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Title: A FAST RSA METHOD FOR FUEL PARTICLE PACKING

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A Fast RSA Method for Fuel Particle Packing

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INTRODUCTION

Several of the concepts under study for Generation-IV reactors are VHTR or HTGR designs with coated particle fuel randomly dispersed within pebbles or fuel compacts [1]. Explicit modeling of the double heterogeneity introduced by the coated particle fuel has involved fixed lattices of particles [2,3], lattices with stochastic displacements of the particles [4], and random arrangements generated using the random sequential addition (RSA) method [5]. In this paper, we discuss the computational characteristics of the RSA method, provide an improved "fast RSA" method, and comment on the application of RSA to the random packing of coated fuel particles.

THE BASIC RSA METHOD

The basic RSA method [6] is sequential and static, in that particles are placed in a container one-at-a-time into a fixed position. The particles are not subsequently moved. For the case of 3D geometry and spherical particles, the maximum attainable particle packing fraction is .38 [7], which is much lower than the values of .74 for a close-packed face-centered cubic lattice, .637 from random packing experiments, and .64 from random close-packing computer experiments based on molecular-dynamics-like algorithms [7].

The basic RSA method for packing N spheres of radius R into a container can be described as:

K = 0
While K < N

- *a. Randomly select a position XYZ within the container (such that XYZ is at least a distance R from the container boundaries)*
- *b. If a sphere centered at XYZ does not overlap any of the previous K-1 spheres, then*
    - *Add XYZ to the list of sphere centers*
    - *Increment K by 1*

  Otherwise,
    - *Reject XYZ*

Because of Step b, checking all previous spheres for non-overlap, the method scales as $O(N^2)$ with the number of spheres. The scaling with packing fraction is nonlinear, such that packing fractions above ~.30 can take very large amounts of computing time (cf. Fig. 2).

AN IMPROVED FAST RSA METHOD

An obvious improvement to the basic RSA method is to modify Step b to check only nearest-neighbor spheres for overlap, rather than an exhaustive check of all previous spheres. This can be readily achieved by defining a lattice with spacing $h \le 2R/\sqrt{3}$. Each lattice box can contain at most 1 sphere center, and only $m=\lfloor R/h \rfloor+1$ neighboring boxes need be checked for overlapping spheres in the ±x, ±y, and ±z directions. Lists are maintained to keep track of the spheres contained in each lattice box as well as the empty lattice boxes. With these modifications, the improved fast RSA method is:

K = 0
While K < N

- *a. Randomly select a lattice box L from the list of empty lattice boxes*
- *b. Randomly select a position XYZ within lattice box L*
- *c. If the sphere centered at XYZ does not overlap any spheres with centers in the m neighboring boxes in the ±x, ±y, and ±z directions (and XYZ is at least a distance R from the container boundary), then*
    - *Add XYZ to the list of sphere centers*
    - *Increment K by 1*
    - *Delete lattice box L from the list of empty lattice boxes*
    - *Assign sphere K as contained within lattice box L*

  Otherwise,
    - *Reject XYZ*

Because previous spheres need be checked for overlap only for a fixed number of neighboring lattice boxes, the improved RSA method scales as $O(N)$ rather than $O(N^2)$ with the number of spheres.

NUMERICAL RESULTS

Both the Basic RSA and Fast RSA methods were tested for sphere volume fractions ranging from 0.01 to 0.32 and numbers of spheres ranging from 1000 to 16000. Outer container volumes included boxes, spheres, and cylinders. All tests were performed on a 2.5 GHz Apple G5 processor using the g95 Fortran-90 compiler with –O3 optimization. Figure 1 shows the total CPU time vs. the number of spheres for two sphere volume fractions, .25 and .30, for both methods with a cubical container. The Basic RSA method clearly shows $O(N^2)$ scaling, with very large increases in CPU time for 1000s of spheres, while the Fast RSA method shows modest linear scaling with large numbers of spheres. The very large nonlinear increase in CPU time with volume fraction is apparent in Figure 2, which shows the total CPU time vs. volume fraction for 8000 and 16000 spheres for both methods with a cubical container. For the Basic RSA method, CPU times become prohibitively large for volume fractions above .30 and numbers of spheres greater than 10000. CPU time for the Fast RSA method also increases nonlinearly with volume fraction, but remains reasonable due to the improved scaling with the number of spheres.

