Optimal parameters for contact detection using a hierarchical grid data structure

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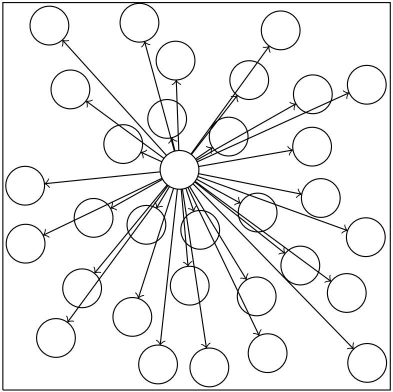
Contact detection

- Basic computational problem in many simulations.
- Straightforward approach requires $O\left(N^2\right)$ collision checks.
- Sophisticated methods use two-phases, for short range forces:
  - Broad phase
    - Coordinate sorting
    - Delaunay triangulations
    - Spatial subdivision
  - Narrow phase

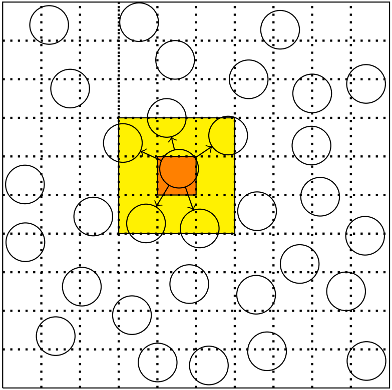


Assumptions

- N Particles (with $N >> 1$)
- Uniform random positions (i.e. no excluded volume effect)
- d-Dimensional periodic box
- Packing fraction ν
- Particle radii probability density function $f(r)$
  - Minimum particle radius r_{min}
  - Maximum particle radius r_{max}
  - Extreme size ratio $\omega = r_{\text{max}} / r_{\text{min}}$

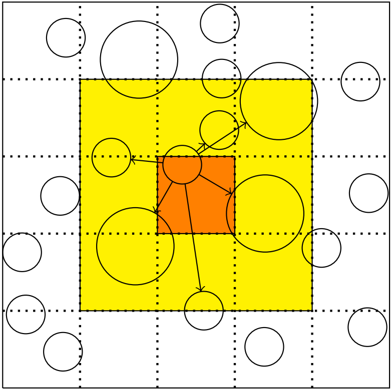
Linked Cell (2D, monodisperse)

- Developed for monodisperse simulations ($\omega = 1$)
- Set cell-size to particle diameter
  $s = 2r$
- Average particles per cell:
  $m = \frac{N}{N_{\text{cells}}} = 4\frac{\nu}{\pi}$
- Potential contacts:
  $T^{\text{cd}} = N n_c m = 18N\frac{\nu}{\pi}$



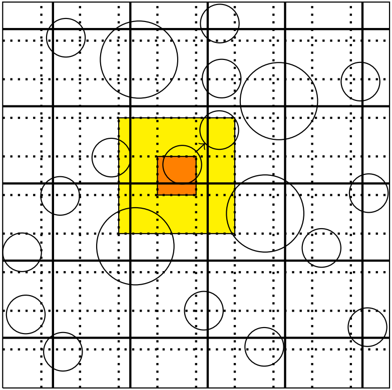
Linked Cell (2D, bi-disperse)

- However for bi-disperse simulations with equal area
- Set cell-size to maximum particle diameter
  $s = 2r_{\text{max}} = 2\omega r_{\text{min}}$
- Average particles per cell:
  $m = 2\frac{\nu}{\pi}\left(1+\omega^2\right)$
- Potential contacts:
  $T^{\text{cd}} = 9N\frac{\nu}{\pi}\left(1+\omega^2\right)$



Hierarchical grid (2D, bi-disperse)

- Use different grids for different sizes
- Set cell-size to maximum particle diameter
  $s_1 = 2r_{\min}, \ s_2 = 2r_{\max}$
- Average particles per cell:
  $m_1 = m_2 = \frac{2\nu}{\pi}$
- Potential contacts: ??



