\alpha, \xi_\beta)$ *and* $\underline{\omega}_{\hat{k}} = \omega_{\alpha\beta}$.

The mass matrix is therefore intrinsically diagonal, *a most useful property in time-stepping schemes for elastodynamics where frequent application of* $\mathbb{M}^{-1}$ *is required.*

Note Internal Forces *After similar but more cumbersome manipulations, the discrete internal forces can be written as*

$$\underline{\boldsymbol{F}}_i^{int,e} = \sum_{l=1}^{d} \sum_{p,q=1}^{d} \boldsymbol{D}_p^T \boldsymbol{G}_{iplq}^e \boldsymbol{D}_q \underline{u}_l^{eh}$$

where $\boldsymbol{G}_{iplq}^e$ *is a block diagonal matrix with*

$$\left\{ G_{iplq}^e \right\}_{\hat{k}\hat{k}} = \left[\sum_{j,m=1}^{d} F_{pj}^{-1e} C_{ijlm} F_{qm}^{-1e} \right]_{(\xi_\alpha, \xi_\beta)} J^e(\xi_\alpha, \xi_\beta) \omega_{\alpha\beta}$$

Remark *The total number of operations in 3D is only* $\propto (N+1)^4$ *thanks to the sum-factorization, and the leading order of storage is* $\propto (N+1)^3$.

Note Alternative Formulation

$$\underline{\boldsymbol{F}}_i^{int,e} = \sum_{j=1}^{d} \tilde{\boldsymbol{D}}_j^T \sum_{l,m=1}^{d} \boldsymbol{C}_{ijlm}^e \, \tilde{\boldsymbol{D}}_m \underline{u}_l^{eh} \underline{J}^e \underline{\omega}$$

$$= \sum_{j=1}^{d} \tilde{\boldsymbol{D}}_j^T \underline{\Sigma}_{ij}^{eh} \underline{J}^e \underline{\omega}$$

where

$$\underline{\Sigma}_{ij}^{eh} := \left(\Sigma_{ij|1}^{eh}, \cdots, \Sigma_{ij|\hat{l}}^{eh}, \cdots, \Sigma_{ij|\mathcal{N}}^{eh} \right)^T$$

$$\underline{\Sigma}_{ij}^{eh} = \sum_{l,m=1}^{d} \boldsymbol{C}_{ijlm}^e \, \tilde{\boldsymbol{D}}_m \underline{u}_l^{eh} = \boldsymbol{K}_{ij}^e \underline{\boldsymbol{u}}^e \quad \rightarrow \quad \underline{\boldsymbol{\Sigma}}^{eh} = \boldsymbol{K}^e \underline{\boldsymbol{u}}^{eh}$$

where $\boldsymbol{K}_{ij}^e$ *is a block-diagonal matrix*

$$\left\{ \boldsymbol{K}_{ij}^e \right\}_{\hat{k}\hat{k}} = span \bigotimes_{k=1}^{d} \left\{ \sum_{m=1}^{d} C_{ijkm} \, \tilde{\boldsymbol{D}}_m \right\} \otimes \hat{\boldsymbol{e}}_k$$

with $\hat{\boldsymbol{e}}_k$ *the canonical vectors.*

Note A velocity-Stress semi-discrete system

This allows to rewrite the discrete dynamical system, taking into account the velocity continuity, e.g. $\underline{\boldsymbol{V}}_L = \boldsymbol{Q}\underline{\boldsymbol{V}}$ *as*

$$\mathbb{M}\dot{\underline{\boldsymbol{V}}}^h = \mathbb{F}^{ext}(t) - \mathbb{F}^{int}\left(\underline{\boldsymbol{\Sigma}}_L^h\left\{\underline{\boldsymbol{U}}_L^h\right\}\right)$$
$$\dot{\underline{\boldsymbol{\Sigma}}}_L^h = \mathbb{K}_L\,\boldsymbol{Q}\underline{\boldsymbol{V}}^h$$

where $\underline{\boldsymbol{\Sigma}}_L^h = \left\{\underline{\Sigma}^{1,h}, \cdots, \underline{\Sigma}^{n_e,h}\right\}^T$

Time discretization

The discrete dynamical system obtained after the space discretization is,

$$\mathbb{M}\underline{\dot{\boldsymbol{V}}}^h = \mathbb{F}^{ext} - \mathbb{F}^{int}\left(\underline{\boldsymbol{U}}^h\right)$$

$$\underline{\dot{\boldsymbol{U}}}^h = \underline{\boldsymbol{V}}^h$$

where $\mathbb{M}$ is the $\left(d \cdot \bar{\mathcal{N}}\right) \times \left(d \cdot \bar{\mathcal{N}}\right)$ diagonal mass matrix.
$\mathbb{F}^{ext}$ and $\mathbb{F}^{int}\left(\underline{\boldsymbol{q}}\right)$ denote the $\left(d \cdot \bar{\mathcal{N}}\right)$ vectors of external and internal forces respectively at the global nodes.

Notation *Let denote now* $\underline{\boldsymbol{q}} = \underline{\boldsymbol{U}}^h$, $\underline{\dot{\boldsymbol{q}}} = \underline{\boldsymbol{V}}^h$, *the* $\left(d \cdot \bar{\mathcal{N}}\right)$ *vector of nodal displacement and nodal velocities,*

Newmark Scheme

The Newmark family of integrators originally given in Newmark (1959), is usually written for a given time discretization $t_n = n\Delta t$ as maps $(\underline{\boldsymbol{q}}_n, \dot{\underline{\boldsymbol{q}}}_n) \longrightarrow (\underline{\boldsymbol{q}}_{n+1}, \dot{\underline{\boldsymbol{q}}}_{n+1})$ by enforcing the semi-discrete momentum equations at time t_{n+1} ; i.e

$$\underline{\boldsymbol{a}}(\underline{\boldsymbol{q}}_{n+1}) = \mathbb{M}^{-1}\left(\mathbb{F}^{ext}(t_{n+1}) - \mathbb{F}^{int}(\underline{\boldsymbol{q}}_{n+1}))\right)$$

$$\underline{\boldsymbol{q}}_{n+1} = \underline{\boldsymbol{q}}_n + \Delta t \dot{\underline{\boldsymbol{q}}}_n + \Delta t^2 \left[\left(\frac{1}{2} - \beta\right)\underline{\boldsymbol{a}}(\underline{\boldsymbol{q}}_n) + \beta \underline{\boldsymbol{a}}(\underline{\boldsymbol{q}}_{n+1})\right]$$

$$\dot{\underline{\boldsymbol{q}}}_{n+1} = \dot{\underline{\boldsymbol{q}}}_n + \Delta t \left[(1-\gamma)\,\underline{\boldsymbol{a}}(\underline{\boldsymbol{q}}_n) + \alpha \underline{\boldsymbol{a}}(\underline{\boldsymbol{q}}_{n+1})\right]$$

where $\gamma \in [0, 1]$ and $\beta \in \left[0, \frac{1}{2}\right]$ specify the method.

