1. Acoustic propagation problem

$$\nabla^2 p(\mathbf{x},t) - \mu(\mathbf{x})\frac{\partial^2 p(\mathbf{x},t)}{\partial t^2} - \zeta(\mathbf{x})\frac{\partial p(\mathbf{x},t)}{\partial t} + s(\mathbf{x},t) = 0 \quad \forall(\mathbf{x},t) \in \Omega \times (0,T], \tag{1}$$

$$p(\mathbf{x},0) = 0 \qquad \forall \mathbf{x} \in \Omega, \tag{2}$$
$$\dot{p}(\mathbf{x},0) = 0 \qquad \forall \mathbf{x} \in \Omega, \tag{3}$$
$$p(\mathbf{x},t) = \bar{p}(\mathbf{x},t) \qquad \forall(\mathbf{x},t) \in \Gamma_D \times (0,T], \tag{4}$$
$$\nabla p(\mathbf{x},t) \cdot \mathbf{n} = \bar{q}(\mathbf{x},t) \qquad \forall(\mathbf{x},t) \in \Gamma_N \times (0,T]. \tag{5}$$

This equation depends on $\mu \in L^2(\Omega)$ and $\zeta \in L^2(\Omega)$. The squared slowness is defined as $\mu(\mathbf{x}) = 1/c^2(\mathbf{x})$, being $c(\mathbf{x})$ the speed of sound in the medium.

The following sets are defined:

$$\begin{aligned}\bar{\mathcal{V}} = \{\varphi(\cdot,t) \in W^{1,m}(\Omega) : \varphi(\mathbf{x},t) = \bar{p}(\mathbf{x},t)\ \forall(\mathbf{x},t) \in \Gamma_D \times (0,T], \\ \varphi(\mathbf{x},0) = \dot{\varphi}(\mathbf{x},0) = 0\ \forall \mathbf{x} \in \Omega\}\ ,\end{aligned} \tag{6}$$

$$\mathcal{V}_0^N = \{\varphi(\cdot,t) \in W^{1,m}(\Omega) : \varphi(\mathbf{x},0) = \dot{\varphi}(\mathbf{x},0) = 0\ \forall \mathbf{x} \in \Omega\}\ , \tag{7}$$

$$\mathcal{V}_T^N = \{\varphi(\cdot,t) \in W^{1,n}(\Omega) : \varphi(\mathbf{x},T) = \dot{\varphi}(\mathbf{x},T) = 0\ \forall \mathbf{x} \in \Omega\}\ , \tag{8}$$

where $W^{1,m}(\Omega)$ is a Sobolev space defined in $\mathbb{R}^2$, such that

$$\frac{1}{m} + \frac{1}{n} = 1, \quad \text{with } 1 \leq m < 2\ . \tag{9}$$

Also, the set Γ_D accounts for nr points at the boundary $\partial\Omega$, where the measures of $\bar{p}$ are typically given:

$$\Gamma_D = \{\mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_{nr}\} \subset \partial\Omega\ . \tag{10}$$

It is considered total reflection on Γ_N, so $\bar{q} = 0$. By using these definitions and the bilinear and linear operators

$$a_k(p,\eta) = \int_0^T \int_\Omega \nabla p \cdot \nabla \eta \;\; \mathrm{d}\Omega \, \mathrm{d}t, \tag{11}$$

$$a_m(\ddot{p},\eta) = \int_0^T \int_\Omega \mu \, \ddot{p}\eta \, \mathrm{d}\Omega \, \mathrm{d}t, \tag{12}$$

$$a_c(\dot{p},\eta) = \int_0^T \int_\Omega \zeta \, \dot{p}\eta \, \mathrm{d}\Omega \, \mathrm{d}t, \tag{13}$$

$$l_0(\eta) = \int_0^T \int_\Omega s\eta \, \mathrm{d}\Omega \, \mathrm{d}t. \tag{14}$$

the variational expression of the wave equation can be stated as finding $p \in \mathcal{V}_0^N$ such that

$$a_m(\ddot{p},\eta) + a_c(\dot{p},\eta) + a_k(p,\eta) = l_0(\eta) \quad \forall \eta \in \mathcal{V}_T^N. \tag{15}$$

2. Inverse problem

Find $p \in \mathcal{V}_0^N$ solution of

$$a_m(\ddot{p},\lambda) + a_c(\dot{p},\lambda) + a_k(p,\lambda) = l_0(\lambda) \quad \forall \lambda \in \mathcal{V}_T^N. \tag{16}$$

2.1. Optimization problem

$$\mathcal{J}_{ST}(p) := \frac{1}{2} \sum_{s=1}^{ns} \int_0^T \sum_{r=1}^{nr} \left(\mathcal{Z}_r(p_s) - p^* \right)^2 \, \mathrm{d}t, \tag{17}$$

$$\mathcal{Z}_r(p_s) := \int_\Omega \delta(\mathbf{x} - \mathbf{x}_r) \, p_s \; \mathrm{d}\Omega, \tag{18}$$

where nr is the number of considered receivers, ns is the number of sources and the function $\mathcal{Z}_r(p)$ yields the value of p at the receiver position $\mathbf{x}_r$.

