TRANSIENT ACOUSTIC WAVEFIELD COMPUTATION - FROM PHYSICS VIA MATHEMATICS TO COMPUTATIONAL PHYSICS

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The **objective** is to construct a **computational discretization** of the (forward) acoustic wave problem that is

- as **coherent** and **internally consistent** as possible
- as **close** as possible to the **physics of the problem**

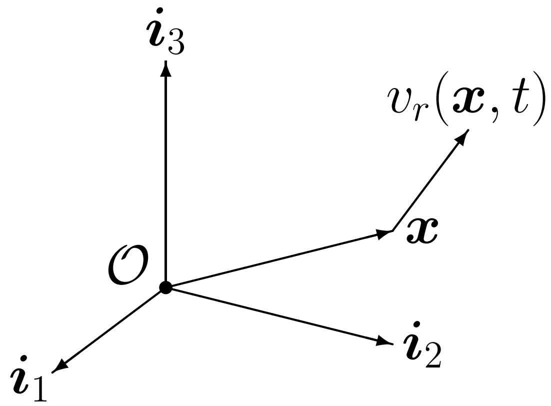
Type of **configuration**:

- piecewise continuous distribution of constitutive parameters
- piecewise continuous volume source distributions

Guideline:

- avoid spatial delta distributions!

Reference frame in $\mathcal{R}^3$



Position vector

$$\boldsymbol{x} \;=\; x_1\boldsymbol{i}_1 + x_2\boldsymbol{i}_2 + x_3\boldsymbol{i}_3$$

Subscript notation and summation convention

$$\rho_{k,r}v_r \;=\; \sum_{r=1}^{3} \rho_{k,r}v_r \quad \text{for } k = 1, 2, 3$$

Cartesian reference frame, subscript notation

The **acoustic wave quantities** are:

$$
\begin{aligned}
p &= \text{acoustic pressure (Pa)} \\
v_r &= \text{particle velocity (m/s)} \\
\theta &= \text{cubic dilatation} \\
\Phi_k &= \text{mass flow density rate } (\text{kg/m}^2 \cdot \text{s})
\end{aligned}
$$

The **acoustic source quantities** are:

$$
\begin{aligned}
f_k &= \text{volume source density of force } (\text{N/m}^3) \\
q &= \text{volume source density of injection rate } (\text{s}^{-1})
\end{aligned}
$$

The **acoustic medium properties** are:

$$
\begin{aligned}
\rho_{k,r} &= \text{volume density of mass } (\text{kg/m}^3) \\
\kappa &= \text{compressibility } (\text{Pa}^{-1})
\end{aligned}
$$

Acoustic wave quantities

- **Acoustic wave equations**:

$$\partial_k p + \partial_t \Phi_k = f_k$$
$$\partial_r v_r - \partial_t \theta = q$$

- **Acoustic compatibility relation**:

$$\int_{\mathcal{S}} \boldsymbol{\epsilon}_{j,m,k} \nu_m \partial_t \Phi_k \mathrm{d}A = \int_{\mathcal{S}} \boldsymbol{\epsilon}_{j,m,k} \nu_m f_k \mathrm{d}A,$$

for any closed surface $\mathcal{S}$ ($\nu_m =$ unit vector along outward normal to $\mathcal{S}$)

Levi-Civita tensor:

$\boldsymbol{\epsilon}_{j,m,k} = \{+1, -1, 0\}$ if $\{j, m, k\}$

{even, odd, no} permutation of $\{1, 2, 3\}$

Acoustic wave equations, compatibility relation

- **Interface boundary condition**:

across any surface of discontinuity in medium properties

$$p = \text{continuous}$$
$$\nu_r v_r = \text{continuous}$$

$\nu_r =$ unit vector along the normal to the interface

- **Compatibility boundary condition**:

across any surface of discontinuity in medium properties or volume source distributions

$$\boldsymbol{\epsilon}_{j,m,k}\nu_m\partial_t\Phi_k - \boldsymbol{\epsilon}_{j,m,k}\nu_m f_k = \text{continuous}$$

