
The University of Queensland School of Earth and Environmental Sciences

Application of Finite Elements in Geophysical Modelling

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Outline

- I) Derive a generic PDE form \rightarrow `PDE Template`
- II) How does this work apply in some geophysical application?
- III) Solution using the Finite Element Method (FEM)

PDE Template

- Generic form of a PDE with coefficient as parameters
 - framework to derive FEM
 - useful for development of software
- Problem: overhead & efficiency vs. flexibility
- See also esys-escript for a more general form:
<https://github.com/esys-escript/esys-escript.github.io/blob/master/user.pdf>

PDE Template

- Potential u
- Gravity force

$$\mathbf{g} = -\nabla u$$

- Gauss' Law

$$\nabla^T \mathbf{g} = -4\pi G \rho$$

- Unknown u
- Pseudo flux \mathbf{F} :

$$\mathbf{F} = -\mathbf{A} \nabla u + \mathbf{X}$$

- `Conservation` Law

$$\nabla^t \mathbf{F} + D u = Y$$

3D Case

- Assume \mathbf{A} as a diagonal matrix:

$$\mathbf{A} = \begin{bmatrix} a_{00} & 0 & 0 \\ 0 & a_{11} & 0 \\ 0 & 0 & a_{22} \end{bmatrix} \quad \mathbf{X} = [X_0, X_1, X_2]^T$$

$$\mathbf{F} = -\mathbf{A}\nabla u + \mathbf{X} \quad \mathbf{F} = \begin{bmatrix} F_0 \\ F_1 \\ F_2 \end{bmatrix} = \begin{bmatrix} -a_{00}\frac{\partial u}{\partial x_0} + X_0 \\ -a_{11}\frac{\partial u}{\partial x_1} + X_1 \\ -a_{22}\frac{\partial u}{\partial x_2} + X_2 \end{bmatrix}$$

3D Case (cont.)

- Conservation condition:

$$\nabla^t \mathbf{F} + D u = Y \quad \frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} + D u = Y$$

PDE Template for Gravity

For the gravity case:

$$\mathbf{g} = -\nabla u$$

$$\nabla^T \mathbf{g} = -4\pi G \rho$$

$$\mathbf{F} = -\mathbf{A} \nabla u + \mathbf{X}$$

$\mathbf{A} = \mathbf{I}$ $\mathbf{X} = \mathbf{0}$

$$\nabla^t \mathbf{F} + D u = Y$$

$D = 0$ $Y = -4\pi G \rho$

$$a_{00} = a_{11} = a_{22} = 1 \text{ and } X_0 = X_1 = X_2 = 0$$

$$D = 0 \text{ and } Y = -4\pi G \rho$$

Formulation of PDE:

- Insert Flux into Conservation condition:

$$-\nabla^t \mathbf{A} \nabla u + D u = -\nabla^t \mathbf{X} + Y$$

- In 2D:

$$-\frac{\partial}{\partial x_0} a_{00} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} a_{11} \frac{\partial u}{\partial x_1} + D u = -\frac{\partial X_0}{\partial x_0} - \frac{\partial X_1}{\partial x_1} + Y$$

Boundary conditions

- Dirichlet-type boundary conditions on Γ_D

$$u = r$$

- Γ_D = top of the domain Ω
- Neumann-type boundary conditions on Γ_N

$$\mathbf{n}^T \mathbf{F} = 0 \longrightarrow \mathbf{n}^T \mathbf{A} \nabla u = \mathbf{n}^T \mathbf{X}$$

- With outer normal field \mathbf{n}
- Γ_N = all other faces of the domain Ω

Magnetic Anomalies

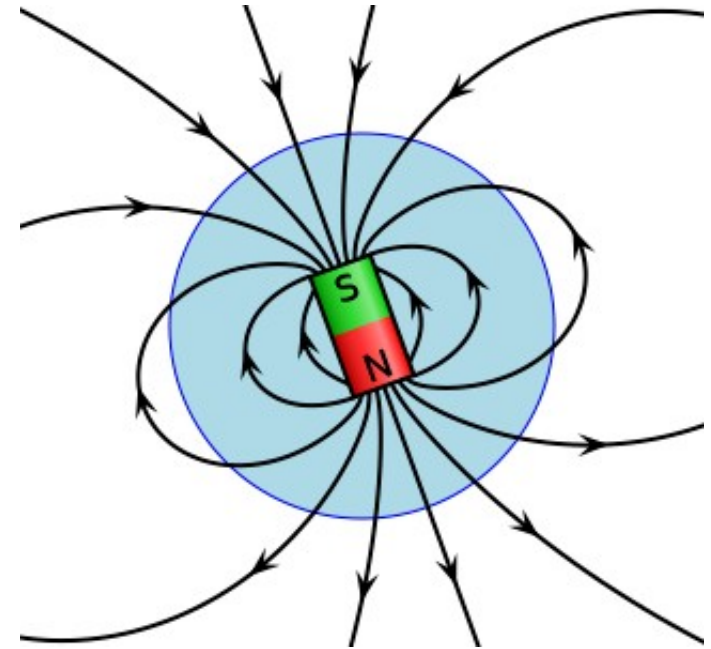
- Magnetic Flux \mathbf{B}_f

$$\mathbf{B}_f = \mathbf{B}_t + \mathbf{M}$$

- Total magnetic field \mathbf{B}_t
 - Background magnetic field \mathbf{B}_b
 - Magnetic field anomaly \mathbf{B}_a

$$\mathbf{B}_t = \mathbf{B}_a + \mathbf{B}_b$$

- Magnetization $\mathbf{M} = k \mathbf{B}_b$ with susceptibility k
 - Here: linearized model, also possible $\mathbf{M} = k \mathbf{B}_t$



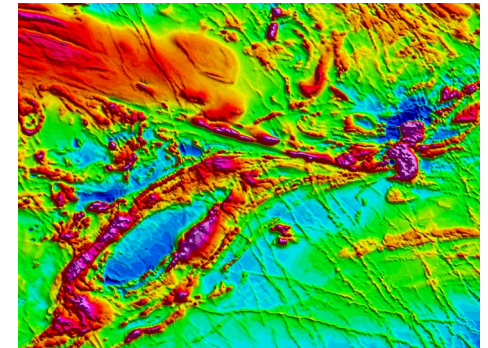
Magnetic Anomalies (cont.)

