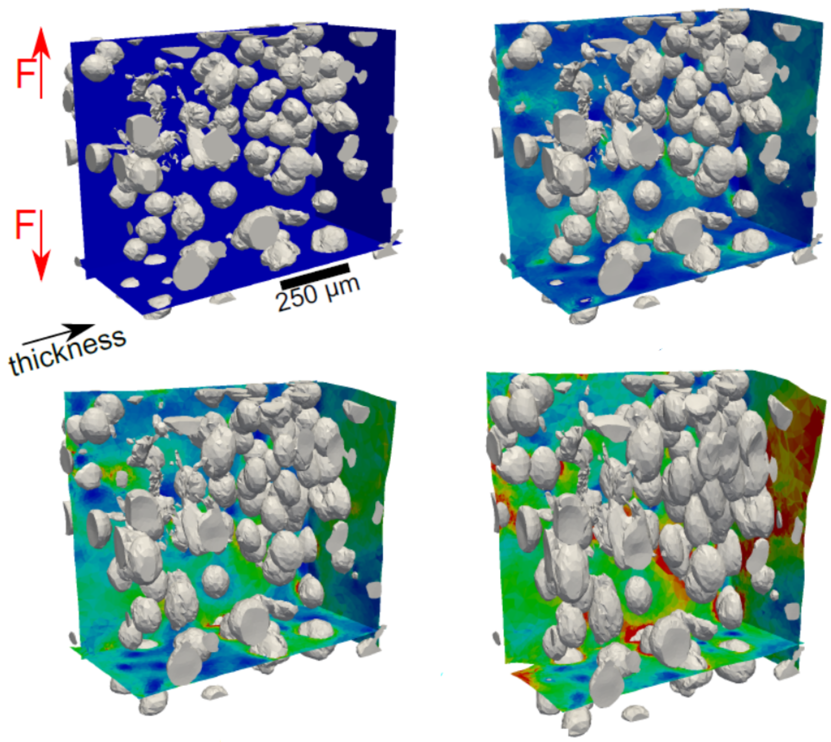
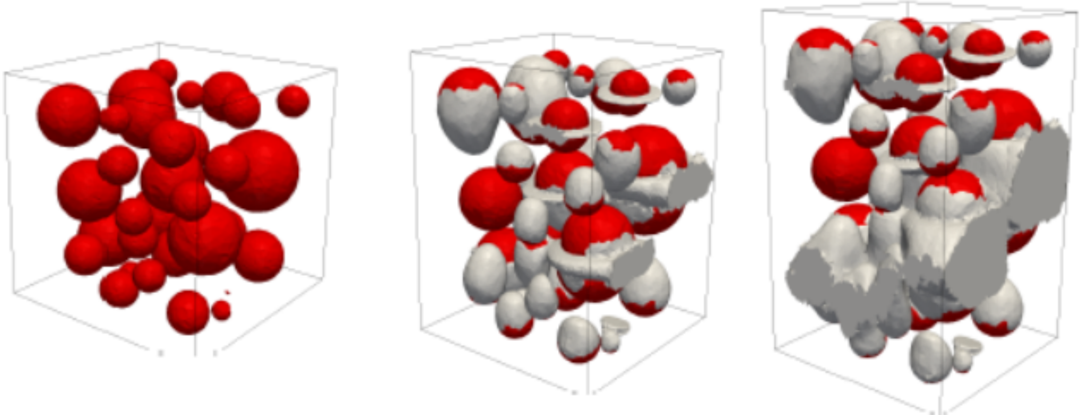
November, 4th 2016

Three-dimensional numerical modeling of ductile fracture mechanisms at the microscale



Modesar SHAKOOR



Advisors:
Pierre-Olivier BOUCHARD
Marc BERNACKI

Context

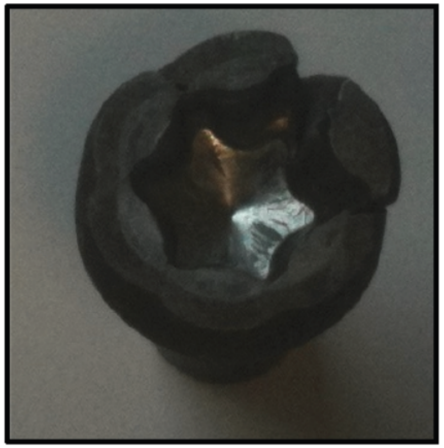
- Damage and failure prediction - arbitrary loading conditions

Connecting rod

[P.-O. Bouchard]

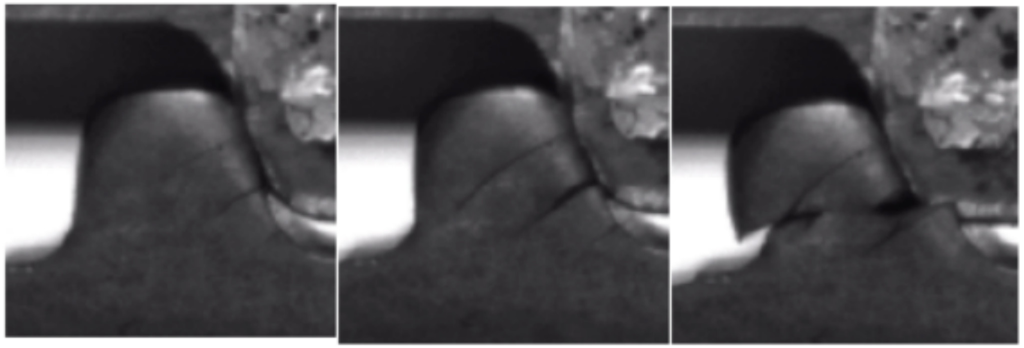
Extrusion

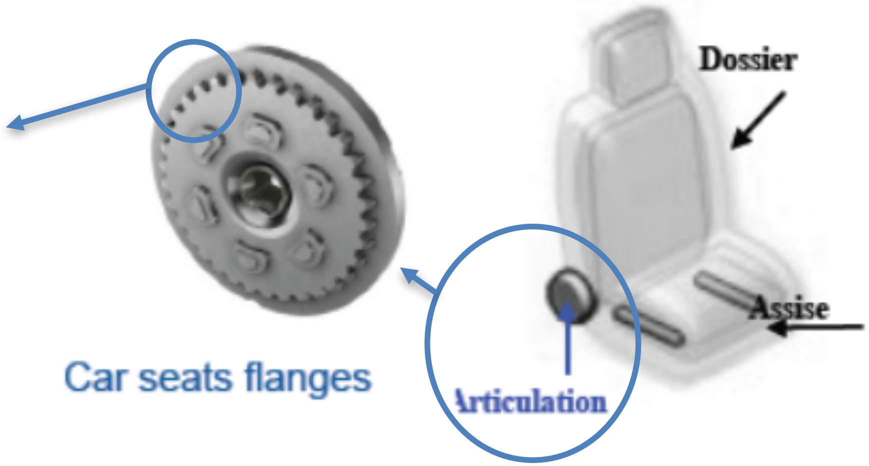
Screw head



Failure during forming

Failure in service

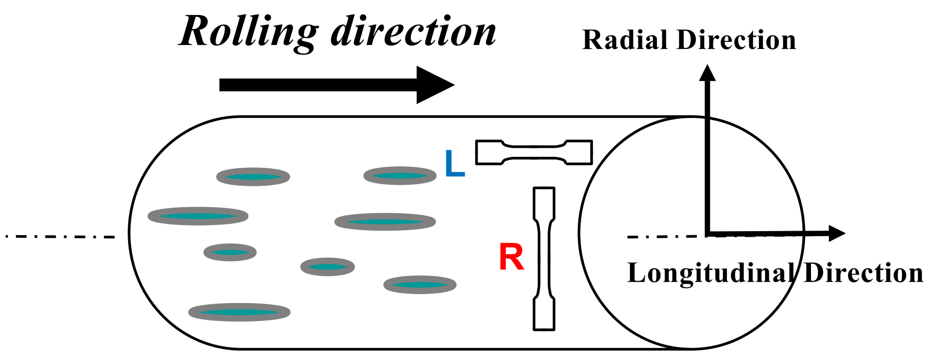


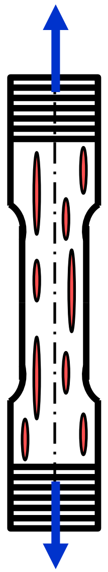


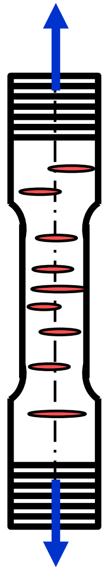
[C. Karolak, *PhD thesis*, 2016]

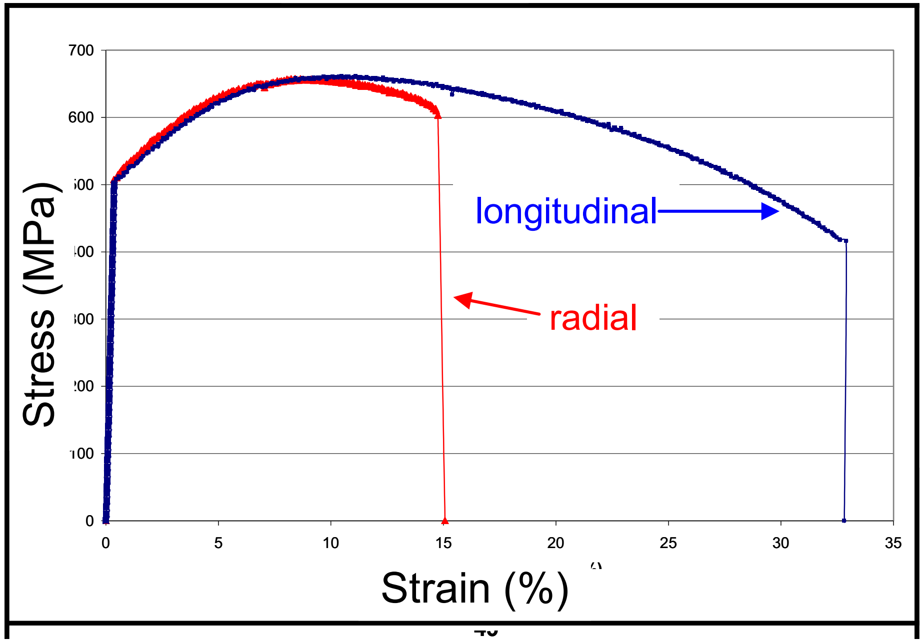
Influence of the microstructure

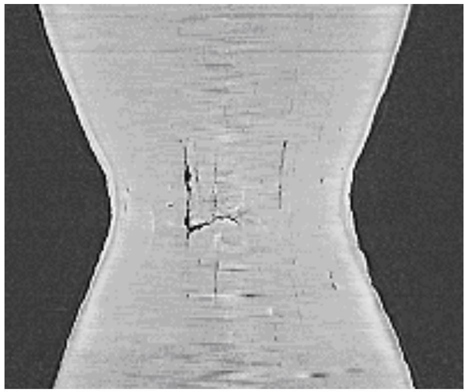
- Cold rolled bainitic steel



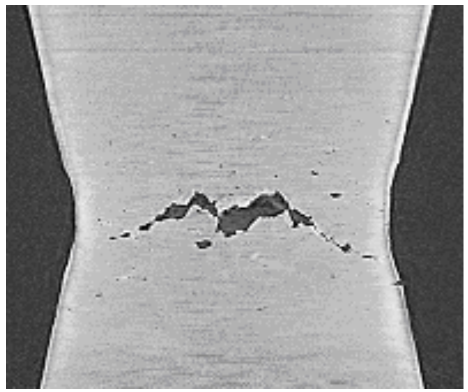








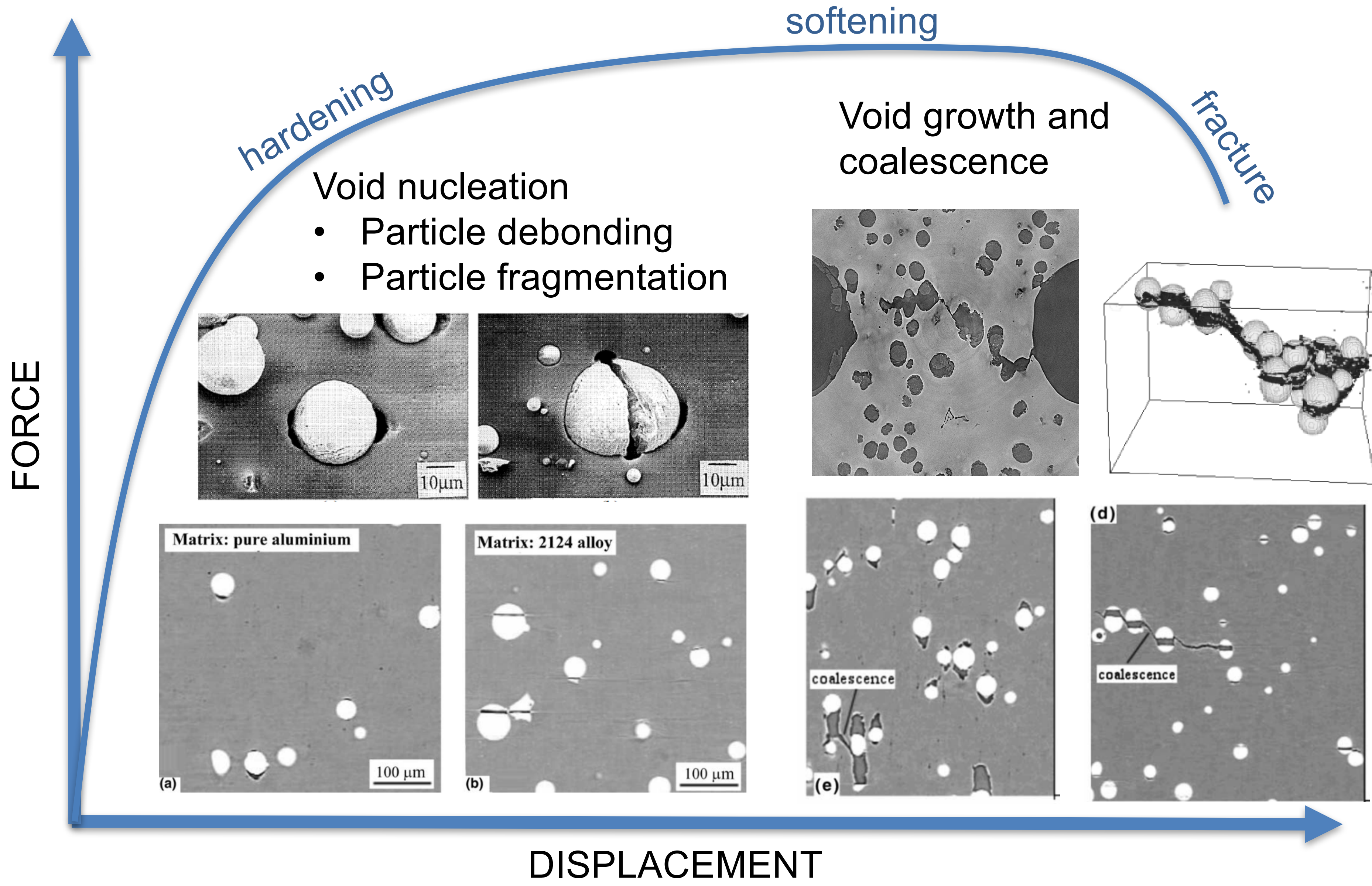
Longitudinal



Radial

P.-O. Bouchard, L. Bourgeon, H. Lachapele, E. Maire, C. Verdu, R. Forestier, R. E. Logé, On the influence of particles distribution and reverse loading on damage mechanisms of ductile steel alloys, *Mater. Sci. Engng. A*, 496: 223–233, 2008

Ductile damage at the microscale



Outline

1. Literature review
   – Damage models
   – Micromechanics
2. Numerical framework
   – Level-Set method
   – Mesh adaptation method
3. Void nucleation and growth
   – Micromechanical models
   – Fracture criteria
   – RVE simulations
4. Void growth and coalescence
   – Meshing real microstructures
   – Applying measured boundary conditions
5. Conclusions and outlook

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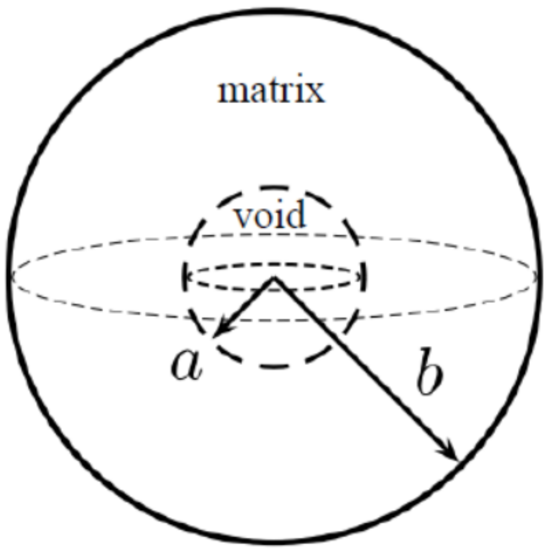
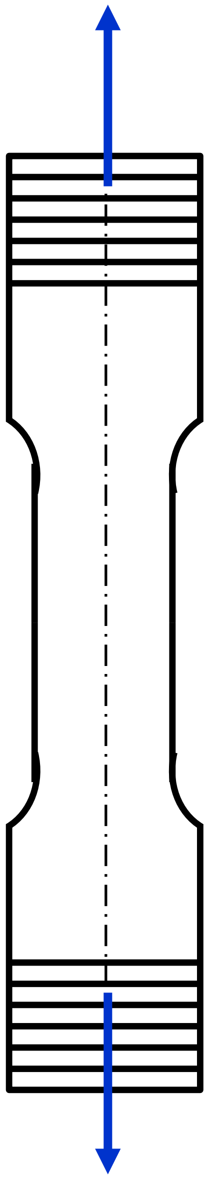
Damage models

- Empirical damage indicators and fracture criteria
  - Latham & Cockcroft 1968
  - Bao & Wierzbicki 2004
- Continuum damage models
  - Kachanov 1958
  - Lemaitre and Chaboche 1978
- Micromechanics-based damage indicators
  - McClintock 1968
  - Rice & Tracey 1969
- Porous plasticity
  - Gurson 1975
  - Tvergaard and Needleman 1984
  - Gologanu, Leblond and Devaux 1993
  - Tekoglu, Leblond and Pardoen 2012

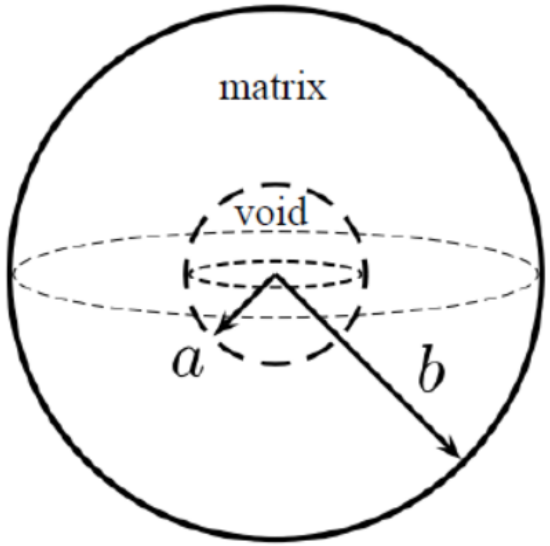
Fracture strain? Porosity? How much? Where?



