

35 Fictitious domain based solvers for particulate flows

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Introduction

In this article we discuss the application of fictitious domain methods to the numerical simulation of incompressible viscous flow with suspended moving particles. The model coupling the Navier-Stokes equations from fluid dynamics with the Newton equations for the particle motion has been extensively studied in the literature (see e.g. [GPH⁺98, GPH⁺00]). Among the problems for its practical application are fluidized beds, sedimentation, a blood flow around artificial heart valve, etc.

The solution method discussed here combines finite element discretizations in space, time discretization by a projection scheme and the method of characteristics [GP92] for the treatment of the convection term. The key points of our method are locally refined locally adapted grids for space discretization and efficient iterative solvers based on fictitious domain methods. The methodologies we follow in this paper were proposed and studied in [Ast78, GK98, MKM86]. We shall show in Section 4, that the concrete choice of the optimal domain embedding is strongly governed by the computational domain topology. Therefore, we focus in our research on simulations with a few solid particles to investigate in details the behavior of iterative solvers for the case of particle collisions.

Formulation of the particulate flow problem

Let $B(t)$, $t > 0$, be the union of a few solid particles suspended in an incompressible viscous fluid occupying the fixed domain Π . The fluid velocity \mathbf{u} and pressure p are solutions of the Navier-Stokes equations

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \frac{1}{\rho} \nabla p &= \mathbf{g} & \text{in } \Omega(t), \\ \nabla \cdot \mathbf{u} &= 0 & \text{in } \Omega(t), \end{aligned} \tag{1}$$

with initial and boundary conditions

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_0 & \text{in } \Omega(0), \\ \mathbf{u} &= \mathbf{g}_0 & \text{on } \partial\Omega(t). \end{aligned} \tag{2}$$

Here $\Omega(t) = \Pi \setminus \bar{B}(t)$ is the domain occupied by the fluid, ρ is the fluid density, ν is the kinematic viscosity and \mathbf{g} is the gravity. Without loss of generalization, we assume that the fluid-particle system is at rest at $t = 0$, i.e. $\mathbf{u}_0 = \mathbf{0}$ and $\mathbf{g}_0 = \mathbf{0}$. For $t > 0$, the particle motion

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satisfies Newton's law:

$$\begin{aligned} m_i \frac{d\mathbf{V}_i}{dt} &= \int_{\partial B_i(t)} \boldsymbol{\sigma} \cdot \mathbf{n} ds + m_i \mathbf{g}, \\ \frac{d}{dt} (\mathbf{I}_i \boldsymbol{\omega}_i) &= \int_{\partial B_i(t)} (\mathbf{x} - \mathbf{O}_i) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) ds, \quad i = 1, \dots, N, \end{aligned} \quad (3)$$

where \mathbf{V}_i , $\boldsymbol{\omega}_i$, m_i , \mathbf{I}_i and \mathbf{O}_i are translational and angular velocities, mass, inertia tensor and centroid of the i -th particle, respectively, $\boldsymbol{\sigma} = \nu \rho (\nabla \mathbf{u} + \nabla^T \mathbf{u}) - p \mathbf{I}$ is the stress tensor and \mathbf{n} is the unit normal vector on the particle boundary $\partial B_i(t)$ pointing outward. We assume that the no-slip boundary condition on $\partial B_i(t)$ holds, namely:

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{V}_i + \boldsymbol{\omega}_i \times (\mathbf{x} - \mathbf{O}_i), \quad i = 1, \dots, N. \quad (4)$$

Problem approximation

We use the Galerkin finite element formulation for the space discretization and finite differences for the time discretization.

Time discretization scheme

Let Δt denote the time step, $t^n = n \Delta t$, $\Omega^n = \Omega(t^n)$, and \mathbf{u}^n , p^n , \mathbf{V}_i^n , $\boldsymbol{\omega}_i^n$, $i = 1, \dots, N$, be approximations of the continuous solution at time t^n . The discretization scheme for problem (1)-(4) includes five steps:

Convection step. For any $\mathbf{x} \in \Omega^n$, we compute the characteristics $\psi(\mathbf{x}, t)$, $t \in [t^{n-1}, t^n]$, ending at \mathbf{x} and set $\mathbf{u}^{n+1/2}(\mathbf{x}) = \mathbf{u}(\psi(\mathbf{x}, t^{n-1}))$.

