Computational & Multiscale Mechanics of Materials



Homogenization with propagation of instabilities through the different scales

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Content

• Introduction

- Multi-scale modelling
- Strain softening issues
- Non-local damage-enhanced mean-field-homogenization

Computational homogenization for cellular materials

Conclusions



- Computational technique: FE²
 - Macro-scale _
 - FE model
 - At one integration point $\overline{\epsilon}$ is know, $\overline{\sigma}$ is sought







- Computational technique: FE²
 - Macro-scale
 - FE model
 - At one integration point $\overline{\epsilon}$ is know, $\overline{\sigma}$ is sought



- Micro-scale
 - Usual 3D finite elements
 - Periodic boundary conditions



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Multi-scale modelling: How?

- Computational technique: FE²
 - Macro-scale
 - FE model
 - At one integration point $\overline{\epsilon}$ is know, $\overline{\sigma}$ is sought
 - Transition
 - Downscaling: $\overline{\epsilon}$ is used to define the BCs
 - Upscaling: $\overline{\sigma}$ is known from the reaction forces
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Multi-scale modelling: How?

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 - Micro-scale
 - Usual 3D finite elements
 - Periodic boundary conditions
 - Advantages
 - Accuracy
 - Generality
 - Drawback
 - Computational time

Ghosh S et al. 95, Kouznetsova et al. 2002, Geers et al. 2010, ...



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Multi-scale modelling: How?

Mean-Field Homogenization

- Macro-scale
 - FE model •
 - At one integration point $\overline{\varepsilon}$ is know, $\overline{\sigma}$ is sought •
- Transition
 - Downscaling: ε is used as input of the MFH model
 - Upscaling: $\overline{\sigma}$ is the output of the MFH model •
- Micro-scale
 - Semi-analytical model ٠
 - Predict composite meso-scale response
 - From components material models
- Advantages
 - Computationally efficient
 - Easy to integrate in a FE code (material model)
- Drawbacks
 - Difficult to formulate in an accurate way
 - Geometry complexity
 - Material behaviours complexity



Mori and Tanaka 73, Hill 65, Ponte Castañeda 91, Suguet 95, Doghri et al 03, Lahellec et al. 11, Brassart et al. 12, ...



Strain softening of the microscopic response

- Finite element solutions for strain softening problems suffer from:
 - The loss the uniqueness and strain localization
 - Mesh dependence



The numerical results change with the size of mesh and direction of mesh







The numerical results change without convergence

• Requires a non-local formulation of the macro-scale problem



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Multi-scale simulations with strain softening

Two cases considered

- Composite materials
 - Mean-field homogenization
 - Non-local damage formulation



- Honeycomb structures
 - Computational homogenization
 - Second-order FE2
 - Micro-buckling



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Non-local damage-enhanced mean-field-homogenization

L. Wu (ULg), L. Noels (ULg), L. Adam (e-Xstream), I. Doghri (UCL)

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One more equation required

$$\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon} : \boldsymbol{\varepsilon}_{\mathrm{0}}$$

Difficulty: find the adequate relations

$$\sigma_{I} = f(\boldsymbol{\varepsilon}_{I})$$

$$\sigma_{0} = f(\boldsymbol{\varepsilon}_{0})$$

$$\boldsymbol{\varepsilon}_{I} = \boldsymbol{B}^{\varepsilon} : \boldsymbol{\varepsilon}_{0}$$