Let us consider a design field function $\phi(\mathbf{x})$ that controls the material property distributions in such a way that

$$\mu \to \mu(\phi) \; , \qquad \zeta \to \zeta(\phi) \; . \tag{19}$$

Standard optimization problem

$$\begin{cases} \underset{\phi}{min} \quad \mathcal{J}_{ST}^{R} = \mathcal{J}_{ST}(p) + \mathcal{R}(\phi), \\ \text{subject to} \\ a_m(\ddot{p},\lambda) + a_c(\dot{p},\lambda) + a_k(p,\lambda) = l_0(\lambda) \qquad \forall p \in \mathcal{V}_0^N, \ \forall \lambda \in \mathcal{V}_T^N. \end{cases} \tag{20}$$

2.2. Sensitivity analysis

Let the Lagrangian functional $\mathcal{L}$ be defined as

$$\mathcal{L}(p,h,\lambda,\eta) = \mathcal{J}_{KV}^{R}(p,h) + a_m(\ddot{p},\lambda) + a_c(\dot{p},\lambda) + a_k(p,\lambda) - l_0(\lambda) \tag{21}$$

with arguments $p \in \mathcal{V}_0^N, \ \ \lambda \in \mathcal{V}_T^N$.

The total variation of $\mathcal{L}$ in directions $[\delta\phi, \delta p, \delta\lambda]$ is given by

$$\delta\mathcal{L} = \frac{\partial \mathcal{L}}{\partial \phi}[\delta\phi] + \frac{\partial \mathcal{L}}{\partial p}[\delta p] + \frac{\partial \mathcal{L}}{\partial \lambda}[\delta\lambda]. \tag{22}$$

The first stationary conditions of $\mathcal{L}$ over direction $\delta\lambda$ provide the already defined *forward propagation problem*:

$$\frac{\partial \mathcal{L}}{\partial \lambda}[\delta\lambda] = a_m(\ddot{p},\delta\lambda) + a_c(\dot{p},\delta\lambda) + a_k(p,\delta\lambda) - l_0(\delta\lambda) = 0 \ \ \forall \delta\lambda \in \mathcal{V}_T^N, \tag{23}$$

Reciprocally, first stationary condition of $\mathcal{L}$ over direction δp provide variational expressions for the so-called *adjoint propagation problem*:

$$\frac{\partial \mathcal{L}}{\partial p}[\delta p] = \frac{\partial}{\partial p}\mathcal{J}_{KV}^{R}[\delta p] + a_m(\delta\ddot{p},\lambda) + a_c(\delta\dot{p},\lambda) + a_k(\delta p,\lambda) = 0 \quad \forall \delta p \in \mathcal{V}_0^N, \tag{24}$$

The adjoint problem in Eq. (24) seek for the field $\lambda \in \mathcal{V}_T^N$ that solve the variational expression:

$$\frac{\partial \mathcal{L}}{\partial p}[\delta p] = \int_0^T \int_\Omega \left(\mu \, \delta p \ddot{\lambda} \ - \zeta \, \delta p \dot{\lambda} + \nabla \delta p \cdot \nabla \lambda + (p - p^*)\delta p \right) \mathrm{d}\Omega \, \mathrm{d}t = 0, \tag{25}$$

where p is the solutions of the forward propagation problem in Eq. (23).