Note More on the Newmark scheme

- **second-order accurate** if and only if $\gamma = 1/2$; *explicit when making* $\beta = 0$;
- *schemes with* $\gamma = 1/2$ *are* variational *and* exact conservation of total angularmomentum *for* $\beta/\gamma = 1/2$ *(symplectic scheme)* ;
- **Courant number** *requires :*

$$\Delta t \leq \Delta t_C = C \frac{h_{min}}{c_{max}} \qquad \Delta t_C \propto \mathcal{O}(n_e^{1/d} N^{-2})$$

- **Minimal dispersion** *requires a certain number of points per dominant wavelength* n_{max} *per dominant wavelength which scales with* c_{min} *:* $h_{disp} \propto \lambda_{dom}/n_{max}$ *with* $n_{max} \approx 5 - 8$

Mid-Point scheme

An alternative time-stepping is provided by the generalized mid-point scheme obtained by enforcing the semi-discrete momentum equations at time $t_{n+\alpha}$ with $\alpha \in [0,1]$, i.e.

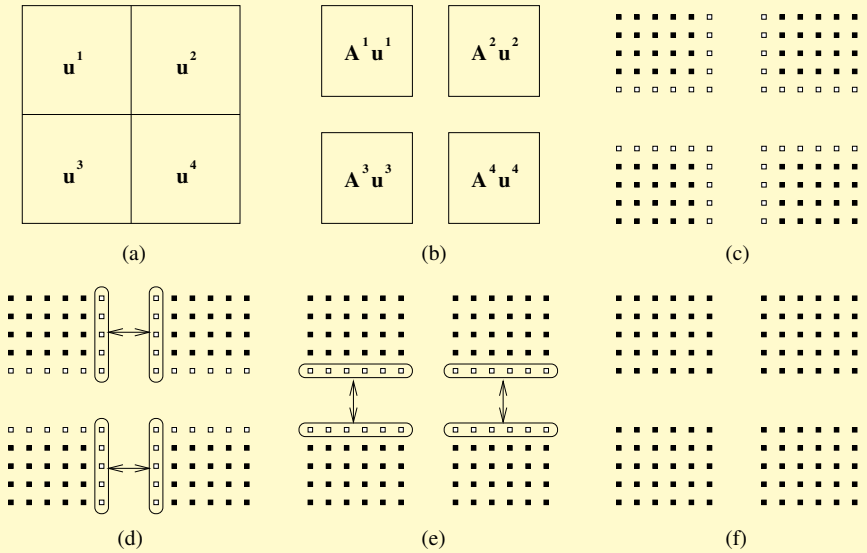
$$\underline{\dot{\boldsymbol{q}}}_{n+1} = \underline{\dot{\boldsymbol{q}}}_n + \Delta t \mathbb{M}^{-1} \left[\{(1-\alpha)\mathbb{F}^{ext}(t_n) + \alpha \mathbb{F}^{ext}(t_{n+1})\} - \mathbb{F}^{int}(\underline{\boldsymbol{q}}_{n+\alpha}) \right]$$

$$\underline{\boldsymbol{q}}_{n+1} = \underline{\boldsymbol{q}}_n + \frac{\Delta t}{2} \left(\underline{\dot{\boldsymbol{q}}}_n + \underline{\dot{\boldsymbol{q}}}_{n+1}) \right)$$

where $\underline{\boldsymbol{q}}_{n+\alpha} = (1+\alpha)\underline{\boldsymbol{q}}_n + \alpha \underline{\boldsymbol{q}}_{n+1}$

Remark *This define a second-order scheme which has also the strong property of being a simplectic scheme that conserves the total linear and angular momentum (for equilibrated loading).*

Parallelisation and Implementation



- ▷ Efficient parallel implementation on distributed memory architectures.
- ▷ Sum-factorization techniques using the tensorial structure of SEM.

Alternative Mid-point scheme

An alternative mid-point time-stepping can be derived from the velocity-stress discrete dynamical system,

$$\underline{\dot{\boldsymbol{q}}}_{n+1} = \underline{\dot{\boldsymbol{q}}}_n + \Delta t \mathbb{M}^{-1} \left[\{(1-\alpha)\mathbb{F}^{ext}(t_n) + \alpha \mathbb{F}^{ext}(t_{n+1})\} - \mathbb{F}^{int}(\boldsymbol{\Sigma}_{n+\alpha}) \right]$$
$$\underline{\boldsymbol{\Sigma}}_{n+1} = \underline{\boldsymbol{\Sigma}}_n + \Delta t \mathbb{K}_L \boldsymbol{Q} \underline{\dot{\boldsymbol{q}}}_{n+1/2}$$

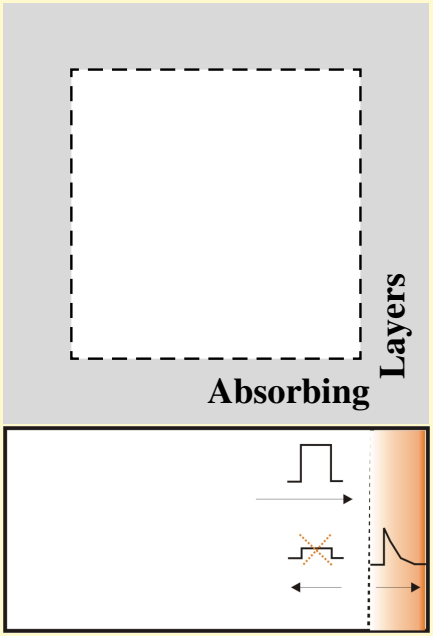
where $\underline{\dot{\boldsymbol{q}}}_{n+\alpha} = (1+\alpha)\underline{\dot{\boldsymbol{q}}}_n + \alpha \underline{\dot{\boldsymbol{q}}}_{n+1}$

Remark *Such a system can be show to be equivalent in a discrete sense to a mixed velocity-stress formulation when approximating the stress field in L^2. Such a formulation allow straightforward implementation of PML.*

