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A new C++ workbench to develop discrete element simulations: GranOO

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Abstract. *Discrete Model is based on the description of the physical state (velocity, position, temperature, magnetic moment, electric potential ..) of a large number of discrete elements that form the media to be studied. It is not based on a continuous description of the media. Thus, it is particularly well adapted to describe media evolution driven by discontinuous phenomena like the description of multi fracturation followed by debris flow like wear study. Recently, the use of discrete model has been widened to face problem encountered with complex rheological behavior and/or multi-physical behavior. Multi-physical problems face complex mathematical formulation because of the mixing of different families of differential equations when continuous approach is chosen. With the discrete model, each particle has a physical state and state evolution is due to local physical particle interaction: it is often much simple to write. To help and promote research in this area, a free platform GranOO has been developed under a C++ environment and is distributed under the GPL license. The main aspect of this platform is presented in this extended abstract and one application is given as example. Details can be found on url www.granoo.org.*

Keywords: discrete element method; DEM; C++; Code development.

1 INTRODUCTION

To study complex phenomena like wear, multi-fracturing, or machining the use of adapted numerical tools to understand and predict the contact behavior is necessary. Finite element method is often used. Its great advantage is due to the fact that it is easy to use and commercial software are widely distributed. But finite element method faces difficulties to describe multi fracturation followed by debris like in wear study. Molecular dynamic methods are more and more used for the study of complex problems. In that field, some open software exists and can be used by a large number of scientists. But the simulated time and space scales are often little compared to the phenomenon scales. In the past ten years, discrete element models have been shown to be an interesting tool to take into account the contact at the right scale and to solve multi physical problems. Unfortunately, discrete element software are often ‘one use software’ and there is a lack of easy to use discrete element model software. The consequence is that studies using discrete element model are restricted due to software difficulties. The GranOO workbench has been developed in order to offer to the scientific community free and easy to use discrete element software. This paper briefly recall the main aspect of the discrete element model developed in GranOO. Then the main aspect of the GranOO workbench is presented and one example is given.

2 THE DISCRETE ELEMENT MODEL

The discrete element method (DEM) can describe quite naturally a granular medium. The development of this method began in the early 1980s [4]. More recently, researchers have adapted this method to study the damage of heterogeneous solids such as concrete [6] or rock [2], and homogeneous materials such as ceramics [13] or silica glass [1]. In these works, the discrete element methods describe the media as an assembly of a great number of interacting elements with cohesive bonds. A failure criterion is introduced to broke the bonds that reach a given value of strain [3] or stress [11]. This process mimics crack formation in a given media. With this method, the main difficulty is:

1. the choice of the constitutive equations of the interaction between discrete elements and
2. the calibration of the parameters of the chosen constitutive equation.

A part of this difficulty was treated for brittle elastic materials [1] and was implemented in the GranOO workbench. The stable branch of the GranOO project uses spherical particles, regular contact laws, beam elements for the joint between discrete elements of a same media and an explicit integration algorithm. This choice is well adapted to:

1. solve dynamic problems with effects at little time scale. This property is induced by the explicit integration algorithm that forces the time step to be small.
2. massive DEM simulations. The sphere shape of the discrete element allows a very fast contact detection.

The discrete element method developed in GranOO is based on the following physical description:

- the discrete element stores the mass, volume, accelerations, velocities and positions, and is able to store other physical properties (magnetic moment, electric potential, etc.),
- the joint stores the rheological behavior and
- the contact stores the interface behavior.

The next section will show how this physical description has been translated into the C++ platform GranOO.

3 ARCHITECTURE

The aim of this object oriented workbench is to provide class libraries that can be used to build the DEM simulation adapted to a specific problem. The GranOO workbench is based on three main C++ libraries that forms the GranOO's API (Application Programming Interface): the geometrical, the DEM and the utility libraries. The utility library, that provides some technical and specific computer engineering tools will not be detailed here.

A DEM simulation involves massively basic geometrical operations. The challenge is to propose an high level C++ class interfaces that model geometrical entities without lowering performances. In the GranOO's geometrical library, the orientations are described by quaternions that is an efficient way to compute angular rotation [10, §2.5]. An originality of this library is to express the coordinates of the geometrical entities along a reference frame. This mechanism allows an fast and easy-to-use changing frame operations for vectors, points, matrix and quaternions and facilitate the writing of complex geometrical problems. The performance of this library was validated through benchmarks in comparison of the linear algebra library *blitz++* [14].

The DEM library provides the classes used to model all the DEM ingredients: discrete elements, bonds, mechanical contacts, thermal contacts, smooth contact processing, optimized contact detection algorithm, etc. This library is the core of the GranOO workbench. It allows to describe and model the physical laws introduced into the DEM simulation.

In addition, the GranOO distribution includes also some useful tools:

- The *cooker* program can be used to create the discrete domains required for the DEM modeling of continuous media. *cooker* itself is an application created thank to the GranOO workbench. It is designed to guarantee users that the discrete domain created has the right coordination number to ensure satisfying isotropic and homogeneous properties [1].
- The *gddviewer* program is a graphical application that can be used to draw the discrete domain at different simulation time steps. It can plot colored drawings of the discrete domain, showing selected physical quantities see figure 1.
- Some Python¹ scripts that help the users to calibrate the microscopic properties, to build discrete domains and to post-treat the data given by a simulation.

