FEMxDEM Multi-Scale Modelling with Second Gradient Regularization

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Outline

1. Introduction
2. Method
   - Newton-Raphson Operator
   - Parallelization
   - Material heterogeneity
   - Second Gradient
3. Results
   - Biaxial test
   - Hollow cylinder

Motivation

Bridge the gap between continuum and discrete approaches

- Take into account the discrete microscale nature of geomaterials.
- Take advantage of continuum approaches

Figure: Geomaterials have a discrete microscale nature

Multiscale FEMxDEM model

- The macroscale consists in a classical FEM approach: Lagamine (Liège University).
- The microscale is a DEM model with PBC (in-house 3SR)

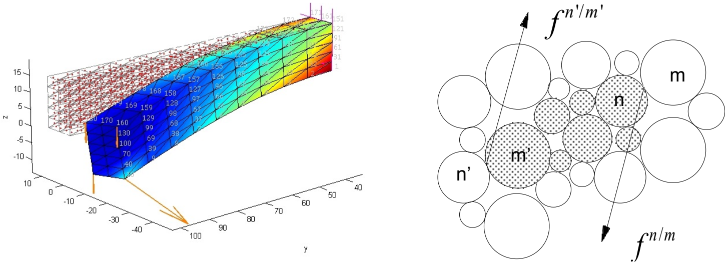


Figure: FEM and DEM model examples

DEM numerical homogenization

- DEM model: molecular dynamics, 400 particles with frictional cohesive contact laws and PBC
- The link between scales is made via numerical homogenization

$$\sigma^f = \frac{1}{S} \sum_{(n,m)\in\mathcal{C}} \vec{f}^{m/n} (\vec{r}^m - \vec{r}^n)$$

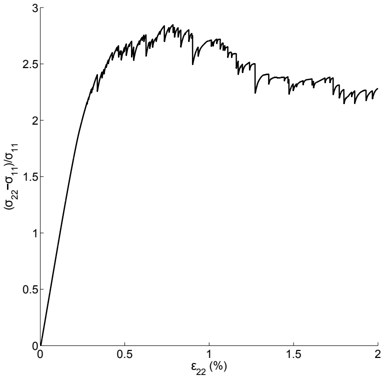
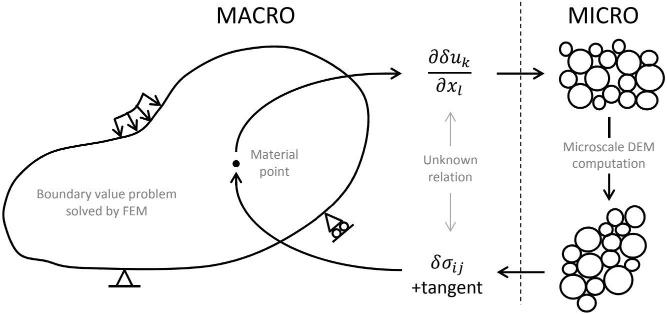


Figure: DEM biaxial test response

Macroscale constitutive modelling

- The obtained constitutive law is injected into the macroscale



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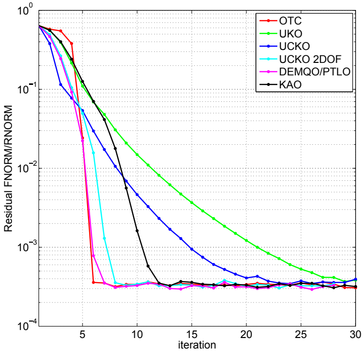
Operator study

The classical Consistent Tangent Operator doesn't work with FEMxDEM, a new operator is needed, tested operators:

- CTO: Consistent Tangent
- AEO: Auxiliary Elastic
- UKO: Upper bound Kruyt
- UCKO: Upper bound Corrected Kruyt
- UCKO 2DOF: Upper bound Corrected Kruyt 2 DOF
- DEMQO: DEM Quasi Static
- PSTLO: PreStressed Truss-Like
- KAO: Kruyt Augmented