The PML in SEM

Efficient absorbing boundary requires

- ▷ a limited zone, within no large increase of computation and storage
- ▷ no impedence constrast at the interface with the elastic bulk
- ▷ an exponential decay of propagating fields



Perfectly matched layer (PML)

Remark PML implementation

Analytic continuation in the complex space. For Cartesian coordinates, the continuation is achieved by

$$\tilde{x}_i = \int_0^{x_i} s_i\left(\zeta, \omega\right) d\zeta$$

where ω is the frequency. Simple expression of s

$$s_i = 1 + i\,\frac{\alpha_i\left(x_i\right)}{\omega}$$

A plane wave $e^{i(\omega t - \mathbf{k}\cdot\mathbf{x})}$ decreases inside the PML, in the x_i direction, by the factor $e^{-\frac{k_i}{\omega}\int \alpha_i(\zeta) d\zeta}$ and is independent of the frequency. The mapping induces a metric change $\tilde{\mathbf{G}} = \mathbf{\Lambda}\,\mathbf{I}_d\,\mathbf{\Lambda}$ where $\mathbf{I}_d$ is the unit metric and

$$\mathbf{\Lambda} = \begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_2 & 0 \\ 0 & 0 & s_3 \end{pmatrix} \qquad \textit{and} \qquad \tilde{\boldsymbol{\nabla}} = \mathbf{\Lambda}^{-1}\,\boldsymbol{\nabla}$$

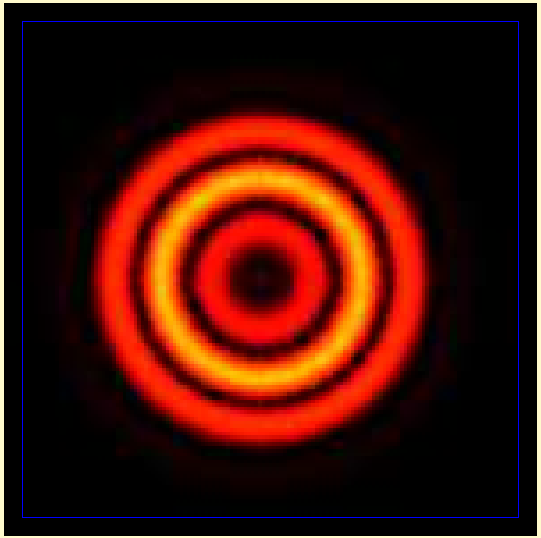
Remark PML implementation

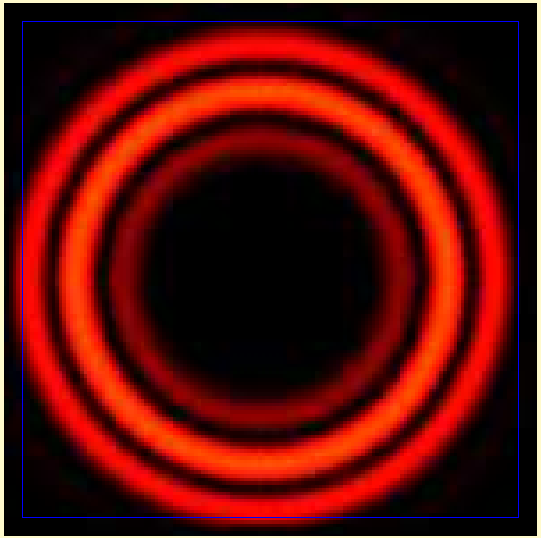
To be efficient in the time domain it requires a first-order equation (velocity-stress formulation).
Components are splitted along the directions of derivatives normal and parallel to the interface between PMLs and bulk (unphysical!)

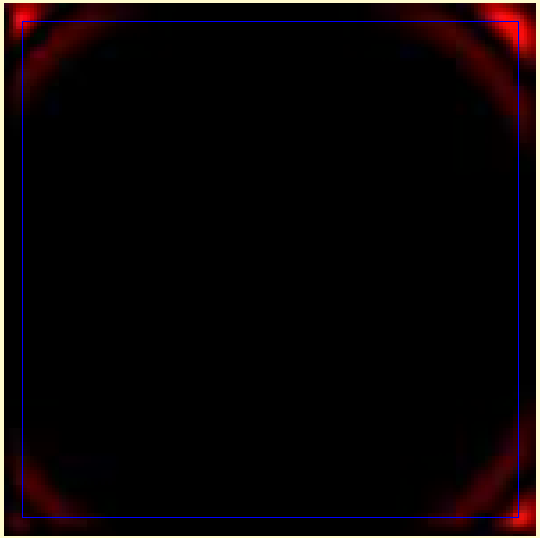
$$\rho(\dot{v}_i^{(m)} + d_m v_i^{(m)}) = \frac{\partial \sigma_{ij}}{\partial x_j}\delta_{jm}$$

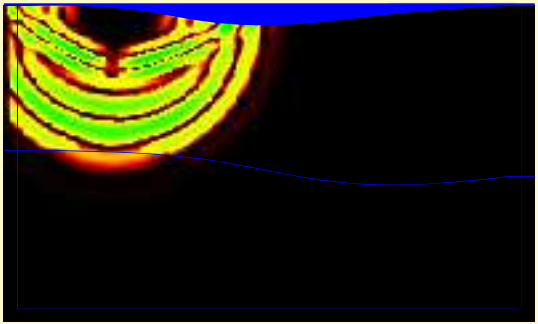
$$\dot{\sigma}_{ij}^{(m)} + d_m \sigma_{ij}^{(m)} = c_{ijkl}\frac{\partial v_l}{\partial x_k}\delta_{km}$$

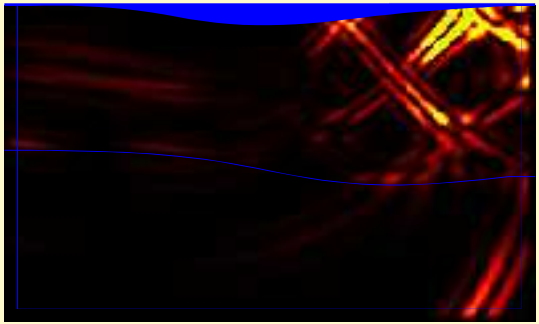
$$v_i = \sum_{m=1}^{3} v_i^{(m)}; \quad \sigma_{ij} = \sum_{m=1}^{3} \sigma_{ij}^{(m)}$$

