Metamaterials and multiphysical couplings [solved with finite elements]

Introduction to finite element modeling for waves and other physical problems with FreeFem++

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Content

Objectives of the lecture

- Basics of the Finite Element Method (FEM)
- Waves (optics, electromagnetism, acoustics) with finite elements
- Show how far you can go with open-source software

Topics:

1. Introduction to the language: domain, mesh, variables, weak form, boundary conditions, solving a linear equation (forced response), obtaining eigenvalues and eigenvectors
2. 2D photonic and sonic crystals (scalar wave equation, periodicity, radiation boundary condition)
3. Guided waves in optical planar waveguides and fibers (weak form, light cone)
4. Vibrations and modes of mechanical and optical resonators (PML, 3D mesh)
5. Acousto-optical coupling in nanophotonics (photoelastic and moving boundary effects, optomechanics)

Partial differential equations (PDE)

A **partial differential equation (PDE)** for the function $u(x, y)$, written as

$$\mathcal{L}u = f$$

over a domain Ω, where $\mathcal{L}$ is a differential operator containing x, y, u, $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial y}$.
Examples:

- **Laplace**'s equation: $-\nabla \cdot (\nabla u) = 0$
- **Poisson**'s equation: $-\nabla \cdot (\epsilon \nabla \phi) = \rho$
- **Helmholtz**'s equation: $-\nabla \cdot (c \nabla u) - k^2 u = 0$

Galerkin's method (*for the dummies*)

Let us consider $\mathcal{L}u = f$ defined over a domain Ω. One can represent (project) u over a base defined by functions w_j, by

$$u(x, y) = \sum_{j=1}^{n} a_j w_j(x, y)$$

where a_j are coefficients (real or complex).
The PDE is projected over the functions w_i

$$\int_\Omega w_i \mathcal{L}u = \int_\Omega w_i f, \forall i = 1...n$$

We get a linear equation

$$A\mathrm{a} = \mathrm{f}$$

with $A_{ij} = \int_\Omega w_i \mathcal{L} w_j$ and $f_i = \int_\Omega w_i f$. The formal solution is $\mathrm{a} = A^{-1}\mathrm{f}$.

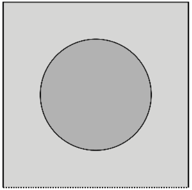
Linear equations

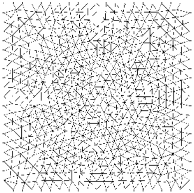
Many programs can solve linear equations. General purpose: Matlab, Octave, Python, Julia. Finite element method: Comsol and FreeFem++.

- Matrix inversion:
$$A^{-1}A = I$$
- Linear problem: find x satisfying
$$A\mathrm{x} = \mathrm{f}$$
- Eigenvalue problem: find (λ, x) satisfying
$$A\mathrm{x} = \lambda\mathrm{x}$$
- Generalized eigenvalue: find (λ, x) satisfying
$$A\mathrm{x} = \lambda B\mathrm{x}$$

Mesh and sub-domains

- We divide a domain Ω in smaller domains where all coefficients of the differential equation are homogeneous.
- One has to decrease the size of the small domains to improve the result. One has to not decrease it to much to avoid infinite calculation time! Compromising / understanding the problem is the key to find the best mesh.





Most common Boundary Conditions: BC

1. A boundary condition which specifies the value of the function itself is a **Dirichlet boundary condition**:

$$u = 0, \text{ or } u = u_0, \text{ on } \sigma$$

2. A boundary condition which specifies the value of the normal derivative of the function is a **Neumann boundary condition**:

$$\frac{\partial u}{\partial n} = 0$$

with n the outgoing normal to the boundary σ.

Additional BC (for a given function f):

1. Robin: $c_0 u + c_1 \frac{\partial u}{\partial n} = f$
2. Mixed: $u = f$ and $c_0 u + c_1 \frac{\partial u}{\partial n} = f \dots$

Finite element space

- Let us consider a domain Ω and its mesh Th. We decide to describe the solution by a finite number of degrees of freedom (*dof*), for example the nodal values u_j^e for the j nodes of the e elements.
- The finite element space Wh is the union of all representable functions by this given choice. Practical important aspect: It is a functional space of finite dimension.
- Representation *inside* a finite element
  $u^e(x, y) = \sum_j N_j^e(x, y) u_j^e$ where $N_j^e(x, y)$ are basis functions.
- For Lagrange elements, P_n, there is continuity of $u(x, y) = \sum_e u^e(x, y)$ between elements. The space derivatives, however, are not continuous!