Micromechanics

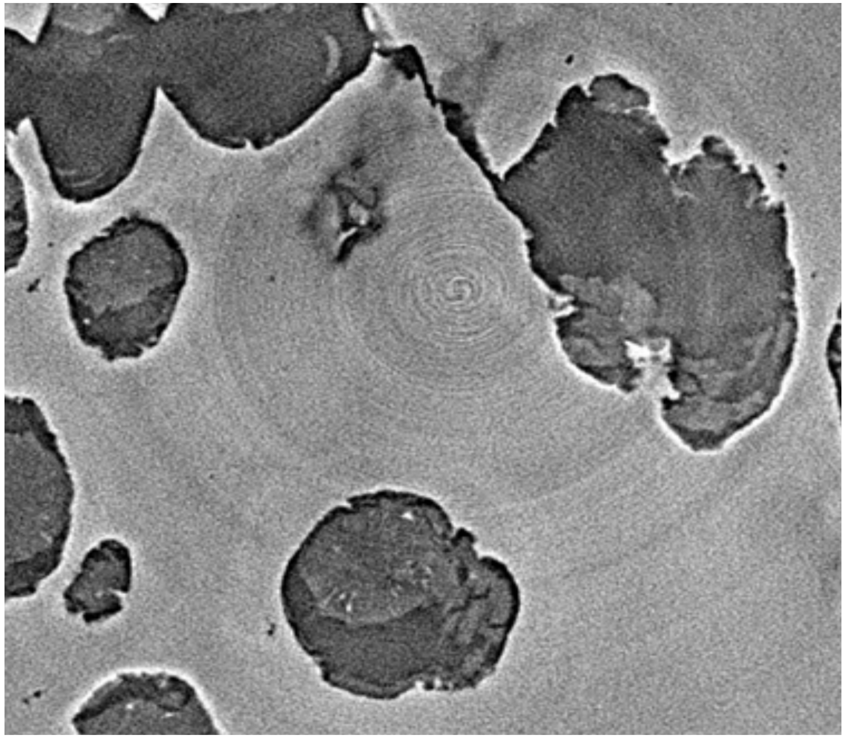


Macro to micro
McClintock, Rice
& Tracey

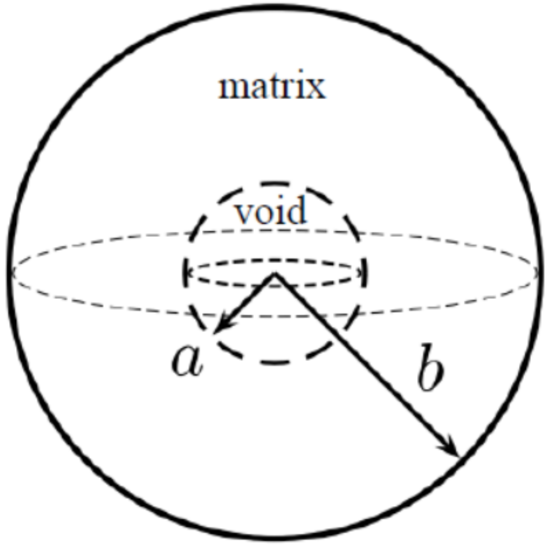


Micro to macro
Gurson

Micromechanics: analytical approaches



?

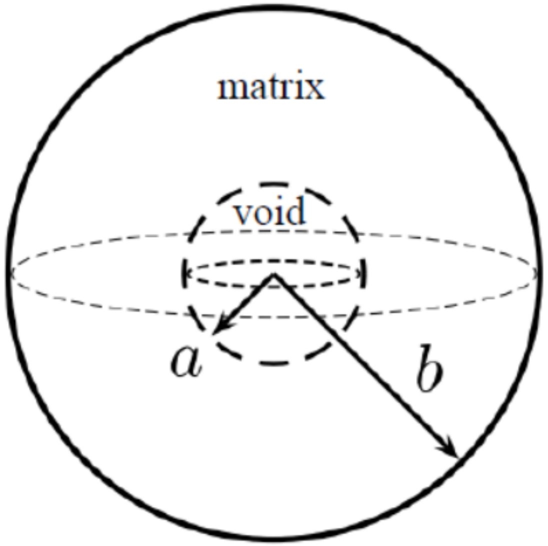


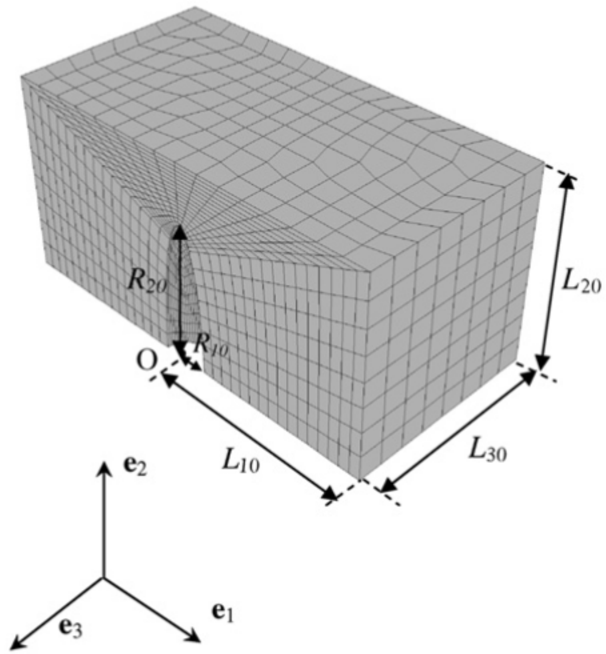
[T.F. Morgeneyer]

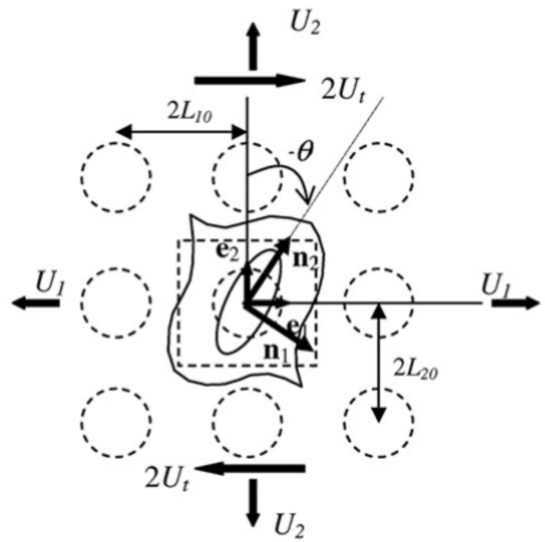
Reality
- Random arrangements of particles & voids
- Random sizes and shapes
- Void nucleation, growth & coalescence
- Complex & non proportional loading paths
- Heterogeneous plasticity and damage in the matrix

Gurson model
- Single void
- Spherical shape
- Only void growth
- Proportional loading, no shear
- Von mises plasticity in the matrix, no damage

Micromechanics: numerical approaches





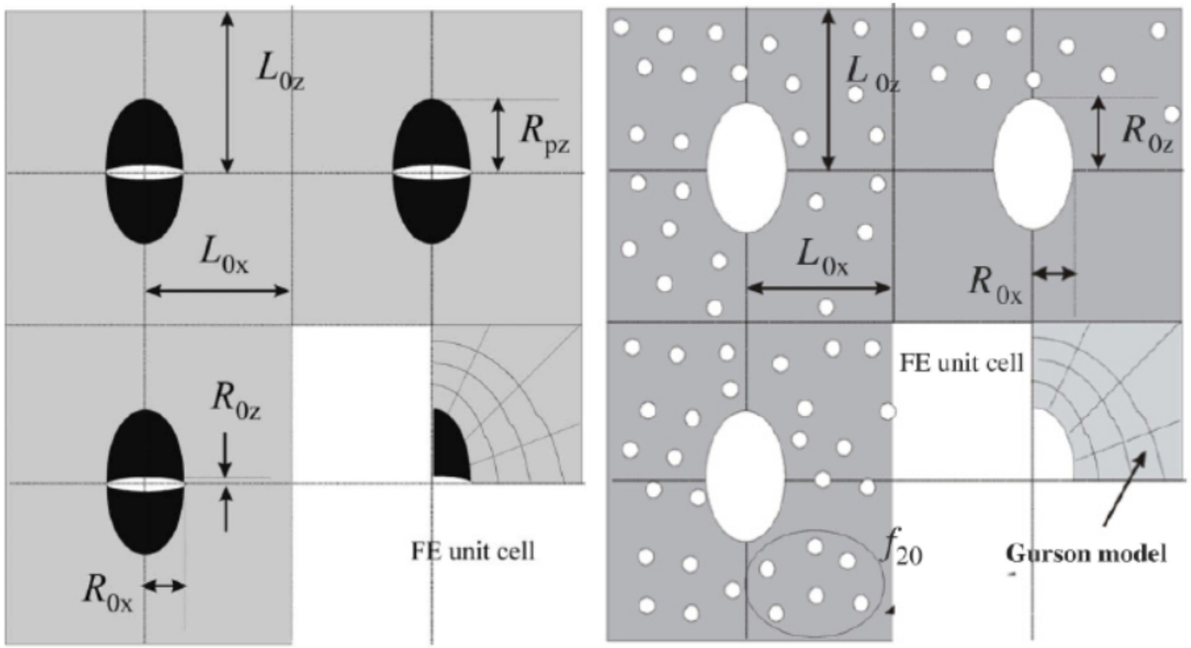


[F. Scheyvaerts, *JMPS*, 2011]

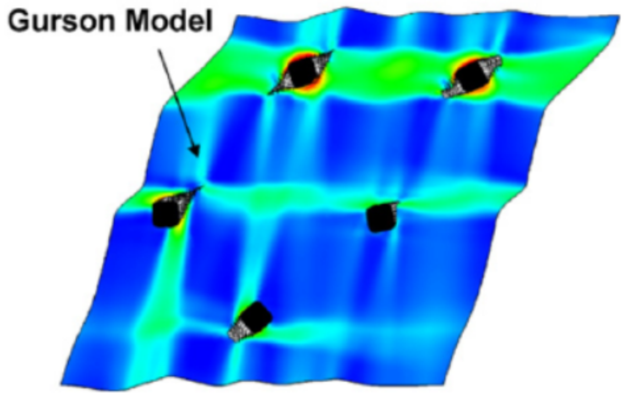
Unit cell approaches

- Periodic arrays of voids or particles
- Ellipsoidal shape
- Void growth & coalescence
- Complex and non proportional loading
- Von mises or porous plasticity in the matrix

Micromechanics: numerical approaches

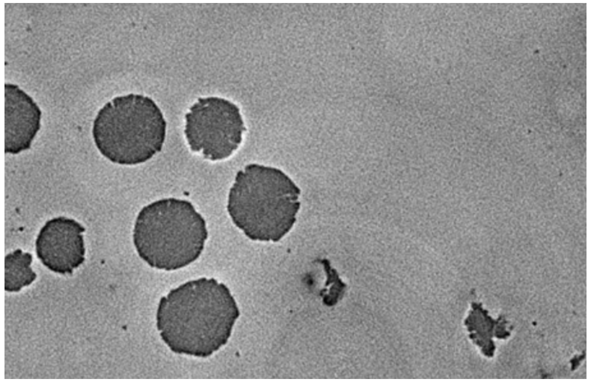


[D. Fabregue and T. Pardoen, *JMPS*, 2008]
[D. Lassance *et al.*, *EFM*, 2006]

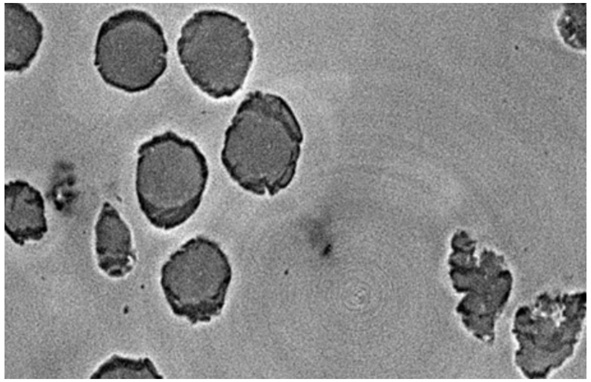


[C. McVeigh *et al.*, *JMPS*, 2007]

Objectives of the present work

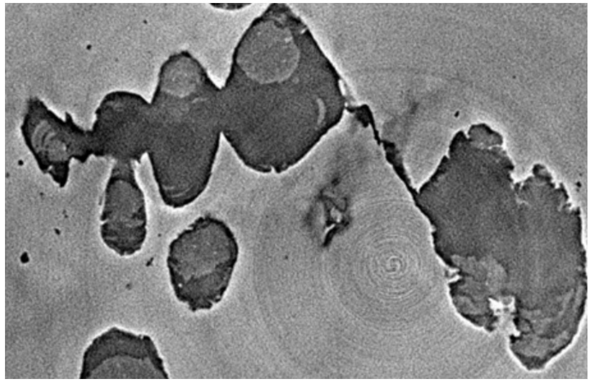


Microstructures of arbitrary size and shape



Particle debonding

Particle fragmentation



Matrix micro-cracking

Large deformations

Complex topological events

Model all micromechanisms simultaneously

More realistic simulations

Comparisons with experiments

Need for an advanced numerical framework

Outline

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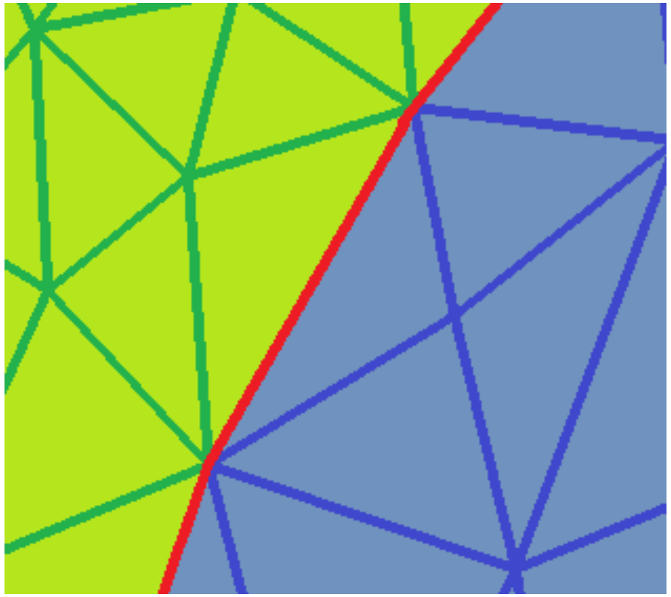
Numerical framework

- Literature review

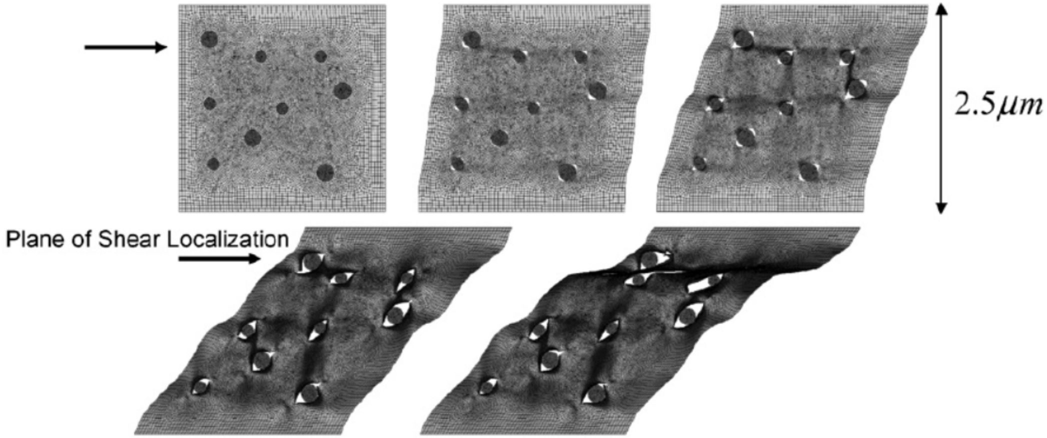


Explicit interface

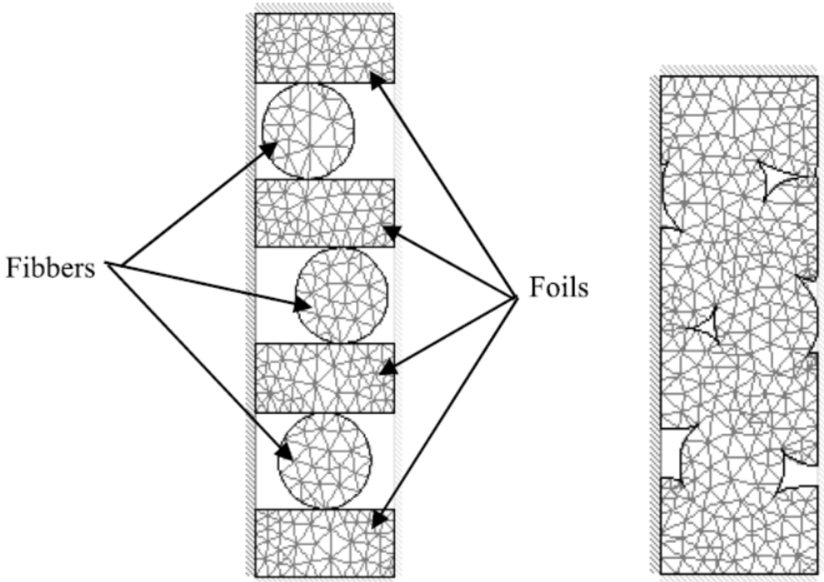
- Remeshing more difficult
- Topological events?

Crack modeling techniques

- Element deletion
- Edge/face splitting



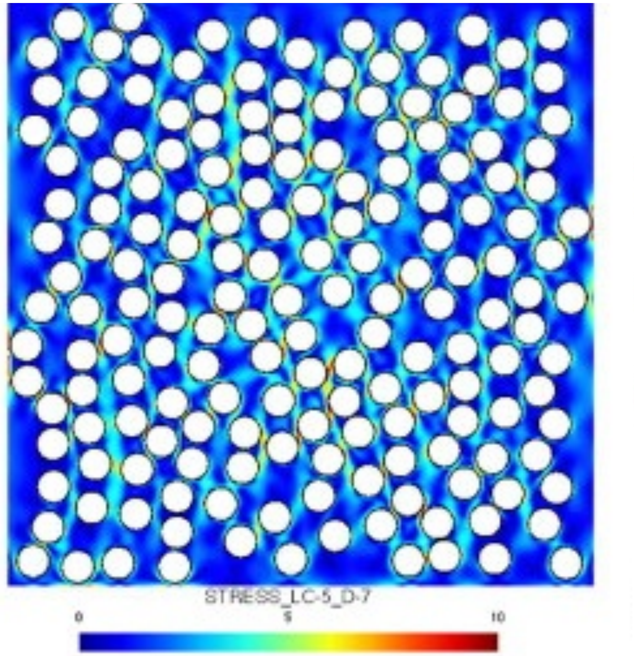
[C. McVeigh *et al.*, *JMPS*, 2007]

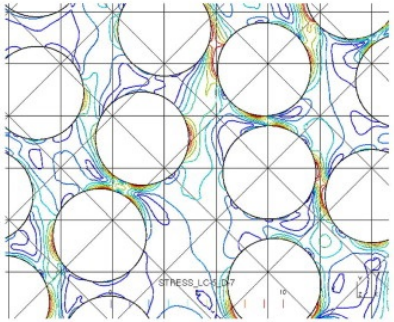


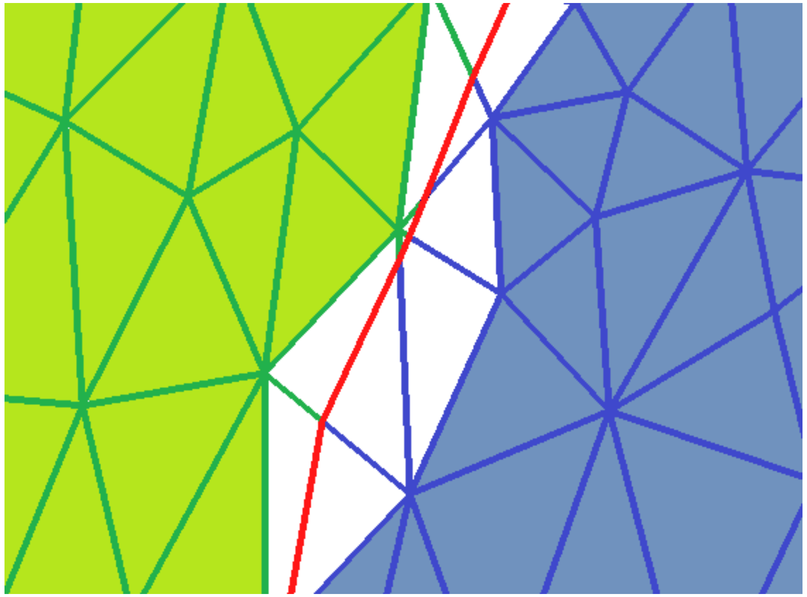
[P.-O. Bouchard *et al.*, *CMAME*, 2000]

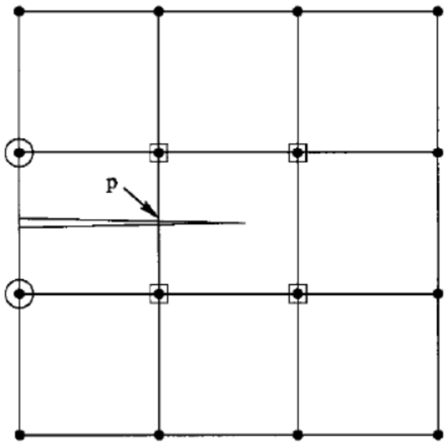
Numerical framework

○ Literature review









[G. Legrain *et al.*, *CMAME*, 2012]

[N. Moës *et al.*, *IJNME*, 1999]

Implicit interface

- Interface modeling? (*e.g.* XFEM)
- Remeshing easier
- Topological events easily handled
- Volume loss