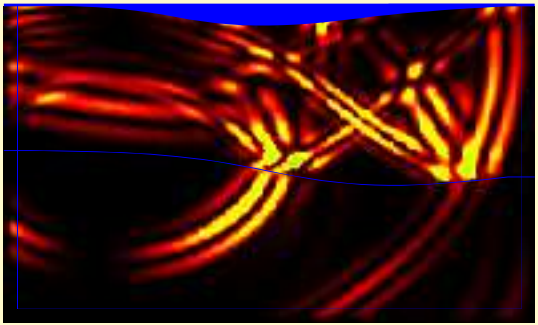


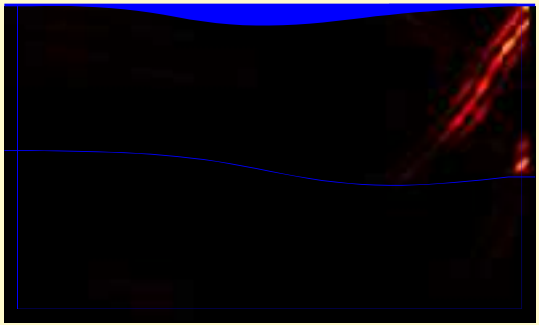




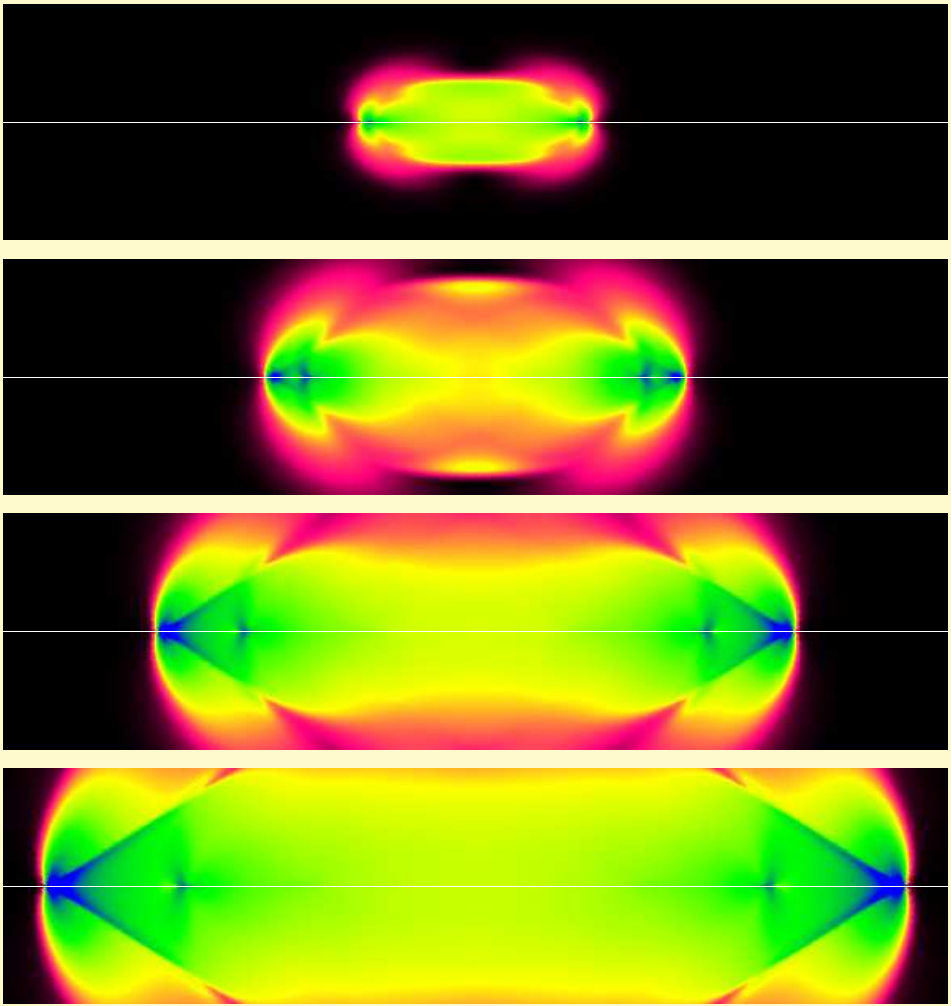




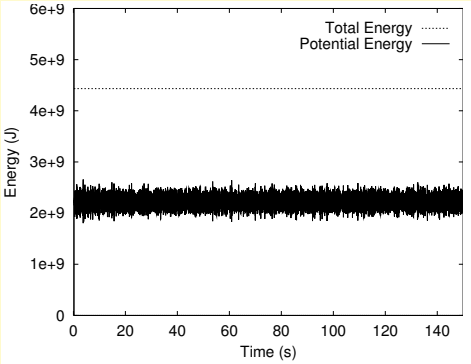




Fracture Dynamics



Energy-Momentum conservation



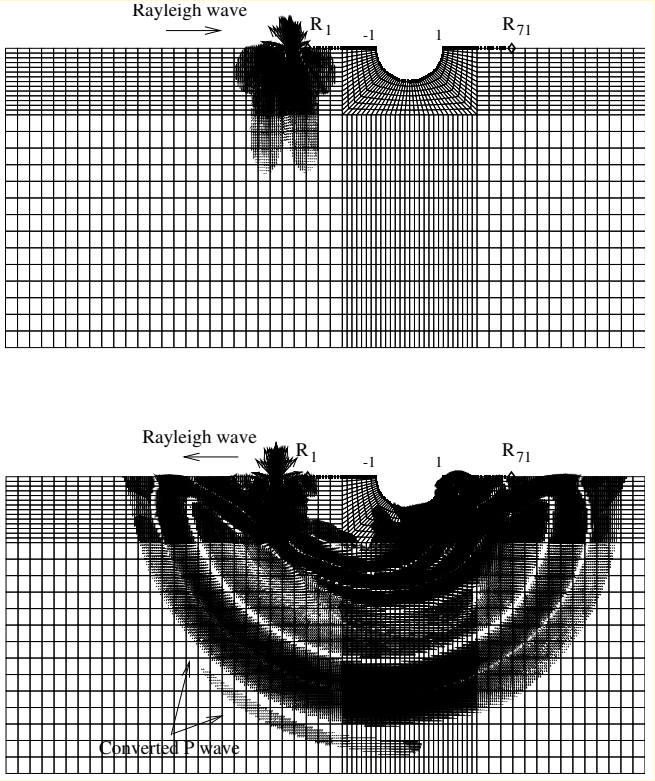
- Kinetic and potential energies :

$$U_k = \frac{1}{2}\mathbf{v}^T \mathcal{M}\, \mathbf{v}$$

$$U_p = \frac{1}{2}\int_{\mathbf{\Omega}} \nabla \mathbf{u}^h : \mathbf{c} : \nabla \mathbf{u}^h \, dV$$

