

A distributed Lagrange multiplier based / fictitious domain method to model acoustic wave propagation in granular media in a fluid

David Imbert and Sean McNamara

Institute of Physics, Rennes (UMR UR1/CNRS 6251)
University of Rennes 1



5-7 December 2011

Summary

- 1 Introduction
- 2 Governing equations
- 3 Computational schemes
- 4 Numerical experiments
- 5 Conclusions

Section contents

- 1 Introduction
 - Granular media & acoustics
 - Modelling
- 2 Governing equations
 - Strong form
 - Weak form
 - Fictitious domain formulation
- 3 Computational schemes
 - Spatial discretization
 - Time discretization
- 4 Numerical experiments
 - Test with 1 grain
 - Test with 2 grains
- 5 Conclusions

Granular media

- Conglomeration of macroscopic discrete particles called grains

Granular media

- Conglomeration of macroscopic discrete particles called grains
- Energy loss whenever grains interact due to friction

Granular media

- Conglomeration of macroscopic discrete particles called grains
- Energy loss whenever grains interact due to friction
- Characteristics of solids, liquids or gas depending on the average energy per grain

Granular media

- Conglomeration of macroscopic discrete particles called grains
- Energy loss whenever grains interact due to friction
- Characteristics of solids, liquids or gas depending on the average energy per grain
- Ubiquitous in nature and industry

Granular media

- **Conglomeration** of macroscopic **discrete** particles called **grains**
- **Energy loss** whenever grains interact due to **friction**
- Characteristics of **solids, liquids or gas** depending on the average energy per grain
- Ubiquitous in **nature** and **industry**

Granular media

- **Conglomeration** of macroscopic **discrete** particles called **grains**
- **Energy loss** whenever grains interact due to **friction**
- Characteristics of **solids, liquids or gas** depending on the average energy per grain
- Ubiquitous in **nature** and **industry**

Examples



Figure: Dunes



Figure: Rice



Figure: Capsules

Acoustics in granular media

- Medium undergoes structural **rearrangements** a long time before being completely stabilized.

Acoustics in granular media

- Medium undergoes structural **rearrangements** a long time before being completely stabilized.
- These events generate acoustic wave sources which can propagate:
 - through the granular medium skeleton when it's a **dry** one
 - both in skeleton and matrix when the granular medium is **submerged**

Acoustics in destabilized granular media

- Louder acoustic signals can be recorded: **avalanche precursors**

Acoustics in destabilized granular media

- Louder acoustic signals can be recorded: **avalanche precursors**
- Experimental acoustic measurements have already been done within the framework of the **StabInGraM ANR** project (*STAbility loss In GRAnular Media*).

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius
 - *interaction forces* are defined according to models:
 - normal force: linear, viscoelastic models...
 - tangential force: Haff & Werner's, Cundall & Strack's models...

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius
 - *interaction forces* are defined according to models:
 - normal force: linear, viscoelastic models...
 - tangential force: Haff & Werner's, Cundall & Strack's models...
 - numerically solve mechanics equations for *point particles*

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius
 - *interaction forces* are defined according to models:
 - normal force: linear, viscoelastic models...
 - tangential force: Haff & Werner's, Cundall & Strack's models...
 - numerically solve mechanics equations for *point particles*
 - *N-body* algorithm which manages a list of particles

Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius
 - *interaction forces* are defined according to models:
 - normal force: linear, viscoelastic models...
 - tangential force: Haff & Werner's, Cundall & Strack's models...
 - numerically solve mechanics equations for *point particles*
 - *N-body* algorithm which manages a list of particles
 - works fine in *vacuum* or *gas*

