1st Yade Workshop

July 15, 2014

Frequently asked questions?(Keywords)
1. DEM Application: computation time; time step(when coupling); testing scale (size); boundary condition; calibration;
2. Numerical methods and modelling techniques, Open-Source development and Complex shapes: size effects; non-spherical interaction;
3. Multi-phase couplings: computation time; time step; external libs (CGAL...);
4. Yade-DEM project meeting, General discussion and Brainstorming: calibration testing; benchmark; parallel (insertion sort collider, verlet distance); external libs;

1 Application of DEM at IMFD Freiberg (by Anton Gladky)

1.1 Outline & Keywords

1. Introduction of TU.BF
2. Processing machine simulations (examples)
2.1 Ball mill simulation (geometry, material properties, operating modes, etc.)
2.2 Screeing machine simulation (geometry, inclination angle, material properties, operating models, grain size, etc..)
2.3 Screw conveyor.(geometry, inclination angle, material properties, operating models, grain size)
2.4 High pressure grinding roller
2.5 Pelletizer
3. Flow Process
3.1 Split-bottom shear cell
3.2 Shear cell scheme

1.2 Questions and Answers

Q1. The maximum number of spheres can be simulate in these examples.
A: less than 200,000
Q2. Is there any non-periodic boundary in cylinder (or asymmetry shape)?
A: ?

Q3. Other ways to define shapes, geometry in Yade?
A: can import data from other software.
Q4: How large the particles can be? (because it's related to time steps when simulating rock falls)
A: doesn't matter (it depends what you want to simulate).
Q5. How close between the simulation results and the real flow materials?
A: It also depends.(on what you simulate and experiment)

2 Multi-scale FEM×DEM Modeling of cohesive-frictional granular materials (by Jacques Desrues)

2.1 Outline & Keywords

What's FEM×DEM
1. Introduction
Bridging scales in geomechanical engineering.
2. Principle: how to couple?
FEM-Gauss points ; code(Lagamine)
DEM-using PBC (periodic boundary condition), REV; code(Gael Combe's work) (the same idea can be found in Jidong Shao, U. HongKong, who using Yade in DEM.)
3. Micro-scale model
the same rules as DEM theory, considering cohesive.
REV size - 400 spheres
4. Examples
4.1 Triaxial tests
4.2 Hollow cylinder (drilling) under different pressures - strain localization
5. Discussion
5.1 different REVs can have different properties. (upscaling non-homogeneous)
5.2 Multi-scale computation
by biaxial compression: observer strain localization; with different mesh precision. (64 elements, 128 elements...)

2.2 Questions and Answers

Q1. the time step of DEM×FEM
Q2. Does the strain localization depend on REV?
A: REV is not localized.
Q3. Mesh dependence on the results
A: Yes. it depends. Nice mesh, nice results.
Q4. Compare with other experiments and simulation method?
A: Yes. DEM×FEM VS only DEM.
Q5. about second gradient regularization, why not to use it both in DEM and FEM ?
A: In progress.

3 Open source DEM-FEM coupling (by Jan Stransky)

3.1 Outline & Keywords

1. Motivation
FEM: PDE ; continuous deformation
DEM: discrete; contact detection
2. MuPIF-Multi-Physic Integration Framework
3. Coupling (1 step DEM 1 step FEM)
3.1 surface coupling (DEM-load− >FEM-displacement− >DEM...)
3.2 FE$\times$DE (Multi-scale) coupling
3.3 contact coupling
4. Future work volume coupling; testing; improvementand extension (currently, the laws are linear)

3.2 Questions and Answers

Q1. about surface coupling, what's the DEM and FEM size.
A: It depends (what you to simulate).
Q2. about facet and spheres, is that possible to use different shape in Yade (non-spherical)
A: currently, nope.
Q3. about the non-spherical particles in the examples, is that the facet contact?
A: No, it's not facet contact.
Q4. a short discussion about optimization of plotting
A: various plotlib, python, C++, etc...
Q5. what's the role of MuPIF in this work?
A: for high level integration .