We use a first order Runge Kutta integration scheme. In the case when the characteristic leaves the domain Ω^n , a special numerical procedure is used to estimate $\psi(\mathbf{x}, t^{n-1})$.

Diffusion step. Using the convected field $\mathbf{u}^{n+1/2}$, we approximate the total time derivative by the first order implicit Euler scheme:

$$\begin{aligned} \frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^{n+1/2}}{\Delta t} - \nu \Delta \mathbf{u}^{n+1} + \frac{1}{\rho} \nabla p^n &= \mathbf{g} \quad \text{in } \Omega^n, \\ \tilde{\mathbf{u}}^{n+1} &= \mathbf{u}^n \quad \text{on } \partial \Omega^n. \end{aligned} \quad (5)$$

Projection step. The computed field $\tilde{\mathbf{u}}^{n+1}$ is projected onto a space of divergent-free functions by solving a Poisson equation for $p^{n+1} - p^n$:

$$\begin{aligned} \mathbf{u}^{n+1} &= \tilde{\mathbf{u}}^{n+1} - \frac{\Delta t}{\rho} \nabla (p^{n+1} - p^n) \quad \text{in } \Omega^n, \\ \nabla \cdot \mathbf{u}^{n+1} &= 0 \quad \text{in } \Omega^n, \end{aligned}$$

with the Dirichlet boundary condition $\mathbf{u}^{n+1} = \mathbf{u}^{n+1/2}$ on $\partial \Omega^n$.

Particle motion step. Using the computed solutions \mathbf{u}^{n+1} and p^{n+1} and the first order Euler scheme, we discretize the motion equations:

$$\begin{aligned} m_i \frac{\mathbf{V}_i^{n+1} - \mathbf{V}_i^n}{\Delta t} &= \int_{\partial B_i(t^n)} \boldsymbol{\sigma}^n \cdot \mathbf{n} ds + m_i \mathbf{g}, \\ \mathbf{I}_i \frac{\boldsymbol{\omega}_i^{n+1} - \boldsymbol{\omega}_i^n}{\Delta t} &= \int_{\partial B_i(t^n)} (\mathbf{x} - \mathbf{O}_i^n) \times (\boldsymbol{\sigma}^n \cdot \mathbf{n}) ds - \boldsymbol{\omega}_i^n \times \mathbf{I}_i \boldsymbol{\omega}_i^n, \\ \mathbf{O}_i^{n+1} &= \mathbf{O}_i^n + \mathbf{V}_i^n \Delta t \end{aligned}$$

In the case of a few moving particles, a collision strategy based on the physics of solid bodies is used [GPH⁺00].

Interpolation step. The new particle positions define the domain Ω^{n+1} for the next time step. We use the finite element interpolation to compute the fluid velocity \mathbf{u}^{n+1} and pressure p^{n+1} in the new domain.

Local adaptive locally fitted grids

The time-discretized problem is approximated by a finite element method. It is quite clear that the meshes used for space discretization are as important as the time discretization schemes and iterative solvers. Indeed the mesh determines the size of the algebraic problem and accuracy of the approximation. Taking this into account leads strongly to choose structured Locally Refined Locally Adapted (LRLA) meshes (see Figure 1).

A LRLA grid is built in three steps. First, a locally refined fully hierarchical grid is constructed in the domain Π to satisfy requirements on the mesh size imposed by the geometry and the discretization. Second, the locally refined mesh is adapted to the particle boundaries to provide the second order of the discretization. Finally, the LRLA grid Π_h is restricted to the computational domain Ω .

The hierarchical structure of the grid allows the use of advanced preconditioners like multigrid methods and provides natural tree data structure which can be used for effective implementation of the interpolation step.

