FEMxDEM double scale approach with second gradient regularization applied to granular materials modeling

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Outline

1 Introduction

2 Method
   • Newton Operator
   • Parallelization
   • Second Gradient

3 Results
   • Random field methods
   • Parametric tests
   • Engineering scale simulation

4 Conclusions
Motivation
Bridge the gap between continuum and discrete approaches

Figure: Numerical modeling dilemma

**Continuum approaches**
- Numerically efficient
- No scale limitations

**Discrete approaches**
- No need of phenomenological laws
- Faithful representation of the microscale
Multiscale coupling

FEM: Lagamine (Liège University)

DEM with PBC (in-house 3SR)

A numerically obtained constitutive law is injected into the material points
Discrete Element Model (DEM)

- Frictional cohesive contact laws
- Periodic Boundary Conditions

Figure: DEM assembly preparation
Discrete Element Model (DEM)

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Figure: DEM assembly preparation

Numerical homogenization

\[ \sigma^f = \frac{1}{S} \sum_{(n,m) \in C} \vec{f}_{m/n} (\vec{r}_m - \vec{r}_n) \]
State of the Art in FEMxDEM

- Early works (Kaneko, 2003; Miehe, 2010; Nitka, 2011)
- Study of anisotropy (Guo and Zhao, 2013; Nguyen, 2013)
- DEM cohesion (Nguyen, 2014)
- Non-local regularization (Liu, 2015)
- 3D microscale (Liu, 2015; Wang and Sun, 2016)
- DEM material heterogeneity (Shahin, 2016)
- Macroscale hydro-mechanical coupling (Wang and Sun, 2016; Guo and Zhao, 2016)
- Full micro-macro 3D (Guo and Zhao, 2016)
Model performance

- **FEMxDEM issues**
  - Bad convergence
  - Computational time

- **Generic issues**
  - Mesh dependency
## Model performance

### FEMxDEM issues
- Bad convergence
- Computational time

### Generic issues
- Mesh dependency

### FEMxDEM proposed solutions
- Alternative Operator
- Parallelization

### Generic proposed solutions
- Regularization
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Link with classical geomechanics FEM codes

We consider the quasi static evolution of a continuous medium which shares features with elastoplasticity and hypoplasticity. The constitutive equation provides the Cauchy stress $\sigma^f$ as a function of the deformation tensor $F^f$ in a loading step:

$$F^f \mapsto \sigma^f = S \left( F^f \right)$$  \hspace{1cm} (1)
Link with classical geomechanics FEM codes

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$$ F^f \mapsto \sigma^f = S \left( F^f \right) \quad (1) $$

The non linear boundary value problem, is solved using the iterative Newton’s method. This needs to differentiate $S$ with respect to $F^f$ (1), the gradient of $S$ is often called the ”consistent operator”, it is denoted by $C$

$$ d\sigma^f = S \left( F^f + df^f \right) - S \left( F^f \right) = C : dF^f + \cdots \quad (2) $$
Link with classical geomechanics FEM codes

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(2)
Determination of the Consistent Operator

Except for some cases for which closed-form expression of the tensor $C$ can be found, the determining of $C$ is performed numerically using a perturbation method:

$$
(C_{ijmn}) = \frac{S_{ij} (F^f + \epsilon \Lambda^{mn}) - S_{ij} (F^f)}{\epsilon}
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Assuming $S$ to be differentiable, that determines $C$
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**Issues**
- Bad convergence
- Computational time
- Mesh dependency

**Proposed solutions**
- Alternative Operator
- Parallelization
- Regularization
Alternative Newton Operators for FEMxDEM:

**Perturbation based operators**
- Consistent Tangent (CTO)
- Auxiliary Elastic (AEO)

**Elastic operators**
- DEM Quasi Static (DEMQO)
- PreStressed Truss-Like (PSTLO)

**Kruyt operators**
- Kruyt Augmented (KAO)
- Upper bound Kruyt (UKO)
- Upper bound Corrected Kruyt (UCKO - UCKO 2DOF)
**Consistent Tangent (CTO)**

