# An Introduction to Finite Element Modelling with ONELAB

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# About modern product development

### Development cycle



### How is testing performed? Physical vs. Numerical

# Test of a car – The physical crash test



Costly (vehicle 250k€, dummy 50-500k€) and time-consuming









• Nowadays, typically more than 100 numerical tests are performed for 1 physical test

Thanks to the finite element method (and related numerical techniques)

• Both testing strategies are complementary





#### Weather forecasting



#### Geophysical modelling





**Biomedical engineering** 





# Steps of a finite element analysis



# Steps of a finite element analysis

- Many commercial software packages are available, that perform all the steps:
  - ANSYS, Abaqus/CATIA/SIMULIA, Siemens
     NX/Nastran/SAMCEF, Altair, ADINA, COMSOL, LS-DYNA, ...
- Several open source packages are also available, but most only implement one step:
  - Code\_Aster, deal.II, CalculiX, Elmer, FEniCS, FreeFem++, OpenFOAM, GetDP, Gmsh, Paraview, ...
- This week: introduction to finite element modelling with ONELAB (<u>http://onelab.info</u>)



- Open source, lightweight interface to finite element software
- The default ONELAB software bundle contains
  - the mesh generator Gmsh (<u>http://gmsh.info</u>)
  - the finite element solver GetDP (<u>http://getdp.info</u>)
- Many other codes (free or not) can be easily interfaced as well
- Download the software bundle now for Windows, Linux, Mac, Android or iOS from <u>http://onelab.info</u>

# Steps of a finite element analysis with ONELAB



# This week – Objective of the course

As an introduction to finite element modelling, we would like you to

- understand,
- model,
- simulate, and
- optimize

a practical device with ONELAB, and learn the basics of the finite element method along the way

The device we chose is a Micro Electro-Mechanical System (MEMS): a Xylophone Bar Magnetometer (XBM)

### This week – Objective of the course



### Xylophone Bar Magnetometer (XBM) Micro Electro-Mechanical System (MEMS)

# This week – Objective of the course

- When an alternating current flows through it, the magnetometer starts to vibrate if it is placed in a magnetic field; the amplitude of the vibration can be used to measure the magnetic field
- To increase sensitivity, the frequency of the current is tuned to excite a resonant mode of the xylophone-type structure
- Modelling should take into account the multiphysics coupling (electromagnetic, mechanical and thermal) and multiple time states (static, transient, harmonic, eigenmodes)

# This week – Schedule

- Monday 10h00-12h00 & 14h00-17h00
  - Basics of the finite element method
- Tuesday 10h00-12h00 & 14h00-17h30
  - Electromagnetics and heat transfer
- Wednesday 10h00-12h00 & 14h00-17h00
  - Mechanics
- Thursday 10h00-12h00 & 14h00-17h30
  - Optimization
- Friday 10h00-13h00
  - Siemens LMS Samtech visit

# **Geometry construction**

- Gmsh uses a Boundary REPresentation (BREP) approach to describe geometrical models:
  - volumes are bounded by surfaces
  - surfaces are bounded by curves
  - curves are bounded by points
- Models can be
  - built interactively using the graphical user interface (which logs all commands in a ".geo" file)
  - scripted directly in ".geo" files
  - imported from external CAD packages

To launch Gmsh, double-click on the <u>icon</u>



 To open an existing geometry, use "File->Open" and select "models/magnetometer/magnetometer.geo"

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 Model parameters are on the left, below the "Geometry", "Mesh" and "Solver" modules



- To change a parameter, simply enter a value or click and slide the mouse across an input field
- In the graphic window:
  - The left mouse button rotates the model and selects objects
  - The middle mouse button (or the mouse wheel, or a two finger zoom gesture) zooms in or out
  - The right mouse button pans (translates)
  - For two- or single-button manipulation:
    - Middle click = Shift+left click
    - Right click = Alt+left click

• Common options can be accessed by double-clicking in the graphic window



 Preset viewports and rotations can also be accessed in the status bar



 A video tutorial showing how to create geometries interactively is available here: <u>http://youtu.be/nkuawZkiu1w</u>



 Let us create a magnetometer model from scratch: select "File->New" and choose a name ("new.geo")

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 Select "Modules->Geometry->Elementary entities-> Add->Point" to create a point

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• Enter coordinates (0,0,0) and press "Add" (or choose the position with the mouse and press "e")



 Press "q" when you are done; placing the mouse on the point will show its attributes



If anything goes wrong, don't worry:

- Select "Modules->Geometry->Remove last script command"
  - This removes the last command that was added to the script "new.geo" and reloads the updated script
- Or select "Modules->Geometry->Edit script"
  - This opens the script in a text editor, where you can remove the erroneous commands or fine-tune the commands that were inserted
  - Then save the file, close the text editor and select Select "Modules->Geometry->Reload"

 Define some variables by selecting "Add->Parameter": w=50e-6, w2=2e-6, l=500e-6, e=2e-6


• Create a line of length "w" by extruding the point with "Translate->Extrude point"; then press "e"



• This is the left side of the magnetometer; Create a surface of width "w" with "Translate->Extrude line"



 Proceed along axis "X" with successive line extrusions of length "w2", "l", "w2" and "w"



 Create the "legs" by extruding by "w" and "-w" along axis "Y"



 Create the volume by extruding all the surfaces ("Ctrl+left click" to select a region) along the "Z" axis



• Note that the parameters are "live": you can change them in the left menu and see the result



 Select "Modules->Geometry->Edit script" to see the transcription of our work so far



 You can edit this file, save it and press "Modules->Geometry->Reload script" to reload it



- The main commands we have used are
  - Point(1) = {0, 0, 0, 1.0};
    - This creates a point with identification number "1", at Cartesian coordinates "(0,0,0)" and with a target mesh size of "1.0" (the size of the finite elements that will be created close to this point)
  - w = DefineNumber[ 50e-6, Name "Parameters/w" ];
    - This creates a variable "w" with default value "50e-6" and ONELAB name "Parameters/w". ONELAB names are provided as paths, which correspond to the tree hierarchy in the graphical user interface.

- Extrude {0, w, 0} { Point{1}; }
  - This extrudes the point "1" and creates a line of length "w" in along the "Y" axis
- Extrude {w2, 0, 0} { Line{2}; }
  - This extrudes the line "2" by "w2" along the "X" axis
- Extrude {0, 0, e} { Surface{5, 25, 9, 29, ...};}
  - This extrudes the listed surfaces along the "Z" axis to create a volume

- The geometry is almost ready to be meshed and used for computing a solution: we just need to group elements in "physical groups"
- We will need one physical group for each region that must be distinguished in the solution process: for example, for each material and for each boundary condition
- For the magnetometer, we define a single "physical volume" (single material) grouping all the elementary volumes and two "physical surfaces" – one for each electrode, where the structure is also clamped



 Click on "Physical groups->Add->Volume", select all volumes, choose a name and press "e"



 Click on "Physical groups->Add->Surface", select the electrodes, choose names and press "e"



• You can inspect all entities (elementary and physical) by selecting Tools->Visibility



• To reset all ONELAB variables to their default value, select "Reset database" in the gear menu



 Many more commands exist in Gmsh: examine in more detail the first tutorials provided in the distribution (in the "tutorial" directory):



 The complete documentation is available on <u>http://gmsh.info</u>

# Mesh generation

 To generate a finite element mesh, select "Modules->Mesh->3D"



- The resulting mesh is
  - as coarse as possible (we set a target mesh size of "1.0" on point 1, for a structure of about 6e-4; notice that there are no units at this stage)
  - made of tetrahedra in the volume, triangles on surfaces and line segments on curves (select "Tools->Statistics" to see the details)

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	Press Update		Gamma	Plot	X-Y	3D	
	Press Update		Rho	Plot	X-Y	3D	
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• Double-click in the graphic window and set the "Global mesh size factor" to 1e-2



 Press "1D", "2D" and "3D" in "Modules->Mesh" to remesh the curves, surfaces and volumes



- For a thin structure like the magnetometer, a regular ("structured") mesh would be more suitable
- Edit the "new.geo" file and modify the Extrude commands by adding "Layers" options to specify explicitly the number of layers of elements to be generated in the extrusion



• Adding "Recombine;" will recombine all triangles into quadrangles and all tetrahedra into hexahedra



#### The final "new.geo" script after removing the comments:

```
Point(1) = \{0, 0, 0, 1.0\};
w = DefineNumber[ 50e-6, Name "Parameters/w" ];
w2 = DefineNumber[ 2e-6, Name "Parameters/w2" ];
1 = DefineNumber[ 500e-6, Name "Parameters/1" ];
e = DefineNumber[ 2e-6, Name "Parameters/e" ];
n1 = 5; n2 = 2; n3 = 50;
Extrude {0, w, 0} { Point{1}; Layers{n1};}
Extrude {w, 0, 0} { Line{1}; Layers{n1}; Recombine;}
Extrude {w2, 0, 0} { Line{2}; Layers{n2}; Recombine; }
Extrude {1, 0, 0} { Line{6}; Layers{n3}; Recombine;}
Extrude {w2, 0, 0} { Line{10}; Layers{n2}; Recombine; }
Extrude {w, 0, 0} { Line{14}; Layers{n1}; Recombine;}
Extrude {0, w, 0} { Line{8}; Layers{n1}; Recombine;}
Extrude {0, -w, 0} { Line{7}; Layers{n1}; Recombine;}
Extrude \{0, -w, 0\} { Line\{15\}; Layers\{n1\}; Recombine; }
Extrude {0, w, 0} { Line{16}; Layers{n1}; Recombine; }
Extrude {0, 0, e} { Surface {5, 25, 9, 29, 13, 37, 17, 33, 21}; Layers {n2};
                    Recombine; }
Physical Volume("Magnetometer") = \{2, 1, 3, 4, 5, 6, 7, 9, 8\};
Physical Surface("Left Electrode") = {76, 120};
Physical Surface("Right Electrode") = {164, 208};
```

- To save the mesh to disk in the default mesh format, select "Modules->Mesh->Save"
- The "File->Save As" menu has many more options to save the mesh in various formats suitable for different solvers, or to export images. Simply choosing a file name with the right extension (e.g. "image.png" for a PNG image) will select the appropriate file format
- You can mesh without the graphical user interface, by opening a terminal and typing: "gmsh new.geo -3"

# Solution computation

## **GetDP solver**

- GetDP is a rather general finite element solver, whose main feature is the closeness between the input data defining discrete problems (written in plain text ".pro" files) and the symbolic mathematical expressions of these problems
- ONELAB uses GetDP both
  - as a "black-box" solver, if a template problem definition is available
  - as a fully customizable solver, when the physical problem definition is written from scratch

- If a template for the given physical problem already exists, simply merge it along with the geometrical description with "File->Merge"
- Simple templates are provided in the "templates" directory



• "File->Merge" the "Electrostatics.pro" template with the magnetometer geometry



• Materials and boundary conditions can be specified interactively on the available physical groups



• Once the parameters are chosen, press "Run" to compute the solution



• We will see later how to exploit the results in the post-processing module



# GetDP solver – Constructing your own model

- In order to construct your own physical model, you need to start with the mathematical description of the physical problem as partial differential equations
- The finite element method allows to solve such partial differential equations in so-called "weak form", after discretization on a mesh
- The next slides provide a short summary of the general approach – you will study details for electromagnetics, heat transfer and mechanics on Tuesday and Wednesday

# GetDP solver – Constructing your own model

 Let us assume that the physical problem we want to solve is modelled by the following partial differential equation on the open set Ω ⊂ R<sup>3</sup>, with homogeneous boundary conditions on the boundary ∂Ω:

div 
$$\alpha(\boldsymbol{x}) \operatorname{grad} u(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega$$
  
 $u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \partial \Omega$ 

• Given  $\alpha(x) > 0$  and f(x), we want to find u(x) everywhere in  $\Omega$ 

GetDP solver – Constructing your own model

- For general  $\Omega$ ,  $\alpha(x)$  and f(x) there is no closed form solution for u(x)
- The main idea behind the finite element method is to look for the solution u(x) such that the partial differential equation is satisfied when tested against well-chosen test functions
- Mathematically, we look for u(x), with u(x) = 0on  $\partial \Omega$ , such that

 $\int_{\Omega} (\operatorname{div} \alpha(\boldsymbol{x}) \operatorname{\mathbf{grad}} u(\boldsymbol{x})) \ u'(\boldsymbol{x}) \ d\Omega = \int_{\Omega} f(\boldsymbol{x}) \ u'(\boldsymbol{x}) \ d\Omega$ 

holds for all appropriately chosen functions  $u'(\boldsymbol{x})$
- The differential operators div and grad should be understood in the distributional sense (think about  $\alpha(x)$  being discontinuous)
- Integrating by parts, the problem becomes: find  $u(\mathbf{x})$  such that

$$-\int_{\Omega} \alpha(\boldsymbol{x}) \operatorname{\mathbf{grad}} u(\boldsymbol{x}) \cdot \operatorname{\mathbf{grad}} u'(\boldsymbol{x}) \, d\Omega = \int_{\Omega} f(\boldsymbol{x}) \, u'(\boldsymbol{x}) \, d\Omega$$

holds for all  $u'(\boldsymbol{x})$ 

• The finite element methods consists in approximating u(x) by  $u_h(x)$  in a finite dimensional function space

• For classical finite elements, this means taking  $u_h(x)$ and the test functions in

 $F^0(\Omega) = \text{span}\{s_1(\boldsymbol{x}), s_2(\boldsymbol{x}), \dots s_N(\boldsymbol{x})\}$ where the basis functions  $s_i(\boldsymbol{x}), i = 1, \dots, N$  are associated with the N vertices of the mesh

 Lowest order basis functions are linear on line, triangle and tetrahedral elements, bilinear on quadrangles and trilinear on hexahedra; their value goes from 1 at the associated vertex, to 0 on the other vertices