Space discretization

Let Ω_h^n be a triangulation of the domain Ω^n . A triangulation $\Omega_{h/2}^n$ is obtained from Ω_h^n by one level of uniform refinement, i.e. by splitting every tetrahedron in Ω_h^n into 8 smaller tetrahedra. Let $V_p \subset H^1(\Omega_h^n)$ be the space of piecewise linear functions with a zero mean value defined on triangulation Ω_h^n . Similarly, let $V_u \subset [H^1(\Omega_{h/2}^n)]^3$ be a space of vector piecewise linear functions defined on triangulation $\Omega_{h/2}^n$. We denote by V_{0u} a subspace of V_u of functions vanishing on $\partial\Omega_h^n$.

The Galerkin finite element formulation of the Diffusion step (5) is to find $\tilde{\mathbf{u}}_h^{n+1} \in V_u$, $\tilde{\mathbf{u}}_h^{n+1} = \mathbf{u}_h^n$ on $\partial\Omega_h^n$, such that

$$\int_{\Omega_h^n} \left(\frac{1}{\nu \Delta t} \tilde{\mathbf{u}}_h^{n+1} \cdot \mathbf{v}_h + \nabla \tilde{\mathbf{u}}_h^{n+1} : \nabla \mathbf{v}_h \right) dx = \int_{\Omega_h^n} \mathbf{f} \cdot \mathbf{v}_h dx \quad \forall \mathbf{v}_h \in V_{0u}, \quad (6)$$

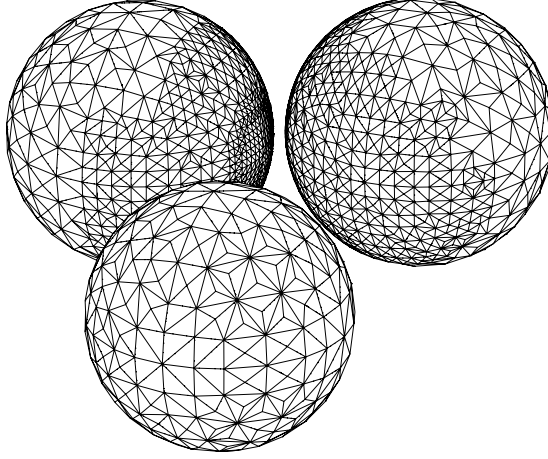


Figure 1: The trace of a LRLA grid on the particle boundaries

where $\mathbf{f} = \frac{1}{\nu}(\mathbf{g} + \frac{1}{\Delta t}\mathbf{u}_h^{n+1/2} - \frac{1}{\rho}\nabla p_h^n)$.

The weak formulation of the Projection step is to find a pair of functions $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in V_u \times V_p$, $\mathbf{u}_h^{n+1} = \mathbf{u}_h^{n+1/2}$ on $\partial\Omega_h^n$, such that

$$\begin{aligned} \int_{\Omega_h^n} \mathbf{u}_h^{n+1} \cdot \mathbf{v}_h dx + \frac{\Delta t}{\rho} \int_{\Omega_h^n} p_h^{n+1} \nabla \cdot \mathbf{v}_h dx &= \int_{\Omega_h^n} \mathbf{f} \cdot \mathbf{v}_h dx, \\ \int_{\Omega_h^n} q_h \nabla \cdot \mathbf{u}_h^{n+1} dx &= 0 \quad \forall (\mathbf{v}_h, q_h) \in V_{0u} \times V_p, \end{aligned} \quad (7)$$

where $\mathbf{f} = \tilde{\mathbf{u}}_h^{n+1} + \frac{\Delta t}{\rho}\nabla p_h^n$.

Fictitious domain method

Both problems (6) and (7) can be solved by fictitious domain methods (FDM). For simplicity of presentation we omit upper indices for unknown variables and computational domain, and assume that the flux satisfies the homogeneous Dirichlet boundary condition. Additionally, let the particles be spheres of the same radius R . We embed Ω into domain Π_δ in such a way that the triangulation Ω_h is a part of a triangulation $\Pi_{\delta h}$. Technically, both Ω_h and $\Pi_{\delta h}$ are traces of the fully hierarchical grid Π_h .

