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A discrete element and finite element coupled scheme for particle-structure interaction

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Abstract. This work presents a computational framework for the simulation of problems wherein discrete solid particles may interact with thin flexible structures, such as beams, shells and membranes. The particles are assumed to be spherical, following a DEM (discrete element method) approach, whereas the flexible structures are described by large displacements/finite rotations kinematics, leading ultimately to large deformations finite element (FEM) formulations. The DEM model is implemented within a Fortran program called PSY (Particle System Analysis Program), and the FEM model within a C++ program called GIRAFFE (Generic Interface Readily Accessible for Finite Elements). Both are in-house codes that have been extensively developed by two of the authors in the past years. The models are coupled in a staggered, implicit way embedded within a time-marching integration scheme wherein the two codes communicate with each other in an efficient, run-time, memory-sharing way that truly boosts up computational performance. The aim of this work is to present the computational scheme devised to couple both models, which ultimately led to a unified project called GIPSY. A few possibilities of such robust DEM-FEM scheme are illustrated by means of numerical examples.

Keywords: Particles, Flexible structures, Particle-Structure interaction, Discrete element method, Finite element method.

1 Introduction

Contact between rigid particles and deformable structures is a recurring phenomenon within several areas of study. It can occur in different ways, such as piles foundation settlement with the soil, conveyor belt ore transport, industrial painting, additive manufacturing, among other examples. It is a complex phenomenon, involving separate (although coupled) physics, with numerous action and reaction forces from multiple contact occurrences, with occasional shear forces (friction), which in turn can damage the material. The way that we can treat the contact physics depends intrinsically on the problem´s geometry. For example, in a conveyor belt transporting grains, there are two different types of material interactions, which are the grains, treated as rigid solid particles, and the conveyor belt, which can be treated as a continuum (structural) shell.

In a general perspective, solid particles are used to describe granular and particulate materials, which Duran [1] defines as an agglomeration of discrete macroscopic solids which are in contact with each other most of the time. It is possible to see these materials in a number of human applications and natural phenomena, such as beach sands, food grains, construction materials, industrial powders and many others. For the study and modeling of these materials, the computer program PSY (Particle Systems Analysis Program) is being developed at the University of São Paulo by Prof. Eduardo M. B. Campello. PSY is conceived to serve as a programming environment and advanced simulation tool. It is written in Fortran 90/95/2003 and is fully based on the object-oriented paradigm, with encapsulation, data processing, polymorphism, inheritance and operator loading. The kinematic and dynamic descriptions of the particles are based on a special formulation of the Discrete Element

Method (DEM), as proposed by Campello [2]–[4], and Campello and Cassares [5].

To allow the study and computational modeling of contact between deformable bodies and, in particular, structures, the computer program GIRAFFE (Generic Interface Readily Accessible for Finite Elements) is being developed at the University of São Paulo by prof. Dr. Alfredo G. Neto. GIRAFFE is a computational platform written in C++ language, also under the object orientated concept, with use of virtual classes. Inside the program there are a number of contact and finite element models implemented for bars, beams, tubes, shells, point masses, rigid bodies, springs and dampers, based on both advanced contact algorithms (see e.g.: Gay Neto and Wriggers [6],[7], and Gay Neto, Pimenta and Wriggers [8]–[10]) and kinematics formulations (see Pimenta, Campello, and Wriggers [11], [12], and Campello, Pimenta, and Wriggers [13]).

The aim of this work is to propose a framework to couple both codes (PSY and GIRAFFE) in an efficient, run-time, memory-sharing way, leading to a unified project called GIPSY. This framework will be a powerful tool for the simulation of problems wherein particle materials interact with thin flexible structures, such as (but not restricted to) particle deposition processes for surface engineering applications, the transport of grains in flexible conveyor belts in the mining industry, particle bombardment systems on membrane and cell structures, 3D manufacturing of flexible electronics, and many others. Throughout the text, italic letters $(a,b,\ldots,\alpha,\beta,\ldots,A,B,\ldots)$ denote scalar quantities, boldface italic letters $(\boldsymbol{a},\boldsymbol{b},\ldots,\boldsymbol{\alpha},\boldsymbol{\beta},\ldots)$ denote vectors and boldface italic capital letters $(\boldsymbol{A},\boldsymbol{B},\ldots)$ denote second-order tensors in a three dimensional Euclidian space.

