Multilevel Summation for Dispersion: A Linear-Time Algorithm for r^{-6} Potentials

D. Tameling, **P. Springer**, **P. Bientinesi**, **A.E. Ismail**

tameling@aices.rwth-aachen.de

arXiv:1308.4005

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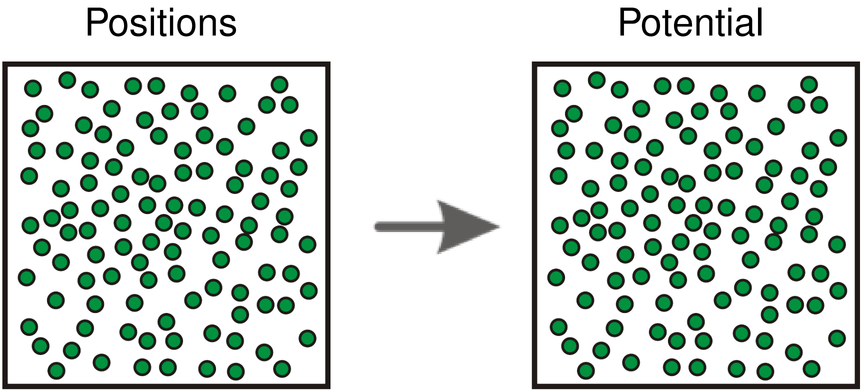
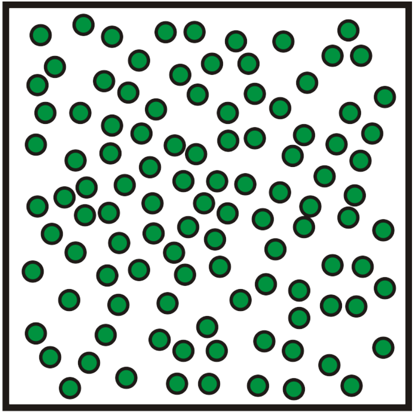
Outline


Positions
Potential

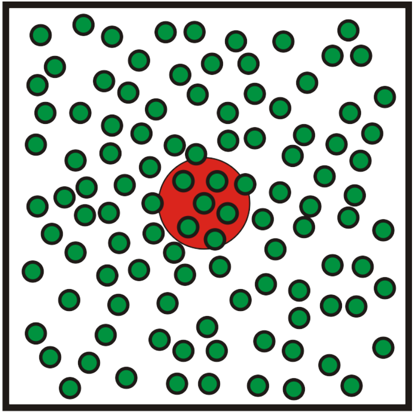


Dispersion potential:

$$V_{disp} = \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ i \neq j}}^{N} \frac{C_{ij}}{r_{ij}^6}$$

- E.g. in Lennard-Jones and Buckingham potentials
- Only attractive interaction between all pairs of atoms

Dispersion Interactions



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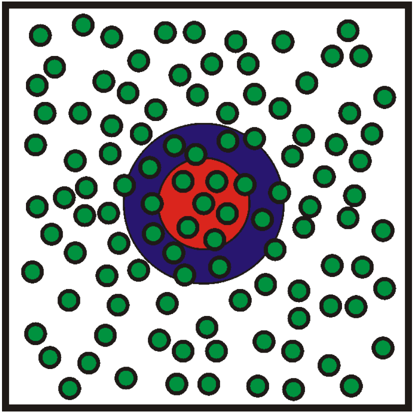

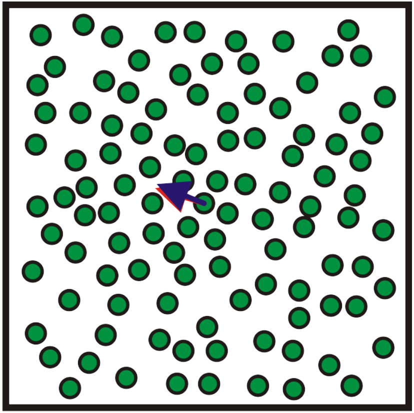

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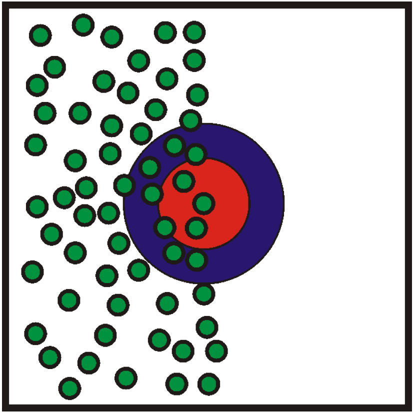

