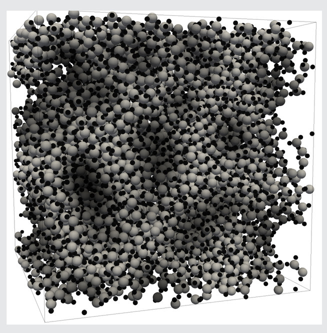
TECHNISCHE UNIVERSITÄT CHEMNITZ

Faculty of Mathematics
Applied Functional Analysis
Franziska Nestler and Michael Pippig

P^{2}NFFT - A versatile framework for computing NFFT based fast Ewald summation

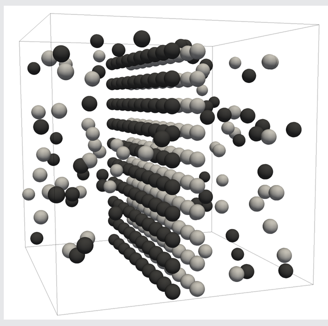
Task

Silica melt



$N = 12960$ charged particles

Cloud-wall



$N = 300$ charged particles

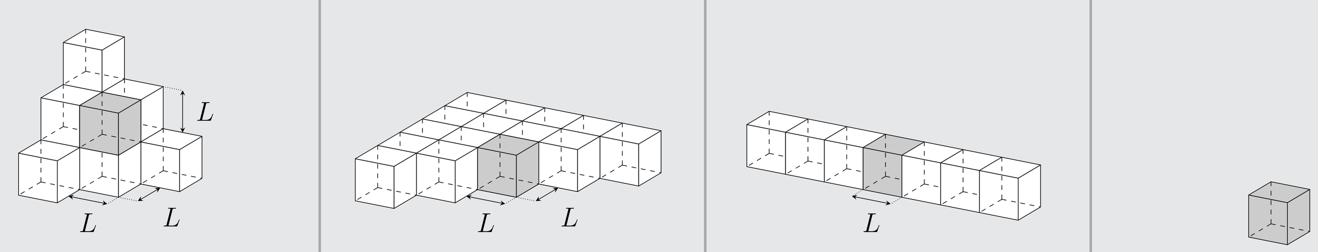
N-body problem

For N particles $\boldsymbol{r}_j = (x_j, y_j, z_j) \in [-L/2, L/2)^3$ with charges q_j compute the Coulomb potential under periodic boundary conditions along the first p dimensions

$$\phi_{\mathcal{S}_p}(\boldsymbol{r}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}_p} \sum_{i=1}^{N}{}' \frac{q_i}{\|\boldsymbol{r}_{ij} + L\boldsymbol{n}\|},$$

where $\boldsymbol{r}_{ij} = (x_{ij}, y_{ij}, z_{ij}) := \boldsymbol{r}_i - \boldsymbol{r}_j \in [-L, L)^3$.

3d-periodic | 2d-periodic | 1d-periodic | 0d-periodic



$\mathcal{S}_3 = \mathbb{Z}^3$ | $\mathcal{S}_2 = \mathbb{Z}^2 \times \{0\}$ | $\mathcal{S}_1 = \mathbb{Z} \times \{0\}^2$ | $\mathcal{S}_0 = \{0\}^3$

Fourier Approximations

Ewald splitting

The identity $\frac{1}{r} = \frac{\mathrm{erfc}(\alpha r)}{r} + \frac{\mathrm{erf}(\alpha r)}{r}$ splits $\phi_{\mathcal{S}_p}(\boldsymbol{r}_j) = \phi^{\mathrm{S}}_{\mathcal{S}_p}(\boldsymbol{r}_j) + \phi^{\mathrm{L}}_{\mathcal{S}_p}(\boldsymbol{r}_j)$ with the short-range part

$$\phi^{\mathrm{S}}_{\mathcal{S}_p}(\boldsymbol{r}_j) = \sum_{\boldsymbol{n}\in\mathcal{S}_p} \sum_{i=1}^{N}{}' q_i \frac{\mathrm{erfc}(\alpha\|\boldsymbol{r}_{ij} + L\boldsymbol{n}\|)}{\|\boldsymbol{r}_{ij} + L\boldsymbol{n}\|} - \frac{2\alpha}{\sqrt{\pi}} q_j$$

and the long-range part

$$\phi^{\mathrm{L}}_{\mathcal{S}_p}(\boldsymbol{r}_j) = \sum_{\boldsymbol{n}\in\mathcal{S}_p} \sum_{i=1}^{N} q_i \frac{\mathrm{erf}(\alpha\|\boldsymbol{r}_{ij} + L\boldsymbol{n}\|)}{\|\boldsymbol{r}_{ij} + L\boldsymbol{n}\|}.$$