4 Simulation of (rock fall) wire meshes with Yade (by Klaus Thoeni)

4.1 Outline & Keywords

1. Introduction
various wires: double-twist, chain-link, **orthogonal**... Nicot(2001)-ASM ring net; Bertrand(2008)
2. Modeling
2.1 The wired model in Yade
define interaction; identify double-twist interaction
pack.hexanet(...)
2.2 Define materials.
WireMat(...)
2.3 EWM-Elementary Wire Model
WireMat(...)

2.4 SDWM-Stochastically Distorted Wire Model
3. How to use
3.1 create Mesh: define material, define engines to initialize
3.2 interaction with other particles
4. Examples
4.1 tension test
4.2 block bouncing on mesh
5. Application
5.1 rock fall protection along high walls
5.2 drapery systems (contact law: FricViscoPM)-experiment VS simulation (nice videos.)
6. Future
6.1 particle-particle contact for wire particles
6.2 better integration of contacts
6.3 better integration of wire particles

4.2 Questions and Answers

Q1. about computation time.
A: step 1: mesh takes not so long; step 2: simulate rock falling takes 14-17 h.
Q2. a short question about test results of single VS double twist .
Q3. Calibration of parameters.
A: use test to calibrate λ_u and λ_F .
Q4. How to calibrate the parameters between rock and mesh
A: dynamic calibration, vibration systems (not sure about the answer)
Q5. can implement twist stiffness, bonding stiffness?
A: Yes
Q6. Is the size of mesh model equal to the real material?
A: not really
Q7. about the time step? (because the mesh is light, soft and the rock is hard)
A: not a real problem.

5 DEM modelling of mass finishing at IWF (by Alexander Eulitz)

5.1 Outline & Keywords

1. Introduction of Mass finishing
process fundaments: process based on motivation of loose abrasive media; workpiece movements; surface roughness improvement.
non-vibrating / vibrating media
focus: fundamental mechanism of surface evolution ; predict surface roughness
2. DEM modelling of Mass finishing
approach 1/2 : simulate number, type and intensity
approach 2/2 : formulation− >calibrate− >validation− >utilization
consider: bounding conditions, contact law; material properties, damping

Calibration: physical (micro-scale); phenomenological (macro-scale)
Calibration: material and material combination; parameters (friction, coefficients,...); damping and restitution (independence between global damping and material damping)
Calibration: obtained by a weighted linear optimization algorithm.
3. Model validation: results agrees.
4. Wish list of Yade:
4.1 model of non-spherical particle
4.2 improve particle-facet contact. (reference radius, facet-facet-sphere interaction)
4.3 static and dynamic (kinetic) friction coefficient
4.4 DEM on GPU better performance with more particles
4.5 VTK recorder: self defined data for export
5. outlook: non-spherical media; lubrication; vibrating bowl; efficiency

5.2 Questions and Answers

Q1. questions about wish list, such as VTK recorder, non-spherical, reference radius.
Q2. A long discussion about damping calibration
Q3. a small question about effects of stiffness of particles.

6 Biphasic particles to simulate fresh previous concrete compaction (by Ricardo Pieralisi)

6.1 Outline & Keywords

1. Introduction
the properties of previous concrete: low quantity of cement paste; inter connected pores; high permeability coefficient
2. Particle definition
2.1 elastic inner core
2.2 viscoelastic external layer
3. Characteristic of the contact
3.1 cement paste bridge (CPB) formation
3.2 CPB considerations (interaction: S-S, S-W)
4. material model
4.1 normal direction: rheological model; force-displacement relationship
4.2 tangential direction
5. Solution process
6. experiments program, validation