Weak Form

- Let us assume that we have made a choice on Wh (for a domain Ω and its mesh Th).
- We replace the initial problem $\mathcal{L}u = f$ by an approximation:
  Find $u \in Wh$ that solves $\int_\Omega w\mathcal{L}u = \int_\Omega wf$ for all test functions $w \in Wh$.
- u and w are uniquely determined by their nodal values $\mathrm{U} = \{u_j^e\}$ and $\mathrm{W} = \{w_j^e\}$.
- There exists a matrix K and a vector B such that

$$\mathrm{W}^T K \mathrm{U} = \mathrm{W}^T \mathrm{B}, \forall \mathrm{W}$$

- Finally we get a linear equation: $K\mathrm{U} = \mathrm{B}$

Practical implementation for any FEM software

1. Define the domain
2. Mesh it
3. Choose the type of elements
4. Define the BC
5. Define the equations (i.e, define their weak form)
6. Choose the solver
7. Solve!
8. Display the results

1D: How does the software solve the problem (Poisson)?

1. Projection of the PDE on test functions

$$-\int_0^1 dx \psi(x) \frac{\partial}{\partial x}\left(\epsilon(x)\frac{\partial \phi(x)}{\partial x}\right) = \int_0^1 dx \psi(x)\rho(x)$$

2. Integration by parts

$$\int_0^1 dx \frac{\partial \psi}{\partial x}\epsilon\frac{\partial \phi}{\partial x} - \left[\psi\epsilon\frac{\partial \phi}{\partial x}\right]_0^1 = \int_0^1 dx \psi\rho$$

3. Application of known BC: $\left[\psi\epsilon\frac{\partial \phi}{\partial x}\right]_0^1$; for example:
   - Dirichlet: $\psi(0) = 0$
   - Neumann: $\frac{\partial \phi(1)}{\partial x} = 0$

2D: How does the software solve the problem (Poisson)?

1. Projection of the PDE on test functions

$$-\int_\Omega dr\psi(r)\nabla\cdot(\epsilon(r)\nabla\phi(r)) = \int_\Omega dr\psi(r)\rho(r)$$

2. Gauss's law

$$\int_\Omega dr\nabla\psi\cdot(\epsilon\nabla\phi) - \int_\sigma dn\psi\epsilon\frac{\partial\phi(r)}{\partial n} = \int_\Omega dr\psi\rho$$

3. Application of BC: $\int_\sigma \psi\epsilon\frac{\partial\phi(r)}{\partial n}$; for example:
   - Dirichlet: $\psi(r) = 0$ over a part of σ
   - Neumann: $\epsilon\frac{\partial\phi(r)}{\partial n} = 0$ on the rest of σ

Eigenvalue problem (summary)

- Let us consider a square (real or complex valued) matrix M of dimension n. An eigenvalue problem with eigenvalue λ and eigenvectors u is an equation of the following form $Mu = \lambda u$ ($\sum_{i=1}^{n} M_{ij} u_j = \lambda u_i$). Eigenvalues are solution of the caracteristic polynomial $|M - \lambda I| = 0$.
- There are exactly n eigenvalues and at most n eigenvectors (*a priori* complex). Eigenvectors are nonzero and thus can always be normalized.
- If M is a real symmetric (or Hermitian) matrix, then eigenvalues are real and eigenvectors are orthogonal.
- Generalized eigenvalue problem: $Au = \lambda Bu$

Artificial crystals

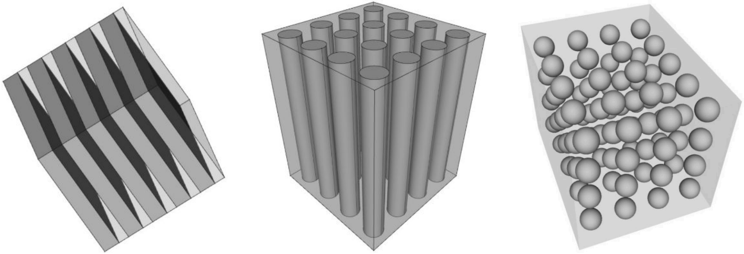


Figure: **Artificial crystals for waves with 1D, 2D, or 3D periodicity**

- Photonic crystal: matrix and Inclusions are dielectrics
- Sonic crystal: matrix is a fluid (e.g., water or air)
- Phononic crystal: matrix is a solid (e.g., steel, silicon, quartz...)
- Inclusions can be void, solid, or fluid

Acoustics (harmonic)

Acoustic equation for pressure p in the harmonic regime with a source term:

$$-\nabla \cdot (\rho^{-1} \nabla p) - \omega^2 B^{-1} p = f$$

with B the elastic modulus (Pa), ρ the density (kg/m^3), and f a source term (1/s^2).

