TECHNISCHE UNIVERSITÄT CHEMNITZ

Faculty of Mathematics
Applied Functional Analysis
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The P²NFFT method
for mixed charge-dipole systems

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Task

N-body problem

Given:

- N_{c} charges $q_j \in \mathbb{R}$ at positions $\boldsymbol{r}_j = (x_j, y_j, z_j)^\top \in \mathbb{R}^3$, $j \in \mathcal{C}$,
- N_{d} dipoles with moments $\boldsymbol{\mu}_j \in \mathbb{R}^3$ at positions $\boldsymbol{r}_j = (x_j, y_j, z_j)^\top \in \mathbb{R}^3$, $j \in \mathcal{D}$.

The particles may be located in a box spanned by three linearly independent vectors $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3 \in \mathbb{R}^3$.

Task: Compute the potentials

$$\phi(j) := \sum_{\boldsymbol{n}\in\mathcal{S}}{}^{*} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \frac{\xi_i}{\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\|} \quad \text{with} \quad \xi_i := \begin{cases} q_i & : i \in \mathcal{C}, \\ \boldsymbol{\mu}_i^\top \nabla_{\boldsymbol{r}_i} & : i \in \mathcal{D}, \end{cases}$$

$\boldsymbol{r}_{ij} := \boldsymbol{r}_i - \boldsymbol{r}_j$, $\boldsymbol{L} := [\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3] \in \mathbb{R}^{3\times 3}$ and $\mathcal{S} \subseteq \mathbb{Z}^3$ (periodic boundary conditions, $\boldsymbol{n} = 0 \Rightarrow i \neq j$).

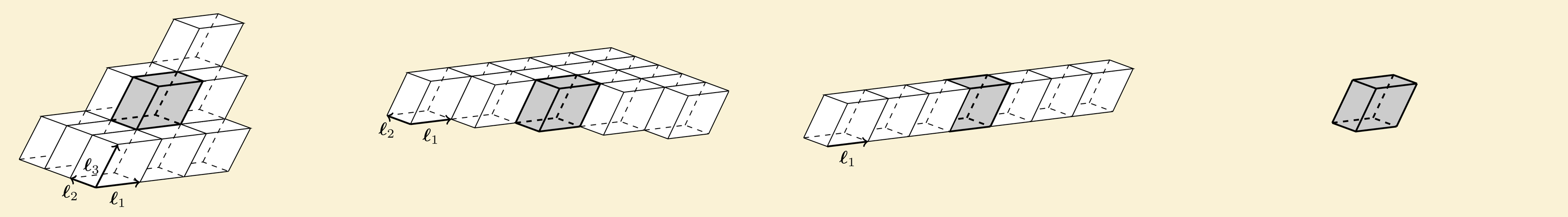
Further quantities of interest:

- fields $\boldsymbol{E}(j) := -\nabla_{\boldsymbol{r}_j}\phi(j)$,
- field gradients $\boldsymbol{G}(j) := -\nabla_{\boldsymbol{r}_j}\nabla_{\boldsymbol{r}_j}^\top\phi(j)$.

Periodic boundary conditions

We consider the following cases.

3d-periodic, $\mathcal{S} = \mathbb{Z}^3$ | 2d-periodic, $\mathcal{S} = \mathbb{Z}^2 \times \{0\}$ | 1d-periodic, $\mathcal{S} = \mathbb{Z} \times \{0\}^2$ | 0d-periodic, $\mathcal{S} = \{0\}^3$



all directions: $\boldsymbol{L} = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & * \end{pmatrix}$

xy-plane: $\boldsymbol{L} = \begin{pmatrix} * & * & 0 \\ * & * & 0 \\ 0 & 0 & 0 \end{pmatrix}$

x-direction: $\boldsymbol{L} = \begin{pmatrix} * & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

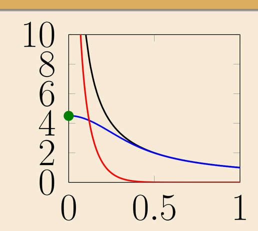
no periodicity: $\boldsymbol{L} = \boldsymbol{0}_{3\times 3}$

Ewald Summation

Ewald-splitting

Split the interactions based on

$$\frac{1}{r} = \frac{\operatorname{erfc}(\alpha r)}{r} + \frac{\operatorname{erf}(\alpha r)}{r} \quad \text{with} \quad \alpha > 0.$$



Short range potentials

$$\phi^{\mathrm{S}}(j) := \sum_{\boldsymbol{n}\in\mathcal{S}}{}^{*} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \frac{\operatorname{erfc}(\alpha\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\|)}{\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\|}$$

Direct via truncation: $\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\| \le r_{\mathrm{cut}}$.