6.2 Questions and Answers

Q1. about fluid transport simulation
A: by using CFD

Q2. How to increase compaction degree?
A: by stress

7 DEM techniques for rock mass and fracture (by Jerome Duriez)

7.1 Outline and Keywords

Introduction: rock hydro-mechanics case studies
1. Rock fall risk assessment
1.1 describe discontinuous
1.2 describe failure in rock
method: from in-situ observation to 3D model
2. Crack propagation analysis (justification of the model)
a pre-existed crack; failure in rock
failure in rock
3. Hydro-mechanical for fluid extraction/injection progress
describe cohesive pro-cracked media; various flow model to couple
this research: 3DEC + YADE
4. Examples: Flow in a fracture network

7.2 Questions and answers

Q1. what's the model in flow fracture?
Q2. about the model, is the media initially dry?
Q3. what's the advantage of this model?
A: it can simulate rock failures.

8 Rock fall impacts on trees and other wooden structures (by Franck Bourrier)

8.1 Outline and Keywords

context: protection against hazard; slope stability; rock falls
1. rock falls: modelling the rock/tree interaction
2. deformation of cylinder elements (grid elements)
cylinder stress-strain relationship; sphere-cylinder interactions
3. DEM model of rock-tree interaction (focus on the rock-stem interaction)
static stem loading; impact on stems
calibration:
3.1 calibration on LE impacts/HE impacts
3.2 comparison of the parameters calibrate OS and impact tests
3.3 model validation
4. conclusion: framework ; calibration

challenge: integrate the effect root system; scale change

8.2 Questions and answers

Q1. Is this in 2D or 3D?
A: fully 3D.
Q2. a short discussion on model calibration. calibrate slope, rockfalls

9 Discrete element modelling of fracture rock (by Jerome Duriez)

9.1 Outline and Keywords

Introduction
introduce properties of rock: deformation; failure
introduce DEM rock modelling: discontinuous; pre-existed cracks
1. DEM modelling of rock matrix
Jointed Cohesive Frictional Particle Model (JCFpm) in yade
1.1 contact bond variant of Potyondy's model
1.2 definition of interacting spheres $\neq$ Potyondy's.
1.3 tangential interaction
1.4 no moment transfer law
2. DEM modelling of rock fracture
2.1 The smooth joint model(SJM, 2008): jointed (cohesive frictional particle model) in Yade
2.2 contact laws for joint interaction (Sliding defined by friction angle and dilatancy angle)
2.3 SJM-JCFpm VS other approaches
3. conclusion

9.2 Questions and answers

Q. what's size effect for individual spheres? A: this model is using uniform spheres.

10 Particle-node: logical separation in W00-DEM (by Vaclav Smilauer)

10.1 Outline and Keywords

1. Introduction of Woo
funding model; customizations; emphasize on industrial process;
dev: generic particle shapes (potential particles);
tight python integration, easier scripting;
non DEM needed-the finite pointset method
2. comparison between in Yade and Woo

2.1 yade conflict particles as: colliding (bboxes); having contacts (shapes); undergoing motion (mass, velocity)
2.2 particles in Woo:
2.2.1 node concept: borrow from yade; assures C_n continuity across element (sharing nodes); important for deformable element
2.2.2 split shape and motion: shape positioned by one or more associated nodes; nodes are shared; each node carry data
2.3 consistency: particles refer their nodes; nodes need to know about their particles
3 advantage and examples
connectivity; anything have a node can move; clumps are not special particles; node define moving

10.2 Questions and answers

Q1. short question about trust-element and computation time
Q2. Is there any comparison with other methods or experiments? No.
Q3. interaction about 3 bodies contact /separation