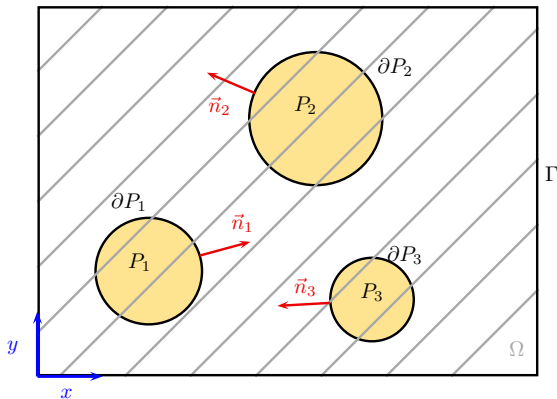
Molecular Dynamics

- *Molecular Dynamics* algorithm [PS05] is often used to simulate movements of interacting particles.
- Main characteristics:
 - *incompressible 2D rigid spheres* characterized by:
 - their center position, velocity and acceleration
 - their radius
 - *interaction forces* are defined according to models:
 - normal force: linear, viscoelastic models...
 - tangential force: Haff & Werner's, Cundall & Strack's models...
 - numerically solve mechanics equations for *point particles*
 - *N-body* algorithm which manages a list of particles
 - works fine in *vacuum* or *gas*
- **Problem:** if the matrix is a *liquid*, sound waves don't only propagate through the packing skeleton, but also through the liquid which is not taken in account by MD

Section contents

- 1 Introduction
 - Granular media & acoustics
 - Modelling
- 2 Governing equations
 - Strong form
 - Weak form
 - Fictitious domain formulation
- 3 Computational schemes
 - Spatial discretization
 - Time discretization
- 4 Numerical experiments
 - Test with 1 grain
 - Test with 2 grains
- 5 Conclusions

Domains



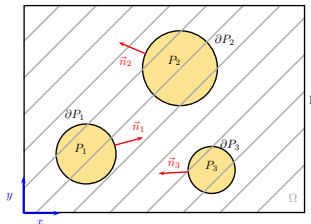
$$P = \bigcup_{i=1}^N P_i$$

Acoustic wave equation

$$\left\{ \begin{array}{ll} \rho_f \frac{\partial \vec{u}}{\partial t} + \nabla p = \vec{0} & \text{in } \Omega \setminus \overline{P(t)} \quad (1) \\ \frac{1}{\rho_f c_f^2} \frac{\partial p}{\partial t} + \nabla \cdot \vec{u} = 0 & \text{in } \Omega \setminus \overline{P(t)} \quad (2) \\ \vec{u} \cdot \vec{n}_i = \vec{U}_i \cdot \vec{n}_i & \text{on } \partial P_i(t) \quad (3) \end{array} \right.$$

perfectly matched layers on Γ

[BG05, GPHJ99]



Newton's second law

$$\left\{ \begin{array}{l} m_{g_i} \frac{d\vec{U}_i}{dt} = \vec{W}_i + \vec{B}_i + \vec{H}_i + \vec{F}_i \\ I_{g_i} \frac{d\omega_i}{dt} = T_i \end{array} \right. \quad (4)$$

(5)

Newton's second law

$$\begin{cases} m_{g_i} \frac{d\vec{U}_i}{dt} = \vec{W}_i + \vec{B}_i + \vec{H}_i + \vec{F}_i \\ I_{g_i} \frac{d\omega_i}{dt} = T_i \end{cases} \quad (4)$$

$$(5)$$

Forces acting on each particle

- weight: $\vec{W}_i = \rho_g V_{g_i} \vec{g}$
- buoyancy: $\vec{B}_i = -\rho_f V_{g_i} \vec{g}$
- hydrodynamic force: $\vec{H}_i = -\int_{\partial P_i(t)} p \vec{n}_i d\vec{n}_i$
- interaction force: $\vec{F}_i = \sum_{j=i}^N (F_{n_{i,j}}^{\vec{}} + F_{t_{i,j}}^{\vec{}})$
or spring force: $\vec{F}_i = -k(y - y_0)$