Example: Loud speaker in a room

- Domain
- BC (pressure, normal acceleration, soft and hard boundary, radiation)?
- Applying a force: Dirichlet or Neumann? Response of the system?
- What is a good mesh for a harmonic problem at a single wavelength λ?
- Change the finite elements; does the solution change?

TE and TM 2D photonic crystal (harmonic)

Maxwell's equations in the harmonic regime lead to:

- TE (transverse electric field)

$$-\nabla \cdot (\nabla E_z) = \epsilon(\omega/c)^2 E_z$$

- TM (transverse magnetic field)

$$-\nabla \cdot (\epsilon^{-1} \nabla H_z) = (\omega/c)^2 H_z$$

with $\epsilon = n^2$ the relative dielectric permittivity and c the speed of light in a vacuum.

Bloch theorem

Helmholtz equation with periodic coefficients: $-\nabla \cdot (c(\boldsymbol{r})\nabla u(\boldsymbol{r})) = \omega^2 u(\boldsymbol{r})$

Theorem (Bloch)

The eigenmodes of the periodic Helmholtz equation are Bloch waves of the form

$$u(\boldsymbol{r}) = \exp(-\imath \boldsymbol{k} \cdot \boldsymbol{r})\tilde{u}(\boldsymbol{r})$$

where $\tilde{u}(\boldsymbol{r})$ is a periodic function with the same periodicity as the crystal and $\boldsymbol{k}$ is the Bloch wave vector.

(Classical) band structure: solve for $\omega(k)$

Weak form of the pressure equation, boundary conditions

- Consider all possible test functions $q(t, \boldsymbol{x})$ belonging to the same finite element space as the pressure and form the scalar products

$$-\int_\Omega \mathrm{d}\boldsymbol{x}\, q \nabla \cdot \left(\frac{1}{\rho} \nabla p \right) + \int_\Omega \mathrm{d}\boldsymbol{x}\, q \frac{1}{B} \frac{\partial^2 p}{\partial t^2} = \int_\Omega \mathrm{d}\boldsymbol{x}\, q f.$$

- Using the divergence theorem, the weak form is

$$\int_\Omega \mathrm{d}\boldsymbol{x}\, \nabla q \cdot \left(\frac{1}{\rho} \nabla p \right) - \int_\sigma \mathrm{d}s\, q \left(\frac{1}{\rho} \nabla p \right) \cdot \boldsymbol{n} + \int_\Omega \mathrm{d}\boldsymbol{x}\, q \frac{1}{B} \frac{\partial^2 p}{\partial t^2} = \int_\Omega \mathrm{d}\boldsymbol{x}\, q f.$$

- External boundary conditions – free: $\left(\frac{1}{\rho} \nabla p \right) \cdot \boldsymbol{n} = 0$; Dirichlet: $p = p_0$
- Continuity between elements of p and $\left(\frac{1}{\rho} \nabla p \right) \cdot \boldsymbol{n}$ (normal acceleration)

Example of an internal source and radiation BC

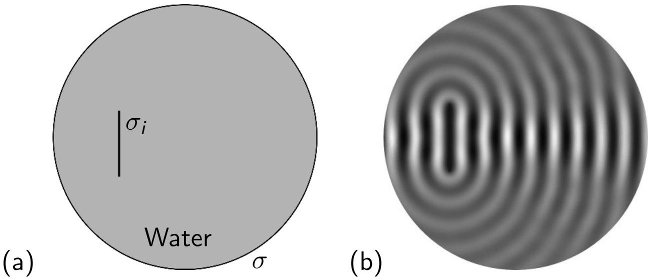


Figure: **Internal source and radiation boundary condition.** (a) The computational domain is a disk of water inside which a linear source is added by prescribing $p = 1$ Pa along internal boundary σ_i. A radiation boundary condition $\left(\frac{1}{\rho}\nabla p\right) \cdot \boldsymbol{n} = -\imath \frac{\omega p}{\rho c}$ is applied at boundary σ. (b) The solution shows the natural diffraction of the acoustic beam radiated from the source. The source dimension is slightly less than 3 wavelengths in water.