- Observed is total magnetic field anomaly b_a is the difference of the intensity of the total magnetic field \mathbf{B}_t and of the background field \mathbf{B}_b :

$$b_a = |\mathbf{B}_t| - |\mathbf{B}_b|$$

- With Linearization

$$b_a = \frac{\mathbf{B}_b^T}{|\mathbf{B}_b|} \mathbf{B}_a .$$



- Task: calculate magnetic field anomaly \mathbf{B}_a from subsurface susceptibility k

Towards a PDE

- magnetic flux \mathbf{B}_f is divergence free:

$$\nabla^t \mathbf{B}_f = 0$$

- With definition of \mathbf{B}_f :

$$\mathbf{B}_f = \mathbf{B}_t + \mathbf{M} \quad \nabla^t \mathbf{B}_b = 0 \quad \longrightarrow \quad \nabla^t (\mathbf{B}_a + k \mathbf{B}_b) = 0$$

- Analogously to gravity: scalar potential u with

$$\mathbf{B}_a = -\nabla u$$


- Leading to PDE

$$-\nabla^t \nabla u = -\nabla^t k \mathbf{B}_b$$

Using the PDE template

- pseudo flux $\mathbf{F} = \mathbf{B}_f - \mathbf{B}_b$

$$\mathbf{F} = -\nabla u + k\mathbf{B}_b$$

$A=I$  $X=k B_b$

$$\mathbf{F} = -\mathbf{A}\nabla u + \mathbf{X}$$

- Also: $D=0$, $Y=0$: $\nabla^t(\mathbf{B}_a + k\mathbf{B}_b) = 0 \xrightarrow{\text{green arrow}} \nabla^t \mathbf{F} + D u = Y$
- Neumann Boundary conditions:

$$\mathbf{n}^T \mathbf{F} = 0 \xrightarrow{\text{green arrow}} \mathbf{n}^T \mathbf{B}_f = \mathbf{n}^T \mathbf{B}_b$$

Magnetotellurics

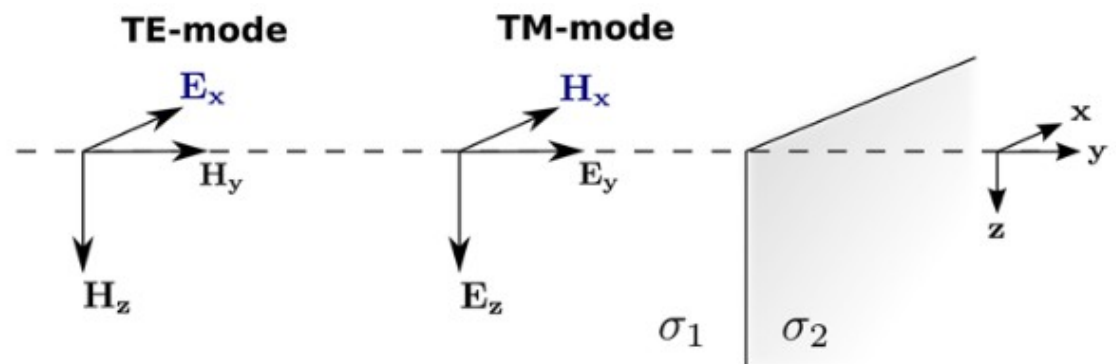
- Maxwell's equations for
 - magnetic field \mathbf{H}
 - electric field \mathbf{E}
 - Conductivity σ , resistivity ρ ($\sigma\rho=1$)
 - Conductivity in air layer $\sigma=0$
 - Angular frequency ω
 - magnetic permeability μ_0

$$\nabla \times \rho \times \nabla \mathbf{H} + \mathbf{j}\mu_0\omega\mathbf{H} = 0$$

$$\nabla \times \nabla \times \mathbf{E} + \mathbf{j}\mu_0\sigma\omega\mathbf{E} = 0$$

2D Model

- no variation along the strike = x-direction
- incoming wave fronts:
 - transverse electric (TE) along E_x
 - $E_y = E_z = 0, H_x = 0$
 - transverse magnetic (TM) along H_x
 - $H_y = H_z = 0, E_x = 0$



TE mode

- Maxwell equation simplifies to

$$-\nabla^T \nabla E_x + \mathbf{j} \omega \sigma \mu_0 E_x = 0$$

- Recover magnetic field component:

$$H_z = -\frac{\mathbf{j}}{\omega \mu_0} \frac{\partial E_x}{\partial x_0} \quad H_y = \frac{\mathbf{j}}{\omega \mu_0} \frac{\partial E_x}{\partial x_1}$$

- Dirichlet boundary conditions
 - Set as E_x from 'air plus homogeneous subsurface'

PDE Template: TE mode

$$u = E_x \quad -\nabla^T \nabla E_x + \mathbf{j}\omega\sigma\mu_0 E_x = 0$$

$$a_{00} = a_{11} = 1 \text{ and } D = \mathbf{j}\omega\sigma\mu_0$$

$$-\frac{\partial}{\partial x_0} a_{00} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} a_{11} \frac{\partial u}{\partial x_1} + Du = -\frac{\partial X_0}{\partial x_0} - \frac{\partial X_1}{\partial x_1} + Y$$

TM mode

- Maxwell equation simplifies to

$$-\nabla^T \rho \nabla H_x + \mathbf{j} \omega \mu H_x = 0$$

- No air-layer required as $\rho = \infty \rightarrow H_x = \text{const}$
- Recover magnetic field component:

$$E_z = \rho \frac{\partial H_x}{\partial x_0} \quad E_y = \rho \frac{\partial H_x}{\partial x_1}$$

- Dirichlet boundary conditions
 - Set as H_x from 'homogeneous subsurface'

PDE Template: TM mode

$$u = H_x, \quad -\nabla^T \rho \nabla H_x + \mathbf{j} \omega \mu H_x = 0$$

$$a_{00} = a_{11} = \rho \text{ and } D = \mathbf{j} \omega \mu_0$$

$$-\frac{\partial}{\partial x_0} a_{00} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} a_{11} \frac{\partial u}{\partial x_1} + Du = -\frac{\partial X_0}{\partial x_0} - \frac{\partial X_1}{\partial x_1} + Y$$