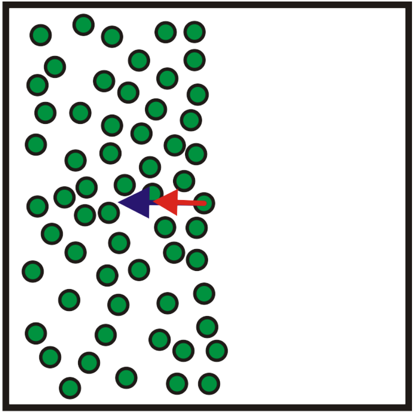

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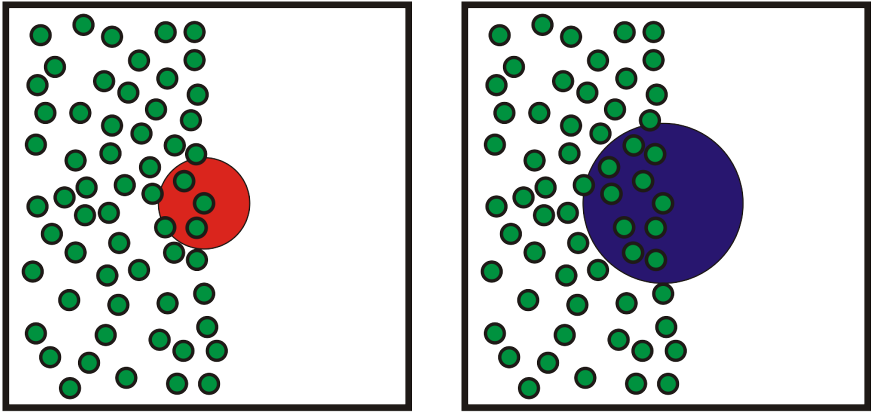
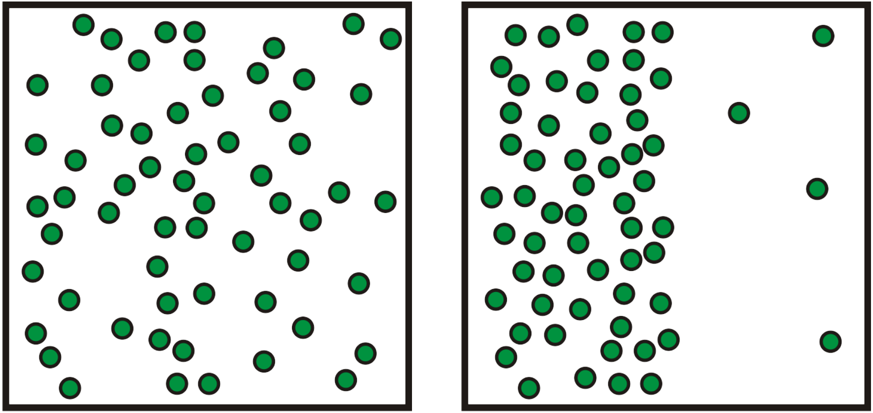
Dispersion Interactions



Dispersion Interactions



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- Direct evaluation $\rightarrow \mathcal{O}\left(N^2\right) \rightarrow$ typically too expensive

Long-Range Methods

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- Standard methods: Ewald Mesh methods
  - Use fast Fourier transforms
  - $\mathcal{O}\left(N \log N\right)$
  - Don't scale well

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  - Don't scale well
- Multilevel Summation method

Multilevel Summation for Dispersion

$$V = \boldsymbol{\xi}^T \ \mathbf{G} \ \boldsymbol{\xi}$$

e.g. $\xi_i = \sqrt{2}\sqrt{\varepsilon_{ii}}\sigma_{ii}^3$

(Lennard-Jones potential with geometric mixing)

$G_{ij} = \frac{1}{r_{ij}^6}$ for $i \neq j$

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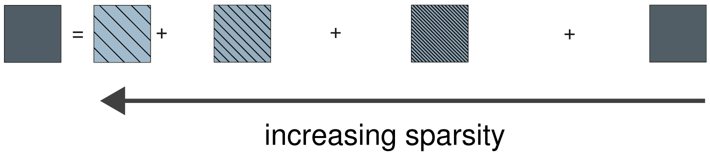
$$V = \boldsymbol{\xi}^T \ \mathbf{G} \ \boldsymbol{\xi}$$