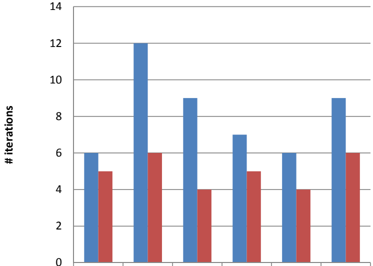
Convergence rates

- The convergence rate of the operators is compared in the initial state and post-peak in a biaxial compression test:



Operators performance

- OTC does not work with FEMxDEM
- Kruyt based operators represent an improvement over the CTO
- DEMQO outperforms the other operators both in the initial state and post-peak



	OTC/ AEO	UKO	UCKO	UCKO 2DOF	DEMQO /PSTLO	KAO
Initial	6	12	9	7	6	9
Post-peak	5	6	4	5	4	6

Figure: Comparison Operators, number of iterations: lower is better

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Element loop parallelization

- The overhead produced by concurrent element integrations is reduced using a shared memory parallelization: OpenMP
- Speedup proportional to the number of cores
- Other Approaches: Massive Parallelization (MPI)

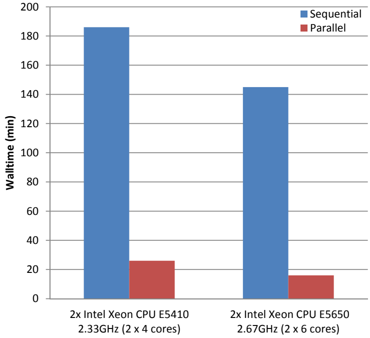

Figure: Parallelization speedup: x7.15 (8 cores), x9.06 (12 cores)

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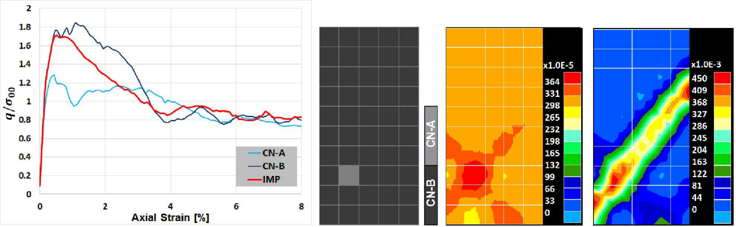
Introducing a material imperfection

- Numerical models are perfectly homogeneous which gives them different properties with respect to real materials
- The FEMxDEM approach provides a natural way to embed material heterogeneity into the model



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

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Second Gradient microstructured materials

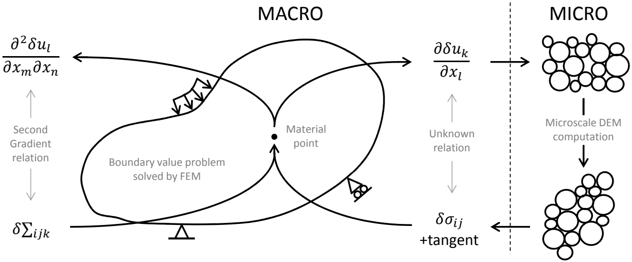
- Second gradient regularization introduces an internal length that regularizes the model.

$$\forall u_i^*, \int_\Omega \sigma_{ij}\epsilon_{ij}^* + \Sigma_{ijk}\frac{\partial^2 u_i^*}{\partial x_j \partial x_k} d\Omega = \int_{\partial\Omega} t_i u_i^* ds \qquad (1)$$

Where u_{ij}^* is the kinematically admissible virtual displacement field, σ_{ij} the stress field, ϵ_{ij} the strain field, Σ_{ijk} the double stress dual of $\frac{\partial^2 u_i^*}{\partial x_j \partial x_k}$, f_i the body forces, $\partial\Omega$ the part of the surface where the forces are known, t_i the surface forces.