Impedance

- Defined as

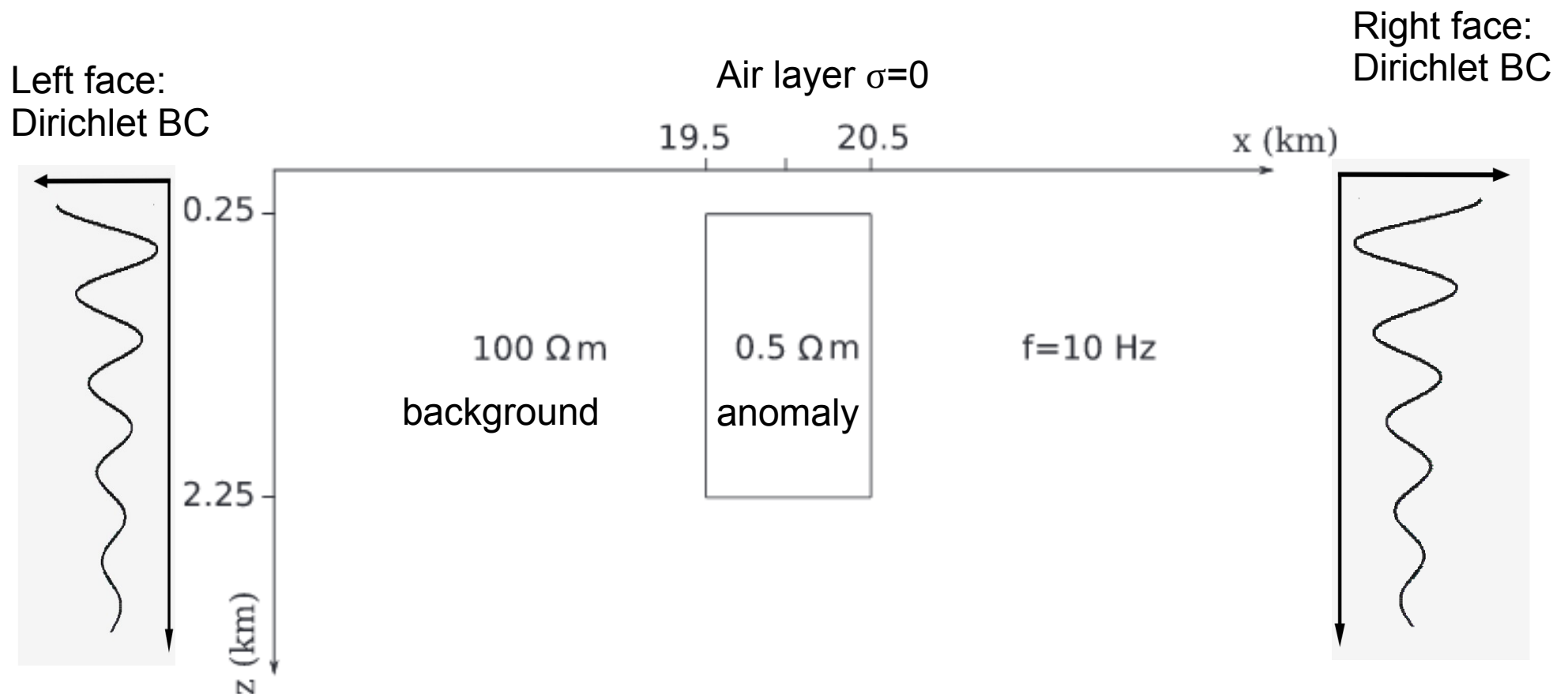
$$Z_{xy}(\omega) = \frac{E_x}{H_y} \quad Z_{yx}(\omega) = \frac{E_y}{H_x}$$

- Expressed on term of apparent resistivity and phase:

$$\rho_a(\omega) = \frac{1}{\omega\mu_0} |Z_{xy}(\omega)|^2 \quad \phi(\omega) = \arctan\left(\frac{Z_{xy}(\omega).imag}{Z_{xy}(\omega).real}\right)$$

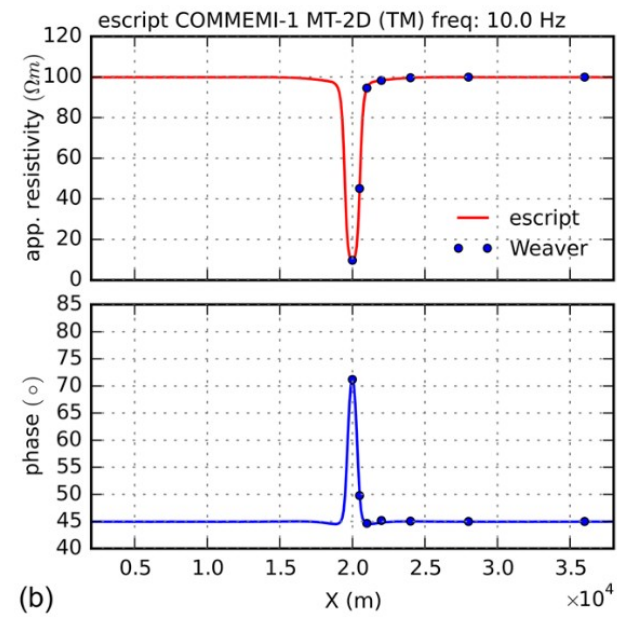
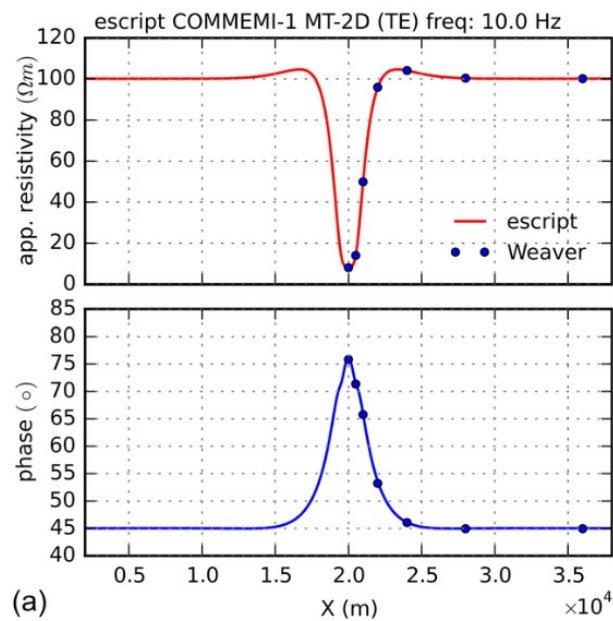
FEM solution

- **Test case:** See <https://doi.org/10.1088/1742-2132/13/2/S59>



Result TE mode

- FEM with 60000 nodes
 - solved with esys-escript in python
- Weaver – reference solution



Seismic

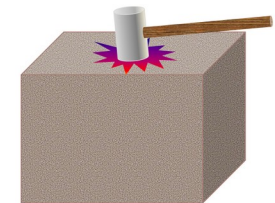
- acoustic wave equation for pressure $p=p(t,\mathbf{x})$

$$\frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} - \nabla^T \nabla p = f(t) \cdot \delta_{\mathbf{x}_s}$$