2 Summary of the DEM model

The main idea behind the DEM for describing the mechanical behavior of a group of solid entities is by understanding and mapping the individual motion of each one of these entities. In this paper's context, the solid entities (or discrete elements) will be called "particles". It is assumed that the particles interact with each other and with its surroundings by means of forces, which can be a combination of contact forces (with both normal and friction components) and non-contact forces (e.g., drag, gravity, electromagnetic repulsion/attraction, etc.). The contact forces are due to collisions and touching with other particles, obstacles, rigids walls and occasionally deformable structures (such as beams and shells). With the aim to estabilish a general framework, we will considerer here only spherical particles. The model herein summarized is described in depth in Campello [2]–[4] and Campello and Cassares [5].

Let us consider a system of N_P particles each with mass m_i, radius r_i and rotation inertia $j_i = 2/5(m_i r_i^2)$, with $i = 1,\ldots,N_P$. The position of a particle will be denoted by vector $\boldsymbol{x}_i$, the velocity by vector $\boldsymbol{v}_i$ and the spin by vector $\boldsymbol{w}_i$, as shown in Figure 1. Motion description of a particle. Point P belongs to the particle's surface.. The rotation vector relative to the beginning of the motion is denoted by $\boldsymbol{\alpha}_i$, whereas the incremental rotation vector is denoted by $\boldsymbol{\alpha}_i^{\Delta}$. Contrary from the usual, we take this vector as being the Rodrigues rotation vector instead of the classical Euler rotation vector. For a detailed account of the rotation description we refer the reader to Campello [4].

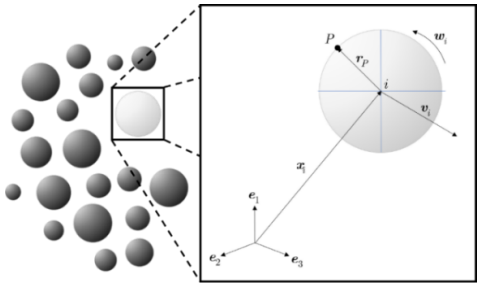


Figure 1. Motion description of a particle. Point P belongs to the particle's surface.

From the Euler's laws, the following equations must hold for each particle at every time instant t,

$$\begin{aligned} m_i\ddot{\boldsymbol{x}}_i &= \boldsymbol{f}_i^{\text{tot}}, \\ j_i\dot{\boldsymbol{w}}_i &= \boldsymbol{m}_i^{\text{tot}}. \end{aligned} \tag{1}$$

Here, we denote $\boldsymbol{f}_i^{\text{tot}}$ as the total force vector acting on the particle and $\boldsymbol{m}_i^{\text{tot}}$ as the total moment vector with respect the particle's center. The superposed dots shown above denote time differentiation. The total force $\boldsymbol{f}_i^{\text{tot}}$ is the sum of the following force contributions,

$$\boldsymbol{f}_i^{\text{tot}} = m_i \boldsymbol{g} + \boldsymbol{f}_i^{\text{drag}} + \boldsymbol{f}_i^{\text{nf}} + \boldsymbol{f}_i^{\text{con,p}} + \boldsymbol{f}_i^{\text{fric,p}} + \boldsymbol{f}_i^{\text{con,str}}, \tag{2}$$

where $\boldsymbol{g}$ is the gravity acceleration vector, $\boldsymbol{f}_i^{\text{drag}}$ is the drag force vector, $\boldsymbol{f}_i^{\text{nf}}$ are the forces due the near-field interactions with others particles, $\boldsymbol{f}_i^{\text{con,p}}$ are the normal forces due to contacts stemming from collisions with other particles as well as obstacles and rigid walls (herein given through Hertz contact theory), $\boldsymbol{f}_i^{\text{fric,p}}$ are the tangential forces due to friction caused by these collisions (herein given through a consistent stick-slip scheme), and $\boldsymbol{f}_i^{\text{con,str}}$ the forces due to contacts with deformable structures (which include both normal and frictional contributions, coming from solution of the particle-structure contact problem as described in section 4). In the same way, the total moment applied on the particle will be given by the sum of the following contributions,