Fourier series along periodic dimensions

Computing the Fourier series of the long-range part $\phi^{\mathrm{L}}_{\mathcal{S}_p}(\boldsymbol{r}_j)$ along periodic dimensions converts $x \to k_x, y \to k_y, z \to k_z$ and yields the well known Ewald formulas.

3dp: $$\phi^{\mathrm{L}}_{\mathcal{S}_3}(\boldsymbol{r}_j) = \sum_{i=1}^{N} q_i \sum_{k_x,k_y,k_z} \Theta^{3\mathrm{d}}\left(\sqrt{k_x^2 + k_y^2 + k_z^2}\right) \mathrm{e}^{\frac{2\pi\mathrm{i}}{L}(k_x x_{ij} + k_y y_{ij} + k_z z_{ij})}$$

2dp: $$\phi^{\mathrm{L}}_{\mathcal{S}_2}(\boldsymbol{r}_j) = \sum_{i=1}^{N} q_i \sum_{k_x,k_y} \Theta^{2\mathrm{d}}\left(\sqrt{k_x^2 + k_y^2}, |z_{ij}|\right) \mathrm{e}^{\frac{2\pi\mathrm{i}}{L}(k_x x_{ij} + k_y y_{ij})}$$

1dp: $$\phi^{\mathrm{L}}_{\mathcal{S}_1}(\boldsymbol{r}_j) = \sum_{i=1}^{N} q_i \sum_{k_x} \Theta^{1\mathrm{d}}\left(|k_x|, \sqrt{y_{ij}^2 + z_{ij}^2}\right) \mathrm{e}^{\frac{2\pi\mathrm{i}}{L}(k_x x_{ij})}$$

0dp: $$\phi^{\mathrm{L}}_{\mathcal{S}_0}(\boldsymbol{r}_j) = \sum_{i=1}^{N} q_i \quad \Theta^{0\mathrm{d}}\left(\sqrt{x_{ij}^2 + y_{ij}^2 + z_{ij}^2}\right)$$

Remaining problem:

How to convert the non-periodic dimensions to Fourier space?

Analytically known Fourier coefficients

The Fourier coefficients and their type of decay are given as follows.

3dp: $$\Theta^{3\mathrm{d}}(k) := \frac{\mathrm{e}^{-\pi^2 k^2/(\alpha^2 L^2)}}{\pi L k^2}$$

2dp: $$\Theta^{2\mathrm{d}}(0, r) := -\frac{2\sqrt{\pi}}{L^2}\left[\frac{1}{\alpha}\mathrm{e}^{-\alpha^2 r^2} + \sqrt{\pi} z\,\mathrm{erf}(\alpha r)\right] \quad \text{type B}$$

$$\Theta^{2\mathrm{d}}(k, r) := \frac{1}{2Lk}\left[\mathrm{e}^{2\pi k r/L}\,\mathrm{erfc}\left(\frac{\pi k}{\alpha L} + \alpha r\right) + \mathrm{e}^{-2\pi k r/L}\,\mathrm{erfc}\left(\frac{\pi k}{\alpha L} - \alpha r\right)\right] \quad \text{type A}$$

1dp: $$\Theta^{1\mathrm{d}}(0, r) := -\frac{1}{L}\left[\gamma + \Gamma(0, \alpha^2 r^2) + \ln(\alpha^2 r^2)\right] \quad \text{type B}$$