Propagation speed c

Source amplitude speed $f(t)$

Source location \mathbf{x}_s

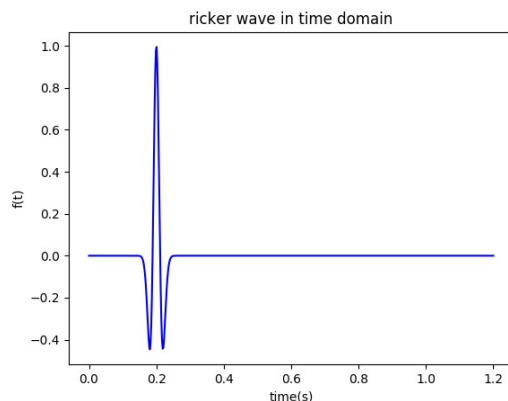


In Frequency Domain

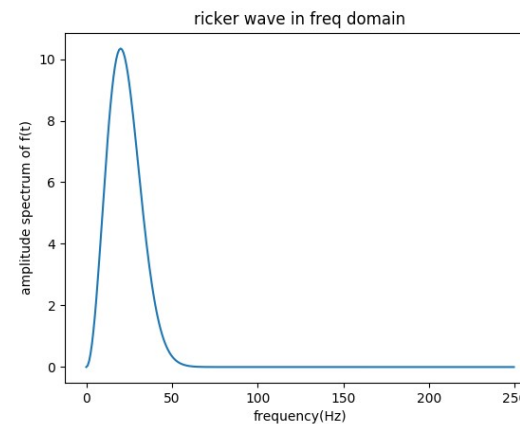
- Apply Fourier Transformation
 - For any angular frequency ω :

$$-\nabla^T \nabla u - k^2 u = f_\omega \delta_{\mathbf{x}_s} \quad k = \frac{\omega}{c}$$

Source amplitude speed $f(t)$

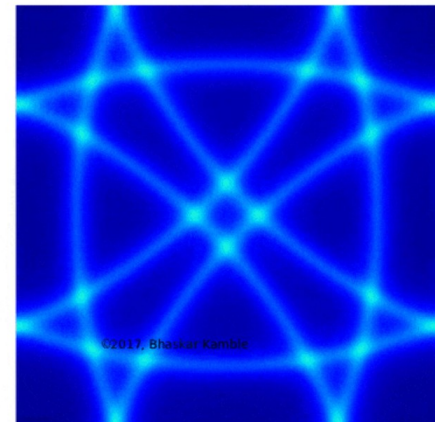


Source Spectrum speed f_ω



Where Are We?

- Boundary conditions?
 - For instance: $u=0$ on boundary
- Wave equation in frequency fits PDE template: $A=I, D=-k^2$ 😊
- But: reflection from boundary
 - As domain is bounded
- Introduce absorption near boundary → eg. PML



PML

- PML = Perfect Matching Layer
- Apply a coordinate transformation:

$$x_i \rightarrow \gamma_i x_i$$

- With

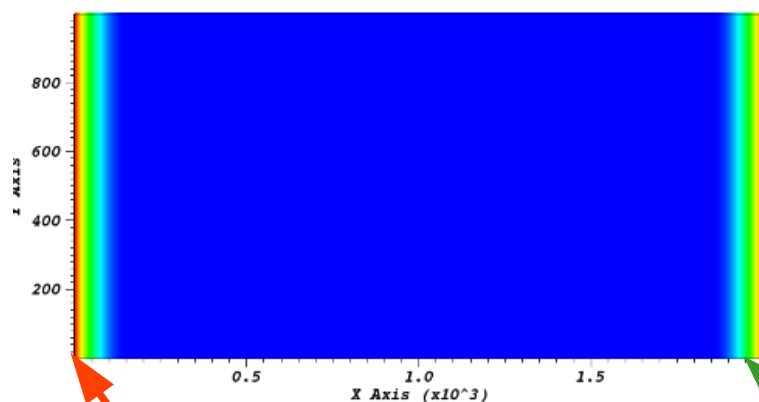
$$\gamma_i = 1 - \mathbf{j} \frac{c \alpha}{\omega} Q_i$$

- absorption strength parameter α
- absorbing functions Q_i : switches on/off absorption

Absorbing Function

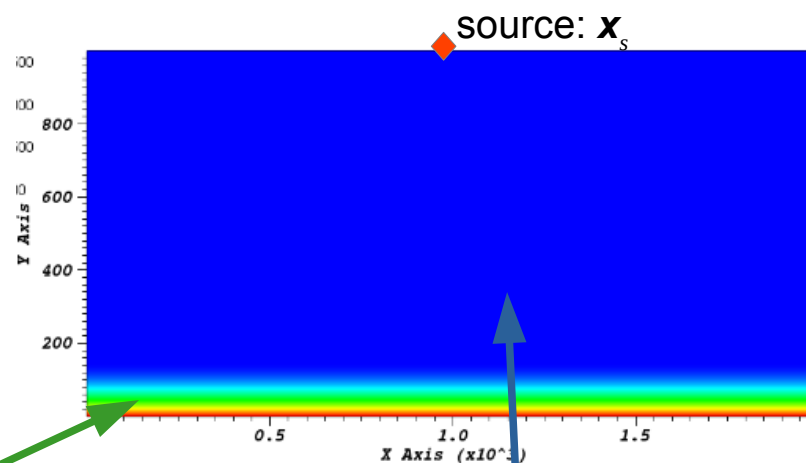
Red: $Q_i=1$, blue: $Q_i=0$

Horizontally: Q_0



Switched on near boundary

Vertically: Q_1



Smooth transition

Switched off in the interior

Wave Equation With PML

$$-\nabla^T \nabla u - k^2 u = f_\omega \delta_{\mathbf{x}_s}$$



$$x_i \rightarrow \gamma_i x_i$$

$$-\frac{1}{\gamma_0} \frac{\partial}{\partial x_0} \frac{1}{\gamma_0} \frac{\partial u}{\partial x_0} - \frac{1}{\gamma_1} \frac{\partial}{\partial x_1} \frac{1}{\gamma_1} \frac{\partial u}{\partial x_1} - k^2 u = f_\omega \delta_{\mathbf{x}_s}$$

Does not fit PDE Template!!!!