$\nu_m =$ unit vector along the normal to the interface

The computational procedure starts from the **domain integrated acoustic equations** (weak form of the acoustic wave equations):

$$\int_{\partial\mathcal{D}} \nu_k p \mathrm{d}A + \int_{\mathcal{D}} \partial_t \Phi_k \mathrm{d}V = \int_{\mathcal{D}} f_k \mathrm{d}V,$$
$$\int_{\partial\mathcal{D}} \nu_r v_r \mathrm{d}A - \int_{\mathcal{D}} \partial_t \theta \mathrm{d}V = \int_{\mathcal{D}} q \mathrm{d}V,$$

where $\partial\mathcal{D}$ is the closed boundary surface of $\mathcal{D}$ and ν_m is the unit vector along the normal to $\partial\mathcal{D}$ oriented away from $\mathcal{D}$.

- Note that **no spatial differentiations** occur in these equations.

The **embedding procedure** amounts to selecting a **target region** of bounded support in an embedding medium (constitutive parameters $\{\rho^{\mathrm{b}}_{k,r}, \kappa^{\mathrm{b}}\}$ for which the Green's functions are known. The **incident wavefield** $\{p^{\mathrm{i}}, v^{\mathrm{i}}_r, \theta^{\mathrm{i}}, \Phi^{\mathrm{i}}_k\}$ is introduced as the wavefield that would be generated by the sources as if they were acting in the embedding; the **scattered wavefield** $\{p^{\mathrm{s}}, v^{\mathrm{s}}_r, \theta^{\mathrm{s}}, \Phi^{\mathrm{s}}_k\}$ is introduced as the **difference** between the **total wavefield** $\{p, v_r, \theta, \Phi_k\}$ and the **incident wavefield**. Hence,

$$\{p, v_r, \theta, \Phi_k\}$$
$$= \{p^{\mathrm{i}} + p^{\mathrm{s}}, v^{\mathrm{i}}_r + v^{\mathrm{s}}_r, \theta^{\mathrm{i}} + \theta^{\mathrm{s}}, \Phi^{\mathrm{i}}_k + \Phi^{\mathrm{s}}_k\}$$

Embedding procedure

The **incident** wavefield satisfies the **wave equations**

$$\partial_k p^{\mathrm{i}} + \partial_t \Phi_k^{\mathrm{i}} \;=\; f_k \quad \text{for all } \boldsymbol{x} \in \mathcal{R}^3$$
$$\partial_r v_r^{\mathrm{i}} - \partial_t \theta^{\mathrm{i}} \;=\; q \quad \text{for all } \boldsymbol{x} \in \mathcal{R}^3$$

the **compatibility relation**

$$\int_{\mathcal{S}} \epsilon_{i,m,k} \nu_m \partial_t \Phi_k^{\mathrm{i}} \mathrm{d}A \;=\; \int_{\mathcal{S}} \epsilon_{i,m,k} \nu_m f_k \mathrm{d}A$$

for any closed surface $\mathcal{S}$, and the **constitutive relations**

$$\Phi_k^{\mathrm{i}} \;=\; \rho_{k,r}^{\mathrm{b}} v_r^{\mathrm{i}}$$
$$\theta^{\mathrm{i}} \;=\; -\kappa^{\mathrm{b}} p^{\mathrm{i}}$$

Embedding procedure (incident wavefield)

The **scattered** wavefield satisfies the **wave equations**

$$\partial_k p^{\mathrm{s}} + \partial_t \Phi_k^{\mathrm{s}} \;=\; 0 \quad \text{for all } \boldsymbol{x} \in \mathcal{R}^3$$
$$\partial_r v_r^{\mathrm{s}} - \partial_t \theta^{\mathrm{s}} \;=\; 0 \quad \text{for all } \boldsymbol{x} \in \mathcal{R}^3$$

the **compatibility relation**

$$\int_{\mathcal{S}} \epsilon_{i,m,k} \nu_m \partial_t \Phi_k^{\mathrm{s}} \mathrm{d}A \;=\; 0$$

