

# Accelerated granular matter simulation

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## Abstract

Modeling and simulation of granular matter has important applications in both natural science and industry. One widely used method is the discrete element method (DEM). It can be used for simulating granular matter in the gaseous, liquid as well as solid regime whereas alternative methods are in general applicable to only one. Discrete element analysis of large systems is, however, limited by long computational time. A number of solutions to radically improve the computational efficiency of DEM simulations are developed and analysed. These include treating the material as a nonsmooth dynamical system and methods for reducing the computational effort for solving the complementarity problem that arise from implicit treatment of the contact laws. This allow for large time-step integration and ultimately more and faster simulation studies or analysis of more complex systems. Acceleration methods that can reduce the computational complexity and degrees of freedom have been invented. These solutions are investigated in numerical experiments, validated using experimental data and applied for design exploration of iron ore pelletising systems.



## Sammanfattning

Modellering och simulering av granulära material har viktiga tillämpningar inom såväl naturvetenskap som i industrin. En vanlig metod är den så kallade diskreta elementmetoden (DEM). Den kan användas för simulering av granulära material i alla dess olika faser - gas, flytande och fast form - medan alternativa metoder i allmänt endast stöder en av faserna. Diskret elementanalys av stora system är dessvärre begränsat av långa beräkningstider. Ett antal lösningar för att dramatiskt öka beräkningseffektiviteten i DEM-simuleringar har utvecklats och analyserats. Dessa inkluderar att beskriva materialet som ett system med icke-slät dynamik och metoder för att öka effektiviteten i beräkningarna av de komplementaritetsproblem som en implicit hantering kontaktlagarna medför. Detta möjliggör tidsintegration med stora tidssteg vilket kan omsättas i fler och snabbare simuleringsstudier eller analys av mer komplexa system. Lösningarna undersöks i numeriska experiment, valideras mot experimentella mätningar och tillämpas för design-utforskning av system inom järnmalmspelletisering.



## Acknowledgements

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# Preface

This thesis consists of an introduction and the following papers:

- I Martin Servin, Da Wang, Claude Lacoursière, Kenneth Bodin, *Examining the smooth and nonsmooth discrete element approaches to granular matter*, Journal for Numerical Methods in Engineering, vol. 97, no. 12, 878-902, 2014.
- II Da Wang, Martin Servin, and Kjell-Ove Mickelsson, *Outlet design optimization based on large-scale nonsmooth DEM simulation*, Powder Technology, vol. 253, pp. 438 - 443, 2014.
- III Da Wang, Martin Servin, Tomas Berglund, Kjell-Ove Mickelsson, and Stefan Rönnbäck, *Parametrization and validation of a nonsmooth discrete element method for simulating flows of iron ore green pellets*, Powder Technology, Powder Technology vol. 283, 475-487, 2015.
- IV Da Wang, Martin Servin, and Tomas Berglund, *Warm starting the projected Gauss-Seidel algorithm for granular matter simulation*, submitted 2015.
- V Martin Servin, and Da Wang, *Adaptive model reduction for nonsmooth discrete element simulation*, submitted 2015.



# 1 Background

Granular matter is collection of discrete macroscopic particles that interact locally by interfacial contact forces that are highly dissipative [1]. Examples are natural grains of corn and minerals and manufactured pharmaceuticals pills and pellets. It has been estimated that more than 50 % of the sales in the world deal with products that involve handling of granular materials at some stage. In most large-scale systems, experiments and measurements are impossible for practical and economical reasons. Modeling and computer simulation is indispensable for deeper understanding of the nature of granular materials and for making radical improvements and innovating entirely new solutions in processing and transportation systems. The nature of granular materials is very complex and rich in phenomena despite the simplicity of the models at grain level. The materials are strongly dissipative and meta-stable with critical phenomena like jamming transitions and avalanches. There is a strong relation between the macroscopic bulk properties and the microscopic properties, such as grain size, shape, friction and elasticity. Granular materials can switch quickly between solid, liquid and gas state [2]. Especially characteristic is the occurrence of strong force chains - that reach through the material and cause arching phenomena that give structural strength. This is fundamental for the design of storage silos, and make grains in an hourglass either jam or flow at steady rate. Another fascinating phenomena is size segregation. When granular materials are excited by periodic perturbation, such as vibration, larger grains move upwards and smaller ones downwards despite having the same mass density. Popularly this is known as the *Brazil nut effect* and explains why the largest nuts are found on the top in a container of mixed nuts. This can be understood as a convection phenomena and make it extremely difficult to produce homogeneous mixtures of granular materials. For many phenomena, it is necessary to explicitly model the individual particles and their interactions. This is most challenging task considering that one cubic meter of sand consists of roughly one billion grains. Each sample can have big variations in the microscopic properties, it can be loosely or densely packed and be influenced in numerous different ways: shaken, rotated, compressed, sheared, suspended in fluid etc. This renders a tremendous large space of possible behaviour to investigate. The goal of this thesis is to provide new knowledge and methods to accelerate the modeling and exploration of complex granular systems using computer simulation.