¹Python is a programming interpreted language, see <http://www.python.org>.

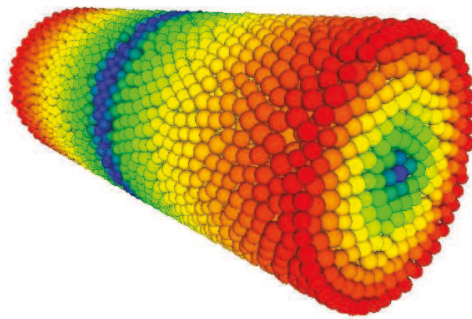


Figure 1: Exemple of discrete domain created with the *cooker* program and drawn by the *gddviewer* program. The discrete cylindrical sample is loaded in a torsion mode where an equal and opposite torque is applied to the faces of the sample. The color scale corresponds to the norm of the discrete element displacements.

4 USAGE

The GranOO workbench is not a software. This is a set of tools and APIs that help the user in the development of a specific numerical DEM experiment with consistency. It is not possible, for the GranOO's developers, to plan all the need wanted by the users for a specific application. By the way, if a user don't find a desired behavior in the GranOO workbench, he could develop it thanks to the tools provided by GranOO. A particular effort was done to felicitate these specific developments. The user could implement its own desired behavior by:

1. using the oriented object architecture and implement a new classes that derive from a class provided by the GranOO's API. This is a very versatile method but it requires knowledge in oriented object and C++ programming.
2. using the *physical properties* mechanism provided by the DEM library. It allows to add dynamically a new comportment and attributes to the discrete elements.
3. using the plug-in mechanism provided by GranOO.

A GranOO's application is considered as a sequence of specific treatments. These treatments are specified inside a plug-in. These plug-ins could be provided by the GranOO workbench or developed by a user. The exhaustive list of standard plugins provided by GranOO is available in the documentation. Examples of standard plug-in are:

- instantiation of beams between selected discrete elements, with given micro mechanical parameters,
- computation of resultant force and torque applied on discrete elements,
- performing the numerical integration to compute linear and angular velocities and positions of discrete elements,
- applying boundary conditions and loadings,
- saving the domain state (C++ serialization of all the objects) in an output file...

The order which these plug-ins are called during the execution of a GranOO's simulation is specified in a separated XML (eXtensible Markup Language) file called *input* file. This input file allows to parametrize in a standard manner an numerical experiment. It resumes, in a human readable format, all the treatments processed during the execution of a simulation.

5 A SCIENTIFIC TOOL

In the GranOO's point of view, the user is also a developer. He develops its own application by using the standard tools provided by the workbench. By the way, GranOO is a powerful tool that gives to the user the possibility to do what-he-wants inside a coherent framework. The programming frame used by GranOO allows an easy integration of these different developments. If a user supposes that its development is interesting for the rest of the community, he could submit its work to the GranOO's developer to integrate it in the standard distribution. This organization, based on the free software philosophy, allows to GranOO to capitalize each personal work in a coherent and documented framework.

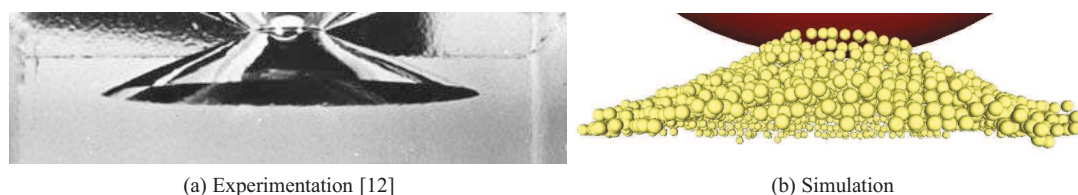


Figure 2: The hertzian cone crack

6 APPLICATION EXAMPLE: THE HERTZIAN CONE CRACK

The hertzian cone (see figure 2a) is produced while loading a brittle solid with a spherical indenter. It was first observed by Hertz [7, 8] in the end of the eighteenth century. This phenomena has been intensively studied; however, computational models are still in discussion [9, 5]. Figure 2b shows the obtained results of the associated DEM simulation. To validate the results, the geometrical characteristics of the numerically hertzian cone crack were compared to the experimentally one. The measures show a good adequation between the numerical results and the experimental observations. This kind of problem shows the ability of the DEM and the associated workbench to deal with non-trivial crack phenomena like the hertzian cone crack problem.

7 CONCLUSION

The GranOO project has conducted to the development of a free workbench for discrete element simulation. The numerical method chosen is well adapted to dynamic and discontinuous problems (dynamic solver, easy contact detection). A methodology has been proposed to solve quantitatively these problems and has been implemented in GranOO. Of course, most of the work to obtain predictive results remains to be done. The goal of the GranOO workbench is to widen the number of scientist that can use DEM simulation to generate fruitful collaboration and improve the level and number of innovation in that field.

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