• Injecting 
$$u(\boldsymbol{x}) \approx u_h(\boldsymbol{x}) = \sum_{i=1}^N u_i s_i(\boldsymbol{x})$$
 in the weak form

$$-\int_{\Omega} \alpha(\boldsymbol{x}) \operatorname{\mathbf{grad}} u(\boldsymbol{x}) \cdot \operatorname{\mathbf{grad}} u'(\boldsymbol{x}) \, d\Omega = \int_{\Omega} f(\boldsymbol{x}) \, u'(\boldsymbol{x}) \, d\Omega$$

and taking for  $u'(\boldsymbol{x})$ :  $s_i(\boldsymbol{x}), i = 1, ..., N$  leads to a system of linear equations, for j = 1, ..., N:

$$-\sum_{i=1}^{N} u_i \int_{\Omega} \alpha(\boldsymbol{x}) \operatorname{\mathbf{grad}} s_i(\boldsymbol{x}) \cdot \operatorname{\mathbf{grad}} s_j(\boldsymbol{x}) d\Omega = \int_{\Omega} f(\boldsymbol{x}) s_j(\boldsymbol{x}) d\Omega$$

• In matrix form, we have

$$\begin{aligned} \mathbf{A}\mathbf{u} &= \mathbf{f} \\ \text{with } \mathbf{A}_{ij} &= -\int_{\Omega} \alpha(\boldsymbol{x}) \operatorname{\mathbf{grad}} s_i(\boldsymbol{x}) \cdot \operatorname{\mathbf{grad}} s_j(\boldsymbol{x}) \, d\Omega \\ \mathbf{u} &= [u_1, u_2, \dots, u_N]^T \\ \mathbf{f} &= [\int_{\Omega} f(\boldsymbol{x}) \, s_1(\boldsymbol{x}) \, d\Omega, \dots, \int_{\Omega} f(\boldsymbol{x}) \, s_N(\boldsymbol{x}) \, d\Omega]^T \end{aligned}$$

This is the system solved by the computer, e.g. using LU factorization

 The matrix A is very sparse, since basis functions associated with distant nodes have disjoint support – leading to many zero integrals

- The implementation in GetDP ".pro" files reflects this problem definition structure:
  - Group{ } defines the domains (i.e.  $\Omega$  and  $\partial \Omega$ )
  - Function{ } defines the functions (i.e.  $\alpha(\boldsymbol{x})$  and  $f(\boldsymbol{x})$  )
  - FunctionSpace{ } and Constraint{ } define the function space (i.e.  $F^0(\Omega)$ ) and associated constraints (u(x) = 0 on  $\partial\Omega$ )
  - Formulation{ } defines the weak form

- Additional objects define
  - Integration methods: Integration{ }
  - Geometrical transformation methods: Jacobian{ }
  - Resolution steps: Resolution{ }
  - Post-processing specifications: PostProcessing{ } and PostOperation{ }

10 objects Top: particular to a particular test-case Bottom: generic for a physical/mathematical model



- 1. Group
  - Regions (physical groups)
  - "Functions" on regions (nodes, edges, edges of tree, ...)

```
Group{
   Air = Region[1]; //simple group (linked with the mesh)
   Core = Region[2];
   Gamma = Region[{3,4}];
   Omega = Region[{Air, Core}]; //combining groups
   nodes = NodesOf[Omega]; //function group
   edgesOfSpanningTree = EdgesOfTreeIn[Omega, StartinOn Gamma];
}
```

- 2. Function
  - Piecewise definition (on groups)
  - Space/time dependent, with arguments
  - For physical characteristics, sources, contraints, ...

```
Function{
    f = 50; //constants
    mu0 = 4.e-7 * Pi;
    mu[Air] = mu0; //piecewise definition
    mu[Core] = mu0 + 1/(100 + 100 * ($1)^6); //argument ($1)
    TimeFct[] = Cos[2*Pi*f*$Time] * Exp[-$Time/0.01]; //current value
}
```

- 3. FunctionSpace
  - List of basis functions associated with nodes, edges, faces or volumes, of various orders
  - Local or nonlocal (fluxes, circulations, ...)

```
FunctionSpace{
    { Name H1; Type Form0; //discrete function space for H1_h
    BasisFunction {
        { Name wi; NameOfCoef fi; Function BF_Node; //``P1 finite elements''
        Support Omega; Entity NodesOf[All]; }
    }
    Constraint {
        { NameOfCoef fi; EntityType NodesOf; NameOfConstraint Dirichlet; }
    }
    }
}
```

#### 3. FunctionSpace

```
//higher-order version
FunctionSpace{
  { Name H1; Type FormO;
    BasisFunction {
      { Name wi; NameOfCoef fi; Function BF_Node; //order 1
        Support Omega; Entity NodesOf[All]; }
      { Name wi2; NameOfCoef fi2; Function BF_Node_2E; //order 2
        Support Omega; Entity EdgesOf[All]; }
    Constraint {
      { NameOfCoef fi; EntityType NodesOf; NameOfConstraint Dirichlet; }
        NameOfCoef fi2; EntityType EdgesOf; NameOfConstraint Dirichlet2; }
```

- 4. Constraint
  - Constraints on FunctionSpace coefficients (boundary, periodicity, initial and gauge conditions, ...)
  - Topology of circuits with lumped elements

```
Constraint{
    { Name Dirichlet; Type Assign; //boundary conditions
    Case {
        { Region Surface0; Value 0; }
        { Region Surface1; Value 1; }
    }
}
```

#### 4. Constraint

```
Constraint{
   //time-dependent or harmonic constraints
   { Name Current; Type Assign;
     Case {
        { Region CurrentLoop; Value 1000; TimeFunction TimeFct[]; }
    }
}
```

```
//network relations between global quantities
```

```
{ Name ElectricalCircuit; Type Network;
Case Circuit {
        { Region E1; Branch {1,2}; }
        { Region R1; Branch {1,3}; }
        { Region L1; Branch {3,2}; }
        { Region C1; Branch {1,2}; }
    }
}
```



- 5. Formulation
  - Symbolic equation builder (bilinear and linear forms, term by term) involving local and nonlocal quantities

```
Formulation{
   { Name Maxwell_e; Type FemEquation;
      Quantity {
         { Name e; Type Local; NameOfSpace Hcurl_h; }
      Equation {
         Galerkin { [1/mu[] * Dof{Curl e}, {Curl e} ];
                           In Omega; Jacobian Jac1; Integration Int1; }
         Galerkin { DtDt [ epsilon[] * Dof{e} , {e} ];
                           In Omega; Jacobian Jac1; Integration Int1; }
  }
                                                                 "Find \boldsymbol{e} \in \boldsymbol{H}_h(\operatorname{curl}; \Omega) such that
                          (\mu^{-1}\operatorname{curl} \boldsymbol{e}, \operatorname{curl} \boldsymbol{e}') + \partial_t^2(\epsilon \boldsymbol{e}, \boldsymbol{e}') = 0, \quad \forall \boldsymbol{e}' \in \boldsymbol{H}_h(\operatorname{curl}; \Omega)
```

- 6. Jacobian
  - Mapping fom reference to solution space
  - Geometrical transformations (axisymmetry, infinite domains, ...)

```
Jacobian{
    { Name Jac1;
    Case { //piecewise defined on groups
        { Region OmegaInf; Jacobian VolSphShell{Rint, Rext}; }
        { Region OmegaAxi; Jacobian VolAxi; }
        { Region All; Jacobian Vol; }
    }
}
```

- 7. Integration
  - Numerical and analytic integration methods
  - Criterion-based selection

```
Integration {
    { Name Int1; Criterion Test[];
    Case {
        { Type Gauss;
        Case {
            { GeoElement Triangle; NumberOfPoints 3; }
        { GeoElement Tetrahedron; NumberOfPoints 3; }
        }
      }
    }
    }
}
```

- 8. Resolution
  - Sequence of solving operations (system generation and solution, time-stepping and nonlinear iterations, multiformulation coupling, ...)

```
Resolution{
    { Name Parabolic;
      System {
         { Name A; NameOfFormulation Parabolic; }
     }
     Operation{
         InitSolution[A];
         TimeLoopTheta[tmin,tmax,dt,1]{
         Generate[A]; Solve[A]; If[Save[]]{ SaveSolution[A]; }
     }
     }
}
```

- 9. PostProcessing
  - Piecewise definition of quantities of interest
  - Local or integral evaluation

```
PostProcessing {
    { Name magfields; NameOfFormulation Dynamic;
    Quantity {
        { Name b;
        Value {
        Local { [ -mu[] * {Grad phi} ]; In OmegaCC; }
        Local { [ mu[] * h ]; In OmegaC; }
      }
    }
}
```

10. PostOperation

 Evaluation and export of post-processing quantities (maps, cuts, ...)

```
PostOperation {
    { Name Map_b; NameOfPostProcessing magfields;
    Operation {
        Print[ b, OnElementsOf Omega, File "b.pos", Format Gmsh ];
        Print[ b, OnLine {{0,0,0}{1,0,0}} {100}, File "b.txt" ];
     }
}
```

#### For our toy problem, the complete "new.pro" file is:

```
Group{
  Omega = Region[1]; Gamma0 = Region[{2,3}];
}
Function{
  alpha[Omega] = 1; f[Omega] = -1;
}
Jacobian {
  { Name Vol; Case { { Region All; Jacobian Vol; } } }
}
Integration {
  { Name I1; Case {
     { Type Gauss; Case { { GeoElement Hexahedron; NumberOfPoints 6; } } }
  }
}
Constraint {
  { Name Dirichlet; Case { { Region Gamma0; Value 0; } } }
}
```

```
FunctionSpace {
  { Name H1 0; Type Form0;
                                                             F^0(\Omega) = \operatorname{span}\{s_1(\boldsymbol{x}), s_2(\boldsymbol{x}), \dots, s_N(\boldsymbol{x})\}
    BasisFunction {
       { Name si; NameOfCoef ui; Function BF Node;
                                                                 u(oldsymbol{x}) pprox u_h(oldsymbol{x}) = \sum_{i=1}^N u_i s_i(oldsymbol{x})
         Support Omega; Entity NodesOf[ All ]; }
    }
    Constraint {
       { NameOfCoef ui; EntityType NodesOf; NameOfConstraint Dirichlet; }
    }
  }
}
Formulation {
  { Name Laplace; Type FemEquation;
    Quantity {
       { Name u; Type Local; NameOfSpace H1 0; }
    }
    Equation {
       In Omega; Jacobian Vol; Integration I1; }
                                                                    -\int_{\Omega}f(\boldsymbol{x})\,u'(\boldsymbol{x})\,d\Omega
       Galerkin { [ - f[], {u} ];
         In Omega; Jacobian Vol; Integration I1; }
    }
                                                                     = 0
  }
```

```
Resolution {
  { Name MyResolution;
    System {
      { Name A; NameOfFormulation Laplace; }
    }
    Operation {
      Generate[A]; Solve[A]; SaveSolution[A];
                                                               Au = f
    }
  }
}
PostProcessing {
  { Name MyPostPro; NameOfFormulation Laplace;
    PostQuantity {
      { Name u; Value { Term { [ {u} ]; In Omega; Jacobian Vol; } } }
    }
  }
}
PostOperation {
  { Name u; NameOfPostProcessing MyPostPro;
    Operation {
      Print[ u, OnElementsOf Omega, File "u.pos" ];
    }
  }
}
```

- Note that Gamma0 in "new.pro" does not actually contain the whole boundary of the magnetometer: the homogeneous Dirichlet boundary condition will only be applied on the electrodes. Question: what happens on the rest of the boundary? (As an exercise, modify "new.geo" to fix this.)
- The complete GetDP documentation is available on <a href="http://getdp.info">http://getdp.info</a>
- We will study the physics and the implementation of electromagnetic, thermal and mechanical formulations on Tuesday and Wednesday

## Post-processing

## Post-processing with Gmsh

- Once you compute a solution by pressing "Run", it is merged and displayed automatically in the graphic window; it is called a "view"
- Check/uncheck the views in "Modules->Postprocessing" to show or hide them
- The Left/Right keyboard arrows allow to navigate in time
- The Up/Down arrows on the keyboard allow to navigate between views
- Click on the arrow next to a view name to access the view options

### Post-processing with Gmsh

 A video tutorial showing how to use basic postprocessing features is available here: <u>http://youtu.be/oS3T8i07wkl</u>



**Electromagnetism and Heat Transfer** 

## Electromagnetic models Different types of field computations

**Electrostatics** — Distribution of electric field due to static charges and/or electric potential difference



- Electrokinetics Distribution of static electric current in conductors
  - **Electrodynamics** Distribution of electric field and electric current in materials (insulating & conducting)



Magnetostatics — Distribution of static magnetic field due to static currents (DC) & permanent magnets





Full wave — Propagation of electromagnetic fields

$$C = \frac{Q}{V} = \frac{\epsilon S}{d}$$







## Electrostatics

Phenomena involving time-independent distributions of charges & fields  $\partial_t b = 0$ 

$\operatorname{curl} \boldsymbol{e} = 0$	boundary conditions
$\operatorname{div} \boldsymbol{d} = q$	$oldsymbol{n}  imes oldsymbol{e} _{\Gamma_e} = 0$
$d = \epsilon e$	$oldsymbol{n}\cdotoldsymbol{j}ert_{\Gamma_j}=0$





in each conducting region imposed potential at boundary

$$\Omega_{c,i}, \ v = v_i \Rightarrow v|_{\Gamma_{c,i}} = v_i$$

## Electrostatics

field next to a 220 kV high voltage line







## Electrokinetics

 $\operatorname{curl} \boldsymbol{e} = 0$  $\operatorname{curl} \boldsymbol{h} = \boldsymbol{j} \Rightarrow \operatorname{div} \boldsymbol{j} = 0$  $\boldsymbol{j} = \sigma \, \boldsymbol{e}$ 

boundary conditions (BCs)

$$n \times e|_{\Gamma_e} = 0$$

$$n \cdot j|_{\Gamma_j} = 0$$

$$\Gamma_{0i}$$

$$\Gamma_{0e,0}$$

$$e=?, j=?$$

$$V = v^1 - v^0$$

electric scalar potential formulation

$$-\operatorname{div}\left(\sigma\operatorname{grad} v\right) = 0, \quad \boldsymbol{e} = -\operatorname{grad} v$$

formulation for the conducting region  $\Omega_c$ 

in each electrode imposed potential

$$\Gamma_{e,i}, v = v_i \Rightarrow v|_{\Gamma_{e,i}} = v_i$$

## Electrokinetics



electric potential distribution

## Electrodynamics

$$\operatorname{curl} \boldsymbol{e} = 0$$
  
$$\operatorname{curl} \boldsymbol{h} = \boldsymbol{j} + \partial_t \boldsymbol{d} \Rightarrow \operatorname{div} (\boldsymbol{j} + \partial_t \boldsymbol{d}) = 0$$
  
$$\boldsymbol{j} = \sigma \, \boldsymbol{e}$$
  
$$\boldsymbol{d} = \epsilon \, \boldsymbol{e}$$

electric scalar potential formulation

$$-\operatorname{div}\left(\sigma \operatorname{grad} v + \epsilon \operatorname{grad} \partial_t v\right) = 0, \quad \boldsymbol{e} = -\operatorname{grad} v$$

