A Domain Decomposition method for granular dynamics using discrete elements and application to railway ballast

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Abstract

The paper is devoted to the development of a non overlapping Domain Decomposition method adapted to granular dynamics. The formulation and the efficiency of such a method are well established for structural mechanics. In order to extend this approach to granular systems a so-called primal splitting of the domain is chosen because it is a less intrusive method for software development. Once the interface problem is defined and the solver is slightly enriched with some extra numerical parameters, the method is tested on railway ballast simulations for improving the maintenance of railway tracks.

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1 Motivations

The simulation of more and more realistic granular media leads to intensive computations. The size of the simulation increases both in term of number of bodies or particles and of duration of the process to be simulated. The increase of the

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computations concerns then both the space and the time, because a granular system presents often a complex dynamic behavior. Indeed dense collections of grains subjected to dynamic loadings require large-scale samples simulated on a long time to capture the local dynamic crises responsible of the global behavior of the system. Many applications involve such dense assemblies as the sand piles, dunes, blocky rocks, powders. We are here specially interested in a class of applications for which the connectivity of the grains remains almost stable during the studied process, as the masonry of monuments (before collapse) or the railway ballast.

The denominations of 'discrete element methods' and 'distinct element methods' (DEM) are commonly used to refer to the pioneering approach of Cundall [11], today implemented in a large range of commercial pieces of software intended to handle non-interpenetrability. Also, because the computation techniques applied in such implementations are close to those of molecular simulations, the denomination of 'molecular dynamics' (MD) method is also used, specially in the domain of granular mechanics [16]. Such an approach is based on regularization strategies both for the dynamics and the interactions between grains. First, the non-interpenetrability constraints are replaced by some stiff 'elastic' repulsion laws which take effect as soon as two members of the system come close to each other. Similarly, frictional contact may be somewhat regularized through the introduction [12] of a local elastic micro-deformation and of viscosity-like effects. The dynamics of the approximate system is then governed by stiff differential equations requiring a very small step-length in a classical explicit integration scheme.

The Non Smooth Contact Dynamics (NSCD) or Contact Dynamics in short, has been developed by J. J. Moreau and M. Jean over the last two decades [21, 29]. It is well suited for our applications as characterized above. It does not use regularization of the nonsmooth frictional contact relations. Numerical simulations thus may to be performed using a fully implicit resolution of the contact forces. At each step of the evolution problem, all kinematic constraints within the packing are simultaneously taken into account along with the equations of motion to determine all contact forces. Using a much larger time step than the MD method, this allows us to deal properly with nonlocal momentum transfers involved in multiple collisions, contrary to the classical DEM that consider the system evolution as a succession of binary collisions.

The parallel computing may be useful for different stages of the calculation in granular simulations: contact detection, partitioning and solver. If a classical MD approach is used, we have no solver and the main effort has to be done on the contact detection phase, see [27, 31] for instance. In this case the partitioning phase has to be parallelized to optimize the load balance of the processors only if a Domain Decomposition strategy is performed [23]. Since we use large time steps with the NSCD approach for simulating granular systems involving moreover a stable connectivity, we focus on the parallelization of a solver which combines the generic NSCD solver identified to a Non Linear Gauss Seidel algorithm [22, 33] (NLGS) and a Domain Decomposition Method (DDM). We resort to a DDM among all the parallel techniques because of two reasons. First, in the long term, a DDM may

provide an automatic numerical homogenization procedure if a multiscale description is performed [24, 17, 26]. A discrete-continuous mixed model may be also defined for a dense granular system which may be viewed as continuous medium at a macroscale. Secondly, in the short term, a pertinent geometric decomposition may at least reduce the computational effort in some subdomains far enough from the solicitation to be in a stable mechanical state.

The first difficulty to deal with a DDM for a granular system is to split the domain into subdomains because the system is discrete and the nonsmoothness occurs within the whole domain and not only on a few surfaces as it is often the case in structural mechanics [8, 15]. Since the system is discrete, we have two possible strategies for splitting the domain. Starting from a box-like partitioning [6] the primal strategy provides a nonsmooth interface, whereas the dual one leads to perfect interfaces. The dual partitioning and the associated solvers require theoretical developments and are investigated in others papers concerning granular mediums [19, 20] and previously tensegrity systems [32] or more general reticulated structures [2]. We opt in this article for the primal partitioning because it is the less intrusive approach for an industrial software. Such a method may be also interpreted as a special renumbering of the contacts.

Secondly the evaluation of the efficiency of a new solver in comparison with the previous one is a difficult topic because a dense granular system is an evolutive nonsmooth problem leading to a large multiplicity of solutions [30]. Consequently we have not relevant error estimates as underlined in [21]. Only the quality of the computation may be appreciated using a set of qualitative indicators as presented in the section 3.

This article is structured as follows. In section 2 the fundamental equations of the Granular Dynamics are presented from the velocity-impulse formulation of the NSCD to the NLGS generic solver. In section 3 the primal partitioning and the resulting coupled DD-NLGS solver are detailed. In section 4 the ability to distribute inhomogeneously the computational efforts into the subdomains of an industrial application is discussed according some qualitative indicators before a first attempt to evaluate the efficiency of the parallel treatment.

The deterioration of railway track under intense train traffics induces various tracks irregularities in the track mainly due to differential settlement. In order to restore the initial geometry of the track, the ballast tamping operation is currently in use and some open point about ballast durability, track deterioration rate have to be investigated in order to optimize maintenance. The opportunities to use Domain Decomposition Methods allows to evaluate an industrial process over a representative portion of railway track for optimize the efficiency of a continuous process in a granular media.

2 Granular dynamics

2.1 Grain dynamics with nonsmooth interactions

The system considered is a collections of rigid bodies submitted to externel efforts and non smooth interaction such as contact and friction. These interactions assumed to be a finite number of ponctual contacts.