FEM for a unit-cell: the band structure of sonic crystals

- Look for Bloch waves in the form $p(\boldsymbol{r}) = \exp(-\imath \boldsymbol{k} \cdot \boldsymbol{r}) \tilde{p}(\boldsymbol{r})$, and consider $\tilde{p}(\boldsymbol{r})$ as the unknown field
- In order to obtain the band structure, it is enough to solve the eigenproblem

$$\omega^2 \int_\Omega d\mathrm{r} \left(\tilde{q}^* \frac{1}{B} \tilde{p} \right) = \int_\Omega d\mathrm{r} \left((\nabla \tilde{q} - \imath \mathrm{k} \tilde{q})^\dagger \frac{1}{\rho} (\nabla \tilde{p} - \imath \mathrm{k} \tilde{p}) \right), \forall \tilde{q}$$

- There is no source term and the boundary integral vanishes identically because of the periodic boundary conditions.
- The wave vector $\boldsymbol{k}$ enters directly the variational formulation, and more precisely the stiffness matrix.

Sonic crystal of cylindrical steel rods in water: band structure

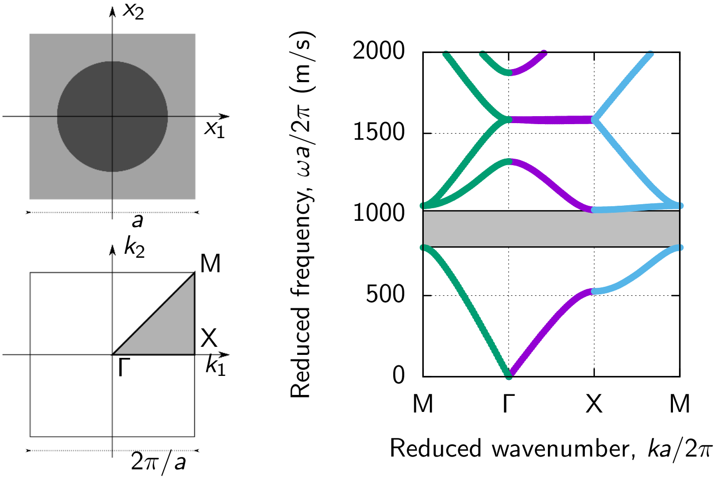
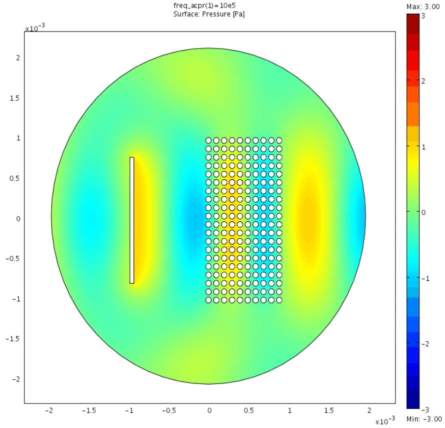


Figure: **2D square-lattice sonic crystal**. $d/a = 0.83$

A square-lattice phononic crystal of steel rods in water: transmission



- Pitch: 100 μm
- Diameter: 70 μm
- Complete band gap: 8-9 MHz
- Plane source emits 1 Pa

Acoustics (eigenvalue problem) for a special case

Acoustical equation in harmonic regime with an axial wavenumber:

$$-\nabla \cdot (\rho^{-1} \nabla p) + (k_z^2 \rho^{-1} - \omega^2 B^{-1}) p = 0$$

with B the elastic modulus (Pa), ρ the density (kg/m^3), and k_z an axial wave number (1/m).

Example: tubular problem

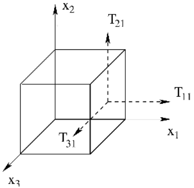
- Domain
- BC (soft and hard boundary)?
- Find the first 5 eigenvalues?
- change k_z: influence of the length of the tube?