Approximation of matrix G:

1. Splitting
2.



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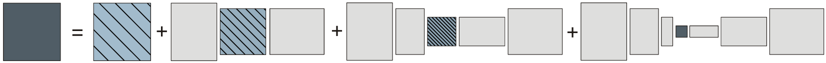

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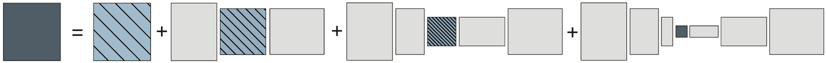
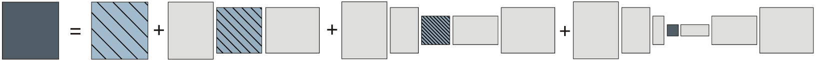
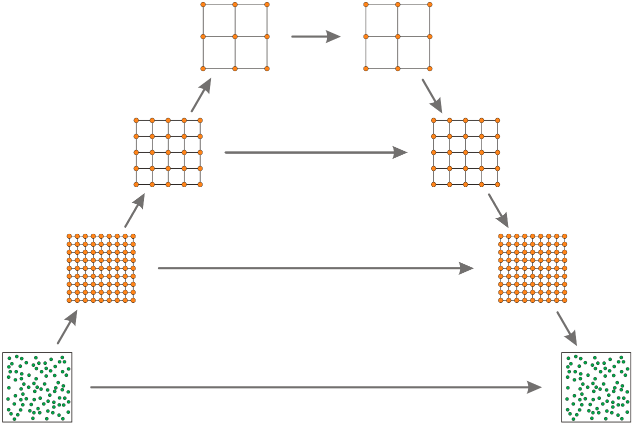
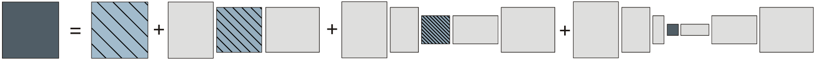


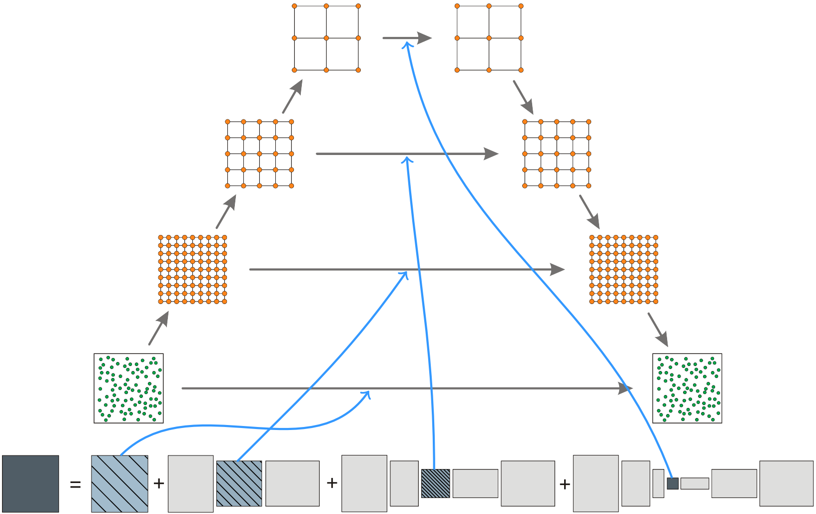
$$\Rightarrow \mathcal{O}(N)$$

Physical Interpretation









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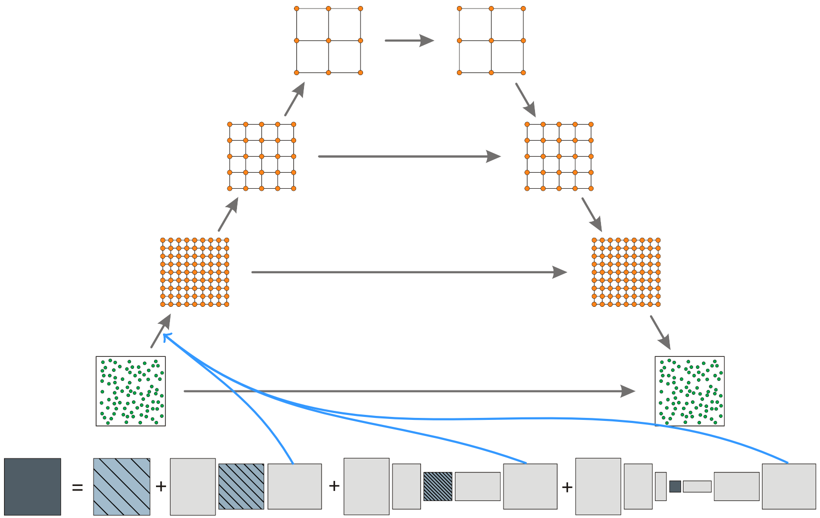