# Electrodynamics




magnetic vector potential formulation

$$\operatorname{curl} \nu \operatorname{curl} \boldsymbol{a} = \boldsymbol{j}_s \,, \quad \boldsymbol{b} = \operatorname{curl} \boldsymbol{a}$$

Possible sources:

- $\boldsymbol{j}_s$  imposed current density in inductor
- $\boldsymbol{b}_s$  remanent induction if magnets
- $\boldsymbol{h}_s$  remanent magnetic field if magnets

# Magnetostatics



# Magnetodynamics

 $\operatorname{curl} \boldsymbol{h} = \boldsymbol{j}$  $\operatorname{curl} \boldsymbol{e} = -\partial_t \boldsymbol{b}$  $\operatorname{div} \boldsymbol{b} = 0$  $\boldsymbol{b} = \mu \boldsymbol{h} + \boldsymbol{b}_s$  $\boldsymbol{j} = \sigma \, \boldsymbol{e} + \boldsymbol{j}_s$ 



magnetic vector potential formulation

$$\operatorname{curl} \nu \operatorname{curl} \boldsymbol{a} + \sigma \left(\partial_t \boldsymbol{a} + \operatorname{grad} v\right) = \boldsymbol{j}_s, \quad \boldsymbol{b} = \operatorname{curl} \boldsymbol{a}$$
$$\boldsymbol{e} = -\operatorname{grad} v - \partial_t \boldsymbol{a}$$
reluctivity  $\nu = \frac{1}{\mu}$ 



## Full wave

 $\operatorname{curl} \boldsymbol{h} = \boldsymbol{j} + \partial_t \boldsymbol{d}$  $\operatorname{curl} \boldsymbol{e} = -\partial_t \boldsymbol{b}$  $\boldsymbol{b} = \mu \boldsymbol{h}$  $\boldsymbol{d} = \epsilon \, \boldsymbol{e}$  $\boldsymbol{j} = \sigma \, \boldsymbol{e}$  total electric field = scattered field + incident field

$$oldsymbol{e} = oldsymbol{e}_s + oldsymbol{e}_{inc}$$
 $oldsymbol{e}_s = (oldsymbol{n} imes oldsymbol{e}) imes oldsymbol{n}$ 

+ Silver-Müller radiation condition at infinity (outgoing waves)

curl 
$$\boldsymbol{e} \times \boldsymbol{n} - \imath k ((\boldsymbol{n} \times \boldsymbol{e}) \times \boldsymbol{n}) =$$
  
curl  $\boldsymbol{e}_{inc} \times \boldsymbol{n} - \imath k ((\boldsymbol{n} \times \boldsymbol{e}_{inc}) \times \boldsymbol{n}), \text{ on } \Gamma$ 

electric or magnetic field formulation

time domain

$$\operatorname{curl}\operatorname{curl}\boldsymbol{e} + \sigma\mu\,\partial_t\boldsymbol{e} + \epsilon\mu\,\partial_t^2\boldsymbol{e} = 0$$
$$\operatorname{curl}\operatorname{curl}\boldsymbol{h} + \sigma\mu\,\partial_t\boldsymbol{h} + \epsilon\mu\,\partial_t^2\boldsymbol{h} = 0$$

frequency domain 
$$\omega = 2\pi f$$
  
 $\Delta \boldsymbol{e} - \imath \omega \sigma \mu \, \boldsymbol{e} + \omega^2 \epsilon \mu \, \boldsymbol{e} = 0$   
 $\Delta \boldsymbol{h} - \imath \omega \sigma \mu \, \boldsymbol{h} + \omega^2 \epsilon \mu \, \boldsymbol{h} = 0$ 



# Model choice

Maxwell's equations & constitutive relations in frequency domain, without sources:

$$\Delta \boldsymbol{e} - \imath \omega \sigma \mu \, \boldsymbol{e} + \omega^2 \epsilon \mu \, \boldsymbol{e} = 0 \qquad \sigma = 0 + \text{no RHS term} \qquad \Delta \boldsymbol{e} + k^2 \, \boldsymbol{e} = 0$$
  
$$\Delta \boldsymbol{h} - \imath \omega \sigma \mu \, \boldsymbol{h} + \omega^2 \epsilon \mu \, \boldsymbol{h} = 0 \qquad k^2 = \omega^2 \epsilon \mu \qquad \Delta \boldsymbol{h} + k^2 \, \boldsymbol{h} = 0$$

Using characteristic lengths

- domain size L skin depth  $\delta = \sqrt{\frac{2}{\omega \sigma \mu}}$ wavelength  $\lambda = \frac{2\pi}{k}$ , wave number  $k = \frac{\omega}{c}$ , speed of light  $c = \frac{1}{\sqrt{\epsilon \mu}}$  allows to write them in non-dimensional form:

$$\left(\frac{3}{L^2} - \frac{2i}{\delta^2} + \frac{4\pi}{\lambda^2}\right)\boldsymbol{e} = 0$$
$$\left(\frac{3}{L^2} - \frac{2i}{\delta^2} + \frac{4\pi}{\lambda^2}\right)\boldsymbol{h} = 0$$

Helmholtz equations

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# Model choice

Non-dimensional numbers

Maxwell's equations

$$\left(\frac{3}{L^2} - \frac{2i}{\delta^2} + \frac{4\pi}{\lambda^2}\right)\boldsymbol{e} = 0$$
$$\left(\frac{3}{L^2} - \frac{2i}{\delta^2} + \frac{4\pi}{\lambda^2}\right)\boldsymbol{h} = 0$$

(	Care and the second	
$g_1 = \left(\frac{\lambda}{L}\right)^2$	$g_1 \gg 1$	uncoupled problem electric/magnetic
$\begin{cases} g_2 = \left(\frac{\delta}{L}\right)^2 \\ \end{pmatrix}$	$g_3 \ll 1$	electrostatics
$\left( g_3 = \left(\frac{\lambda}{\delta}\right)^2 \right)$	$g_3 \gg 1$	electrokinetics
	$g_3 \approx 1$	electrodynamics
tions	$g_2 \gg 1$	magnetostatics
e = 0	$g_2 \lesssim 1$	magnetodynamics
h = 0	$g_1 \lesssim 1$	full wave
	$g_1 \rightarrow 1$	HF asymptotics

EM model	governing equations
electrostatics	$\operatorname{curl} \boldsymbol{e} = 0, \ \operatorname{div} \boldsymbol{d} = q$ $\boldsymbol{d} = \epsilon  \boldsymbol{e}$
electrokinetics	$\operatorname{curl} \boldsymbol{e} = 0, \ \operatorname{div} \boldsymbol{j} = 0$ $\boldsymbol{j} = \sigma  \boldsymbol{e}$
electrodynamics	$\operatorname{curl} \boldsymbol{e} = 0, \ \operatorname{div} (\boldsymbol{j} + \partial_t \boldsymbol{d}) = 0$ $\boldsymbol{j} = \sigma  \boldsymbol{e}, \ \boldsymbol{d} = \epsilon  \boldsymbol{e}$
magnetostatics	$\operatorname{curl} oldsymbol{h} = oldsymbol{j} \ , \ \operatorname{div} oldsymbol{b} = 0 \ oldsymbol{b} = \mu  oldsymbol{h} \ , \ oldsymbol{h} =  u  oldsymbol{b}$
magnetodynamics	$\operatorname{curl} \boldsymbol{h} = \boldsymbol{j}, \ \operatorname{curl} \boldsymbol{e} = -\partial_t \boldsymbol{b}, \ \operatorname{div} \boldsymbol{b} = 0$ $\boldsymbol{b} = \mu \boldsymbol{h}, \ \boldsymbol{j} = \sigma \boldsymbol{e}$
full wave	$\operatorname{curl} \boldsymbol{h} = \boldsymbol{j} + \partial_t \boldsymbol{d}, \ \operatorname{curl} \boldsymbol{e} = -\partial_t \boldsymbol{b}, \ \operatorname{div} \boldsymbol{b} = 0$ $\boldsymbol{b} = \mu \boldsymbol{h}, \ \boldsymbol{j} = \sigma \boldsymbol{e}, \ \boldsymbol{d} = \epsilon \boldsymbol{e}$

# **Continuous mathematical structure**

# Maxwell's equations

grad 
$$f_0 \equiv \nabla f_0 = (\partial_x, \partial_y, \partial_z) f_0$$
  
curl  $f_1 \equiv \nabla \times f_1 \equiv (\partial_x, \partial_y, \partial_z) \times f_1$   
div  $f_2 \equiv \nabla \cdot f_2 \equiv (\partial_x, \partial_y, \partial_z) \cdot f_2$ 

$$\begin{aligned} \operatorname{curl} \boldsymbol{h} - \partial_t \boldsymbol{d} &= \boldsymbol{j} \\ \operatorname{curl} \boldsymbol{e} + \partial_t \boldsymbol{b} &= 0 \\ \operatorname{div} \boldsymbol{b} &= 0 \\ \operatorname{div} \boldsymbol{d} &= q \end{aligned} \qquad \begin{aligned} \boldsymbol{b} &= \mathcal{B}(\boldsymbol{e}, \boldsymbol{h}) &= \mu \boldsymbol{h} \ (+\boldsymbol{b}_s) \\ \boldsymbol{d} &= \mathcal{D}(\boldsymbol{e}, \boldsymbol{h}) &= \epsilon \boldsymbol{e} \ (+\boldsymbol{d}_s) \\ \boldsymbol{j} &= \mathcal{J}(\boldsymbol{e}, \boldsymbol{h}) &= \sigma \boldsymbol{e} \ (+\boldsymbol{j}_s) \end{aligned}$$

v 0-form = scalar, continuous field  $\mathbf{p}$   $\mathbf{p$ 

## Square integrable vector fields Useful definitions

The solutions of Maxwell's equations belong to spaces of square integrable scalar and vector fields  $L^2(\Omega)$  and  $L^2(\Omega)$ . They are defined by

$$L^{2}(\Omega) = \left\{ u : \int_{\Omega} u^{2}(\boldsymbol{x}) \, d\boldsymbol{x} < \infty \right\}$$
$$L^{2}(\Omega) = \left\{ \boldsymbol{u} : \int_{\Omega} \|\boldsymbol{u}(\boldsymbol{x})\|^{2} \, d\boldsymbol{x} < \infty \right\}$$

The scalar product of  $u, v \in L^2(\Omega)$  and  $u, v \in L^2(\Omega)$  is defined by

$$(u, v)_{\Omega} = \int_{\Omega} u(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}$$
 and  $(\boldsymbol{u}, \boldsymbol{v})_{\Omega} = \int_{\Omega} \boldsymbol{u}(\boldsymbol{x}) \cdot \boldsymbol{v}(\boldsymbol{x}) d\boldsymbol{x}$ 

The norm of  $u \in L^2(\Omega)$  and  $\boldsymbol{u} \in \boldsymbol{L}^2(\Omega)$  is defined by

$$\|u\|_{L^{2}(\Omega)} = (u, u)_{\Omega}^{1/2} = \left[\int_{\Omega} u^{2}(x) \, dx\right]^{1/2}$$
$$\|u\|_{L^{2}(\Omega)} = (u, u)_{\Omega}^{1/2} = \left[\int_{\Omega} \|u(x)\|^{2} \, dx\right]^{1/2}$$



square integrable scalar & vector fields: field + field with differential operator

$$H_f^1(\Omega) = \{ u \in L^2(\Omega) : \operatorname{grad} u \in L^2(\Omega), u|_{\Gamma_f} = u_f \}$$
$$H_f(\operatorname{curl}; \Omega) = \{ u \in L^2(\Omega) : \operatorname{curl} u \in L^2(\Omega), n \times u|_{\Gamma_f} = n \times u_f \}$$
$$H_f(\operatorname{div}; \Omega) = \{ u \in L^2(\Omega) : \operatorname{div} u \in L^2(\Omega), n \cdot u|_{\Gamma_f} = n \cdot u_f \}$$
$$f = e \text{ or } h$$

# Classification of 2<sup>nd</sup> order PDEs

EM problems involve linear second order partial differential equations (PDE), for the unknown field u and the source function f(x,y), that can be written (2D):

$$\mathcal{L}(u) = a\frac{\partial^2 u(x,y)}{\partial x^2} + b\frac{\partial^2 u(x,y)}{\partial x \partial y} + c\frac{\partial^2 u(x,y)}{\partial y^2} + d\frac{\partial u(x,y)}{\partial x} + e\frac{\partial u(x,y)}{\partial y} + gu = f$$

with coefficients *a*, *b*, *c*, *d*, *e*, *g* are functions of *x*, *y*, but they can also depend on *u* (nonlinear PDE), homogeneous if f=0, inhomogeneous if  $f \neq 0$ 

