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A Collective Dynamics-based Method for Initial Pebble Packing in Pebble Flow Simulation

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ABSTRACT

In the simulation of pebble flow in Pebble Bed Reactors (PBR), high-fidelity methods, such as Discrete Element Methods (DEM) and Computational Fluid Dynamics (CFD) methods, are usually employed to simulate the dynamic process of pebbles circulation, accounting for the pebble-to-pebble, pebble-to-reflector wall and pebble-to-fluid interactions. To obtain a realistic model of pebble distribution around dynamic equilibrium state of pebble flow, the simulation based on high-fidelity methods normally resists brute force computation. However, if an initial dense packing of pebbles can be provided, which is close to realistic packing at equilibrium state and can be easily implemented without much computational effort, the long time high-fidelity simulation can be considerably more efficient and take much less time to reach dynamic equilibrium state. In this paper, a collective arrangement method based on a dynamics model is developed to generate an initial pebble distribution at a quasi-equilibrium state. In the new method, pebble positions are generated firstly by a fast sequential process in the full core allowing overlapping, and then a simplified normal contact force model is adopted in the initialization for eliminating the pebble overlap. The adopted model provides an adaptive way to account for the situations in which multiple pebbles are overlapped and different contact forces should be applied for different ratios of overlapping depth and sphere size, thus speeding up the initialization without loss of reliability and making the approach feasible for variable size sphere packing. Moreover, an intermittent vibration function, as an optional process, can be provided to further densify the packing depending on different applications. Comparisons with other existing random packing methods for initialization are made. It is shown that the developed method not only exhibits unique significance and good computation efficiency in speeding up the pebble flow simulation, but also presents desirable potential in other applications as a general packing algorithm for packing uniform- or variable-size spheres in a large container.

Key Words: Pebble bed reactor, random close packing, discrete element method, packing fraction, porosity

1. INTRODUCTION

Recently, pebble bed gas-cooled reactors (PBR) have received much attention as a promising candidate for Gen IV reactor designs. About 15K TRISO fuel particles are embedded in a spherical fuel pebble and over 450K fuel pebbles circulate within the pressure vessel in a typical reactor configuration. Such a design has many advantages in fuel burnup, online refueling capability and inherent passive safety feature [1]. Accurate modeling of pebble flow in reactor core is essential to evaluate the neutronic, thermal-hydraulic and safety performances.

Normally, pebble circulation in reactors can be modeled as a dense spherical granular flow driven by gravity. Discrete element methods (DEM) are widely used [2, 7, 14, 18] to model the sphere contact mechanics and predict the long-term dynamic behavior of granular flow. Due to the complicated physical interactions, including pebble-to-pebble, pebble-to-reflector wall, and pebble-to-fluid, as well as the high-fidelity physical models used for friction and drag forces, the dynamic simulation using DEM and other coupled fluid dynamics methods is computationally intensive and it normally takes much longer time to reach the dynamic equilibrium state for pebble flow, which represents a realistic packing model of pebbles. However, if a quasi-equilibrium state pebble packing can be provided as an initial packing for further fully dynamic simulation, it can greatly relieve the heavy computational burden and increase the overall efficiency in granular flow simulation, thus an equilibrium state can be obtained quickly. In order to speed up the high-fidelity dynamic simulation, the quasi-equilibrium state packing should satisfy: (1) it should present similar packing fraction distribution to the equilibrium/realistic state produced by further high-fidelity simulation, where the maximum packing fraction can be up to around 64%, representing a Random Close Packing (RCP) [4, 5, 9]; (2) it can be generated in a very cheap way without costing too much computational effort; (3) its efficiency should be nearly independent of geometry complexity. Based on these requirements, a fast, efficient random packing method needs to be developed that accounts for the large pebble quantity, the complexity of reactor core geometry, as well as the high packing fraction of pebbles.