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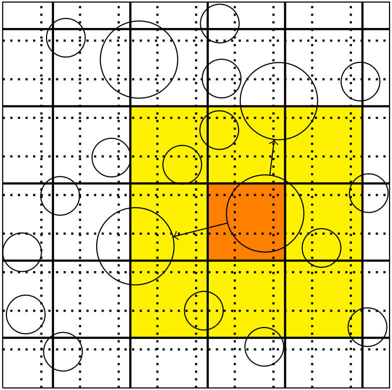
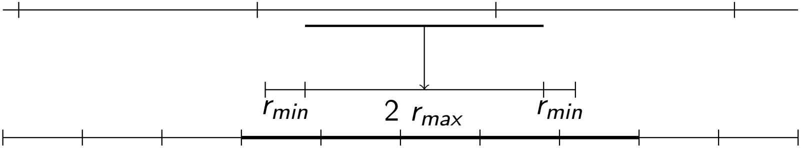


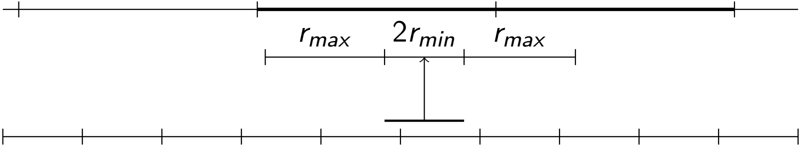
Top-Down vs. Bottom-Up

Top-Down:



5 Cells have to be checked, on average this is $(2+\omega)^d$.

Bottom-Up:



2 cells have to be checked, on average this is $\left(2+\frac{1}{\omega}\right)^d$.

Polydisperse systems (1)

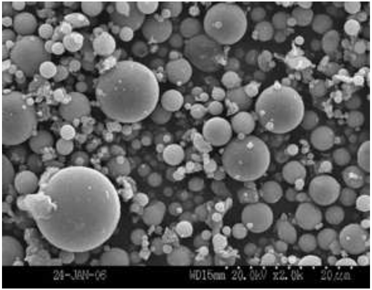


Figure: Kentucky Fly Ash.
[University of Kentucky]

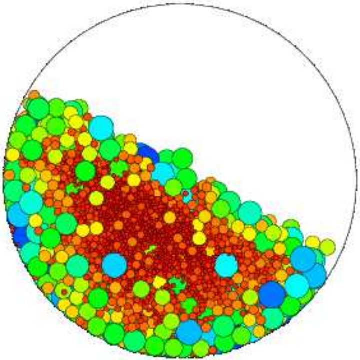
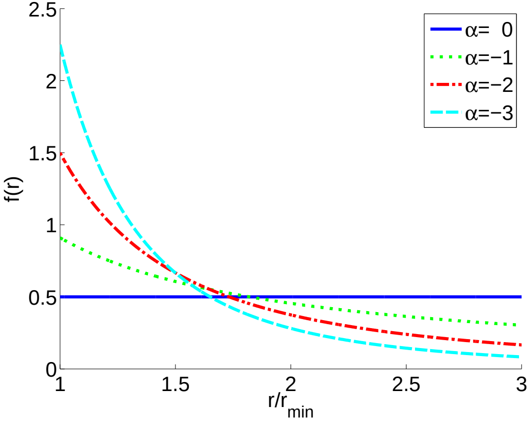


Figure: Poly-dispersed segregation in a rotating drum.
[S. Gonzalez]

Polydisperse systems (2)

What to do when the system is polydisperse, e.g:

$$f\left(r\right) = Cr^{\alpha} \text{ for } r_{\min} \leq r \leq r_{max} \tag{1}$$



Infinite number of different sizes, so use infinite different grids?

Overhead of the hierarchical grid

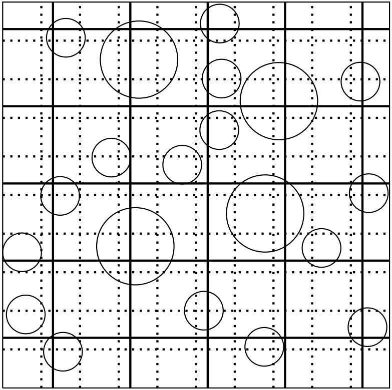
Due to multiple grids, more cells have to be accessed:

- Single level checks
- Cross level checks

Total computational time:

$$T = T^{\mathrm{cd}} + KT^{\mathrm{ca}} \qquad (2)$$

Throughout the rest of this talk $K = 0.2$



Task

Find optimal number of levels L and the corresponding cell sizes s_h, given particle size distribution $f(r)$, dimensionality d, packing fractions ν and K, such that the expected computational time T is minimal.