## 2 Computational Granular Dynamics

There is a multitude of methods for simulating granular materials [4]. One widely used method is the discrete element method (DEM). It can be used for simulating granular matter in the gaseous, liquid as well as solid regime whereas alternative methods are in general applicable to only one regime. With DEM, and other particle based methods, the characteristic dynamics of granular materials emerges naturally

through the collective behaviour of the interacting particles and with direct relation to the microscopic properties. Resolving the systems at grain level come with considerable computational cost, however. At large enough scales it becomes intractable to use DEM. In the time of writing this thesis, the largest reported number of particles in a scaling experiment with a nonsmooth discrete element method is  $2.8 \times 10^{10}$  non-spherical particles and  $1.1 \times 10^{10}$  contacts using peta-scale supercomputers with almost 500 thousands processor cores [3]. To increase the size further, reduce computational time or the need for supercomputers, a more coarse model must be used. Essentially there are two alternatives to DEM: cellular automata models and continuum mechanics. Cellular automata models make use of a regular lattice where each grid cell attain a certain state that represent the local state of the granular media. The system evolves in time by a set of rules that determine the new state of each cell in terms of the current state of the cell and the states of the neighbouring cells. Cellular automata models have been applied mostly to granular gases, described by kinetic theory and with the automata rules derived from statistical collision models. This has for instance helped explaining transport and pattern formation of sand dunes [5]. On large enough length scales it is reasonable to treat the granular material using continuum mechanics, either as a solid, liquid or a multiphase model [1]. Simulations based on these models involve solving partial differential equations discretised using finite elements, finite differences or meshfree methods. Each discrete unit typically represent many thousand or millions of particles. For natural reasons the continuum models fail at phenomena that occur on the length scales approaching the particle diameter. The main challenge is to find constitutive laws that relate the stress and strain fields that are of general validity. Predicting and handling the transitions between elastic, plastic and viscous behaviour is particularly difficult. Discrete element methods play a central role in this development as detailed analysis can be made of the relationships between stress, strain and microscopic particle properties.

## 2.1 Discrete Element Method (DEM)

The discrete element method was developed in the late 1960s by Cundall and Stracks [6] as an extension of molecular dynamics to model macroscopic slightly deformable solid grains. Each particle is modeled as a rigid body. The bodies interact via viscoelastic contact forces obeying the Coulomb friction law. For a rigid body,  $a$ , the notations  $\vec{\mathbf{x}}_{[a]}$ ,  $\vec{\mathbf{v}}_{[a]}$ ,  $\vec{\mathbf{f}}_{[a]}$  and  $m_{[a]}$  are used for position, velocity, force and mass, and  $\vec{\mathbf{e}}_{[a]}$ ,  $\vec{\boldsymbol{\omega}}_{[a]}$ ,  $\vec{\boldsymbol{\tau}}_{[a]}$  and  $\mathbf{I}_{[a]}$ , for orientation, angular velocity, torque and inertia tensor. These are combined into generalised position, velocity, force and mass, denoted  $\mathbf{x}_{[a]}$ ,  $\mathbf{v}_{[a]}$ ,  $\mathbf{f}_{[a]}$  and  $\mathbf{M}_{[a]}$ , with  $\mathbf{v}_{[a]} = (\vec{\mathbf{v}}_{[a]}^T, \vec{\boldsymbol{\omega}}_{[a]}^T)^T$  etc. and  $\mathbf{M}_{[a]} = \text{diag}(m_{[a]}\mathbf{1}_{3 \times 3}, \mathbf{I}_{[a]})$ . These are in turn collected in full system state vectors  $\mathbf{x} = (\mathbf{x}_{[1]}, \mathbf{x}_{[2]}, \dots)$ ,  $\mathbf{v} = (\mathbf{v}_{[1]}, \mathbf{v}_{[2]}, \dots)$  etc. Contact forces and velocities may be decomposed in the directions of contact normals,  $\vec{\mathbf{n}}$  and tangents,  $\vec{\mathbf{t}}$ , see Fig.1. The gap function  $g(\mathbf{x})$  measures the magnitude of overlap between the contacting bodies. The equations of motion follows

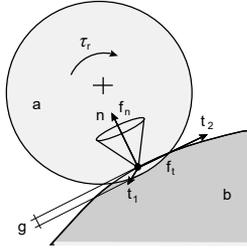


Figure 1: Illustration of the contact between two particles  $a$  and  $b$ .