Kinematic equations & initial conditions

$$\left\{ \begin{array}{l} \frac{d\vec{X}_i}{dt} = \vec{U}_i \\ \frac{d\theta_i}{dt} = \omega_i \end{array} \right. \quad (6)$$

$$(7)$$

Kinematic equations & initial conditions

$$\begin{cases} \frac{d\vec{X}_i}{dt} = \vec{U}_i \\ \frac{d\theta_i}{dt} = \omega_i \end{cases} \quad (6)$$

$$(7)$$

Initial conditions:

$$\begin{aligned} \vec{u}|_{t=0} &= \vec{u}_0 & p|_{t=0} &= p_0 \\ \vec{U}_i|_{t=0} &= \vec{U}_{i,0} & \omega_i|_{t=0} &= \omega_{i,0} \\ \vec{X}_i|_{t=0} &= \vec{X}_{i,0} & \theta_i|_{t=0} &= \theta_{i,0} \end{aligned}$$

Combined spaces

Combined velocity space

$$\mathbb{U} = \{(\vec{u}, \vec{U}, \omega) | \vec{u} \in [L^2(\Omega \setminus \overline{P(t)})]^2, \vec{U} \in \mathbb{R}^2, \omega \in \mathbb{R} \quad (8)$$

$$\vec{u} \cdot \vec{n} = \vec{U} \cdot \vec{n} \text{ on } \partial P(t)\}$$

Combined variation space

$$\mathbb{V} = \{(\vec{v}, \vec{V}, \xi) | \vec{v} \in [L^2(\Omega \setminus \overline{P(t)})]^2, \vec{V} \in \mathbb{R}^2, \xi \in \mathbb{R} \quad (9)$$

$$\vec{v} \cdot \vec{n} = \vec{V} \cdot \vec{n} \text{ on } \partial P(t)\}$$

Combined equation of motion

Principle [GPHJ99]

Combine:

- wave equation in the fluid
- Newton's second law for grains

Combined equation of motion

Principle [GPHJ99]

Combine:

- wave equation in the fluid
- Newton's second law for grains

by performing the symbolic operation:

$$\int_{\Omega \setminus \overline{P(t)}} (1) \cdot \vec{v} \, d\vec{x} + (4) \cdot \vec{V} + (5) \xi = 0$$

$$\rho_f \frac{\partial \vec{u}}{\partial t} + \nabla p = 0 \quad (1)$$

$$m_g \frac{d\vec{U}}{dt} - (\rho_g - \rho_f) V_g \vec{g} + \int_{\partial P(t)} p \vec{n} \, d\ell - \vec{F} = 0 \quad (4)$$

$$I_g \frac{d\omega}{dt} - T = 0 \quad (5)$$

Fictitious domain method

Basic idea [GPP94]

- **Extend** the problem from $\Omega \setminus \overline{P(t)}$ to all of Ω in two steps:
 - 1 obtain an analogous combined equation of motion for $P(t)$ using a **rigid body motion constraint**: $\vec{u} = \vec{U}$ in $P(t)$
 - 2 add it to equation in $\Omega \setminus \overline{P(t)}$ to get the combined equation of motion **for all Ω**

Fictitious domain method

Basic idea [GPP94]

- **Extend** the problem from $\Omega \setminus \overline{P(t)}$ to all of Ω in two steps:
 - ① obtain an analogous combined equation of motion for $P(t)$ using a **rigid body motion constraint**: $\vec{u} = \vec{U}$ in $P(t)$
 - ② add it to equation in $\Omega \setminus \overline{P(t)}$ to get the combined equation of motion **for all Ω**
- Force the solution to **satisfy conditions** on $\partial P(t)$ and inside $P(t)$
 - ① remove the constraints from the combined velocity space (8)
 - ② enforce them as a side constraint using **Lagrange multipliers**

Fictitious domain method

Basic idea [GPP94]

- **Extend** the problem from $\Omega \setminus \overline{P(t)}$ to all of Ω in two steps:
 - ① obtain an analogous combined equation of motion for $P(t)$ using a **rigid body motion constraint**: $\vec{u} = \vec{U}$ in $P(t)$
 - ② add it to equation in $\Omega \setminus \overline{P(t)}$ to get the combined equation of motion **for all Ω**
- Force the solution to **satisfy conditions** on $\partial P(t)$ and inside $P(t)$
 - ① remove the constraints from the combined velocity space (8)
 - ② enforce them as a side constraint using **Lagrange multipliers**