Second Gradient in a Boundary Value Problem

- The first gradient relation is kept intact, the regularization is added with a second order constitutive relation



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Biaxial test with a first gradient constitutive relation

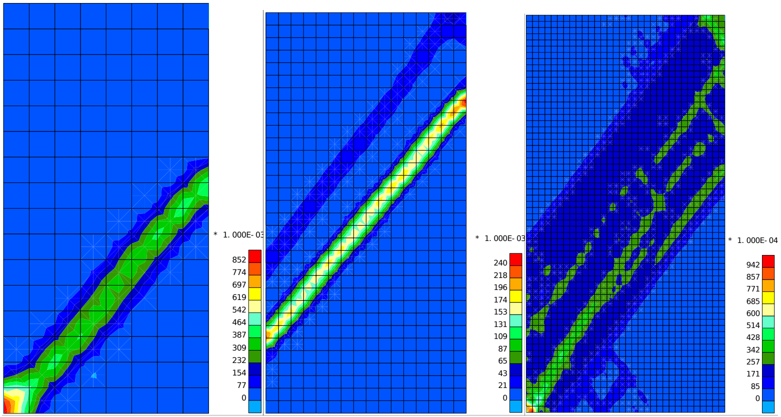

Figure: 128, 512, and 2048 element biaxial compression tests. The localization presents mesh sensitivity, this violates the separation of scales

Biaxial test enriched with Second Gradient

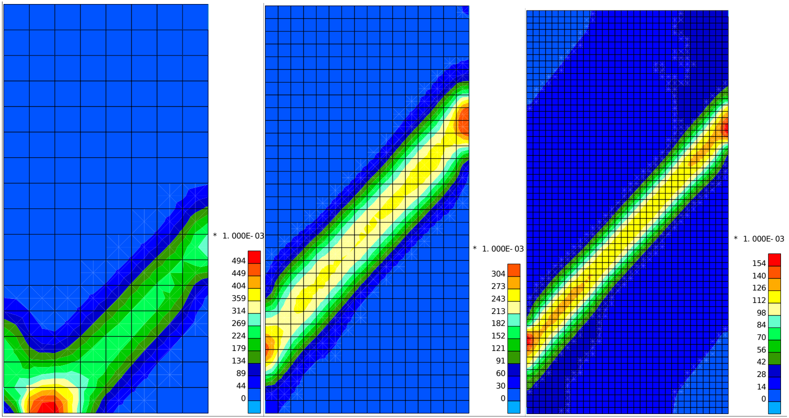

Figure: 128, 512, and 2048 elements biaxial compression tests. The internal length introduced by Second Gradient regularizes the solution

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Hollow cylinder with Second Gradient

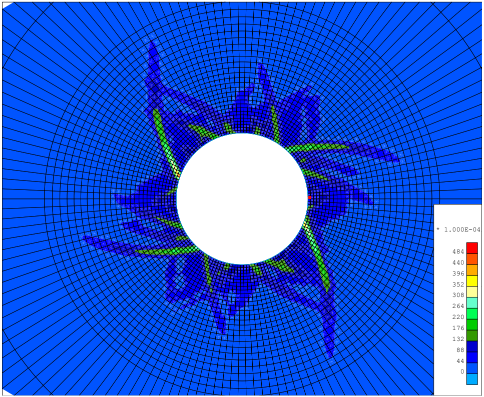

Figure: Localization around the gallery. FEM: 4950 elements, 18900 nodes, 66297 DOF

Figure: 400 particles DEM microscale at the end of the loading

Summary

- A FEMxDEM approach allows to use a constitutive law built in the microscale
- Parallelization allows the model to compete with classical FEM aproaches.
- A Second gradient regularization assures the separation of scales.
  - Outlook
    - 3D microscale is expected to bring richer constitutive behabiour
    - The model can be calibrated with microscale data from experiments

Thanks!!!