Now, given the set $\{p, \lambda\}$ satisfying Eq. (23) and Eq. (25), one has the equivalences

$$\mathcal{J}_{ST}^{R}(p) = \mathcal{L}(p, \lambda), \tag{26}$$

$$\frac{d}{d\phi}\mathcal{J}_{ST}^{R}[\delta\phi] = \frac{\partial \mathcal{L}}{\partial \phi}[\delta\phi], \tag{27}$$

By operating such a derivative considering the dependence in Eq. (19), one has

$$\frac{d}{d\phi}\mathcal{J}_{ST}[\delta\phi] = \int_{\Omega}\left(\int_{0}^{T}\frac{\partial \mu}{\partial \phi}[\delta\phi]\ddot{p}\lambda + \frac{\partial \zeta}{\partial \phi}[\delta\phi]\dot{p}\lambda\ \mathrm{d}t\right)\mathrm{d}\Omega, \tag{28}$$

which after some simplification and integration by parts leads to

$$\frac{d}{d\phi}\mathcal{J}_{ST}[\delta\phi] = -\int_{\Omega}\frac{\partial \mu}{\partial \phi}[\delta\phi]\mathcal{S}_{\mu}\, d\Omega - \int_{\Omega}\frac{\partial \zeta}{\partial \phi}[\delta\phi]\mathcal{S}_{\zeta}\, d\Omega, \tag{29}$$

where $\mathcal{S}_{\mu}$ and $\mathcal{S}_{\zeta}$ are called *sensitivity fields*:

$$\mathcal{S}_{\mu} = \int_{0}^{T}\dot{p}\dot{\lambda}\ \mathrm{d}t, \tag{30}$$

$$\mathcal{S}_{\zeta} = \int_{0}^{T}p\dot{\lambda}\ \mathrm{d}t. \tag{31}$$

We recall that, when more than a single source case is being used ($s > 1$) we have to include the summation over each source case:

$$\mathcal{S}_{\mu} = \sum_{s=1}^{ns}\int_{0}^{T}\dot{p}_s\dot{\lambda}_s\ \mathrm{d}t, \tag{32}$$

$$\mathcal{S}_{\zeta} = \sum_{s=1}^{ns}\int_{0}^{T}p_s\dot{\lambda}_s\ \mathrm{d}t, \tag{33}$$

where $p_s, \dot{p}_s, \lambda_s, \dot{\lambda}_s$... are the corresponding fields associated to the s-load case.

3. Level set based material model

For the sake of simplicity, consider first the distribution of the squared-slowness μ and the following definitions:

$$\phi(\mathbf{x}) \in [-1, 1], \tag{34}$$

$$H(\phi) = \begin{cases} 1 & \text{if } \phi(\mathbf{x}) \geq 0 \\ 0 & \text{otherwise} \end{cases}, \tag{35}$$

$$\mu(\phi) = \mu_1 H(\phi) + \mu_2(1 - H(\phi)). \tag{36}$$

The derivative of this material model with respect to ϕ is

$$\frac{\partial \mu}{\partial \phi} = (\mu_1 - \mu_2)\frac{\partial H}{\partial \phi} = \bar{\mu}\frac{\partial H}{\partial \phi}, \tag{37}$$

$$\frac{\partial H}{\partial \phi} = \delta(\phi), \tag{38}$$

where $\bar{\mu} = \mu_1 - \mu_2$ is the *contrast* of the material property between regions and $\delta(\phi)$ the Dirac function. Recalling Eq. (29) and substituting above material model for both μ and ζ one has

$$\frac{d}{d\phi}\mathcal{J}_{ST}[\delta\phi] = -\int_{\Omega} \left(\bar{\mu}\,\mathcal{S}_\mu + \bar{\zeta}\,\mathcal{S}_\zeta\right) \delta(\phi)\,\delta\phi \,\mathrm{d}\Omega. \tag{39}$$

or

$$\mathcal{S} = \bar{\mu}\,\mathcal{S}_\mu + \bar{\zeta}\,\mathcal{S}_\zeta. \tag{40}$$

4. Optimization procedure: reaction-diffusion problem

The following Tikhonov regularization term is used in Eqs. (20):

$$\mathcal{R}(\phi) = \int_{\Omega} \tau ||\nabla\phi||^2 \,\mathrm{d}\Omega. \tag{41}$$

The rate of change of the design function $\phi(\mathbf{x})$ with respect to the *pseudo-time* θ is equal to the gradient of the regularized objective function:

$$\frac{\partial \phi}{\partial \theta} = -\frac{d}{d\phi}\mathcal{J}^R_{ST}. \tag{42}$$

The evaluation of the Eq. (42) leads to

$$\frac{\partial \phi}{\partial \theta} = \tau\nabla^2\phi - \frac{d}{d\phi}\mathcal{J}_{ST}, \tag{43}$$

which is also referred to as Allen-Cahn equation.