A concrete choice of the domain Π_δ depends on the topology of Ω . We assume that $\Omega \subset \Pi_\delta \subset \Pi$ and parameter δ characterizes the value of embedding. In other words it will be the thickness of a spherical layer $B_i(t^n) \cap \Pi_\delta$, i.e., $0 \leq \delta \leq R$. Thus $\Pi_0 = \Omega$ and $\Pi_R = \Pi$. Let $\gamma = \partial\Pi_\delta \setminus \partial\Pi$ be a part of the boundary $\partial\Pi_\delta$ living inside particles. Note that $\gamma = \emptyset$ when $\delta = R$.

FDM with distributed Lagrange multipliers

Following [GK98] we replace (6) by the equivalent saddle point problem with *distributed Lagrange multipliers*: find $(\mathbf{u}_h, \boldsymbol{\lambda}_h) \in W_u \times W_\lambda$:

$$\begin{aligned} \int_{\Pi_\delta} \left(\frac{1}{\nu \Delta t} \mathbf{u}_h \cdot \mathbf{v}_h + \nabla \mathbf{u}_h : \nabla \mathbf{v}_h \right) dx + \int_{\Pi_\delta \setminus \bar{\Omega}_h} \left(\frac{1}{\nu \Delta t} \boldsymbol{\lambda}_h \cdot \mathbf{v}_h + \nabla \boldsymbol{\lambda}_h : \nabla \mathbf{v}_h \right) dx &= \int_{\Omega_h} \mathbf{f} \cdot \mathbf{v}_h dx, \\ \int_{\Pi_\delta \setminus \bar{\Omega}_h} \left(\frac{1}{\nu \Delta t} \mathbf{u}_h \cdot \boldsymbol{\mu}_h + \nabla \mathbf{u}_h : \nabla \boldsymbol{\mu}_h \right) dx &= 0 \quad \forall (\mathbf{v}_h, \boldsymbol{\mu}_h) \in W_u \times W_\lambda, \end{aligned}$$

where $W_u \subset H^1(\Pi_\delta, \partial\Pi_\delta)$ and $W_\lambda \subset H^1(\Pi_\delta \setminus \bar{\Omega}_h, \gamma)$ are subspaces of piecewise linear functions vanishing on $\partial\Pi_\delta$ and γ , respectively. In algebraic form it reads:

$$\begin{pmatrix} A_u & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}. \quad (8)$$

By dividing the components of the solution u into separate groups denoted by u_1 and u_2 we obtain a useful block representation of the stiffness matrix. The subvectors u_1 and u_2 corresponds to the mesh nodes from the mesh domains Ω_h and $\Pi_{\delta h} \setminus \Omega_h$, respectively. By reordering the vector u according to this partitioning the linear system (8) can be written in the block form

$$\begin{pmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} & B_2^T \\ 0 & B_2 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \lambda \end{pmatrix} = \begin{pmatrix} f_1 \\ 0 \\ 0 \end{pmatrix}. \quad (9)$$

One of the main results of [GK98] is that the subvector u_1 is the solution to (6). Indeed, the matrix B_2 is symmetric and positive definite. Thus, eliminating $u_2 = 0$ from the first block equation, we end up with an algebraic problem equivalent to (6). It turns out that the linear system (9) can be solved much more easily than the reduced system. By introducing the new variable $\tilde{\lambda} = B_2 \lambda$, we simplify (9):

$$A \begin{pmatrix} u_1 \\ u_2 \\ \tilde{\lambda} \end{pmatrix} \equiv \begin{pmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} & I_2 \\ 0 & I_2 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \tilde{\lambda} \end{pmatrix} = \begin{pmatrix} f_1 \\ 0 \\ 0 \end{pmatrix}, \quad (10)$$

where I_2 is the identity matrix. This problem can be solved iteratively with a preconditioner H proposed in [GK98]:

$$H = \begin{pmatrix} H_{11} & H_{12} & 0 \\ H_{21} & H_{22} & 0 \\ 0 & 0 & B_2 \end{pmatrix} \equiv \begin{pmatrix} H_u & 0 \\ 0 & B_2 \end{pmatrix}.$$