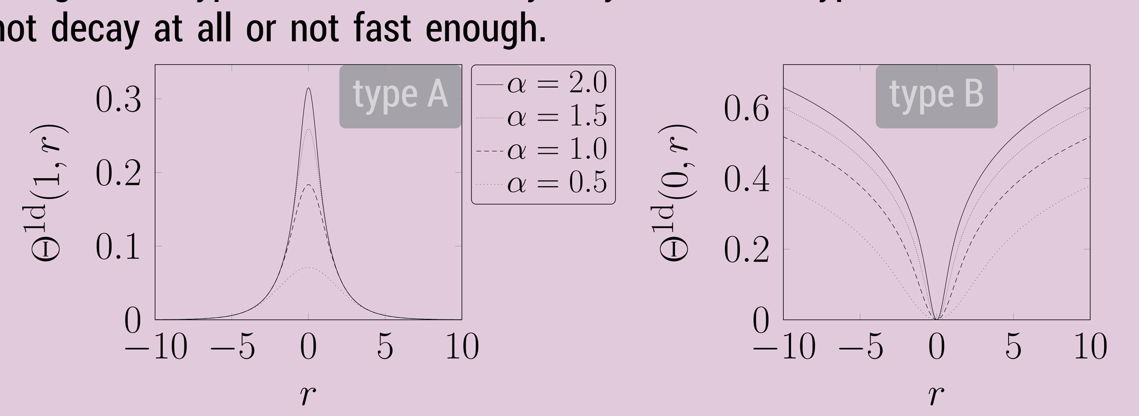
$$\Theta^{1\mathrm{d}}(k, r) := \frac{1}{L} K_0\left(\frac{\pi^2 k^2}{\alpha^2 L^2}, \alpha^2 r^2\right) \quad \text{type A}$$

0dp: $$\Theta^{0\mathrm{d}}(r) := \frac{\mathrm{erf}(\alpha r)}{r} \quad \text{type B}$$

All of these functions asymptotically tend to zero as $\frac{1}{k^2}\mathrm{e}^{-k^2}$ for $k \to \infty$, which justifies truncation of the Fourier series along periodic dimensions.

Decay of type A and B

The decay of the smooth functions $\Theta^{p\mathrm{d}}(k, r)$ for $r \to \infty$ falls into two categories. Type A functions decay very fast, while type B functions do not decay at all or not fast enough.



Type A Fourier approximation

If $\Theta^{p\mathrm{d}}(k, r)$ is neglible for $|r| \geq h \geq 2L$, we can use its h-periodization instead and apply the Poisson summation formula. E.g., in the 2d-periodic case we have

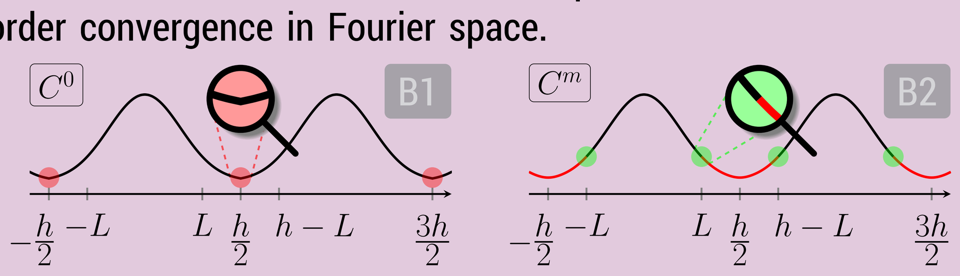
$$\Theta^{2\mathrm{d}}(k, z) \approx \sum_{n\in\mathbb{Z}} \Theta^{2\mathrm{d}}(k, z + hn) = \frac{1}{h}\sum_{k_z\in\mathbb{Z}} \widehat{\Theta}^{2\mathrm{d}}\left(k, \frac{k_z}{h}\right) \mathrm{e}^{\frac{2\pi\mathrm{i}}{h} k_z z},$$

where the analytically known, continuous Fourier transform of $\Theta^{2\mathrm{d}}(k, \cdot)$ fulfills $\widehat{\Theta}^{2\mathrm{d}}(k, v) \sim \frac{1}{v^2}\mathrm{e}^{-v^2}$ for $v \to \infty$.

Type B Fourier approximations

But what if $\Theta^{p\mathrm{d}}(k, r)$ does not decay fast enough?

Type B1: A first attempt is to repeat $\Theta^{p\mathrm{d}}(k, r)$ with period $h \geq 2L$. But the kink at $r = \pm h$ implies a rather slow 2nd order convergence in Fourier space.



Type B2: Instead, we construct an interpolating polynomial within $[L, h - L]$ that fits the first m derivatives of $\Theta^{p\mathrm{d}}(k, r)$ at $r = \pm L$. Then, the convergence rate will be $m + 2$.