$$\boldsymbol{\varepsilon}_{I} = \boldsymbol{\varepsilon}_{0}$$

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Mean-Field Homogenization for different materials Linear materials ω_{I} inclusions Materials behaviours • $\boldsymbol{\sigma}_{\mathrm{I}} = \overline{\boldsymbol{C}}_{\mathrm{I}} : \boldsymbol{\varepsilon}_{\mathrm{I}}$ $\boldsymbol{\sigma}_{\mathrm{0}} = \overline{\boldsymbol{C}}_{\mathrm{0}} : \boldsymbol{\varepsilon}_{\mathrm{0}}$ ω_0 composite ? Mori-Tanaka assumption $\boldsymbol{\varepsilon}^{\infty} = \boldsymbol{\varepsilon}_{0}$ Use Eshelby tensor • $\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon} (\mathrm{I}, \overline{\boldsymbol{C}}_{\mathrm{O}}, \overline{\boldsymbol{C}}_{\mathrm{I}}) : \boldsymbol{\varepsilon}_{\mathrm{O}}$ matrix with $\boldsymbol{B}^{\varepsilon} = [\boldsymbol{I} + \boldsymbol{S} : \overline{\boldsymbol{C}}_{0}^{-1} : (\overline{\boldsymbol{C}}_{1} - \overline{\boldsymbol{C}}_{0})]^{-1}$ 3 alg $\sigma \wedge$ Non-linear materials Define a Linear Comparison Composite inclusions • Common approach: incremental tangent • composite $\Delta \boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon} \left(\mathrm{I}, \overline{\boldsymbol{C}}^{\mathrm{alg}}, \overline{\boldsymbol{C}}^{\mathrm{alg}} \right) : \Delta \boldsymbol{\varepsilon}_{\mathrm{0}}$ matrix: $\pmb{\sigma}_{0}$ ₹ 3 $\Delta \boldsymbol{\varepsilon}_0$ $\Delta \overline{\boldsymbol{\varepsilon}}$ $\Delta \boldsymbol{\mathcal{E}}_{\mathrm{I}}$

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- Material models
 - Elasto-plastic material
 - Stress tensor $\boldsymbol{\sigma} = \boldsymbol{C}^{\text{el}} : (\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^{\text{pl}})$
 - Yield surface $f(\boldsymbol{\sigma}, p) = \boldsymbol{\sigma}^{eq} \boldsymbol{\sigma}^{Y} R(p) \le 0$
 - Plastic flow $\Delta \varepsilon^{\rm pl} = \Delta p N$ & $N = \frac{\partial f}{\partial \sigma}$
 - Linearization $\delta \sigma = C^{\text{alg}} : \delta \varepsilon$





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 - Local damage model
 - Apparent-effective stress tensors $\boldsymbol{\sigma} = (1 D)\hat{\boldsymbol{\sigma}}$
 - Plastic flow in the effective stress space
 - Damage evolution $\Delta D = F_D(\varepsilon, \Delta p)$







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- Finite element solutions for strain softening problems suffer from:
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The numerical results change with the size of mesh and direction of mesh





The numerical results change without convergence

- Implicit non-local approach [Peerlings et al 96, Geers et al 97, ...]
 - A state variable is replaced by a non-local value reflecting the interaction between neighboring material points

$$\widetilde{a}(\mathbf{x}) = \frac{1}{V_{\rm C}} \int_{V_{\rm C}} a(\mathbf{y}) w(\mathbf{y}; \mathbf{x}) \mathrm{d}V$$

Use Green functions as weight w(y; x)

 \implies $\widetilde{a} - c\nabla^2 \widetilde{a} = a \implies$ New degrees of freedom

Workshop "Multiscale simulations"



- Material models
 - Elasto-plastic material
 - Stress tensor $\boldsymbol{\sigma} = \boldsymbol{C}^{\text{el}} : (\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^{\text{pl}})$
 - Yield surface $f(\boldsymbol{\sigma}, p) = \boldsymbol{\sigma}^{eq} \boldsymbol{\sigma}^{Y} R(p) \le 0$
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 - Linearization $\delta \sigma = C^{\text{alg}} : \delta \varepsilon$
 - Local damage model
 - Apparent-effective stress tensors $\boldsymbol{\sigma} = (1 D)\hat{\boldsymbol{\sigma}}$
 - · Plastic flow in the effective stress space
 - Damage evolution $\Delta D = F_D(\boldsymbol{\varepsilon}, \Delta p)$
 - Non-Local damage model
 - Damage evolution $\Delta D = F_D(\varepsilon, \Delta \widetilde{p})$
 - Anisotropic governing equation $\widetilde{p} \nabla \cdot (\boldsymbol{c}_{g} \cdot \nabla \widetilde{p}) = p$
 - Linearization

2014 -

$$\delta \boldsymbol{\sigma} = \left[(1 - D) \boldsymbol{C}^{\text{alg}} - \hat{\boldsymbol{\sigma}} \otimes \frac{\partial F_D}{\partial \boldsymbol{\varepsilon}} \right] : \delta \boldsymbol{\varepsilon} - \hat{\boldsymbol{\sigma}} \frac{\partial F_D}{\partial \tilde{\boldsymbol{p}}} \delta \tilde{\boldsymbol{p}}$$