Newton's law

$$\begin{aligned}\dot{\mathbf{x}}_{[a]} &= \mathbf{v}_{[a]} \\ \dot{\mathbf{v}}_{[a]} &= \mathbf{M}_{[a]}^{-1} \mathbf{f}_{[a]}(\mathbf{x}, \mathbf{v})\end{aligned}\quad (1)$$

where the force on particle  $a$  is the sum of all contact forces acting on it plus external forces,  $\mathbf{f}_{[a]} = \mathbf{f}_{\text{ext}} + \sum_{b \in \mathcal{N}_c(a)} \mathbf{f}_{[ab]}$ . A common force model is the nonlinear Hertz model that follows from the theory of linear viscoelastic materials. Friction is usually modeled as a spring in the tangential direction. The tangential spring extension is computed by integrating the slide velocity, and the force is projected onto the friction cone to obey the Coulomb law. Similarly, rolling resistance is modeled as torque that counteract relative rolling motion, also limited by a Coulomb-like law. For spherical particles, the contact forces are:

$$\begin{aligned}\vec{\mathbf{f}}_{\mathbf{n}} &= k_{\mathbf{n}} (g^{3/2} + cg^{1/2}\dot{g}) \vec{\mathbf{n}} \\ \vec{\mathbf{f}}_{\mathbf{t}} &= \text{proj}_{\mu|\vec{\mathbf{f}}_{\mathbf{n}}|} \left( - \int k_{\mathbf{t}} \vec{\mathbf{u}}_{\mathbf{t}} dt \right) \\ \vec{\tau}_{\mathbf{r}} &= \text{proj}_{\mu_{\mathbf{r}}|\vec{\mathbf{f}}_{\mathbf{n}}|} \left( - \int k_{\mathbf{r}} \vec{\mathbf{w}}_{\mathbf{t}} dt \right)\end{aligned}\quad (2)$$

where  $\vec{\mathbf{u}}_{\mathbf{t}}$  and  $\vec{\mathbf{w}}_{\mathbf{t}}$  are the tangential relative velocity and relative angular velocity at the contact point. The normal stiffness and damping coefficients are  $k_{\mathbf{n}} = E\sqrt{2d}/3(1-\nu^2)$ , where  $E$  is the Young's modulus,  $\nu$  is the Poisson ratio,  $d = (d_{[a]}^{-1} + d_{[b]}^{-1})^{-1}$  is the effective diameter, the dissipation coefficient is  $c = 4(1-\nu^2)(1-2\nu)\eta/15E\nu^2$ , and the material viscosity constant is  $\eta$ . For the friction spring coefficient,  $k_{\mathbf{t}}$ , and rolling resistance coefficient,  $k_{\mathbf{r}}$ , there are no such relations to fundamental material parameters and they must be determined from experiments. A DEM simulation consists of numerical integration of Eq. (1), which are ordinary differential equations (ODE). However, due to the occurrence of contact events and of the friction law in (2), the force is in general not differentiable in time. High-order integration algorithms are therefore not applicable [7]. Instead, the semi-implicit Euler or Verlet algorithm is a common choice, although the ODEs are very stiff and the time-step  $\Delta t$  become limited by the time-scale given by the elastic interaction time  $\sqrt{m/k_{\mathbf{n}}}$ . The simulation algorithm of DEM involve contact detection, force computation and velocity and position update,  $(\mathbf{x}_i, \mathbf{v}_i) \rightarrow (\mathbf{x}_{i+1}, \mathbf{v}_{i+1})$  from time  $t_i$  to  $t_{i+1} = t_i + \Delta t$ .

## 2.2 Nonsmooth Discrete Element Method (NDEM)

The nonsmooth contact dynamics method was introduced in the late 1980s by J. J. Moreau [8,9] and further developed by Jean [10] and others. In the case of rigid bodies this is also known as the nonsmooth discrete element method (NDEM) [7] and can be understood as an implicit version of DEM using convex analysis to remedy the fact that the contact laws cannot be written as simple mappings of position and velocity to force. In the nonsmooth DEM, impacts and frictional stick-slip transitions are considered as instantaneous events making the velocities discontinuous in time. The contact forces and impulses are modeled in terms of kinematic constraints and complementarity conditions between force and velocity, e.g., by the Signorini-Coulomb law for unilateral non-penetration and dry friction. The contact network becomes strongly coupled and any dynamic event may propagate through the entire system instantaneously. The benefit of nonsmooth DEM is that it allows integration with much larger simulation step-size than for smooth DEM and thus potentially faster. There are several equivalent formulations of NDEM. The formulation in terms of multibody dynamics in descriptor form will be used here [12] and with constraint stabilization [13]. The explicit contact force in Eq. (1) is replaced by a constraint forces  $\mathbf{G}_c^T \boldsymbol{\lambda}_c$  with Lagrange multiplier  $\boldsymbol{\lambda}_c$  and Jacobian matrix  $\mathbf{G}_c$ . The constraint force is implicitly given by the contact laws expressed as kinematic constraints in form of algebraic equations, inequalities or complementarity conditions. One advantage of this particular formulation is that it is automatically unified with the framework of multibody system dynamics for articulated mechanisms and power transmission systems. The constrained equations of motion can be written