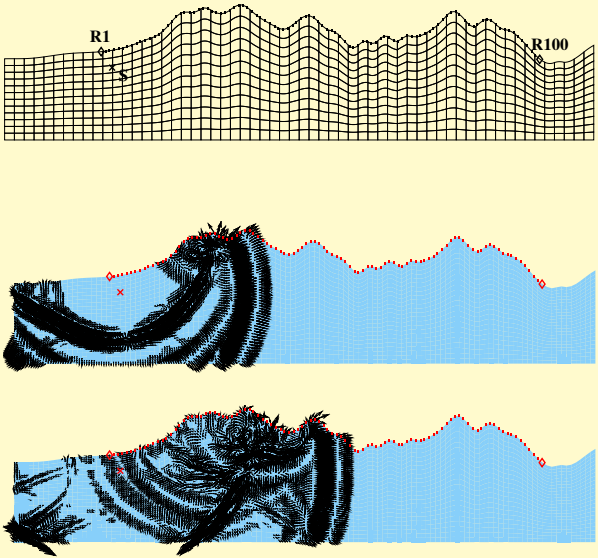
- The domain : $1600 \times 1600m$ with 484 spectral elements. $c_L = 3200m.s^{-1}$ and $c_T = 184.5m.s^{-1}$ and $\rho = 2200kg.cm^{-3}$. $f_c = 15Hz$
- Time step $\Delta t = 1.5ms$ and 10^5 time steps.
- *total energy constant while kinetic and potential energies are exhanging.*

Semi-Circular Canyon



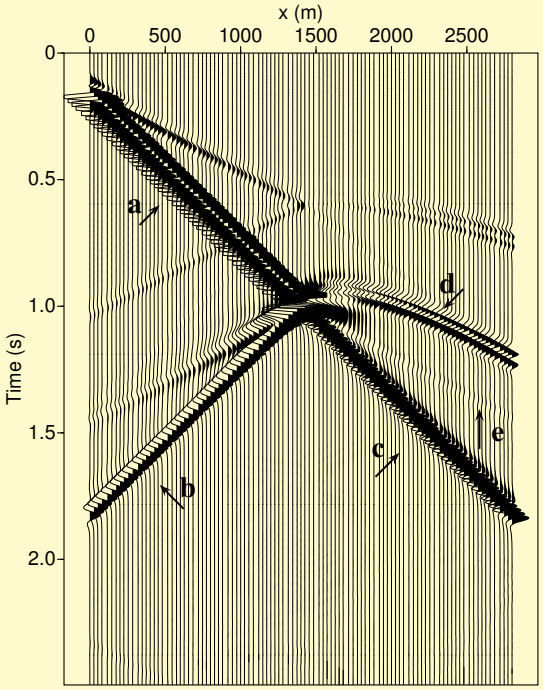
- Model : $c_L = 2000m.s^{-1}$, $c_T = 1000m.s^{-1}$, $\rho = 1000kg.m^{-3}$;
  radius of the canyon $r = 1000m$.
- Incident Rayleigh wave for an elastic half space : snapshots at $t = 3s$ and $t = 6s$.
- Horizontal component of the incident Rayleigh wave :
  Ricker with $f_{dom} = 1Hz$.
- Mesh : 1960 elements, with $N = 5$, number of nodes 49596. Propagation for $8s$ with $\Delta t = 1.25ms$.
- 71 receivers at the free surface $x \in [-3km, 3km]$
- *Diffraction pattern when the wave hits the canyon.*

Surface Topography

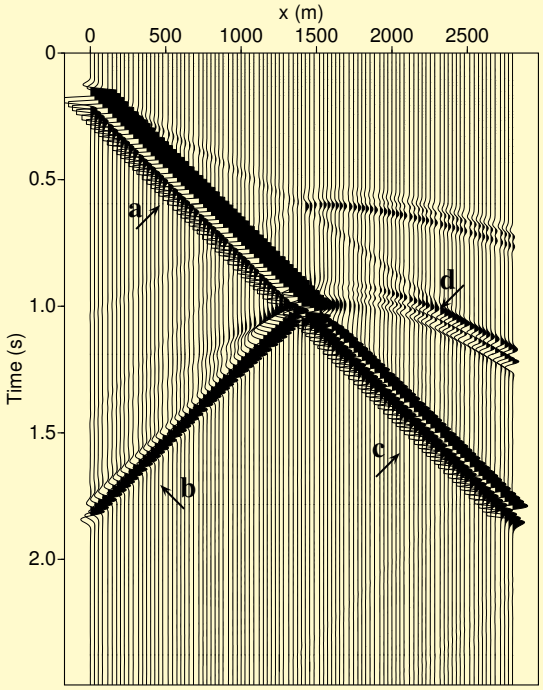


- Topography from the Peruvian Andes (courtesy TotalElf).
- Elastic half-space : $c_p = 3200m.s^{-1}$, $c_s = 1848m.s^{s-1}$, $\rho = 2200kg.m^{-3}$.
- Explosive source near the free surface, $f_c = 12Hz$.
- Width of the model $5500m$, mean height of the topography $1300m$.
- 60×12 elements, $46,657$ points.
- 5000 time steps and $\Delta t = 0.30ms$
- *Strong diffracted phases and conversion from Rayleigh to body waves*