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Problem

- We want the fibres to get unloaded during the matrix damaging process
 - For the incremental-tangent approach

$$\Delta \boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon} \Big(\mathrm{I}, (1-D) \overline{\boldsymbol{C}}_{0}^{\mathrm{alg}}, \overline{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{alg}} \Big) : \Delta \boldsymbol{\varepsilon}_{0}$$

- To unload the fibres ($\boldsymbol{\varepsilon}_{\mathrm{I}} < 0$) with such approach would require $\overline{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{alg}} < 0$
- We cannot use the incremental tangent MFH
- We need to define the LCC from another stress state





• Idea

- New incremental-secant approach
 - Perform a virtual elastic unloading from previous solution
 - Composite material unloaded to reach the stress-free state
 - Residual stress in components







• Idea

- New incremental-secant approach
 - Perform a virtual elastic unloading from previous solution
 - Composite material unloaded to reach the stress-free state
 - Residual stress in components
 - Apply MFH from unloaded state
 - New strain increments (>0)

$$\Delta \boldsymbol{\varepsilon}_{\mathrm{I}/0}^{\mathrm{r}} = \Delta \boldsymbol{\varepsilon}_{\mathrm{I}/0} + \Delta \boldsymbol{\varepsilon}_{\mathrm{I}/0}^{\mathrm{unload}}$$

- Use of secant operators

$$\Delta \boldsymbol{\varepsilon}_{\mathrm{I}}^{\mathrm{r}} = \boldsymbol{B}^{\varepsilon} \left(\mathrm{I}, (1-D) \overline{\boldsymbol{C}}_{0}^{\mathrm{Sr}}, \overline{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{Sr}} \right) : \Delta \boldsymbol{\varepsilon}_{0}^{\mathrm{r}}$$

Possibility of have unloading

$$\left[\begin{array}{c} \Delta \boldsymbol{\varepsilon}_{\mathrm{I}}^{\mathrm{r}} > 0 \\ \Delta \boldsymbol{\varepsilon}_{\mathrm{I}} < 0 \end{array} \right]$$



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Mesh-size effect

- Fictitious composite
 - 30%-UD fibres
 - Elasto-plastic matrix with damage
- Notched ply

2014 -





Laminate plate with hole Carbon-fibres reinforced epoxy _ 60%-UD fibres • Elasto-plastic matrix with damage • - $[-45_2/45_2]_{\rm S}$ staking sequence 4.68±0.05 damage (0/83) $39.60 \pm 0.35 \bigcirc 0000$ 0,0316 0,001 220 40 300 damage (0/83) ¥ x 0.0316 0,001



- Laminate plate with hole (2)
 - Carbon-fibres reinforced epoxy _
 - 60%-UD fibres •
 - Elasto-plastic matrix with damage •
 - $[-45_2/45_2]_{\rm S}$ staking sequence











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Computational homogenization for cellular materials



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Challenges

- Micro-structure
 - Not perfect with non periodic mesh

How to constrain the periodic boundary conditions?





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Challenges ۲

- Micro-structure _
 - Not perfect with non periodic mesh



How to constrain the periodic boundary conditions?

- Thin components ٠
- Experiences micro-buckling









Challenges

- Micro-structure
 - Not perfect with non periodic mesh



How to constrain the periodic boundary conditions?

- Thin components
- Experiences micro-buckling



- Transition
 - Homogenized tangent not always elliptic
 - Localization bands



How can we recover the solution unicity at the macro-scale?





Challenges

- Micro-structure
 - Not perfect with non periodic mesh



How to constrain the periodic boundary conditions?

- Thin components
- Experiences micro-buckling



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How can we recover the solution unicity at the macro-scale?

- Macro-scale
 - Localization bands



- How to remain computationally efficient
- \implies How to capture the instability?