Much effort has been made by many researchers for random packing of spheres at high packing fractions since last century [3-16]. Generally, packing algorithms can be classified into two models: sequential model [11, 13-16] and collective model [7, 8, 10, 12]. In the sequential model, spheres are generated one by one (or group by group) based on certain rules that ensure the randomness of packing and no overlapping between spheres. Most sequential approaches use a constructive method, in which newly inserted sphere is usually positioned randomly within the domain or layer by layer [11]. Typical examples are trial method [7], sedimentation techniques [11] and domain triangulation [14]. Sequential models are easily implemented but difficult to precisely control the total sphere quantity or reach high packing fractions, especially for the case of uniform-size sphere packing within a complex geometry. In the collective model, all the spheres are generated randomly, allowing overlapping, and then collective rearrangement is performed to eliminate the overlapping. The rearrangement process can either be moving spheres apart [8], compress loosely packed spheres [12], or adjusting the sphere diameters [8, 10]. Compared with sequential models, collective models are usually more time-consuming for dense packing but can control the total sphere quantity or packing fraction in a better way. From the perspective of physics, random packing algorithms can also be classified into geometry-based model [8, 10, 12-14] and dynamics-based model [7, 15, 16]. A geometry-based model, for example, the sequential trial method mentioned above, does not account for any realistic forces. While dynamics-based models adopt artificial or realistic forces to perform the sphere rearrangement, which are closer to real physics but more computationally intensive compared with the geometry-based models. Many engineers use the DEM simulation itself for the initialization [7, 14], by firstly generating loosely packed spheres and then densifying the packing through realistic forces. This approach is effective but extremely costly due to the intensive computation requirement for DEM. Another dynamics-based approach is the gravitational deposition, which belongs to the sequential model [14]. In this model, spheres are dropped into the container one by one and then find their equilibrium positions by gravity and

normal contact forces. As pointed out above, as a sequential model, the gravitational sediment method cannot precisely control the packing fraction within a confined space.

In this paper, a collective dynamics-based method is developed to obtain a quasi-equilibrium state packing of pebbles, which provides an initial packing for further high-fidelity simulation of coupled pebble flow and coolant fluid flow in a PBR. Both initial packing and dynamic flow simulation have been implemented in PEBFD, a recently developed code at RPI [21]. In the new method for initial packing, pebble positions are firstly generated randomly within the core using Random Sequential Addition (RSA) [22] and allowing overlapping. Then a simplified normal contact model is adopted to move overlapped pebbles apart using a nearest neighbor search technique [7]. Intermittent vibration and final gravitational deposition can be optional to further densify the packing. The dynamics-based nature of this method brings a result closer to the equilibrium/realistic pebble arrangement in PBR, while the simplified normal contact model and nearest neighbor search technique greatly speed up the simulation. Packing statistics is given and comparison with other existing method is made to show the efficiency of this method. Example of variable-sized pebble packing is also presented to illustrate the potential of the methodology.

2. Methodology Description

2.1. Algorithm description

For a given container, pre-determined packing fraction ϕ and a priori sphere radius distribution, the total number of spheres N can be easily calculated. The algorithm first uniformly and randomly generates N sphere centers using the RSA approach. By now multiple overlapping among spheres are inevitable. Then the overlaps among neighboring pebbles and the boundary breach are computed from the pebble center coordinates. Based on the calculated overlapping and boundary violation information, a simplified normal contact force model is employed to move the pebbles to a new configuration, and all other forces like pebble friction, coolant drag and pebble gravity are removed throughout the process in order to speed up the initialization without loss of reliability. In this way the pebble overlapping is eliminated iteratively while all the pebbles are constrained within the container boundary.