Crack modeling techniques

- X-FEM

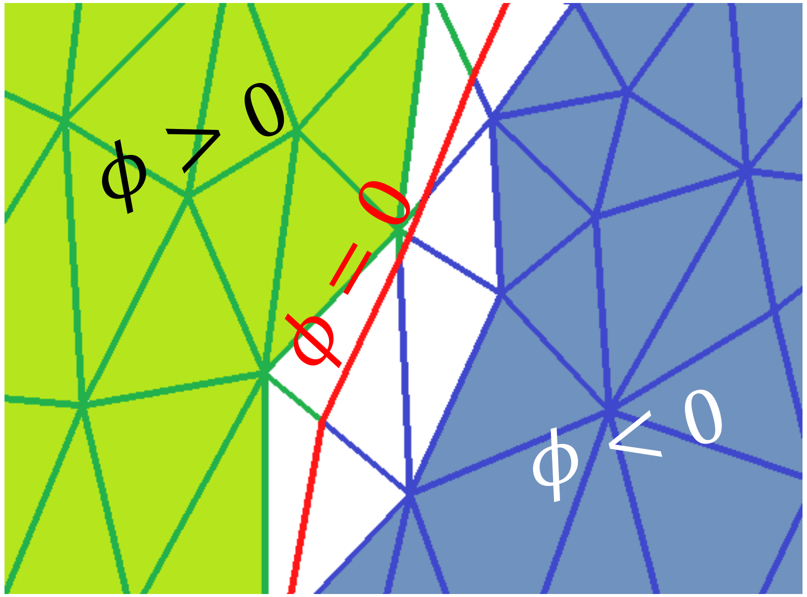
Numerical framework

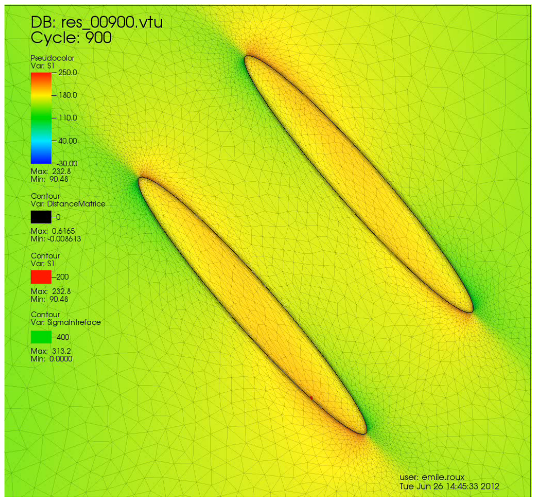
- Literature review: previous work at CEMEF

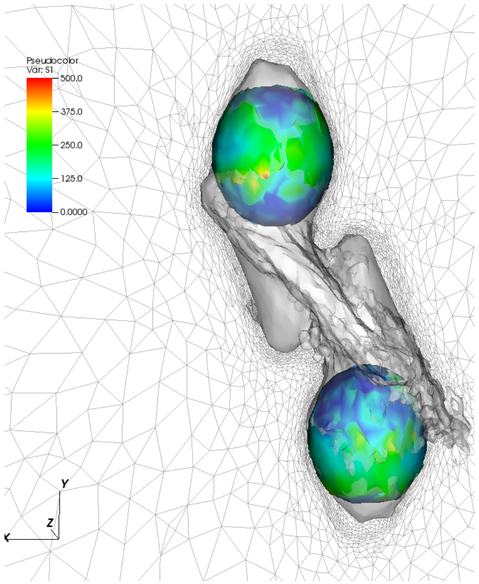
Level-Set method

$$\forall x \in \Omega, \phi_i(x) = \begin{cases} d(x, \partial\Omega_i), x \in \Omega_i \\ -d(x, \partial\Omega_i), x \notin \Omega_i \end{cases}$$

[S. Osher and J.A. Sethian, *JCP*, 1988]







Implicit interface

- Interface modeling more difficult
- Remeshing easier
- Topological events easily handled
- Volume loss

Crack modeling techniques

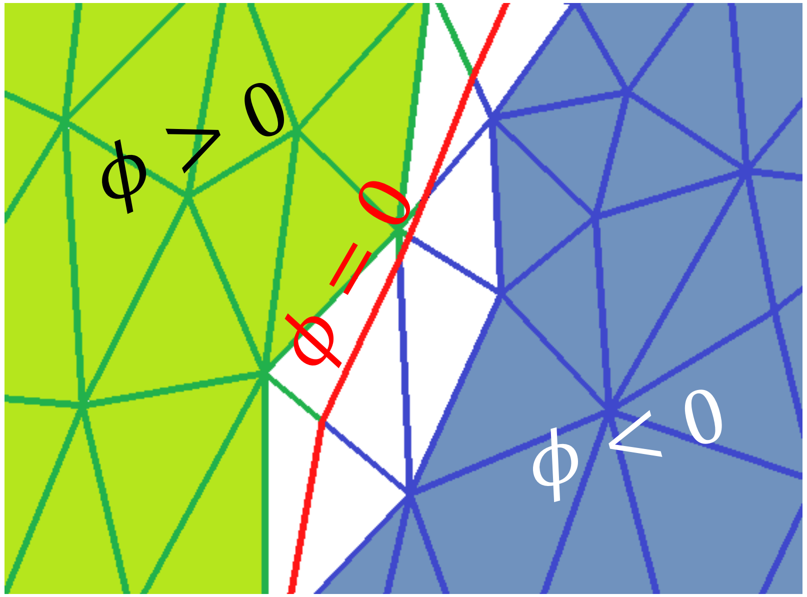
- Region deletion

E. Roux, M. Shakoor, M. Bernacki, P.-O. Bouchard. A new finite element approach for modelling ductile damage void nucleation and growth – analysis of loading path effect on damage mechanisms. *Engineering Fracture Mechanics*, 22:075001, 2014

Numerical framework

○ Literature review: previous work at CEMEF

Void growth



Implicit interface

- Interface modeling more difficult
- Remeshing easier
- Topological events easily handled
- Volume loss

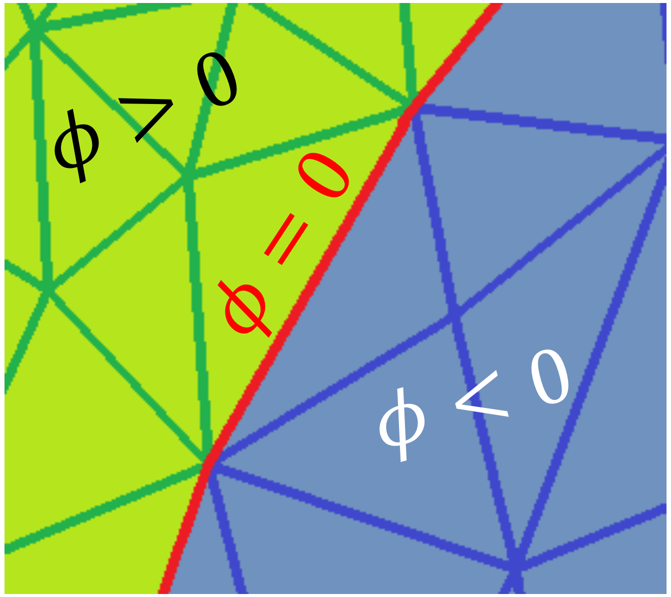
Crack modeling techniques

- Region deletion

E. Roux, M. Bernacki, P.-O. Bouchard. A level-set and anisotropic adaptive remeshing strategy for the modeling of void growth under large plastic strain. *Computational Materials Science*, 68, 32-46, 2013

Numerical framework

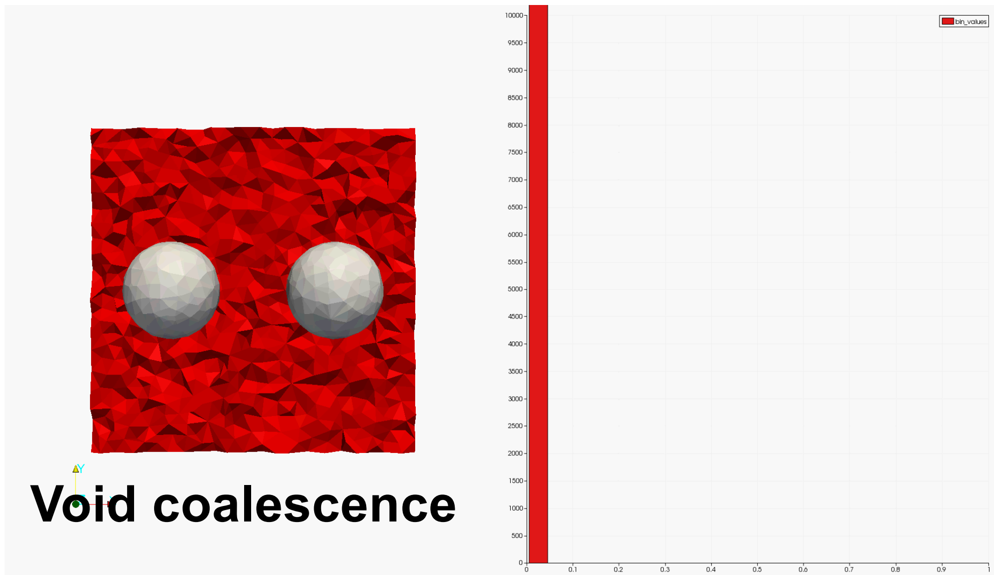
- New developments: body-fitted remeshing



Explicit interface

- Interface modeling easier
- New remesher
- Topological events handled
- Volume conservation

Void growth



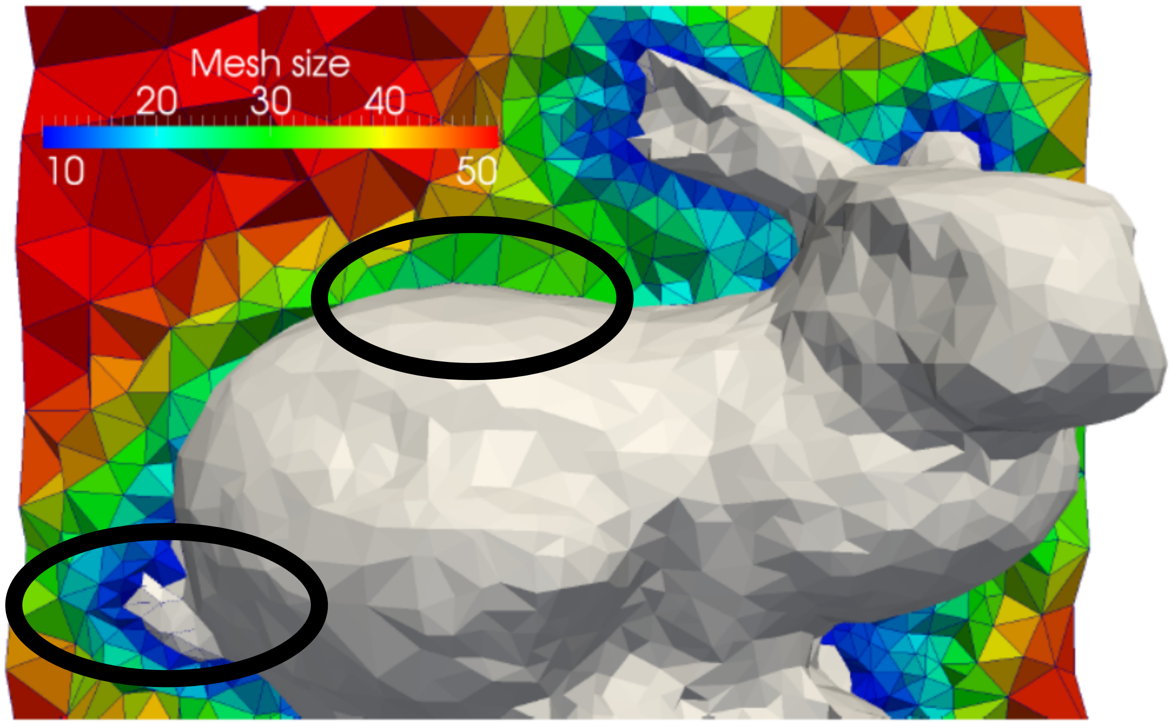
Void coalescence

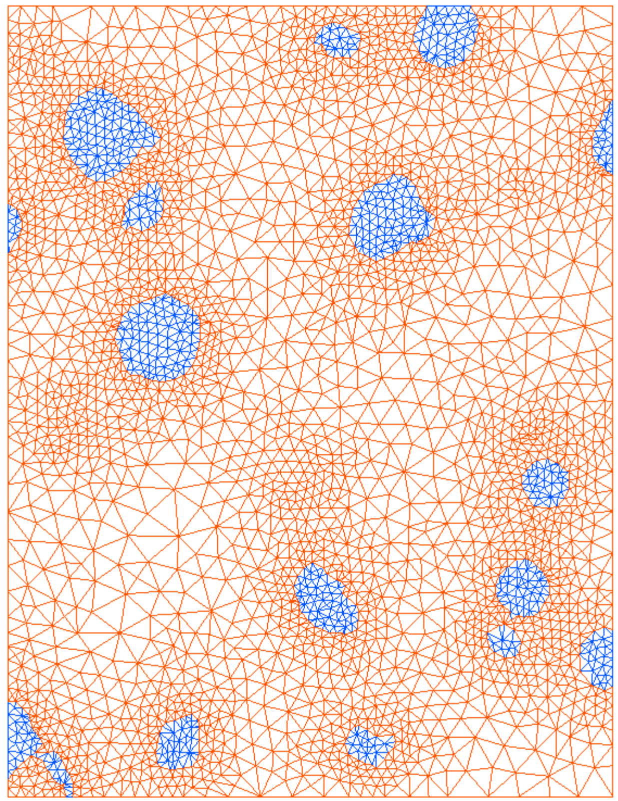
M. Shakoor, P.-O. Bouchard, M. Bernacki. An adaptive level-set method with enhanced volume conservation for simulations in multiphase domains. *International Journal for Numerical Methods in Engineering*, Article In Press, 2016

Numerical framework

- New developments: geometric error based remeshing

Local mesh refinement → Geometric error → Level-Set functions

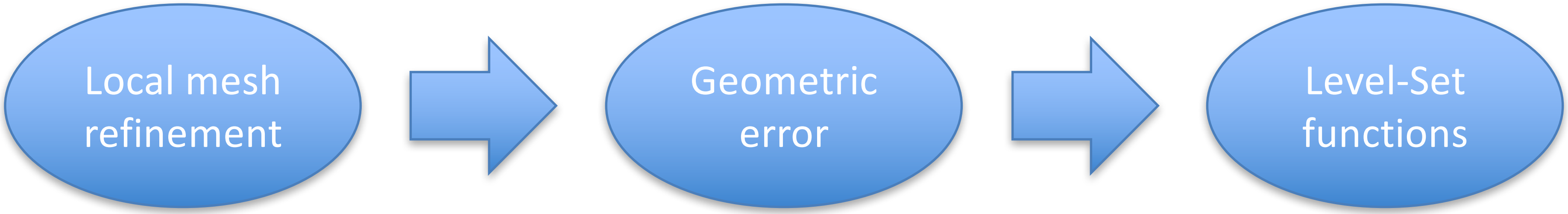




M. Shakoor, M. Bernacki, P.-O. Bouchard. A new body-fitted immersed volume method for the modeling of ductile fracture at the microscale: Analysis of void clusters and stress state effects on coalescence. *Engineering Fracture Mechanics*, 147, 398-417, 2015

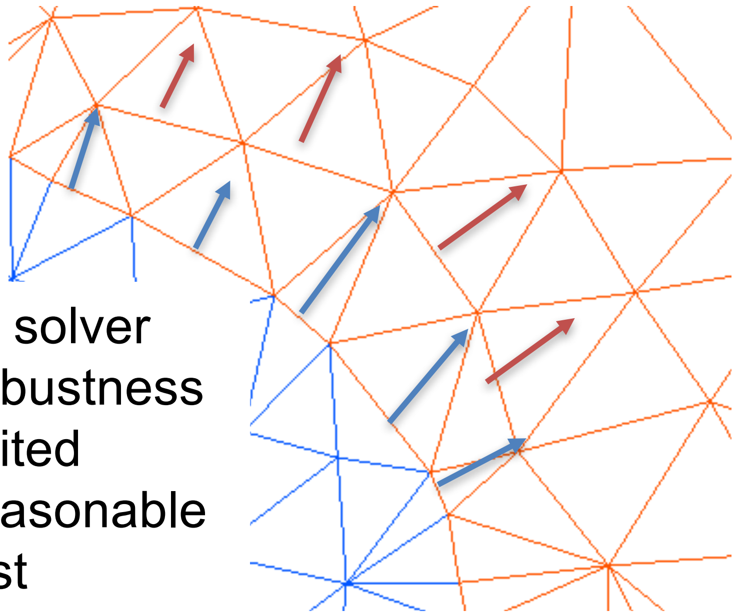
Numerical framework

- New developments: level-set reinitialization



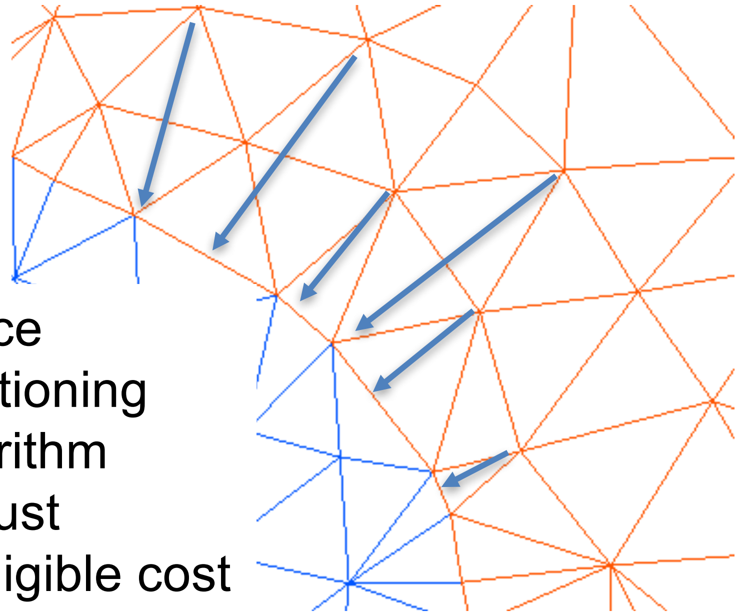
Need to keep distance property

Previous work: indirect methods



- FE solver
- Robustness limited
- Reasonable cost

New development: direct method



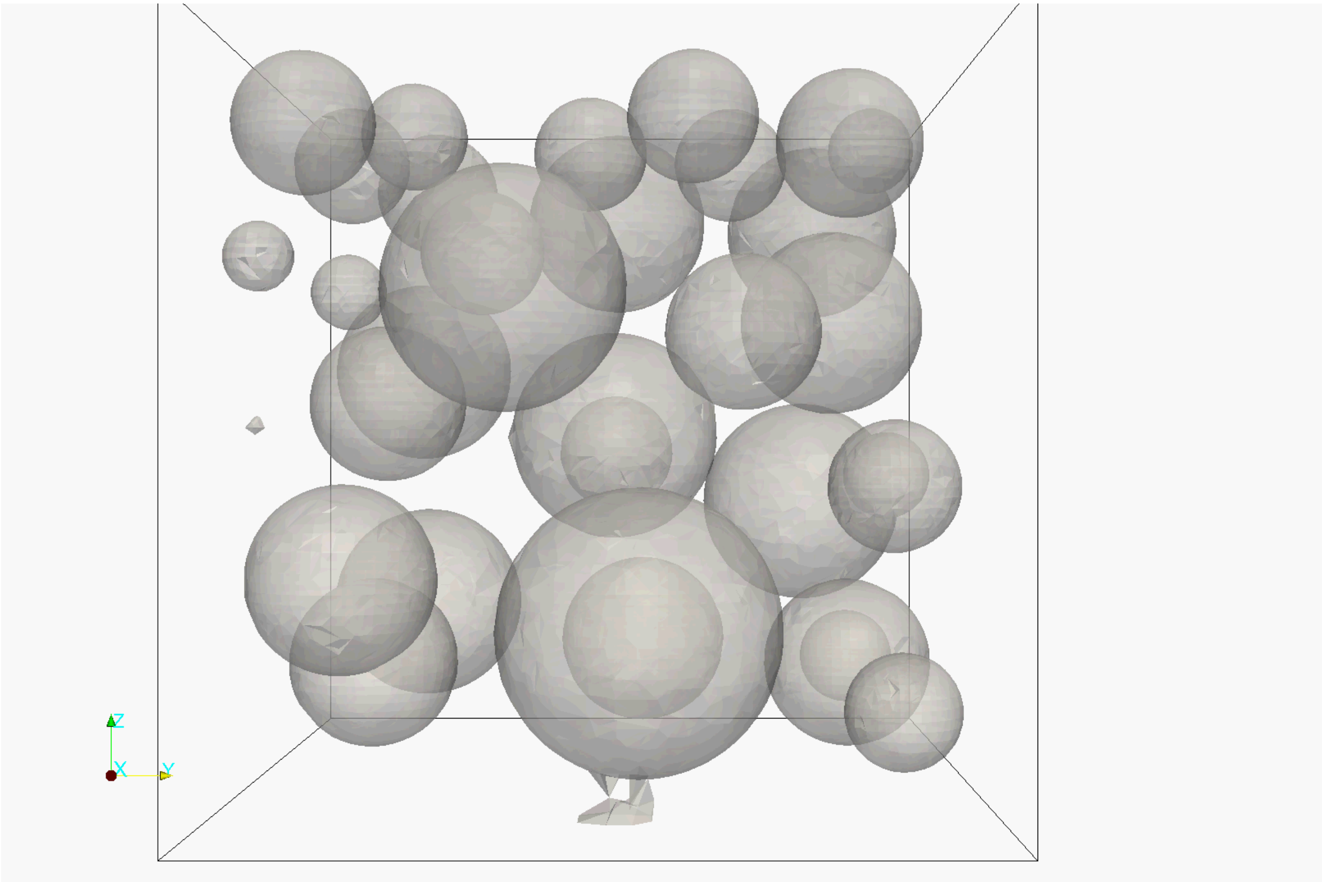
- Space partitioning algorithm
- Robust
- Negligible cost