Lemma 1 (Glowinski, Kuznetsov (1998)) *Let H_u be spectrally equivalent to A_u^{-1} ($H_u \sim A_u^{-1}$). Then $(A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1} \sim B_2$ and $H \sim A^{-1}$.*

Note that A_u is a matrix form of the operator $-\Delta + \frac{1}{\nu\Delta t}$ in Ω_h with Dirichlet boundary conditions. One of the possible choices for H_u is a multigrid preconditioner, for example, the BPX preconditioner [BPX90]. It is most efficient when the grid is fully hierarchical. Recall that the construction of Ω_h is already based on a fully hierarchical grid Π_h . From this viewpoint we have to take $\Pi_\delta = \Pi$. On the other hand spectral properties of HA depend on δ and may be deteriorated for larger values of δ . The maximal embedding guaranteeing independence with respect to δ is determined by the particle radius R and the distance d between two neighboring particles. Let $\|\cdot\|_{1,\omega}$ be a norm given by

$$\|\mathbf{u}_h\|_{1,\omega}^2 = \int_\omega \left(\frac{1}{\nu\Delta t} |\mathbf{u}_h|^2 + |\nabla \mathbf{u}_h|^2 \right) dx.$$

Let \mathbf{u}_{1h} and \mathbf{u}_{2h} be finite element counterparts of subvectors u_1 and u_2 , respectively. Given a function \mathbf{u}_{2h} we define its norm-preserving extension \mathbf{u}_{1h} in such a way that $\mathbf{u}_{1h} = \mathbf{u}_{2h}$ on γ . The following quantity plays the crucial role in the general theory of fictitious domain methods (see, for example, [MKM86]):

$$c = \max_{\mathbf{u}_{2h} \neq 0} \min_{\mathbf{u}_{1h}} \frac{\|\mathbf{u}_{1h}\|_{1,\Omega_h}^2 + \|\mathbf{u}_{2h}\|_{1,\Pi_\delta \setminus \bar{\Omega}_h}^2}{\|\mathbf{u}_{2h}\|_{1,\Pi_\delta \setminus \bar{\Omega}_h}^2}. \quad (11)$$

Lemma 2 (Marchuk, Kuznetsov, Matsokin (1986)) *Let c be as above. Then $\text{cond}(H_u A_u) \lesssim c$.*

Reasonable estimates of c can be obtained by analyzing collision of two particles. Let d be the distance between these particles.

Lemma 3 *The parameter c is independent of d , δ and R when either (a) $\sqrt{\nu\Delta t} \lesssim R$ and $\sqrt{\nu\Delta t} \lesssim d$ or (b) $\delta \lesssim d$.*

The proof is based on the norm preserving finite element extension theorem [Ast78, Nep91, Wid87] and scaling arguments.

An important corollary from Lemma 3 is that when particles are close to each other a severe restriction is imposed on δ . Therefore grid $\Pi_{\delta h}$ has only a few fully hierarchical levels. Fortunately, we are solving the singular perturbed elliptic problem for which the BPX preconditioner leads to a well conditioned coarse grid problem.

FDM for the Neumann boundary value problem

The saddle point problem (7) from the Projection step in the algebraic form reads:

$$A \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} M_u & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}. \quad (12)$$

Consider a block diagonal matrix

$$H = \begin{pmatrix} H_u & 0 \\ 0 & H_p \end{pmatrix},$$

where

$$H_u \sim M_u^{-1} \quad \text{and} \quad H_p \sim (BM_u^{-1}B^T)^{-1}.$$

By using arguments similar to that in the proof of Lemma 1, we can show that the matrix H is spectrally equivalent to the stiffness matrix A . The simplest choice for H_u is the diagonal lumping of mass matrix M_u . The Schur complement $BM_u^{-1}B^T$ is spectrally equivalent to a discrete Laplace operator in Ω with Neumann boundary conditions. Such boundary conditions allow us to construct a very simple preconditioner proposed by Astrakhantsev [Ast78].