$$\boldsymbol{m}_i^{\text{tot}} = \boldsymbol{m}_i^{\text{fric,p}} + \boldsymbol{m}_i^{\text{con,str}}, \tag{3}$$

where $\boldsymbol{m}_i^{\text{fric,p}}$ is the moment generated by the friction forces from other particles (and obstacles and rigid walls) and $\boldsymbol{m}_i^{\text{con,str}}$ is the moment generated by the friction forces from the neighboring structures. Numerical time integration of equation (1) provides the particles' motion. This is done here by the integration algorithm proposed in Campello [3], which has both implicit and explicit versions. In this work, we adopted the explicit version only, since the inter-particle contacts inherently require a very small time-step, thus rendering the implicit version unnecessary. For the sake of conciseness, the integration algorithm will be omitted here.

3 Summary of the FEM model

The structures´ deformation (we are mainly interested in beams and shells here, the latter of which membranes are a special case) are here described by the advanced kinematics models (accounting for large deformations and finite rotations) of Campello, Pimenta and Wriggers [14], Pimenta, Campello, and Wriggers [11]-[12], Gay Neto [15] (in which the geometrically-exact rod model is employed for dynamics of slender long offshore risers, with contact with the seabed), and Ota et al. [16] (in which the geometrically-exact shell model is employed for dynamics, using the Newmark's (implicit) integration scheme and the principle of virtual work). Beams are treated as isoparametric elements with 2 or 3 nodes each, and shells with the triangular element so-called T6-3i (incompatible, quadratic in displacements and linear in rotations, see Campello, Pimenta, and Wriggers [14], and Campello [17]). The time integration is done by the implicit Newmark method (with possibility to consider structural damping, in this case, of Rayleigh type, as presented for this context by Ota et al. [16]).

4 Particle-structure and structure-structure contact

For particle-structure contact, the contact formulation basis adopted here is that of Gay Neto, Pimenta, and Wriggers. Accordingly, for particle-beam interactions, we follow a simple strategy in which the beams are assumed to be of circular cross section, and treated as a set of spheres (of same radius of the beam´s cross section) whose centers lie on the beam's axis. This approximation to the beam's geometry is adopted *only for the sake of contact detection*, and not for the beam´s kinematics. The advantage of this approach is the simplicity of the contact detection scheme (which amounts to a sphere-sphere contact), thereby sparing the solution to a minimum distance problem, which could be untenable for large multi-particle systems. It has been successfully used by the authors as it can be seen in Gay Neto and Campello [19]. GIRAFFE also may handle more complex contact models between beams (see, e.g., Gay Neto and Wriggers [7] and Gay Neto, Pimenta and Wriggers [8]–[10]).

For particle-shell interactions, in turn, the contact model here adopted is that of Neto, Pimenta, and Wriggers [8]. This amounts to contact between two surfaces, the first one being given by a spherical shape Γ_S, with radius r (herein representing the boundary of a spherical particle of the DEM model), and the second one being a general surface Γ, representing the surface of the shell. The model is an enhanced master-slave contact, considering as the slave point the spherical surface Γ_S of the particle (with its rigid body movement attached to the movement of the particle´s center) and as the master the Γ surface of the shell. Accordingly, in order to describe the

configuration evolution of the slave surface, six degrees of freedom (DOFs) are required, so, for a time interval between any two successive configurations, "i" and "$i+1$", the 6-dimensional vector $\boldsymbol{d}_S^{\Delta}$ is used to handle the slave surface's DOFs.