$$\mathbf{M}\dot{\mathbf{v}} = \mathbf{f}_{\text{ext}} + \mathbf{G}_c^T \boldsymbol{\lambda}_c + \mathbf{G}_j^T \boldsymbol{\lambda}_j \quad (3)$$

$$\varepsilon_j \boldsymbol{\lambda}_j + \eta_j \mathbf{g}_j + \tau_j \mathbf{G}_j \mathbf{v} = 0 \quad (4)$$

$$\text{law}[\mathbf{v}, \boldsymbol{\lambda}_c] = \text{true} \quad (5)$$

where (4) is a generic constraint equation that may model kinematic joints and motors. With  $\varepsilon_j, \tau_j = 0$  and  $\eta_j = 1$ , it becomes an ideal holonomic constraint  $\mathbf{g}(\mathbf{x}) = 0$ . For  $\varepsilon_j, \eta_j = 0$  and  $\tau_j = 1$ , the constraint become an ideal Pfaffian constraint  $\mathbf{G}\mathbf{v} = 0$ . With  $\varepsilon_j, \eta_j, \tau_j \neq 0$  it represent a generic constraint with compliance and damping. Eq. (5) represent the contact laws that are imposed on the system, for instance the Signorini-Coulomb and rolling resistance law

$$0 \leq \varepsilon_n \boldsymbol{\lambda}_n + \mathbf{g}_n + \tau_n \mathbf{G}_n \mathbf{v} \perp \boldsymbol{\lambda}_n \geq 0 \quad (6)$$

$$\gamma_t \boldsymbol{\lambda}_t + \mathbf{G}_t \mathbf{v} = 0, \quad |\boldsymbol{\lambda}_t| \leq \mu_t |\mathbf{G}_n^T \boldsymbol{\lambda}_n| \quad (7)$$

$$\gamma_r \boldsymbol{\lambda}_r + \mathbf{G}_r \mathbf{v} = 0, \quad |\boldsymbol{\lambda}_r| \leq r \mu_r |\mathbf{G}_n^T \boldsymbol{\lambda}_n| \quad (8)$$

where the contact constraint (c) have been decomposed into normal (n), tangential friction (t) and rolling constraint (r). Eq. (6)-(7) are the Signorini-Coulomb conditions with constraint regularization and stabilization terms  $\varepsilon_n, \tau_n$  and  $\gamma_t$ . With  $\varepsilon_n = 0$  and  $\tau_n = 0$ , Eq. (6) state that bodies should be separated or have zero overlap,  $\mathbf{g}_n(\mathbf{x}) \geq 0$ ,

and if so the normal force should be non-cohesive,  $\lambda_n \geq 0$ . With  $\gamma_t = 0$ , Eq. (7) state that contacts should have zero relative slide velocity,  $\mathbf{G}_t \mathbf{v} = 0$ , provided that the friction force remain bounded by the Coulomb friction law with friction coefficient  $\mu_t$ . Eq. (8) similarly constrains relative rotational motion of contacting bodies, provided the constraint torque do not exceed the rolling resistance law with coefficient  $\mu_r$  and contact radius  $r$ . The Lagrange multiplier become an auxiliary variable to solve for, in addition to position and velocity. The regularization and stabilization terms,  $\varepsilon$  and  $\gamma$ , introduce compliance and dissipation when constraints are violated. Regularized constraints may be viewed as Legendre transforms of a potential and Rayleigh dissipation function of the form  $U_\varepsilon(\mathbf{x}) = \frac{1}{2\varepsilon} \mathbf{g}^T \mathbf{g}$  and  $\mathcal{R}_\gamma(\mathbf{x}, \mathbf{v}) = \frac{1}{2\gamma} (\mathbf{G}\mathbf{v})^T (\mathbf{G}\mathbf{v})$  [15, 16]. This is a key point to map the constraint parameters to conventional force models, such as the Hertz contact law.