According to Hertzian contact mechanics, for two spheres P_i and P_j with radius r_i and r_j, relative normal velocity $\vec{\boldsymbol{v}}_n(i,j) = (\vec{\boldsymbol{V}}_i - \vec{\boldsymbol{V}}_j)\bullet\vec{\boldsymbol{n}}_\mathrm{ij}$ and overlapping depth δ_ij, the realistic normal contact forces $\boldsymbol{F}_\mathrm{n}$ is :

$$\vec{\boldsymbol{F}}_\mathrm{n}(i,j) = \sqrt{\frac{r_\mathrm{i} r_\mathrm{j}}{r_\mathrm{i} + r_\mathrm{j}}}\left(k_\mathrm{n}\delta_\mathrm{ij}^{\,1.5} - \gamma_\mathrm{n}\delta_\mathrm{ij}^{\,0.5} v_\mathrm{n}\right)\vec{\boldsymbol{n}}_\mathrm{ij}, \quad (1)$$

where k_n and γ_n are material elastic and viscoelastic constant separately, and $\vec{\boldsymbol{n}}$ is the unit normal vector.

Different from the high-fidelity simulation, the initialization algorithm does not have to account for all the realistic physics. Therefore a simplified and linearized contact model is adopted:

$$\vec{\boldsymbol{T}}(\mathrm{i},\mathrm{j}) = K_\mathrm{p}\sqrt{r_\mathrm{ij}}\,\delta_\mathrm{ij}\vec{\boldsymbol{n}}_\mathrm{ij}, \quad (2)$$

where $r_{ij} = \frac{r_i r_j}{r_i + r_j}$, K_p is a constant associated with the pebble elasticity and usually much less than the true value of k_n.

For a pebble with radius r_i and breach the feasible core region boundary by δ_i, similar normal contact force $\boldsymbol{W}$ (i) can be formulated:

$$\vec{\boldsymbol{W}}(\mathrm{i}) = \sqrt{r}_{\mathrm{i}} K_w \delta_{\mathrm{i}} \vec{\boldsymbol{n}}_{\mathrm{i}} , \qquad (3)$$

where K_w is a constant associated with the boundary elasticity.

The total contact force acting on the i^{th} pebble $\boldsymbol{F}$(i) is the vector summation of $\boldsymbol{T}$(i) and $\boldsymbol{W}$(i) among all contacts:

$$\boldsymbol{F}(i) = \sum_j \boldsymbol{T}(i, j) + \boldsymbol{W}(i) . \qquad (4)$$

And the move direction and distance for i^{th} pebble is:

$$\Delta X(i) = K_V F(i) / r_i^3 , \qquad (5)$$

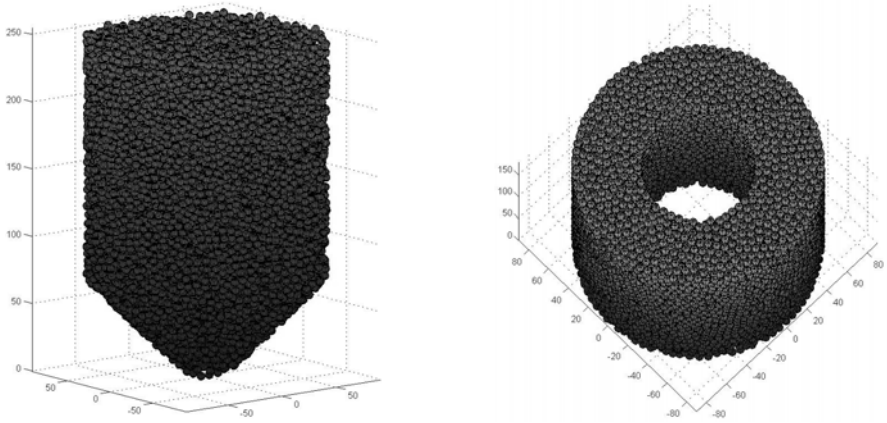
where K_v is a constant.