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki. An efficient and parallel level set reinitialization method – Application to micromechanics and microstructural evolutions. *Applied Mechanical Modelling*, 39:23-24, 7291-7302, 2015

Numerical framework

Illustration of numerical capabilities

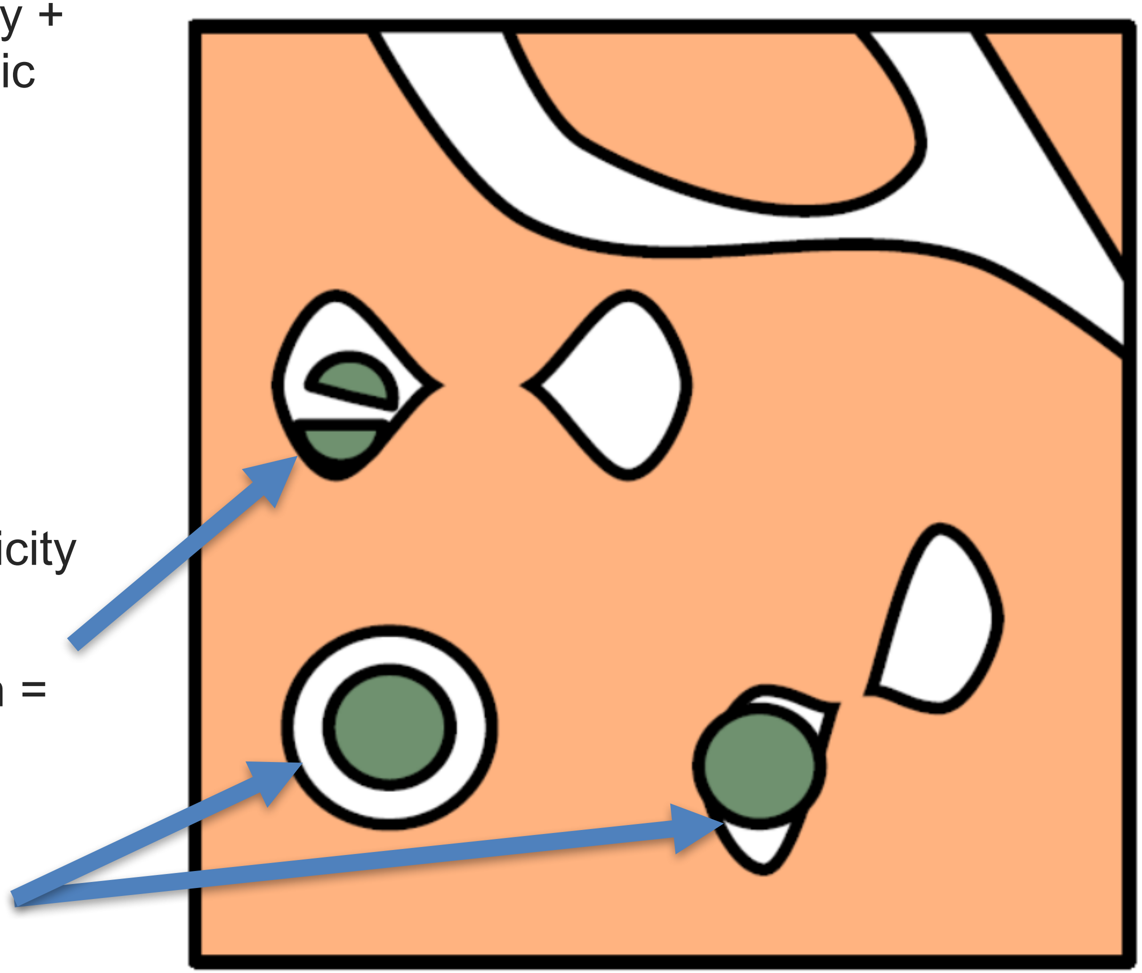
- Level-set method + explicit interfaces
- Geometric error based mesh refinement + level-set reinitialization
- Remeshing for large deformations & topological events



Outline

Micromechanical models

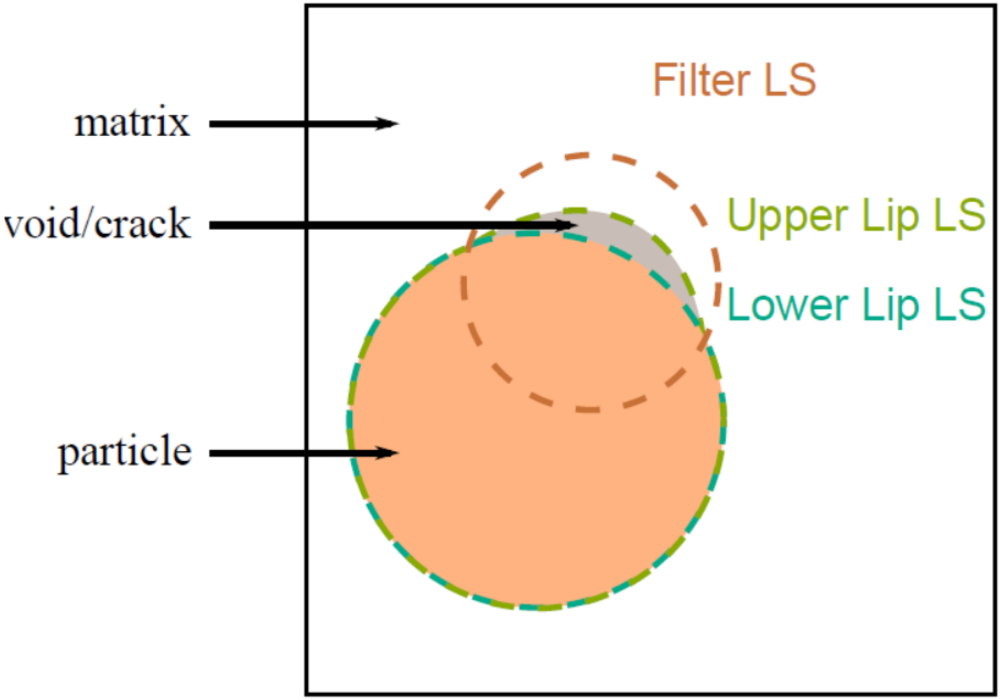
- Matrix = linear isotropic elasticity + von Mises plasticity with isotropic hardening
- Particles = linear isotropic elasticity
- Particles fragmentation criterion = maximum principal stress σ_1
- Particles debonding criterion = normal stress σ_n



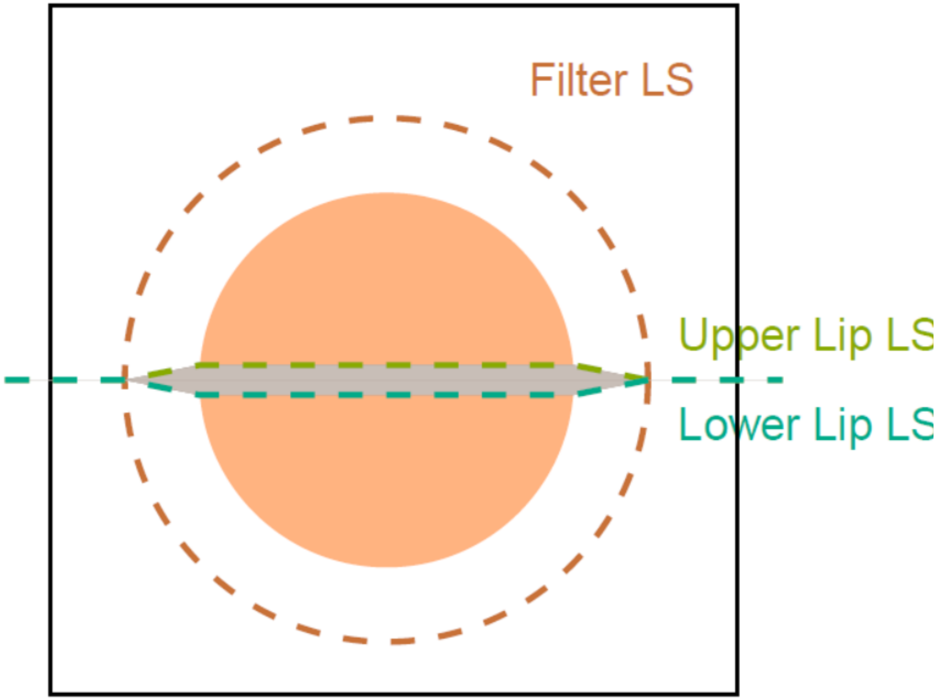
Fracture criteria

- Level-set functions to define crack geometry
- Dynamic meshing of new interfaces

Broken interface
Normal stress criterion

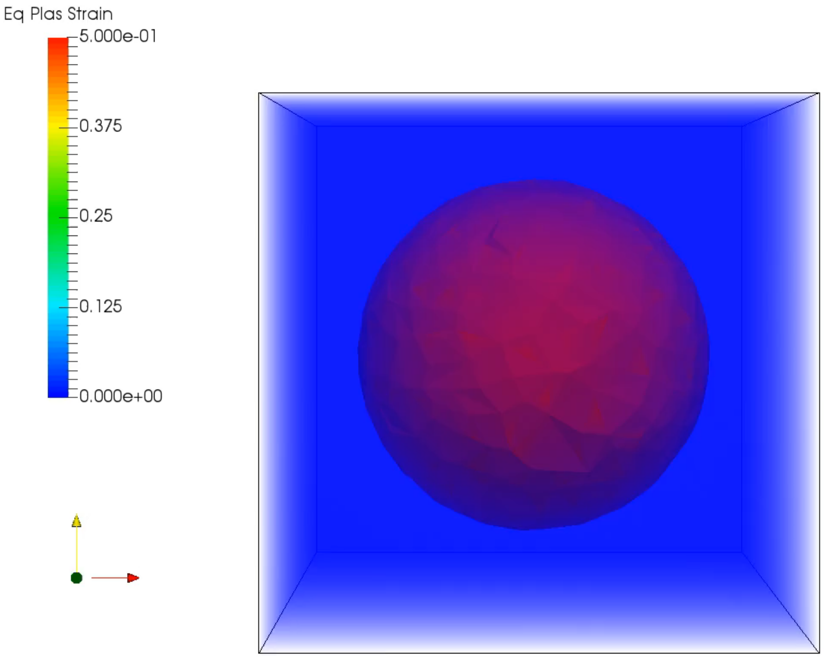


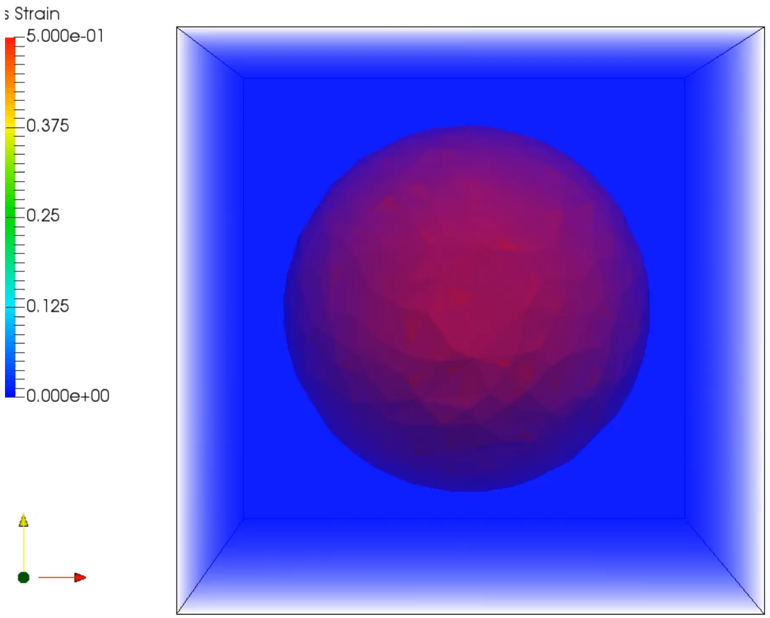
Broken inclusion
Maximum principal stress



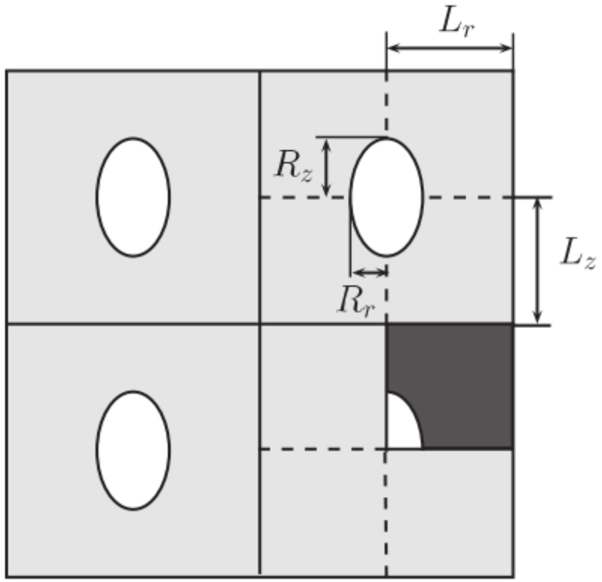
Unit cell simulations

- Single particle RVE, particle density ~ 20%
- Particle harder than matrix



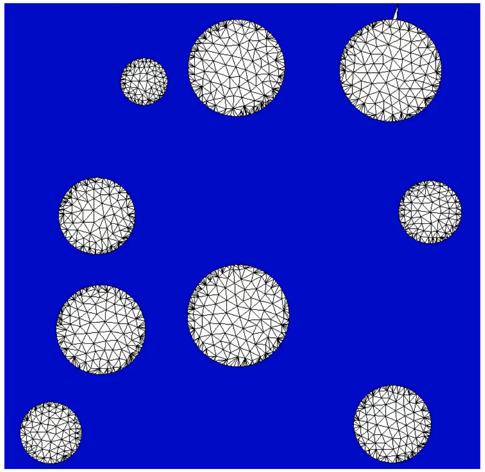


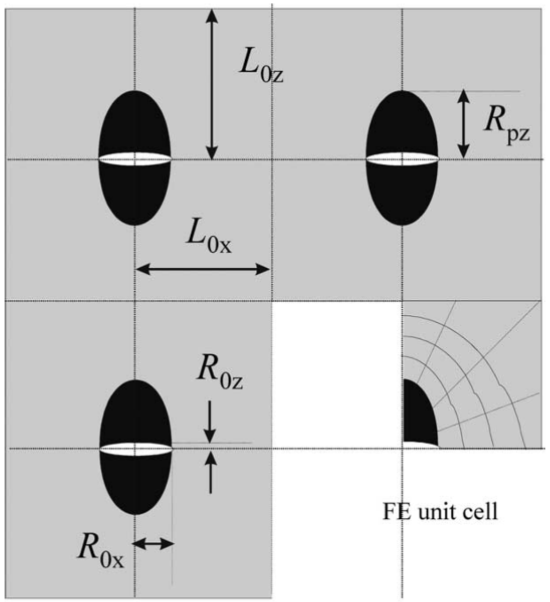
Multi-voids or multi-particles RVEs



[Lecarme *et al.*, *IJP*, 2011]

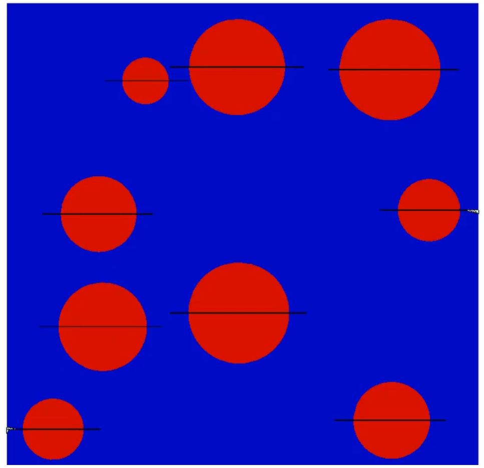
Voids instead of particles





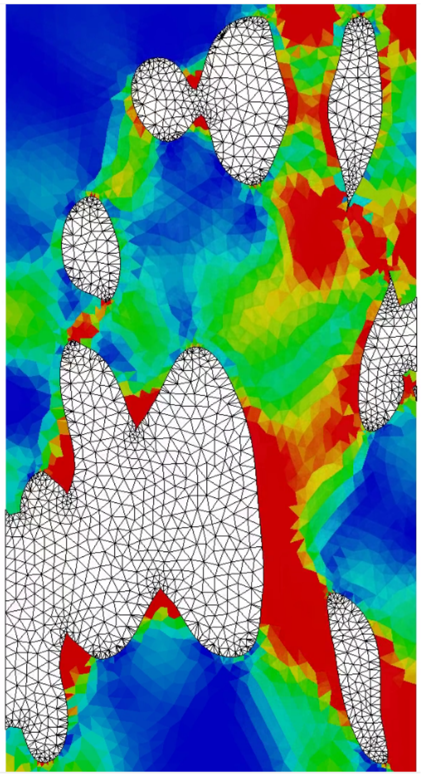
[D. Lassance *et al.*, *EFM*, 2006]