### 2.2.1 Time integration of NDEM

The numerical time integration scheme used in this thesis is based on the SPOOK stepper [16] derived from a discrete variational principle for the augmented system  $(\mathbf{x}, \mathbf{v}, \lambda, \dot{\lambda})$  and applying a semi-implicit discretization. The stepper is linearly stable and  $\mathcal{O}(\Delta t^2)$  accurate for constraint violations [16] and involve solving a mixed complementarity problem (MCP) or equivalent quadratic programming problem (QP) [17]

$$\begin{aligned} \mathbf{H}\mathbf{z} + \mathbf{b} &= \mathbf{w}_l - \mathbf{w}_u \\ 0 &\leq \mathbf{z} - \mathbf{l} \perp \mathbf{w}_l \geq 0 \\ 0 &\leq \mathbf{u} - \mathbf{z} \perp \mathbf{w}_u \geq 0 \end{aligned} \quad (9)$$

where

$$\mathbf{H} = \begin{bmatrix} \mathbf{M} & -\mathbf{G}_n^T & -\mathbf{G}_t^T & -\mathbf{G}_r^T \\ \mathbf{G}_n & \Sigma_n & 0 & 0 \\ \mathbf{G}_t & 0 & \Sigma_t & 0 \\ \mathbf{G}_r & 0 & 0 & \Sigma_r \end{bmatrix} \quad (10)$$

$$\mathbf{z} = \begin{bmatrix} \mathbf{v}_{i+1} \\ \lambda_{n,i+1} \\ \lambda_{t,i+1} \\ \lambda_{r,i+1} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -\mathbf{M}\mathbf{v}_i - \Delta t \mathbf{M}^{-1} \mathbf{f}_{\text{ext}} \\ \frac{4}{\Delta t} \Upsilon_n \mathbf{g}_n - \Upsilon_n \mathbf{G}_n \mathbf{v}_i \\ 0 \\ 0 \end{bmatrix} \quad (11)$$

The solution vector  $\mathbf{z}$  contains the new velocities at time  $t_{i+1}$  and the Lagrange multipliers  $\lambda_n$ ,  $\lambda_t$  and  $\lambda_r$ . A factor  $\Delta t$  has been absorbed in the multipliers such that the constraint force reads  $\mathbf{G}^T \lambda / \Delta t$ . The upper and lower limits,  $\mathbf{u}$  and  $\mathbf{l}$  in Eq. (9), follow from the Signorini-Coulomb and rolling resistance law with the friction and rolling resistance coefficients  $\mu_t$  and  $\mu_r$ . Since the limits depend on the solution, this is a partially nonlinear complementarity problem.  $\mathbf{w}_l$  and  $\mathbf{w}_u$  are temporary slack variables. The diagonal matrices  $\Sigma_n$ ,  $\Sigma_t$ ,  $\Sigma_r$  and  $\Upsilon_n$  are related to the constraint

parameters are as follows

$$\begin{aligned}
\Sigma_n &= \frac{4}{\Delta t^2} \frac{\varepsilon_n}{1 + 4\frac{\tau_n}{\Delta t}} \mathbf{1} \\
\Sigma_t &= \frac{\gamma_t}{\Delta t} \mathbf{1} \\
\Sigma_r &= \frac{\gamma_r}{\Delta t} \mathbf{1} \\
\Upsilon_n &= \frac{1}{1 + 4\frac{\tau_n}{\Delta t}} \mathbf{1}
\end{aligned} \tag{12}$$

Since the stepping scheme (9) is an implicit method the time-step is no longer restricted to the viscoelastic time-scale of the normal force. Instead, it is limited by the tolerance in acceptable constraint satisfaction. Typically, a time-step many orders in magnitude larger than for smooth DEM can be used. The precise mapping of the parameters in Eq. (12) to material parameters are addressed in Paper I and IV in this thesis. Increasing the parameters  $\varepsilon$ ,  $\gamma$  and  $\tau$  make the contacts more compliant. This improve the solvability of the MCP. The stiffness go to infinity in the limit of  $\varepsilon, \gamma, \tau \rightarrow 0$ .

## 2.2.2 Projected Gauss-Seidel (PGS) Solver

The computational properties of the solution algorithms for NDEM simulations is largely open questions. There are no general proofs of existence and uniqueness of solutions and few theoretical results on convergence and numerical stability [14]. The nonlinear projected Gauss-Seidel (PGS) algorithm is widely popular because of its low computational cost per iteration, small memory footprint and smooth distribution of truncation errors that favour stable simulation. The Schur complement form of Eq. (9) is

$$(\mathbf{GM}^{-1}\mathbf{G}^T + \Sigma)\lambda_{i+1} = \mathbf{q} - \mathbf{GM}^{-1}\mathbf{p} \tag{13}$$

subject to law $[\mathbf{v}_{i+1}, \lambda_{i+1}] = \text{true}$ ,  $\mathbf{p} = \mathbf{M}\mathbf{v}_i + \mathbf{f}_{\text{ext}}$ , and  $\mathbf{q} = [(\Upsilon\mathbf{G}_n\mathbf{v}_i - \frac{4}{\Delta t}\Upsilon\mathbf{g})^T, 0, 0]^T$  and the velocity update reads

$$\mathbf{v}_{i+1} = \mathbf{v}_i + \Delta t\mathbf{M}^{-1}\mathbf{f}_{\text{ext}} + \mathbf{M}^{-1}\mathbf{G}^T\lambda_{i+1} \tag{14}$$