From the homogeneous case with constant coefficients, we get

$$\begin{vmatrix} ax^{2} + bxy + cy^{2} + dx + ey + g = 0 \\ ab/2 & c & e/2 \\ d/2 & e/2 & g \end{vmatrix} = (ac - b^{2}/4)g + bed/4 - cd^{2}/4 - ae^{2}/4$$

$$\begin{cases} b^2 - 4ac < 0 & \text{elliptic} \Rightarrow \text{steady-state problems} \\ b^2 - 4ac = 0 & \text{parabolic} \Rightarrow \text{diffusion problems} \\ b^2 - 4ac > 0 & \text{hyperbolic} \Rightarrow \text{propagation problems} \end{cases}$$

Circle

Ellipse

**Parabola** 

Hyperbola

# Classification of 2<sup>nd</sup> order PDEs (cont'd)

elliptic e.g. electrostatics  $e = -\operatorname{grad} v, \ d = \epsilon e$   $-\Delta v = -\frac{\partial^2 v(x, y, z)}{\partial x^2} - \frac{\partial^2 v(x, y, z)}{\partial y^2} - \frac{\partial^2 v(x, y, z)}{\partial z^2} = \frac{q}{\epsilon}$   $n \times e|_{\Gamma_e} = 0$  $n \cdot d|_{\Gamma_d} = 0$ 

#### parabolic e.g. magnetodynamics

$$\begin{aligned} \operatorname{curl} \nu \operatorname{curl} \boldsymbol{a} + \sigma \left( \partial_t \boldsymbol{a} + \operatorname{grad} \boldsymbol{v} \right) &= \boldsymbol{j}_s \,, \quad \boldsymbol{b} = \operatorname{curl} \boldsymbol{a} \\ \boldsymbol{n} \times \boldsymbol{h}|_{\Gamma_h} &= 0 \\ \boldsymbol{n} \cdot \boldsymbol{b}|_{\Gamma_h} &= 0 \end{aligned} \qquad \boldsymbol{a}(t = t_0) = \boldsymbol{a}_0 \end{aligned}$$

#### hyperbolic e.g. full wave in time domain

$$\operatorname{curl}\operatorname{curl}\boldsymbol{e} + \sigma\mu\,\partial_t\boldsymbol{e} + \epsilon\mu\,\partial_t^2\boldsymbol{e} = 0 \qquad \boldsymbol{e}(t = t_n) = \boldsymbol{e}_n$$
$$\boldsymbol{n} \times (\boldsymbol{e}^{tot} - \boldsymbol{e}^{inc}) + \sqrt{\frac{\mu}{\epsilon}}\,\boldsymbol{n} \times (\boldsymbol{n} \times (\boldsymbol{h}^{tot} - \boldsymbol{h}^{inc})) = 0 \qquad \boldsymbol{e}(t = t_{n-1}) = \boldsymbol{e}_{n-1}$$

# Strong and weak formulations

## **notation** $(u, v)_{\Omega} = \int_{\Omega} u \cdot v \, \mathrm{d}\Omega$ $\langle u, v \rangle_{\Gamma} = \int_{\Gamma} u \cdot v \, \mathrm{d}\Gamma$

#### **Strong formulation**



#### Weak formulation

 $\checkmark \mathcal{L} \text{ differential operator of order } n$ 

- $\checkmark \ \mathcal{L}^* \text{ adjoint of } \mathcal{L}$
- $\checkmark~\mathcal{B}$  differential operator imposing BC
- $\checkmark \ f \ \text{function in } \Omega, \ g \ \text{function on } \Gamma = \partial \Omega$
- $\checkmark u$  unknown function
- $\checkmark Q_g$  linear function of v

find u so that

$$(u, \mathcal{L}^* v)_{\Omega} - (f, v)_{\Omega} + \int_{\Gamma} Q_g(v) \, ds = 0, \ \forall v \in V(\Omega)$$

Continuous system  $\Rightarrow \infty \times \infty$ Discrete system  $\Rightarrow N \times N$  $\Rightarrow$  numerical solution

#### Green formulae

$$(\mathcal{L}u, v)_{\Omega} - (u, \mathcal{L}^*v)_{\Omega} = \int_{\Gamma} Q(u, v) ds$$

 $\boldsymbol{Q}$  bilinear function of  $\boldsymbol{u}$  and  $\boldsymbol{v}$ 

 $egin{aligned} & ext{grad-div type} \ & (m{v}, ext{grad}\,u)_\Omega+( ext{div}\,m{v},u)_\Omega=\langle u,\hat{n}\cdotm{v}
angle_\Gamma \ & ext{curl-curl type} \ & (m{v}, ext{curl}\,m{w})_\Omega-( ext{curl}\,m{v},m{w})_\Omega=\langlem{v} imes\hat{n},m{w}
angle_\Gamma \end{aligned}$ 

# Strong and week formulations (cont'd)

e.g. strong electrostatic formulation  $e = -\operatorname{grad} v, \ d = \epsilon e$ 

$$\begin{split} -\Delta v &= -\frac{\partial^2 v(x,y,z)}{\partial x^2} - \frac{\partial^2 v(x,y,z)}{\partial y^2} - \frac{\partial^2 v(x,y,z)}{\partial z^2} = \frac{q}{\epsilon} \quad \Rightarrow \begin{cases} \mathcal{L} &= -\Delta \\ f &= \frac{q}{\epsilon} \\ u &= v \end{cases} \\ u &= v \end{cases} \\ \mathbf{n} \times \mathbf{e}|_{\Gamma_e} &= 0 \\ \mathbf{n} \cdot \mathbf{d}|_{\Gamma_d} &= 0 \end{split}$$

#### e.g. weak electrostatic formulation

$$\int_{\Omega} -\Delta v \cdot w \, \mathrm{d}\Omega = \int_{\Omega} \left( -\operatorname{div} \left( \operatorname{grad} v \right) \right) \cdot w \, \mathrm{d}\Omega = \int_{\Omega} \frac{q}{\epsilon} \, w \, \mathrm{d}\Omega$$

$$v \cdot \operatorname{grad} u + u \operatorname{div} v = \operatorname{div} \left( u v \right)$$
Green formula:
integrating by parts
$$\int_{\Omega} \left( -\operatorname{div} \left( w \operatorname{grad} v \right) + \operatorname{grad} v \cdot \operatorname{grad} w \right) \mathrm{d}\Omega = \int_{\Omega} \frac{q}{\epsilon} \, w \, \mathrm{d}\Omega$$

# Constraints

 $\mathcal{L}u = f \text{ in } \Omega$  $\mathcal{B}u = g \text{ on } \Gamma$ 

- Local constraints
  - boundary conditions (BCs) on local fields at the boundary of the domain
    - their choice influences the final solution
    - they can be exploited to reduce the computational domain
  - interface conditions (ICs): coupling of fields between subdomains
- Global constraints
  - Flux or circulations of fields to be fixed (current, voltage, e.m.f., m.m.f, charge)
  - Flux or circulations of fields to be connected (circuit coupling)

# Boundary conditions (BCs)

 $\mathcal{L}u = f \text{ in } \Omega$  $\mathcal{B}u = g \text{ on } \Gamma$ 

• Dirichlet BCs: fix the unknown at the boundary to a given value

$$u|_{\Gamma} = u_0 \left\{ \begin{array}{l} = 0, \text{ homogeneous BC} \\ \neq 0, \text{ inhomogeneous BC} \end{array} \right.$$

• Neumann BCs: fix the normal derivative of the unknown at the boundary to a given value

$$\frac{\partial u(\boldsymbol{x})}{\partial n} = w(\boldsymbol{x}), \ \boldsymbol{x} \text{ on } \Gamma$$

• Mixed BCs: a combination of Dirichlet and Neumann BCs $\frac{\partial u(\boldsymbol{x})}{\partial n} + f_1(\boldsymbol{x})u = f_2(\boldsymbol{x}), \ \boldsymbol{x} \text{ on } \Gamma$  $f_1(\boldsymbol{x})u \text{ and } f_2(\boldsymbol{x}) \text{ explicitly known}$ 

Boundary conditions (BCs) (cont'd)

 $\mathcal{L}u = f \text{ in } \Omega$  $\mathcal{B}u = g \text{ on } \Gamma$ 

• Periodic BCs: fixing the unknown at the boundary to a given value

$$u(\boldsymbol{x}_0) + C_1 u(\boldsymbol{x}_1) = C_2, \quad \boldsymbol{x}_0 \text{ on } \Gamma_0, \ \boldsymbol{x}_1 \text{ on } \Gamma_1$$

or 
$$\frac{\partial u(\boldsymbol{x}_0)}{\partial n} + C_1' \frac{\partial u(\boldsymbol{x}_1)}{\partial n} = C_2', \quad \boldsymbol{x}_0 \text{ on } \Gamma_0, \ \boldsymbol{x}_1 \text{ on } \Gamma_1$$

• Floating BCs: unknown fixed to a value that still has to be determined, often related to global boundary conditions

#### $\mathbf{Dirichlet} \ \mathbf{BC}$





#### Neumann BC





## BCs — symmetry



### symmetry axis

normal component of induction = zero

half model!

#### symmetry axis





# Discrete mathematical structure Whitney elements

## Discrete mathematical structure

Replace the continuous spaces (infinite dimension) by discrete spaces (finite dimension)

# Finite elements

- set of linearly independent test and trial functions (also called basis/shape functions and weighting functions)
- commonly piecewise polynomial
- defined at a structured grid or an unstructured mesh
- compact support
- scalar or vectorial functions



# Finite elements geometry defined by nodes



# The Whitney elements

Finite element  $(\mathcal{G}, \Sigma, S)$ :

- $\checkmark\,$  geometrical element  ${\cal G}$
- $\checkmark \ \Sigma = \text{set of } N \text{ Dofs}$
- $\checkmark S$  function of finite dimension N

Let us consider a mesh of  $\Omega$  formed by geometrical elements  $\mathcal{G}$  with nodes  $\mathcal{N}$ , edges  $\mathcal{E}$ , faces  $\mathcal{F}$ , volumes  $\mathcal{V}$ ,



The Whitney elements of order p are expressed as

$$\boldsymbol{w}_{n_0,\dots,n_p} = p! \sum_{j=0}^p (-1)^m \varsigma_{n_m} \operatorname{grad} \varsigma_{n_0} \times \dots \times \operatorname{grad} \varsigma_{n_{m-1}} \times \operatorname{grad} \varsigma_{n_{m+1}} \times \dots \times \operatorname{grad} \varsigma_{n_p}$$

with  $\varsigma_n(x)$  barycentric weight of x with respect to node n in  $\mathcal{G}$ 

## The Whitney elements of order 0 Nodal elements



$$w_n = \varsigma_n$$
  
with  $n \in \mathcal{N}$  (node set)  
span space  $W^0(\mathcal{G})$ 

The interpolation of a function u is given by

$$I(u) = \sum_{x_i \in \mathcal{N}} u_i w_i$$
  
with  $u_i = \alpha_i(u) = u(x_i)$ 

 $\overline{\tilde{0}}$ 

# The Whitney elements of order 1 Edge elements



$$\boldsymbol{w}_{e} = \boldsymbol{w}_{\{m,n\}} = \varsigma_{m} \operatorname{grad} \varsigma_{n} - \varsigma_{n} \operatorname{grad} \varsigma_{m},$$
  
with  $e \in \mathcal{E}$  (edge set)  
span space  $W^{1}(\mathcal{G})$ 

The interpolation of a function  $\boldsymbol{u}$  is given by

$$\begin{split} I(\boldsymbol{u}) &= \sum_{e \in \mathcal{E}} u_e \boldsymbol{w}_e \\ \text{with } u_e &= \alpha_e(\boldsymbol{u}) = \int_e \boldsymbol{u} \cdot d\boldsymbol{l} \ , \ \forall e \in \mathcal{E} \end{split}$$

- $\checkmark$  Dof = circulations of field along edges of mesh
- $\checkmark\,$  discretisation of 1-forms, e.g.  $h,\,e$
- $\checkmark\,$  tangential component continuous across faces
- $\checkmark$  circulation of  $w_e = 1$  along edge e, 0 across other edges  $N_{F,m\tilde{n}}$

 $N_{F,n\widetilde{m}}$ 

n

 $w_e$ 

 $u_{e}$ 

# Whitney elements of order 2 Face elements

 $\frac{2-\text{form } k}{\text{facet BF}} 2(\varsigma$ 

$$\begin{split} \boldsymbol{w}_{f} &= \boldsymbol{w}_{\{l,m,n\}} = \\ 2\left(\varsigma_{l} \operatorname{grad} \varsigma_{m} \times \operatorname{grad} \varsigma_{n} - \varsigma_{m} \operatorname{grad} \varsigma_{l} \times \operatorname{grad} \varsigma_{n} + \varsigma_{n} \operatorname{grad} \varsigma_{l} \times \operatorname{grad} \varsigma_{m}\right) \\ & \text{with } f = \{l,m,n\} \in \mathcal{F} \text{ (face set)} \\ & \text{span space } W^{2}(\mathcal{G}) \end{split}$$

The interpolation of a function  $\boldsymbol{u}$  is given by



 $\checkmark$  Dof = flux through faces of mesh

 $\checkmark\,$  discretisation of 2-forms, e.g.  $b,\,j$ 

 $\checkmark\,$  normal component continuous across interfaces

✓ flux of  $w_f = 1$  across face, 0 across other faces of G

## Whitney elements of order 3 Volume elements

 $w_{v} = w_{\{k,l,m,n\}} = 6 \left(\varsigma_{k} \operatorname{grad} \varsigma_{l} \times \operatorname{grad} \varsigma_{m} \times \operatorname{grad} \varsigma_{n} - \varsigma_{l} \operatorname{grad} \varsigma_{k} \times \operatorname{grad} \varsigma_{m} \times \operatorname{grad} \varsigma_{n} + \varsigma_{n} \operatorname{grad} \varsigma_{k} \times \operatorname{grad} \varsigma_{k} \times \operatorname{grad} \varsigma_{k} \times \operatorname{grad} \varsigma_{l} \times \operatorname{grad} \varsigma_{m} - \varsigma_{n} \operatorname{grad} \varsigma_{k} \times \operatorname{grad} \varsigma_{l} \times \operatorname{grad} \varsigma_{m} \right)$ 

with  $v = \{k, l, m, n\} \in \mathcal{V}$  (volume set) span space  $W^3(\mathcal{G})$ 



The interpolation of a function u is given by

$$I(u) = \sum_{v \in \mathcal{V}} u_v w_v$$
  
with  $u_v = \alpha_v(u) = \int_v u \, dv$ 

- $\checkmark\,$  piecewise constant functions
- $\checkmark$  Dof = integration over its volume
- $\checkmark\,$  discretisation of densities

 $\checkmark \sum w_v = 1$  over the volume of  $\mathcal{G}$  , 0 over other volumes



✓ Nodal elements: Conforming finite elements (in  $\mathcal{H}^1(\Omega)$ ) interpolate scalar fields that are continuous across any interface. Discretisation of scalar quantities: potentials  $\varphi$ , v, temperature...

