Fast Ewald summation for mixed periodic boundary conditions based on the nonuniform FFT

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The 3d-NFFT (FFT for nonequispaced data)

Notation

- define the torus $\mathbb{T} := \mathbb{R}/\mathbb{Z} \simeq [-{}^1\!/_2, {}^1\!/_2)$
- for $M \in 2\mathbb{N}$ set $\mathcal{I}_M := \{-{}^M\!/_2, \dots, {}^M\!/_2 - 1\}^3 \subset \mathbb{Z}^3$

NFFT: $$f(\boldsymbol{x}_j) := \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_j} \qquad \boldsymbol{x}_j \in \mathbb{T}^3, j = 1, \dots, N$$

Complexity: $\mathcal{O}(|\mathcal{I}_M| \log |\mathcal{I}_M| + N)$

[Dutt, Rokhlin 1993] [Beylkin 1995]
[Potts, Steidl, Tasche 2001] [Greengard, Lee 2004]

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$$\text{adjoint NFFT:} \quad h(\boldsymbol{k}) := \sum_{j=1}^{N} f_j \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}_j} \qquad \boldsymbol{k} \in \mathcal{I}_M$$

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Coulomb interactions, mixed periodicity

Let N charges $q_j \in \mathbb{R}$ at positions $\boldsymbol{x}_j \in [-L/2, L/2]^3$ be given.
Coulomb interaction energy ($\boldsymbol{x}_{ij} := \boldsymbol{x}_i - \boldsymbol{x}_j$) s.t. periodic boundary conditions:

$$E := \frac{1}{2} \sum_{j=1}^{N} q_j \phi(\boldsymbol{x}_j) \quad \text{with} \quad \phi(\boldsymbol{x}_j) := \sum_{\boldsymbol{n} \in \mathcal{S}} \sum_{\substack{i=1 \\ i \neq j \text{ if } \boldsymbol{n} = \boldsymbol{0}}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij} + L\boldsymbol{n}\|},$$

where $\mathcal{S} \subset \mathbb{Z}^3$. Forces: $\boldsymbol{F}(\boldsymbol{x}_j) := -\nabla_{\boldsymbol{x}_j} \phi(\boldsymbol{x}_j)$.

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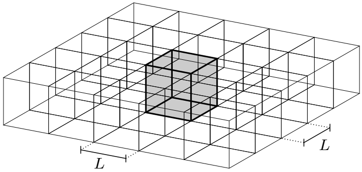
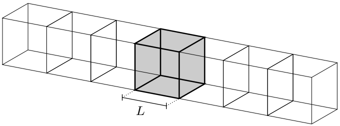
2d-periodic: $\mathcal{S} := \mathbb{Z}^2 \times \{0\}$.



1d-periodic: $\mathcal{S} := \mathbb{Z} \times \{0\}^2$.



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Fast particle mesh methods	**3dp**	**2dp**	**1dp**	**0dp**
P3M [Hockney, Eastwood 1988]	✓	✗	✗	✗
PME [Darden et al. 1993], SPME [Essmann et al. 1995]	✓	✗	✗	✗
Non-smooth approximated 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^2NFFT [Nestler, Pippig, Potts 2013, 2015]	✓	✓	✓	✓

Other methods

Multigrid [Brandt, Hackbusch, Trottenberg 1977], FMM [Greengard, Rokhlin 1987]

Ewald summation

Apply the well known Ewald splitting

$$\frac{1}{r} = \frac{\operatorname{erfc}(\alpha r)}{r} + \frac{\operatorname{erf}(\alpha r)}{r}$$

with $r := \|\boldsymbol{x}_{ij} + L\boldsymbol{n}\|$ and obtain

$$\phi(\boldsymbol{x}_j) = \sum_{\boldsymbol{n}\in S} \sum_{\substack{i=1 \\ i\neq j \text{ if } \boldsymbol{n}=\boldsymbol{0}}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij} + L\boldsymbol{n}\|}$$

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- short range part can be obtained via direct evaluation after truncation