Its evolution is described with its velocity and its rotation rate, and since it involves nonsmooth effects with velocity jumps, a scheme which is not built on the derivability and continuity of velocity equations is used. Because of the very large number of contacts involved in a dense granular media, a time-stepping scheme is chosen rather than an event-driven one, which would lead to a too small time step. Such a scheme, on a time slab $]t_i, t_{i+1}[$ involves a discretized equation of dynamics with impulses in its right-hand side [28, 29]:

$$M(V - V^i) = R^d + R \tag{1}$$

where M stores the mass and inertia matrix, V is the velocity (and rotation rate) at t_{i+1}, V^i is the previous velocity at t_i. R^d is the prescribed impulse on the studied time slab, and R is the resulting impulse arising from the contact interactions. In the following, (1) will denote the assembly of the nonsmooth dynamics of all the grains.

For each potential contact α between two grains, the non penetration condition enforces a positive gap: $g_\alpha \geq 0$. The relative velocity is denoted v_α. It can be derived from the kinematics of the neighboring grains with a global-to-local operator H_α as $v_\alpha = H_\alpha^T V$. The assembly for all the potential contacts reads: $v = H^T V$. The dual quantity is the assembly of the impulses on the grains, from the impulse in the interactions r_α as: $R = Hr$.

Moreau's Lemma [29] allows to express the Signori conditions at each contact with relative velocities and impulses for the normal part, denoted with a subscript n (non penetration and no adhesion), and Coulomb friction model for the tangential part, denoted with a subscript t, as:

$$\begin{cases} \text{if } g > 0, \quad r = 0 \\ \text{if } g = 0, \quad 0 \leq v_n \perp r_n \geq 0 \text{ and } \begin{cases} \text{if } \|v_t\| = 0, \quad \|r_t\| \leq \mu r_n \\ \text{if } \|v_t\| \neq 0, \quad r_t = -\mu r_n v_t / \|v_t\| \end{cases} \end{cases} \tag{2}$$

(these conditions are assumed to be expressed on each contact α separately). In the following, they are gathered and formally expressed as a non-univoque and non differentiable expression of the form: $\mathcal{R}(r, v) = 0$.

2.2 Reference problem

The reference problem can be expressed in the reduced dynamics form by inverting the system (1) (it is block diagonal for each grain, and even diagonal if the

velocities are expressed at mass centers, and rotation rates in each principal inertial basis) and using the operators H and H^T, to get, at each time step:

$$v = v^d + Wr \tag{3}$$

$$\mathcal{R}(r, v) = 0 \tag{4}$$

where $W = H^T M^{-1} H$ is the Delassus operator, and the given quantity is $v^d = H^T(M^{-1}R^d + V^i)$. The unknowns are the couples of impulse and relative velocity at each potential contact (r, v).

Once solved, the positions are updated with an integration scheme, the contact detection is performed (the potential contacts may evolve from a time step to another), and the next time step is searched for. As already specified, we are concerned herein in the parallelization of the solver but not of the contact detection phase, though this may be costly too, but for which several existing methods are already available, see [7] for instance.

2.3 Non Linear Gauss Seidel solver

A nonlinear Gauss-Seidel (NLGS) applied to the reference problem (3), (4) on the current time step is the following:

- Initialization: compute the "free" velocity by solving dynamics on each grain: $V_{\text{free}} = M^{-1}R^d$, and $v^d = H^T(V_{\text{free}} + V^i)$; for each contact α, extract $W_{\alpha\alpha} = \sum_j H_{j\alpha}^T M_j^{-1} H_{j\alpha}$ where the sum is performed on the grains j connected to the contact α.

- Iterate: for each contact α, solve

$$W_{\alpha\alpha} r_\alpha - v_\alpha = -v_\alpha^d - \sum_{\beta \neq \alpha} W_{\alpha\beta} r_\beta \tag{5}$$

$$\mathcal{R}(r_\alpha, v_\alpha) = 0 \tag{6}$$

  To do so, the right hand side is evaluated as follows; for each grain j connected to the contact α, solve the dynamical equation: $M_j V_j = \sum_{\beta \neq \alpha} H_{j\beta} r_\beta$ and assemble the contributions: $\sum_j H_{j\beta}^T V_j$. Once the right hand side is computed, the current iterate can be solved explicitly for the normal contact part. For the tangential part, if the search direction $W_{\alpha\alpha}$ is diagonal, the solution is explicit as well; if not, a small non linear system has to be solved in 3D, for instance with a generalized Newton method [1] . Once each contact has been dealt with, the loop is performed again. Such an iteration is called a sweeping iteration because the set of contacts is swept.

The iterations are performed till a convergence criterion is satisfied. For large-scale industrial problems, the selection of a pertinent termination criterion is still an open question [21]. A check on the penetration residual at contact, and a stationary condition, are usually part of it.

The overall implicit solver is known as Non Smooth Contact Dynamics (NSCD) and is implemented into the LMGC90 platform [13] All the subsequent developments are also performed in the same platform.

3 Domain Decomposition solver

To address the case of large-scale problems, a partitioning strategy belonging to the domain decomposition methods (DDM) is selected. In this Section, a non overlapping DDM [9] is designed for the case of discrete problem that exhibits several non smoothness: the dynamics of a rigid body collection, and the frictional contact and impact interactions between them. Moreover, since an evolution problem is settled, the configuration (connectivity between grains with potential contact detection) may change at each time step. Previous studies have addressed the case of discrete static problems with unilateral conditions and compliance, as well as a fixed configuration (case of tensegrity structures) [32, 2], and also granular dynamics with a different DDM design [19, 20]. Indeed, the proposed DDM in this article deals with an algebraic partitioning of the reference problem (3) allowed by the chosen partitioning described in the following.

3.1 Geometric and algebraic partitioning

The proposed geometric partitioning relies on a graph partitioning, cf. [25] for instance, using the coordinates of the vertices: a box-like partitioning is used herein [6] that allows to get a locality of data useful for a parallel implementation. This feature is an add-on when compared to the previous study [33] and will allow an algorithm design that is suited to both shared and distributed memory architectures.