✓ Edge elements: Curl-conforming finite elements (in  $H(\text{curl}; \Omega)$ ) ensure the continuity of the tangential component of the field. Discretisation of the magnetic field h, the magnetic vector potential a or the electric field e.

$$\hat{n} \times (\boldsymbol{h}_2 - \boldsymbol{h}_1)|_S = \boldsymbol{j}_s$$
$$\hat{n} \times (\boldsymbol{e}_2 - \boldsymbol{e}_1)|_S = 0$$



✓ Face elements: Div-conforming finite elements (in  $H(\text{div}; \Omega)$ ) ensure the continuity of the normal component of the interpolated field. Discretisation of the magnetic flux density **b**, the current density **j** or the electric flux density **d**.  $\hat{n} = V$ 

$$\partial S \qquad \hat{r} \qquad \int_{S} \mathbf{b} \cdot \hat{n} \, ds = 0$$

$$\int_{S} \mathbf{b} \cdot \hat{n} \, ds = \int_{V} \rho \, dv$$

$$\int_{S} \mathbf{d} \cdot \hat{n} \, ds = \int_{V} \rho \, dv$$

$$\hat{n} \cdot (\mathbf{b}_{2} - \mathbf{b}_{1})|_{S} = 0$$

$$\hat{n} \cdot (\mathbf{d}_{2} - \mathbf{d}_{1})|_{S} = \rho_{s}$$

✓ Volume elements: Finite elements in  $L^2(\Omega)$  do not impose any continuity (discontinuous) between elements on the interpolated field. Discretisation of quantities that may vary from one element to the other e.g. the electric charge density  $\rho$ .

$$\int_{S} \boldsymbol{d} \cdot \hat{n} \, ds = \int_{V} \rho \, dv$$

# Electrokinetic formulation and discretization

# Electrostatics



Phenomena involving time-independent distributions of charges & fields


### Electrostatics





### Spatial discretization — electrostatics

### Weighted residual approach

$$-\operatorname{div}\left(\epsilon \operatorname{grad} v\right) = q \quad \text{ in } \Omega$$

We integrate the equation weighted by test functions  $w_i(\boldsymbol{x})$  over the whole domain:

$$\int_{\Omega} \left( -\operatorname{div} \left( \epsilon \operatorname{grad} v \right) \right) w_i d\Omega = \int_{\Omega} q \, w_i \, d\Omega \,, \qquad \forall w_i(\boldsymbol{x})$$

 $w_i(\boldsymbol{x})$  weighting or test functions

## Spatial discretization — electrostatics (II)

 $\forall w_i(\boldsymbol{x})$ 

**Weak formulation** 

search wiki vector calculus

$$\int_{\Omega} \left( -\operatorname{div}\left(\epsilon \operatorname{grad} v\right) \right) w_{i} \, \mathrm{d}\Omega = \int_{\Omega} q \, w_{i} \, \mathrm{d}\Omega$$

$$\downarrow \mathbf{v} \cdot \operatorname{grad} u + u \operatorname{div} \mathbf{v} = \operatorname{div}\left(u\mathbf{v}\right) \quad \text{integration by parts}$$
Green formula
$$\int_{\Omega} \left( -\operatorname{div}\left(w_{i}\epsilon \operatorname{grad} v\right) + \epsilon \operatorname{grad} v \cdot \operatorname{grad} w_{i} \right) \mathrm{d}\Omega = \int_{\Omega} q \, w_{i} \, \mathrm{d}\Omega$$

$$\downarrow \int_{\Omega} \operatorname{div} \mathbf{a} \, \mathrm{d}\Omega = \oint_{\partial\Omega} \mathbf{a} \, \mathrm{d}\Gamma \quad \text{divergence theorem}$$

$$\int_{\partial\Omega} w_{i}(-\epsilon \operatorname{grad} v) \, \mathrm{d}\Gamma + \int_{\Omega} \epsilon \operatorname{grad} v \cdot \operatorname{grad} w_{i} \, \mathrm{d}\Omega = \int_{\Omega} q \, w_{i} \, \mathrm{d}\Omega$$

only the first derivative of the electric potential is now required

### Spatial discretization — electrostatics (III)



### Spatial discretization — electrostatics (IV)

$$v = \sum_{j} u_j s_j$$
 with  $s_j(\boldsymbol{x}) = 0$  at  $\Gamma_{Dirichlet}$ 

 $s_j(\mathbf{x})$  shape functions  $u_j$  unknowns, degrees of freedom

Ritz-Galerkin method $s_j(\boldsymbol{x}) = w_j(\boldsymbol{x})$ Petrov-Galerkin method $s_i(\boldsymbol{x}) \neq w_i(\boldsymbol{x})$ 

$$\int_{\Omega} \epsilon \operatorname{grad} v \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega = \int_{\Omega} q \, w_i \, \mathrm{d}\Omega$$

$$\sum_j u_j \int_{\Omega} \epsilon \operatorname{grad} w_j \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega = \int_{\Omega} q \, w_i \, \mathrm{d}\Omega \longrightarrow$$

$$= k_{ij} = f_i$$

matrix system  $[k_{ij}][u_j] = [f_i]$ 

### -////-

### Electrokinetics

Phenomena involving time-independent (static) currents in conductors



### Electrokinetics



### Spatial discretization — electrokinetics

### Weighted residual approach

$$-\operatorname{div}\left(\sigma \operatorname{grad} v\right) = 0 \quad \text{ in } \Omega_c$$

We integrate the equation weighted by test functions  $w_i(\boldsymbol{x})$  over the whole domain:

$$\int_{\Omega} \left( -\operatorname{div} \left( \sigma \operatorname{grad} v \right) \right) w_i d\Omega = 0, \qquad \forall w_i(\boldsymbol{x})$$

 $w_i(\boldsymbol{x})$  weighting or test functions

### Spatial discretization — electrokinetics (II)

Weak formulation 
$$\forall w_i(\boldsymbol{x})$$
  

$$\int_{\Omega} \left( -\operatorname{div} (\sigma \operatorname{grad} v) \right) w_i \, \mathrm{d}\Omega = 0$$

$$\mathbf{v} \cdot \operatorname{grad} u + u \operatorname{div} \boldsymbol{v} = \operatorname{div} (u\boldsymbol{v}) \quad \text{integration by parts} \quad \text{Green formula}$$

$$\int_{\Omega} \left( -\operatorname{div} (w_i \sigma \operatorname{grad} v) + \sigma \operatorname{grad} v \cdot \operatorname{grad} w_i \right) \mathrm{d}\Omega = 0$$

$$\int_{\Omega} \operatorname{div} \boldsymbol{a} \, \mathrm{d}\Omega = \oint_{\partial\Omega} \boldsymbol{a} \, \mathrm{d}\Gamma \quad \text{divergence theorem}$$

$$\int_{\partial\Omega} w_i (-\sigma \operatorname{grad} v) \, \mathrm{d}\Gamma + \int_{\Omega} \sigma \operatorname{grad} v \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega = 0$$

only the first derivative of the electric potential is now required

### Spatial discretization — electrokinetics (III)



## Spatial discretization — electrokinetics (IV)

$$v = \sum_{j} u_j s_j$$
 with  $s_j(\boldsymbol{x}) = 0$  at  $\Gamma_{Dirichlet}$ 

 $s_j(\mathbf{x})$  shape functions  $u_j$  unknowns, degrees of freedom

**Petrov-Galerkin method** 

**Ritz-Galerkin method** 

$$s_j(\boldsymbol{x}) = w_j(\boldsymbol{x})$$
  
 $s_j(\boldsymbol{x}) \neq w_j(\boldsymbol{x})$ 

$$\int_{\Omega} \sigma \operatorname{grad} v \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega = 0$$

$$\sum_{j} u_j \int_{\Omega} \sigma \operatorname{grad} w_j \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega = 0 \qquad \longrightarrow \qquad \begin{bmatrix} \operatorname{matrix system} \\ [k_{ij}][u_j] = [0] \end{bmatrix}$$

$$= k_{ij}$$
Source via constraints

Source via constraints in U vector (potential at electrodes)

### Function space – electric scalar potential

$$v = \sum_{n \in \mathcal{N}} v_n s_n$$



x





## Electrokinetic formulation: build equation!

```
Formulation {
   { Name Electrokinetics_v ; Type FemEquation ;
     Quantity {
        { Name v ; Type Local ; NameOfSpace Hgrad_v_EleKin ; }
     Equation {
       Galerkin { [ sigma[] * Dof{d v} , {d v} ] ;
          In DomainC_Ele ; Jacobian Vol ; Integration GradGrad ; }
                                                                weighing function
                            basis function
              \int_{\partial\Omega} w_i(-\sigma \operatorname{grad} v) \,\mathrm{d}\Gamma + \int_{\Omega} \sigma \operatorname{grad} v \cdot \operatorname{grad} w_i \,\mathrm{d}\Omega = 0
                                irichlet constraint
Constraint {
  { Name ElectricScalarPotential ;
     Case {
       { Region Dirichlet0 ; Value 0. ; }
        { Region Dirichlet1 ; Value V_imposed ; }
```

```
w_j(x,y)
Function space – temperature
T = \sum T_n s_n
    n{\in}\mathcal{N}
FunctionSpace{
  { Name Hgrad_T; Type FormO; //discrete function space for H1_h
    BasisFunction {
      { Name sn; NameOfCoef Tn; Function BF_Node; // ``P1 FEs''
        Support Domain_The; Entity NodesOf[All]; }
    Constraint {
      { NameOfCoef Tn; EntityType NodesOf; NameOfConstraint Temperature; }
                     Constraint {
                       { Name Temperature ;
                         Case {
                           { Region Dirichlet0 ; Value 20. ; }
                           { Region Dirichlet1 ; Value 20. ; }
```

## Thermal formulation: build equation!

```
Formulation {
   { Name Thermal_T ; Type FemEquation ;
      Quantity {
        { Name T ; Type Local ; NameOfSpace Hgrad_T ; }
        { Name v ; Type Local ; NameOfSpace Hgrad_v_EleKin ; }
      Equation {
        Galerkin { [ kappa[] * Dof{d T} , {d T} ];
                       In Domain_The; Integration GradGrad ; Jacobian Vol ; }
        Galerkin { DtDof[ rhoc[] * Dof{T} , {T} ];
                       In Domain_The; Integration GradGrad ; Jacobian Vol ; }
        Galerkin { [-1/sigma[] * SquNorm[sigma[]*{d v}], {T} ];
                       In Domain_The ; Integration GradGrad ; Jacobian Vol ; }
 \begin{cases} \begin{cases} \kappa \operatorname{grad} T \cdot \operatorname{grad} w_i \, \mathrm{d}\Omega_T + \int_{\Omega_T} \rho_T \, c_p \, \partial_t T \cdot w_i \, \mathrm{d}\Omega_T + \int_{\Omega_T} Q_v \cdot w_i \, \mathrm{d}\Omega_T \end{cases} \\ \end{cases}
```

```
\rho c_p \partial_t T = \operatorname{div} (\kappa \operatorname{grad} T) + Q_v Heat conduction equation
```

### **Coupling: Electrokinetic + thermal resolution**



# **Mechanics and Elasticity**

#### Magnetometer = Electromagnetism + Elasticity



#### classical Electromagnetism

Vector fields:  $\vec{B}, \vec{H}, \vec{J}, \dots$ Vector analysis: div, curl, grad Assumes Euclidean space



Euclidean metric

classical Elasticity Displacement field  $\vec{u}$ Symmetric tensors  $\varepsilon$ ,  $\sigma$ Assumes Euclidean space

### Magnetometer = Electromagnetism + Elasticity

classical Electromagnetism

Vector fields:  $\vec{B}, \vec{H}, \vec{J}, \dots$ Vector analysis: div, curl, grad Assumes Euclidean space



classical Elasticity Displacement field  $\vec{u}$ Symmetric tensors  $\varepsilon$ ,  $\sigma$ Assumes Euclidean space

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Euclidean metric

- Classical Elasticity and classical Electromagnetism assume a Euclidean metric
- ◊ This assumption
  - engineers background
  - hides the central role of metric
  - electromagnetic world and elasticity world cannot communicate (no common concepts, the door is locked)
  - forbids clear electromechanical concepts (Maxwell stress tensor, electromagnetic forces)
  - forbids clear sensitivity analysis (cf tomorrow)

### Magnetometer = Electromagnetism + Elasticity

classical Electromagnetism Vector fields:  $\vec{B}, \vec{H}, \vec{J}, \dots$ Vector analysis: div, curl, grad





classical Elasticity Displacement field  $\vec{u}$ Symmetric tensors  $\varepsilon$ ,  $\sigma$ Assumes Euclidean space

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Euclidean metric

- One could have done a classical introduction, boring,
- We are going to open the door and see how the two worlds communicate
- Closer to research
- Define the metric tensor and demonstrate its fundamental role (giant step to understand curved spaces and general relativity)
- $\diamond~$  Show that all physical quantities we need are tensors of various kinds
- ◊ Finally, review the elastic part of the magnetometer model.