11 Extended use of periodic boundary conditions (by Jan Stransky)

11.1 Outline and Keywords

1. motivation: breaking periodicity in material simulation
PUC− >SEPUC− >extension; Wang tilings; Tiling algorithms; Stochastic Wang cubes
Application: Homogenization of Alpora foam;
2. periodic packing
periodic boundary conditions: interaction found also with periodic images of other particles
3. semi-periodic packing
4. "Wangization" of semi-periodic cell
5. conclusion and summary:
5.1 Wang's boundary condition works
5.2 Extended bitmask type needed
5.3 algorithm easily extensible to 3D
6. Future : Extension to 3D; polydisperse packings PSD; different shape of 3D;

11.2 Questions and answers

Q1. what's the advantage?
depend on what you want; much flexible ;
Q2. about the periodic units, do they have the same mechanism behavior?
depend on the requirements; the aim of this model is only for building a data

structures, (according to the customer's requirements). it's still not used to do real simulation.
Q3. if there is some discipline for each periodic cell ?
in this model, they have the same fixed size.

12 Inconsistencies of contact force models and impossible elasticity of 3D granular material (by Bruno Chareyre)

12.1 Outline and Keywords

1. Introduction
contact kinematics /what's shear ? ; Cundall's model; ratcheting effect
2. 2D problem/ Ratcheting cycle
2.1 corrected equations of McNamara et al: the relative displacement is a function of rotations wrt contact normal; with the elastic potential
2.2 why is path dependence bad?
2.3 Yet another set of equations
compare with Cundall, PFC...
3. Path dependence in 3D (no solution)
4. conclusion (A 3D packing has always internal mechanisms)

13 open-source development (by Anton Gladky and Remi Cailletaud)

13.1 Outline and Keywords

Anton:
A very interesting GIT-Statistic: history, activity, website-statistic, current development, miscellaneous...
Also some interesting question: yade-daily is yade-weekly; the default parameters for installation...
Remi:
Yade: continuous integration, doc and wiki
Automatic build, test and release; hardware; builders; web view; Documentation and Wiki;

14 DEM-membrances: membrances finite element in Woo (by Vaclav Smilauer)

14.1 Outline and Keywords

1. Motivation
2. Corotational formulation of FEM;
3. best fit Corotational frame (element-local coordinates):

position and orientation: frame origin; frame xy plane; rotation around z
4. rotations:
element rotation WRT initial element-node orientation ; store initial per-node rotation difference; calculate current node rotation; break for rotation $> \pi$. but that is hardly small strain.
5. plant element (constant strain triangle, CST)
6. bending element (discrete Krichhoff triangle, DKT)
7. total generalized model forces
superposed contributions: CST forces; DKT forces; hydrostatic pressure P acting on the current element area; contact force and torques
8. Woo-specific considerations: time-step; no element-level damping, purely elastic behavior

15 DEM simulation of ballast oedometrict test (by Jan Stransky)

1. Motivation and experiment
2. Grain shape
2.1 Polyhedron: convex Polyhedron is intersection of half-spaces; use CGAL library to manipulate polyhedrons, compute convex-ghulls etc. 2.2 Randomly-shaped polyhedral ballast grains
2.3 Controlling polyhedral shape
3. Contact force
3.1 Necessary algorithms: contact detection; magnitude of normal force; magnitude of shape force; normal direction and point of action
3.2 Calculation of intersecting polyhedron
4. Comparison and conclusion
simple method to generate convex randomly shaped grains;
possibility to control aspect of grains
repulsive force estimated from volume of intersection polyhedron
normal direction estimated from least-square fitting of shells intersection by plane
crushing of grain can be simply done in geometrical sense, problem is to develop correct criterion

16 Grids element in Yade-DEM as connected cylinders: from develop to use (by Francois Kneib)

16.1 Outline and Keywords

1. construction of grid elements
1.1 internal behavior
internal behavior of the whole beam as described highly depends on the inter-element distance

solution: need to adjust all stiffness to the Beam Theory
1.2 external interaction
need of a new specific set of classes to handle external contacts and avoid rugosity. force dispatching between the two nodes of a cylinder according to the contact position-¿need to write specific contact law
2. How to use
show a short script to use GridNode/GridConnection.