Let L be a matrix spectrally equivalent to the discrete Laplace operator on Π_h with Neumann boundary conditions. Let us divide mesh nodes into two separate groups. The first group includes nodes from the mesh domain Ω_h . The second group contains the remainder of the nodes. According to this partitioning matrix L can be written in the block form

$$L = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}.$$

One of the main results of [Ast78] is that the Schur complement $S_{11} = L_{11} - L_{12}L_{22}^{-1}L_{21}$ is spectrally equivalent to the discrete Laplace operator in Ω_h with Neumann boundary conditions. Therefore we set $H_p = S_{11}^{-1}$. Obviously that action of H_p on a vector p is reduced to solving a linear system with matrix L and the right-hand side $(p, 0)^T$. One of the possible choices for L is a multigrid preconditioner, for example, the BPX preconditioner.

Numerical experiments

For the simulation we used 27 identical balls of radius $R = 0.01m$ centered at nodes of a $3 \times 3 \times 3$ cubic grid with the mesh step size $5R/2$ (see Figure 2). The particles were placed in a parallelepiped with the square base $0.12m \times 0.12m$ and height $0.23m$ filled with a glycerin. We have chosen particles with density twice as large as the fluid density. The particle positions at times $t = 0s$, $t = 0.23s$ and $t = 0.31s$ are shown on Figure 2. The variable time step strategy was chosen to minimize the number of time steps. The total simulation required 64 time steps with about 520000 degrees of freedom for velocity and 65000 for the pressure.

A very interesting symmetric aggregation of particles in triples is observed after a few collisions between particles. Despite decreasing the distance between particles, we did not change the embedding domain Π . The number of iterations for solving the singular perturbed problem (6) with the BPX preconditioner has been changed from 18 to 30 when distance between particles has been changed from $5R/2$ to $R/5$ (the minimal allowed distance). We expect that the new embedding strategy described above will decrease the number of iterations and allow us a more detailed numerical analysis of particles collisions.

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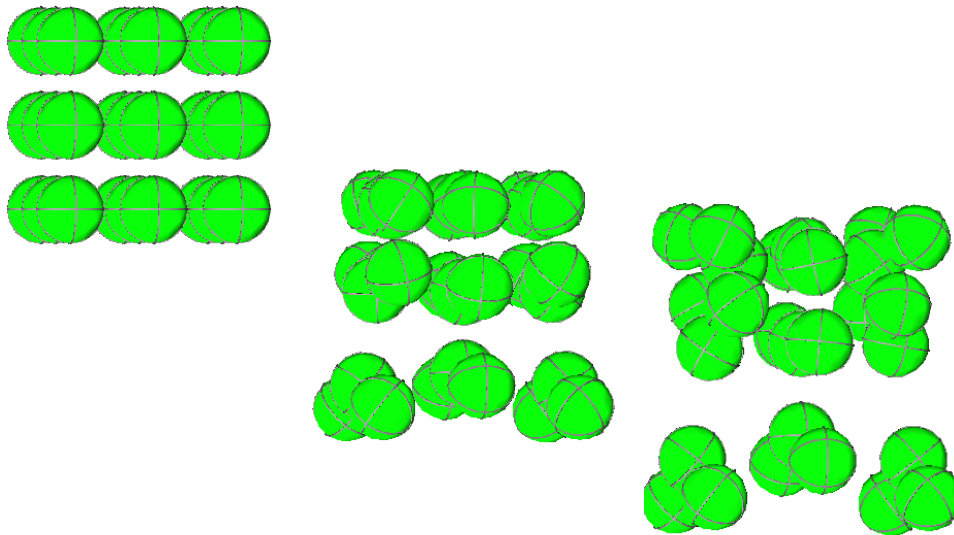


Figure 2: The motion of the cubic structure of spheres

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