for any closed surface $\mathcal{S}$, and the **'constitutive relations'**

$$\begin{aligned}
\Phi_k^{\mathrm{s}} \;&=\; \rho_{k,r} v_r^{\mathrm{s}} + (\rho_{k,r} - \rho_{k,r}^{\mathrm{b}}) v_r^{\mathrm{i}} \\
&=\; \rho_{k,r}^{\mathrm{b}} v_r^{\mathrm{s}} + (\rho_{k,r} - \rho_{k,r}^{\mathrm{b}}) v_r \\
\theta^{\mathrm{s}} \;&=\; -\kappa p^{\mathrm{s}} - (\kappa - \kappa^{\mathrm{b}}) p^{\mathrm{i}} \\
&=\; -\kappa^{\mathrm{b}} p^{\mathrm{s}} - (\kappa - \kappa^{\mathrm{b}}) p
\end{aligned}$$

Embedding procedure (scattered wavefield)

Source-type integral representations:

$$p^{\mathrm{i,s}}(\boldsymbol{x},t) = \int_{\mathcal{D}^{\mathrm{i,s}}} \{ \mathsf{C}_t[G^{p,q}(\boldsymbol{x},\boldsymbol{x}',\cdot), q^{\mathrm{i,s}}(\boldsymbol{x}',\cdot)] + \mathsf{C}_t[G^{p,f}_k(\boldsymbol{x},\boldsymbol{x}',\cdot), f^{\mathrm{i,s}}_k(\boldsymbol{x}',\cdot)]\}\mathrm{d}V(\boldsymbol{x}')$$

$$\text{for all } \boldsymbol{x} \in \mathcal{R}^3,$$

$$v_r^{\mathrm{i,s}}(\boldsymbol{x},t) = \int_{\mathcal{D}^{\mathrm{i,s}}} \{ \mathsf{C}_t[G^{v,q}_r(\boldsymbol{x},\boldsymbol{x}',\cdot), q^{\mathrm{i,s}}(\boldsymbol{x}',\cdot)] + \mathsf{C}_t[G^{v,f}_{r,k}(\boldsymbol{x},\boldsymbol{x}',\cdot), f^{\mathrm{i,s}}_k(\boldsymbol{x}',\cdot)]\}\mathrm{d}V(\boldsymbol{x}')$$

$$\text{for all } \boldsymbol{x} \in \mathcal{R}^3,$$

- $G^{\cdot}_{\cdot}$ = Green's function (point-source solution)

$$f^{\mathrm{i}}_k = f_k, \ q^{\mathrm{i}} = q \quad (\text{support} = \mathcal{D}^{\mathrm{i}})$$

and

$$\left.\begin{aligned} f^{\mathrm{s}}_k &= -(\rho_{k,r} - \rho^{\mathrm{b}}_{k,r})\partial_t v_r \\ q^{\mathrm{s}} &= -(\kappa - \kappa^{\mathrm{b}})\partial_t p \end{aligned}\right\} \text{support } = \mathcal{D}^{\mathrm{s}}$$

Source-type integral representations

The position vector in the **simplex** $\boldsymbol{\Sigma}$ with **vertices** $\{\boldsymbol{x}(0), \boldsymbol{x}(1), \boldsymbol{x}(2), \boldsymbol{x}(3)\}$ and **vectorial areas** $\{\boldsymbol{A}(0), \boldsymbol{A}(1), \boldsymbol{A}(2), \boldsymbol{A}(3)\}$ can in a symmetrical fashion be expressed as

$$x_m = \sum_{I=0}^{3} \lambda(I, \boldsymbol{x}) x_m(I)$$

where the **barycentric coordinates** of $\boldsymbol{x}$ are

$$\lambda(I, \boldsymbol{x}) \;=\; 1/4 - (1/3V)(x_m - b_m)A_m(I)$$
$$\text{for } I = 0, 1, 2, 3$$

with the **barycenter** $b_m = \frac{1}{4}\Sigma_{I=0}^{3} x_m(I)$.

