Journal of Computational Physics 313 (2016) 662–673

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Application of a force field algorithm for creating strongly correlated multiscale sphere packings

Thomas Zauner

Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

ARTICLE INFO

Article history:
Received 22 August 2015
Received in revised form 13 February 2016
Accepted 15 February 2016
Available online 19 February 2016

Keywords:
Sphere packing
Discrete-Element-Method
Porous media
Lattice-Boltzmann

ABSTRACT

This work presents a protocol driven force field algorithm, used to create multiscale correlated dense sphere packings. It was developed as part of a tool chain for the reconstruction of realistic multiscale porous rock samples. It overcomes limitations of Monte-Carlo or deposition based approaches, that are quite common in this field and were used previously. The new algorithm can create large, low porosity sphere packings with radius distributions covering two decades. Highly correlated structures that model pore clogging and sedimentation can be generated. To achieve this, an adequate force field and proper termination strategies are necessary. By changing the algorithm parameters in a controlled way during the simulation, a complex protocol driven process can be established. The implementation of the algorithm targets large parallel computer platforms to perform simulations with more than 10 million spheres. This article includes an application of the algorithm used to generate a highly polydisperse sphere packing with roughly 10^6 spheres and radii from 1 to 100 μm. The continuum description of this packing is discretized at resolutions from 0.25 to 1 μm and investigated using geometric and statistical characterizations and results from Lattice-Boltzmann flow simulations. These resolution dependent results affirm that reliable, predictive calculations for multiscale porous microstructures depend on the availability of large realistic continuum models. To obtain such models the algorithm presented herein can be used as a starting point.

1. Introduction

The demand for a new sphere packing algorithm arose from the task of generating large 3D models for multiscale porous rocks from experimental X-ray, synchrotron or optical images [1–4]. Therein sphere packings are the starting point for the model reconstruction and the following analysis of the discretized data-set. The available implementation [3] exhibited limitations when used for large systems with more than 10 million spheres or multiscale packings with size distributions covering more than one decade. Therefore a new, more flexible and efficient, algorithm using a different methodology was sought after. Various approaches exist like Monte-Carlo (MC), rejection based, algorithms that try to generate a valid packing by repeatedly inserting objects into an existing packing [3]. Also there exist Monte-Carlo algorithms that start from a random packing and repeatedly modify the packing following a stochastic rule set to generate a desired target packing. Some hard sphere packing algorithms [5,6] combine a loose, initially MC generated, packing with a compression (boundary shrinking) technique. So called "force based" approaches [7] use predefined interactions between the spheres to modify a

E-mail address: zauner@icp.uni-stuttgart.de.

http://dx.doi.org/10.1016/j.jcp.2016.02.038

packing after starting from a random or lattice based packing. These interaction based algorithms can be discrete (time-stepping) or continuous (event-based) in time and either discrete in space, i.e. use a spatial lattice, or continuous in space. The algorithm presented here is closest related to the lineage of time-discrete continuous-space numerical methods called "discrete-element-method" (DEM) [8–10] in granular systems or "molecular dynamics" [11,5] in chemical and biological systems. There exist many commercial [12–14], free [15,16] or academic [17] DEM implementations. These DEM packages mainly focus on simulating physical processes in granular systems, like granular flow, particle sedimentation, material wear and fracturing. The implementation presented herein focuses on the original target of creating large sphere packings with different sphere types, and constraints like given size distributions, maximal allowed overlaps or other spacial correlations. Compared to the DEM implementations mentioned above, this allows the usage of less accurate numerical schemes, a more flexible force-field and a protocol driven behavior that enables the algorithms to cope with the large sphere numbers that are necessary to create laboratory sized highly polydisperse samples. In sections 2 and 3 of the article the algorithm and its implementation are discussed. Section 4 presents an application that generates a multiscale sphere packing using a complex simulation protocol. Various characterizations and calculations for the discretized date set of this packing are carried out in Section 5.