Method

- Use a linear cell size distribution:

$$s_h = 2r_{\min}\left(1 + h\frac{\omega - 1}{L}\right)$$

- Use an exponential cell size distribution:

$$s_h = 2r_{\min}\omega^{\frac{h}{L}}$$

- Use a cell size distribution where the number of particles per cell is constant[1] :

$$m_h = m_{h+1}$$

- Use a minimization algorithm

[1] Ogarko and Luding 2012.

Results

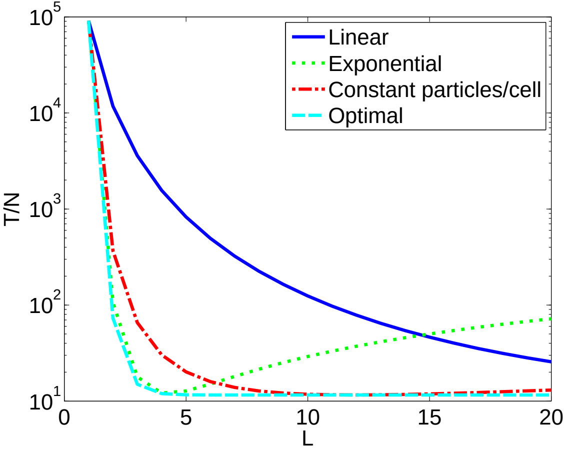


Figure: Computational effort of the HGrid algorithm as a function of the number of levels, L, for different cell-size distributions, using $\alpha = -3$, $\omega = 100$, $d = 3$, $\nu = 0.7$ and $K = 0.2$.

Mercury DPM

MERCURYDPM

Code for performing discrete particle simulations.[2]

- Hierarchical grid contact detection
- Built in coarse-graining statistical package
- Simple C++ implementation

Developed at the University of Twente.

[2] Thornton et al. 2012; Weinhart et al. 2012; Thornton et al. 2013; Krijgsman and Luding 2013.

Comparison with DPM (1)

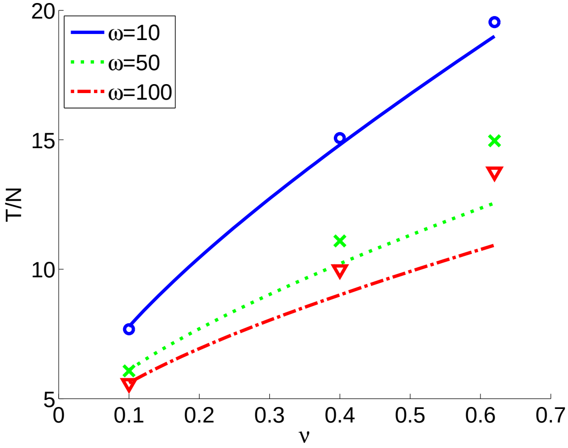


Figure: Comparison of the estimated HGrid computational effort (lines) versus that for a real DPM system (markers), using $\alpha = -3$, $N = 1000001$, $d = 3$, $K = 0.2$ and Optimal cell-size distribution.

Comparison with DPM (2)

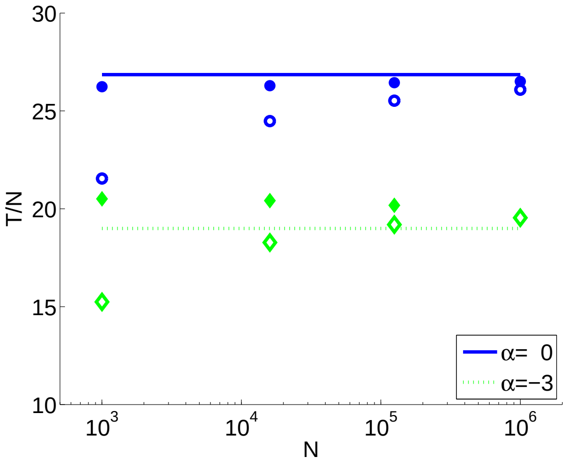


Figure: Comparison of the estimated HGrid computational effort (lines) versus that for a DPM system (markers), using $\omega = 10$, $\nu = 0.62$, $d = 3$, $K = 0.2$ and Optimal cell-size distribution.

Conclusions

- The HGrid algorithm greatly reduces the time spend for contact detection in polydisperse systems
- Performance of the algorithm depends on the chosen parameters
- Ideally a minimization routine is used to find optimal parameters
- Otherwise cell-sizes should be chosen according to the constant particles per cell method
- For highly polydisperse flow the excluded volume effect becomes important