3D elasticity: deformations and strain

- Let us consider a point $\mathbf{x}$ with its coordinates (x_1, x_2, x_3). $u_i(\mathbf{x} + d\mathbf{x}) = u_i(\mathbf{x}) + \frac{\partial u_i}{\partial x_j} dx_j$ at the first order. $\frac{\partial u_i}{\partial x_j}$ is the displacement gradient.
- One can split this gradient into a symmetric part (S_{ij}) and an antisymmetric part as follows $\frac{\partial u_i}{\partial x_j} = S_{ij} + AS_{ij}$, $S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ and $AS_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$
- The symmetric part gives the deformation or **strain** and the antisymmetric part the local rotations.
- The dilation is given by $S = S_{11} + S_{22} + S_{33} = \nabla \cdot \mathbf{u}$.
- Terms S_{11}, S_{22} and S_{33} are longitudinal strains and $S_{ij}, i \neq j$, are transverse strains.

3D Elasticity: Stresses

- 3 independent constraints can be applied on a surface: a traction-compression and two shear constraints.



- On the face of the cube normal to x_1, the force per unit of surface is $T_{11} + T_{21} + T_{31}$. T_{ij} is a rank-two symmetric tensor called the **stress tensor**. For a surface denoted by its normal n, the traction is given by the vector $T_{ij}n_j$.
- Dynamical (or Navier) equation (with f_i the internal forces): $\frac{\partial T_{ij}}{\partial x_j} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2}$

3D elasticity: Hooke's law

- For small deformations Hooke's law can be expressed as :

$$T_{ij} = c_{ijkl} S_{kl}$$

  i/e. the stress is proportional to the strain.
- c_{ijkl} is a 4th order tensor, called elasticity tensor. It has *a priori* $3^4 = 81$ components. Assuming symmetry of T_{ij} and S_{kl} implies that $c_{jikl} = c_{ijkl}$ et $c_{ijkl} = c_{ijlk}$. reducing it to 36 independent components.
- Adding the major symmetry $c_{ijkl} = c_{klij}$ only 21 components are left.

3D elasticity: Notations

$$(11) \longrightarrow 1; (22) \longrightarrow 2; (33) \longrightarrow 3$$

$$(23) = (32) \longrightarrow 4; (13) = (31) \longrightarrow 5; (12) = (21) \longrightarrow 6$$

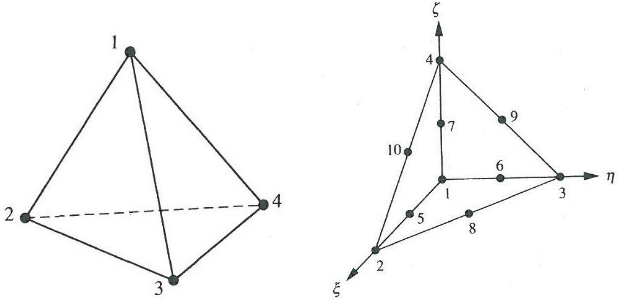
$$T_I = T_{ij}; c_{IJ} = c_{ijkl}; T_I = c_{IJ} S_J$$

$$S_1 = S_{11}; S_2 = S_{22}; S_3 = S_{33}; S_4 = 2S_{23}; S_5 = 2S_{13}; S_6 = 2S_{12}$$

Matériaux	Classe	Rigidités (10^{10} N/m^2)						ρ (10^3 kg/m^3)
cub. ou isotrope		c_{11}	c_{12}	c_{44}				
AsGa	$\bar{4}3m$	11.88	5.38	2.83				5.307
SiO_2	isotrope	7.85	1.61	3.12				2.203
Si	$m3m$	16.56	6.39	7.95				2.329
hexagonal		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}		
PZT-4	trans. iso.	13.9	7.8	7.4	11.5	2.6		7.5
ZnO	$6mm$	21.0	12.1	10.5	21.1	4.2		5.676
trigonal		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}	
Al_2O_3	$\bar{3}m$	49.7	16.3	11.1	49.8	14.7	-2.3	3.986
$LiNbO_3$	$3m$	20.3	5.3	7.5	24.5	6.0	0.9	4.7
quartz α (SiO_2)	32	8.7	0.7	1.2	10.7	5.8	-1.8	2.648

3D Mesh

- In 2D one can mesh the domain using triangles.
- In 3D one may use tetrahedrons.



Vector finite elements

- Let's consider a vector field (u_1, u_2, u_3).
- A domain Ω and its mesh Th. One describes the solution by a finite number of DOF
- A vector finite space of elements Wh is a finite set of representable functions by this choice.
- Representation *in* a finite element
  $u_i^e(x, y) = \sum_j N_j^e(x, y) u_{ij}^e$ where $N_j^e(x, y)$ are basis functions as in the scalar case.
- For Lagrange elements, P_n, the continuity $u_i(x, y) = \sum_e u_i^e(x, y)$ between elements is preserved.