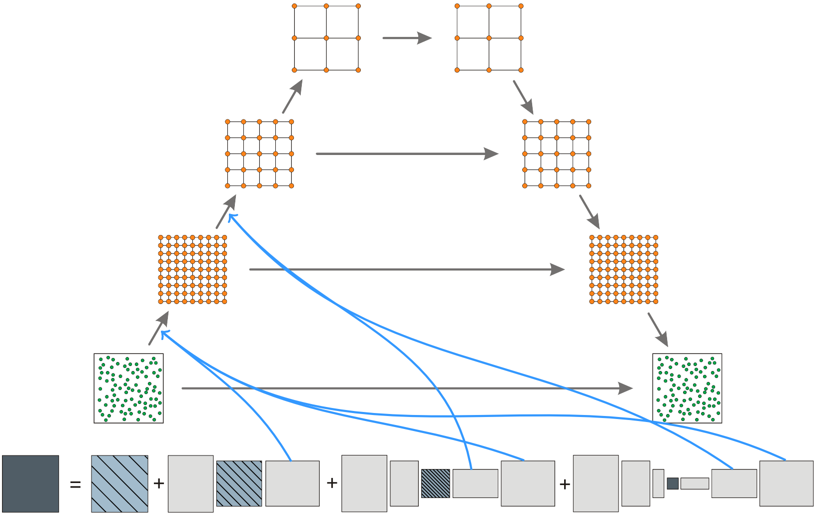

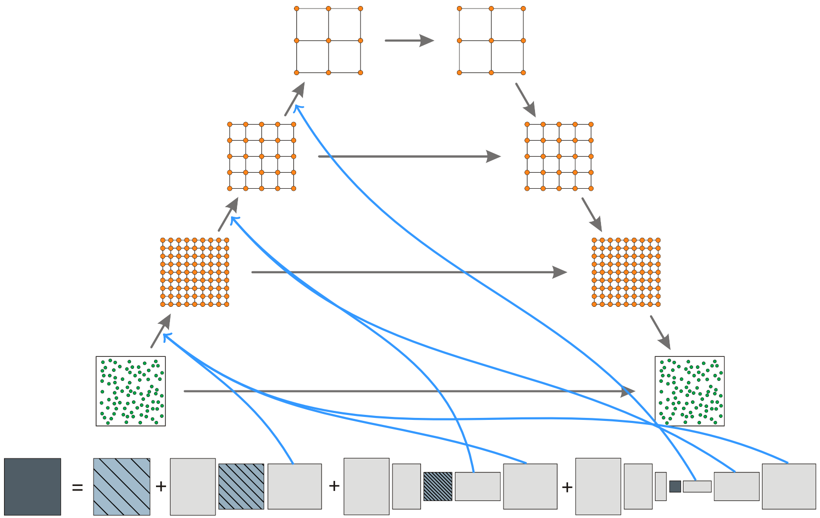

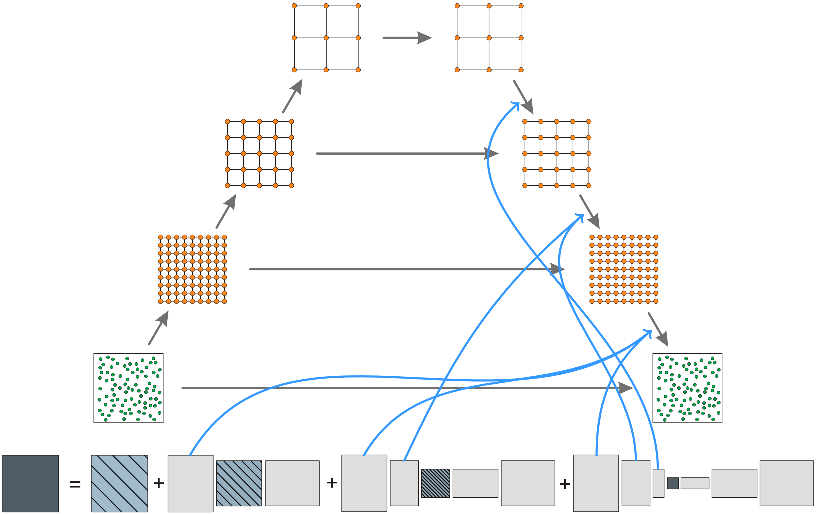

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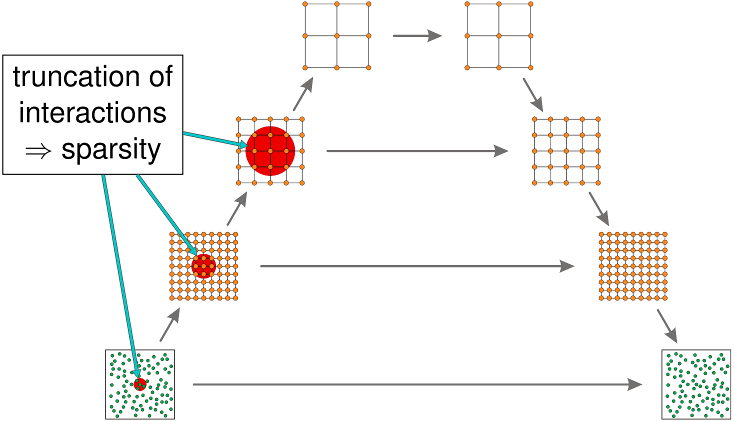