This problem can be written as

$$\begin{cases} \frac{\partial\phi}{\partial\theta} = \tau\nabla^2\phi - \frac{d}{d\phi}\mathcal{J}_{ST} & \forall(\mathbf{x},\theta) \in \Omega\ \times (0,\Theta], \\ \nabla\phi\cdot\mathbf{n} = 0 & \forall(\mathbf{x},\theta) \in \Gamma_N\ \times (0,\Theta], \\ \phi = c_t & \forall(\mathbf{x},\theta) \in \Gamma_D\ \times (0,\Theta], \\ \phi(\mathbf{x},0) = \phi_0 & \forall\mathbf{x} \in \Omega, \end{cases} \tag{44}$$

considering c_t a constant and Θ the pseudo-time period of the reaction-diffusion.

5. Spatial and temporal discretization

5.1. Spatial (FEM) discretization

Consider $\mathbf{N}$ the vector of Finite Element (FE) quadrilateral-bilinear interpolation functions and $\mathbf{p}$, $\dot{\mathbf{p}}$, $\ddot{\mathbf{p}}$ and $\boldsymbol{\lambda}$ the vectors of nodal values corresponding to the respective fields.

$$p(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\mathbf{p}(t), \qquad \dot{p}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\dot{\mathbf{p}}(t), \qquad \ddot{p}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\ddot{\mathbf{p}}(t), \tag{45}$$

$$\lambda(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\boldsymbol{\lambda}(t). \tag{46}$$

Also, the gradient of the pressure field can be written as

$$\nabla p \simeq \mathbf{B}\mathbf{p}\,, \qquad \mathbf{B} = \nabla\mathbf{N}. \tag{47}$$

The final discrete form of $\mathcal{P}_1$ is written as

$$\mathbf{M}\ddot{\mathbf{p}} + \mathbf{C}\dot{\mathbf{p}} + \mathbf{K}\mathbf{p} = \mathbf{f} \qquad \forall t \in (0,T], \tag{48}$$

where

$$\mathbf{M}(\phi) = \int_\Omega \mu(\phi)\,\mathbf{N}^T\mathbf{N}\,\mathrm{d}\Omega, \tag{49}$$

$$\mathbf{C}(\phi) = \int_\Omega \zeta(\phi)\,\mathbf{N}^T\mathbf{N}\,\mathrm{d}\Omega, \tag{50}$$

$$\mathbf{K} = \int_\Omega \mathbf{B}^T\mathbf{B}\,\mathrm{d}\Omega, \tag{51}$$

$$\mathbf{f} = \int_\Omega s\mathbf{N}\,\mathrm{d}\Omega. \tag{52}$$

For the adjoint problem, the procedure is analogous. Considering the Eq. (25), and the additional approximations

$$\dot{\lambda}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\dot{\boldsymbol{\lambda}}(t), \qquad \ddot{\lambda}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\ddot{\boldsymbol{\lambda}}(t), \tag{53}$$

$$\dot{\eta}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\dot{\boldsymbol{\eta}}(t), \qquad \ddot{\eta}(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\ddot{\boldsymbol{\eta}}(t), \tag{54}$$

$$\delta p(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\delta\mathbf{p}(t), \tag{55}$$

$$\delta h(\mathbf{x},t) \simeq \mathbf{N}(\mathbf{x})\delta\mathbf{h}(t), \tag{56}$$

one has the final discrete form:

$$\mathbf{M}\ddot{\boldsymbol{\lambda}} - \mathbf{C}\dot{\boldsymbol{\lambda}} + \mathbf{K}\boldsymbol{\lambda} = -\mathbf{f}_a \qquad \forall t \in (0,T], \tag{57}$$

The adjoint force $\mathbf{f}_a$ considers the solution field $\mathbf{p}$ and the experimental data $\mathbf{p}^*$, then

$$\mathbf{f}_a = \mathbf{p} - \mathbf{p}^*. \tag{58}$$

5.2. Time discretization

A discrete solution given by Newmark's method is first introduced by the Eqs. (59-62) for a generic problem set $\{\mathbf{u},\mathbf{v},\mathbf{a}\}$, that is,

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t\mathbf{v}_n + \Delta t^2\left[\left(\frac{1}{2}-\beta\right)\mathbf{a}_n + \beta\mathbf{a}_{n+1}\right], \tag{59}$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + \Delta t\left[(1-\gamma)\,\mathbf{a}_n + \gamma\mathbf{a}_{n+1}\right], \tag{60}$$

$$\mathbf{M}\mathbf{a}_0 + \mathbf{C}\mathbf{v}_0 + \mathbf{K}\mathbf{u}_0 = \mathbf{f}_0, \tag{61}$$

where the solution $\mathbf{a}_{n+1}$ is given by

$$\begin{aligned}(\mathbf{M} + \gamma\Delta t\mathbf{C} + \beta\Delta t^2\mathbf{K})\mathbf{a}_{n+1} =& \mathbf{f}_{n+1} - \mathbf{C}\left[\mathbf{v}_n + (1-\gamma)\,\Delta t\mathbf{a}_n\right] \\ & -\mathbf{K}\left[\mathbf{u}_n + \Delta t\mathbf{v}_n + \left(\frac{1}{2}-\beta\right)\Delta t^2\mathbf{a}_n\right].\end{aligned} \tag{62}$$

The time march procedure presented above is used to solve all forward and adjoint problems.