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$$\sum_{\boldsymbol{n}\in S} \sum_{i=1}^{N} q_i \frac{\operatorname{erf}(\alpha\|\boldsymbol{x}_{ij} + L\boldsymbol{n}\|)}{\|\boldsymbol{x}_{ij} + L\boldsymbol{n}\|} - \frac{2\alpha}{\sqrt{\pi}} q_j$$

- short range part can be obtained via direct evaluation after truncation
- $\lim\limits_{r\to 0} \frac{\operatorname{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}} \Rightarrow$ substract self potential
- write the long range part as a sum in Fourier space

Ewald summation

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

- write the long range part as a sum in Fourier space

Ewald summation s.t. 2d-periodic boundary conditions

Long range part under 2d-periodic b.c. [Grzybowski, Gwóźdź, Bródka 2000]

We write $\boldsymbol{x}_{ij} = (\tilde{\boldsymbol{x}}_{ij}, x_{ij,3})$ and obtain

$$\phi^{\mathrm{L}}(\boldsymbol{x}_j) = \sum_{\boldsymbol{k}\in\mathbb{Z}^2\setminus\{\boldsymbol{0}\}} \sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\tilde{\boldsymbol{x}}_{ij}/L} \Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3}) \quad - \quad \sum_{i=1}^{N} q_i \Theta^{\mathrm{p2}}(0, x_{ij,3})$$

2d Fourier series

$\boldsymbol{k} = \boldsymbol{0}$ part

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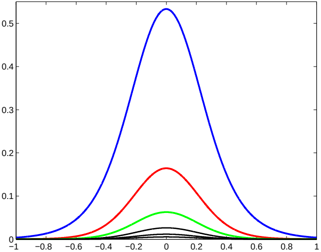

$\Theta^{\mathrm{p2}}(k, r)$

$k = 1$

$k = \sqrt{2}$

$k = \sqrt{3}$

$\dots$

$$\frac{\mathrm{e}^{2\pi k r/L}}{2Lk} \operatorname{erfc}\left(\frac{\pi k}{\alpha L} + \alpha r\right) + \frac{\mathrm{e}^{-2\pi k r/L}}{2Lk} \operatorname{erfc}\left(\frac{\pi k}{\alpha L} - \alpha r\right)$$

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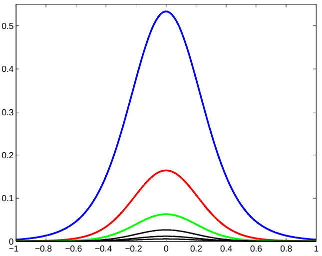

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$\ldots$

$$\frac{\mathrm{e}^{2\pi k r/L}}{2Lk}\operatorname{erfc}\left(\frac{\pi k}{\alpha L}+\alpha r\right) + \frac{\mathrm{e}^{-2\pi k r/L}}{2Lk}\operatorname{erfc}\left(\frac{\pi k}{\alpha L}-\alpha r\right)$$

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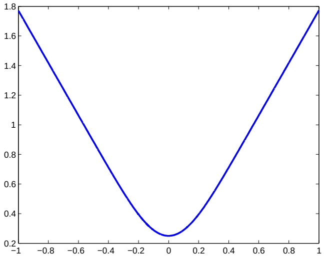
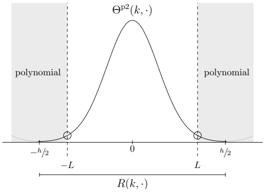


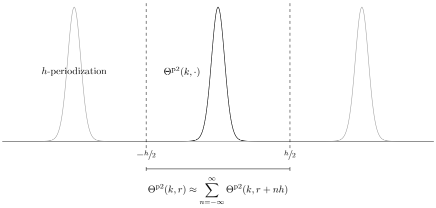
$$\Theta^{\mathrm{p2}}(0,r) = \frac{2\sqrt{\pi}}{\alpha L^2}\mathrm{e}^{-\alpha^2 r^2} + \frac{2r\pi}{L^2}\operatorname{erf}(\alpha r)$$

Approximation by Fourier sums

$k = 0$ and small $k \neq 0$



$k \neq 0$ large enough



Choose an appropriate period $h > 2L$:

- embed $\Theta^{\mathrm{p2}}(k,\cdot)$ into a smooth function $R(k,\cdot)$ (regularization)
- interpolate the derivatives at the boundary up to order $p \in \mathbb{N}$
- approximate function by FFT

- approximate the function by its h-periodic version
- use analytical Fourier coefficients (Poisson summation formula)

Result: $$\Theta^{\mathrm{p2}}(k,r) \approx \sum_{l=-M_3/2}^{M_3/2-1} \hat{b}_{k,l} \mathrm{e}^{2\pi \mathrm{i} l r/h} \quad , r \in [-L, L].$$

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- For each $k = \|\boldsymbol{k}\|$ and $M_3 \in 2\mathbb{N}$ large enough we have:

$$\Theta^{\mathrm{p2}}(k, x_{ij,3}) \approx \sum_{l=-M_3/2}^{M_3/2-1} \hat{b}_{k,l} \mathrm{e}^{2\pi\mathrm{i}l x_{ij,3}/h}$$

(precompute by FFT or use analytical Fourier transform)

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$$\phi^{\mathrm{L}}(\boldsymbol{x}_j) \approx \sum_{\boldsymbol{k}\in\mathcal{I}_M} \sum_{l=-M_3/2}^{M_3/2-1} \hat{b}_{\|\boldsymbol{k}\|,l} \left(\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\begin{bmatrix}k_1\\k_2\\l\end{bmatrix}\cdot\hat{\boldsymbol{x}}_i} \right) \mathrm{e}^{-2\pi\mathrm{i}\begin{bmatrix}k_1\\k_2\\l\end{bmatrix}\cdot\hat{\boldsymbol{x}}_j}$$

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Parameter choice

Consider the case of a cubic box: $\boldsymbol{x}_j \in [-L/2, L/2]^3$, $j = 1, \dots, N$.
Choose the NFFT mesh size as follows:

	2d-periodc		3d-periodic
	periodic dims.	non periodic dim.	periodic dims.
box length	L	$h := 2L + \delta$	L
# grid points	M	$M_3 := 2M + P$	M

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If the parameters are chosen appropriately, the achieved rms errors are comparable:

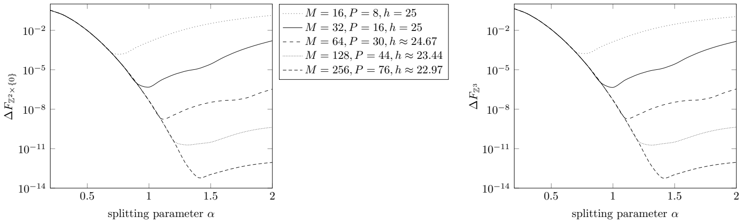

Figure: Achieved rms force errors for the 2d-periodic (left) compared to the 3d-periodic (right) case. ($L = 10$, $N = 300$)

Results for large particle systems

Idea: Tune parameters for a **small** system and use the same parameters.

N	L	M	P	$2M+P$	h	rms force error 2d-periodic	rms force error 3d-periodic
300	10	16	8	40	25	1.3771e-04	1.6261e-04
2400	20	32	8	72	45	1.5115e-04	1.6261e-04
19200	40	64	8	126	85	1.5815e-04	1.6261e-04
153600	80	128	8	264	165	1.6192e-04	1.6261e-04
1228800	160	256	8	520	325	1.6415e-04	1.6261e-04

Table: Achieved rms force errors and applied parameters for particle systems of different size. We use the same splitting parameter α as well as the same near field cutoff.

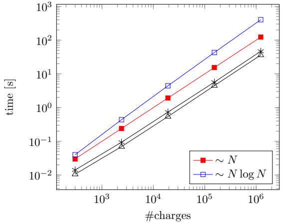

Figure: Comparison of the computation times (2dp: $*$, 3dp: $\triangle$).

Conclusion

- new approach to fast Ewald summation under mixed boundary conditions: [Nestler, Pippig, Potts, J. Comput. Phys. 2015]
  - 2d-periodic: Ewald + fast summation in 1d
  - 1d-periodic: Ewald + fast summation in 2d

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Thank you for your attention!

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