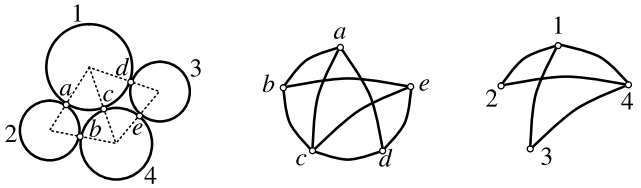

Figure 1: Left: a simple connectivity between grains (1 to 4) with potential contacts (a to e). Middle: the corresponding dual graph. Right: the corresponding primal graph.

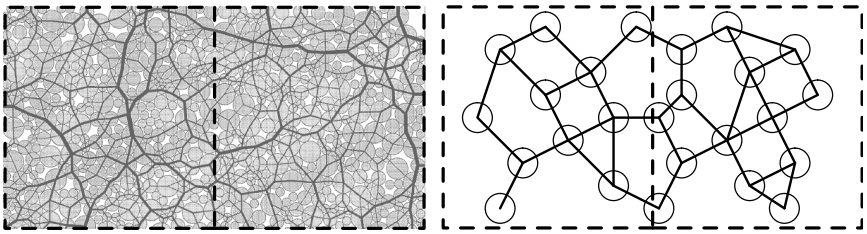

Figure 2: Box-decomposition of a 2D granular media (left) and its principle (right)

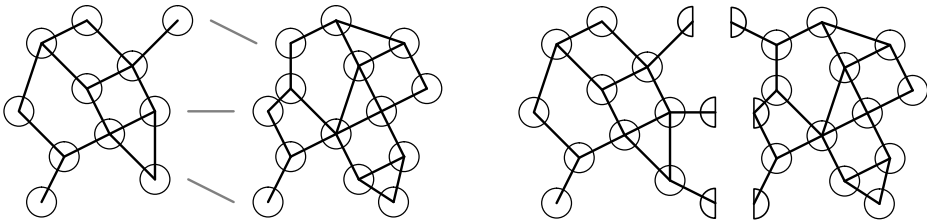

Figure 3: Primal decomposition (left) with links as interface, dual decomposition (right) with nodes as interface

Considering the granular system as an assembly of nodes (grains) and links (potential contact interactions detected at a particular time step), two splittings can be considered, Figures 1, 2 and 3:

- If a graph is defined with nodes as vertices, and links as edges (the primal graph), the nodes can be split among the subdomains (considering their center of mass coordinates, and the box-like decomposition of the domain);
- If a graph is defined with links as vertices, and nodes as edges (the dual graph), the links can be split among the subdomains (considering the coordinates of the barycenter of the two grains that posses a potential interaction, and the box-like decomposition of the domain), as in [20].

We choose herein to use the primal splitting. In such a case a node belongs to only one subdomain, and the global interface is constituted with links that traduces an interaction between two nodes belonging to different subdomains. The behavior of this interface is therefore non smooth, and non smoothness is also located within each subdomain for the internal links (between two nodes belonging to the same subdomain).

The DDM allows to define quasi-independent blocks via a geometrical splitting of the domain. A subdomain is therefore a granular system itself, coupled with its neighbor by specific boundary conditions arising from a global interface. As soon as these boundary conditions are known (within each DDM iteration), a subdomain resolution is a granular independent problem, and can reuse an existing solver technology on a particular processor. The global interface treatment is also

a standard resolution, but dealing only with links behavior since no node is located in this interface.

We choose herein to consider the global interface treatment in a specific step to produce a synchronized algorithm. An other solution could be to parallelize the interface treatment by splitting itself into different processors [14], but this would lead to an asynchronous treatment. Two arguments are used to motivate our choice:

- The global interface treatment is expected to be cheap due to the interface nature (this will be justified in the numerical results Section);
- Since the granular dynamics problem is a multi-valued problem, an asynchronous algorithm will produce a different local solution at each run [33].

The algebraic partitioning of the reference problem (3) is performed in the following. Since a partition of nodes is performed, each node belongs to one subdomain only. Therefore, all the node-based fields (grain velocity, grain impulse) can be split accordingly. Let E and E' denote two subdomains for sake of simplicity; one gets:

$$V = \begin{bmatrix} V_E \\ V_{E'} \end{bmatrix} \qquad \text{and} \qquad R = \begin{bmatrix} R_E \\ R_{E'} \end{bmatrix} \tag{7}$$

The case of link-based quantities is somehow different. Indeed, since links can be internal ones (denoted with a subscript E for a subdomain E) and links on the global interface (denoted with a subscript Γ), the relative velocities and the interaction impulses are split as:

$$v = \begin{bmatrix} v_E \\ v_{E'} \\ v_\Gamma \end{bmatrix} \qquad \text{and} \qquad r = \begin{bmatrix} r_E \\ r_{E'} \\ r_\Gamma \end{bmatrix} \tag{8}$$

The dynamical evolution of the grains on the subdomain E is therefore:

$$M_E V_E = M_E V_E^i + R_E^d + R_E + R_{E\Gamma} \tag{9}$$

R_E is the assembly of internal interaction impulses, while $R_{E\Gamma}$ is the assembly, at the subdomain E level, of the impulses of Γ acting on E ($E\Gamma$ denotes the local interface of subdomain E, i.e. a part of the larger global interface Γ). A consistent splitting of the operator H leads to the following admissibility conditions. Note that since each subdomain is independent from each other, the block decomposition of H into h can be used as well:

$$R_E = H_E r = h_E r_E \qquad \text{and} \qquad R_{E\Gamma} = H_{E\Gamma} r = h_{E\Gamma} r_\Gamma \tag{10}$$

Γ can be seen as a particular subdomain constituted of interactions but no grains. Similarly, one gets:

$$v_E = H_E^T V = h_E^T V_E \qquad \text{and} \qquad v_\Gamma = \sum_E H_{E\Gamma}^T V = \sum_E h_{E\Gamma}^T V_E \tag{11}$$