Fictitious domain method

Basic idea [GPP94]

- **Extend** the problem from $\Omega \setminus \overline{P(t)}$ to all of Ω in two steps:
 - ① obtain an analogous combined equation of motion for $P(t)$ using a **rigid body motion constraint**: $\vec{u} = \vec{U}$ in $P(t)$
 - ② add it to equation in $\Omega \setminus \overline{P(t)}$ to get the combined equation of motion **for all Ω**
- Force the solution to **satisfy conditions** on $\partial P(t)$ and inside $P(t)$
 - ① remove the constraints from the combined velocity space (8)
 - ② enforce them as a side constraint using **Lagrange multipliers**

In order to keep:

- physical variables in all Ω
- Lagrange multipliers variables in $P(t)$

Section contents

- 1 Introduction
 - Granular media & acoustics
 - Modelling
- 2 Governing equations
 - Strong form
 - Weak form
 - Fictitious domain formulation
- 3 Computational schemes
 - Spatial discretization
 - Time discretization
- 4 Numerical experiments
 - Test with 1 grain
 - Test with 2 grains
- 5 Conclusions

Meshes

- 2 domains of definition : Ω (static) and $P(t)$ (time-dependent)

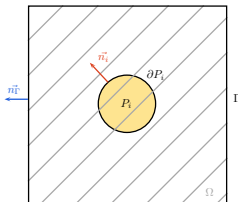


Figure: Domain

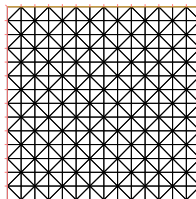


Figure: \mathcal{T}_{Ω_h}

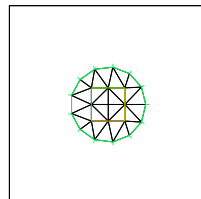


Figure: \mathcal{T}_{P_h}

Meshes

- 2 domains of definition : Ω (static) and $P(t)$ (time-dependent)
- \Rightarrow 2 meshes :
 - a **regular** grid \mathcal{T}_{Ω_h} for rectangular domain Ω
 - an **unstructured** grid \mathcal{T}_{P_h} for the grains

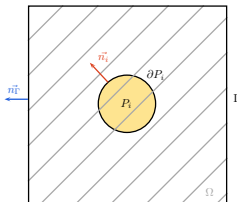


Figure: Domain

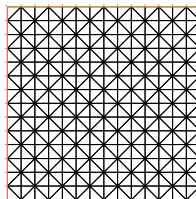


Figure: \mathcal{T}_{Ω_h}

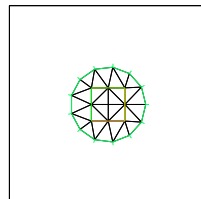


Figure: \mathcal{T}_{P_h}

Meshes

- 2 domains of definition : Ω (static) and $P(t)$ (time-dependent)
- \Rightarrow 2 meshes :
 - a **regular** grid \mathcal{T}_{Ω_h} for rectangular domain Ω
 - an **unstructured** grid \mathcal{T}_{P_h} for the grains
- mesh sizes are related by a condition : $h_P = \kappa h_\Omega$ with $1 < \kappa < 2$ which come from results on problems involving Lagrange multipliers [Bab73] (best results are obtained with $\kappa \approx 1.3$)