A Little Trick

- Multiply by $\gamma_0\gamma_1$:

$$-\gamma_1 \frac{\partial}{\partial x_0} \frac{1}{\gamma_0} \frac{\partial u}{\partial x_0} - \gamma_0 \frac{\partial}{\partial x_1} \frac{1}{\gamma_1} \frac{\partial u}{\partial x_1} - \gamma_0 \gamma_1 k^2 u = f_\omega \delta_{\mathbf{x}_s}$$

- Notice: $\gamma_1 = \gamma_1(x_1)$ and $\gamma_0 = \gamma_0(x_0)$

$$-\frac{\partial}{\partial x_0} \frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} \frac{\gamma_0}{\gamma_1} \frac{\partial u}{\partial x_1} - \gamma_0 \gamma_1 k^2 u = f_\omega \delta_{\mathbf{x}_s}$$



- Works also in 3D

PDE Template

$$-\frac{\partial}{\partial x_0} \frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} \frac{\gamma_0}{\gamma_1} \frac{\partial u}{\partial x_1} - \gamma_0 \gamma_1 k^2 u = f_\omega \delta_{\mathbf{x}_s}$$



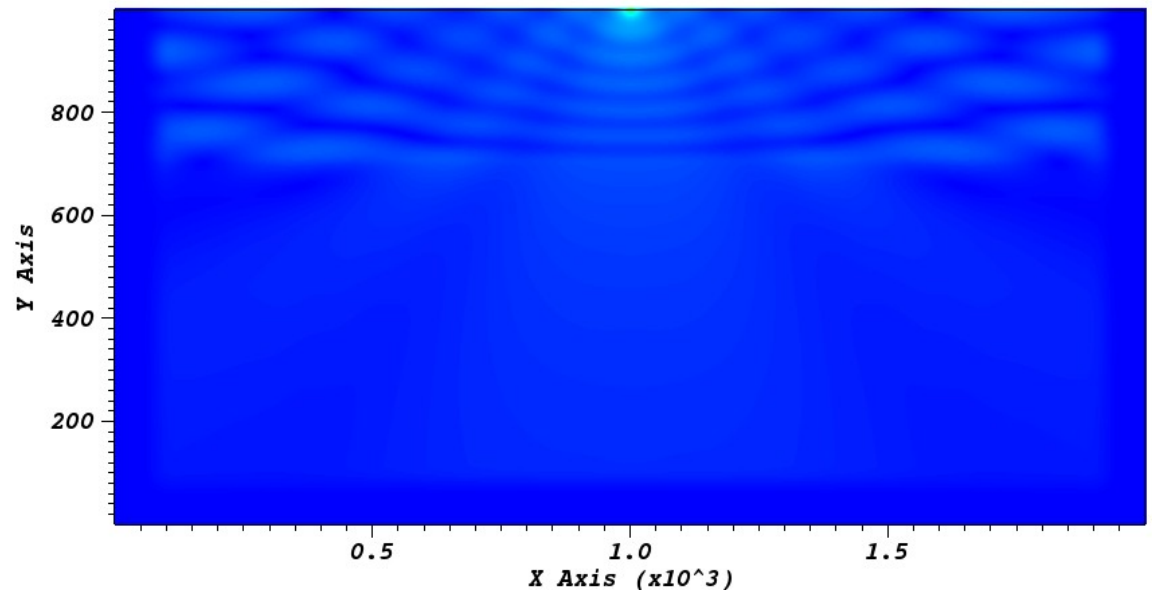
$$a_{00} = \frac{\gamma_1}{\gamma_0}, a_{11} = \frac{\gamma_0}{\gamma_1}, D = -\gamma_0 \gamma_1 k^2 \text{ and } Y = f_\omega \delta_{\mathbf{x}_s}$$

with Neumann boundary conditions

Example

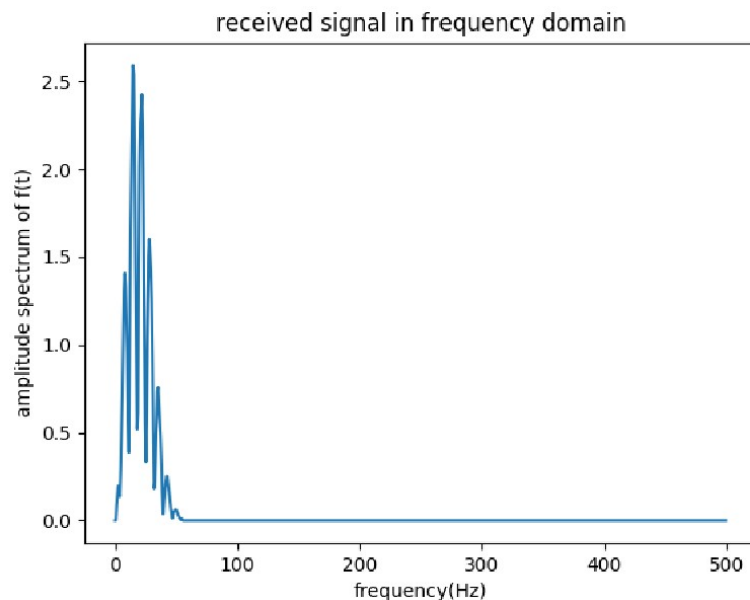
- Single reflector 2000m/s vs 3000m/s @ 300m
- 2000x1000 elements with edge length $h=1$
- PML: $\alpha=0.5$, layer thickness = 150m

Wave field u for 20Hz

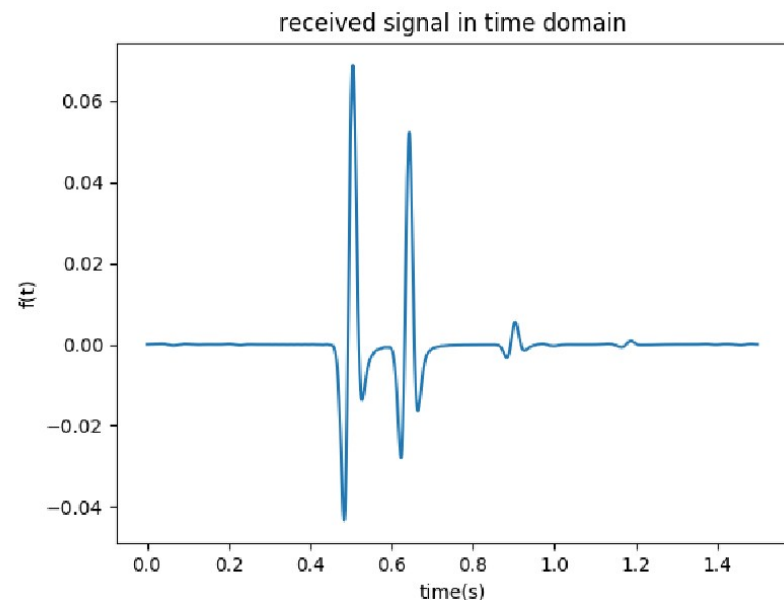


Example (cont.)