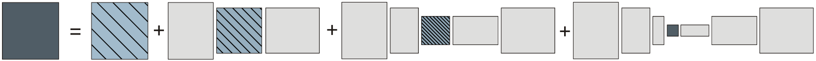
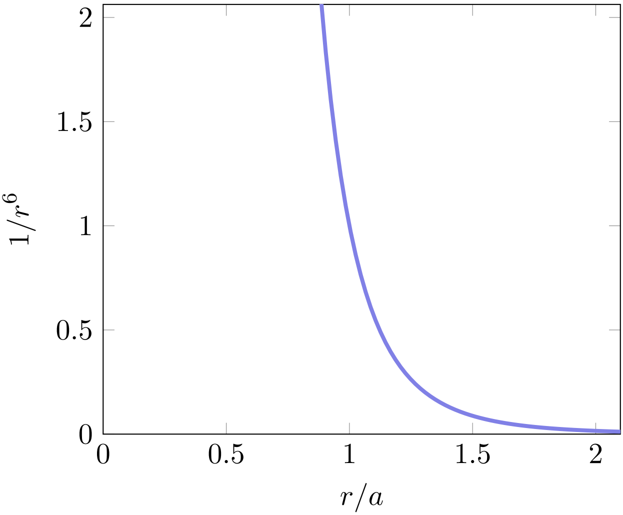




Dispersion Potential



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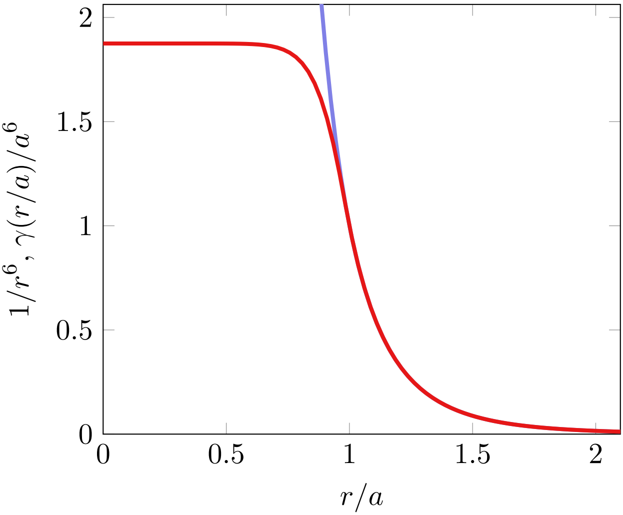