Pre-fragmented particles

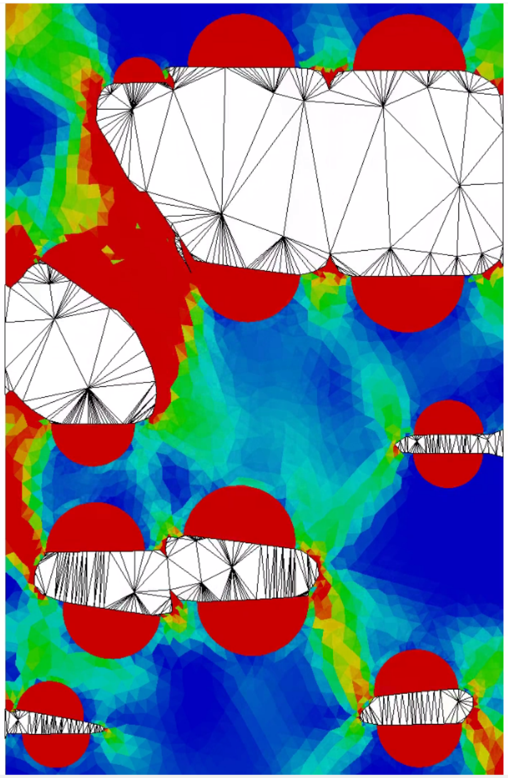


Importance of void nucleation modeling

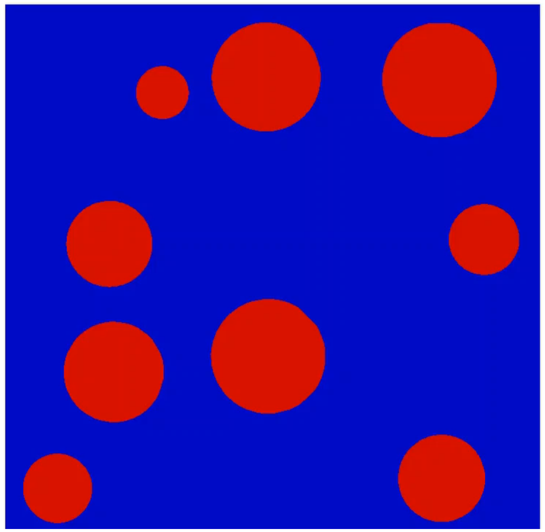
- Influence on micromechanisms



Voids instead
of particles



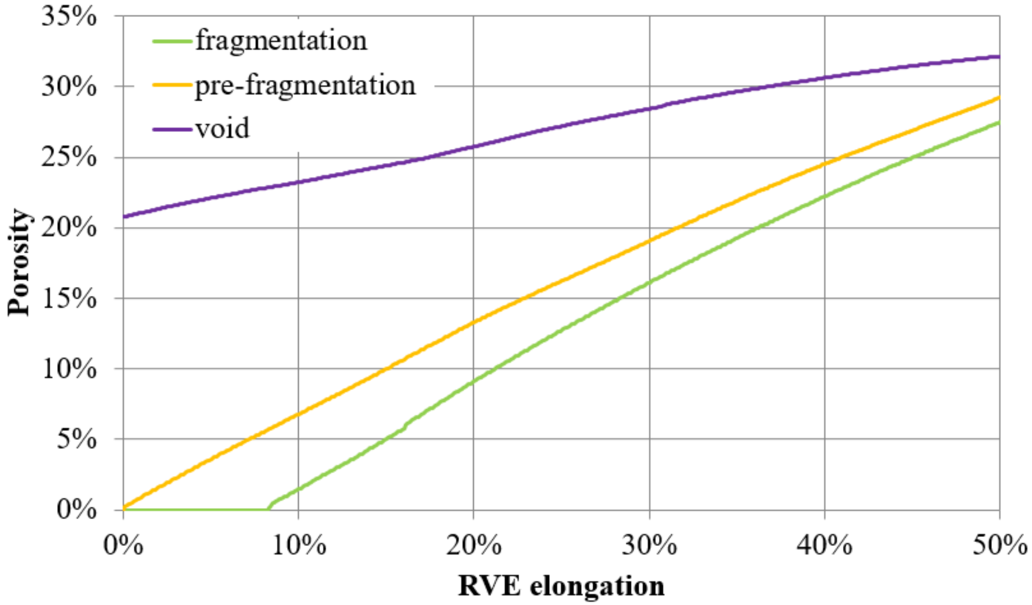
Pre-fragmented
particles

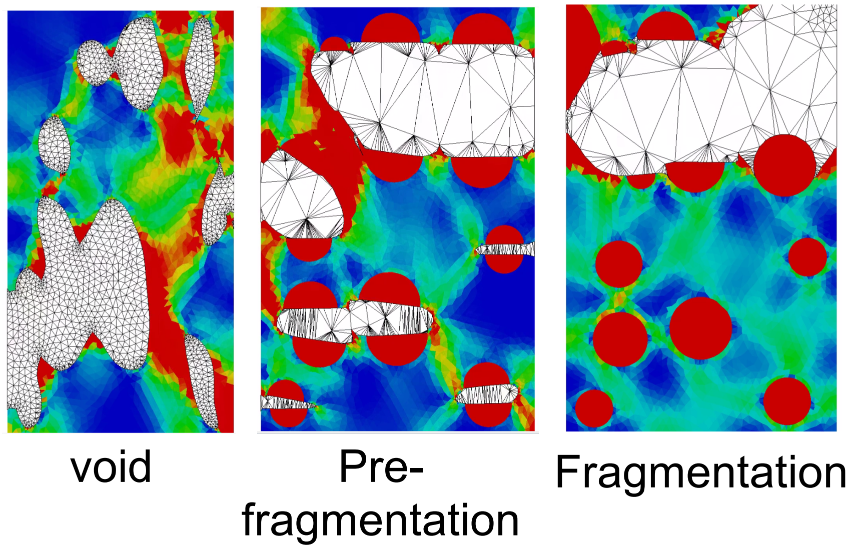


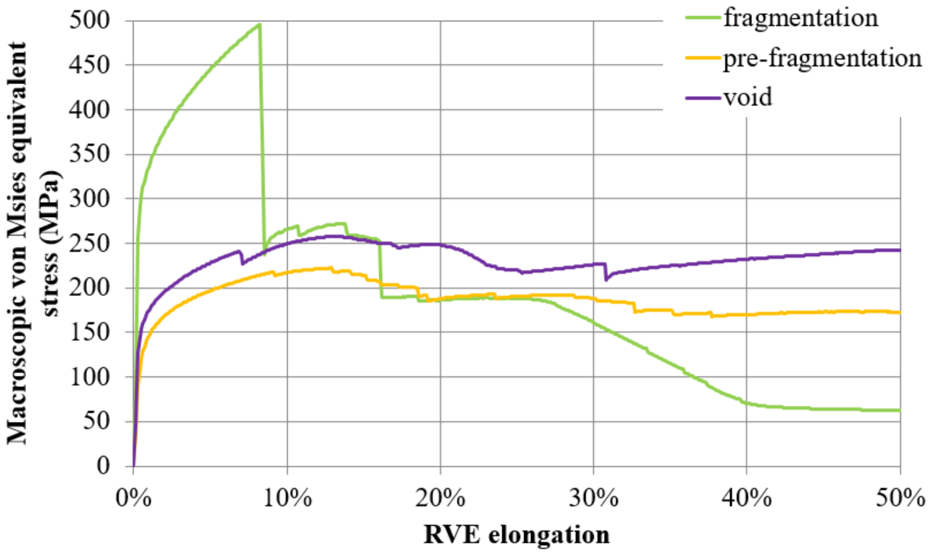
Fragmentation
criterion

Importance of void nucleation modeling

- Influence on macroscopic quantities of interest



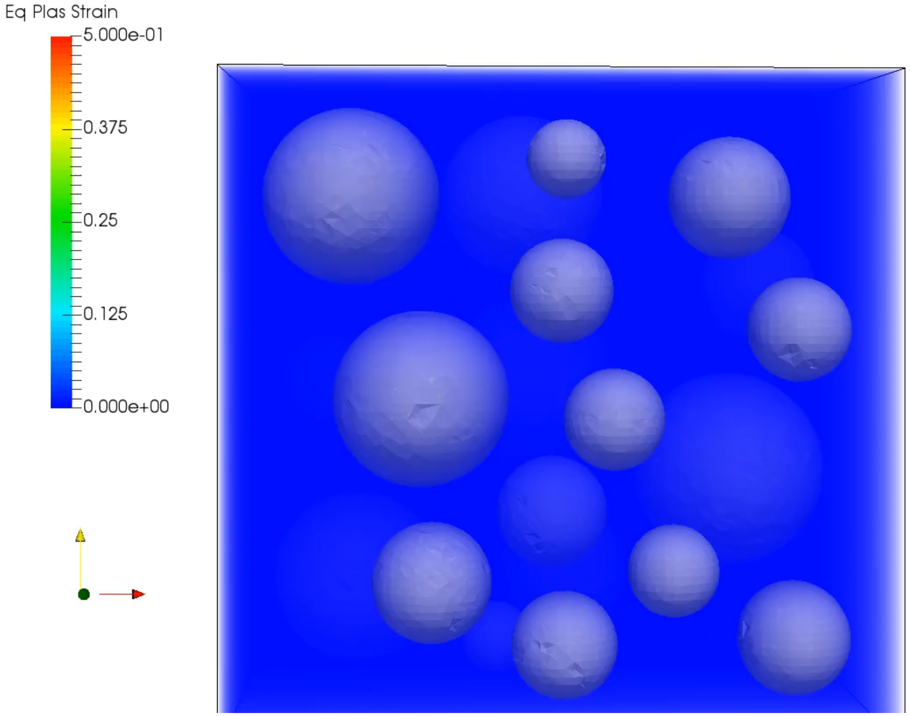


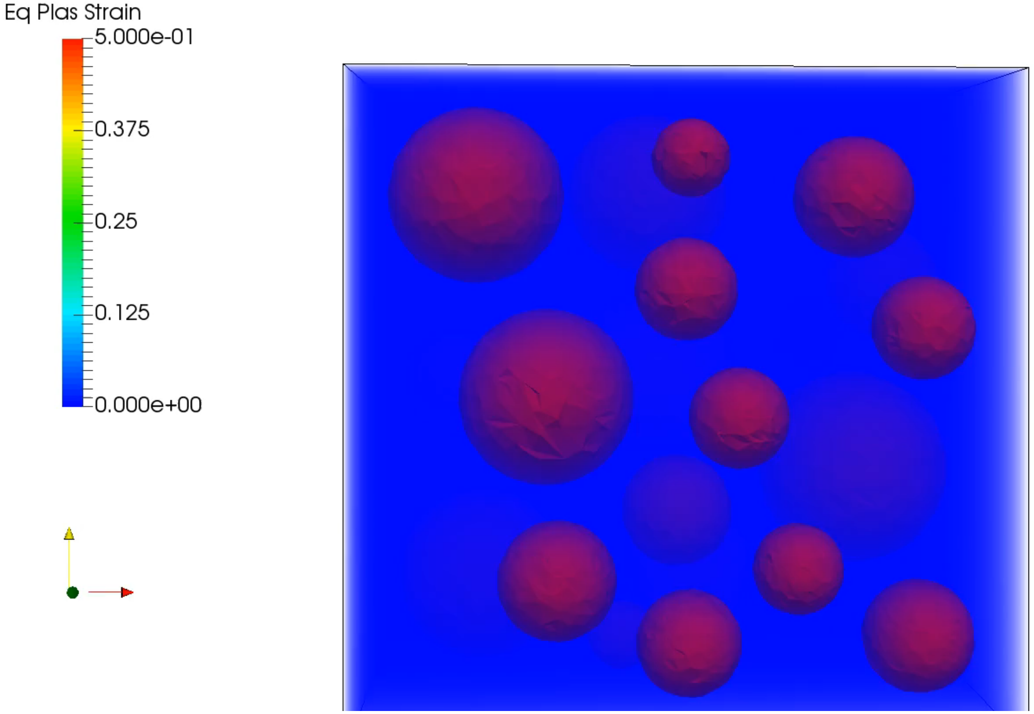


- Strength underestimated for small plastic strain
- Ductility overestimated for large plastic strains

Importance of void nucleation modeling

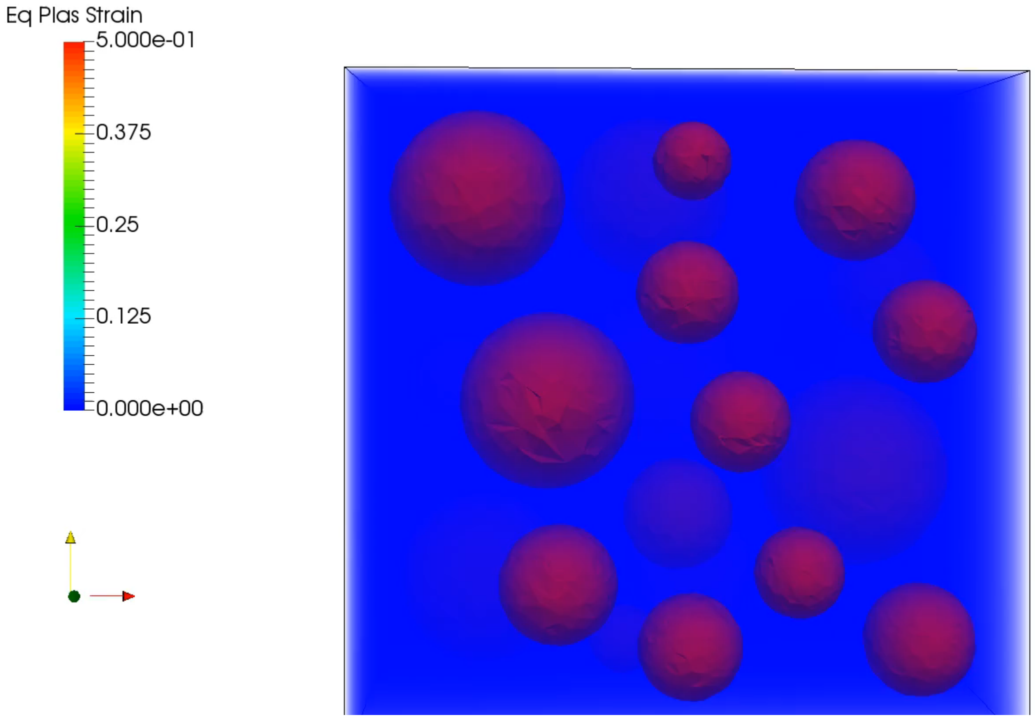
- RVE size 165 µm, 33 voids, vertical tension, macroscopic stress triaxiality ratio 0.33





Conclusions on unit cell calculations

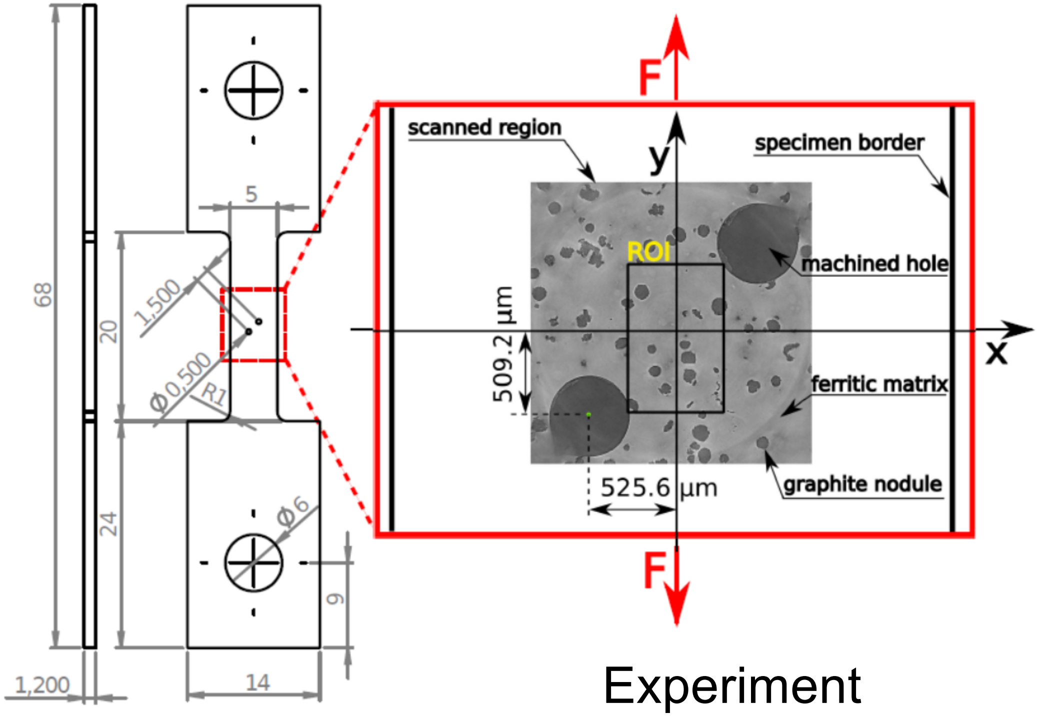
- Unit cell simulations accounting for
  - Large microstructures
  - Random sizes
  - Random arrangements
- Simulations revealed
  - Influence of particles on void growth
  - Influence of void nucleation on void coalescence
- Comparison with experiments require
  - Meshing real microstructures
  - Realistic boundary conditions
  - Local error measurements



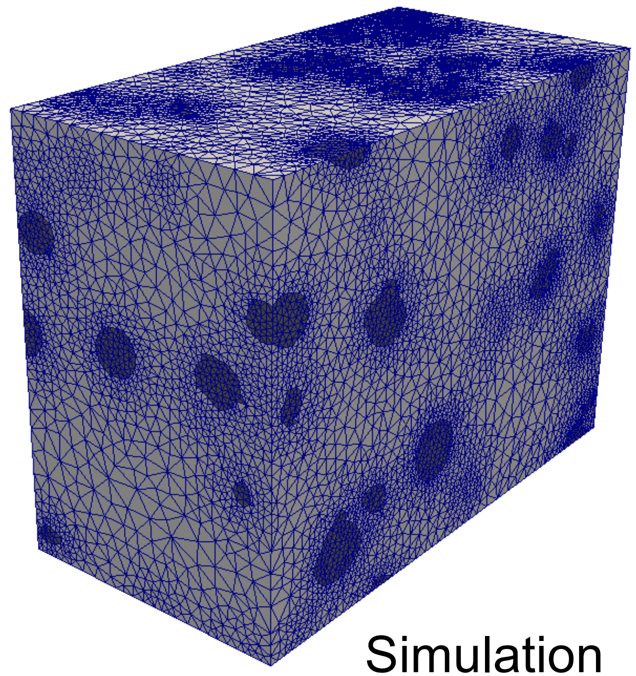
Outline

Validation of simulations

- Standard approach



Experiment

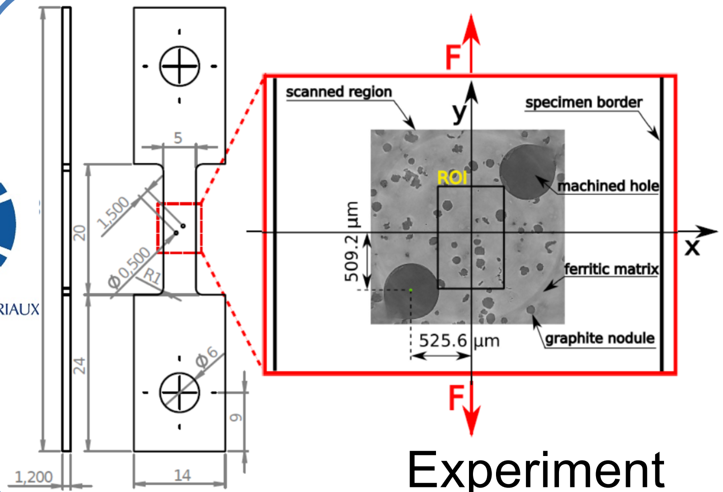


Simulation

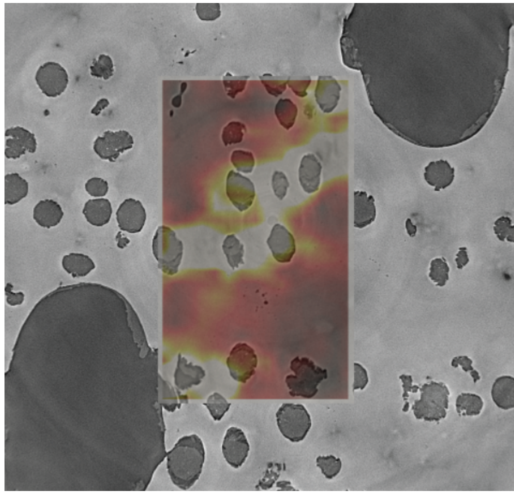
Boundary conditions?
Not periodic!
Not homogeneous!