Using equations (2)-(5), the pebbles are moved to a new configuration, and these procedures will be repeated until the maximum overlap is less than the threshold value. This methodology does not assure that the maximum or average overlapping for a certain iteration step is improved over the previous one, but it will be convergent after several steps. To interpret the robust convergence performance of the algorithm qualitatively, it can be considered that the pebble configuration with overlapping has elastic potential energy stored which is not a ground state, and the simplified contact force will drive the pebbles to a new configuration without overlap, which corresponds to one of the feasible lowest energy states. For high packing fractions (greater than 62%), it is possible that the algorithm will converge to a jammed state which corresponds to a local minimum and still has overlapping. In such a case, auxiliary techniques, such as vibration or shaking, are needed to shift the configuration away from the jamming. And since the pebble size is taken into account in the algorithm, it can handle both uniform-sized and variable-sized packing problems desirably.

2.2. Results for PBR initialization

Two PBR configurations are used to pack pebbles inside using the developed algorithms. For the first example (Fig. 1a), 33K pebbles are randomly initialized within a cylindrical PBR with radius of 90cm and height of 180cm and with a 45 degrees conic bottom, which has the packing fraction of 62.9%. For the second example (Fig. 1b), the initialization of 20K pebbles is performed within an annular core with the outer radius 90cm, inner radius 40cm and 180cm in height, which has the same packing fraction of 62.5%. All the pebbles have a uniform radius of 3cm.

To make a comparison with the gravitational deposition model, codes using both methods are developed. A comparison of CPU performance (on Pentium IV PC) for both models in packing 25K pebbles in a cylindrical container is given in Table I.



(a) Cylindrical core with conic bottom (b) Annular core

Figure 1 Cylindrical and annular PBR initialization

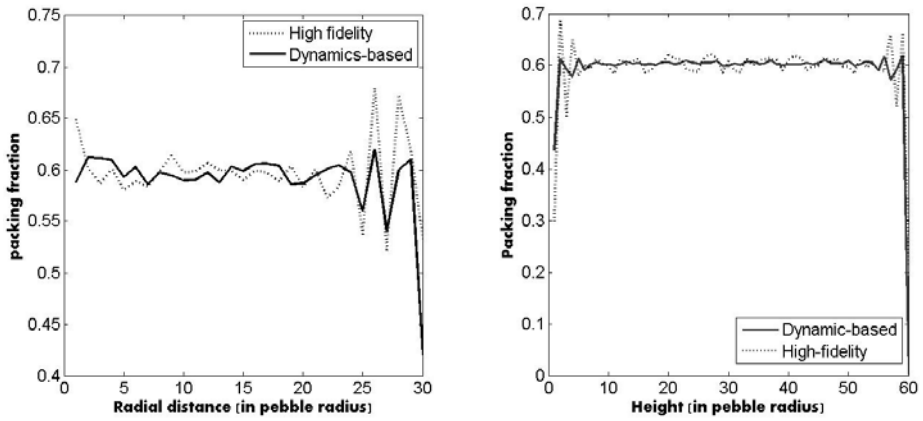
Table I. CPU time of initialization for different methods (25K pebbles)

Packing fraction	55%	58%	60%	61.5%	62.5%	>63%
Dynamic-based Approach	30s	150s	~450s	~840s	~4000s	N/A
Gravitational Deposition	580s	~670s	~800s	~1060s	N/A	N/A

From table I we can see that the developed method is much faster than the gravitational deposition at packing fractions less than 60%, but the CPU time increases significantly with the packing fraction, and it is hard to achieve packing fractions that are greater than 63%, if no other densification techniques, such as vibration, are used. For gravitational deposition, the upper limit of packing fraction is around 62.5% and the packing density does not have too much impact on the CPU time. For the realistic PBR, due to the large friction coefficient of graphite pebbles (μ~0.7), the actual packing fraction is usually less than 61% [2, 6, 18], which is the range that dynamic-based method is much faster than deposition method.