### Elasticity

- 2 formulations for Elasticity
  - full general geometric approach (large strains, finite strain, nonlinear elasticity)
  - $\diamond~$  linear elasticity, infinitesimal strain: linearization of the latter (complicated  $\rightarrow$  simple)



www.quia.com, www.ifam.rwth-aachen.de

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#### Pathway to tensors

This all relies on a chain of basic mathematical concepts

- continuous medium (manifold)
- $\diamond$  curve
- $\diamond$  vector
- $\diamond$  covector
- $\diamond$  tensors

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#### $\text{Manifold} \rightarrow \text{curve}$

#### Manifold:

- Analogy: sponge
- continuous set of points
- $\diamond$  no defined distance between points <> rigid boby
- ◊ no tearing, no creation of voids, ...
- $\diamond$  Infinitely many curves pass through each point *P* of  $\Omega$



#### $Curve \rightarrow tangent \ vector$





$$C(\lambda) = \{x^{i}(\lambda)\}, \lambda \in [A, B]$$
$$= \{x(\lambda), y(\lambda), z(\lambda)\}$$
$$\vec{V}(\lambda) = \{\frac{dx^{i}}{d\lambda}(\lambda)\}$$
$$= \{\frac{dx}{d\lambda}, \frac{dy}{d\lambda}, \frac{dz}{d\lambda}\}$$
$$= \{V^{x}, V^{y}, V^{z}\}$$

$$\vec{r}(t) = \{x^{i}(t)\}, t \in [A, B]$$
$$= \{x(t), y(t), z(t)\}$$
$$\vec{v}(t) = \{\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt}\}$$
$$= \{v^{x}, v^{y}, v^{z}\}$$

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http://math.etsu.edu/multicalc/prealpha/Chap1/Chap1-7/9-7-1.gif http://i.stack.imgur.com/VOPuE.png

F. Henrotte, C. Geuzaine, R. Sabariego, E. Kuci

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#### Curve $\rightarrow$ tangent vector



- $\diamond$  Infinitely many curves pass through each point *P* of  $\Omega$
- ♦ Each curve has its *tangent vector*  $\vec{V} = \{V^x, V^y, V^z\}$  in *P*
- ♦ the set of all tangent vectors at *P* is the tangent space  $T_P Ω$ , a linear space
- $\diamond$  if the curve is a trajectory, and the curve parameter  $\lambda$  is the time *t*, the tangent vector is the velocity
- Note the upper (contravariant) indices for vector components

#### Vector $\rightarrow$ covector

- A covector field is a quantity that makes sense when integrated over a curve (circulation)
- ♦ Examples: force field  $\vec{f}$ , gravity field  $m\vec{g}$ , electric field  $\vec{E}$ , magnetic field  $\vec{H}$

#### **Mechanical work**

the curve  $C(P_A, P_B) = \{x^k(t)\}$  is a trajectory from  $P_A$  to  $P_B$ 

$$W = \int_{C(P_A, P_B)} \vec{f} \cdot d\vec{C}$$
 conventional vector representation  
$$= \int_{C(P_A, P_B)} f_i dC^i$$
 note the lower (covariant) indices for  $\vec{f}$   
$$= \int_A^B f_i \frac{dx^i}{dt} dt$$
 using the parametrisation of the curve, implicit sum

#### $\textit{Vector} \rightarrow \textit{covector}$

#### Potential gravitational energy

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### $\begin{array}{l} \text{Vector} \rightarrow \text{covector} \\ \text{Ampere law} \end{array}$



$$I = \oint_{C} \vec{H} \cdot d\vec{C} \qquad \vec{B} = \mu_{0}\vec{H} = \oint_{C} H_{i} dC^{i}$$
$$= \oint_{C} H_{i} \frac{dx^{i}}{d\lambda} d\lambda = \int_{C} (H_{x} \frac{dx}{d\lambda} + H_{y} \frac{dy}{d\lambda} + H_{z} \frac{dz}{d\lambda}) d\lambda$$

http://agni.phys.iit.edu/ vpa/images/mag1.jpg, https://c1.staticflickr.com/3/2481/3789856303\_7d9f858c0a.jpg

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#### Vector and covectors $\rightarrow$ tensors

- Vectors: velocities or tangent vectors of curves
- Covectors: physical quantities that make sense when integrated over a curve or a trajectory
- ♦ distinguished by covariant or contravariant indices A vector: { $V^x$ ,  $V^y$ ,  $V^z$ } A covector: { $\alpha_x$ ,  $\alpha_y$ ,  $\alpha_z$ }
- covector = first example of a tensor, the simplest one, a tensor with one vector argument and zero covector argument:

$$\alpha(\vec{V}) = \alpha_i V^i \in \mathbb{R}$$

contraction of repeated indices, one covariant, one contravariant

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#### Tensors: a general definition

 Generalisation of the principle of contraction for *m* vector arguments and *n* covector arguments:

$$T(\vec{V},\ldots\vec{W},\alpha,\ldots,\beta) = T_{i\ldots j}^{k\ldots l} V^{i}\ldots W^{j}\alpha_{k}\ldots\beta_{l}$$

Linearity for all arguments, e.g. for the first one

$$T(a\vec{V}+b\vec{W},\dots)=aT(\vec{V},\dots)+bT(\vec{W},\dots)$$

- ◊ To the classroom: "Cite tensors..."
- In tensor analysis, tensors are NOT always 2 dimensional arrays of numbers!
- Scalars, vectors and covectors are the simplest tensor types

#### Tensors: transformation matrices

◇ Tensors with one vector argument (m = 1) and one covector argument (n = 1) are transformation matrices

$$T(\vec{V},\alpha) = T_i^k V^i \alpha_k$$

- ◇ They have 9 independent components  $T_i^k$  (9 terms at the right-hand side of the above identity, due to implicit sums)
- ♦ Contracting the transformation matrix with its vector argument,  $T(\vec{V},.)$ , gives a tensor with one covector argument, i.e. a new vector
- ♦ Contracting the transformation matrix with its covector argument,  $T(., \alpha)$ , gives a tensor with one vector argument, i.e. a new covector
- Hence the name transformation matrix. Summary so far

. . .

m	n	
0	0	scalar field
0	1	vector field
1	0	covector field
1	1	transformation matrix

#### Tensors with several arguments of the same nature

 Tensors with 2 vector arguments have also 9 independent components *T<sub>ij</sub>* (like transformations matrices)

$$T(\vec{V},\vec{W})=T_{ij}V^iW^j.$$

 When there are at least two arguments of the same nature, the order of the arguments matters in general

$$\mathcal{T}(ec{V},ec{W})=\mathcal{T}_{ij}V^iW^j
eq \mathcal{T}(ec{W},ec{V})=\mathcal{T}_{ij}W^iV^j.$$

 The behaviour under swapping arguments of the same nature allows to define very important tensor subclasses: symmetric and antisymmetric tensors

#### Symmetric tensors

A symmetric tensor verifies

$$T(\vec{V}, \vec{W}) = T(\vec{W}, \vec{V}) \quad \forall \vec{V}, \vec{W}$$

♦ The above condition holds in particular for the basis vectors  $\vec{e}_x = \{\delta_x^i\} = \{1, 0, 0\}, \ \vec{e}_y = \{\delta_y^i\} = \{0, 1, 0\}, \ \vec{e}_z = \{\delta_z^i\} = \{0, 0, 1\}.$ ♦ Hence

$$T(\vec{e}_x,\vec{e}_y)=T(\vec{e}_y,\vec{e}_x)\Rightarrow T_{xy}=T_{yx}$$

This yields in total 3 non trivial independent relationships

$$T_{xy} = T_{yx}$$
 ,  $T_{yz} = T_{zx}$  ,  $T_{zx} = T_{xz}$ 

- Symmetric tensors with 2 vector arguments have thus only 6=9-3 independent components.
- ♦ Examples: metric tensor g, deformation tensor  $\varepsilon$

#### Antisymmetric tensors

Another important class of tensors are the antisymmetric tensor:

$$T(\vec{V}, \vec{W}) = -T(\vec{W}, \vec{V}) \quad \forall \vec{V}, \vec{W}$$

 Components with repeated indices of antisymmetric tensors always vanish

$$T(\vec{e}_x, \vec{e}_x) = -T(\vec{e}_x, \vec{e}_x) \Rightarrow T_{xx} = -T_{xx} \Rightarrow T_{xx} = 0$$

Antisymmetry yields in total 6 non trivial independent relationships

$$T_{xx} = 0 \quad , \quad T_{yy} = 0 \quad , \quad T_{zz} = 0$$
$$T_{xy} = -T_{yx} \quad , \quad T_{yz} = -T_{zx} \quad , \quad T_{zx} = -T_{xz}$$

- Antisymmetric tensors with 2 vector arguments have thus 3=9-6 independent components, like vectors and covectors.
- $\diamond$  Examples: current density  $\vec{J}$ , magnetic flux density  $\vec{B}$

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#### Flux density



- A flux density associates a number to a facet made of 2 nonparallel vectors
- The flux is zero if the two vectors are parallel
- The flux changes sign if the vectors are swapped
- $\Rightarrow$  a flux density is an antisymmetric tensor with 2 vector arguments (*m* = 2, *n* = 0)
- It has 3 components like a vector or a covector...

https://inspirehep.net/record/1281391/files/multivectors\_good2.png

### Volume density



- A volume density associates a number to a parallelepiped made of 3 nonparallel vectors
- The number is zero if the any two vectors out of the three are parallel (flat parallelepiped)
- The number changes sign if any two vectors are swapped (negative volume according to the right-hand rule)
- $\diamond$  ⇒ a volume density is an antisymmetric tensor with 3 vector arguments (m = 3, n = 0)
- o How many independent components has such a tensor?

http://www.wackerart.de/mathematik/geometric\_algebra/trivector.gif < 🗆 🕨 < 🖻 🕨 < 🖹 🕨 🤹 🖘 🦉
# Volume density

♦ A tensor with 3 vector arguments (m = 3, n = 0) has 27 independent components (27 terms in the sum):

$$T(\vec{U},\vec{V},\vec{W})=T_{ijk}U^{i}V^{j}W^{k}$$

 A volume density ρ is a fully antisymmetric tensor with 3 vector arguments

$$\rho(\vec{U},\vec{V},\vec{W}) = -\rho(\vec{V},\vec{U},\vec{W}) = -\rho(\vec{U},\vec{W},\vec{V})\dots \quad \forall \vec{U},\vec{V},\vec{W}$$

and so on for any argument permutation

- ♦ All 21 components with a repeated index vanish: e.g.  $\rho_{xxy} = 0$
- Only 6 components exist with no repeated indices, for which one has 5 relationships

$$\rho_{xyz} = \rho_{yzx} = \rho_{zxy} = -\rho_{xzy} = -\rho_{zyx} = -\rho_{yxz}$$

 Antisymmetric tensors with 3 vector arguments have thus only 1 independent components, like a scalar field

# **Differential forms**

- Differential forms of order *m* are completely antisymmetric tensors with *m* vector arguments and zero covector arguments
- Originate from the theory of integration over geometrical regions
- $\diamond~$  Stokes theorem: duality with the boundary operator  $\partial~$

$$\int_{\Omega} \, \mathrm{d}\alpha = \int_{\partial\Omega} \alpha$$

$$\int_{C(P_{A},P_{B})} \operatorname{grad} f \cdot d\vec{C} = f|_{\partial C(P_{A},P_{B})} = f(P_{B}) - f(P_{A})$$
$$\int_{S} \operatorname{curl} \vec{f} \cdot d\vec{S} = \int_{\partial S} \vec{f} \cdot d\partial \vec{S}$$
$$\int_{V} \operatorname{div} \vec{f} \, dV = \int_{\partial V} \vec{f} \cdot d\partial \vec{V} = \int_{\partial V} \vec{f} \cdot \vec{n} \, d\partial V$$

Accurate mathematical representation of electromagnetic fields

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### Differential forms: shape functions

т		
0	0-form	scalar function
1	1-form	covector field, circulation density
2	2-form	flux density
3	3-form	volume density



т		
0	0-form	scalar function
1	1-form	covector field, circulation density
2	2-form	flux density
3	3-form	volume density

The value of the shape function  $v_i$  of node *i* of the mesh is 1 at node *i*, and zero at all other nodes of the mesh.



http://www.iue.tuwien.ac.at, http://mooseframework.org

т		
0	0-form	scalar function
1	1-form	covector field, circulation density
2	2-form	flux density
3	3-form	volume density

The circulation of the shape function k is 1 over edge k of the mesh, and zero over all other edges of the mesh.



http://www.iue.tuwien.ac.at/phd/nentchev/node40.html, http://www.iue.tuwien.ac.at/phd/nentchev/node43.html

F. Henrotte, C. Geuzaine, R. Sabariego, E. Kuci

Mechanics and elasticity with Onelab

т		
0	0-form	scalar function
1	1-form	covector field, circulation density
2	2-form	flux density
3	3-form	volume density

The flux of the shape function k is 1 across facet k of the mesh, and zero across all other facets of the mesh.



т		
0	0-form	scalar function
1	1-form	covector field, circulation density
2	2-form	flux density
3	3-form	volume density

The integral of the shape function k is 1 over element k of the mesh, and zero over all other elements of the mesh. Draw it...

