Parallel hierarchical multiscale modeling of granular media by coupling FEM and DEM with open-source codes Escript and YADE

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YADE download page: https://launchpad.net/yade
Escript download page: https://launchpad.net/escript-finley
mpi4py download page (optional, require MPI): https://bitbucket.org/mpi4py/mpi4py

Tested platforms: Desktop with Ubuntu 10.04, 32 bit; Server with Ubuntu 12.04, 14.04, 64 bit; Cluster with Centos 6.2, 6.5, 64 bit;

1. Work on the YADE side

The version of YADE should be at least rev3682 in which Bruno added the `stringToScene` function. Before installation, I added some functions to the source code (in "yade" subfolder). But only one function ("Shop::getStressAndTangent" in "./pkg/dem/Shop.cpp") is necessary for the FEM/DEM coupling, which returns the stress tensor and the tangent operator of a discrete packing. The former is homogenized using the Love's formula and the latter is homogenized as the elastic modulus. After installation and we get the executable file: yade-*versionNo.* We then generate a .py file linked to the executable file by "ln yade-*versionNo* yadeimport.py". This .py file will serve as a wrapped library of YADE. Later on, we will import all YADE functions into the python script through "from yadeimport import *" (see **simDEM.py** file).

Open a python terminal. Make sure you can run:

```
import sys
sys.path.append('where you put yadeimport.py')
from yadeimport import *
Omega().load('your initial RVE packing, e.g. 0.yade.gz')
```

If you are successful, you should also be able to run:

```
from simDEM import *
```

2. Work on the Escript side

No particular requirement. But make sure the modules are callable in python, which means the main folder of Escript should be in your PYTHONPATH and LD_LIBRARY_PATH. The modules are wrapped as a class in **msFEM*.py**.

Open a python terminal. Make sure you can run:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Rectangle
```

(**Note:** Escript is used for the current implementation. It can be replaced by any other FEM package provided with python bindings, e.g. FEniCS (http://fenicsproject.org). But the interface files (**msFEM*.py**) need to be modified.)

3. Example tests

After Steps 1 & 2, one should be able to run all the scripts for the multiscale analysis. The initial RVE packing (default name “**0.yade.gz**”) should be provided by the user (e.g. using YADE to prepare a consolidated packing), which will be loaded by **simDEM.py** when the problem is initialized. The sample is initially uniform as long as the same RVE packing is assigned to all the Gauss points in the problem domain. It is also possible for the user to specify different RVEs at different Gauss points to generate an inherently inhomogeneous sample.

While **simDEM.py** is always required, only one **msFEM*.py** is needed for a single test. For example, in a 2D (3D) dry test, **msFEM2D.py** (**msFEM3D.py**) is needed; similarly for a coupled hydro-mechanical problem (2D only, saturated), **msFEMup.py** is used which incorporates the **u**—*p* formulation. Multiprocessing is used by default. To try MPI parallelization, please set *useMPI=True* when constructing the problem in the main script. Example tests given in the “examples” subfolder are listed below.
(**Note:** The provided initial RVE packings ***.yade.gz** need to be renamed to **0.yade.gz**. One may need to generate his/her own initial RVE packing, as **0.yade.gz** could be machine/version-dependent.)

1. 2D drained biaxial compression test on dry dense sand (**biaxialSmooth.py**)
   Note: Test description and result were presented in Ref. [1].
2. 2D passive failure under translational mode of dry sand retained by a rigid and frictionless wall (**retainingSmooth.py**)
   Note: Rolling resistance model (CohFrictMat) is used in the RVE packing. Test description and result were presented in Ref. [4].
3. 2D half domain footing settlement problem with mesh generated by Gmsh (**footing.py**, **footing.msh**)
   Note: Rolling resistance model (CohFrictMat) is used in the RVE packing. Six-node triangle element is generated by Gmsh with three Gauss points each. Test description and result were presented in Ref. [4].
4. 3D drained conventional triaxial compression test on dry dense sand using MPI parallelism (**triaxialRough.py**)
   Note1: The simulation is very time consuming. It costs ~4.5 days on one node using multiprocessing (16 processes, 2.0 GHz CPU). When *useMPI* is switched to *True* (as in the example script) and four nodes are used (80 processes, 2.2 GHz CPU), the simulation costs less than 24 hours. The speedup is about 4.4 in our test.

Note2: When MPI is used, mpi4py is required to be installed. The MPI implementation can be either MPICH or Open MPI. The file "**mpipool.py**" should also be placed in the main folder. Our test is based on openmpi-1.6.5. Test description and result were presented in Ref. [6].

5. 2D globally undrained biaxial compression test on saturated dense sand with changing permeability using MPI parallelism (**undrained.py**)
   Note: Test description and result were presented in Ref. [5].

References:

1. Guo, N. and Zhao, J. (2014) A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media. International Journal for Numerical Methods in Engineering 99(11), 789-818. DOI: 10.1002/nme.4702.
2. Guo, N. (2014) Multiscale characterization of the shear behavior of granular media. PhD Thesis, The Hong Kong University of Science and Technology, Hong Kong.
3. Zhao, J. and Guo, N. (2015) The interplay between anisotropy and strain localisation in granular soils: a multiscale insight. Géotechnique, under review.
4. Guo, N. and Zhao, J. (2015) Multiscale insights into classic geomechanics problems. International Journal for Numerical and Analytical Methods in Geomechanics, under review.
5. Guo, N. and Zhao, J. (2015) Parallel hierarchical multiscale modelling of hydro-mechanical problems for saturated granular soil. International Journal for Numerical Methods in Engineering, in preparation.
6. Guo, N. and Zhao, J. (2015) 3D multiscale analysis of strain localization in granular media. International Journal of Solids and Structures, in preparation.