Classic perturbation approach:

\[
(C_{ijmn}) = \frac{S_{ij}(F^f + \epsilon \Lambda^{mn}) - S_{ij}(F^f)}{\epsilon}
\]

**Auxiliary Elastic (AEO) (Nguyen, 2013)**

Average of the CTO over several macroscopic loading steps
Elastic operators

**DEM Quasi Static (DEMQO)**

Based on numerical homogenization of an elastic DEM

\[
(C_{ijmn})^{DEMQO} = \frac{S_{ij}^E (\epsilon \Lambda^{mn})}{\epsilon}
\]  

**PreStressed Truss-Like (PSTLO) (Caillerie)**

It treats the DEM as a prestressed linearelastic truss with additional rotational degrees of freedom in the nodes

\[
d\sigma = \frac{1}{|\mathbf{Y}|} \sum_{c \in \mathcal{C}} \delta^i_c d\mathbf{\bar{f}}^c \otimes \mathbf{\bar{Y}}^i + \sigma \circ F^{-T} \circ dF^T - \left( F^{-T} : dF \right) \sigma
\]
Kruyt operators

Kruyt Augmented (KAO) (Caillerie)
UKO with prestresses and rotational degrees of freedom

Upper bound Kruyt (UKO) (Kruyt & Rothenburg, 1998)

\[
\frac{1}{|Y_a|} \sum_{c \in C} (l^c)^2 \left( k_n (\bar{e}^c \otimes \bar{e}^c) \otimes (\bar{e}^c \otimes \bar{e}^c) + k_t (\bar{t}^c \otimes \bar{e}^c) \otimes (\bar{t}^c \otimes \bar{e}^c) \right)
\]  
(6)

Upper bound Corrected Kruyt (UCKO - UCKO 2DOF)
Calibrations of the UKO to fit a CTO
The convergence rate of the operators is compared in the initial state and post-peak in a biaxial compression test:
Operators performance

- **Perturbation** based operators perform well in the initial stages.
- **Kruyt** operators are more robust in the post-peak part.
- **Elastic** operators combine good performance before and after the stress peak.

![Figure: Operators comparison: number of iterations](chart.png)

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The elastic operators overcome the issues giving good stability and convergence velocity.

**Figure:** Operators comparison: number of iterations
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The evaluation of $S$ is issued from a DEM homogenization:

$$F^f \mapsto \sigma^f = S(F^f)$$
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$$F^f \rightarrow \sigma^f = S \left( F^f \right)$$

### Issues
- Bad convergence
- Computational time
- Mesh dependency
FEMxDEM drawbacks

The evaluation of $S$ is issued from a DEM homogenization:

$$F^f \mapsto \sigma^f = S(F^f)$$

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Element loop parallelization

Amdahl’s law (Amdahl, 1967)

\[ S(n) = \frac{1}{B + \frac{1}{n}(1 - B)} \]  \hspace{1cm} (7)

\[ \lim_{B \to 0} S(n) = n \]  \hspace{1cm} (8)

- S: speedup
- n: number of cores
- B: non parallelizable part

Other Approaches: Massive Parallelization: MPI (Desrues)

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

Theorem

*Commutative Law of Addition:*

\[ a + b = b + a \]
Numerical randomness

Does not apply!

Commutative Law of Addition:
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Commutative Law of Addition:

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Figure: Simulated numerical error
Numerical randomness

Does not apply!

Commutative Law of Addition:
\[ a + b = b + a \]

Figure: Simulated numerical error

Figure: Different possible solutions of the same BVP. Cumulative second invariant of strain
The parallelization provides an effective speedup of the model, becoming this competitive with classical FEM codes.
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First order FEM

**Figure:** Non objectivity of the model
First order constitutive relation

Balance equation in virtual power formulation:

$$\forall u_i^*, \int_{\Omega} \sigma_{ij} \varepsilon_{ij}^* d\Omega = \int_{\partial \Omega} t_i u_i^* ds$$ \hspace{1cm} (9)

Where $u_i^*$ is the kinematically admissible virtual displacement field, $\sigma_{ij}$ the stress field, $\varepsilon_{ij}^*$ the virtual strain field, $\partial \Omega$ the surface of $\Omega$, $t_i$ the surface forces
First order constitutive relation