The condensed dynamics on each subdomain and interface leads to an algebraic splitting of the reference problem (3):

$$\begin{bmatrix} v_E \\ v_{E'} \\ v_\Gamma \end{bmatrix} = \begin{bmatrix} v_E^d \\ v_{E'}^d \\ v_\Gamma^d \end{bmatrix} + \begin{bmatrix} W_E & 0 & W_{E\Gamma} \\ 0 & W_{E'} & W_{E'\Gamma} \\ W_{\Gamma E} & W_{\Gamma E'} & W_\Gamma \end{bmatrix} \begin{bmatrix} r_E \\ r_{E'} \\ r_\Gamma \end{bmatrix} \tag{12}$$

where

$$\begin{aligned} v_E^d &= h_E^T(V_E^i + M_E^{-1} R_E^d) \\ v_\Gamma^d &= \sum_E h_{E\Gamma}^T(V_E^i + M_E^{-1} R_E^d) \\ W_E &= h_E^T M_E^{-1} h_E \\ W_{E\Gamma} &= W_{\Gamma E}^T = h_E^T M_E^{-1} h_{E\Gamma} \end{aligned}$$

and

$$W_\Gamma = \sum_E h_{E\Gamma}^T M_E^{-1} h_{E\Gamma} \tag{13}$$

Note that due to the diagonal character (at least per block, corresponding to each grain) of M_E, and to the fact that $h_{E\Gamma}$ is a signed boolean matrix with at most one non null entry per column (an interface link is at most connected to one grain in a subdomain), W_Γ is almost a diagonal matrix (the slighly not diagonal character came from possible rows in $h_{E\Gamma}$ with more than one non null entry: a grain may have more than one interface link). Therefore, it is expected that the interface problem, dealing with left-hand-side W_Γ will not be costly.

3.2 DD-NLGS algorithm

A typical Jacobi splitting of a coupled system naturally leads to a parallel treatment of the resolution. With the previous algebraic splitting, a bloc Gauss-Seidel will also lead to a parallel treatment of all the subdomains. Since we wish to sequentialize the treatment of the global interface to obtain a synchronous algorithm, we propose the following Gauss-Seidel-like splitting of the previous problem (12):

$$\begin{aligned} &\begin{bmatrix} W_E^L & 0 & 0 \\ 0 & W_{E'}^L & 0 \\ W_{E\Gamma} & W_{E'\Gamma} & W_\Gamma^L \end{bmatrix} \begin{bmatrix} r_E \\ r_{E'} \\ r_\Gamma \end{bmatrix} - \begin{bmatrix} v_E \\ v_{E'} \\ v_\Gamma \end{bmatrix} = \\ &= - \begin{bmatrix} v_E^d \\ v_{E'}^d \\ v_\Gamma^d \end{bmatrix} - \begin{bmatrix} (W_E - W_E^L) & 0 & W_{E\Gamma} \\ 0 & (W_{E'} - W_{E'}^L) & W_{E'\Gamma} \\ 0 & 0 & (W_\Gamma - W_\Gamma^L) \end{bmatrix} \begin{bmatrix} r_E \\ r_{E'} \\ r_\Gamma \end{bmatrix} \end{aligned} \tag{14}$$

where the superscript L refers to the lower diagonal part (including the diagonal).

To close the problem (at each time step), one has to add the constitutive behavior of the interactions, i.e.

$$\mathcal{R}(r_E, v_E) = 0, \quad \mathcal{R}(r_{E'}, v_{E'}) = 0 \quad \text{and} \quad \mathcal{R}(r_\Gamma, v_\Gamma) = 0 \tag{15}$$

The corresponding generic program is described in Algorithm 1. This algorithm is suited to a shared memory parallelization via compiler directives (typically, OpenMP paradigm [10]); for a distributed memory, data synchronization should be ensured by ad hoc communications between processors to exchange information (typically, with MPI library), but this is not detailed herein. For sake of simplicity, we choose herein to perform a domain partitioning at each time step to cope with connectivity modifications (new contact detection at each time step).

There are two additional parameters when compared to a sequential algorithm: the number of sub-iterations n and m. Due to the previously mentioned quasi-diagonal character of W_Γ, one could choose $m = 1$. The frequency of interface updating, i.e. the parameter n, has to be chosen from experiments. This is the goal of the following tests.

Algorithm 1 DD–NLGS

```
Loop on time steps
for i = 1, 2 ... do
  position prediction and potential contact detection
  Domain partitioning
  Parallel loop on subdomains
  for E = 1, 2 ... n_SD do
    Compute free velocities per subdomain E
  end for
  Loop on DDM iterations
  for j = 1, 2 ... n_DDM do
    Parallel loop on subdomains
    for E = 1, 2 ... n_SD do
      NLGS resolution per subdomain E, with n sweeping iterations
      Compute error contribution of subdomain E
    end for
    NLGS resolution on global interface Γ, with m sweeping iterations
    Compute error contribution of interface Γ
    Assemble error contributions, to check for loop termination
  end for
  Parallel loop on subdomains
  for E = 1, 2 ... n_SD do
    Compute nodal quantities (velocities and position updates)
  end for
end for
```

The first numerical study aim to settle recommendations for the choice of the additional parameters n and m. Consequently with the previously mentioned sparsity of W_Γ, we first select $m = 1$. The proposed test case concerns a slice of a ballasted railway containing 28 608 ballast grains (polyhedra) and an average of 120 500 frictional contact interactions between grains, with a friction coefficient