Validation of simulations

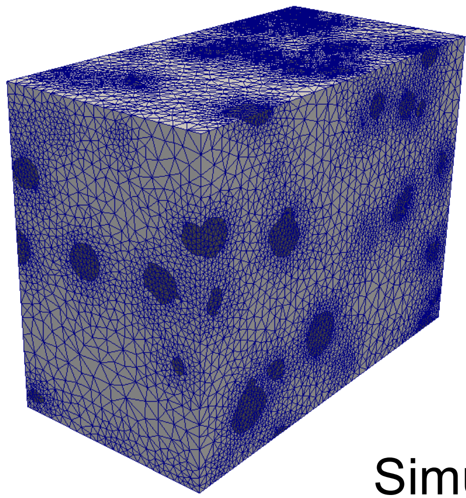
- Proposed approach



Experiment



Digital Volume Correlation

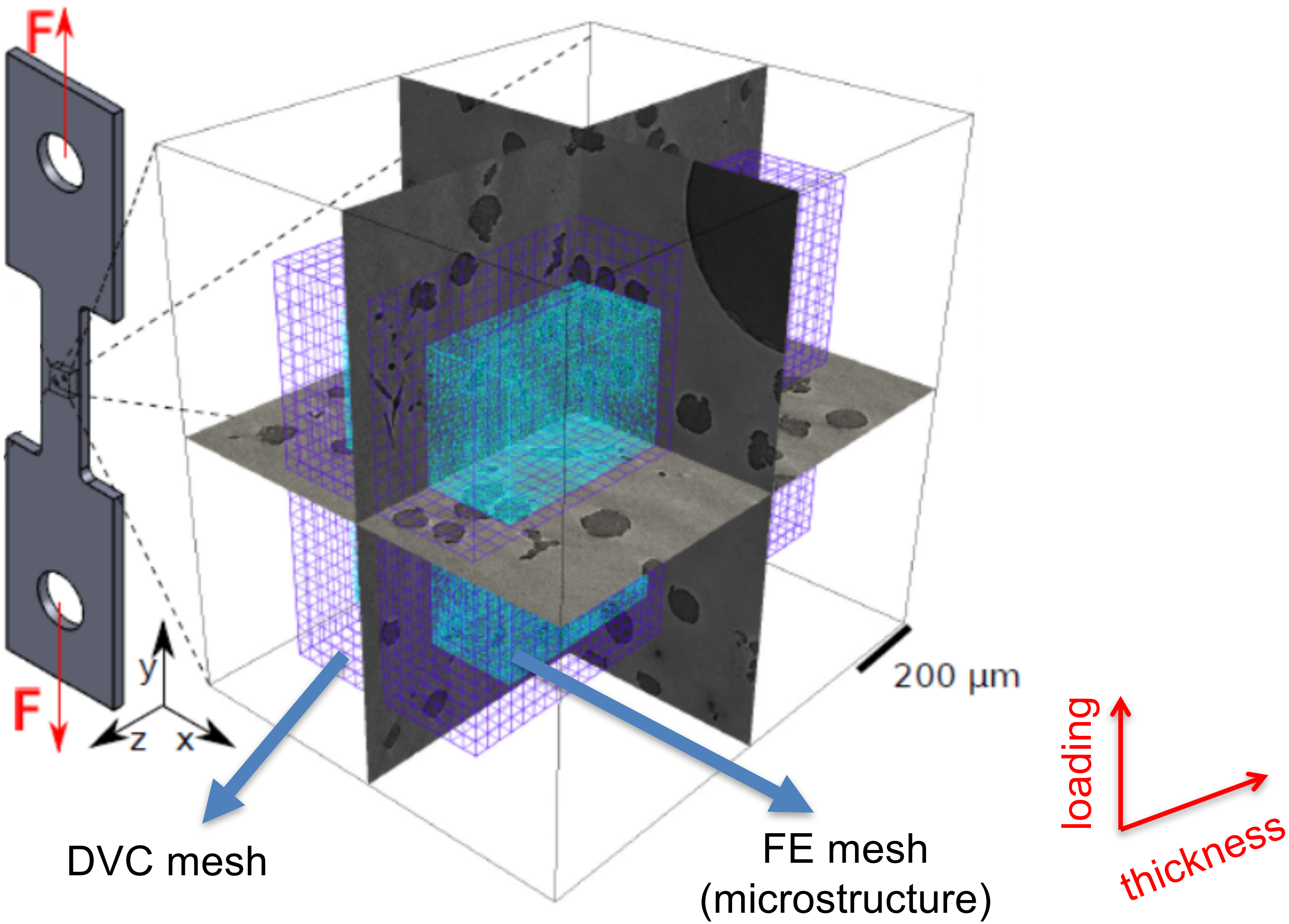


Simulation

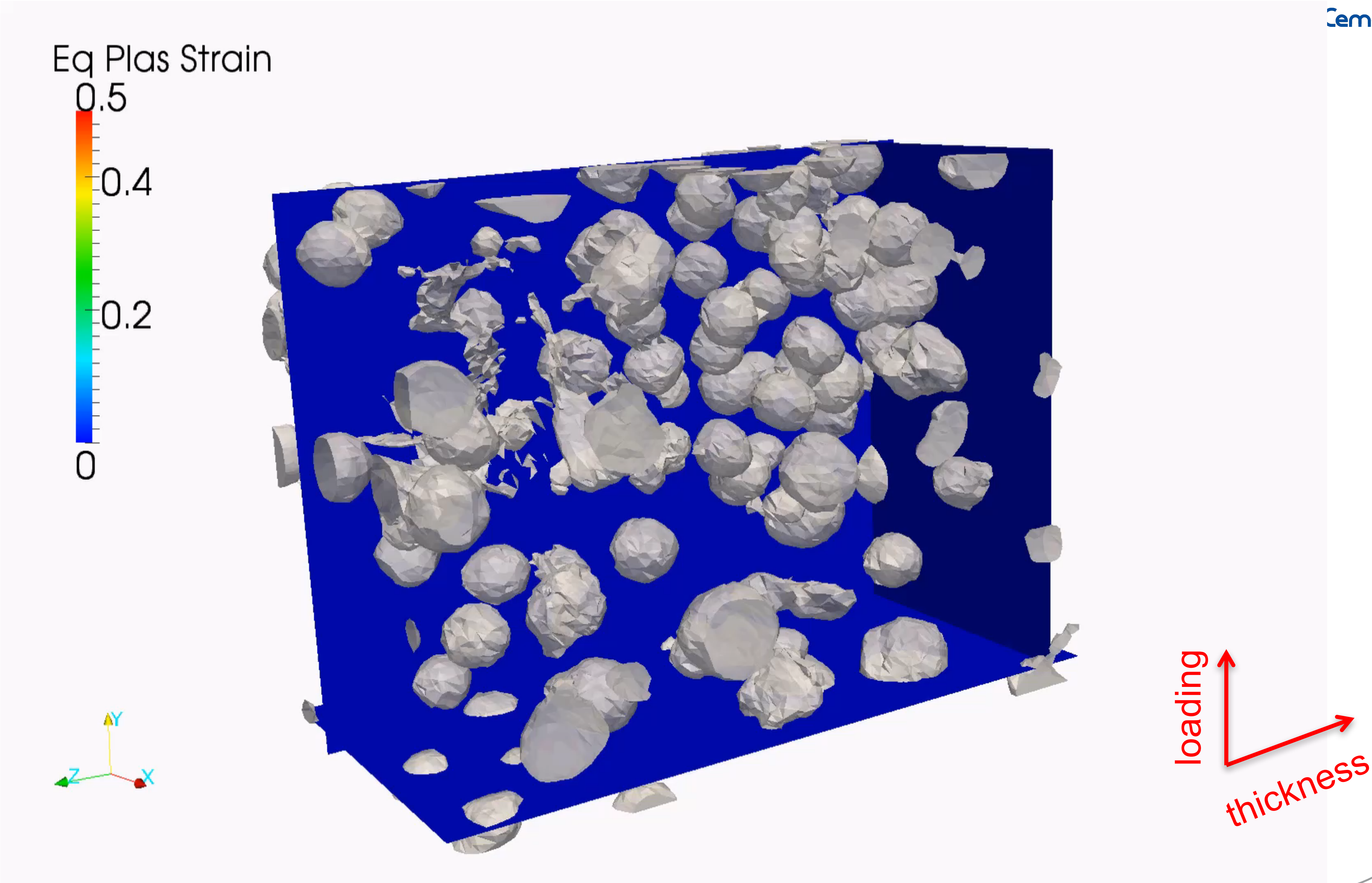
- Real microstructure meshed
- Measured boundary conditions
- Local error measurements between simulations and experiments

A. Buljac, M. Shakoor, J. Neggers, M. Bernacki, P.-O. Bouchard, L. Helfen, T. F. Morgeneyer, F. Hild. Numerical Validation Framework for Micromechanical Simulations based on Synchrotron 3D Imaging, Computational Mechanics, Submitted, 2016

DVC-measured boundary conditions

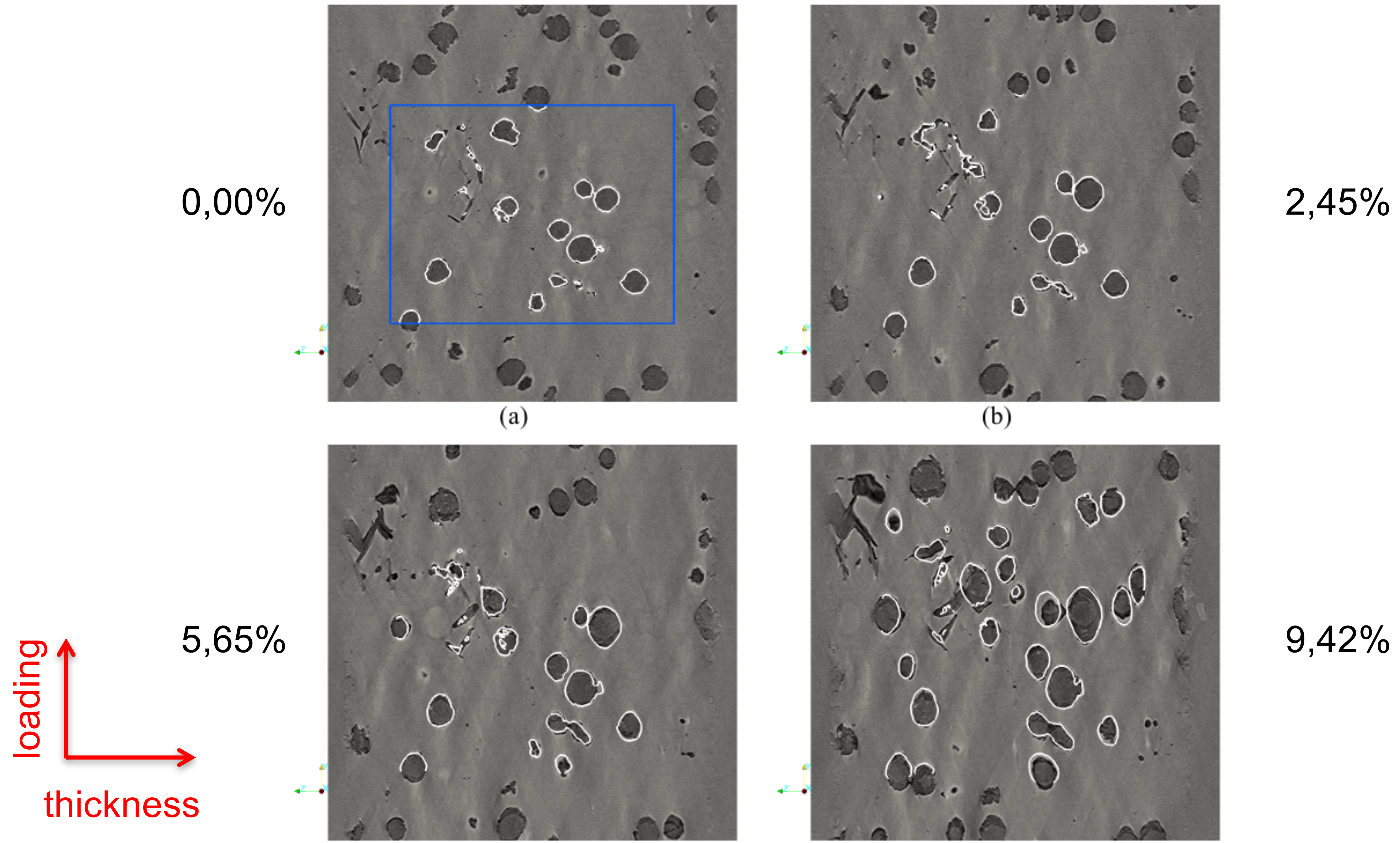


Validation of simulations based on 3D imaging



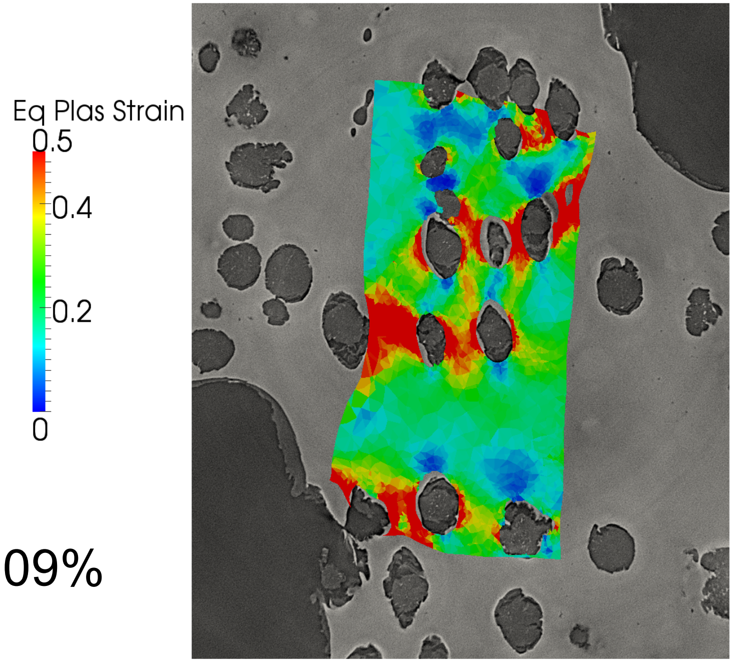
M. Shakoor, A. Buljac, J. Neggers, F. Hild, T. F. Morgeneyer , L. Helfen, M. Bernacki, P.-O. Bouchard. On the choice of boundary conditions for micromechanical simulations based on synchrotron 3D imaging, *IJSS*, Submitted, 2016

Validation of simulations based on 3D imaging



(a) (b) (c) (d)

Validation of simulations based on 3D imaging



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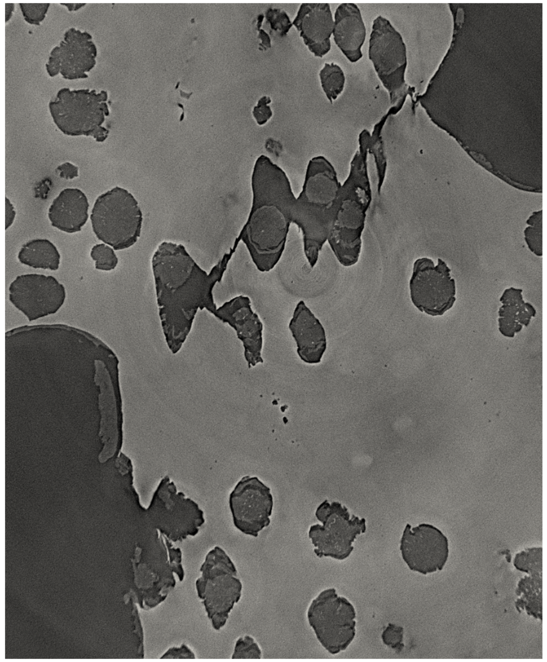

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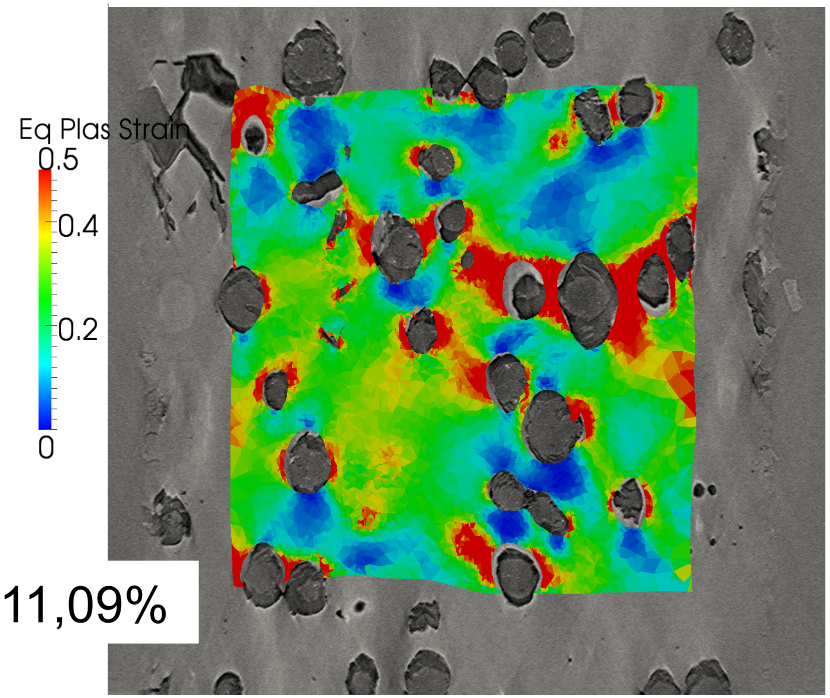

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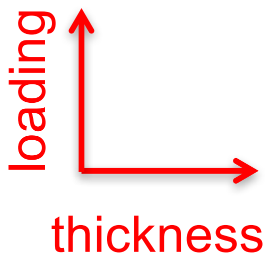
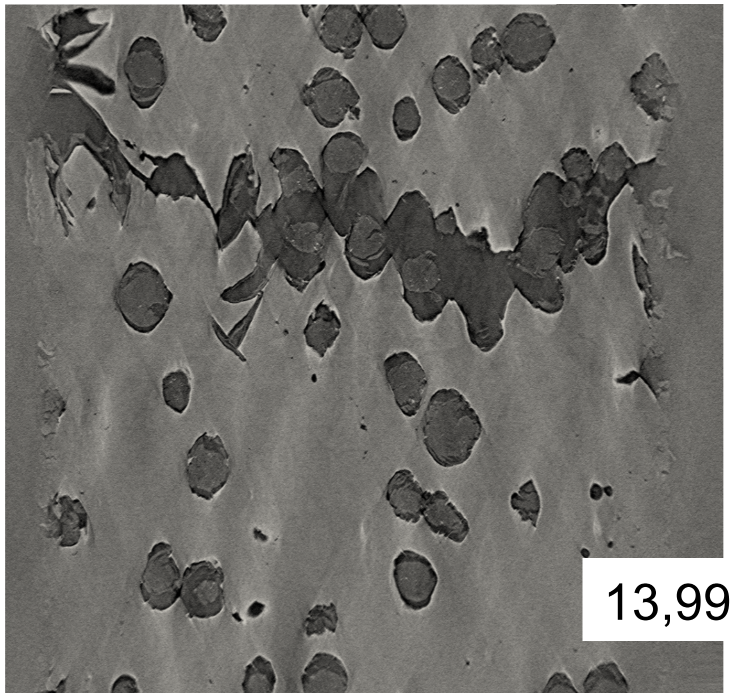




13,99%

Outline

1. Literature review
   - Damage models
   - Micromechanics
2. Numerical framework
   - Level-Set method
   - Mesh adaptation method
3. Void nucleation and growth
   - Micromechanical models
   - Fracture criteria
   - RVE simulations
4. Void growth and coalescence
   - Meshing real microstructures
   - Applying measured boundary conditions
5. Conclusions and outlook

Conclusions

Numerical methods

- New remesher: explicit interfaces with large deformations
- New level-set reinitialization method
- Large 3D microstructures Parallel computing
- Crack initiation and propagation

Ductile fracture applications

- Random particle size and arrangement
- Void nucleation modeling
- Large plastic strains, void growth & coalescence
- Real microstructures
- DVC-measured boundary conditions

Outlook

○ Prospects

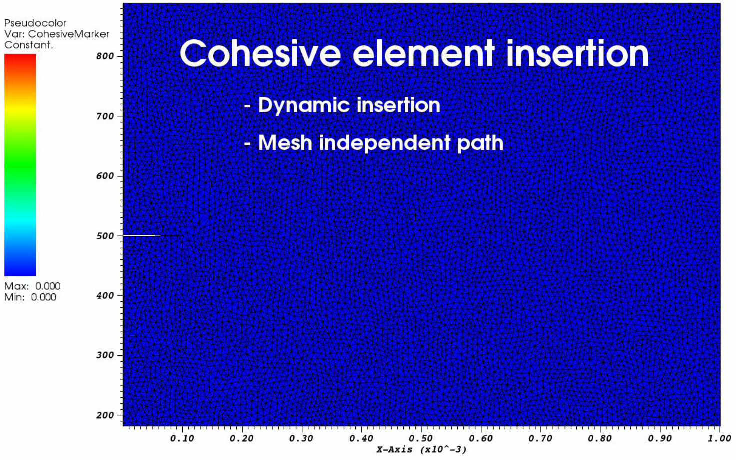
- Identification of material parameters
- Constitutive models for matrix and particles

○ Prospects: PhD of Victor Navas (2015-2018)

- Non local GTN damage model in the matrix
- Influence of non-monotonic loading paths

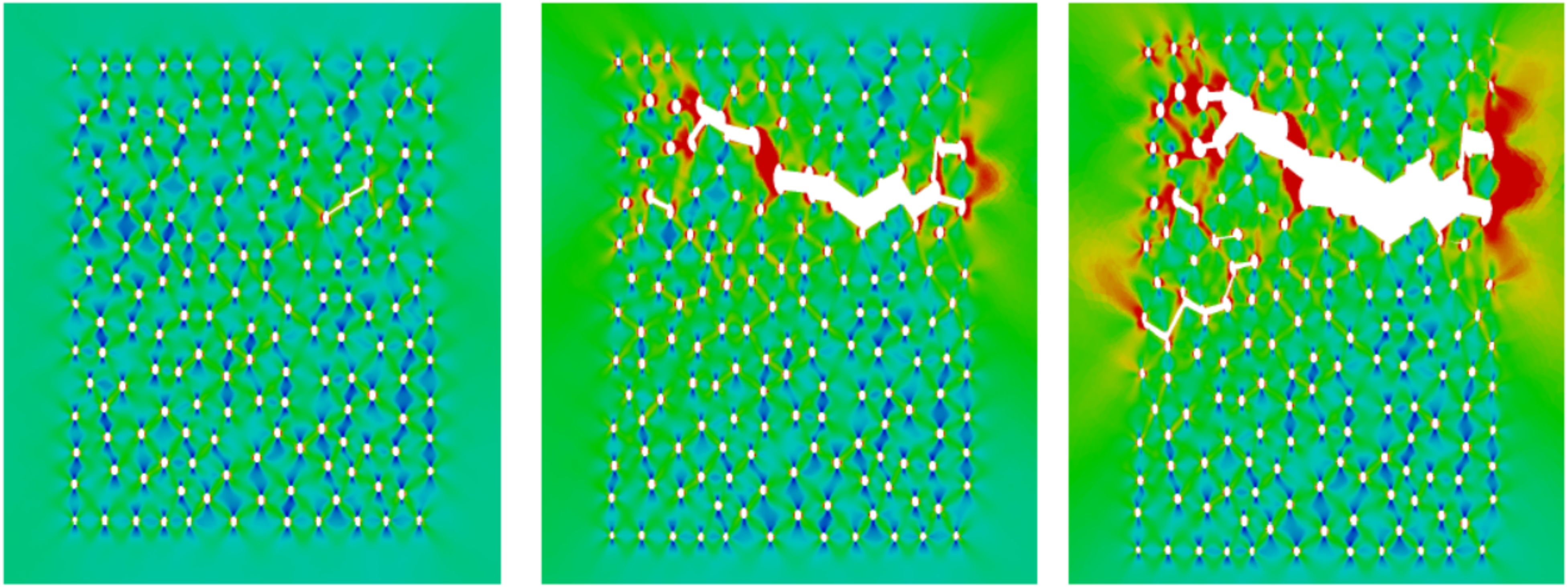
○ Prospects: work of Daniel Pino Muñoz

- Dynamically inserted cohesive zone elements
- Particle debonding & fragmentation
- To be coupled to present developments and tested in 3D