Surface Topography

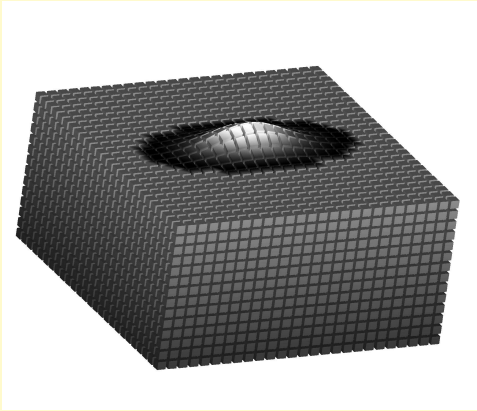


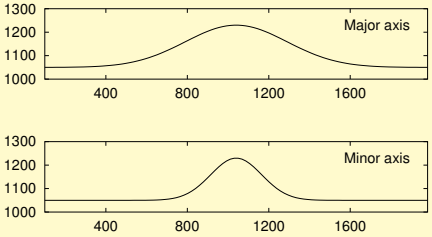
Ux component



Uz component

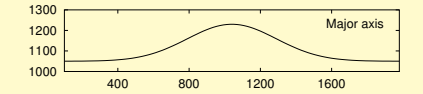
3D-Topography

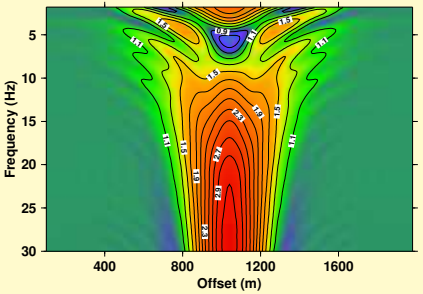


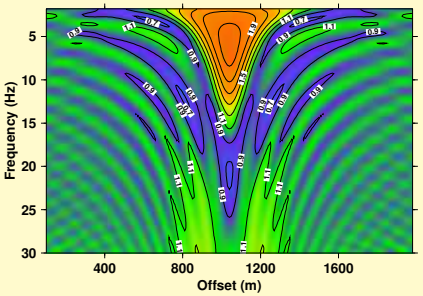


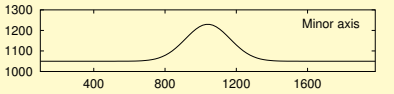
- ▷ Bi-variate Gaussian topography : $h_{max} = 180m$, $\sigma_x = 250m$, $\sigma_y = 125m$
- ▷ Incident vertical S-wave, $\lambda_s = h$ and $f_c = 10.2Hz$, polarized along the minor axis.

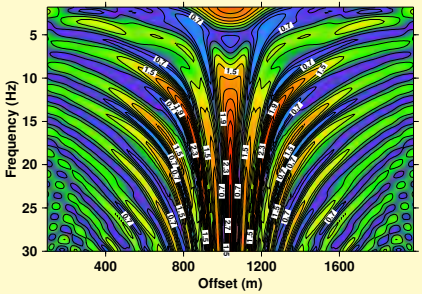
3D Topography : Transfer function

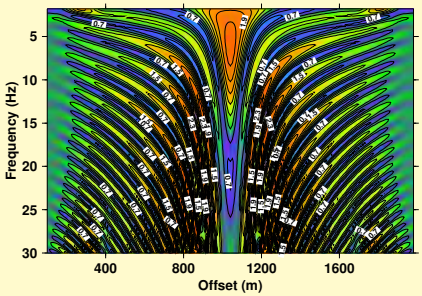




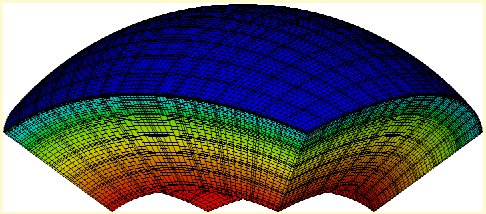


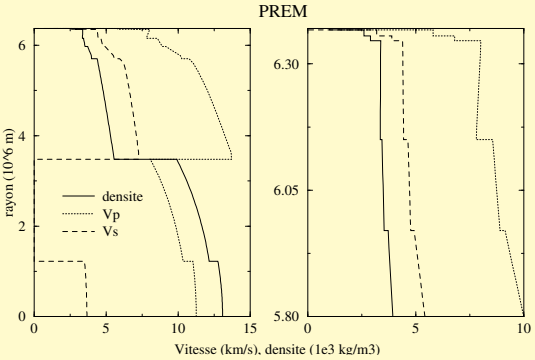


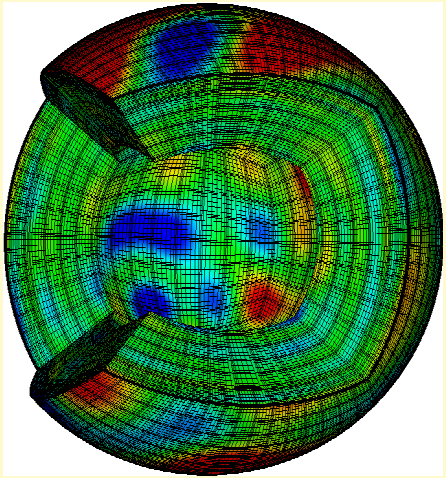




Reference Earth Models

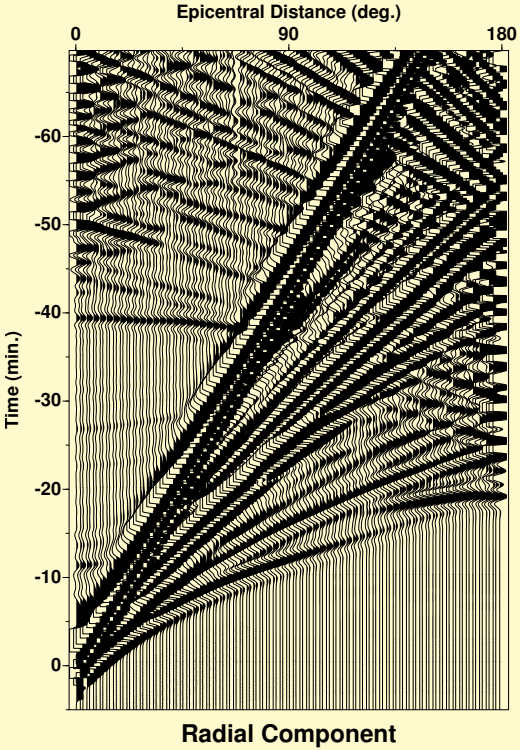


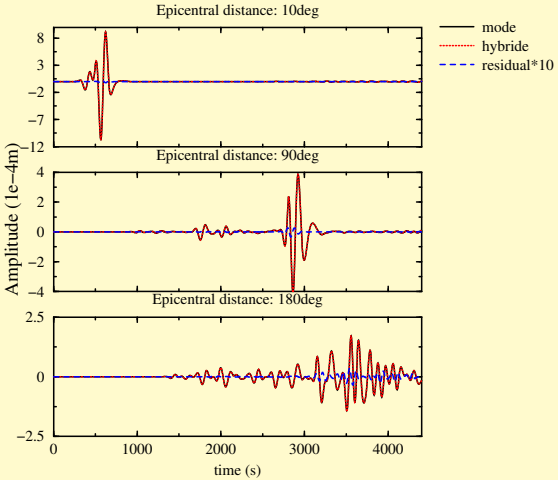




SAW12D model

Validation dans PREM





Note **Orthogonal polynomials** $\bar{\Lambda} = [-1, 1]$ *and* $\Lambda =]-1, 1[$. *The sequence of polynomial functions* $\{p_k\}_{k=0}^{\infty}$, *where* p_k *is of degree* k, *is a* `system of orthogonal polynomials` *with respect to the weight* $w(\xi) > 0, \forall \xi \in \Lambda$ *if,*