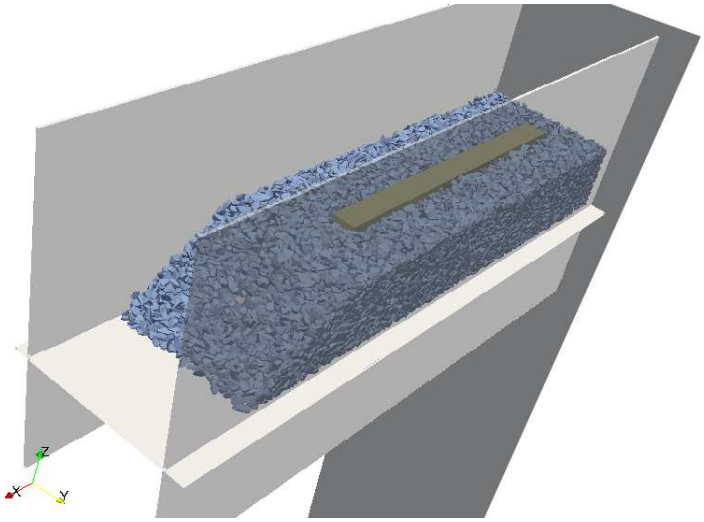

Figure 4: The first test case. One slice of a ballasted railway with one sleeper (only half of the slice is modeled here)

$\mu = 0.7$. The grains are also in contact with a sleeper with a friction coefficient $\mu_s = 2$. Finally, there are 3 planes delimiting the sample, and one plane for the ground, each with a friction coefficient $\mu_p = 0.8$. Figure 4 illustrates the initial state. This study investigates the behaviour of ballast grain under the dynamic track stabilizer which simulate during a few second a railway traffic to restore the initial level of lateral resistance of track before tamping operation [3]. The loading is a vertical descending force on the sleeper with an amplitude 120 kN, and a lateral speed prescribed on the same sleeper, in the Y direction with an amplitude 0.237 m/s at a frequency of 30 Hz, but only the beginning of the evolution is computed since the studied time interval is $[0, T]$ with $T = 0.02$ s (it is discretized in time with 100 time steps).

The reference solution is obtained with 100 sweeping iterations within each time step on the whole domain. For the domain-decomposed problem, $3 \times 3 \times 3$ subdomains are used, and we check several cases with a variable n and a variable number of DDM iterations n_{DDM}, while maintaining an overall number of sweepings $n \times n_{\text{DDM}}$ roughly constant: ($n_{\text{DDM}} = 100$, $n = 1$), ($n_{\text{DDM}} = 50$, $n = 2$), ($n_{\text{DDM}} = 33$, $n = 3$) and ($n_{\text{DDM}} = 25$, $n = 4$). To check the obtained solution in each case, several physical quantities of interest for the ballast [34, 5]) are used:

- the inertia parameter $I = \dot{\varepsilon}\sqrt{m/(dp)}$, measuring the quasistatic character of the problem [18], where d and m are the average size and mass of the grains, p the average pressure, and $\dot{\varepsilon}$ the mean strain rate.
- the spleeper settlement δ, i.e. the vertical displacement of the sleeper,
- the number of single contacts between grains n_1,

- the compactness c, which is the solid fraction of the sample (the ratio between the sum of the volumes of the grains in the sample and the volume of the sample).

The time evolution of these quantities is reported on Figure 5 for the different cases. All of them leads to the same conclusion: The most accurate solution (for a roughly constant cost in terms of computer operations) is obtained with $n = 1$. This conclusion holds for several decompositions with a different number of subdomains: $1 \times 1 \times 1$ (reference problem), $2 \times 2 \times 1$, $2 \times 2 \times 2$, $3 \times 3 \times 3$, $4 \times 4 \times 4$ and $5 \times 5 \times 5$ subdomains. In each case, with ($n_{\text{DDM}} = 100$, $n = 1$) the obtained solution is comparable: the number of single contacts varies only by $0.44\,\%$, the compactness by $0.004\,\%$. The vertical settlement of the sleeper varies by $2\,\%$ and the maximal deviation is obtained from the inertia parameter ($6\,\%$); the evolution of these last two quantities are depicted on Figure 6.

Note that even the solution obtained with $n_{\text{DDM}} = 100$ and $n = 1$, however close to the reference for the above quantities of interest, does not reproduce exactly the reference solution. Indeed, this granular problem has a plurality of solutions and even a modification in the contact ordering for the iteration may lead to a different local solution [30]. For checking that such a local solution is feasible, several error indicators are computed, such as the relative residual interpenetration in volume to ensure a good numerical solution. An example of this numerical indicator is presented in Figure 7, for the case with 125 subdomains. The other global physical quantities (such as compactness, vertical settlement...) are the quantities of interest to select the optimal parameters n and n_{DDM}, to avoid bias in physical results and to allow a sensitivity analysis on the physical parameters of the process (frequency and amplitude of the sollicitation).

As a partial conclusion, the number of synchronization points with the interface has to be sufficiently large to ensure the coupling between the subdomains. Indeed, from a parallel efficiency point of view, one would prefer to increase granularity by allowing the subdomain to maintain a large number of local computations without exchanging data with the interface. In the following, we privileged the convergence rate for the solution by selecting $n = 1$.

4 Numerical results

4.1 Qualitative study on the tamping process

The first numerical investigation focused on the influence of the number of solver iterations per subdomain which can be fixed by considering the mechanical constraint imposed to the granular sample. In our case we suppose that the tamping of the first sleeper dop not modify the ballast behaviour far from the tamped one. The industrial tamping process consist of three phases after the sleepers have been lifted :

- The tamping tines are inserted around the sleepers,

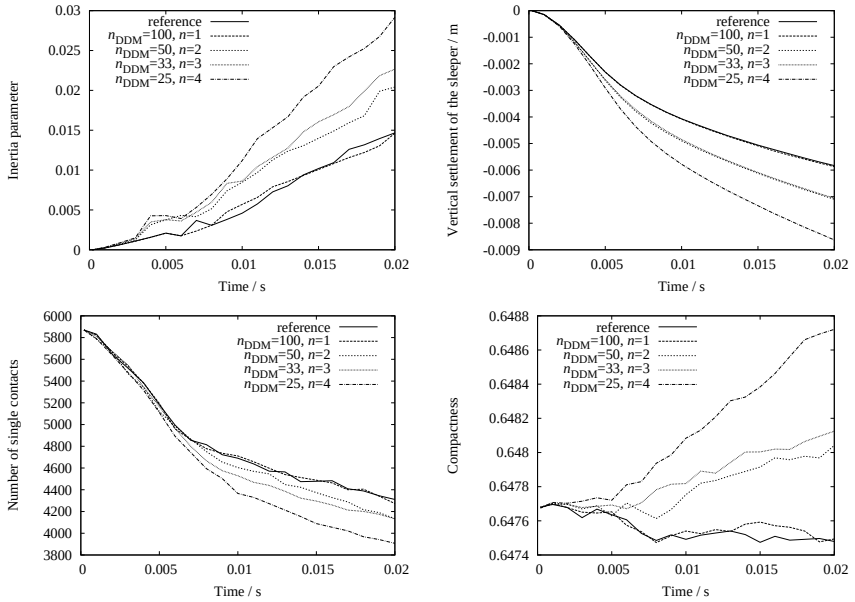

Figure 5: Case with 9 subdomains. Comparisons of several strategies on 4 physical quantities