- Recover signal at 500m off source
 - Sampled at 1ms



(a) Power spectrum



(b) Time signal

- By Ao Chang using esys-escript

FEM solver for the PDE template

- Follow what we did for gravity
 - Define node and elements
 - Element = connect vertices with nodes
 - Define the local basis function N_i
 - linked to FEM basis ϕ_p^h
 - Get Local Element matrices
 - Evaluate PDE with local basis functions N_i ← Here comes in the PDE template
 - Assemble local element matrices to linear system
 - Insert Dirichlet conditions
 - Solve the linear system of equations

→ Done

PDE To Linear System

`strong` form of PDE:

$$-\nabla^T \nabla u = -4\pi G \rho .$$



For PDE template ?

`Weak` form of PDE:

$$\int_{\Omega} \nabla^T v^h \nabla u^h d\mathbf{x} = \int_{\Omega} (-4\pi G) \rho v^h d\mathbf{x}$$



Local element matrices: $S_{ij}^E = \int_E \nabla^T N_i \nabla N_j d\mathbf{x}$ for $i, j = 0, \dots, 3$ $b_i^E = \int_E (-4\pi G) \rho N_i d\mathbf{x}$ for $i = 0, \dots, 3$



Global system of linear equations:

$$\mathbf{S}^h \mathbf{U}^h = \mathbf{b}^h$$

Weak Form PDE Template

- Conservation law

$$\nabla^t \mathbf{F} + D u = Y$$

- Multiply by v and integrate:

$$\int_{\Omega} v (\nabla^t \mathbf{F} + D u - Y) d\mathbf{x} = 0$$

- Again: apply generalized Green's first identity to pseudo-flux:

$$\int_{\Omega} v \nabla^T \mathbf{F} d\mathbf{x} = - \int_{\Omega} \nabla^T v \mathbf{F} d\mathbf{x} + \int_{\partial\Omega} v \mathbf{n}^T \mathbf{F} ds$$

- Boundary integral is zero as

- Neumann condition: $\mathbf{n}^T \mathbf{F} = 0$
- Dirichlet boundary condition: where $u=r \rightarrow v=0$

Weak Form PDE Template (cont.)

- So we get:

$$\int_{\Omega} (v (D u - Y) - \nabla^T v \mathbf{F}) d\mathbf{x} = 0$$

- Recall: 'pseudo-flux $\mathbf{F} = -\mathbf{A} \nabla u + \mathbf{X}$
- Finally: the 'weak' form of the PDE template

$$\int_{\Omega} (\nabla^T v \mathbf{A} \nabla u + D v u) d\mathbf{x} = \int_{\Omega} (\mathbf{X}^T \nabla v + Y v) d\mathbf{x}$$

Weak Form PDE Template (cont.)

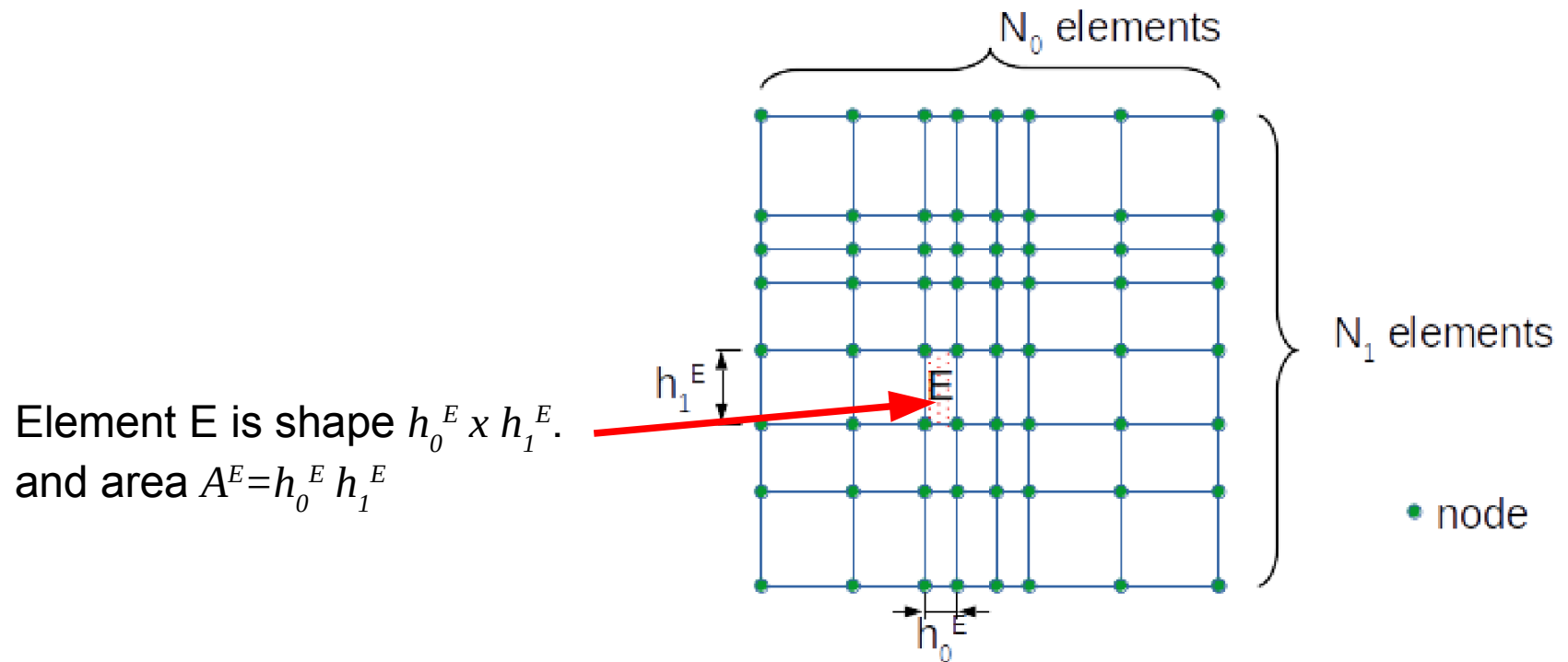
- This is how it looks in the 2D case:

$$\int_{\Omega} \left(a_{00} \frac{\partial v}{\partial x_0} \frac{\partial u}{\partial x_0} + a_{11} \frac{\partial v}{\partial x_1} \frac{\partial u}{\partial x_0} + D v u \right) d\mathbf{x} = \int_{\Omega} \left(X_0 \frac{\partial v}{\partial x_0} + X_1 \frac{\partial v}{\partial x_1} + Y v \right) d\mathbf{x}$$

