La DDM, les éléments discrets et LMGC90

V. Visseq, A. Martin, P. Alart, D. Dureisseix

JUL - LMGC90

Mai 22 2012

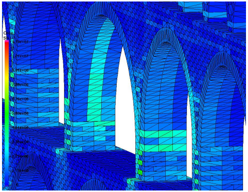
Motivation of parallel computing

Decrease CPU time computations (currently workable) :

- reduce the analysis time
- perform parametric studies

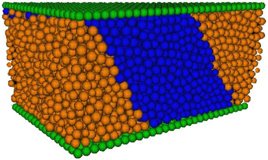
Perform larger and more complex simulations :

- number of particles increases
- shape of discrete elements becomes more complex



[Nîmes Aqueduc - LMGC90]

[Railway Ballast - LMGC90]

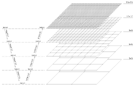


[Third Body - LaMCoS]

HPC strategies

Multigrid methods :

- several scales



Multiprocessing - Shared memory architecture :

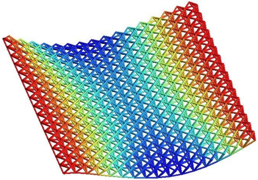
- OpenMP : “Open MultiProcessing”
- Splitting of loops among processors

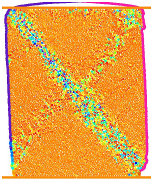
Multiprocessing - Distributed memory architecture :

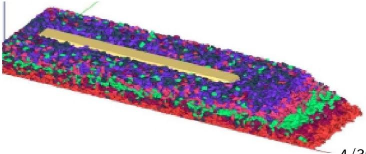
- MPI : “Message Passing Interface”
- Domain decomposition

Parallel computing and LMGC90

- M. Renouf [2004] : “Optimisation Numérique et Calcul Parallèle pour la simulation des milieux divisés bi- et tri-dimensionnels”
- S. Nineb [2007] : “Modélisation et outils numériques en mécanique non-régulière et applications à la tenségrité”
- D. Iceta [2010] : “Simulation numérique de la dynamique des systèmes discrets par décomposition de domaine et application aux milieux granulaires”
- T.M.P. Hoang [2011] : “Décomposition de domaine dans la simulation par éléments discrets en utilisant le calcul parallèle à mémoire partagé pour des applications ferroviaires”







Outlines

Subsection

Particularities of the NSCD framework

Non-smoothness

- Non regular behavior at contact (e.g. complementary law) :

$$\mathcal{R}(v, r) \text{ true}$$

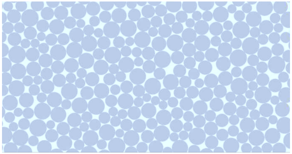
- Number of contacts greater than the number of particles
- Appearance and disappearance of contacts over the process

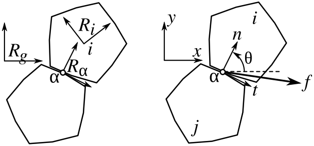
Discreteness / Multibody dynamics

- Dynamics of discrete elements over the time slab $[t_i, t_{i+1}]$:

$$MV - R = R^d \text{ (rigid particles)}$$
$$MV + \int_{t_i}^{t_{i+1}} KUdt - R = R^d \text{ (deformable particles)}$$

- Reorganization of particles during the evolution process
- Large/elongated particles





v : relative velocity at contact
r : impulse at contact
V : velocity of body (translational and rotational degrees of freedom)
R : resultant impulse on a body

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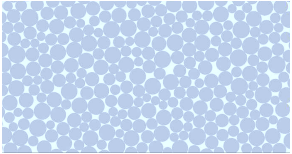

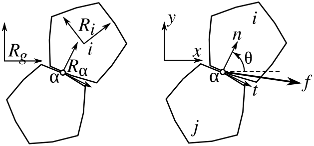

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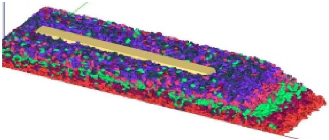

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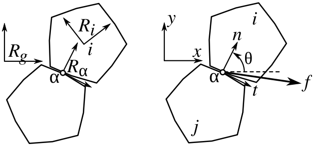

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Particularities of the NSCD framework