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# Tensors: overview

т	n	S/A	
0	0		scalar field
0	1		vector field
1	0		covector field
1	1		transformation matrix
2	0	S	metric tensor $g$ , deformation tensor $\varepsilon$
2	0	А	flux density $\vec{B}$ , displacement current $\vec{D}$
0	2	S	(stress tensor $\sigma$ )
3	0	А	volume density $\rho$

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# Tensors: partial antisymmetrization

- Partially antisymmetrized tensors are also possible
- $\diamond\,$  The force density  $\rho^{\vec{F}}$  is a covector valued volume density

$$\vec{F} = \int_{V} 
ho^{\vec{F}} dV$$

- It is a tensor with 4 vector arguments, antisymmetrised with respect to the first 3 only.
- $\diamond~$  The stress tensor  $\sigma$  is a symmetric tensor with two covector arguments in

$$\boldsymbol{W} = \boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \boldsymbol{\sigma}^{ij} \boldsymbol{\varepsilon}_{ij}$$

 But the stress tensor σ is a tensor with three vector arguments, antisymmetrized over the first 2, when regarded as a surface density of force, or a flux of momentum.

$$\vec{F} = -\int_{S} \sigma \cdot d\vec{S} = -\int_{S} \sigma \cdot \vec{n} \, dS$$

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### Tensors: overview

- Physical quantities are tensor fields with well-defined arguments and symmetry properties
- Partially antisymmetrized tensors are also possible
- Many confusions in Euclidean space: vector, covectors, flux densities, covector densities have all 3 components, and are all regarded as "vectors" in vector analysis, despite their very different tensorial natures

# Elasticity: equilibrium equation

$$\vec{F} = -\int_{S} \sigma \cdot d\vec{S} = -\int_{S} \sigma \cdot \vec{n} \, dS \qquad (*)$$



Hence, for free, the **equilibrium equation** which is a purely gometric statement, directly derived from the geometrical nature of  $\sigma$  and of force densities:

$$\operatorname{div} \sigma + \rho^{\vec{F}} = \mathbf{0}$$

### Finite strain elasticity: placement map



F. Henrotte, C. Geuzaine, R. Sabariego, E. Kuci

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# Finite strain elasticity: placement map



- Material manifold: sponge
- Euclidean space: ruler, notion of distance between points

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 $\diamond$  placement map  $\chi$ : description of motion

### Metric tensor

- ◊ The metric tensor g is a symmetric tensor with two vector arguments
- ♦ The coefficients  $g_{ij}(x, y, z)$  may depend on position (curved space)
- ◊ Defines the distance on a manifold
- ◊ Used in mesh generation also

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# Length of a curve

#### **General case**

- ♦ Consider a curve  $C(P_A, P_B)$  from  $P_A$  to  $P_B$  with tangent vector  $\vec{V}$
- The idea is to integrate a unit tangent vector along the curve to measure its length
- Normalized tangent vector, using the metric tensor g

$$ec{t} = rac{ec{V}}{\sqrt{g(ec{V},ec{V})}}$$

- ♦ Density of curve length is the covector  $g(\vec{t})$ , using again g
- Length of the curve

$$L_C = \int_{C(P_A, P_B)} g(\vec{t})$$

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# Distance between two points $P_A$ and $P_B$

- ◊ Among all curves between P<sub>A</sub> and P<sub>B</sub>, the geodesic is the one with the minimal length
- $\diamond$  The distance between  $P_A$  and  $P_B$  is the length of the geodesic

$$d(P_A, P_B) = \min_C L_C = \min_C \int_{C(P_A, P_B)} g(\vec{t})$$



http://math.etsu.edu/multicalc/prealpha/Chap3/Chap3-7/GeoProof.gif 💿 🕨 🗧 🕨 🛓 📀 🗨

# Distance between two points $P_A$ and $P_B$

#### Euclidean case

In the Euclidean space, everything is more simple

- ◊  $g_{ij} = \delta_{ij}$  using Cartesian coordinates
- Geodesics are straigth lines
- The space is flat, distance depends only on end points

$$d(P_A, P_B) = \sqrt{(x_B - x_A)^2 + (y_B - y_A)^2 + (z_B - z_A)^2}$$

$$\diamond \ \vec{t} = \frac{\vec{v}}{|\vec{v}|}$$

◊ and the metric appears explicitly nowhere...

# Placement map $\chi$



- Material manifold
- ◊ Euclidean space
- ♦ Placement map  $\chi$ : description of motion
- o the placement map is a smooth invertible mapping
- It is sufficient to map all tensor quantities as well

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# Finite strain, another byproduct of g

Cauchy-Green tensor:  $\rightarrow$  distance in the reference configuration

 $C = \chi g$ a non trivial metric tensor $= F^T F$ F is the jacobian matrix of  $\chi$ 

#### Green tensor

$$\begin{split} E &= \frac{1}{2}(\chi g - g) & \text{general expression} \\ &= \frac{1}{2}(C - \mathbb{I}) & \text{in Euclidean space}, g = \mathbb{I}, g_{ij} = \delta_{ij} \\ E_{ij} &= \frac{1}{2}(\frac{du^k}{dx^i}\delta_{ki} + \frac{du^k}{dx^i}\delta_{kj} + \frac{du^k}{dx^i}\frac{du^k}{dx^j}) & \delta_{ki} \text{ factors needed to balance indices} \end{split}$$

Infinitesimal strain: linearisation of E for small deformations

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{du^k}{dx^j} \delta_{ki} + \frac{du^k}{dx^i} \delta_{kj} \right) \stackrel{!}{=} \frac{1}{2} \left( \frac{du^i}{dx^j} + \frac{du^j}{dx^i} \right) = \frac{1}{2} \left( (\nabla u) + (\nabla u)^T \right)$$

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# Hooke law

- ♦ Last piece of the elastic model: the constitutive relationship  $\sigma(\nabla u)$  or  $\sigma(\varepsilon)$
- We now proceed in Euclidean space, and stop balancing covariant and contravariant indices (classical elasticity). Implicit summation remains on repeated indices.
- Classically, Hooke tensor with 81 components, then simplifying assumptions

$$\sigma_{ij} = H_{ijkl}\varepsilon_{kl}$$

- A more intuitive approach is to decompose the 9 dimensional space of 3x3 tensors into relevant geometric subspaces
- ♦ Let *A* be a 3x3 tensor, I be the identity tensor. One has

$$\underset{\text{dim=9}}{A} = \underset{\text{dim=5}}{\text{dev}(A)} + \underset{\text{dim=1}}{\mathbb{I}} \underset{\text{dim=3}}{\text{vol}(A)} + \underset{\text{dim=3}}{\text{antisym}(A)}$$

# Hooke law

$$\underset{\text{dim}=9}{A} = \underset{\text{dim}=5}{\text{dev}(A)} + \underset{\text{dim}=1}{\mathbb{I}} \underset{\text{dim}=3}{\text{vol}(A)} + \underset{\text{dim}=3}{\text{atisym}(A)}$$

with

$$sym(A) = \frac{1}{2}(A + A^{T})$$
  
antisym(A) =  $\frac{1}{2}(A - A^{T})$  rotations  
$$vol(A) = \frac{1}{3}\sum_{k}A_{kk} = \frac{1}{3}trace(A)$$
 compression/dilatation  
$$dev(A) = sym(A) - I vol(A)$$
 shear

Hooke law (linear isotropic material) is then just a linear relation between the different subspaces:

 $vol(\sigma) = 3K \ vol(\nabla u)$ 3K = bulk modulus $dev(\sigma) = 2G \ dev(\nabla u)$ 2G = shear modulusantisym $(\sigma) = 0$ rotations yield no stress

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### Hooke law

$$\begin{split} \sigma &= \operatorname{dev}(\sigma) + \mathbb{I} \operatorname{vol}(\sigma) + \operatorname{antisym}(\sigma) \\ &= 2G \operatorname{dev}(\nabla u) + 3K \,\mathbb{I} \operatorname{vol}(\nabla u) + 0 \\ &= (3K - 2G)\mathbb{I} \operatorname{vol}(\nabla u) + 2G \operatorname{sym}(\nabla u) \\ &= 3\lambda \mathbb{I} \operatorname{vol}(\nabla u) + 2\mu \operatorname{sym}(\nabla u) \\ &= \lambda \mathbb{I} \operatorname{trace}(\nabla u) + 2\mu \operatorname{sym}(\nabla u) \end{split}$$

$$3\lambda = 3K - 2G = \frac{3E\nu}{(1+\nu)(1-2\nu)}$$
$$2\mu = 2G = \frac{E}{1+\nu}$$
$$3\lambda + 2\mu = 3K = \frac{E}{1-2\nu}$$
$$\lambda + 2\mu = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$$

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#### Inverse Hooke law

$$vol(\nabla u) = \frac{1}{3K} vol(\sigma)$$
$$dev(\nabla u) = \frac{1}{2G} dev(\sigma)$$
$$antisym(\sigma) = 0$$

3K = bulk modulus

2G =shear modulus

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rotations yield no stress

$$\nabla u = \operatorname{dev}(\nabla u) + \mathbb{I} \operatorname{vol}(\nabla u) + \operatorname{antisym}(\nabla u)$$
$$= \frac{1}{2G} \operatorname{dev}(\sigma) + \frac{1}{3K} \mathbb{I} \operatorname{vol}(\sigma) + \operatorname{antisym}(\nabla u)$$
$$= (\frac{1}{3K} - \frac{1}{2G}) \mathbb{I} \operatorname{vol}(\sigma) + \frac{1}{2G} \sigma + \operatorname{antisym}(\nabla u)$$

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#### Inverse Hooke law

$$\varepsilon = \nabla u - \operatorname{antisym}(\nabla u) = \left(\frac{1}{3K} - \frac{1}{2G}\right) \mathbb{I} \operatorname{vol}(\sigma) + \frac{1}{2G} \sigma$$
$$= -\frac{\nu}{E} \operatorname{trace}(\sigma) \mathbb{I} + \frac{1+\nu}{E} \sigma$$

- $\diamond \ \nabla u$  cannot be expressed uniquely from  $\sigma$
- $\diamond$  antisym( $\nabla u$ ) must be obtained another way
- Lagrange multiplier in stress formulation

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Use course notes to write down Hooke law under the matrix form

$$\begin{pmatrix} \sigma_{XX} \\ \sigma_{Xy} \\ \sigma_{Xz} \\ \sigma_{yx} \\ \sigma_{yx} \\ \sigma_{yy} \\ \sigma_{yz} \\ \sigma_{zz} \\ \sigma_{zy} \\ \sigma_{zz} \end{pmatrix} = (?) \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial z} \\ \frac{\partial v}{\partial y} \\ \frac{\partial v}{\partial z} \\ \frac{\partial v}{\partial y} \\ \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial y} \\ \frac{\partial w}{\partial y} \\ \frac{\partial w}{\partial z} \end{pmatrix}$$

- Where is this to be found in the Magetometer model files (filename, line number)?
- ◊ Check and compare.

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- Where is the coupling magnetic force defined in the Magetometer model files (filename, line number)?
- ◊ Write down its algebraic expression.
- What is the name of this force?

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- ◇ The magnetometer bar can be regarded as a beam with rectangular cross section and flexural rigidity  $EI = Eab^3/12$ , where *a* is the width and *b* the thickness of the beam.
- So Find different ways to double the rigidity of the beam.
- Make a static Onelab analysis and compare the obtained deflections with the reference situation.

- Still in the static case, how can you double the deflection by modifying the applied voltage?
- How can you double the deflection by modifying electric conductivity of the magnetometer bar?

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# Optimization

# Design problem

# Statement of the design problem

• Starting point: existing CAD model of a bridge



• Use FEM to account for the real geometry



 "Optimal design" should find automatically the structure that minimizes the bridge deflection (for a given load F and support conditions)!

# Selection of design variables

# Shape optimization

• Start with an existing CAD (from a previous design)



- Design variables are the parameters of existing CAD
  - radius of a circle
  - major/minor axis of ellipse
  - position of nurbs control point

Shape optimization

 Each value of design variables provides a novel geometry that must be re-meshed



• A FEM analysis can then be applied to obtain the physical solution for the new geometry



# **Topology optimization**

- Start from scratch with a block of material (steel)
  - with know loading and support conditions
  - without any initial guess of the initial structure



- What would be the "best" structure that
  - respects the loading and support conditions?
  - minimises the deflection?
  - uses only a given fraction of the initial volume?

# **Topology optimization**

Typically define 1 design variable/ FE as the material (e.g. steel) density that can be either 0 (void) or 1 (solid)

- In practice there are millions of FE for finer mesh
  - Impossible to check each combination since a FEM analysis is required for each of them
  - Relaxation of the problem: design variables vary continuously from 0 to 1 -> much more efficient!
# **FEM-analysis setting**

• The physical behavior of the system is provided by PDEs written in a strong form (linear elastic model)

div 
$$\sigma(\epsilon) + \mathbf{g} = 0$$
 in  $\Omega$   
 $\sigma(\epsilon) = C_{ijkl} \epsilon_{kl} \mathbf{e}_i \mathbf{e}_j^T$  in  $\Omega$   
 $\mathbf{z} = 0$  on  $\partial \Omega$ 

• The problem is equivalently written in a weak form with a residual

$$r(\tau, \mathbf{z}^{\star}, \bar{z}) \equiv \int_{\Omega} \left( \sigma(\epsilon^{\star}) : \nabla \bar{z} - \mathbf{g} \cdot \bar{z} \right) \mathbf{d}\Omega = 0, \quad \forall \bar{z} \in Z_{z}^{0}$$

• The solution z\* of the system depends implicetly and nonlinearly on design variables, i.e. on geometry through the FE mesh.

• Application of FEM in a mesh with N nodes, leads to the solution of linear system of algebraic equations

$$\bar{\mathbf{z}}^T \left( \mathbf{K}(\tau) \mathbf{z}^* - \mathbf{g}(\tau) \right) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

- z(Nx1) is the unknown field vector defined in each node of the FE mesh
- K(NxN) is the stiffness matrix of the physical problem
- g(Nx1) is a loading term (takes into account sources)

 Application of FEM in a mesh with N nodes, leads to the solution of (non)linear system of algebraic equations

$$\bar{\mathbf{z}}^T \Big( \mathbf{K}(\tau) \mathbf{z}^{\star}(\tau) - \mathbf{g}(\tau) \Big) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

- z(Nx1) is the unknown field vector defined in each node of the FE mesh
- K(NxN) is the stiffness matrix of the physical problem
- g(Nx1) is a loading term (takes into account sources)

• FEM leads to the solution of (non)linear system of algebraic equations (in a mesh with N nodes)

$$\bar{\mathbf{z}}^T \Big( \mathbf{K}(\tau) \mathbf{z}^{\star}(\tau) - \mathbf{g}(\tau) \Big) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

- where z(Nx1) is the unknown field vector
- K(NxN) is the stiffness matrix of the physical problem
- g(Nx1) is a loading term (takes into account sources)
- The system is usually solved using the Newton-Raphson method

Mathematical formulation of the optimization problem

## **Optimization Problem Formulation**

- Find the n design variables  $\tau$  that
  - minimize the internal energy of the structure
  - while using only a fraction lpha of the initial volume  $V_0$

$$\min_{\tau} \quad \frac{1}{2} \int_{\Omega} \sigma(\epsilon^{\star}) : \epsilon^{\star} \, \mathbf{d}\Omega$$

$$s.t. \quad V(\tau) \leq \alpha V_0,$$

$$\tau_i^{min} \leq \tau_i \leq \tau_i^{max}, \ i = 1, \dots, n$$

$$r(\tau, \mathbf{z}^{\star}, \overline{\mathbf{z}}) = 0, \ \forall \overline{\mathbf{z}} \in Z_z^0.$$

- Consideration of real CAD with the FEM constraint!
- Bound constraints on design variables.