The PGS algorithm can be considered as a fixed-point linear iteration scheme computing the increments of  $\lambda_{i+1}$  and  $\mathbf{v}_{i+1}$  using Eq. (13) and (14) repeatedly while projecting the solution to maintain the nonlinear contact law at each iteration step. After integrating the velocities and positions an impact stage follows. It include solving a similar MCP with the Newton impact law  $\mathbf{G}_n\mathbf{v}_+ = -e\mathbf{G}_n\mathbf{v}_-$ .

### 3 Accelerated DEM Simulation

The time required for simulating  $t_{\text{real}}$  seconds of evolution using DEM is the product of the number of time-steps and the computational time for each step

$$t_{\text{comp}} = \frac{t_{\text{real}}}{\Delta t} \cdot [t_{\text{col}} + t_{\text{solve}} + t_{\text{aux}}] \quad (15)$$

with time serially separated in collision detection ( $t_{\text{col}}$ ), solver ( $t_{\text{solve}}$ ) and auxiliary processing time ( $t_{\text{aux}}$ ). In conventional smooth DEM the computations of force, velocity and position update are very cheap and parallelises well. Collision detection is therefore the main computational bottleneck such that  $t_{\text{comp}}^{\text{DEM}} \propto N_{\text{p}}/S_{\parallel}^{\text{DEM}}$ , where  $S_{\parallel}^{\text{DEM}}$  is the parallel speedup. In NDEM, the solver is the main computational bottleneck. When using a PGS solver, the computational time scale as  $t_{\text{comp}}^{\text{NDEM}} \propto N_{\text{p}}^{1+\gamma_{\epsilon}}/\epsilon S_{\parallel}^{\text{NDEM}}$  depending on error tolerance  $\epsilon$ . The scaling exponent,  $\gamma_{\epsilon} > 0$ , reflect that the number of PGS iterations depend on the system size, connectivity and error tolerance as  $N_{\text{it}} \propto N_{\text{p}}^{\gamma}/\epsilon$  [25]. The auxiliary process time include overheads for communication, memory management and processing of the DEM data structures that is necessary for post-processing or for optimisation of the other computational steps. It is interesting to study the relative computational time of the smooth and nonsmooth DEM

$$\frac{t_{\text{comp}}^{\text{DEM}}}{t_{\text{comp}}^{\text{NDEM}}} \propto \epsilon N_{\text{p}}^{-\gamma_{\epsilon}} \frac{\Delta t_{\text{NDEM}}}{\Delta t_{\text{DEM}}} \quad (16)$$

The following general observations can be made from this expression. The conventional smooth DEM is increasingly favourable in the limit of large systems ( $N_{\text{p}} \rightarrow \infty$ ) and high accuracy ( $\epsilon \rightarrow 0$ ). The relative efficiency of nonsmooth DEM increase with material stiffness and with slow dynamics, since  $\Delta t_{\text{DEM}} \lesssim \sqrt{m/k} \rightarrow 0$  when  $k \rightarrow \infty$  and  $\Delta t_{\text{NDEM}} \lesssim \epsilon d/u_{\text{n}}$ . To accelerate DEM simulations is to diminish the terms in Eq. (15). The following approaches have been identified:

#### Adaptive time-step and number of iterations

Depending on the requirements of the simulation and on the material parameters, a considerable speedup can be achieved by simply making the best choice between smooth and nonsmooth DEM. When NDEM is used, additional speedup can be gained by adjusting time-step size and number of iterations to the desired error tolerance and dynamic state of the granular material.

#### Parallelisation

The parallelisation of DEM subsystems that are weakly or not at all connected to each other is easy to implement, and has almost ideal scaling. Parallelisation of collision detection and PGS solver is more difficult but a well developed area [3, 18] and implemented in the software used in the thesis.

## Convergence

There are several ways to improve the convergence of the PGS solver, either modify it or replace it entirely by alternative solvers, such as the accelerated projected gradient descent method [19] or the proximal point method [20]. With increased convergence less number of iterations can be used to reach the same level of accuracy and a speedup is gained if the computational cost of the modification is not too large. This is highly experimental work since there are few theoretical results on existence, uniqueness, stability and convergence of MCP and QP solvers for nonsmooth dynamics [14]. Modifications of the PGS algorithm include successive over-relaxation (SOR) and warm-starting based on some expectation of the solution.