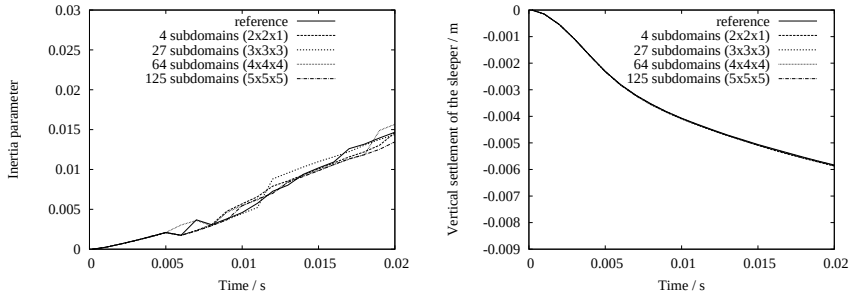

Figure 6: Case with $n_{\text{DDM}} = 100$ and $n = 1$. Influence of the number of subdomains

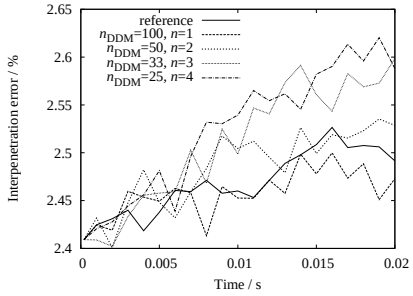

Figure 7: Case with 125 subdomains. Evolution of the error indicator (relative volume interpenetration violation)

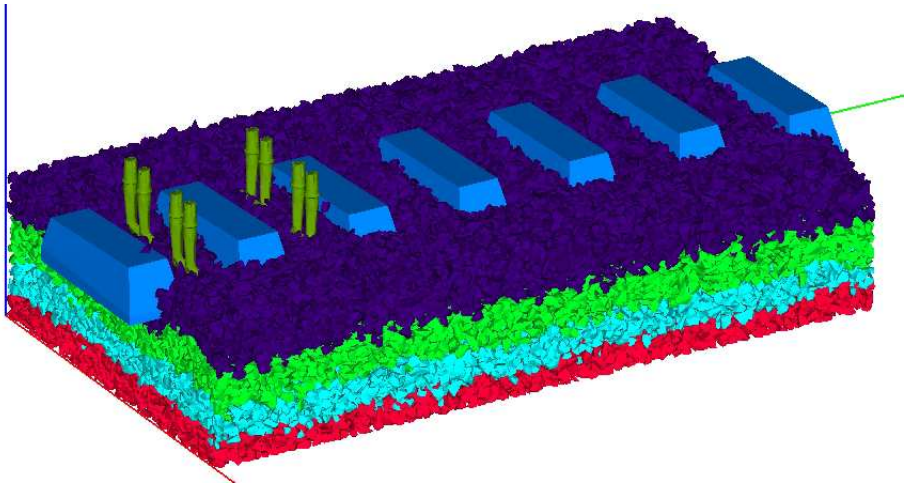

Figure 8: A railway slice of seven sleepers with tamping tines

- Then the tamping tines squeeze the ballast to fill the voids under the sleeper,
- Finally the tamping tines are removed.

The simulation of such a process allows to perform parametric studies to evaluate the influence of different parameters. For instance a previous study [5] underlined the importance of the first phase which contributes to fifty percent of the final compaction gain. The simulations showed also that low speeds of penetration improve the final compaction gain.

We focus attention on the first phase but applied to a large scale problem representing a long railway slice with seven sleepers. (In the long term the process has to be simulated sequentially or simultaneously on several sleepers for both accelerating and improving the maintenance.) The tamping tines are inserted around the second sleeper. The railway slice now contains 90 000 grains and around 300 000 contacts. The domain is split into seven subdomains under the seven sleepers according to the Figure 8. The main objective is here to test the possibility to reduce the computations in the subdomains far from the tamping tines. For that we perform five multidomain computations with different sweeping iteration number per subdomain according to Table 1. To carry on such a strategy starting from the Algorithm 1, the parameters are fixed as follows: $n_{DDM} = 800$, $n = 1$, $m = 1$. But for some subdomains (4 to 7 for the Run1 for instance) $n = 0$ as soon as $j > 700$ as illustrated in Table 1. The reference run requires 800 sweepings for all the subdomains whereas three runs require a decreasing sweeping number from the sleeper 4 to the sleeper 7. The last run is quite special with a small sweeping number for the sleeper 4 and a slightly increasing number for the following ones.