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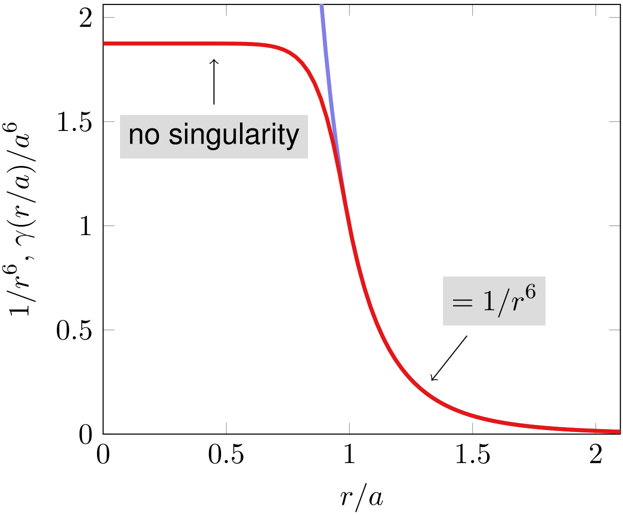

Local & Grid-Based Part

$$\frac{1}{r^6} = \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right) \longleftarrow$$

calculation with short-range method

$= 0$ for $r \geq a$

$$+ \frac{1}{a^6}\gamma\left(\frac{r}{a}\right) \longleftarrow$$

approximation with grids

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Local & Grid-Based Part

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calculation with short-range method

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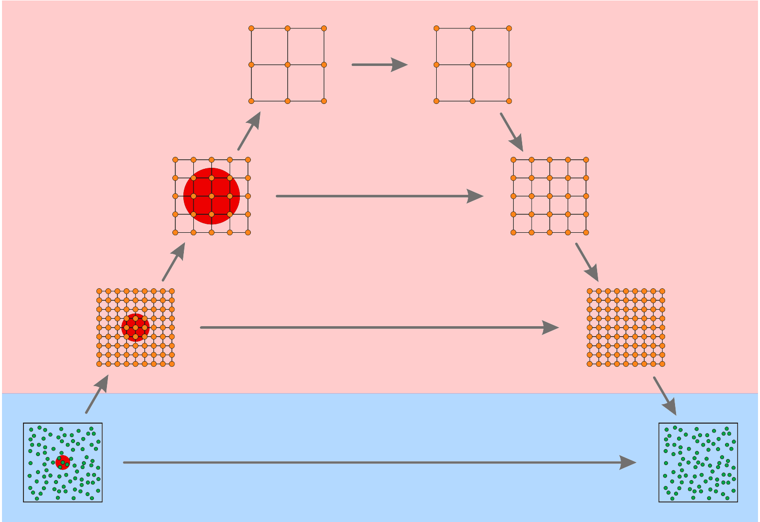
approximation with grids

Example for smoothing function γ:

$$\gamma(x) = \begin{cases} \frac{15}{8} - \frac{5}{4}x^{12} + \frac{3}{8}x^{24} & \text{for } x < 1 \\ \frac{1}{x^6} & \text{for } x \geq 1 \end{cases}$$



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$$\frac{1}{r^6} = \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right)$$

$$+ \frac{1}{a^6}\gamma\left(\frac{r}{a}\right)$$

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Local & Grid-Based Part

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$$\frac{1}{r^6} = \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right)$$

$$+ \frac{1}{a^6}\gamma\left(\frac{r}{a}\right) - \frac{1}{(2a)^6}\gamma\left(\frac{r}{2a}\right)$$

$$+ \frac{1}{(2a)^6}\gamma\left(\frac{r}{2a}\right)$$

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Local & Grid-Based Part

$$\frac{1}{r^6} = \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right)$$

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$$+ \frac{1}{(2a)^6}\gamma\left(\frac{r}{2a}\right) - \frac{1}{(4a)^6}\gamma\left(\frac{r}{4a}\right)$$