$$(p_k, p_l)_{L^2_w(\Lambda)} := \int_{-1}^{1} w(\xi) p_k(\xi)\, p_l(\xi)\, d\xi = \gamma_k \delta - kl$$

where $p_k = \|p_k\|^2_{L^2_w(\Lambda)}$ *depends on the polynomial degree.*

Remark *if* $\{p_k\}_{k=0}^{\infty}$ *is a family of orthogonal polynomials in* $\bar{\Lambda}$ *with respect to the weight function* w, *then* `the zeros of the polynomial` p_k *are real, simple and located in* Λ.

Remark *For a family of orthogonal polynomials* $\{p_k\}_{k=0}^{\infty}$ *with respect to the weight function* w, *we have the three-terms recursion relation :*

$$p_{k+1}(x) = (a_k + b_k x) p_k(x) - c_k p_{k-1}(x)$$

with a_k,b_k *and* c_k *coefficients depending on the degree* k *and on the family of orthogonal polynomials.*

Note **Sturm-Liouville problem and spectral accuracy**

A regular Sturm-Liouville Problem is an `eigenvalue problem` *of the form :*

$$-\frac{d}{dx}\left[p(x)\frac{du}{dx}(x)\right] + q(x)u(x) = \lambda(x)w(x)u(x)$$

where $w(x)$ is non negative integrable weight function, and $p(x)$ and $q(x)$ real valued functions. $p(x)$ is a continuous, non negative and bounded function over Λ, and continuous at both end (± 1), wheras $q(x)$ is continuous, non negative and bounded in Λ.
`If p vanishes at one boundary at least, the Sturm-Liouville problem is singular.`

Remark *Gotlieb and Orzag have shown that if u is* `expanded in a series of eigensolutions of a singular Sturm-Liouville problem`*, then the coefficients of the expansion decay faster than algebraically in k. This is the* **spectral accuracy property**.

Note Jacobi polynomials

The only polynomial eigenvalue of a singular Sturm-Liouville problem are the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ *with* $\alpha, \beta > -1$.

They are solutions of

$$-\frac{d}{dx}\left[(1-x^2)w^{(\alpha,\beta)}\frac{d}{dx}P_n^{(\alpha,\beta)}(x)\right] = \lambda_n^{(\alpha,\beta)}P_n^{(\alpha,\beta)}(x)$$

with $w^{(\alpha,\beta)} = (1-x)^\alpha(1+x)^\beta$ *and* $\lambda_n^{(\alpha,\beta)} = n(n+\alpha+\beta+1)$.

Remark *They satisfy the Rodrigue's formula*

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left[(1-x)^{n+\alpha}(1+x)^{n+\beta}\right]$$

- $(\alpha = \beta = 0) \longrightarrow$ **Legendre polynomials** : $L_k(x)$
- $(\alpha = \beta = 1/2) \longrightarrow$ **Chebyshev polynomials** : $T_k(x)$
- $(\alpha = \beta = -1/2) \longrightarrow$ **Chebyshev polynomials** : $U_k(x)$

Note **Legendre polynomials**

Solutions, with $w = 1$ *and* $(\alpha, \beta = 0)$*, of*

$$-\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}L_k(x)\right] = k(k+1)L_k(x)$$

The family of Legendre polynomials is an orthogonal family

$$(L_k(\xi), L_l(\xi))_{L^2(\Lambda)} = \int_{-1}^{1} L_k(\xi)\, L_l(\xi)\, d\xi = \gamma_k \delta_{kl}$$

Remark *In contrast with Chebyshev polynomials,* `no compact analytical expression` *exist for* $L_k(x)$*. Best computed with a three-term recursion relationship,*

$$L_0(x) = 1 \qquad \text{and} \qquad L_1(x) = x$$
$$(k+1)L_{k+1}(x) = (2k+1)\, x\, L_k(x) - k\, L_{k-1}(x)$$

Finally, the important relationship obtained by Maday and Bernardi,

$$(2k+1)l_k(x) = L'_{k+1}(x) - L'_{k-1}(x)$$

Note Gauss-Lobatto-Legendre Quadratures

Let $\Xi_{N+1} := \{-1 = \xi_0 < \cdots < \xi_N = 1\}$, *denote* $N+1$ *quadrature nodes, generated as the solution of* $(1-x^2)\frac{d}{dx}L_N(x) = 0$, *then*

$$\int_{-1}^{1} \phi(\xi)\, dxi = \sum_{k=0}^{N} \omega_k \phi(\xi_k) \qquad \forall \phi(\xi) \in \mathbb{P}_{2N-1}$$

with $\omega_k = \frac{2}{N(N+1)} \frac{1}{(L_N(\xi_k))^2} > 0$

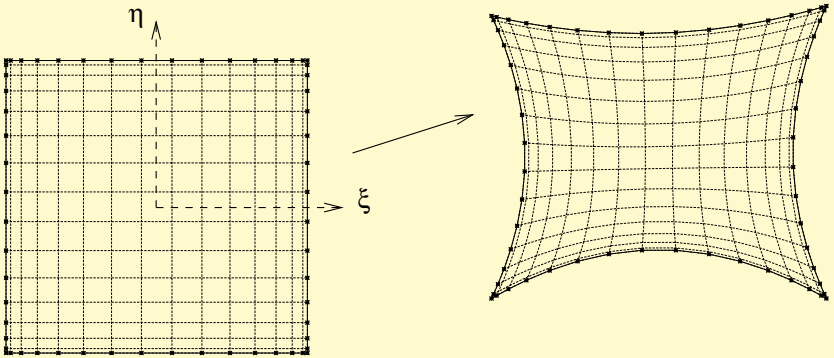
Remark *Locations of the zeros of* L'_N *can be estimated*

$$-1 \leq -\cos\left(\frac{k-1/2}{N-1/2}\right) \leq \xi_k \leq -\cos\left(\frac{k}{N-1/2}\right) \leq 1$$