Weak form for 3D elasticity (1)

1. Elastodynamic equation:

$$-\nabla T + \rho \frac{\partial^2 \mathrm{u}}{\partial t^2} = \mathrm{f}$$

2. Projection on the vector test fonctions v:

$$-\int_\Omega \mathrm{v} \cdot \nabla T + \int_\Omega \mathrm{v} \cdot \rho \frac{\partial^2 \mathrm{u}}{\partial t^2} = \int_\Omega \mathrm{v} \cdot \mathrm{f}$$

3. Divergence theorem:

$$\int_\Omega \nabla \mathrm{v}\, T - \int_\sigma \mathrm{v} \cdot T_n + \int_\Omega \mathrm{v} \cdot \rho \frac{\partial^2 \mathrm{u}}{\partial t^2} = \int_\Omega \mathrm{v} \cdot \mathrm{f}$$

Weak form for 3D elasticity (2)

1. Hooke's law: $T_I = c_{IJ} S_J$ with $S = \nabla \mathrm{u}$

$$\int_\Omega S(\mathrm{v})_I c_{IJ} S(\mathrm{u})_J - \int_\sigma \mathrm{v} \cdot T_n + \int_\Omega \mathrm{v} \cdot \rho \frac{\partial^2 \mathrm{u}}{\partial t^2} = \int_\Omega \mathrm{v} \cdot \mathrm{f}$$

2. BC: $\int_\sigma \mathrm{v} \cdot T_n$ is known:
   - Dirichlet: $\mathrm{v} = 0$ on a part of σ (clamped)
   - Neumann: $T_n = 0$ on the remaining part σ (stress free)
3. monochromatic case (or harmonic excitation)

$$\int_\Omega S(\mathrm{v})_I c_{IJ} S(\mathrm{u})_J - \int_\sigma \mathrm{v} \cdot T_n - \omega^2 \int_\Omega \mathrm{v} \cdot \rho \mathrm{u} = \int_\Omega \mathrm{v} \cdot \mathrm{f}$$

Example: Bending of a beam under gravity

- Clamped silicon beam.
- bending by gravity in the static case.
- Visualization of the deformation.

Eigenmode of a beam

- Clamped on two sides.
- neglect gravity
- Find the eigenmodes
- influence of the BC?

Multiphysics: coupling of different physical problems

- Many physical models are coupled and many phenomena or even moduli depend on one another
  - Electro-optics, magneto-optics
  - Piezoelectricity
- Equations are linked by constitutive relation
- *One must consider a vector finite element space containing all unknowns of the problem.*

Example: piezoelectricity

- Direct piezoelectric effect: an electric polarization is induced by a deformation.
- Inverse piezoelectric effect: an applied electric field induces a deformation of the crystal lattice.
- The piezoelectric effect only appears in non centro-symmetric crystals.
- Coupled equations (e_{kij}: piezoelectric tensor)

$$T_{ij} = c_{ijkl} S_{kl} - e_{kij} E_k ; D_i = e_{ikl} S_{kl} + \epsilon_{ij} E_j$$

- Electric field derives from a potential : $E_i = -\frac{\partial \phi}{\partial x_i}$
- In contracted form:

$$T_I = c_{IJ} S_J - e_{kI} \phi_{,k} ; D_i = e_{iJ} S_J + \epsilon_{ij} \phi_{,j}$$

Indirect coupling of physical models

- Many different situations lead to coupled multiphysics models
  - A system can perform a distant action on another system, for instance a force...
  - If a physical quantity induces a deformation of the system, then the geometry and the mesh must change, and thus the solution can change even there was no direct coupling in the equation...
- There is no simple rule to decide how to solve the problem: a coupling model has to be improvised!

Some useful integral theorems

V a volume, S a surface enclosing the volume. $\oint$ stands for an integral over a **closed** surface or contour.

- Gradient theorem

$$\int_V dV \; \nabla f = \oint_S \mathrm{n} \; f dS$$

- Gauss theorem (or divergence theorem)

$$\int_V dV \; \nabla \cdot \mathrm{f} = \oint_S dS \; \mathrm{n} \cdot \mathrm{f}$$

- Rotational theorem

$$\int_V dV \; \nabla \times \mathrm{f} = \oint_S dS \; \mathrm{n} \times \mathrm{f}$$