Final approximation

In summary, we can write the truncated series as

$$\phi^{\mathrm{L}}_{\mathcal{S}_p}(\boldsymbol{r}_j) \approx \sum_{i=1}^{N} q_i \sum_{\boldsymbol{k}\in\mathcal{M}} c^{p\mathrm{d}}_{\boldsymbol{k}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_{ij}},$$

where $\boldsymbol{k} = (k_x, k_y, k_z)$ runs in a finite 3d mesh $\mathcal{M}$.

P^{2}NFFT

Short-range evaluation

If the particles are sufficiently homogeneously distributed, the short-range part $\phi^{\mathrm{S}}_{\mathcal{S}_p}(\boldsymbol{r}_j)$ can be computed directly within $\mathcal{O}(N)$ operations.

Long-range evaluation

The approximated long-range part is evaluated by non-equispaced fast Fourier transforms (NFFT) within $\mathcal{O}(N \log N)$ operations.

adjoint 3d-NFFT: $$S_{\boldsymbol{k}} := \sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i}$$

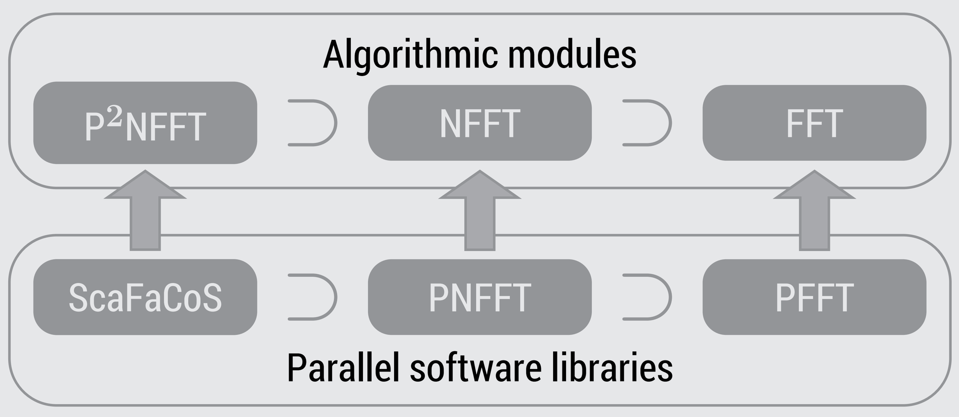
3d-NFFT: $$\phi^{\mathrm{L}}_{\mathcal{S}_p}(\boldsymbol{r}_j) \approx \sum_{\boldsymbol{k}\in\mathcal{M}} c^{p\mathrm{d}}_{\boldsymbol{k}} S_{\boldsymbol{k}} \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j}$$

Historical context

Fast particle-mesh algorithms	3dp	2dp	1dp	0dp
P3M [Hockney, Eastwood 1988]	✓	✗	✗	✗
PME [Darden et al. 1993]	✓	✗	✗	✗
SPME [Essmann et al. 1995]	✓	✗	✗	✗
Type B1 approximated fast Ewald [Martyna et al. 2002]	✗	✓	✓	✓
Gaussian split Ewald [Shan et. al 2004]	✓	✗	✗	✗
NFFT based fast summation [Nieslony, Potts, Steidl 2004]	✗	✗	✗	✓
NFFT based fast Ewald [Hedman, Laaksonen 2006]	✓	✗	✗	✗
Spectrally accurate Ewald [Lindbo, Tornberg 2011, 2012]	✓	✓	✗	✗
P^{2}NFFT [Nestler, Pippig, Potts 2013, 2015]	✓	✓	✓	✓