The master surface is parameterized using a vector $\boldsymbol{c} = [\,\zeta \quad \theta\,]^{\mathrm{T}}$, which contains the convective coordinates ζ and θ of points of the surface that are candidate to establish contact with Γ_{S}. In the general form, the master surface is dependent on an N-dimensional vector $\boldsymbol{d}_M$, containing N values of generalized coordinates, representing the DOFs related to the Γ surface's motion in space, such that we may write $\Gamma = \widehat{\Gamma}(\boldsymbol{c},\boldsymbol{d}_M)$. The contact problem can be seen as the search for a point of convective coordinates $\bar{\boldsymbol{c}} = [\,\bar{\zeta} \quad \bar{\theta}\,]^{\mathrm{T}}$ which has the minimum distance to the particle's center $\boldsymbol{x}_C$, with fixed set of DOFs. We assume that Γ is smooth, such that its tangent directions are given by $\Gamma_{,\zeta}$, and $\Gamma_{,\theta}$. The minimum distance problem between the two bodies can be defined through the following orthogonality relation,

$$\boldsymbol{r} = \begin{cases} \Gamma_{,\zeta} \cdot (\boldsymbol{x}_C - \Gamma) = 0 \\ \Gamma_{,\theta} \cdot (\boldsymbol{x}_C - \Gamma) = 0 \end{cases}, \tag{4}$$

which is solved here through a Newton-Raphson scheme, furnishing the coordinates $\bar{\boldsymbol{c}}$. To test for possible penetration, we resort to the gap function $\mathbf{g}_n$ given by,

$$\mathbf{g}_n = (\boldsymbol{x}_C - \Gamma) - r\boldsymbol{n}\,, \tag{5}$$

providing a scalar quantity $g_n = (\boldsymbol{x}_C - \Gamma)\cdot\boldsymbol{n} - r$ which is then used as the contact detector. If contact occurs, the corresponding force contribution must be included into the weak form of the shell, as well as into the total force vector of the particle. To enforce the non-penetration condition, and thus account for the normal contribution in the weak form, we resort to the penalty method and define the following contact potential

$$W_n = \frac{1}{2}\varepsilon_n \mathbf{g}_n \cdot \mathbf{g}_n\,, \tag{6}$$

where ε_n is the normal penalty parameter ("normal contact stiffness"). This leads to the following contribution into the shell weak form,

$$\delta W_n = \varepsilon_n \mathbf{g}_n \cdot \delta\mathbf{g}_n\,. \tag{7}$$

where $\delta\mathbf{g}_n = (\delta\boldsymbol{x}_C - \delta\Gamma_n) - r\delta\boldsymbol{n}$.

For beam-beam interactions, in turn, we follow the simple strategy proposed in Gay Neto, Pimenta, and Wriggers [18].

5 Coupled DEM-FEM solution scheme

The models summarized previously are implement in our in-house codes PSY [20] (for DEM analysis of particle systems), written in Fortran language, and GIRAFFE [21] (for FEM and contact analyses of structures), written in C++. Here, the FEM solution loop is taken as the "host" loop (although the DEM loop could likewise be taken), and thereby GIRAFFE is taken as the "host code", being responsible for handling all the input data, such as all environment conditions, forces, boundary conditions, material properties and solution parameters (i.e., time step size, converge tolerance, etc.). To couple the codes in an efficient manner, we made use of the C/C++ and Fortran interoperability, enabling full (on-time, memory-sharing) communication between the codes. In the end, a unified project called GIPSY was attained.

An earlier version of this code coupling was implemented previously through the use of input and output text files. In such scheme, at every time step of the solution GIRAFFE writes a results file (containing the current positions, velocities, angles and spins of the beams and shells, as well as their occasional contact forces with the particles) and calls PSY, which then reads it as an input file. PSY then computes the new positions, velocities, angles and spins of the particles and passes all these data back to GIRAFFE through another results file, which is then read by GIRAFFE, refeeding the solution. Thereafter, the particles are kept frozen in space until the convergence of the current time step is achieved. This process is repeated for each time step. In the new coupling scheme proposed here, which makes extensive use of the interoperability between the code languages, we no longer need text files and thus were able to come up with an incredibly more efficient coupling between the codes.