Long range potentials

$$\phi^{\mathrm{L}}(j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \frac{\operatorname{erf}(\alpha\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\|)}{\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\|}$$

Continuous, fast decay in Fourier space.

Self potentials

$$\phi^{\mathrm{self}}(j) = \begin{cases} -2\alpha\sqrt{\pi}^{-1} q_j & : j \in \mathcal{C}, \\ 0 & : j \in \mathcal{D}. \end{cases}$$

Subtract far field contributions with $\|\boldsymbol{r}_{ij} + \boldsymbol{L}\boldsymbol{n}\| = 0$.

Fourier space representation of the long range parts

Periodic directions: Compute analytical Fourier transform (Poisson summation). Exponential decrease for $\|\boldsymbol{k}\| \to \infty$ or $|k| \to \infty$:

3dp: $$\phi^{\mathrm{L}}(j) = \sum_{\boldsymbol{k}\in\mathbb{Z}^3} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \Theta^{\mathrm{p3}}_{\boldsymbol{k},\alpha}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{L}^{-1}\boldsymbol{r}_{ij}}$$

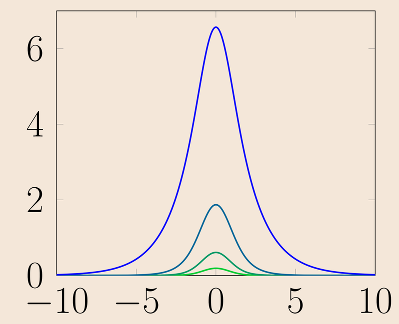
2dp: $$\phi^{\mathrm{L}}(j) = \sum_{\boldsymbol{k}\in\mathbb{Z}^2} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \Theta^{\mathrm{p2}}_{\boldsymbol{k},\alpha}(|z_{ij}|)\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{L}_{xy}^{-1}(x_{ij},y_{ij})^\top}$$

1dp: $$\phi^{\mathrm{L}}(j) = \sum_{k\in\mathbb{Z}} \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \Theta^{\mathrm{p1}}_{k,\alpha}\left(\sqrt{y_{ij}^2 + z_{ij}^2}\right) \mathrm{e}^{2\pi\mathrm{i}k^\top\boldsymbol{L}_x^{-1}x_{ij}}$$

0dp: $$\phi^{\mathrm{L}}(j) = \sum_{i=1}^{N_{\mathrm{c}}+N_{\mathrm{d}}} \xi_i \Theta^{\mathrm{p0}}_{\alpha}\left(\sqrt{x_{ij}^2 + y_{ij}^2 + z_{ij}^2}\right)$$

Influence of nonperiodic directions: Fourier coefficients depend on particle distances regarding the nonperiodic dimensions.

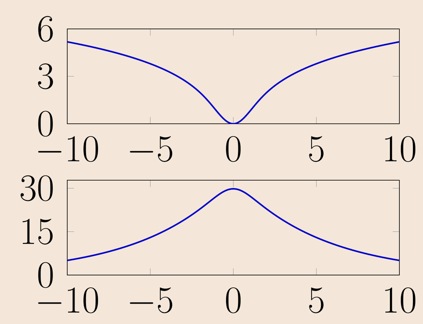
Involved functions



$\Theta^{\mathrm{p2}}_{\boldsymbol{k},\alpha}(\cdot)$, $\Theta^{\mathrm{p1}}_{k,\alpha}(\cdot)$: $\boldsymbol{k}$ or k large enough.

Type A (left): Very fast decay.

Type B (right): No decay at all or not fast enough.

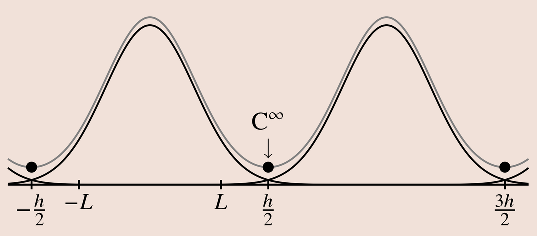


$\Theta^{\mathrm{p2}}_{\boldsymbol{k},\alpha}(\cdot)$, $\Theta^{\mathrm{p1}}_{k,\alpha}(\cdot)$: $\boldsymbol{k}$ or k small; $\Theta^{\mathrm{p0}}_{\alpha}(\cdot)$.

Fourier Approx.

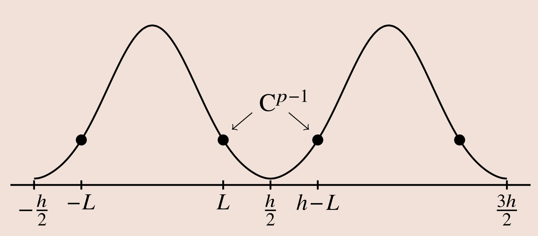
Periodization approaches (nonperiodic dimensions)

One-dimensional setting: Approximate a given nonperiodic function over $[-L, L]$ by a trig. polynomial. Different techniques may be applied for functions of type A and B, respectively.