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Issues

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Issues
- Bad convergence
- Computational time
- Mesh dependency

Proposed solutions
- Alternative Newton Operator
- Parallelization
- Regularization
Second Gradient microstructured materials

Second gradient regularization introduces an internal length that regularizes the model

$$\forall u_i^*, \int_{\Omega} \sigma_{ij} \varepsilon_{ij}^* + \sum_{ijk} \frac{\partial^2 u_i^*}{\partial x_j \partial x_k} \ d\Omega = \int_{\partial\Omega} t_i u_i^* \ ds$$

- First order term

where $\Sigma_{ijk}$ is the double stress dual of $\frac{\partial^2 u_i^*}{\partial x_j \partial x_k}$
Second Gradient microstructured materials

Second gradient regularization introduces an internal length that regularizes the model

\[ \forall u^*_i, \int_\Omega \sigma_{ij} \epsilon_{ij}^* + \sum_{ijk} \frac{\partial^2 u^*_i}{\partial x_j \partial x_k} d\Omega = \int_{\partial \Omega} t_i u^*_i ds \]

- First order term
- Second order term

where \( \Sigma_{ijk} \) is the double stress dual of \( \frac{\partial^2 u^*_i}{\partial x_j \partial x_k} \)
Second Gradient in a Boundary Value Problem

As it is a local model, it can be injected in the material points in the same way as the first gradient relation is

\[
\frac{\partial^2 \delta u_l}{\partial x_m \partial x_n} = \delta \Sigma_{ijk}
\]

Boundary value problem solved by FEM

MACRO

\[
\frac{\partial \delta u_k}{\partial x_i} = \delta \sigma_{ij}
\]

Unknown relation

MICRO

Microscale DEM computation
Biaxial test enriched with Second Gradient

Figure: 128, 512, and 2048 elements biaxial compression tests
With the Second Gradient enrichment the model becomes objective. This allows to use any mesh refinement.

The code is ready to be used in real scale problems.
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Introduction: Symmetry breaking

- Material properties in numerical models are spatially homogeneous unless the contrary is defined.
- The use of a catalyzer to break the symmetry can improve the model performance, both physically and numerically.

Figure: A CT scan of a sand sample (Andò, 2013)
Punctual imperfection

The DEM microstructure has a strong influence on the results

Figure: Homogeneous (a) Defect (b). Second invariant of strain
Full field DEM random variability

**Figure:** (a) FEMxDEM and pure DEM responses under a biaxial loading. (b) and (c), cumulative deviatoric strain field (Shahin, 2016)
The FEMxDEM approach provides a natural way to embed material heterogeneity into the model.
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The outer radius has an influence on the results, a compromise size is chosen.

Figure: Radius=50, 100 and 200 m

Figure: Outer radius=50, 100 and 200 m. Cumulative second invariant of strain

M.S. research project
Nurisa, 2015
DEM allows to tune the coordination independently from the density

Figure: Coordination number = 4.10, 3.67 and 3.14. Cumulative second invariant of strain

The model can cope with any macroscopic boundary conditions

Figure: Stress ratio $\sigma_{0H} : \sigma_{0V} = 1:1$, 1:1.3 and 1:2. Cumulative second invariant of strain
Intrinsic anisotropy

Figure: DEM preparation

Figure: Precharge 0%, 0.3% and 0.6%. Cumulative second invariant of strain
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Hollow cylinder with Second Gradient

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

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

- Real scale simulations are possible thanks to the second gradient and parallelization
- FEMxDEM allows to calibrate the model directly from the microscale
General Conclusions

- A FEMxDEM approach allows to use a constitutive law built via numerical homogenization in the DEM microscale.
- An alternative Newton operator provides the model with good convergence rate and robustness.
- Parallelization allows the model to compete with classical FEM approaches in terms of walltime.
- A Second gradient regularization assures the mesh independence.
- Real scale problems with fine meshes can be considered.
Perspectives

- Calibration of the microscale with experimental data
- 3D microscale can bring a richer constitutive behaviour
- More complex microscale with massive parallelization (MPI)
Thanks!!!