Reduced dynamics

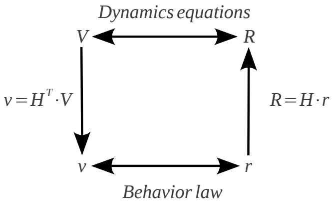
- Dynamics+compatibility conditions, reads :

$$Wr - v = v^d$$

with Delassus operator :

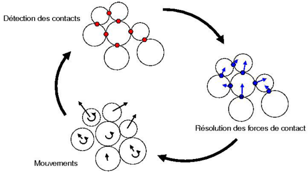
$$W = H^T M^{-1} H \text{ (rigid particles)}$$
$$W = H^T \left(M + h^2 \theta^2 K \right)^{-1} H \text{ (deformable particles)}$$

- Delassus operator symmetric and a priori non-invertible
  $\rightarrow$ multiple admissible solutions
  $\rightarrow$ iterative resolution (NLGS, CPG, etc...)



Algorithm 1 NSCD algorithm

for $i = 1, \ldots, N$ **do**
  Contact detection
  while (convergence criterion not satisfied) **do**
    Iterative resolution
    $$\begin{cases} Wr - v = -v^d \\ \mathcal{R}(v, r) = 0 \end{cases}$$
  end while
  Update grain positions
end for



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   ... Non-Smooth Contact Domain Decomposition (NSCDD)
   - Non-smooth contact dynamics
   - DDM strategy
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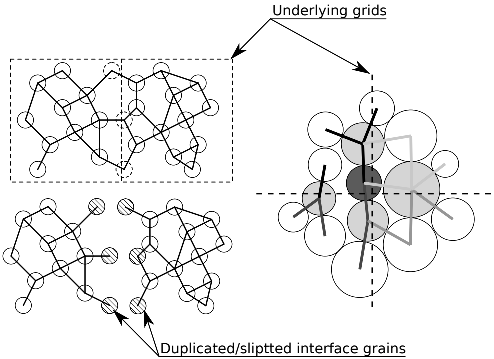
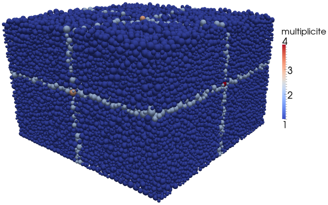
Domain partitioning strategy

Idea : isolate non-smoothness within the subdomains



[Partitioning Examples]



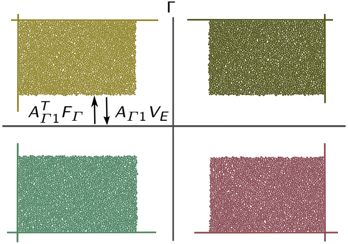
[Multiplicity of grains - 55 000 spheres sample]

Algebraic distribution of masses and inertia of grains according to the multiplicity m^i of the grain i : internal ($m^i = 1$), face ($m^i = 2$), corner ($m^i > 2$).
$\rightarrow$ Partition of Unity method

FETI-like formulation and NSCDD algorithm

- In each subdomain E the problem is identical to the global one
- Interconnecting conditions added to "glue" neighboring subdomains
- FETI-like formulation with F_Γ a multiplier field
- The reduced problem, with $X = \sum_E A_{\Gamma E} M_E^{-1} A_{\Gamma E}^T$

$$\sum_{E=1}^{n_{sd}} A_{\Gamma E} V_E = 0$$

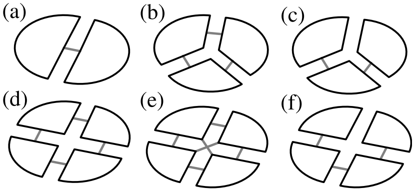


$$\left.\begin{array}{l} W_E r_E - v_E - \hat{A}_{\Gamma E}^T F_\Gamma = -v_E^d \\ \mathcal{R}(v_E, r_E) = 0 \end{array}\right\} E = 1, \ldots, n_{sd}$$
$$X F_\Gamma - \sum_{E=1}^{n_{sd}} \hat{A}_{\Gamma E} r_E = \hat{f}$$

Interface grains and Partition of Unity

$$X^i = \sum_{E=1}^{n_{sd}} A^i_{\Gamma E} (M^i_E)^{-1} (A^i_{\Gamma E})^T$$

$$X^i = \sum_{E=1}^{n_{sd}} (M^i_E)^{-1} L^i_E = (M^i_E)^{-1} L^i$$



$$L^i = \begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & 2 & -1 \\ & & -1 & 2 \end{bmatrix}$$