At the algorithmic level, the main idea behind the coupling is to have a staggered scheme: at every time step, the FEM solver treats the particles as fixed geometric entities in space, with positions, angles, velocities and spins given from the previous converged time step computed by PSY. It then computes the new state of the beams and shells and passes them back to the DEM solver (including the occasional contact forces between particles and beams as well as particles and shells), which in turn treats the beams and shells as fixed in space and computes the motion of the particles, within the time step. Whenever the particles make contact with the structures, GIRAFFE computes the corresponding reaction forces and moments and passes them to PSY (with opposite sign) through the vectors $\boldsymbol{f}_i^{\text{con,str}}$ and $\boldsymbol{m}_i^{\text{con,str}}$ of equations (2) and (3), respectively, leading to new displacements, rotations, velocities and spins experienced by the particles. Such procedure is detailed in Gay Neto, and Campello [19].

6 Numerical examples

In this section, we will provide two numerical simulations to validate and illustrate the applicability of our new coupling scheme. For time integration, the same time step was adopted on both DEM and FEM solutions. In all examples, the convergence tolerance within the Newton iterations was $Tol = 10^{-8}$, for both unbalanced forces and moments (and incremental displacements and rotations) in the FEM solver. No tolerance was needed on the DEM solver since the explicit version of the method is being used.

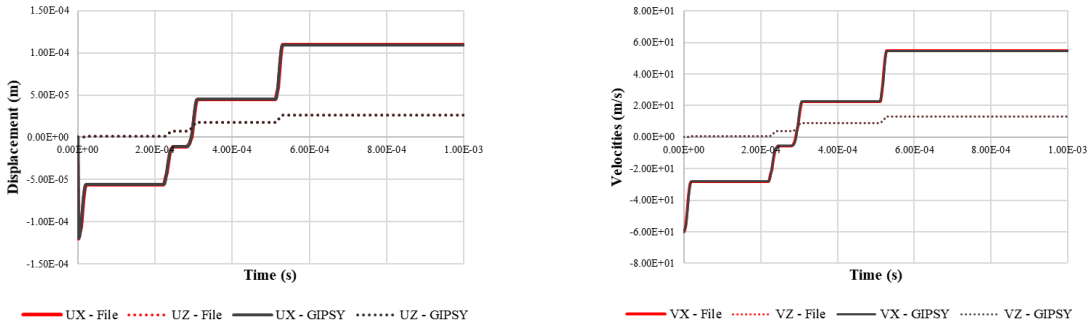
6.1 Single particle interacting with a flexible rod

To validate the new scheme, as a benchmark problem we adopted the single particle interaction with a flexible rod, as provided by Gay Neto, and Campello [19]. Fig. 2 shows some snapshots of the simulation. The particle has a radius of $r_P = 0.01\,\text{m}$, mass density $\rho_P = 1300\,\text{kg/m}^3$, Young's modulus of $E_P = 10$ GPa and Poisson's coefficient of $\upsilon_P = 0.45$. The rod, in turn, has a cross-sectional radius of $r_{\text{rod}} = 2.5\,\text{cm}$, length $L = 5$ cm, mass density $\rho_{\text{rod}} = 8000$ kg/m³ and elastic properties $E_{\text{rod}} = 210\,\text{GPa}$ and $\upsilon_P = 0.3$. The particle has an initial velocity of $\boldsymbol{v}(0) = (-60, 0, 0)$ [m/s], and the rod has its displacements and rotations fixed at the base.

time 0.00 s time 0.00015 s time 0.0003 s time 0.0006 s time 0.0008 s

Figure 2. Snapshots of the motion at some selected time instants.

A time step size of $\Delta t = 2 \times 10^{-6}$ s is adopted, being the final time $t_f = 0.01$ s. The penalty parameter for rod-particle contact is $\varepsilon_n = 1.41 \times 10^7$ N/m. The rod is discretized with 10 3-node finite elements.



(a) Particle's displacements (b) Particle's velocities

Figure 3. Validation results.

As it can be seen from Fig. 3, the results from the present and earlier coupling schemes are *exactly the same*.

Worth mentioning that, in the previous (i.e., coupling by file) implementation, this example takes 98.23 s to complete in a standard, single-core laptop computer, whereas in the new approach it takes only 39.40 s, an increase of about 250 % on the program's performance. *This increase will be much higher for large particle systems*.