- Next: break integration down to elements

A More General Grid

- Allow for rectangular shaped elements
- Nodes are not are **not equally** spaced anymore



Modified local basis functions

Modifications relative to square case

$$N_0(x_0, x_1) = \frac{1}{A_E} (c_0 + h_0 - x_0) \cdot (c_1 + h_1 - x_1)$$

$$N_2(x_0, x_1) = -\frac{1}{A_E} (c_0 + h_0 - x_0) \cdot (c_1 - x_1)$$

$$N_1(x_0, x_1) = -\frac{1}{A_E} (c_0 - x_0) \cdot (c_1 + h_1 - x_1)$$

$$N_3(x_0, x_1) = \frac{1}{A_E} (c_0 - x_0) \cdot (c_1 - x_1)$$

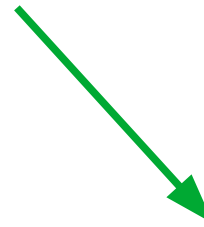
Local Element Matrices

- This gives the local element matrices:

$$\int_{\Omega} (\nabla^T v \mathbf{A} \nabla u + D v u) d\mathbf{x} = \int_{\Omega} (\mathbf{X}^T \nabla v + Y v) d\mathbf{x}$$



$$S_{ij}^E = \int_{\Omega} (\nabla^T N_i \mathbf{A} \nabla N_j + D N_i N_j) d\mathbf{x}$$



$$b_i^E = \int_{\Omega} (\mathbf{X}^T \nabla N_i + Y N_i) d\mathbf{x}$$

The 2D case

- Assume: coefficients are constant at each element

$$S_{ij}^E = a_{00}^E \cdot \int_E \frac{\partial N_i}{\partial x_0} \frac{\partial N_j}{\partial x_0} d\mathbf{x} + a_{11}^E \cdot \int_E \frac{\partial N_i}{\partial x_1} \frac{\partial N_j}{\partial x_1} d\mathbf{x} + D^E \cdot \int_E N_i N_j d\mathbf{x}$$

$$b_i^E = X_0^E \cdot \int_E \frac{\partial N_i}{\partial x_0} d\mathbf{x} + X_1^E \cdot \int_E \frac{\partial N_i}{\partial x_1} d\mathbf{x} + Y^E \cdot \int_E N_i d\mathbf{x}$$

Evaluation

- For instance:

$$\int_E \frac{\partial N_i}{\partial x_0} \frac{\partial N_j}{\partial x_0} d\mathbf{x} = \frac{A^E}{(h_0^E)^2} \hat{S}_{ij}^{1,00}$$

For edge length $h=1$

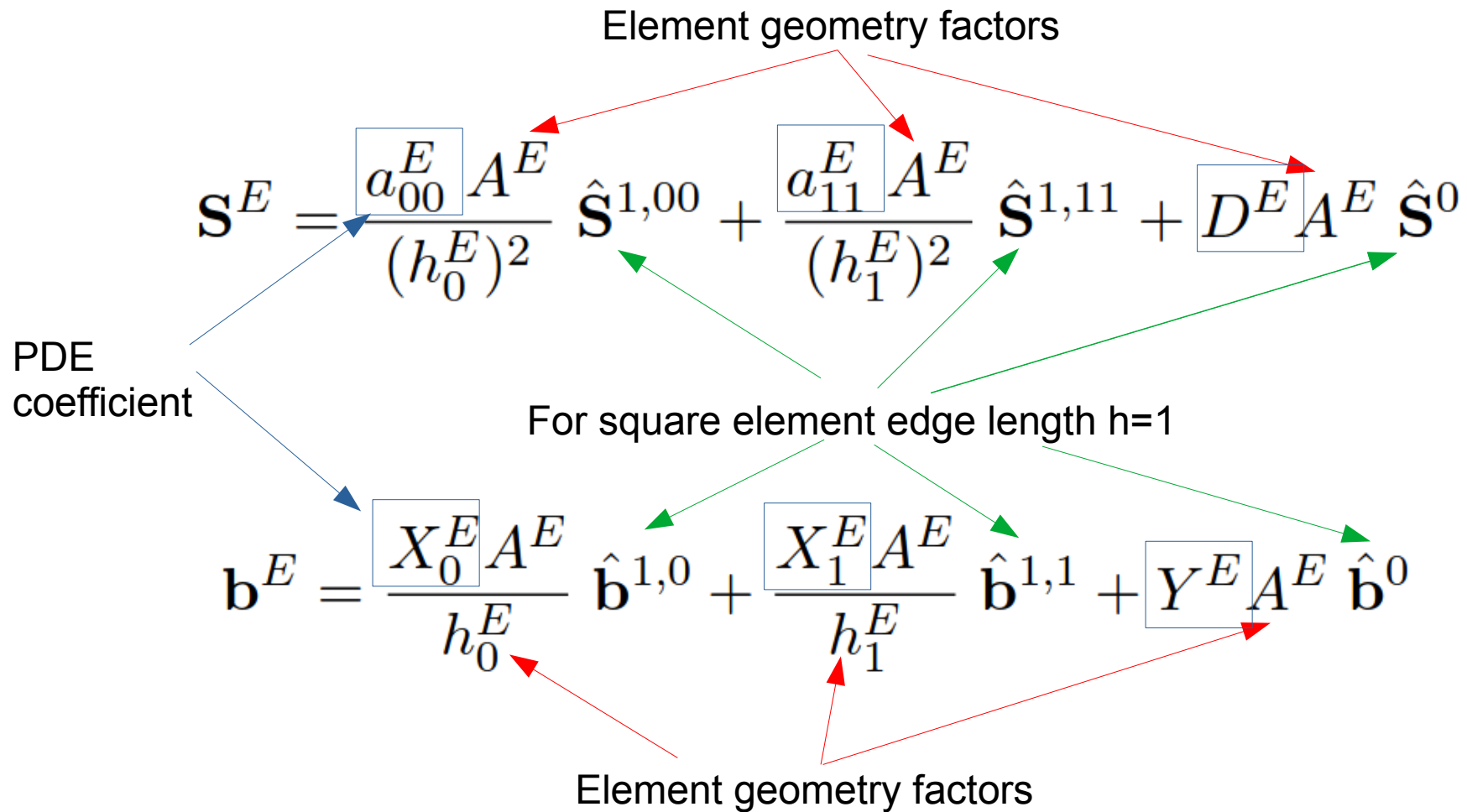
$$\hat{\mathbf{S}}^{1,00} = \begin{bmatrix} \frac{1}{3} & -\frac{1}{3} & \frac{1}{6} & -\frac{1}{6} \\ -\frac{1}{3} & \frac{1}{3} & -\frac{1}{6} & \frac{1}{6} \\ \frac{1}{6} & -\frac{1}{6} & \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{6} & \frac{1}{6} & -\frac{1}{3} & \frac{1}{3} \end{bmatrix}.$$