We fix the number of sweeping iterations because we do not have relevant error estimates to control the computation. The quality of the computation is appreciated according to a set of qualitative indicators mixing error estimates and quantities of

Table 1: Distribution of the sweeping number per subdomains (sleepers)

Sleeper #	1	2	3	4	5	6	7
Reference	800	800	800	800	800	800	800
Run 1	800	800	800	700	700	700	700
Run 2	800	800	800	700	600	500	400
Run 3	800	800	800	700	500	300	200
Run 4	800	800	800	100	200	300	400

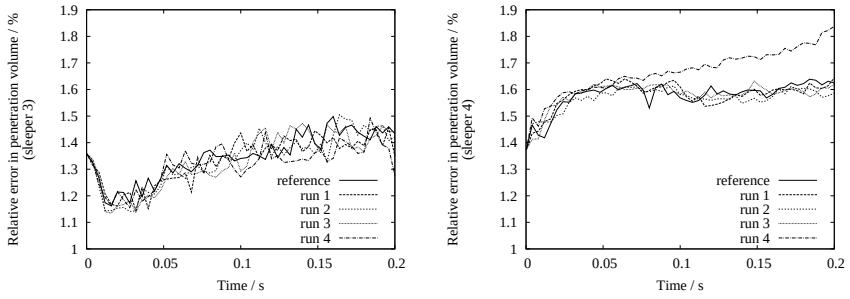

Figure 9: Volume error (interpenetration) under the sleepers 3 and 4, for the 5 runs

mechanical interest. Three of them are discussed in the following: the volume error quantifying the geometrical interpenetration, the compactness c, the inertia parameter discriminating dynamic versus quasistatic regime.

The more interesting results concern the sleepers 3 and 4 and the run 4. In Figure 9 the interpenetration error remains admissible (less than $2\,\%$) in the two subdomains and for all the runs except under the fourth sleeper and for the run 4. That means that 100 sweepings are not sufficient to avoid interpenetration, but this error is not propagated toward the neighboring subdomain 3.

In Figure 10 the evolution of the compacteness is given. The main difference occurs yet with the run 4. The compactness is overestimated under the sleeper 4 and underestimated under the sleeper 3. Then the lack of computation under the sleeper 4 perturbs this indicator also under the sleeper 3.

In Figure 11 the inertia parameter is compared under the same sleepers. This indicator is slightly perturbed by the lack of iterations of the run 4 under the sleeper 4 where the regime remains quasistatic during the process. On the contrary this parameter is clearly modified at the end of the process under the sleeper 3 where it is overestimated.

This study shows the possibility to distribute the computational effort according to solicitation but with some precautions. The number of sweepings cannot be drastically reduced in a subdomain weakly loaded but close to a strongly loaded subdomain.

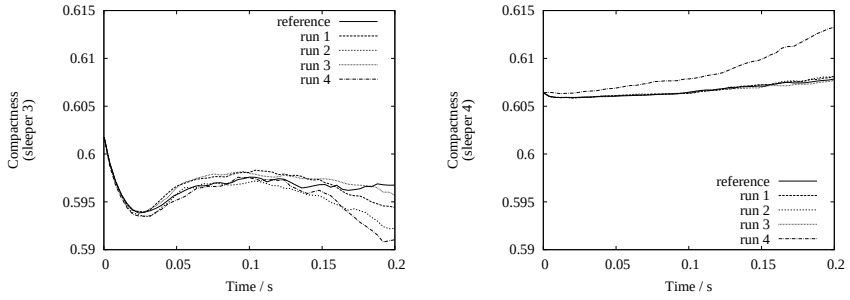

Figure 10: Compactness under the sleeper 3 and 4, for the 5 runs

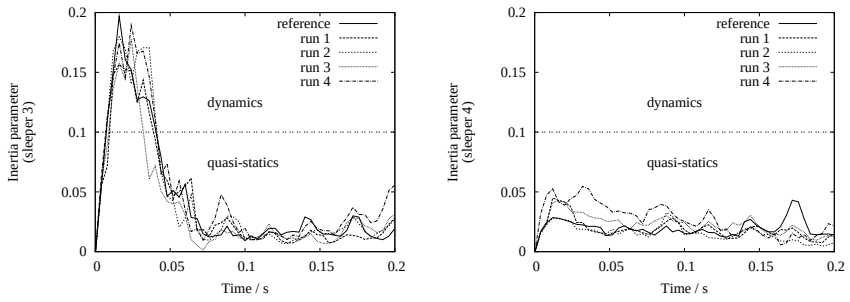

Figure 11: Inertia parameter under the sleeper 3 and 4, for the 5 runs

4.2 Parallelization strategy with OpenMP

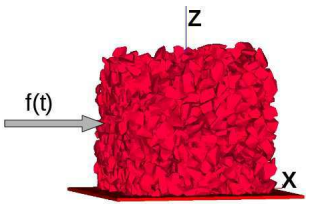

Figure 12: Sample with 2 000 grains and an harmonic force

In this Section, we analyze the efficiency of the parallelization strategy with OpenMP [10] on the previous DD–NLGS algorithm.

The analysis focused on a confined sample of polyhedral grains submitted to an harmonic force. The sample is contained in an open cubic box of $50\,\mathrm{cm}$ edge. One of the wall is submitted to an harmonic force along X direction : $f(t) = F_{\max}(1 - \sin \omega t)$ with $F_{\max} = 5\,\mathrm{kN}$, a frequency of $5\,\mathrm{Hz}$, and a time interval $[0, 0.02\,\mathrm{s}]$ discretized in 100 time steps. The mechanical behavior of such a sample under an harmonic driving force is analyzed with more details in [4].

Herein, to estimate the effect of the parallelization on the resolution part, we use one sweeping iteration ($n = m = 1$) but a large number of DDM iterations ($n_{\text{DDM}} = 10\,000$).

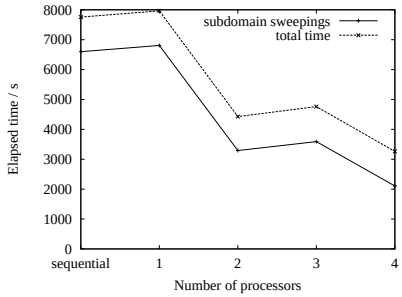

Figure 13: Execution time of the sample split into 4 subdomains

A first decomposition with $n_{\text{SD}} = 2\times2\times1 = 4$ subdomains is tested. The computation is performed on a 2 Dual-Core processor machine, i.e. with a resource of a maximum of 4 processors. The reference case (sequential) and the 4-subdomain decomposition are tested with different numbers of processors (1 to 4). Figure 13 reports the elapsed time spent for the sole treatment of subdomains and for the total simulation, along with the number of processors. With 4 subdomains, the elapsed time in the parallel region is approx. 80 % of the total computation time.