The zeros of L'_N *tend to accumulate at the end points of* Λ, *a cosine expansion show that the node spacing* $\propto 1/N^2$ *near the end points and* $\propto N$ *in the middle.*

Remark *The inner products can be approximated as*

$$(w,u)_N := \sum_{k=0}^{N} \omega_k w(\xi_k) u(\xi_k) = (w,u)_{L^2(\Lambda)}\,; \forall u(x), w(x) \in \mathbb{P}_{2N-1}$$



Remark *In the reference domain* $\square = [-1,1]^{n_d}$*, the quadrature is the tensor product of the 1D-GLL quadrature, defining a grid* $\bigotimes_{i=1}^{n_d} \Xi_{N+1}^{i}$ *of quadrature nodes.*

Note Spectral approximation

Consider the family of orthogonal Legendre polynomials $L_{k\,k=0}^{\infty}$ *as a basis of* $L^2(\Lambda)$*, then*

$$u(\xi) := \sum_{k=0}^{\infty} \hat{u}_k L_k(\xi) \quad \hat{u}_k = \frac{2k+1}{2} \int_{-1}^{1} u(x) L_k(\xi)\, d\xi \quad \forall u \in L^2(\Lambda)$$

Let $P_N u$ *be the formal series truncated at degree* N

$$P_N u(\xi) = \sum_{k=0}^{N} \hat{u}_k L_k(\xi) \quad \textit{with} \quad \lim_{N\to\infty} \|u - P_N u\|_{L^2(\Lambda)} = 0$$

Note Discrete Spectral Transforms and interpolation

$I_N u$ the Lagrange interpolation of u at $N+1$ GLL nodes

$$I_N u(\xi) := \sum_{k=0}^{N} \tilde{u}_k L_k(\xi) \quad with \quad (I_n u)(\xi_k) = u(\xi_k)\ \forall \xi_k \in \Xi_{N+1}$$

Noting that $(u,v)_N = (I_N u, v)_N, \forall v \in L^2(\Lambda)$, then

$$\tilde{u}_k = \frac{1}{\gamma_k^{(N)}} \sum_{j=0}^{N} \omega_j u(\xi_j) L_k(\xi_j) \quad and \quad I_N u(\xi) = \sum_{j=0}^{N} u(\xi_j)\psi_j(\xi)$$

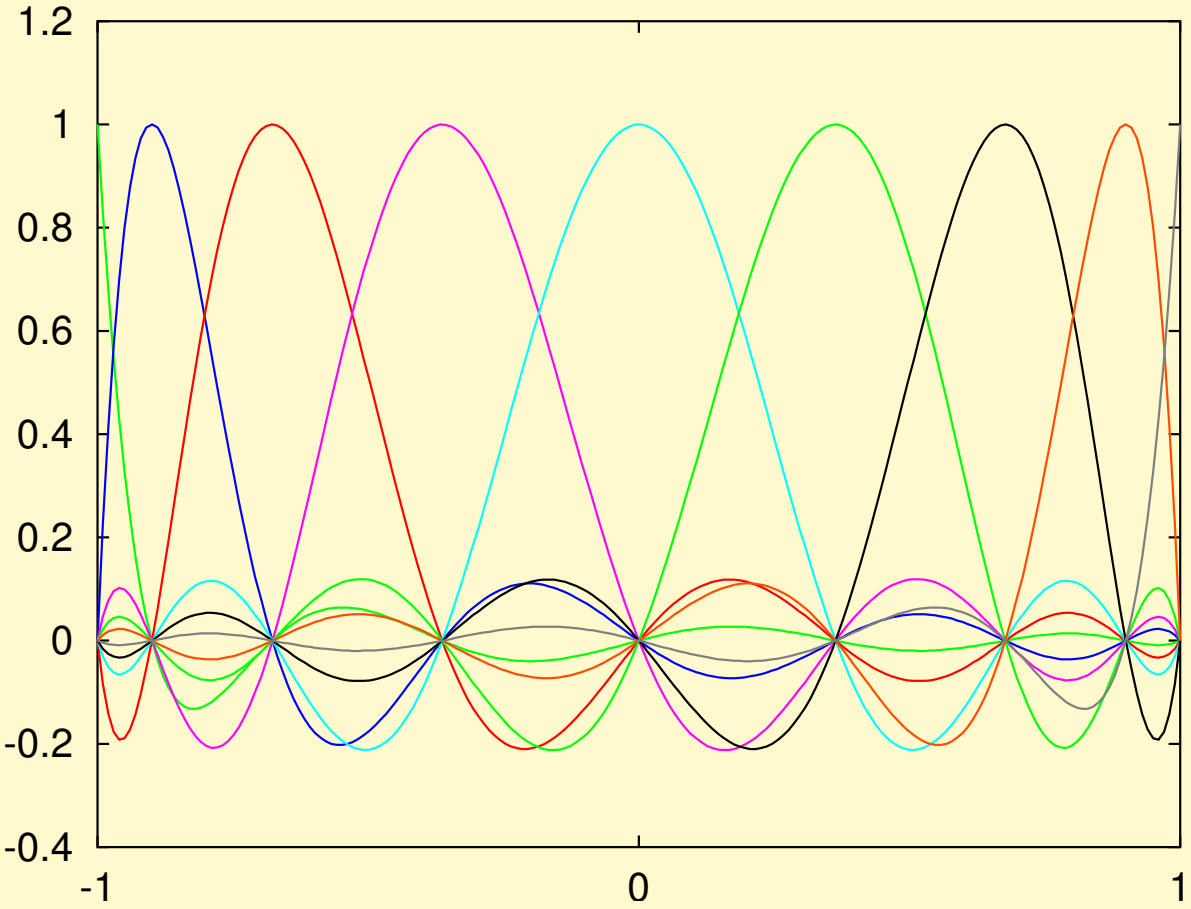
with

$$\psi(\xi_j) := \omega_j \sum_{l=0}^{N} \frac{1}{\gamma_l^{(N)}} L_l(\xi_j) L_l(\xi)\ with\ \psi_j(\xi_k) = \delta_{jk}$$

For Legendre polynomials

$$\psi_j(\xi) = -\frac{N}{N(N+1)} \frac{(1-\xi^2)L'N(\xi)}{(\xi-\xi_j)L_N(\xi_j)}$$

$I_N u(\xi) = P_N u(\xi) + R_N u(\xi)$ with $R_N u$ the aliasing error.


1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-1
0
1

Fin