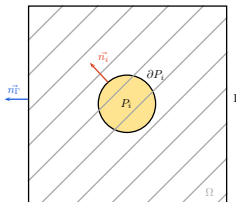


Figure: Domain

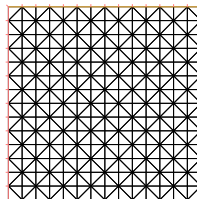


Figure: \mathcal{T}_{Ω_h}

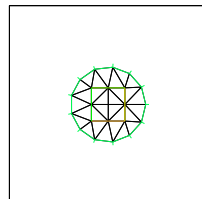


Figure: \mathcal{T}_{P_h}

Finite dimensional spaces

- Choice of approximation functions for each space :

$$\mathbb{Q}_h = \{q_h \in H^1(\Omega), q_h|_K \in P_1 \ \forall K \in \mathcal{T}_{\Omega_h}\} \quad (10)$$

$$\mathbb{W}_h = \{\vec{v}_h \in [L^2(\Omega)]^2, \vec{v}_h|_K \in RT_0 \ \forall K \in \mathcal{T}_{\Omega_h}\} \quad (11)$$

$$\Lambda_h = \{\vec{\mu}_h \in [L^2(\Omega)]^2, \vec{\mu}_h|_K \in RT_0 \ \forall K \in \mathcal{T}_{P_h}\} \quad (12)$$

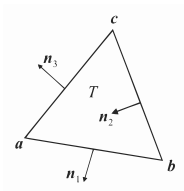


Figure: Raviart-Thomas element RT_0 [Hec]

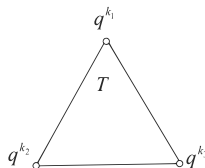


Figure: Lagrangian element P_1 [Hec]

Extra mesh for point-particles variables

- Solution functions \vec{U} and test functions \vec{V} are part of \mathbb{R}^2
- A priori FreeFEM++ can't handle those

Extra mesh for point-particles variables

- Solution functions \vec{U} and test functions \vec{V} are part of \mathbb{R}^2
- A priori FreeFEM++ can't handle those

Trick

- Use a 3rd grid $\mathcal{T}_{P_{d_h}}$ with only 1 triangle including the grain (triangle's incircle)
- Choose a P_0 constant Lagrangian finite element
- Then correct the area with the factor

$$\frac{\pi}{\sqrt{27}}$$

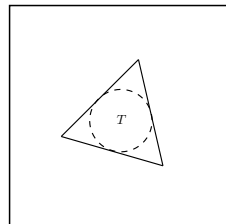


Figure: $\mathcal{T}_{P_{d_h}}$

Operator splitting

- Time-discretization using **Finite Differences Method**
- Final system is complete but too difficult to solve directly

Operator splitting

- Time-discretization using **Finite Differences Method**
- Final system is complete but too difficult to solve directly

Idea

Decouple operators that propagate wave and move the grains from the operators that enforce conditions in $P(t)$.

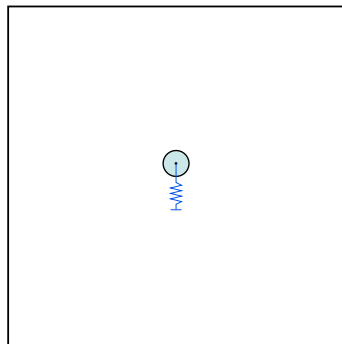
- Marchuk's fractional step [Mar90]

Section contents

- 1 Introduction
 - Granular media & acoustics
 - Modelling
- 2 Governing equations
 - Strong form
 - Weak form
 - Fictitious domain formulation
- 3 Computational schemes
 - Spatial discretization
 - Time discretization
- 4 Numerical experiments
 - Test with 1 grain
 - Test with 2 grains
- 5 Conclusions

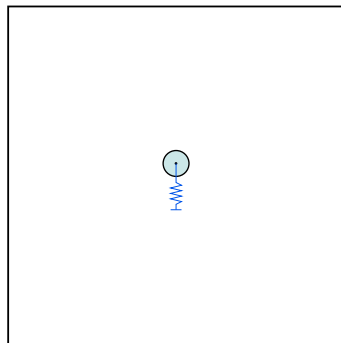
1 grain

- Fixed to a spring with a stiffness k



1 grain

- Fixed to a spring with a stiffness k
- Moved forward from its equilibrium position



Parameters

- Medias:

c_f	1,500 m/s
c_g	5,300 m/s
ρ_f	1.0 g/cm ³
ρ_g	2.4 g/cm ³

- Domains size:

Ω	5 × 5 cm
r	2 mm

- Forces:

\vec{g}	0 m/s ²
\vec{F}	$-k(y - y_0)$

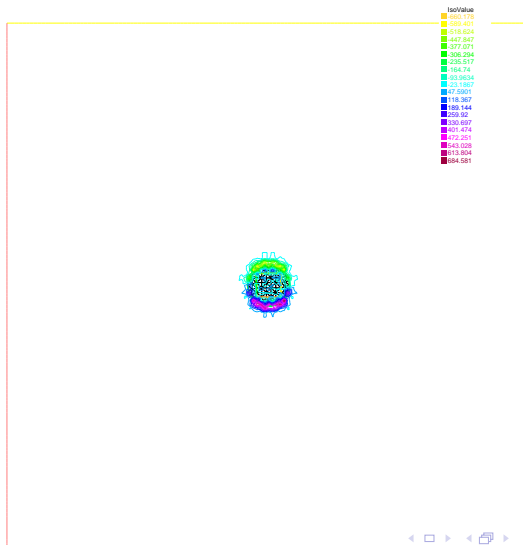
- Spring eigenfrequency:

$f_{0_{res}}$	0.2 MHz
---------------	---------

- Discretization:

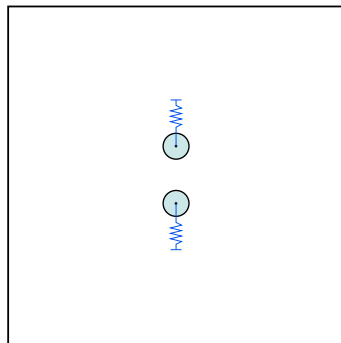
$N_x \times N_y$	136 × 136
N_t	346
Δx	0,37 mm
Δt	43 ns

Acoustic pressure field: 1 grain



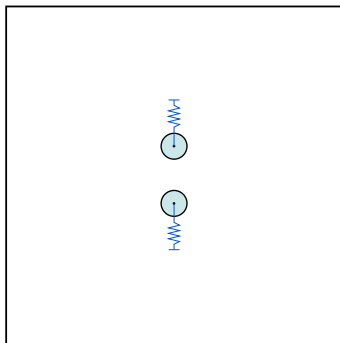
2 grains

- Both fixed to their own spring with the stiffness k



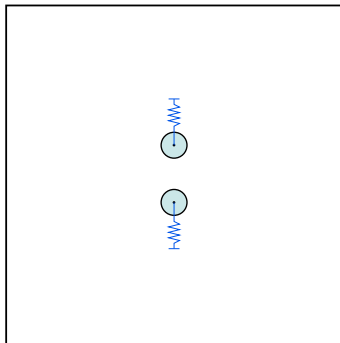
2 grains

- Both fixed to their own spring with the stiffness k
- The bottom one is moved forward from its equilibrium position



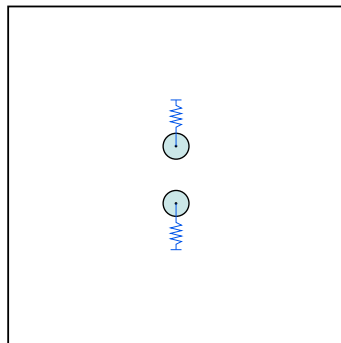
2 grains

- Both fixed to their own spring with the stiffness k
- The bottom one is moved forward from its equilibrium position
- The top one is at its equilibrium position