[(c) and (f) cases]

$$L^i = \left[\begin{array}{cccc|c} 2 & -1 & & & 1 \\ -1 & \ddots & \ddots & & \\ & \ddots & 2 & -1 & \\ & & -1 & 2 & 1 \\ \hline 1 & & & 1 & 2 \end{array}\right]$$

[(b) and (d) cases]

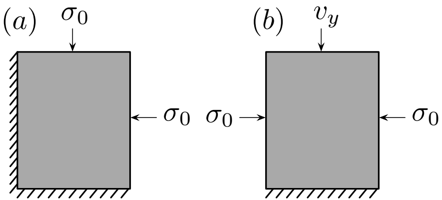
$$X^i \Delta F^i_\Gamma = \sum_{E=1}^{n_{sd}} A^i_{\Gamma E} \bar{V}^i_E \quad \Leftrightarrow \quad \Delta F^i_\Gamma = (L^i)^{-1} M^i_E \sum_{E=1}^{n_{sd}} A^i_{\Gamma E} \bar{V}^i_E$$

Subsection

Validation of NSCDD according to the physics of granular media

Perform a realistic test on the LMGC90 platform

Test of the robustness of the DDM approach : Biaxial loading up to a cumulative vertical strain $\varepsilon_1 = 0.35$ of a dense packing composed of 12000 disks



Boundary conditions for (a) isotropic and (b) biaxial compactions

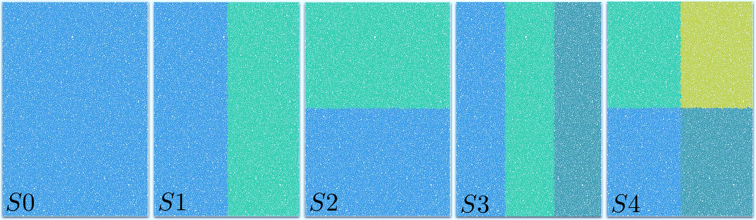
Error estimation

How to evaluate influence of DDM on the solution of such a test ?

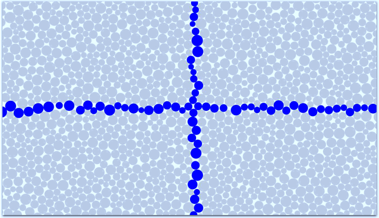
Considered decompositions

Biaxial loading of a dense packing composed of 12000 disks :

Examples of decomposition at the initial state (a) and zoom at the intersection of the four subdomains of case $S4$ (b)

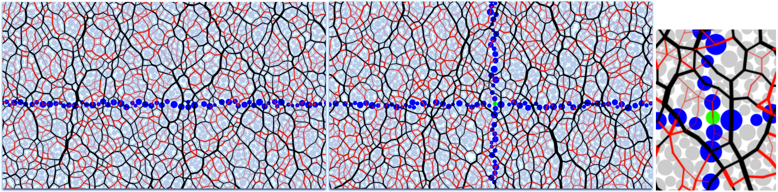


(a)

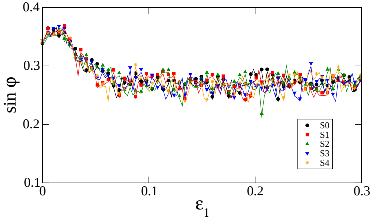

(b)

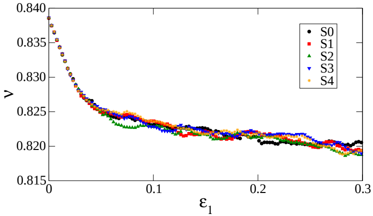
Global behavior and micromechanical structure

Force chains on parts of S2 and S4



Friction angle $\sin\varphi$ as a function of ϵ_1 - Solid fraction ν as a function of ϵ_1





Subsection

Sequential Multi-Domain implementation

Why a sequential implementation of parallel algorithm ?