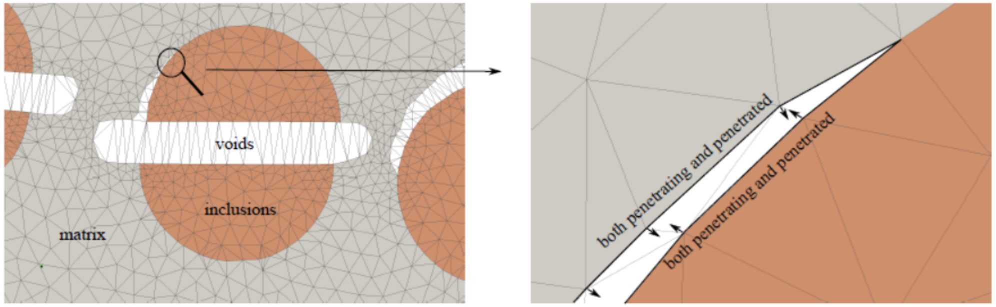
Matrix micro-cracking

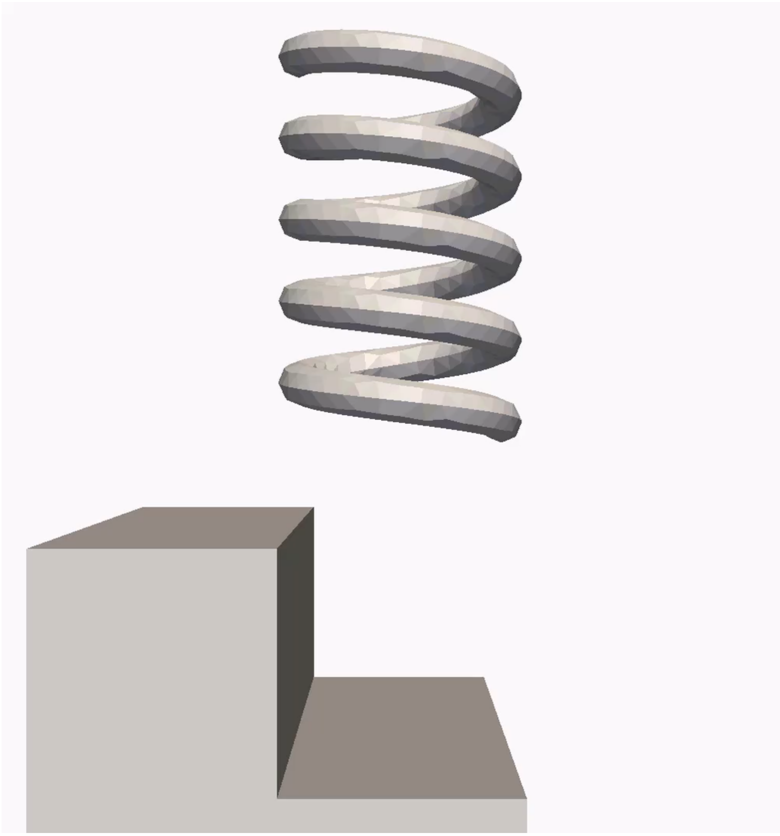
- Model the damage-to-fracture transition with matrix micro-cracking criteria
- Present developments to be extended to 3D and validated against experiments

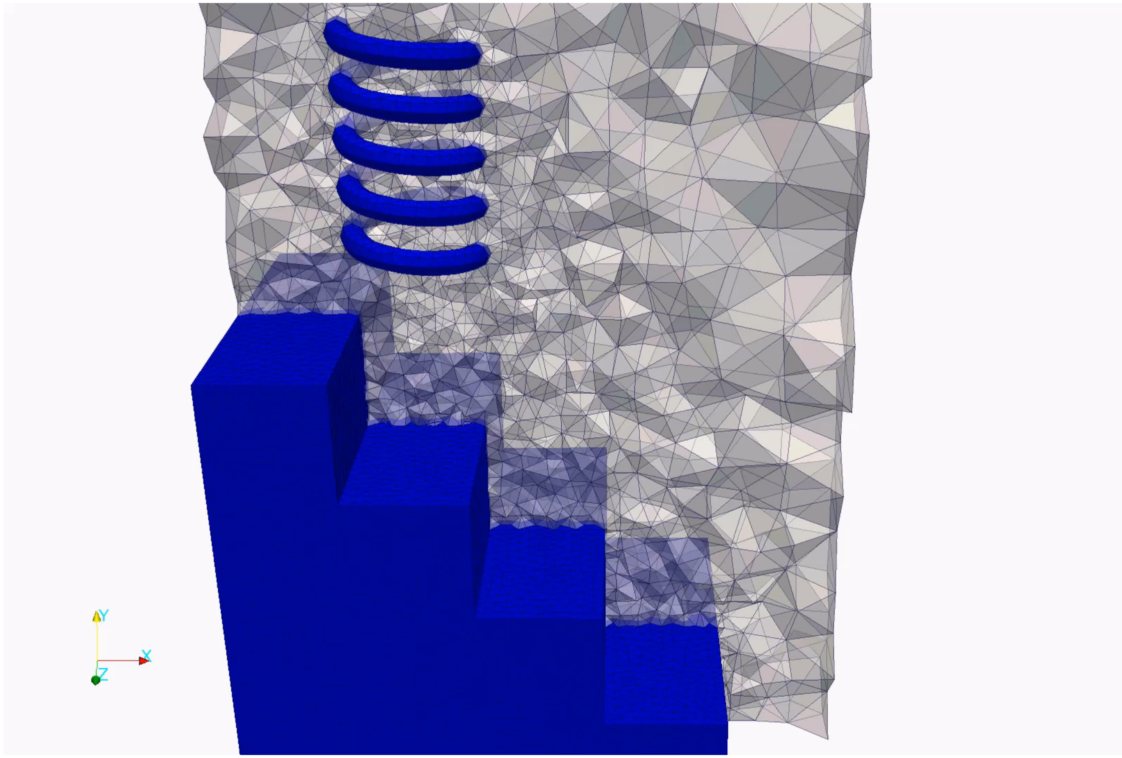


Contact mechanics

- Handling contact events between crack lips
- New and very promising contact detection algorithm
- Contact formulation to be improved

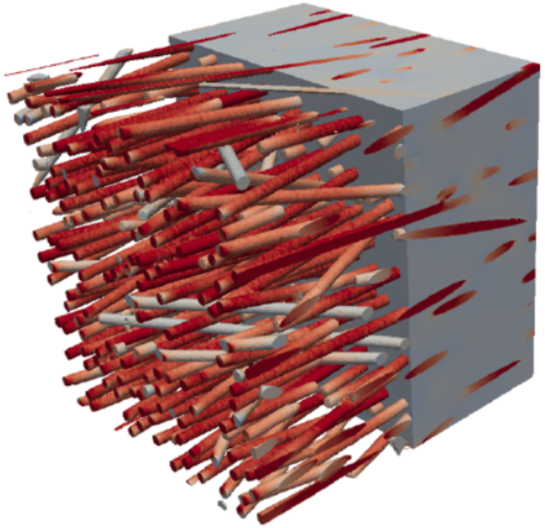


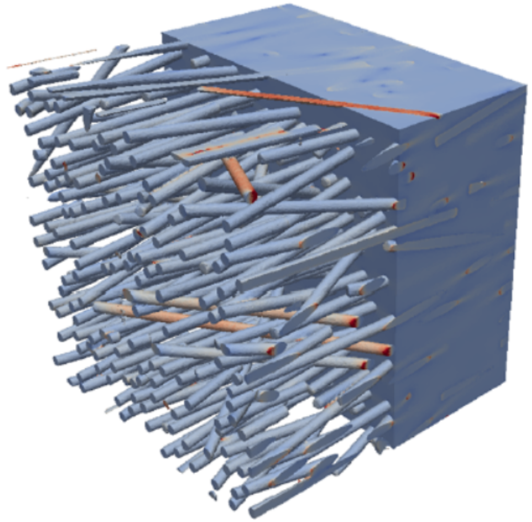




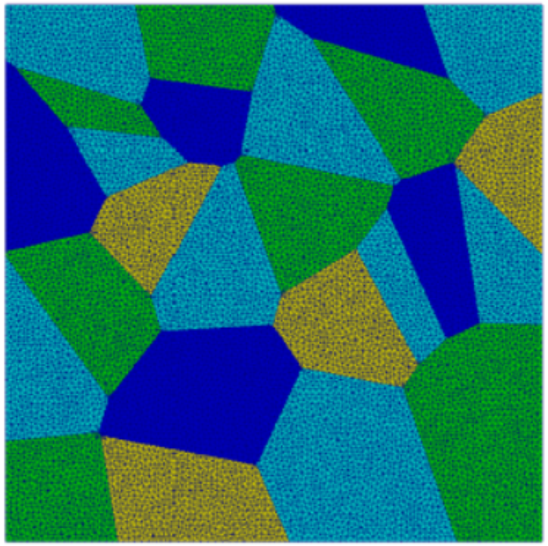
Other materials

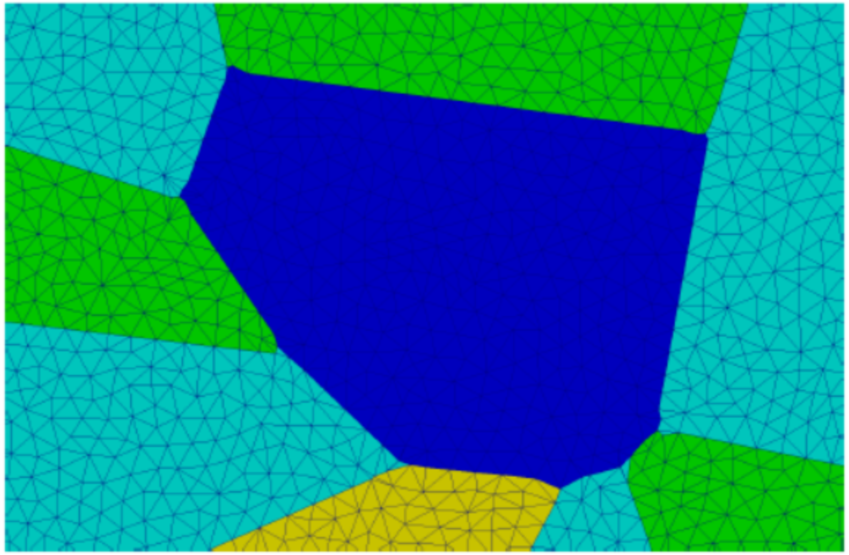
- Fiber-reinforced polymer composites (work of Ivan Coppo - 2016)





- Polycrystals





B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki. New finite element developments for the full field modeling of microstructural evolutions. *Computational Materials Science*, 109, 388-398, 2015

Cemef

MINES ParisTech

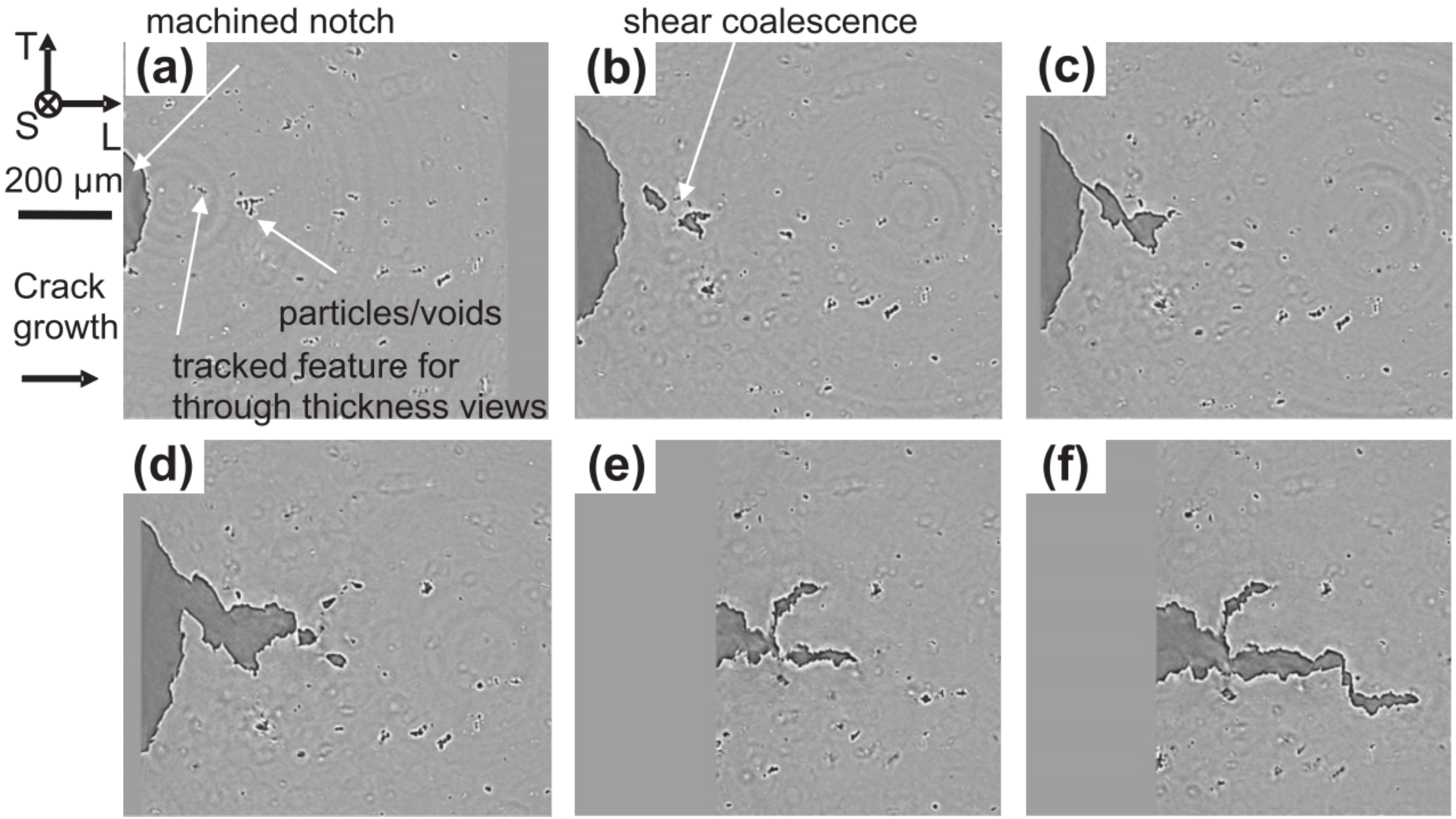
PROJET FINANCÉ PAR L'ANR - PROJECT FUNDED BY THE ANR

ANR

COMINSIDE

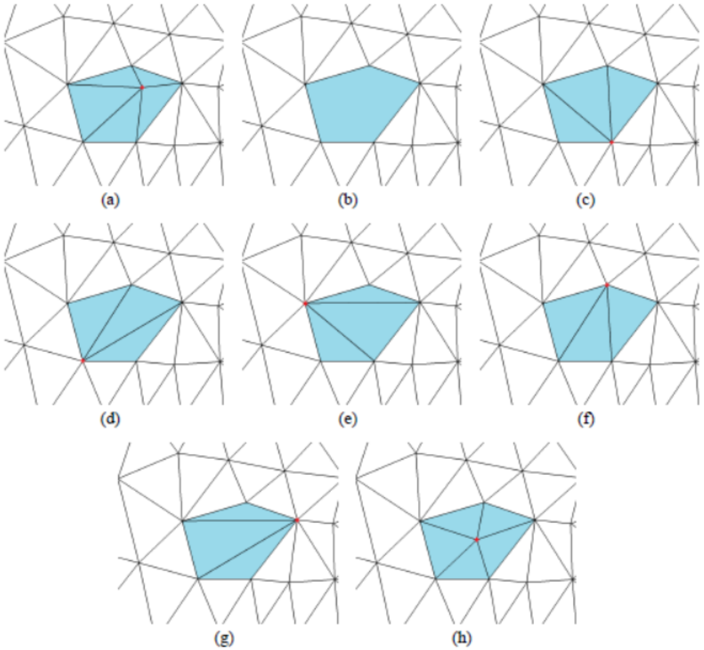
Ductile fracture

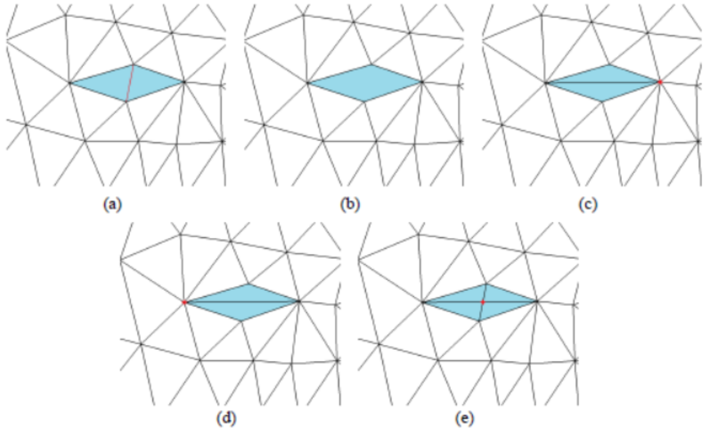
- Aluminum 2XXX alloy

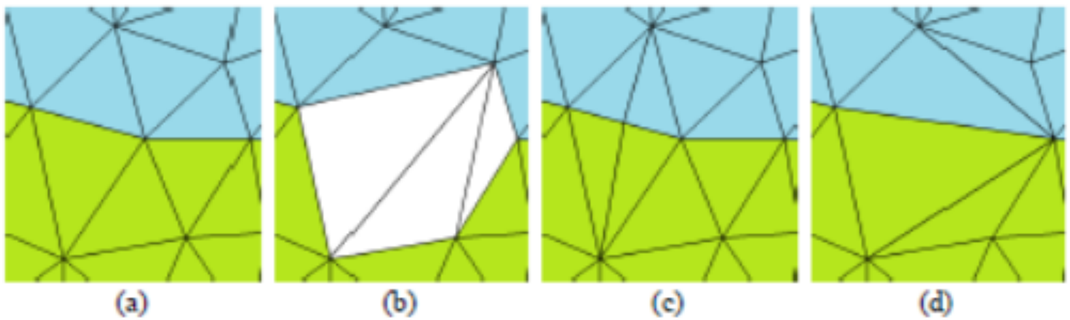


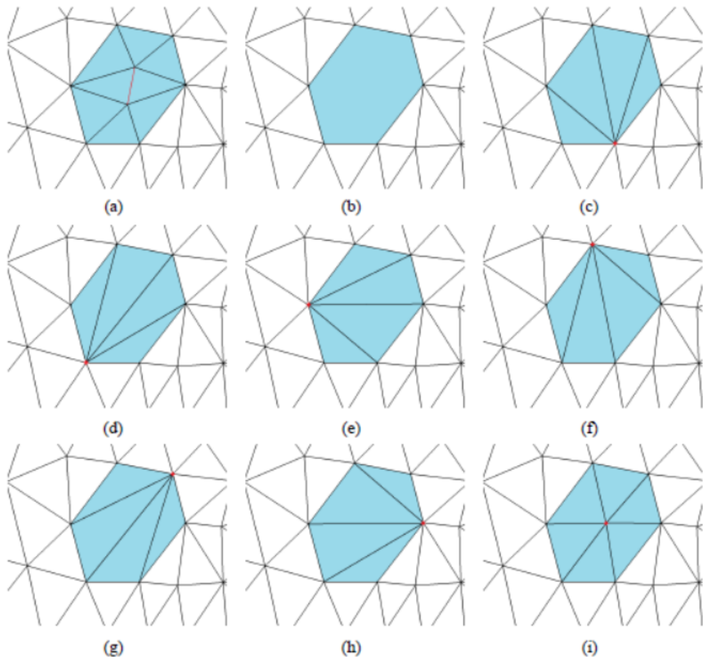
[T.F. Morgeneyer et al., *Scripta Materialia*, 2011]