17 An extension of the grid model (by Klaus Thoeni)

17.1 Outline and Keywords

1. Introduction: Modeling of deformable facets/membrances; modelling of non-spherical particles; modelling of deformable bodies
2. Merging grids and facets: PFacet
GridNodes− >GridConnections(Cylinders)− >PFacet
Contact handing: Sphere-PFacet
Sphere-insidePFacet: use barycentric coordinates to check if inside; create virtual sphere at contact point
3. How to use: show a short script
4. Some interesting examples: modelling of structural elements/bucking phenomena; modelling of bouncing ball; modelling a membrance pull-out test ; a fascinating video of fishing

17.2 Questios and answers

Q1. how to determine the properties of membrance?
A: this model does still not define membrance property.
Q2. what's the interaction of facet and nodes ?
A: facet follows the nodes.
Q3: Is that possible the thickness of the membrance is zero? yes

18 DEM-LBM coupling (by Luc Sibille)

18.1 Outline and Keywords

description of the solid phase at the particle scale (DEM)
description of the fluid in the inter-particle space (LBM)
Solid phase: contact stiffness; contact friction angle; contact adhesion;
Fluid phase: fluid viscosity; position of each particle (explicitly described)
1. LBM
Based on the probability density or distribution function;
The BGK (Bhatnagar-Gross-Krook, 1954) collision operator;
Transfer of momentum from the solid particles to the fluid at solid boundaries
Force applied by the fluid on the solid

2. 2D example: hydraulic heave
LBM time step is automatically computed and DEM time step adjusted according to LBM one.
script available in trunk/example; show post-processing and visualization
3. Some limitations:
incompressible flow assumption and conservation of mass, momentum and energy hold for low Mach number and small density variations
fluid viscosity depends on time and space discretization.

18.2 Questions and answers

Q1. Has this model handled flow couple with solid?
Q2. computation time? 2-5 days
Q3. how fine the mesh? and what's inside the solid ?
Q4. about time step.

19 DEM model of the pendular state

19.1 DEM of unsaturated flow (by Caroline Chalak)

1. Introduction
The total force applied on the particle is the sum of both contact force and capillary force: $F_{tot} = F_{cont} + F_{cap}$
2. DEM modelling of pendular state
2.1 DEM modelling of one meniscus
The shape of the meniscus is determined by Young-Laplace equation.
Non dimensional analysis : in order to make a dimensionless study, all the variables are normalized.
Integration and solving of Laplace equation.
2.2 During simulation
The set of solution is discretized using Delaunay triangulation.
Interpolation
two types of Interpolation are used to solve a pendular water bridge during a simulation: s-based interpolation (parameters: the suction; the distance between particles; the ratio of the radii of connected particles); v-based interpolation (parameters: the volume of the meniscus; the distance between particles; the ratio of the radii of connected particles).
The menisci can be formed between 2 particles in contact in the case of imbibition, and between distant grains also in the case of drainage.
2.3 Limitation of the model
The model is not valid when the menisci starts to overlap.
3. The roughness of the grain
by assuming that the radii of the grains for the capillary law is different than that the radii taken into account in the contact law
4. Interfaces
based on the work of Morrow (1969) for rigid grains.

19.2 capillary bridge models (Anton Gladky)

1. Implemented CBMs:
comparison between capillary bridge models and Willett's experiments and rabinovich's experiments.
2. Willett's
show some results of DEM-simulations of split-bottom shear-cell
2.1 Willett's full
2.2 Willett's reduced
3. rabinovich's
Further steps: liquid migration model; SPH-DEM; CFD-DEM;