- mimic behavior of multiprocessing environment
- study algorithmic properties of NSCDD without messages between processors
- overcome technical aspects of the MPI implementation

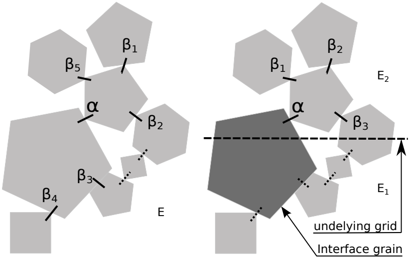
Sequential Multi-Domain on the LMGC90 software

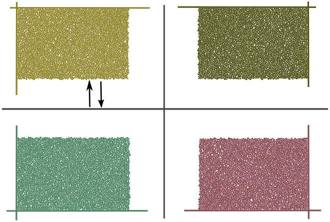
- duplication of the LMGC90 sequential database according to the number of subdomains
- independent resolutions of the reduced dynamics for each subdomains

Time consuming analysis

Main characteristics of the simulations according to the tested decompositions

	$S0$	$S1$	$S2$	$S3$	$S4$
Total elapsed time	262 $10^3 s$	239 $10^3 s$	235 $10^3 s$	258 $10^3 s$	251 $10^3 s$
Total number of NSCDD iterations	164.5 10^5	164.1 10^5	164.1 10^5	166.4 10^5	166.0 10^5
Number of $W_{\alpha\beta}$	418 10^3	380 10^3	341 10^3	366 10^3	303 10^3





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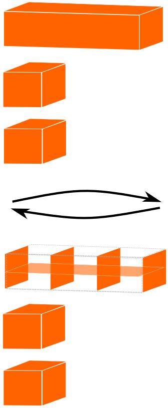
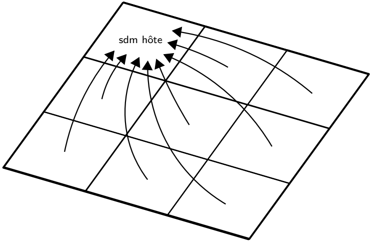
NSCDD main stages : sequential, exchanges and parallel

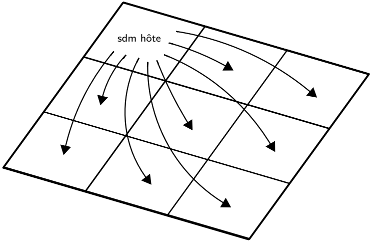
- Rough detection & Domain partitioning
- Fine detection
- Intermediary solving stages
- Exchanges between processors
- Interface gluing stage
- NLGS resolution
- Update



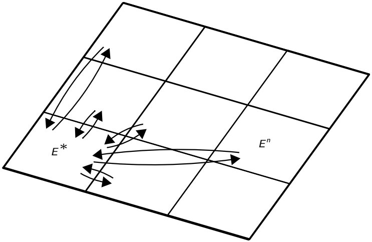
MPI exchanges

Centralized exchanges scheme





Decentralized exchanges scheme



$$\sum_E \underline{\underline{A}}_{\Gamma_{E^*}E} \underline{\underline{M}}_E^{-1} \underline{\underline{A}}^T_{\Gamma_{E^*}E} \cdot \Delta \underline{F}_{\Gamma_{E^*}} = \sum_E \underline{\underline{A}}_{\Gamma_{E^*}E} \underline{V}_E$$

$$\underline{\underline{X}} \cdot \Delta \underline{F}_\Gamma = \sum_E \underline{\underline{A}}_{\Gamma E} \underline{V}_E$$

$$\Leftrightarrow \sum_{E^*} \underline{\underline{B}}^T_{\Gamma_{E^*}\Gamma} \underline{\underline{X}}_{\Gamma_{E^*}} \Delta \underline{F}_{\Gamma_{E^*}} = \sum_{E^*} \underline{\underline{B}}_{\Gamma E^*} \underline{\underline{D}}_{E^*} \underline{\underline{B}}^T_{\Gamma_{E^*}E^*} \sum_E \underline{\underline{A}}_{\Gamma_{E^*}E} \underline{V}_E$$

Performances of the two schemes

Numerical parameters :

- $N_{Time\ Steps} = 500$
- $\Delta t = 10^{-2} s$
- $F_0 = 60\ 10^3 N$
- $Freq_{Repart} = 10 Time\ Steps$
- $Freq_{Out} = 250 Time\ Steps$
- $Norm_{Type} = QM/16$
- $Norm_{Type} = Quad$
- $Tol = 1.6610^{-4}$