$$+ \frac{1}{(4a)^6}\gamma\left(\frac{r}{4a}\right)$$

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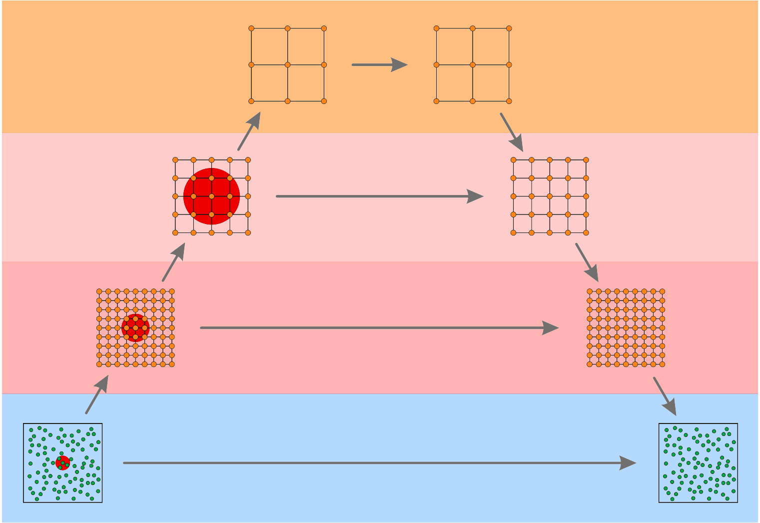
$$
\begin{aligned}
\frac{1}{r^6} &= \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right) \\
&+ \frac{1}{a^6}\gamma\left(\frac{r}{a}\right) - \frac{1}{(2a)^6}\gamma\left(\frac{r}{2a}\right) \\
&+ \frac{1}{(2a)^6}\gamma\left(\frac{r}{2a}\right) - \frac{1}{(4a)^6}\gamma\left(\frac{r}{4a}\right) \\
&+ \cdots + \\
&+ \frac{1}{(2^{l-1}a)^6}\gamma\left(\frac{r}{2^{l-1}a}\right)
\end{aligned}
$$

$$g_0(r) = \frac{1}{r^6} - \frac{1}{a^6}\gamma\left(\frac{r}{a}\right)$$

$$g_k(r) = \frac{1}{2^{6(k-1)}a^6}\gamma\left(\frac{r}{2^{(k-1)}a}\right) - \frac{1}{2^{6k}a^6}\gamma\left(\frac{r}{2^k a}\right) \text{ for } k = 1, \ldots, l-1$$

$$g_l(r) = \frac{1}{2^{6l-6}a^6}\gamma\left(\frac{r}{2^{l-1}a}\right)$$

Multilevel Summation method

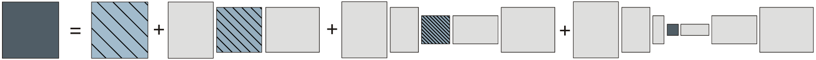


$$\frac{1}{r^6} = g_0 + g_1 + g_2 + \cdots + g_{l-1} + g_l$$

Approximation of g_i

$$\frac{1}{r^6} = g_0 + g_1 + g_2 + \cdots + g_{l-1} + g_l$$

$$\frac{1}{r^6} \approx g_0 + \mathcal{I}_1 \left[g_1 + \mathcal{I}_2 \left[g_2 \ldots + \mathcal{I}_{l-1} \left[g_{l-1} + \mathcal{I}_l \left[g_l \right] \right] \ldots \right] \right]$$



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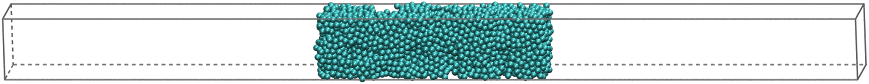
Simulations



4000 particles
Lennard-Jones potential with geometric mixing
$11.01\sigma \times 11.01\sigma \times 176.16\sigma$ with periodic boundaries

results compared with high precision calculation using the Ewald method

Study influence of

- cutoff a
- spacing of finest grid h

Accuracy

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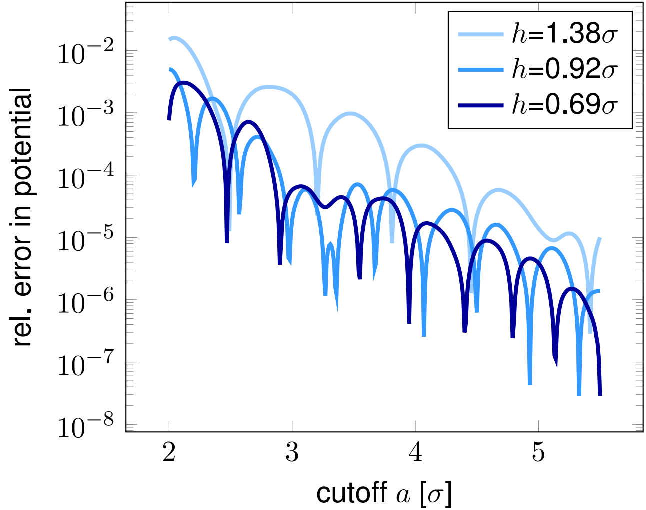