Modularized algorithm structure

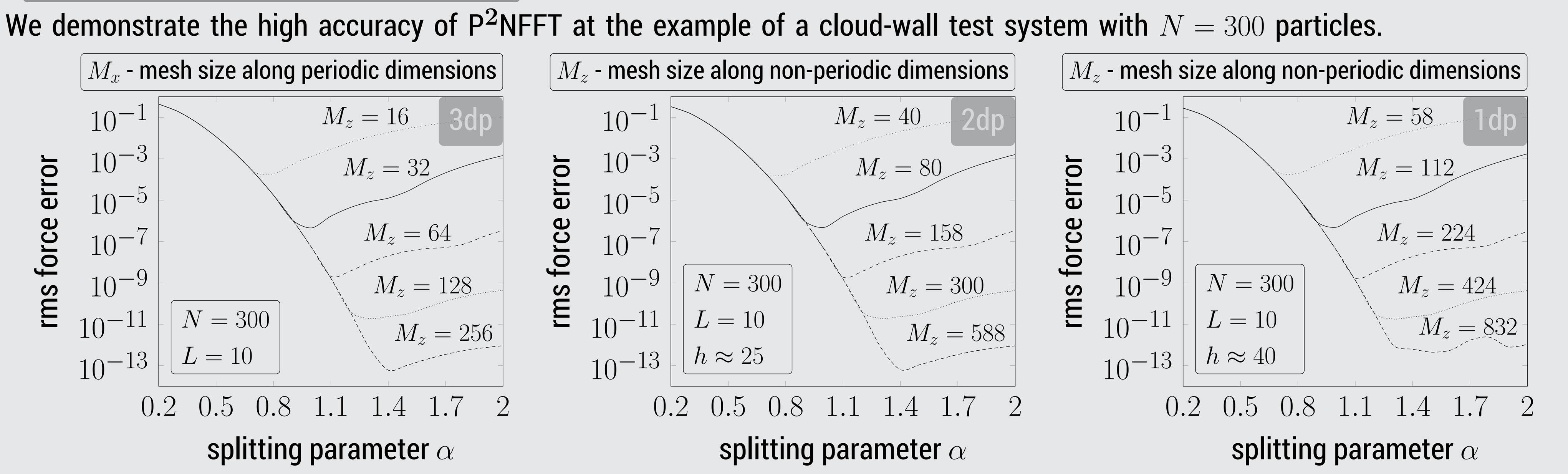
One of the benefits of the P^{2}NFFT is its highly modularized structure. All the performance critical steps are encapsulated and can be implemented by existing software libraries.



Numerical Results

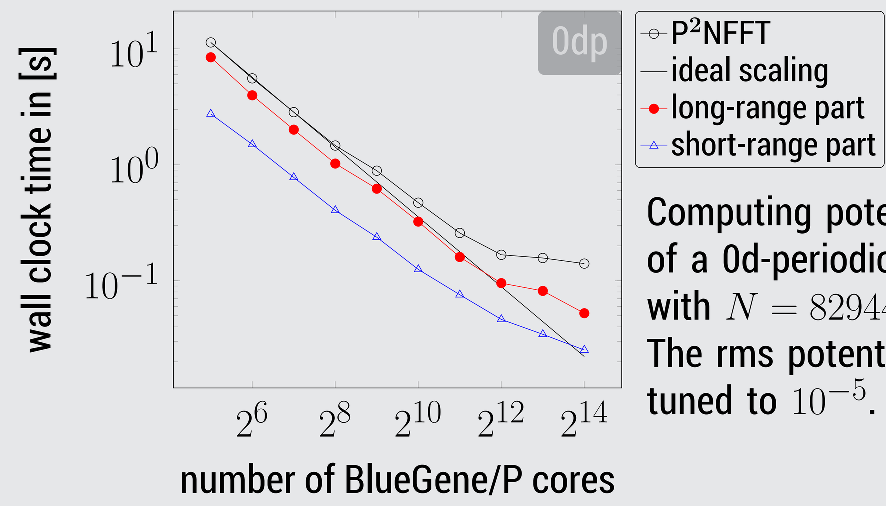
High accuracy independent of periodicity

We demonstrate the high accuracy of P^{2}NFFT at the example of a cloud-wall test system with $N = 300$ particles.



Massive parallelism

The P^{2}NFFT software library was designed for massive parallelism with distributed memory. We demonstrate the scalabilty on a BlueGene/P up to 16384 cores.



Computing potential and field of a 0d-periodic silica melt with $N = 829440$ particles. The rms potential error was tuned to 10^{-5}.

Visit our software page or join us at Github!
www.tu-chemnitz.de/~mpip/software.php.en
www.github.com/mpip

Franziska Nestler
franziska.nestler@mathematik.tu-chemnitz.de
www.tu-chemnitz.de/~nesfr

Michael Pippig
michael.pippig@mathematik.tu-chemnitz.de
www.tu-chemnitz.de/~mpip