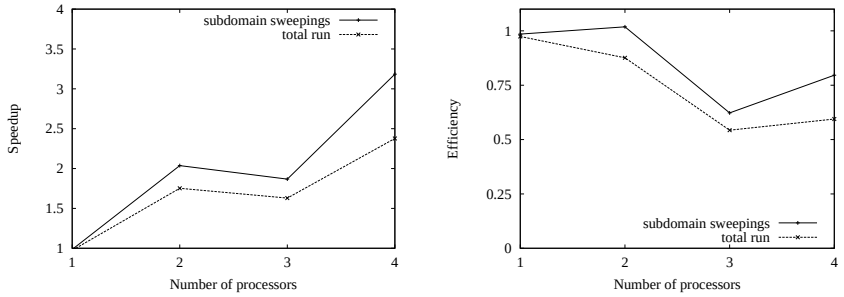

Figure 14: Performance of the parallelization with 4 subdomains

To assess the parallelization, the speedup is defined as: $S_p = T_s/T_p$ where T_s is the execution time of the sequential algorithm and T_p is the execution time of the parallel algorithm on p processors. The ideal speedup is obtained when $S_p = p$. The efficiency is: $E_p = S_p/p$ and is typically in the range $[0, 1]$. Both are depicted in Figure 14.

For the parallel region of the code, the case of 2 running cores gets the best efficiency. For 4 cores, it is still of $78\,\%$. However, a low efficiency is obtained for 3 cores; indeed, the unbalance of the amount of computation is large, since one processor is idle when the 3 remaining ones have been assigned to 1 subdomain

each. Of course, the parallel ratio of the overall code is less that that of the parallel region, and the efficiency is lower for the total run ($E_p = 60\,\%$ for $p = 4$). Indeed, the interface treatment, contact detection, decomposition of the domain are still sequential parts of the code.

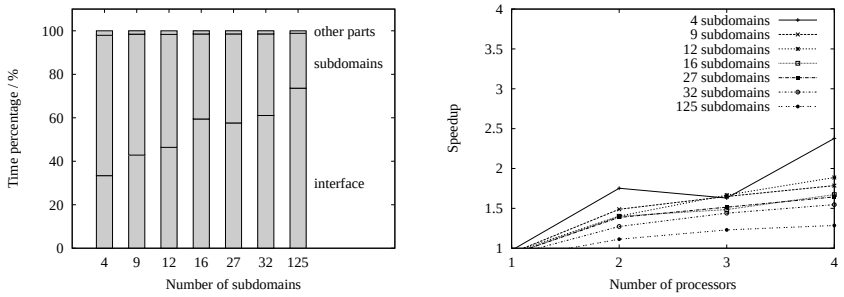

Figure 15: Influence of the number of subdomain, for a fixed number of processors ($p = 4$). Left: percentage of elapsed time spent on different parts of the code; right: speedups

Since the number of DDM iterations n_{DDM} is large, the cost is dominated by the interface and subdomain treatments; Figure 15 (left) reports the percentage of time spent in these different regions of the code, with different numbers of subdomains n_{SD}.

Table 2: Total elapsed time for several splittings

Number of subdomains	Total elapsed time / s				
n_{SD}	sequential	1 proc.	2 proc.	3 proc.	4 proc
$4 = 2 \times 2 \times 1$	7757	7964	4427	4761	3263
$9 = 3 \times 3 \times 1$	8168	8322	5279	4772	4412
$12 = 2 \times 3 \times 2$	8082	8268	5597	4724	4180
$16 = 1 \times 4 \times 4$	8320	8482	5608	5291	4707
$27 = 3 \times 3 \times 3$	8315	8477	5665	5189	4788
$32 = 4 \times 2 \times 4$	8413	8571	6168	5459	5088
$125 = 5 \times 5 \times 5$	8824	8974	7044	6381	6106

Indeed, when increasing the number of subdomains, the size of the interface increases along with its dedicated percentage of time. Since the treatment of the interface is a sequential part in the algorithm, the speedup is expected to decrease when increasing the number of subdomains, though a better load balancing is obtained when the number of subdomains is a multiple of the number of processors. This is reported in Table 2 and Figure 15 (right).

5 Conclusions

The improvement of industrial process or the increase of knowledge of the physical behavior of granular material require usage of numerical simulations which can produce a large volume of data for deep post-processing [5]. The analysis of granular simulations give some orientation to characterize the mechanical behavior, but the variability of the system behavior under the external solicitations remains a hard task to solve. The development of numerical methods with parallelism is also an opportunity to perform statistical study of large sample.

The DDM approach proposed in this paper allows to decrease computational efforts by using parallel algorithm without any difference with a sequential approach. The application of the approach on several railway industrial process currently used for maintenance gives the opportunity to qualify quickly the influence of some parameters. The tamping operation has been investigated on a portion of railway track and we can exhibit the influence of the process on other sleepers and the variability of compaction gain. This parameter is crucial to obtain the lowest differential settlement under cyclic loading and to propose orientations to decrease maintenance cost.

Since we choose only one sweeping iteration per DDM iteration ($n = 1$) to privilege a higher convergence rate, the best performances are obtained when the interface is as small as possible, because it is a bottleneck for parallelization (of course a fine grain parallelization of the interface treatment at the contact level would also be possible). Usually it leads to select a small number of subdomains, i.e. equal to the number of processors. To avoid a load unbalance among the subdomains, a first criteria could be to have a similar number of contact per subdomain, and therefore to use a direct partitioning of the potential contact graph to split the grains in subdomains. Up to now, only a geometric box decomposition has been used, with good results if the granulometry and the density of the granular sample is uniform. The first results have been obtained in parallel on a small sample, and on a small number of processors. The treatment of a larger problem, say the full industrial tamping process on the seven-sleeper case, and eventually with a larger number of processors, will be required to completely validate the proposed strategy on a multicore environment.

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