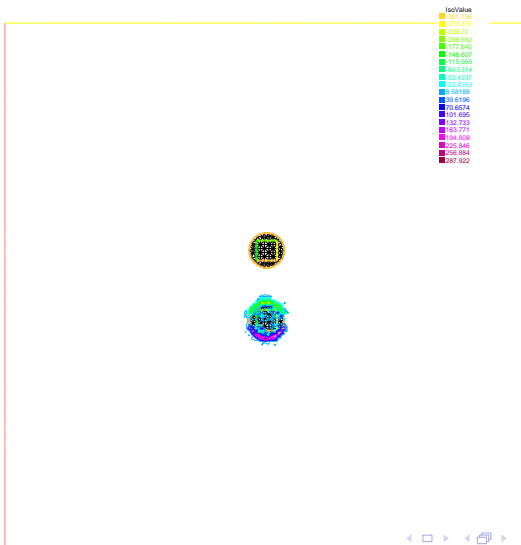


2 grains

- Both fixed to their own spring with the stiffness k
- The bottom one is moved forward from its equilibrium position
- The top one is at its equilibrium position
- Parameters are unchanged



Acoustic pressure field: 2 grains



Mechanical energy of each grain

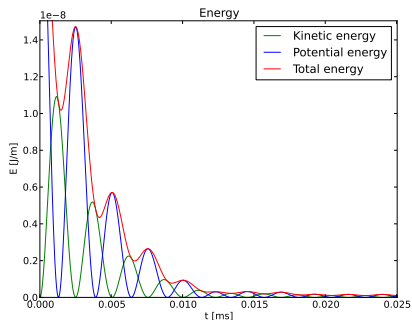


Figure: Bottom grain

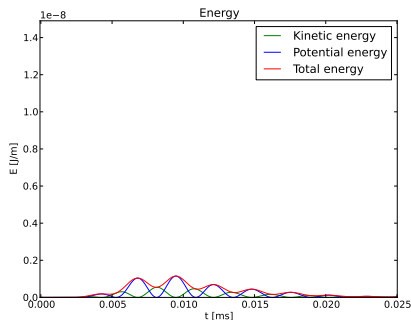


Figure: Top grain

Section contents

- 1 Introduction
 - Granular media & acoustics
 - Modelling
- 2 Governing equations
 - Strong form
 - Weak form
 - Fictitious domain formulation
- 3 Computational schemes
 - Spatial discretization
 - Time discretization
- 4 Numerical experiments
 - Test with 1 grain
 - Test with 2 grains
- 5 Conclusions

Conclusions & Outlook

● Conclusions

- Molecular Dynamic's philosophy preserved (infinite velocity inside the grain, elasticity in interaction forces)
- Good geometry representation of the grains
- *Perfectly Matched Layer* version done

Conclusions & Outlook

1 Conclusions

- Molecular Dynamic's philosophy preserved (infinite velocity inside the grain, elasticity in interaction forces)
- Good geometry representation of the grains
- *Perfectly Matched Layer* version done

2 Outlook

- Stability analysis of the scheme
- Contact forces
- Granular packing modelling
- Simulate acoustic emission of a destabilized granular medium
- Parallel version

References



I. Babuska.

The Finite Element Method with Lagrange multipliers.
Numerische Mathematik, 20:179–192, 1973.



V. A. Bokil and R. Glowinski.

An operator splitting scheme with a distributed Lagrange multiplier based fictitious domain method for wave propagation problems.
Journal of Computational Physics, 205:242–268, May 2005.



R. Glowinski, T.-W. Pan, T. I. Hesla, and D. D. Joseph.

A distributed Lagrange multiplier/fictitious domain method for particulate flows.
International Journal of Multiphase Flow, 25(5):755–794, August 1999.



R. Glowinski, T.-W. Pan, and J. Periaux.

A fictitious domain method for Dirichlet problem and applications.
Computer Methods in Applied Mechanics and Engineering, 111(3-4):283 – 303, 1994.



F. Hecht.

FreeFEM++.
Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie, third edition.



G. I. Marchuk.

Splitting and alternating direction methods.
In P.G. Ciarlet and J.L. Lions, editors, *Finite Difference Methods (Part I) - Solution of Equations in R (Part 1)*, volume 1 of *Handbook of Numerical Analysis*, pages 197 – 462. Elsevier, 1990.



T. Pöschel and T. Schwager.

Computational granular dynamics: models and algorithms.
Springer-Verlag, 2005.