20 DEM-fluid coupling applied to bed load transport (by Raphael Maurin)

20.1 Outline and Keywords

1. Introduction
part of the sediment transport in "contact" with the bed $->$rolling, sliding, salting;
Turbulent flow, dynamic phenomenon;
In link with river/mountain stream/coasted sediment transport
incompressible understanding/prediction
2. Numerical Model
Idea: particle scale; simple fluid description
Model Principle:
fluid phase: momentum balance; code: Fortran + Boost python ; particle phase: DEM ; code: Yade
3. Experimental context: measure transport equilibrium; particle tracking
4. Conclusion: coupling yade with simple turbulent fluid description, in the framework of sediment transport; Model able to reproduce well experimental results
Perspectives: other experimental confirmation; 3D analysis of the phenomenon; segregation

20.2 Questions and answers

Q1. what the parameters of flow?
A: surface tension
Q2. about computation time
Q3. the considerations about time steps during coupling?
A: the coupling doesn't run on every time step.

21 Micromechanical modelling of liquefaction sensible sands (by Anton Gladky)

21.1 Outline and Keywords

1. Model type 1: complex periodic model
periodic model with clumps, dynamic simulation and liquid bridges (instability)
2. Model type 2: stress path

21.2 Questions and answers

Q1. Is there any mesh existed in SPH?
SPH is a meshless model
Q2. Is there any nodes inside the particles? (not sure with the answer)

22 DEM-CFD coupling (by Bruno Chareyre)

22.1 Outline and Keywords

1. Pore scale Finite Volume
1.1 main methods to couple DEM with fluid flow:
sub-particles scale for the fluid (DNS-DEM, LB-DEM, SPH-DEM...)
continuum scale for the fluid (CFD-DEM)
1.2 DEM-PFV has a fluid scale of the order of the particles sizes, aiming: A compromise in terms of computational cost vs. accuracy of per-particle forces
An efficient integration scheme for strong poromechanical coupling
2. A closer look at how the fluid flows
DEM-DNS simulation enables detailed study of fluid flow at the micro-scale
3. Incompressible Stokes Flow
A discrete analog of the equations of continuum (Biot's) poromechanics.
The coupling term leads to instantaneous long range interactions between the particles
Semi-implicit scheme implemented in Yade-DEM
4. Benchmark tests
4.1 Permeability predictions: experiments on mixtures of two-sized glass beads compared to PFV and empirical/semi-empirical relations.
4.2 Consolidation problem: Time evolution of a saturated medium under external load

22.2 Questions and answers

Q1. a short question about time step.
Q2. quasi-static or dynamic simulation? compressible or not ?
Q3. a long discussion about different libs for coupling. CGAL, Eigen3, openblas...

23 PFV + Stokesian dynamic for flowing fluid-grain mixtures: Yade and rheology of dense suspenses (by Donia Marzougui)

23.1 Outline and Keywords

Motivation: sheetflow
immersed granular material:
solid-solid interactions and solid-fluid interactions; rheology of the material: simple shear test.
viscous ratio and volume fraction vs viscous number
1. DEM-fluid model including lubrication forces
1.1 hydrodynamic interactions
Long-range interaction: DEM-PFV; Short-range interactions: lubrication theory
1.2 computing cycle
2. rheology of dense suspensions
2.1 configuration:
Numerical configuration: shearflow; experimental: configuration of Boyer
2.2 rheology
3. how to use and conclusion
show some scripts

23.2 Questions and answers

Q1. compare with experiment, what's the results?
Q2. about calibration. A: No calibration for this model
Q3. about the computation time
Q4. only periodic boundary condition?