2. Force field algorithm

2.1. Overview

A time-discrete, continuous space, soft-sphere force field simulation is used to generate the sphere packing. The discrete simulation steps are $s \in [1, \dots, s^{\max}]$. The bounded region $\Omega \subset \mathbb{R}^3$ contains the spheres s_i, $i = 1, \dots, N$ with spatial positions $\vec{x}_i^s \in \Omega$, radii $r_i^s \in \mathbb{R}$, masses $m_i \in \mathbb{R}$ and types $g_i \in \{1, \dots N_g\}$. For each sphere pair (s_i, s_j) a symmetric overlap

$$\sigma_{ij}^s = \frac{r_i^s + r_j^s - dx_{ij}^s}{r_i^s + r_j^s - |r_i^s - r_j^s|}$$

with $dx_{ij}^s = |\vec{x}_i^s - \vec{x}_j^s|$ is defined. A maximal allowed overlap $\sigma_{g_i}^{\max} \in \mathbb{R}$ is specified for each sphere type. Every step a force acting on each sphere is calculated, depending on position, type and interaction constants. Then the spheres are propagated to new positions using a damped velocity-Verlet integrator as the discretized law of motion. A sphere s_i is considered to be converged, if $0 < \max_{i \neq j}(\sigma_{ij}) \leq \sigma_{g_i}^{\max}$. The system is said to have converged at a final step $s_f \in \mathbb{N}$ if this holds for all spheres. A converged system represents a valid packing.

2.2. System setup and initialization

Either the total number of spheres N or the point density must be specified at startup. The system is then populated uniformly with spheres at random positions $\vec{x}_i^0$. For each sphere type a size distribution must be specified to generate the initial radii r_i^0 of the spheres. This distribution can be:

- **Discrete** $P(r_i^0 = r) = \sum_j \delta(r - r_j) P'(r_j)$ with δ the Dirac delta function. A list of allowed $r_j \in \mathbb{R}$ and associated $P'(r_j) \in [0, 1]$ must be specified with $\sum_j P'(r_j) = 1$.
- **Constant and continuous**, with upper and lower bound, $P(r_i^0 = r) = 1/(r_{g_i}^{\max} - r_{g_i}^{\min})$. Here only the two values $r_{g_i}^{\min} \in \mathbb{R}$ and $r_{g_i}^{\max} \in \mathbb{R}$ for each sphere type must be specified.
- **Exponential and continuous**, $P(r_i^0 = r) = \frac{\alpha \exp(-\alpha r)}{(\exp(-\alpha r_{g_i}^{\min}) - \exp(-\alpha r_{g_i}^{\max}))}$ with given $r_{g_i}^{\min}$, $r_{g_i}^{\max} \in \mathbb{R}$ for each sphere type, and with $\alpha \in \mathbb{R}$ shared among all sphere types.

Once the system is initialized with spheres the simulation iterates between force-, propagation, and termination-steps until it reaches a termination condition, i.e. all spheres are converged, or another termination condition applies.

2.3. Force field and force step

Within this step the force on each sphere is calculated as the sum of pairwise interaction forces

$$\vec{f}_i^s = \sum_{j \in W_i^{s-1}} \vec{f}_{ij}(dx_{ij}^{s-1}, r_i^{s-1}, r_j^{s-1}; k_i)$$

where k_i is an interaction constant that needs to be specified and W_i^s is the set of interaction partners for the sphere s_i. The sets W_i^s, used in the time step s, are updated in a previous propagation step, but not necessarily the step $s - 1$, see section 3.3. The maximal allowed overlap $\sigma_{g_i}^{\max}$ is connected to a minimal acceptable distance $dx_{\min,ij}^{s-1} = r_i^{s-1} + r_j^{s-1} - \sigma_{g_i}^{\max}(r_i^{s-1} - r_j^{s-1} - |r_i^{s-1} - r_j^{s-1}|)$. Also there is a maximal allowed distance $dx_{\max,ij}^{s-1} = r_i^{s-1} + r_j^{s-1}$ for an isolated pair to