Remeshing algorithm

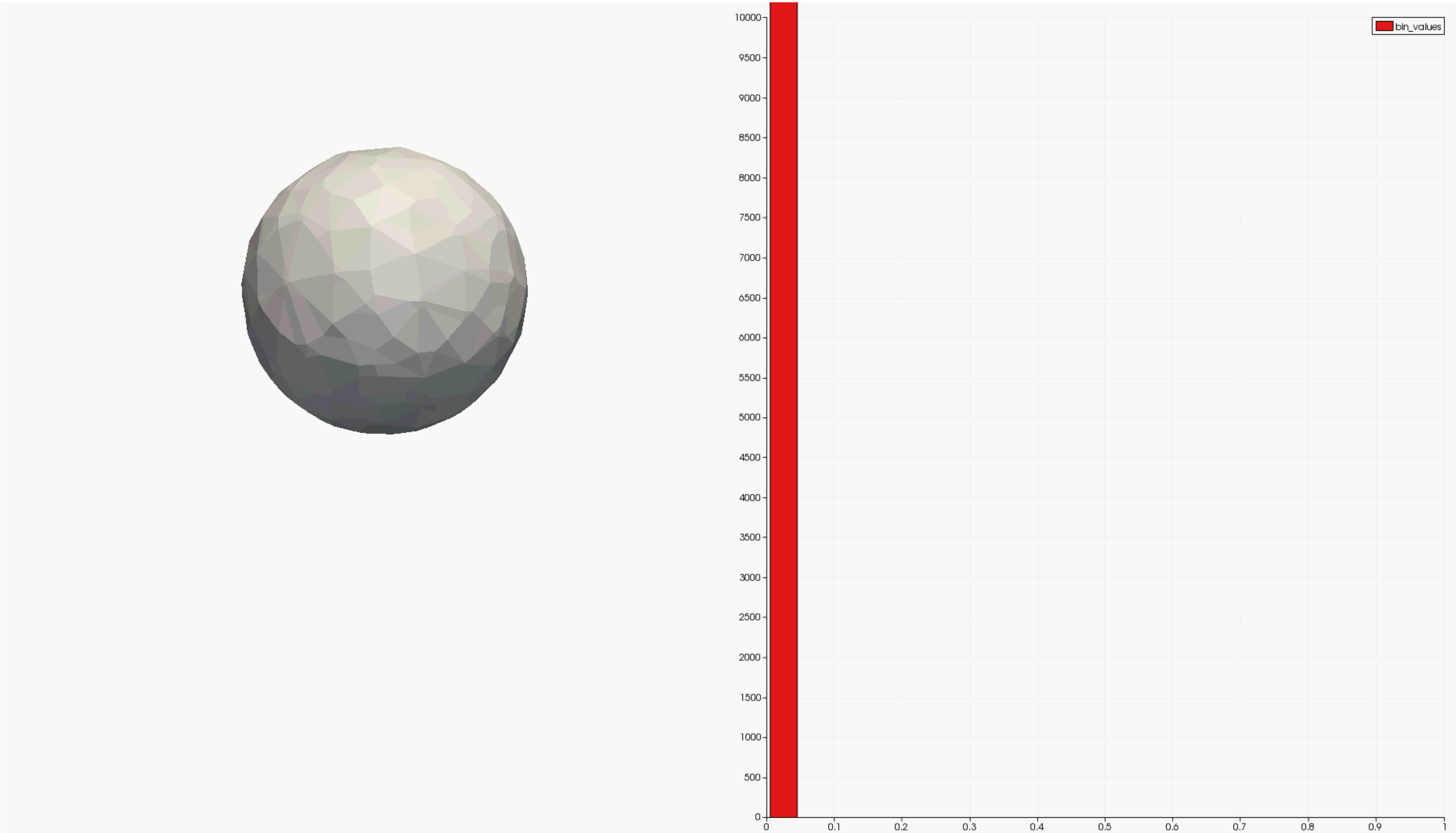








Complex topological events

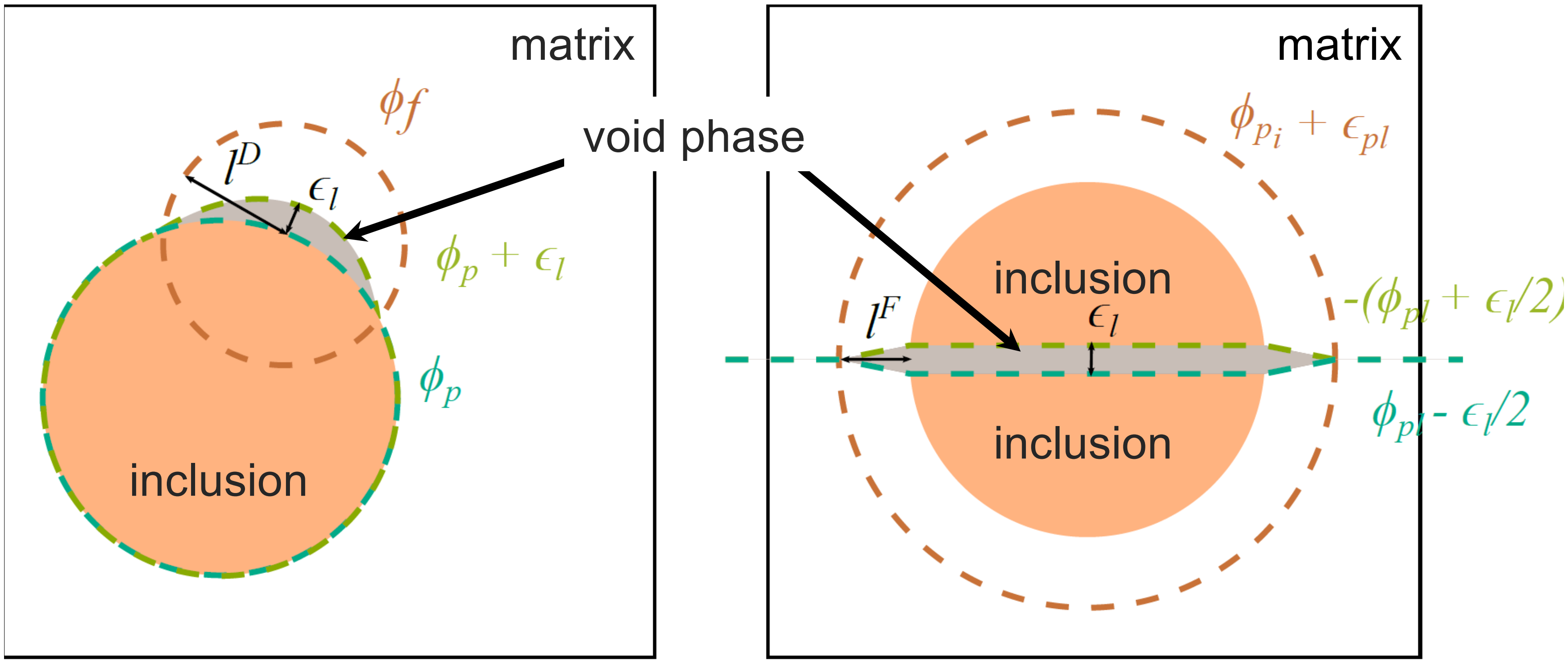


Particle debonding and fragmentation

- Filter level-set function to select elements affected by crack
- Crack lips level-set functions to introduce free surfaces
- Modifies level-set functions associated to the matrix, voids and particles

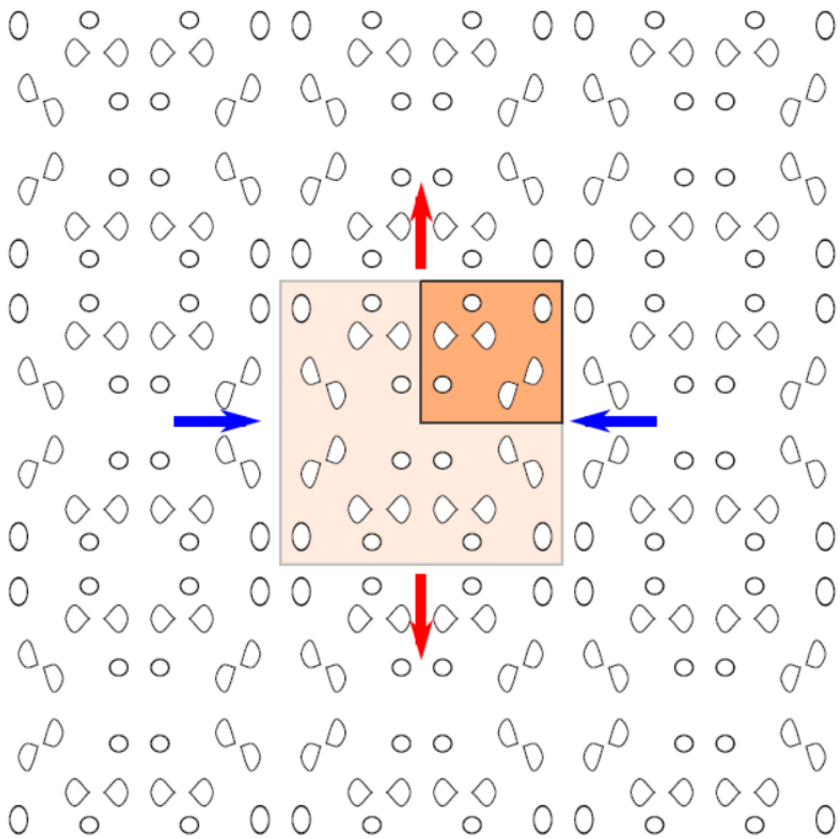
Broken interface
Normal stress criterion

Broken inclusion
Maximum principal stress



Boundary conditions for RVE simulations

- Periodic boundary conditions
- Axisymmetric loading
- Imposed macroscopic **strain** and **stress triaxiality ratio**
- Macroscopic = averaged on the Representative Volume Element (RVE)



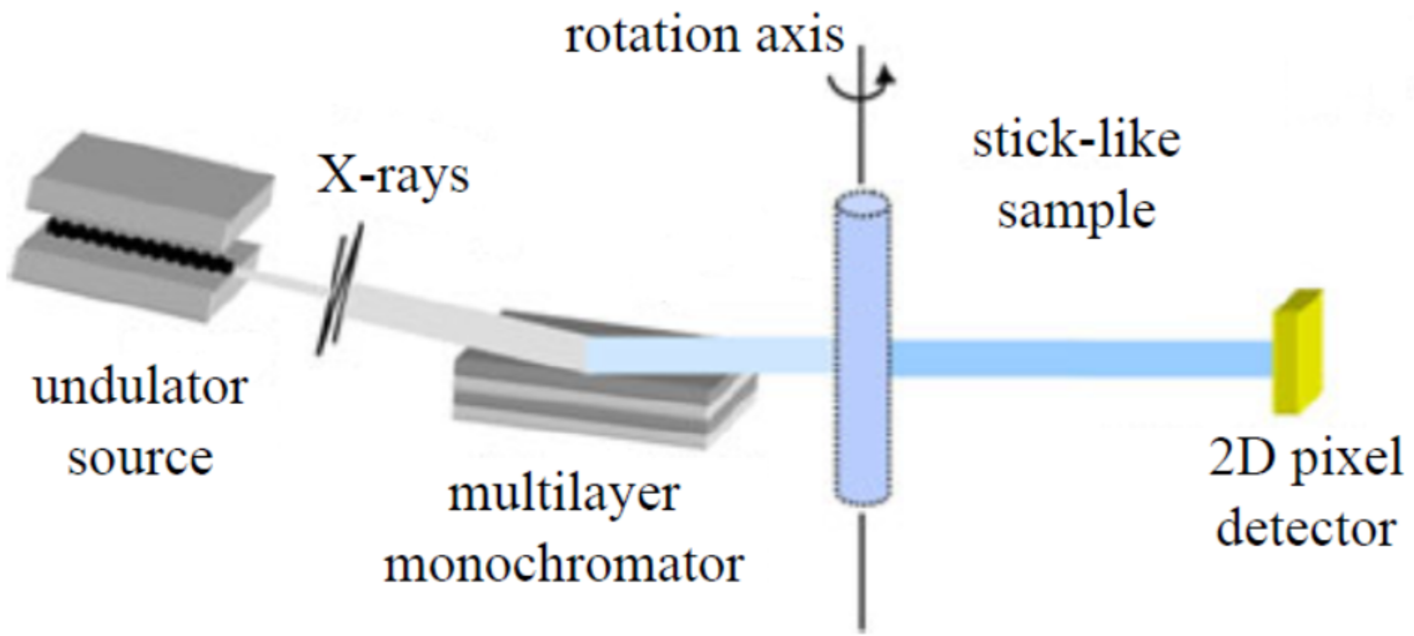
macroscopic stress triaxiality ratio

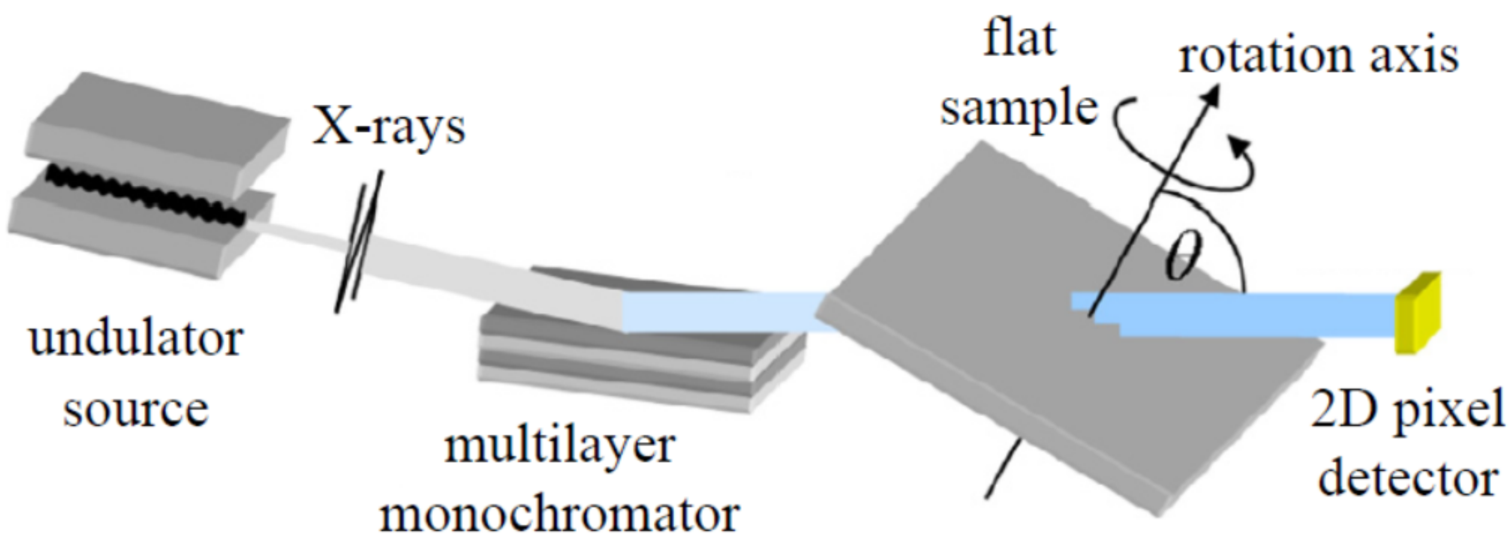
mean macroscopic stress

$$\eta = \frac{\Sigma_m}{\overline{\Sigma}}$$

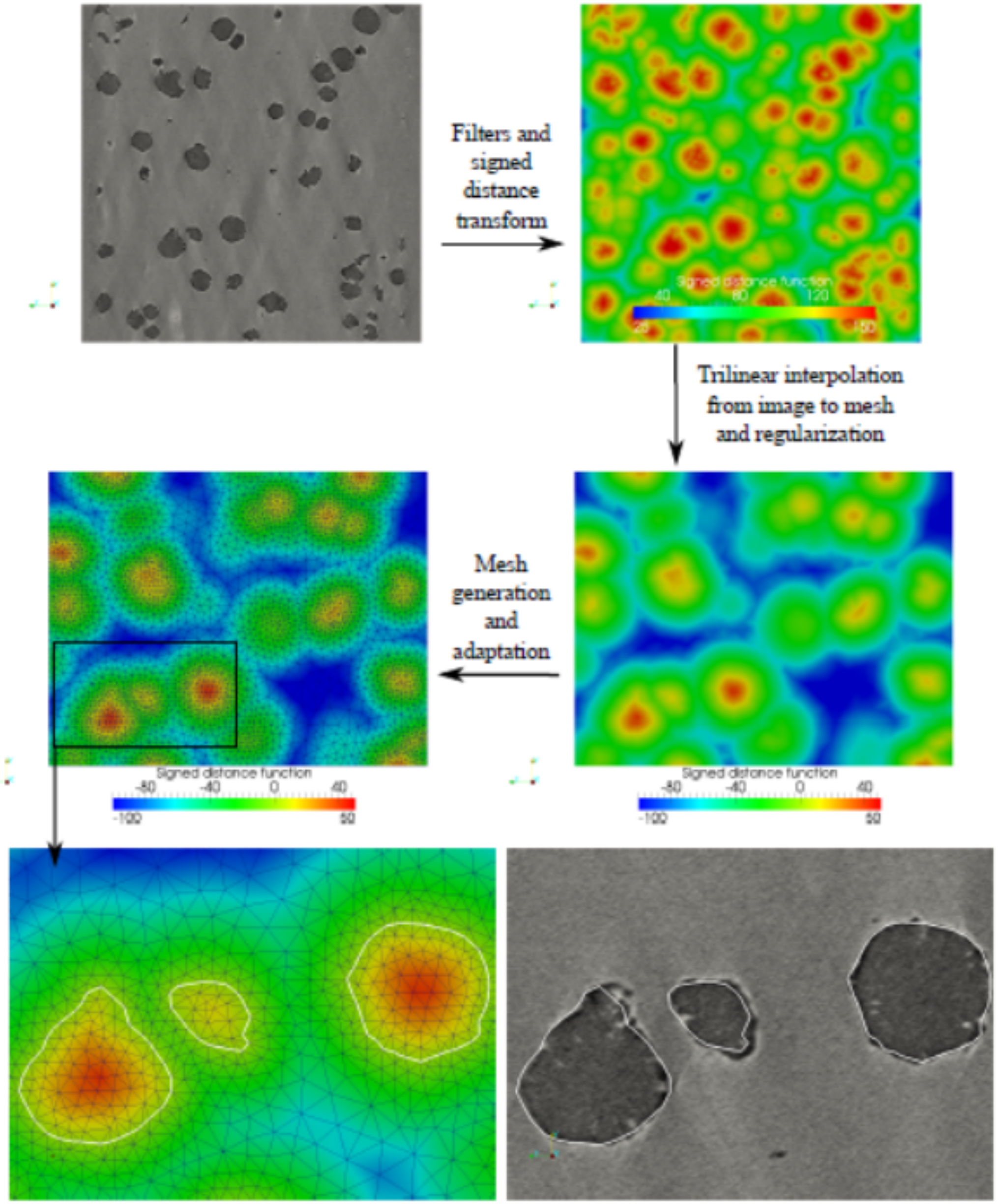
macroscopic von Mises equivalent stress

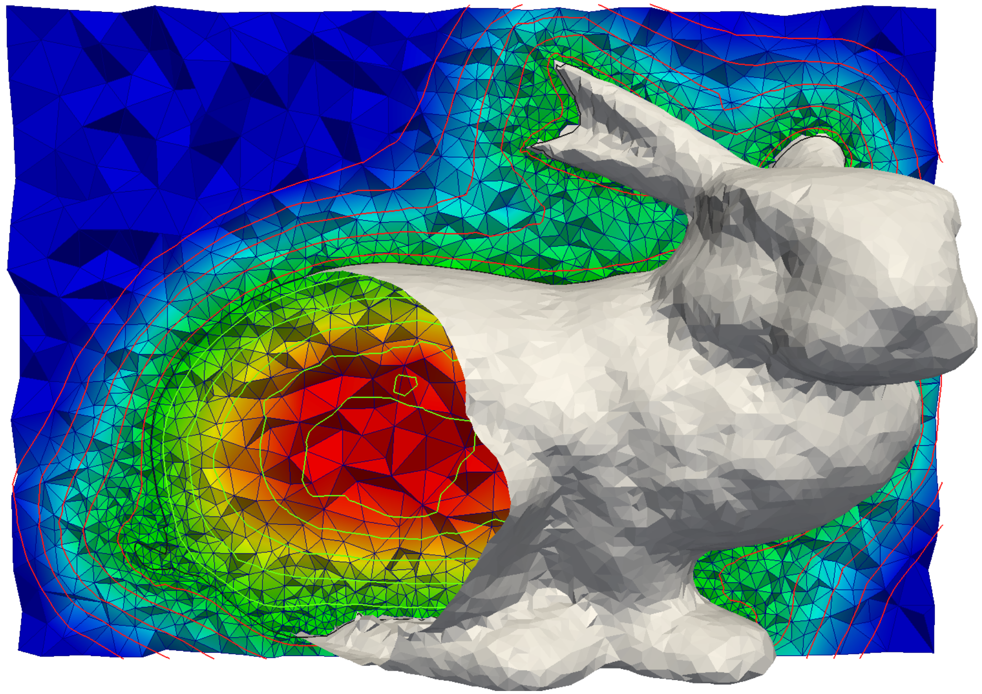
Laminography





Meshing arbitrary geometries





[Stanford Bunny]