## Model reduction

Another way to accelerate the computations is to reduce the model complexity by somehow lowering the number of degrees of freedom in the system. This is known as model reduction and is widely used in solid and fluid mechanics, dynamical systems and control theory [21, 22]. Replacing a DEM model with a finite element model based on a continuum approximation of the same system is an example of this but is in general not applied to accelerate DEM simulations.

# 4 The Iron Ore Pelletising Process

The work presented in this thesis was inspired and motivated by the need for deeper understanding and specialised simulation tools for the processing of iron ore into pellets at the company LKAB. The pelletising process produces spherical pellets 9 – 16 mm in diameter from ore material. The process consists of the following main stages [24], illustrated in Fig. 2. Comminuted fine size ore, *finer*, is first mixed with binder material. Agglomeration into soft ore balls, *green ore pellets*, occur in balling circuits, where fines, water and undersized pellets are circulated through rotating drums. The main agglomeration mechanisms are nucleation, layering, coalescence and breakage. The green pellets leave the drum through an outlet and are size distributed through a roller sieve, see Fig. 3. Under-sized particles are fed back to the drum. Over-sized pellets are crushed and mixed with the fines. The balling process can be controlled by regulating the drum velocity and feed rate of fine material, binding agencies and moisture. On-size pellets are conveyed to the induration furnace where they form hard pellets by oxidation and sintering. After being cooled, the pellets are ready for further transportation by train and ship. A typical iron ore balling circuit have drum diameter ranging between 3 – 5 m, 8 – 10 m long and circulate about 400 – 1200 ton/h producing 100 – 300 ton/h of on-size pellets. For an optimal performance, the material flow on the wide belt conveyor beneath the outlet and onto the sieve need to be as homogeneous in space and time as possible. The right image in Fig. 3 is an example of a failed outlet design that would cause substantial loss in productivity or poor pellet quality.

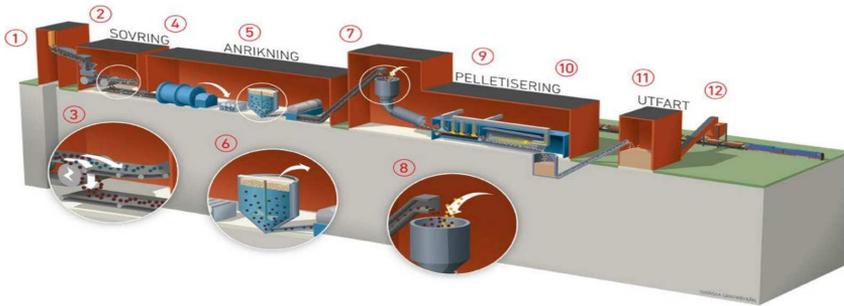


Figure 2: Illustration of the iron ore pelletising process. The balling process occur between step 7 and 9. Image courtesy of LKAB.

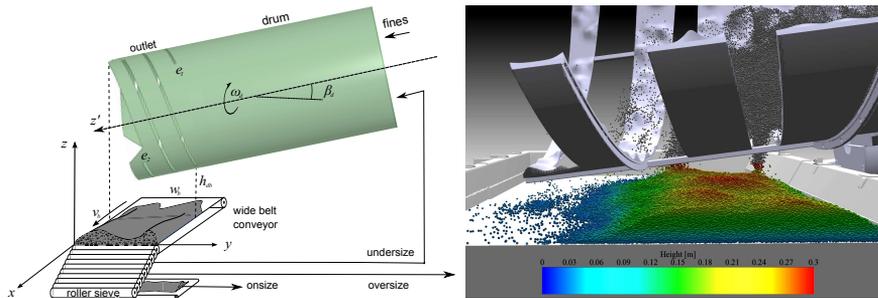


Figure 3: Illustration of the balling circuit and application of NDEM simulation to exploration of outlet designs.

## 5 Simulation Software

The project has involved a substantial amount of implementation work and numerical experiments. This has been carried out using a combination of the simulation software AgX Dynamics [23] and a series of prototype codes were developed and managed by the author. This code has been a mixture of C++, Python, Lua and Matlab scripts. AgX Dynamics is a software library supporting multidomain dynamics simulation for industrial and scientific applications. It is particularly well suited for realtime interactive simulation involving contacting rigid multibody systems. One large area of applications is heavy machinery simulators. AgX Dynamics also has a number of solutions for computer aided design and engineering. This include a module for modeling and simulation of granular materials and bulk handling systems. The core library include a direct solver for quadratic programming problems using a block pivot method with highly optimised algorithms and data structures for multibody systems with contacts and nonsmooth dynamics. A parallelised version of the PGS

algorithm using spatial partitioning for granular materials is implemented. The direct and iterative solvers can be run as coupled hybrid solvers.