6.2 Particles moving through a flexible shell

In this model problem, we analyze the motion of grains over a thin-walled surface, the cross-section of which is shown in Fig. 4. This example explores the contact between particles with a flexible structure, modeled using shell finites elements. The resulting surface was composed of 3000 triangular elements, with 6 nodes each, leading to a problem with 6161 nodes. The thickness of the surface is 1 mm, and its material is aluminum, with an elastic modulus of 70GPa, Poisson ratio of 0.3, and mass density of 2700 kg/m³. The nodes from one of surface's tips have both translations and rotations constrained, while all others are free as in a cantilever. The struct geometry was based on the example shown on Gay Neto, Pimenta, and Wriggers [8].

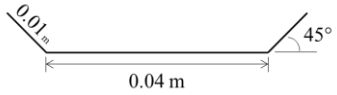


Figure 4. Surface's cross-section.

Initially, the particles are placed into a rigid container. A total of 2080 particles with a 1 mm radius are present, with $E_P = 1\,\text{MPa}$, $\upsilon_P = 0.3$ and $\rho_P = 2000$ each. Gravity acts downwards with a magnitude of $g = 9.81\,\text{m/s}$. The penalty parameter used for the surface-particle contacts was $\varepsilon_n = 2.98 \times 10^2\,\text{N/m}$, and the time step was $\Delta t = 1 \times 10^{-4}\,\text{s}$. The Fig. 5 shows some snapshots of the simulation.

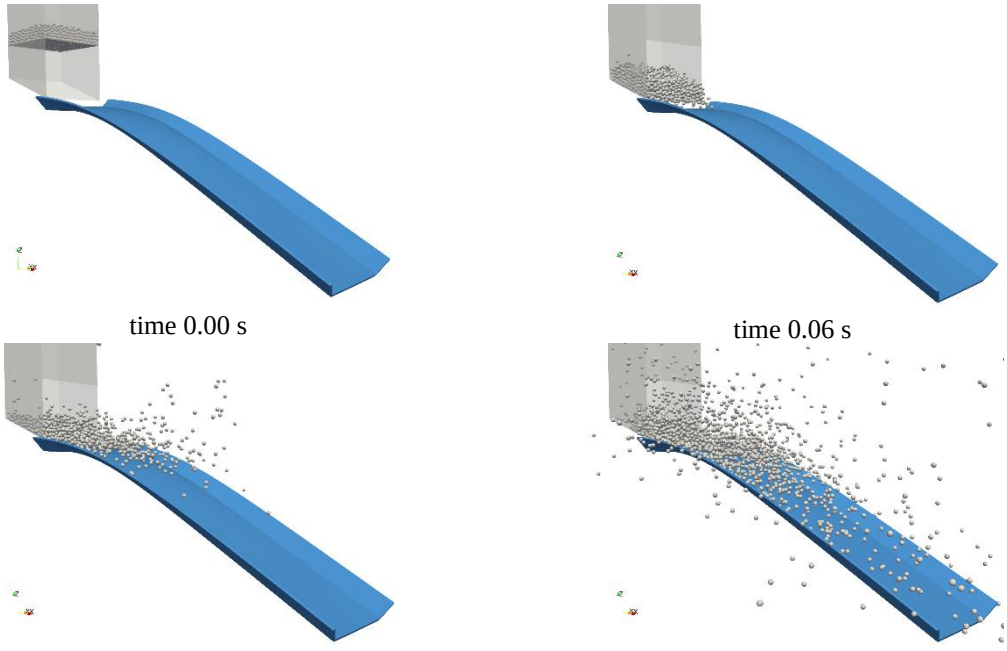


Figure 5. Snapshots of the motion at some selected time instants of the 2nd example.

7 Conclusions

The main purpose of this work was to present an efficient coupling framework for problems wherein particles may interact with flexible surfaces. As it has been shown from the first numerical example, the new scheme based

on the interoperability between C++ and Fortran languages proved to give us the very same results as from the earlier coupling scheme, while attaining a very significant boost in performance. The contact method proved to handle properly the motion of both discrete and continuum materials, allowing multiple contact between each other. More elaborate examples are under work by the authors.

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