## **Optimization Problem Formulation**

- For each design variable (or configuration) au
  - Mesh the structure (for shape optimization)
  - Run FEM analysis (time consuming) : z\*
  - evaluate objective and constraints (postprocessing)

$$\min_{\tau} \quad \frac{1}{2} \int_{\Omega} \sigma(\epsilon^{\star}) : \epsilon^{\star} \, \mathbf{d}\Omega$$

$$s.t. \quad V(\tau) \leq \alpha V_0,$$

$$\tau_i^{min} \leq \tau_i \leq \tau_i^{max}, \ i = 1, \dots, n$$

$$r(\tau, \mathbf{z}^{\star}, \mathbf{\bar{z}}) = 0, \ \forall \mathbf{\bar{z}} \in Z_z^0.$$

- Implicit and nonlinear dependence of z\* on  $\, au$ 
  - each function depends implicitely and nonlinearly on  $\,\tau\,$
  - time consuming evaluation since FEM is required
- Practically, there can be mil. of au and inequalities!

Optimizer – resolution of the optimization problem

## Optimizer

 The functions in the optimization problem depend <u>implicitly</u> and <u>nonlinearly</u> on design variables (possibly very large number).



 How can we find the minimum of that function (assuming that we have only 1 design variable)?

## Gradient-free optimizer

- Naturally converges to the global optimum!
- #function evaluations for a naïve method is  $\frac{n!}{n!(n!-m!)}$
- For a small optimization problem,

$$n = 10, m = 5:252$$
  
 $n = 20, m = 10:185000$   
 $n = 100, m = 50:10^{29}$ 

- Impossible to explore the whole space with a naive method!
- Clever algorithms that can explore the design space are required!

## Gradient-based optimizer

- Idea: At a given point  $\tau^i$  run a FEM analysis to evaluate the function and its derivative  $\tau^i$ .
- Then compute an explicit model (sort of Taylor) of the function (in which function evaluations do not take time compared to FEM!).



#### Gradient-based optimizer

 Once the optimum of the explicit model at a given point is found, a new explicit model is built at that point and the procedure is repeated until convergence to the real optimum.



• Stay always feasible during iterations and higher convergence rate than gradient-free methods!

Application: optimal design of a bridge

# Optimal design of a bridge

• Shape optimization approach



• Topology optimization approach (0-blue, 1-red)



• Fortunately the classical bridge is recovered!

# Sensitivity analysis

#### Introduction

 "Sensitivity" is the derivative of a performance function f (appearing in the optimization problem) w.r.t. a design variable

$$\frac{\mathrm{d}}{\mathrm{d}\tau}f(\tau,\mathbf{z}^{\star}(\tau)) = ?$$

• The performance function depends on the solution  $\mathbf{z}^{\star}$  of the physical problem (at equilibrium)

$$\bar{\mathbf{z}}^T \Big( \mathbf{K}(\tau) \mathbf{z}^{\star}(\tau) - \mathbf{g}(\tau) \Big) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

K<sup>-1</sup> is a NxN matrix with N number of nodes in mesh
 -> obtained during the resolution of the problem!

## Finite difference method

• First order Taylor approximation of  $f(\tau, \mathbf{z}^{\star}(\tau))$ 

 $\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) \approx \frac{f\left(\tau + \delta\tau, \mathbf{z}_{\tau+\delta\tau}^{\star}\right) - f\left(\tau, \mathbf{z}^{\star}\right)}{\delta\tau}$ 

• What is  $z_{\tau+\delta\tau}^{\star}$ ? Solve anew the linear problem with the perturbed geometry (with perturbed mesh)

$$\bar{\mathbf{z}}^T \Big( \mathbf{K}(\tau + \delta \tau) \mathbf{z}_{\tau + \delta \tau}^{\star} - \mathbf{g}(\tau + \delta \tau) \Big) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

- Pros/Cons
  - Simplest method to compute the sensitivity
  - Very slow when the  $\#\tau$  is large since  $\#\tau$  additional FEM are required!

Analytic approach – direct method

Sensitivity of the performance function

$$\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \frac{\partial f}{\partial z^{\star}} \frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau} ?$$

• Requires determining  $\frac{dz^{\star}}{dz}$ 

$$\bar{\mathbf{z}}^T \frac{\mathrm{d}}{\mathrm{d}\tau} \Big( \mathbf{K}(\tau) \mathbf{z}^{\star}(\tau) - \mathbf{g}(\tau) \Big) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

• We end up with a linear system for  $\frac{d\mathbf{z}^{\star}}{d\mathbf{z}}$ 

$$\bar{\mathbf{z}}^T \Big( \mathbf{K}(\tau) \underbrace{\frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau}}_{\mathrm{d}\tau} + (\frac{\partial \mathbf{K}}{\partial \tau} \mathbf{z}^{\star} - \frac{\partial \mathbf{g}}{\partial \tau}) \Big) \stackrel{\mathrm{d}\tau}{=} 0, \forall \bar{\mathbf{z}} \in Z_z^0$$

•  $\mathbf{K}^{-1}$ known as equilibrium of physical system enforced

• with a loading depending only on design variable

Analytic approach – adjoint method

• Sensitivity of the performance function

$$\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \frac{\partial f}{\partial z^{\star}} \frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau} ?$$

$$\frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau} \text{ is obtained from the direct method}$$

$$\underbrace{\frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau}}_{\mathrm{d}\tau} = \mathbf{K}^{-1} \left(\frac{\partial \mathbf{K}}{\partial \tau} \mathbf{z}^{\star}(\tau) - \frac{\partial \mathbf{g}}{\partial \tau}\right)$$

• The latter is injected into the sensitivity equation  $\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \frac{\partial f}{\partial \mathbf{z}^{\star}} \cdot \mathbf{K}^{-1} \left(\frac{\partial \mathbf{K}}{\partial \tau} \mathbf{z}^{\star}(\tau) - \frac{\partial \mathbf{g}}{\partial \tau}\right)$  Analytic approach – adjoint method

• Derivative of the function

$$\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \mathcal{N}\left(\frac{\partial \mathbf{g}}{\partial \tau} - \frac{\partial \mathbf{K}}{\partial \tau}\mathbf{z}^{\star}\right)$$

• Where  $\lambda$  is the solution of the linear adjoint system

$$\bar{\lambda}^T \left( \mathbf{K} \left( \boldsymbol{\lambda} - \frac{\partial f}{\partial \mathbf{z}} (\mathbf{z}^\star) \right) = 0, \forall \bar{\lambda} \in Z_\lambda^0$$

- $\mathbf{K}^{-1}$ known as equilibrium of physical system enforced
- with a loading depending only on the function

Discussion (real problem:  $\#\tau >>$ ,#f >>)

• Direct method

$$\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \frac{\partial f}{\partial z^{\star}} \frac{\mathrm{d}\mathbf{z}^{\star}}{\mathrm{d}\tau}$$

- Back-substitution for each design variable  $\bar{\mathbf{z}}^T \left( \mathbf{K}(\tau) \frac{\mathrm{d}\mathbf{z}^*}{\mathrm{d}\tau} + \left( \frac{\partial \mathbf{K}}{\partial \tau} \mathbf{z}^* - \frac{\partial \mathbf{g}}{\partial \tau} \right) \right) = 0, \forall \bar{\mathbf{z}} \in Z_z^0$
- Use only when  $\#\tau \ll \#f$  !
- Adjoint method

$$\frac{\mathrm{d}f}{\mathrm{d}\tau}(\tau, \mathbf{z}^{\star}) = \frac{\partial f}{\partial \tau}(\tau, \mathbf{z}^{\star}) + \lambda^{T} \left(\frac{\partial \mathbf{g}}{\partial \tau} - \frac{\partial \mathbf{K}}{\partial \tau} \mathbf{z}^{\star}\right)$$

- Back-substitution for each performance function  $\bar{\lambda}^T (\mathbf{K} \lambda + \frac{\partial f}{\partial \mathbf{z}} (\mathbf{z}^{\star})) = 0, \forall \bar{\lambda} \in Z_{\lambda}^0$
- Use only when  $\#\tau >> \#f!$
- $\mathbf{K}^{-1}$ <u>known</u> as equilibrium of physical system enforced!

Tutorial – Shape optimization of the magnetometer fundamental frequency

# Physical problem

• Eigenmode at a given  $f_0$  frequency



- Design problem
  - change the existing geometry
  - in order to set  $f_0$  to a desired frequency  $f_0^d$
  - How can we do this?

## Shape optimization

- Choice of design variable(s)
  - Support length, or width, or position?
  - Relevant variables should give high sensitivity!
- Formulation of the optimization problem
  - First try

$$\min_{\tau_{min} \le \tau \le \tau_{max}} |f_0(\tau) - f_0^d|$$

• Second try

$$\min_{\tau_{min} \le \tau \le \tau_{max}} (f_0(\tau) - f_0^d)^2$$



## Shape optimization

- Solve the unconstrained optimization problem for  $\tau$  set as support position

$$\min_{\tau_{min} \le \tau \le \tau_{max}} (f_0(\tau) - f_0^d)^2$$

- The problem is solved with the onelab-based optimization code written in Python (optdriver.py).
- Hint: check graphically if the optimizer finds the correct optimum by plotting the objective.

## **Onelab-based optimization**



**Optimization algorithm:** (handle both shape and topology optimization)

Initialize design variables (user input)

Loop (until convergence to an optimum) ...

- Set the CAD (design variables) and mesh the CAD
- Analysis (FEM): evaluate performance functions
- Sensitivity analysis (FEM): evaluate the gradient of performance functions
- Call optimizer: update the design variables

Onelab-based optimization (Gmsh/GetDP)

• Define the objective as a function (.pro) and add the desired fundamental frequency in onelab database

```
Function {
    // desired fundamental frequency (onelab parameter)
    DefineConstant[
       f0d = {1e5, Name StrCat("Desired fundamental frequency [Hz]")}
    ];
    // fundamental frequency
    f0[] = $EigenvalueReal/(2*Pi);
    // objective function
    objective[] = SquNorm[ f0[] - f0d];
}
```

## Onelab-based optimization (Gmsh/GetDP)

 Call the objective function "objective[]" in the postprocessing associated with the elastic model.

Call the post-operation

```
// Send the objective function in Onelab database
PostOperation {
    { Name Mec ; NameOfPostProcessing Elasticity3D;
    Operation {
        Print[ objective, OnRegion Domain, TimeStep 0,
            SendToServer "Output/diffEigenFreqNorm" ];
    }
    }
}
```

## **Onelab-based optimization (Python)**

- Create a onelab client and specify the problem
  - Objective and design variables as defined in onelab
  - Onelab parameters defining the model (e.g.  $f_0^d$ )
  - Resolution used in .pro

```
# Create a onelab client
clientOnelab = onelab.client(__file__)
if clientOnelab.action == 'check': exit(0)
# Set options for both optimization problem and CAD/FEM model
options = setOptions(clientOnelab,{
    'CADFEMOptions':{
        'Input/0Type of analysis':0,
        'Optimization/Desired natural frequency [Hz]':2.5e05},
    'file':clientOnelab.getPath('magnetometer'),
    'resolution': 'Analysis',
    'objective': 'Output/diffEigenFreqNorm',
    'constraints':[],
    'designVariables':['Input/Geometry/5Support position [m]'],
    'iterMax':50
})
```

**Onelab-based optimization (Python)** 

• Specify the starting value, lower ( $\tau_{min}$ ) and upper bounds ( $\tau_{max}$ )

```
# Starting value of design variables
desVar = [1.5e-04]
# Lower and upper bounds of design variables
lowerBoundDesVar = [6.0e-05]
upperBoundDesVar = [2.0e-04]
# Upper bound of constraints
```

```
# Upper bound of constraints
upperBoundConstr = []
```

#### Create an optimization solver (mma)

```
# Create an optimizer client
clientOpt = mma.client({
    'm':options['m'],
    'xmin':lowerBoundDesVar,'xmax':upperBoundDesVar,
    'asyinit':0.2,'asyincr':0.8,'asydecr':0.3
})
```

Solve the optimization problem

## Run shape optimization ...

\$ gmsh optdriver.pyv 1		
===	Optimization Problem	
Model sett * "Optim * "Input * "Input Design var * "Input Performanc * Object Stop crite Design v Maximum	ing zation/Desired fundamental frequency [Hz]" 'Geometry/00Mesh size factor " '0Type of analysis " lables (n:1) 'Geometry/5Support position [m] " e functions (m:0) lve :"Output/diffEigenFreqNorm" ra ariables tol. : 1e-06 number of iterations : 50	: 250000.0 : 1 : 0 : 6.00e-05<=1.50e-04<=2.00e-04
It. 1,x It. 2,x It. 3,x It. 4,x It. 5,x It. 6,x It. 7,x	<pre>1: 1.500e-04, f0: 7.609e+09, change: 1.495e-0 1: 1.351e-04, f0: 3.596e+09, change: 2.265e-0 1: 1.124e-04, f0: 3.048e+08, change: 1.780e-0 1: 9.465e-05, f0: 8.853e+06, change: 6.870e-0 1: 1.015e-04, f0: 5.935e+06, change: 1.235e-0 1: 1.003e-04, f0: 1.476e+06, change: 2.674e-0 1: 1.000e-04, f0: 1.476e+06, change: 2.674e-0</pre>	5 5 6 7 7

## Shape optimization results