5.3. Reaction-diffusion discretization

The level set and its gradient are, respectively, represented by

$$\phi(\mathbf{x},\theta) \simeq \mathbf{N}(\mathbf{x})\boldsymbol{\Phi}(\theta), \qquad \dot{\phi}(\mathbf{x},\theta) \simeq \mathbf{N}(\mathbf{x})\dot{\boldsymbol{\Phi}}(\theta), \tag{63}$$

$$\nabla\phi(\mathbf{x},\theta) \simeq \mathbf{B}(\mathbf{x})\boldsymbol{\Phi}(\theta)\ . \tag{64}$$

The variation of ϕ and its gradient are then

$$\delta\phi(\mathbf{x},\theta) \simeq \mathbf{N}(\mathbf{x})\delta\boldsymbol{\Phi}(\theta), \tag{65}$$

$$\nabla\delta\phi(\mathbf{x},\theta) \simeq \mathbf{B}(\mathbf{x})\delta\boldsymbol{\Phi}(\theta). \tag{66}$$

Moreover, one can write the sensitivity field in the discrete form as

$$\mathcal{S} \simeq \mathbf{N}(\mathbf{x})\boldsymbol{S}. \tag{67}$$

By applying the Eq. (40) the array of sensitivity parameters $\boldsymbol{S}$ takes the form

$$\boldsymbol{S} = -\bar{\mu}\int_0^T (\dot{\mathbf{p}} \circ \dot{\boldsymbol{\lambda}})\,\mathrm{d}t - \bar{\zeta}\int_0^T (\mathbf{p} \circ \dot{\boldsymbol{\lambda}})\,\mathrm{d}t, \tag{68}$$

where the operator $\circ$ represents the Hadamard product : $(\mathbf{a}\circ\mathbf{b})_i = a_i b_i\ ,\ i = 1, ..., \mathrm{ndof}$.

The development of the discrete form of the reaction-diffusion leads to

$$\mathbf{K}_L\Phi + \mathbf{C}_L(\dot{\Phi} + \boldsymbol{S}) = 0, \tag{69}$$

where

$$\mathbf{K}_L = \int_\Omega \tau\mathbf{B}^T\mathbf{B}\,\mathrm{d}\Omega, \qquad \mathbf{C}_L = \int_\Omega \mathbf{N}^T\mathbf{N}\,\mathrm{d}\Omega. \tag{70}$$

The time discretization considering the pseudo-time is performed by means of a finite difference scheme as

$$\dot{\Phi} = \left.\frac{\partial\Phi}{\partial\theta}\right|_{n+1} \approx \frac{\Phi_{n+1} - \Phi_n}{\Delta\theta}, \tag{71}$$

and consequently

$$\mathbf{K}_L\Phi_{n+1} + \mathbf{C}_L\left(\frac{\Phi_{n+1} - \Phi_n}{\Delta\theta} + \boldsymbol{S}\right) = 0. \tag{72}$$

By applying the trapezoidal integration rule to calculate $\boldsymbol{S}$, calling $\mathbf{g}_1(t) = -(\dot{\mathbf{p}} \circ \dot{\boldsymbol{\lambda}})$ and $\mathbf{g}_2(t) = -(\mathbf{p} \circ \dot{\boldsymbol{\lambda}})$, one can find

$$\begin{aligned}\boldsymbol{S} &= \bar{\mu} \int_0^T \mathbf{g}_1(t)\,\mathrm{d}t + \bar{\zeta} \int_0^T \mathbf{g}_2(t)\,\mathrm{d}t \\ &\simeq \bar{\mu} \sum_{n=0}^{N_{\text{steps}}} \frac{1}{2}\big(\mathbf{g}_1(t_n) + \mathbf{g}_1(t_{n+1})\big)\Delta t + \bar{\zeta} \sum_{n=0}^{N_{\text{steps}}} \frac{1}{2}\big(\mathbf{g}_2(t_n) + \mathbf{g}_2(t_{n+1})\big)\Delta t,\end{aligned} \tag{73}$$

in which N_{steps} is the total number of time steps and Δt has a constant value.