In order to obtain the spatial statistics of the packing, it is necessary to calculate the radial distribution function (RDF) and axial distribution function. Accurate distribution functions should be calculated based on the exact local packing fractions using Voronoi diagram [2, 17]. But usually an approximate approach is used to obtain these functions [2]. The core can be divided into 30 annular zones, each of which is one pebble radius in thickness. And the RDF is obtained by counting the accumulative volume of pebbles in each zone using the analytical formula given in [19]. As for the axial distribution function, it can be calculated by dividing the core into horizontal layers with equal height and summing up the pebbles' volume in each layer using sphere cap volume formula. The results comparing dynamics-based initialization and high-

fidelity method (which employs other initialization techniques and verified by previous computational and experimental work [2, 6, 18, 20]) are given in Figure 2. It can be seen that the dynamics-based initialization method basically keeps track of the realistic PBR packing statistics in the operation condition (given by high-fidelity simulation), except for the area near the boundary as the pebble friction in the realistic case drastically changes the local packing fractions near the wall [2, 4, 6, 18]. Similarity between two RDFs and axial distribution functions means the computational time would be decreased appreciably if the high-fidelity simulation starts with the pebble distribution generated by the developed initialization method.



(a) Radial distribution (b) Axial distribution

Figure 2: Radial and axial packing fraction distributions

2.3. Sphere packing with variable size

Since in the algorithm the radius impact is taken into account, this method can solve both discrete non-uniform-sized sphere packing and continuous-variable-sized sphere packing. To illustrate the method capability to deal with packing of variable sphere size, an example of 1400 spheres packed within a 30cm radius and 60cm height cylinder is given in Figure 3. The spheres have two sizes, r_1=3cm and r_2=2cm and this size variation does not have much impact on the CPU time. The ratio of the maximum pebble radius $r_{\max}$ to the minimum radius $r_{\min}$ can be as high as $r_{\max}/r_{\min}=10$ without affecting the computation efficiency too much. It is hard for gravitational deposition method to deal with this case because deposition method accomplishes the packing layer by layer, and the smallest spheres are possible to permeate through layers which makes the deposition inefficient.

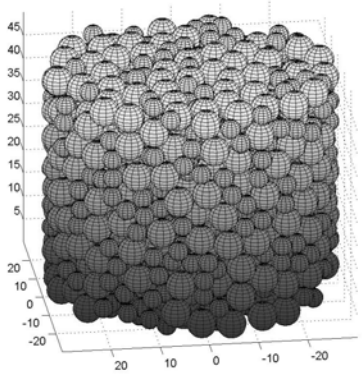


Figure 3: Non-uniform sized pebble packing

3. CONCLUSIONS

A collective dynamic-based sphere packing method is developed and applied to providing an initial packing of pebbles at quasi-equilibrium state for high-fidelity simulation of pebble flow in Pebble Bed Reactors. In the new method, pebbles are packed by first using a sequential RSA model to produce random dense packing, allowing overlapping. And then enlightened by the normal contact calculation used in high-fidelity simulation, a simplified virtual contact force is adopted to repel the spheres overlapped with each other and finally eliminate the overlapping. Due to its dynamics-based nature, the radial and axial packing fraction distribution functions of pebbles packed by the developed method are similar to the ones obtain by using the high-fidelity simulation for an operating PBR, thus showing that the developed initial packing method can speed up further high-fidelity simulation in approaching equilibrium state.

A comparison with an existing packing method, gravitational deposition method, has shown the developed method is much more efficient in providing an initial packing of pebbles at the range of packing fractions that actual PBRs usually have. Because the method accounts for the pebble radius, it can treat both uniform sized packing and variable sized packing, making it advantageous over deposition method. For every iteration step, it does not need to compare all the overlaps and choose a worst one, hence the computation load is smaller than other traditional collective packing method. Finally the dynamics-based nature enables the method to deal with complex constraints and boundary conditions desirably, which is very useful for complicated PBR core geometry. In order to obtain higher packing fractions such as the random close packing, further densification techniques is necessary such as the intermittent vibration treatment.

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