- Recover solution unicity: second-order FE²
 - Macro-scale
 - High-order Strain-Gradient formulation

 $\overline{\mathbf{P}}(\overline{\mathbf{X}}) \cdot \nabla_0 \overline{\mathbf{Q}}(\overline{\mathbf{X}}) : (\nabla_0 \otimes \nabla_0) = 0$

- Partitioned mesh (//)
- Transition
 - Gauss points on different processors
 - Each Gauss point is associated to one mesh and one solver

- Micro-scale
 - Usual continuum

$$\mathbf{P}(\mathbf{X}) \cdot \nabla_0 = 0$$





- Micro-scale periodic boundary conditions
 - Defined from the fluctuation field

$$w = u - (\overline{F} - I) \cdot X + \frac{1}{2} (\overline{F} \otimes \nabla_0) : (X \otimes X)$$

- Stated on opposite RVE sizes

$$\begin{cases} w(X^+) = w(X^-) \\ \int_{\partial V^-} w(X) d\partial V = 0 \end{cases}$$

Can be achieved by constraining opposite nodes

Foamed materials

- Usually random meshes
- Important voids on the boundaries

Honeycomb structures

Not periodic due to the imperfections







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- Micro-scale periodic boundary conditions (2) ۲
 - New interpolant method





Boundary node Control node

- Use of Lagrange, cubic spline .. interpolations
- Fits for
 - Arbitrary meshes
 - Important voids on the RVE sides ٠
- Results in new constraints in terms of the boundary and control nodes displacements

$$\widetilde{\pmb{C}} \ \widetilde{\pmb{u}}_b - \pmb{g}(\overline{\pmb{\mathsf{F}}},\overline{\pmb{\mathsf{F}}} \otimes \pmb{\nabla_0}) {=} 0$$



- Discontinuous Galerkin (DG) implementation of the second order continuum
 - Finite-element discretization
 - Same discontinuous polynomial approximations for the
 - **Test** functions φ_h and
 - **Trial** functions $\delta \varphi$
 - Definition of operators on the interface trace:
 - Jump operator:
 - Mean operator:



- · Continuity is weakly enforced, such that the method
 - Is consistent
 - Is stable
 - Has the optimal convergence rate





• Second-order FE2 method

Macro-scale second order continuum

$\overline{\mathbf{P}}(\overline{X}) \cdot \nabla_0 - \overline{\mathbf{Q}}(\overline{X}) : (\nabla_0 \otimes \nabla_0) = 0$

- Requires C¹ shape functions on the mesh
- The C^1 can be weakly enforced using the DG method

$$a(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = a^{\text{bulk}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) + a^{\text{PI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) + a^{\text{QI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = b(\delta\overline{\boldsymbol{u}})$$



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• Usual volume terms

$$a^{\text{bulk}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = \int_{\overline{V}} [\overline{\mathbf{P}}(\overline{\boldsymbol{u}}):(\delta\overline{\boldsymbol{u}}\otimes \boldsymbol{\nabla}_{\mathbf{0}}) + \overline{\mathbf{Q}}(\overline{X}):(\delta\overline{\boldsymbol{u}}\otimes \boldsymbol{\nabla}_{\mathbf{0}}\otimes \boldsymbol{\nabla}_{\mathbf{0}})]dV$$



Second-order FE2 method

Macro-scale second order continuum

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- Weak enforcement of the C^0
 - Continuity
 - Consistency
 - Stability

between the finite elements

$$a^{\mathrm{PI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = \int_{\partial_{I}\overline{V}} \begin{bmatrix} \llbracket \delta\overline{\boldsymbol{u}} \rrbracket \cdot \langle \overline{\mathbf{P}} - \overline{\mathbf{Q}} \cdot \nabla_{0} \rangle \cdot \overline{N} + \llbracket \overline{\boldsymbol{u}} \rrbracket \cdot \langle \overline{\mathbf{P}}(\delta\overline{\boldsymbol{u}}) - \overline{\mathbf{Q}}(\delta\overline{\boldsymbol{u}}) \cdot \nabla_{0} \rangle \cdot \overline{N} + \\ \llbracket \overline{\boldsymbol{u}} \rrbracket \otimes \overline{N} : \langle \frac{\beta_{P}}{h_{s}} \mathbf{C}^{\mathbf{0}} \rangle : \llbracket \delta\overline{\boldsymbol{u}} \rrbracket \otimes \overline{N} \end{bmatrix} dV$$

Allows efficient parallelization as elements are disjoint



• Second-order FE2 method

Macro-scale second order continuum

$\overline{\mathbf{P}}(\overline{X}) \cdot \nabla_0 \overline{\mathbf{Q}}(\overline{X}): (\nabla_0 \otimes \nabla_0) = 0$

- Requires C¹ shape functions on the mesh
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$$a(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = a^{\text{bulk}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) + a^{\text{PI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) + a^{\text{QI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}) = b(\delta\overline{\boldsymbol{u}})$$