- Property ($\delta(I, J) =$ Kronecker symbol):

$$\lambda(I, \boldsymbol{x}(J)) = \delta(I, J)$$

Barycentric coordinates

The **scalar nodal expansion** in $\mathbf{\Sigma}$ is used for the

- **acoustic pressure**

and the

- **cubic dilatation**:

$$\{p, \theta\}(\boldsymbol{x}, t) = \sum_{I=0}^{3} A^{p,\theta}(I, t)\lambda(I, \boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \mathbf{\Sigma}$$

where

$$A^{p,\theta}(I, t) = \{p, \theta\}(\boldsymbol{x}(I), t) \quad \text{for } I = 0, 1, 2, 3$$

are the values at the vertices of $\mathbf{\Sigma}$.

Scalar nodal expansion in simplex

The **vectorial face-element expansion** is used for the **particle velocity**:

$$v_r(\boldsymbol{x},t) \;=\; \sum_{I=0}^{3} A_r^v(I,t)\lambda(I,\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \boldsymbol{\Sigma},$$

where

$$A_r^v(I,t) \;=\; v_r(\boldsymbol{x}(I),t) \quad \text{for } I = 0,1,2,3$$

To satisfy the **interface boundary conditions**, we work with the numbers (projections along the normals to the faces)

$$\alpha^v(I,J,t) \;=\; v_r(\boldsymbol{x}(I),t)A_r(J)$$

with $\alpha^v(I,I,t) = 0$. Then,

$$v_r(\boldsymbol{x}(I),t) \;=\; -\frac{1}{3V}\sum_{J=0}^{3} \alpha^v(I,J,t)[x_r(J) - x_r(I)]$$

Vectorial face-element expansion

The **vectorial edge-element expansion** is used for the **mass flow density rate**:

$$\Phi_k(\boldsymbol{x},t) = \sum_{I=0}^{3} A_k^{\Phi}(I,t)\lambda(I,\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \boldsymbol{\Sigma}$$

where

$$A_k^{\Phi}(I,t) = \Phi_k(\boldsymbol{x}(I),t) \quad \text{for } I = 0,1,2,3$$

To satisfy the **compatibility boundary conditions**, we work with the numbers (projections along the edges)

$$\alpha^{\Phi}(I,J,t) \ = \ \Phi_k(\boldsymbol{x}(I),t)[x_k(J) - x_k(I)]$$

with $\alpha^{\Phi}(I,I) = 0$. Then,

$$\Phi_k(\boldsymbol{x}(I),t) = -\frac{1}{3V}\sum_{J=0}^{3} \alpha^{\Phi}(I,J,t)A_k(J)$$

Vectorial edge-element expansion

The **computational procedure** consists of the following steps:

- Substitute the expansions in

- • Domain integrated acoustic equations
- • Compatibility relations

- Invoke

- • Interface boundary conditions
- • Compatibility boundary conditions

- • Satisfy Constitutive relations

- pointwise exactly for constant coefficients
- in least square integrated sense for (linearly) varying coefficients

- • Satisfy Causality conditions

Computational procedure

The **Causality condition** is invoked by relating the values of

• p^{s} and • v_r^{s} on the boundary $\partial\mathcal{D}$ of the domain $\mathcal{D}$ of computation

to the values of

$$\left.\begin{array}{l} \bullet\ f_k^{\mathrm{s}} \;=\; -(\rho_{k,r} - \rho_{k,r}^{\mathrm{b}})\partial_t v_r \\ \bullet\ q^{\mathrm{s}} \;=\; -(\kappa - \kappa^{\mathrm{b}})\partial_t p \end{array}\right\} \text{support } = \mathcal{D}^{\mathrm{s}}$$

in the scattering region (contrast region) $\mathcal{D}^{\mathrm{s}}$ via the source type integral representations.

Computational procedure (causality condition)

The computational procedure results in an overdetermined

- **linear system of ordinary differential equations**

that describes the

- **time evolution** of the **system of expansion coefficients**.

This system remains to be solved by an appropriate optimization technique.

Time evolution of expansion coefficients

Checks on the computational results are furnished by

- comparison with **canonical problems** with an **analytical solution**
- checking **reciprocity** via the **time-domain reciprocity theorem of the time convolution type**

Checks on the computational results