24 Coupling the DEM and a pore-scale model of two-phase flow (by Chao Yuan)

24.1 Outline and Keywords

1. Introduction
objective: assign pore-scale model to simulate drainage process; investigate capillary pressure- saturation relationship
assumption: air-water system; solid perfect wetting; quasi-static regime
2. Pore geometry
2.1 Network
use Regular Triangulation to upscale from a pore unit to a dense packing
2.2 pore body and pore throat
3. Model of drainage
3.1 Entry capillary pressure
based on MS-P method, follows from the balance of forces for pore throat sec-

tion
3.2 drainage and trapping (consider trapping or not)
3.3 boundary conditions (consider invade from side boundary or not)
4. Model tests
4.1 test REV, boundary conditions, residual saturation...; comparison with experiment
4.2 capillary force and deformation: shrinking/swelling during drainage (oedometer condition)

24.2 Questions and answers

Q. Is the tessellation necessary ?
A: not really. we can also use other triangulation methods to assign decomposition. But using the network of PFV, it would be much easier to couple with other PFV model (such as dynamic flow, pendular regime...)

25 Hydrofracturing rocks

25.1 Outline and Keywords

Aim: get an inside at hydraulic fracturing (HF) in rock with pre-existing cracks framework
1. 1st coupling
local conductance multiplied by a factor on all facets of cells that contain less 4 "bonded edges"
For each cell: for pairs of vertices compared to interactions: if less than 4 interactions per cell remain cohesive: cell assigned as "cracked"
2. 2nd coupling
Enhanced Flow Engine for flow in rock and rockmass;
Local conductance treated on facets;
parallel plates model(cubic law) to describe flow in fractures

25.2 Questions and answers

Q1. what's the size of example, (or how many spheres) ? A: a small scale
Q2. Is the crack a plane?

26 what happened to the insertion sort collider? (by Bruno Chareyre)

26.1 Outline and Keywords

1. IS Collider
Bzr3000
Small scale optimizations (example1)

example 2: Skip 50% of the bound inversions: -min vs. min ; -max vs. max
different logic: the collider doesn't care when bboxes are separating
Skip 50% of the bound inversions again: max vs. min
overall 75% of the inversions are skipped
String based on actual motion instead of abs.value of max velocity + Motion-based update of the sweep length
2. Parallel IS Collider
parallel sorting algorithms are notorious and well documented in online contents
this case is specific, due to the highly pre-ordered lists
cutting the lists in smaller chunks naively scales almost linearly(!) for large N
almost all the other loops are parallelized(except for the erase loop)
running the 3 axis in parallel could be also tested

26.2 Questions and answers

Q1. about verlet distance (VD)
If the sphere doesn't move at all, the bbox will shrink during the running.
Q2. the optimization of VD.
the default VD=1.5
Q3. a short discussion about definition of VD. the VD for big and small spheres
Q4. if the velocity of small and big spheres are very different, what's the VD and bboxes?
Q5. what's the logic of VD for periodic boundary condition?

27 Performance Benchmarking with YADE (by Klaus Thoeni and Alexander Eulitz)

1. Motivation How many threads should a simulation use?
which kind of hardware is the right? A lot of cores at low frequency (AMD) or some cores with higher frequency (Intel) ?
Does Yade benefit from Hyperthreading ?
How good is Yade parallelized?
which architecture is better AMD or Intel ?
2. system specifications
3. Tests
yade versions: not parallel(version1) and parallel Collider (version2)
test1: checkPerf.py; results are average of 10 simulations
test2: checkPerf.py; results are average of 3 simulations; multiplication for number of iterations; add simulation with 1 million particles
4. show how to do those tests; show a series of results (a huge series of tests)
5. Performance Benchmarking 2013-short conclusion:
Because of OpenMP implementation Yade should benefit from an increasing number of CPU cores
Surprisingly shorter simulation times are only achieved for rather small number of cores (depending on simulation setup between 4 and 7)
Possible explanation: increasing communication and synchronization effort; OpenMP

is not implemented for all Engines.
6. Performance Benchmarking 2014:
Major changes in implementation of insertion sort collider ;
Meanwhile openBlas broke multicores operations
Also show a huge series of tests and results (Hyperthreading, Serial (old) collider/Hyperthreading, Parallel collider; Hyperthreading, scaling of the Parallel collider...)
7. Performance Benchmarking 2014 –j vs. –cores
-j set NUM_OMPTHREADS
use: yadedaily -j4
specified number of cores is at good usage but assignment of threads to cores varies
-cores allocates threads to specified (virtual) cores
use: yadedaily –core "0,1,2,3"
start yade with 4 threads AND one master thread of the first specific core
partly only 2 or 3 threads are used. First one is always active.
Dynamic Performance Benchmark