DISCUSSION

The Basic RSA and improved Fast RSA methods for sphere packing were tested over a range of sphere volume fractions and numbers of spheres. The Fast RSA method provides $O(N)$ scaling with the number of spheres, rather than $O(N^2)$ scaling for the Basic RSA method, and gives significant computational speedups when many thousands of spheres need to be randomly positioned.

For practical application of the RSA method to the random packing of coated fuel particles, either the Basic or Fast RSA methods can be used when the sphere volume fraction is small (<.3) or when the number of spheres to be randomly packed is not too large (<10,000). In [8], for example, 9394 fuel kernels were packed into an HTGR pebble with a fuel kernel volume fraction of only .0576. With such a low volume fraction, CPU time for either the Basic or Fast RSA method is less than 1 second. In [4,5], where 6050 fuel kernels were packed into a VHTR cylindrical fuel compact with a kernel volume fraction of .289, the Basic and Fast RSA required less than 10 seconds. Thus for current designs of coated fuel particle systems, the Basic RSA method is quite adequate for random sphere positioning due to the modest combination of sphere volume fraction and number of spheres.

If, however, the basic specifications for coated particle fuel were to change, for example by reducing the enrichment and using more fuel kernels of the same size, or by using larger fuel kernels in the same sized pebble or compact, then the volume fraction or number of spheres may grow into the regime where the Fast RSA method may be required to achieve reasonable computing times. Application of the RSA method to other areas, such as random vapor bubbles in a liquid, may also require the use of the Fast RSA method.

ACKNOWLEDGEMENT

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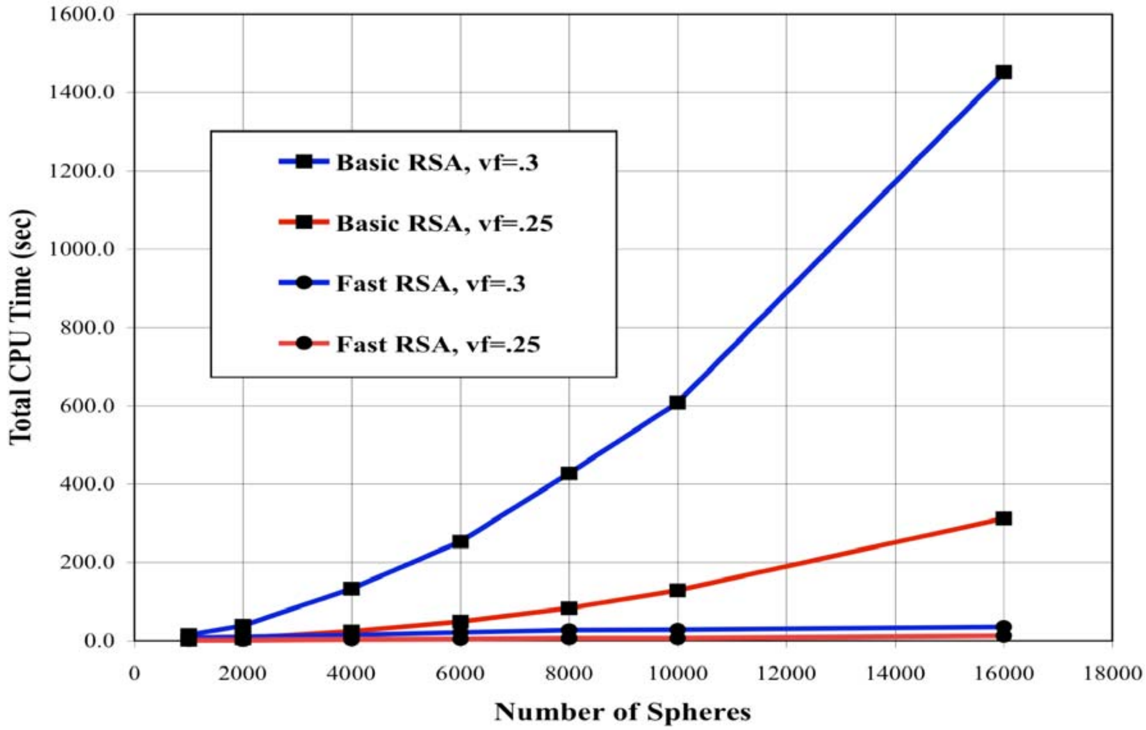