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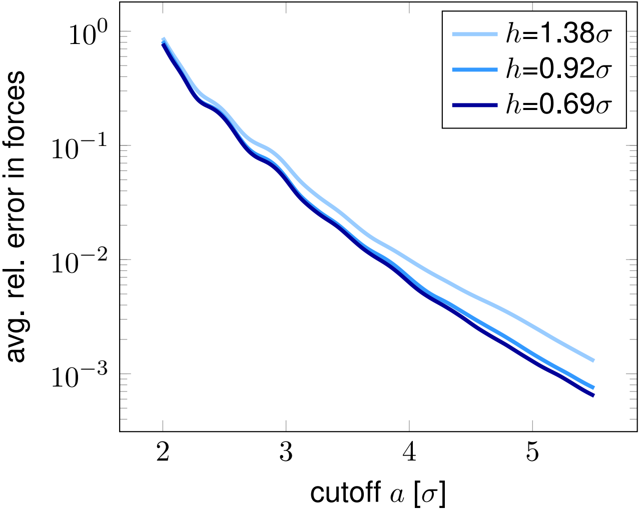
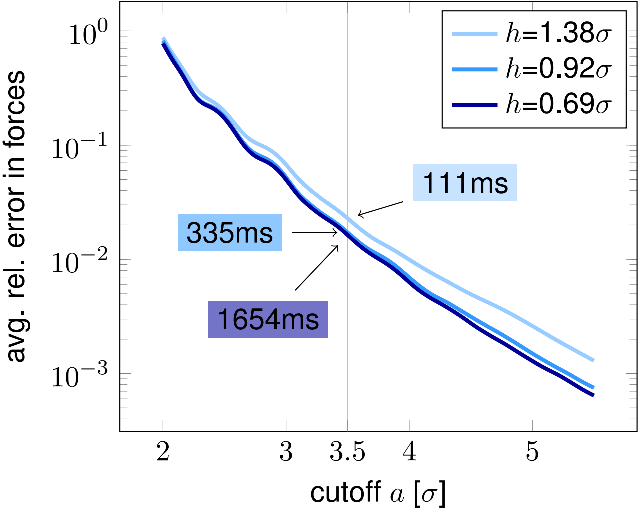
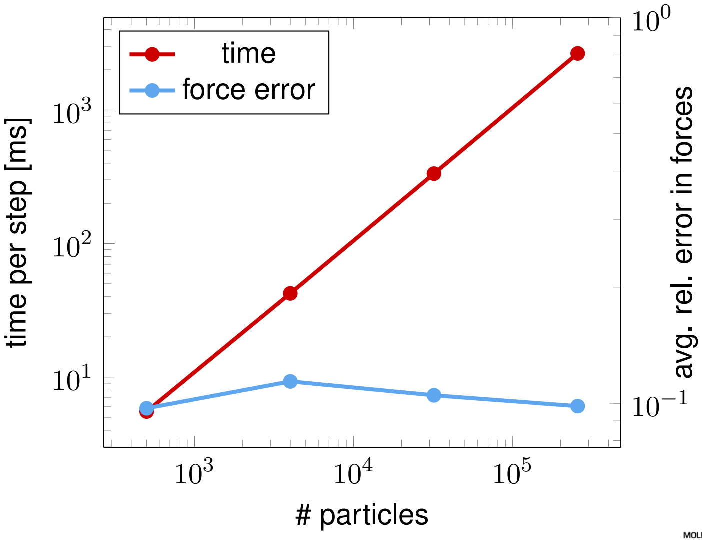

h=1.38σ
h=0.92σ
h=0.69σ
10^0
10^{-1}
10^{-2}
10^{-3}
avg. rel. error in forces
2
3
4
5
cutoff a [σ]

Accuracy



avg. rel. error in forces
10^0
10^{-1}
10^{-2}
10^{-3}
h=1.38σ
h=0.92σ
h=0.69σ
111ms
335ms
1654ms
2
3
3.5
4
5
cutoff a [σ]


time
force error
time per step [ms]
avg. rel. error in forces
10^1
10^2
10^3
10^{-1}
10^0
10^3
10^4
10^5
particles

Conclusions

- We adapted the Multilevel Summation to dispersion interactions
- The accuracy of the Multilevel Summation increases as the cutoff a increases and the finest grid spacing h decreases
- Preliminary performance measurements were done
- The linear complexity can be demonstrated with a serial, prototype implementation

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