27.1 Questions and answers

Q1. a very long discussion on the comparison of testing results .
Q2. What happen in the simulation test?
A: just gravity. More spheres, less iterations, in order to make the same benchmark series.
Q3. From the test results, how many cores should be chosen?
A: depends on how many spheres to simulate, it's not always the more cores used, the better simulation running.
Q4. About the computation time of difference parts of the Engine.
A: It's not always that InsertionSortCollider cost most computation time.
Q5. What's the difference between "-j" and "-core" ?
Q6. What's the roles of cores, threads and Hyperthreading in OpenMP?

28 DEM on GPU (by Vaclav Smilauer)

28.1 Outline and Keywords

1. Introduction
What's (GP)GPU? use the computing power of Graphics Processing Units (GPU) for General Purposes (GP) instead of just graphics.
specific massively parallel architecture: same code run over thousands of different data.
CUDA: nVidia proprietary, nVidia-GPU only; more high-level API
OpenGL: cross-device (GPU, CPU,...), standard, relatively low-level
2. OpenGL architecture
device/compute unit/processing element
corresponding 3 types of memory (64KB, 512KB, 4GB).
division of labor: all data/work-group/work-item

3. DEM on (GP)GPU
3.1 GPGPU features: massive parallel performance; predictable memory access is the key; local/shared memory capacity rather low; all processing elements (cores) on the compute unit must execute the same code; if you branch, others wait
3.2 DEM requirements: relatively parallel; unpredictable (moving particles) and non-local memory access necessary; lots of local data; lots of branching necessary (different shapes)
4. implementation: implement math routines; DEM with spheres, walls, clumps, two contact model; collision detection still on the CPU; date in global memory; python wrapper
5. lessons learned:
OpenCL platforms are buggy. buggy: nVidia < AMD < Intel
hard to write code without assuming memory sizes
GPGPUs are great for tasks with strong locality
the hyper was greater than the truth
GPGPU is not usable for DEM

29 Compilation on MS Windows (by Vaclav Smilauer)

29.1 Outline and Keywords

1. Windows platforms
no good shell; no integrated set of development tools; no ABI, library packages, standard header locations
2. Compilation for Windows
cross-compilation on Linux-MXE object (doesn't support python) ;use Microsoft Visual Studio (bad support for C++11); use Windows port of GCC: MinGW=w64 (recompile all libs by yourself);
3. prepare libs
tons of libs, little workarounds and patches: MinGW-w64, MSYS(shell), Python2.7, cmake, VTK, ...
4. compile and run Woo

30 The P2PCD project, survey of DEM software, project management, Editorial strategy, funding the project and consulting actives (by Bruno Chareyre)

30.1 P2PCD:

the bridge the vectorization gap in the research on non-spherical DEM particle models
Q. what kind of vectorization?

30.2 survey of DEM software

Q. compare with PFC3D, yade has the problem of "save" and "load".

30.3 Editorial strategy

reorganize the chapters: reference paper for per chapter; the contributions of people.
about citing problem, refer to other project, like CGAL
Boosting citation, boosting paper citation, delete/add authors

30.4 Next Yade Workshop

More participants, more open, better to combine with international conference

31 Linking external libraries (by Anton Gladky)

show a very details of how to link external libraries

32 Yade Wiki, Yade's documentation discussion and Brainstorming

1. add link to example script or add minimal python code for each contact law
2. add status/quick info auto-table to contact laws

More details about Brainstorming can be found on: https://yade-dem.org/wiki/Brainstorming