## 6 Thesis Contribution and Future Work

A short description of the findings of the thesis' papers is given below. All papers have multiple authors and a short description of the main contribution by the author of the thesis is therefore included. All papers have been written in close collaboration and with good opportunity to provide input to and influence the development of the manuscripts.

### Paper I

In this paper the computational properties of smooth and nonsmooth DEM are compared and a regularized version of NDEM based on the Hertz-Mindlin contact law is introduced, thus relating the NDEM solver parameters directly to fundamental material parameters. It has the both the conventional DEM and NDEM as limit cases. The required number of iterations needed to obtain a certain error tolerance is investigated in order to understand the true performance of NDEM in relation to accuracy and material properties. A surprising finding is that the required number of iterations do not always grow with the number of bodies in the system. Analogously to the Jansen effect of pressure saturating with depth in a granular column, due to force arching, also the required number of iterations can saturate and become independent of system size.

**My contribution:** development of a prototype NDEM simulation code with Hertzian contact model and PGS solver; setup and management of simulation system and post-processing pipeline; data analysis; establishing the convergence formula.

### Paper II

NDEM simulation is shown to be a feasible tool for exploring the geometric design space of ore pellet balling drums. This is formulated as a design optimization problem. The objective function take the material distribution on the conveyor belt as input. A downscaled drum with a two-parameter outlet design is considered. Over 2000 simulations of different design are run with the identical drum flow to find an optimal shape. The conclusions include that the design principle is fundamentally flawed, as the design can be optimal only for a specific flow rate. It is also observed that the spherical idealization of the particles and absence of rolling resistance lead to significant disagreement between the simulated and observed pile formation.

**My contribution:** modeling of the balling circuit; setup and management of a system for batch simulations and post-processing; analysis and summary of simulation result.

### Paper III

The practical steps of parameter identification, verification and validation of NDEM is described and applied to iron ore green pellets and the balling circuit. Also, the contact model is extended to include constraint based rolling resistance. The validation tests of simulated bulk behaviour show a good agreement with measurements of material flow in the balling plant. The sensitivity to model and solver parameters are investigated. This reveals that the results are very sensitive to rolling resistance and outlet geometry but not particularly sensitive to elasticity, friction coefficient and pellet diameter. It is also found that the application allows for surprisingly large time-step. Although this introduce big errors to a significant fraction (17 %) of the contacts the effect on the bulk flow is negligible.

**My contribution:** identification of material parameters and material flow from optical measurements; modeling and analysis of verification and validation systems; implementation and testing of rolling resistance model.

### Paper IV

The possibility and efficiency of applying warm-starting to the PGS solver in NDEM simulation is investigated. Two methods are proposed - *history based* and *model based* - and tested. It is found that warm-starting based on the history can significantly reduce the required number of iterations. This primarily improve the convergence of friction forces and rolling resistance. A speedup between 2 to 5 can be achieved.

**My contribution:** joint work in developing the two warm-starting methods; prototype implementation; modeling, simulation and analysis of the column, pile and drum experiments.

### Paper V

This paper presents a model order reduction technique for DEM simulations. Algorithms to substitute rigid aggregate bodies adaptively for collections of contacting particles that collectively co-move as rigid bodies are developed, as well as methods to refine the aggregates to smaller parts when necessary. The complexity of the reduced system can be many times smaller than the original. Two methods for predicting refinement are studied: contact event split and background trial solve split. The method has potential to accelerate NDEM simulations by 5 – 50 times for reduction levels of 70 – 95 %, if the computational overhead can be kept below given thresholds.

**My contribution:** algorithm development and prototype development of merge-split algorithms; joint work in development of split conditions; simulation and analysis to identify parameters and artefacts; investigate advantage and drawback of each merge-split method.

## Future Work

There are many interesting questions and ideas to pursue in future work. When it comes to the application of iron ore pelletising systems, it is unclear how the presence of fine material and moisture affect the bulk behaviour of ore green pellets. It is also not clear how a mixture of fines and ore green pellets are efficiently modeled and simulated in a nonsmooth DEM framework - if at all possible. In reality, the ore green pellets are plastic and it is also an open question how to extend the NDEM contact model to this. On the computational modeling side, there are also many attractive continuations. In most real granular systems the solid, liquid and gaseous phase are simultaneously present and they typically benefit from different simulation modes, e.g., smooth versus nonsmooth DEM, size of time-step, number of iterations or change of solver. Ideally one should apply different iteration count, time-step and DEM-smoothness in different parts of the system and adaptively change this in order to focus the computational power to the part where it is needed the most. This point at asynchronous time-integration of the NDEM equations and the use of model order reduction interleaved in the PGS iterations. It is also clear that full use of model order reduction require extension from rigid to deformable aggregates.

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