Element Matrix Calculation

$$\mathbf{S}^E = \frac{a_{00}^E A^E}{(h_0^E)^2} \hat{\mathbf{S}}^{1,00} + \frac{a_{11}^E A^E}{(h_1^E)^2} \hat{\mathbf{S}}^{1,11} + D^E A^E \hat{\mathbf{S}}^0$$

$$\mathbf{b}^E = \frac{X_0^E A^E}{h_0^E} \hat{\mathbf{b}}^{1,0} + \frac{X_1^E A^E}{h_1^E} \hat{\mathbf{b}}^{1,1} + Y^E A^E \hat{\mathbf{b}}^0$$

Let's take a closer look



Dirichlet-Type Boundary condition

- When node q has a Dirichlet condition:
 - overwrite row p with equation:

$$S_{qp}^h = \delta_{qp}$$

- And in right hand side

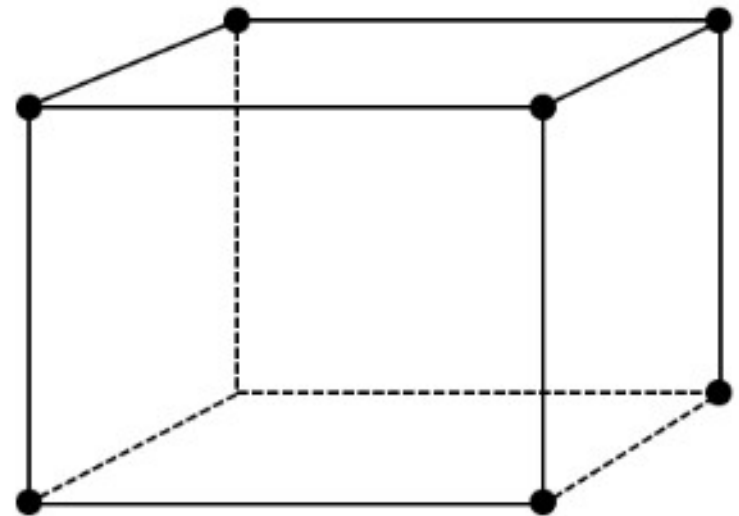
–

$$b_q^h = r(\check{\mathbf{x}}_q)$$

Extension into 3D

- Now an element has 8 vertices = 8 FEM nodes
 - Define link: element vertices \rightarrow FEM nodes
 - Define local basis N_0, \dots, N_7
 - Calculate

$$\hat{S}^{1,00}, \hat{S}^{1,11}, \hat{S}^{1,22} \text{ and } \hat{S}^0$$



Anisotropy

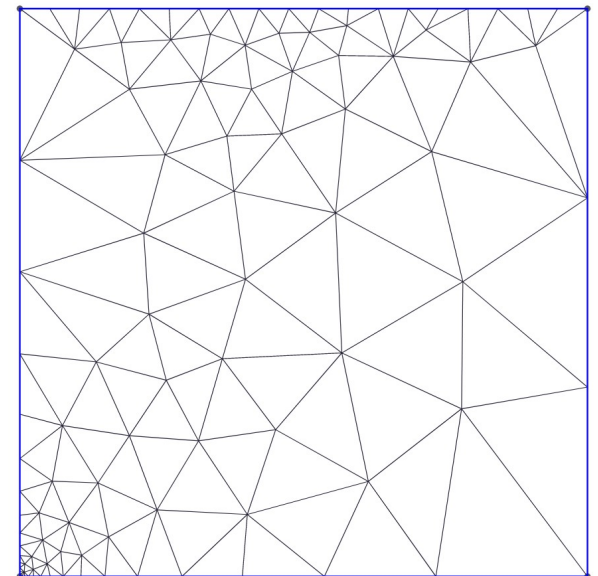
- PDE template with full coefficient matrix \mathbf{A} :

$$\mathbf{A} = \begin{bmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{bmatrix} \text{ with } a_{01} \neq 0 \text{ or } a_{10} \neq 0$$

- for instance modelling anisotropic conductivity
- Introduces mixed derivatives of v and u in weak form
- An element level requires $\int_E \frac{\partial N_i}{\partial x_0} \frac{\partial N_j}{\partial x_1} d\mathbf{x}$

Other Element Shapes

- For instance triangles or tetrahedrons
 - Allows for local refinement
- Modification analogously to 3D
 - Construct local basis N_0, N_1, N_2
 - Link Vertex \rightarrow FEM node
 - Element matrix calculation
 - Not only stretching + **rotation**

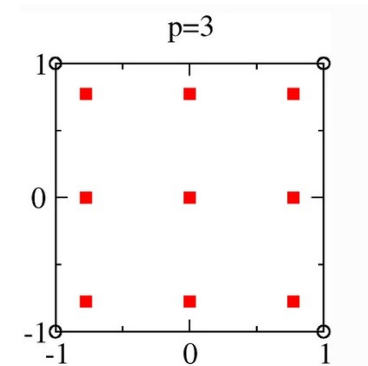


Numerical Integration

- Assumption: PDE coefficient constant across element.
- Better resolution of PDE coefficient on element?
- Apply numerical integration on each element E:

$$\int_E f(\mathbf{x}) d\mathbf{x} \approx \sum_k \omega_k^E f(\mathbf{q}_k^E)$$

- Integration nodes \mathbf{q}_k^E
- Integration weights ω_k^E



Numerical Integration (Cont.)

- Evaluate element matrices using numerical integration:

$$\int_E D N_i N_j d\mathbf{x} \approx \sum_k D_k^E \omega_k^E N_i(\mathbf{q}_k^E) N_j(\mathbf{q}_k^E) = A^E \sum_k D_k^E \hat{S}_{kij}^0$$

PDE coefficient at integration points q_k^E

Element geometry factor

$\omega_k^E N_i(\mathbf{q}_k^E) N_j(\mathbf{q}_k^E)$
For edge length 1

- Warning: This requires more memory and compute time.