Figure 1. Scaling of total CPU time vs. the number of spheres for the Basic and Fast RSA methods, for volume fractions .25 and .3, with a cubical container.

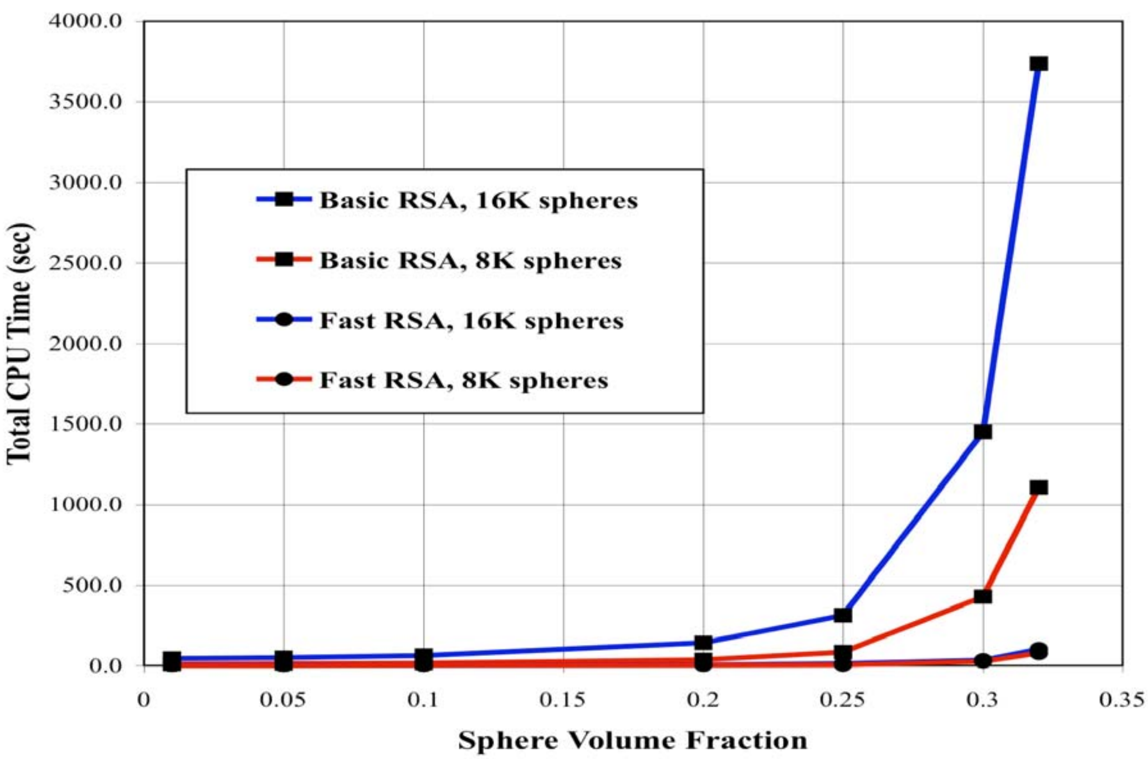

Figure 2. Scaling of total CPU time vs. sphere volume fraction for the Basic and Fast RSA methods, for 8000 and 16000 spheres, with a cubical container.