- Weak enforcement of the $\ensuremath{\mathbb{C}}^1$
 - Continuity
 - Consistency
 - Stability

between the finite elements

$$a^{\mathrm{QI}}(\overline{\boldsymbol{u}},\delta\overline{\boldsymbol{u}}\,) = \int_{\partial_{I}\overline{V}} \begin{bmatrix} \left[\delta\overline{\boldsymbol{u}}\otimes\nabla_{\mathbf{0}} \right] \cdot \langle \overline{\mathbf{Q}} \rangle \cdot \overline{N} + \left[\overline{\boldsymbol{u}}\otimes\nabla_{\mathbf{0}} \right] \cdot \langle \overline{\mathbf{Q}}(\delta\overline{\boldsymbol{u}}) \rangle \cdot \overline{N} + \right] \\ \left[\overline{\boldsymbol{u}}\otimes\nabla_{\mathbf{0}} \right] \otimes \overline{N} : \langle \frac{\beta_{P}}{h_{s}} \mathbf{J}^{\mathbf{0}} \rangle : \left[\delta\overline{\boldsymbol{u}}\otimes\nabla_{\mathbf{0}} \right] \otimes \overline{N} \end{bmatrix} dV$$

Allows efficient parallelization as elements are disjoint



Capturing instabilities

- Macro-scale: localization bands
 - Path following method on the applied loading

 $a(\overline{\boldsymbol{u}}, \delta \overline{\boldsymbol{u}}) = \overline{\mu} \, b(\delta \overline{\boldsymbol{u}})$

• Arc-length constraint on the load increment

$$\bar{h}(\Delta \bar{\boldsymbol{u}}, \Delta \bar{\mu}) = \frac{\Delta \bar{\boldsymbol{u}} \cdot \Delta \bar{\boldsymbol{u}}}{\bar{X}_0^2} + \Delta \bar{\mu}^2 - \Delta L^2 = 0$$





Capturing instabilities

- Macro-scale: localization bands
 - Path following method on the applied loading

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- Micro-scale
 - Path following method on the applied boundary conditions

$$\widetilde{\boldsymbol{C}} \ \widetilde{\boldsymbol{u}}_b - \boldsymbol{g}(\overline{\mathbf{F}}, \overline{\mathbf{F}} \otimes \boldsymbol{\nabla}_{\mathbf{0}}) = 0$$

$$\begin{cases} \overline{\mathbf{F}} = \overline{\mathbf{F}}_0 + \mu \,\Delta \overline{\mathbf{F}} \\ \overline{\mathbf{F}} \otimes \boldsymbol{\nabla}_{\mathbf{0}} = (\overline{\mathbf{F}} \otimes \boldsymbol{\nabla}_{\mathbf{0}})_0 + \mu \,\Delta (\overline{\mathbf{F}} \otimes \boldsymbol{\nabla}_{\mathbf{0}})_0 \end{cases}$$

Arc-length constraint on the load increment

$$h(\Delta \boldsymbol{u}, \Delta \boldsymbol{\mu}) = \frac{\Delta \boldsymbol{u} \cdot \Delta \boldsymbol{u}}{X_0^2} + \Delta \mu^2 - \Delta l^2 = 0$$





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- Compression of an hexagonal honeycomb
 - Elasto-plastic material



- Comparison of different solutions
 - Full direct simulation

Multiscale with different macro-meshes





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- Compression of an hexagonal honeycomb (2)
 - Captures of the softening onset
 - Captures the softening response
 - No macro-mesh size effect







Conclusions

- Non-local damage-enhanced mean-field-homogenization
 - MFH with damage model for the matrix material
 - Non-local implicit formulation
 - Can capture the strain softening
 - More in
 - 10.1016/j.ijsolstr.2013.07.022
 - 10.1016/j.ijplas.2013.06.006
 - 10.1016/j.cma.2012.04.011
 - 10.1007/978-1-4614-4553-1_13
- Computational homogenization for foamed materials
 - Second-order FE² method
 - Micro-buckling propagation
 - General way of enforcing PBC
 - More in
 - <u>10.1016/j.cma.2013.03.024</u>
 - <u>10.1016/j.commatsci.2011.10.017</u>
- Open-source software
 - Implemented in GMSH
 - <u>http://geuz.org/gmsh/</u>