Recollement sur l'interface globale				
n_{sdm}	Découpage : x,y,z	Temps CPU	Efficiency	Echanges "in loop"
1	1 1 1	7207 s	1	0 %
3	3 1 1	5526 s	0.44	31.3 %
4	2 2 1	4225 s	0.43	35.6 %
8	2 2 2	3985 s	0.23	58.3 %
Recollement sur les interfaces locales				
n_{sdm}	Découpage : x,y,z	Temps CPU	Efficiency	Echanges "in loop"
1	1 1 1	7068 s	1	0 %
3	3 1 1	3326 s	0.71	14.0 %
4	2 2 1	2222 s	0.80	9.1 %
8	2 2 2	1454 s	0.61	18.4 %

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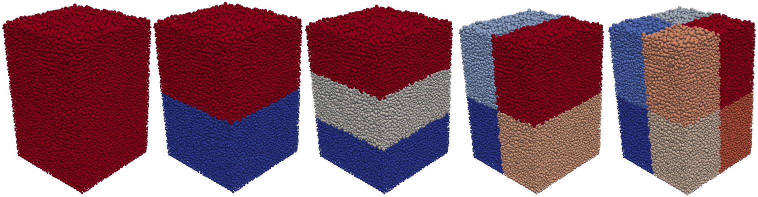
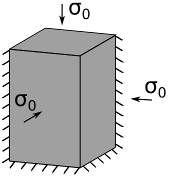
3D NSCDD simulation using MPI library

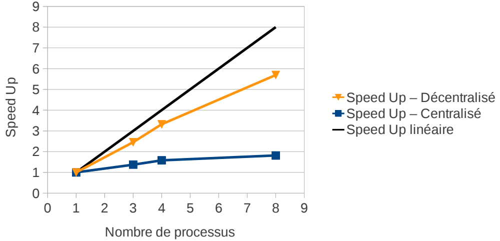
Triaxial loading of a dense packing composed of 55000 disks :

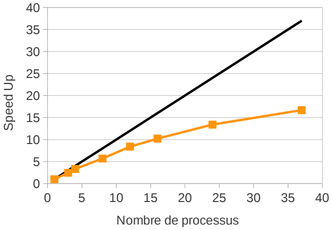
Set of samples to study parallel performances of the NSCDD implementation, with message passing between processors, on the LMGC90 platform

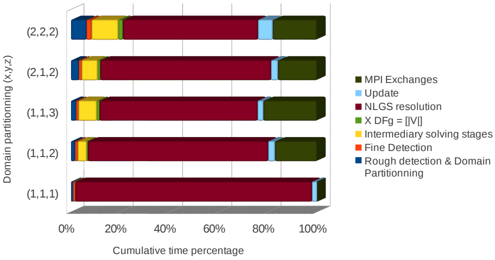


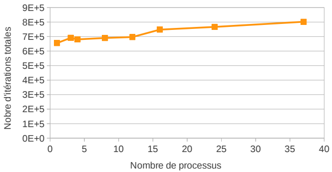


Performances & time consuming analysis









Conclusion

NSCDD a scalable DDM approach for contact dynamics

- Implemented in the LMGC90 plateform
- 2D granular media (Disks)
- 3D masonry (Polyhedra) and granular media (Spheres)

Physical meaning of solutions

- Global behavior and micromechanical 2D structure in accordance with physics of granular materials
- Triaxial compaction under going

The DDM as model coupling framework

Coupling of :

- deformable and rigid discrete elements
- continuum (homogenized/regularized media ?) and discrete models

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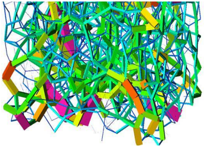
Thank you for your attention !



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[2] D. Dureisseix and C. Farhat, "A numerically scalable domain decomposition method for the solution of frictionless contact problems" in Int. J. Numer. Meth. Eng., 50(12) :2643–2666, 2001.

[3] P. Alart, D. Iceta, and D. Dureisseix, "A nonlinear domain decomposition formulation with application to granular dynamics", Comput. Methods. Appl. M., 205-208(0) :59 – 67, 2012.

[5] E. Azéma and F. Radjaï, "Stress-strain behavior and geometrical properties of packings of elongated particles", Phys. Review E, 81, 053014, 2010.

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