Type A: The function is sufficiently small outside a comparatively small interval $[-\frac{h}{2}, \frac{h}{2}]$. Use analytical Fourier transform:

$$f(x) \approx \sum_{n\in\mathbb{Z}} f(x + hn) \approx \frac{1}{h} \sum_{|k|\le M} \hat{f}\left(\frac{k}{h}\right) \mathrm{e}^{2\pi\mathrm{i}kx/h}$$



Type B: Construct an interpolating polynomial within $[L, h - L]$ that fits the derivatives of f up to a certain degree.

Approximate via FFT: $$\tilde{f}(x) \approx \sum_{|k|\le M} \hat{b}_k\, \mathrm{e}^{2\pi\mathrm{i}kx/h}$$

Higher dimensions: The generalization in case of **Type A** functions is straight forward. The periodization approach **Type B** is possible in a similar fashion for radial kernels $f = f(\|\boldsymbol{x}\|)$.

Final Fourier approximations

Periodic dimensions: Exponential decrease for $\|\boldsymbol{k}\| \to \infty$ or $|k| \to \infty \Rightarrow$ truncate Fourier series.
Nonperiodic dimensions: Apply appropriate periodization approaches to the involved functions.

Result: $$\phi^{\mathrm{L}}(j) \approx \sum_{\boldsymbol{\kappa}\in\mathcal{M}} \hat{b}_{\boldsymbol{\kappa}} \left(\sum_{i\in\mathcal{C}} q_i\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_i} + \sum_{i\in\mathcal{D}} \boldsymbol{\mu}_i^\top \nabla_{\boldsymbol{r}_i} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_i} \right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_j} \qquad \mathcal{M} \subset \mathbb{Z}^3 \text{ finite}$$

	Indices	Fourier coefficients	Approach	Scaled positions $\check{\boldsymbol{r}}_i$
3dp:	$\boldsymbol{\kappa} = \boldsymbol{k}$	$\hat{b}_{\boldsymbol{k}} = \Theta^{\mathrm{p3}}_{\boldsymbol{k},\alpha} = \delta_{\boldsymbol{k},\boldsymbol{0}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{L}^{-\top}\boldsymbol{k}\|^2/\alpha^2}}{\pi V\|\boldsymbol{L}^{-\top}\boldsymbol{k}\|^2}$	analytic FT	$\boldsymbol{L}^{-1}\boldsymbol{r}_i$
2dp:	$\boldsymbol{\kappa} = (\boldsymbol{k}, l)$	Compute $\hat{b}_{\boldsymbol{k},l}$ via periodization of each function $\Theta^{\mathrm{p2}}_{\boldsymbol{k},\alpha}(\lvert\cdot\rvert)$	$\|\boldsymbol{k}\|$ small: **Type B** (1d-FFT) $\|\boldsymbol{k}\|$ large: **Type A** (analytic)	$\operatorname{diag}(\boldsymbol{L}_{xy}, h)^{-1}\boldsymbol{r}_i$
1dp:	$\boldsymbol{\kappa} = (k, \boldsymbol{l})$	Compute $\hat{b}_{k,\boldsymbol{l}}$ via periodization of each function $\Theta^{\mathrm{p1}}_{k,\alpha}(\|\cdot\|)$	$\lvert k\rvert$ small: **Type B** (2d-FFT) $\lvert k\rvert$ large: **Type A** (analytic)	$\operatorname{diag}(\boldsymbol{L}_x, h, h)^{-1}\boldsymbol{r}_i$
0dp:	$\boldsymbol{\kappa} = \boldsymbol{l}$	Approximate $\Theta^{\mathrm{p0}}_{\alpha}(\|\cdot\|) = \frac{\operatorname{erf}(\alpha\|\cdot\|)}{\|\cdot\|}$	**Type B** (3d-FFT)	$\operatorname{diag}(h, h, h)^{-1}\boldsymbol{r}_i$

Tools

NFFT

Approximate the function values

$$f(\boldsymbol{r}_j) := \sum_{\boldsymbol{k}\in\mathcal{M}} \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{r}_j}$$

for arbitrary $\boldsymbol{r}_j \in \mathbb{T}^3$, $j = 1, \ldots, N$.
Complextiy: $\mathcal{O}(|\mathcal{M}| \log |\mathcal{M}| + N)$

Gradient NFFT

Approximate the gradients

$$\nabla f(\boldsymbol{r}_j) := 2\pi\mathrm{i} \sum_{\boldsymbol{k}\in\mathcal{M}} \boldsymbol{k}\hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{r}_j}$$

for arbitrary $\boldsymbol{r}_j \in \mathbb{T}^3$, $j = 1, \ldots, N$.
Complextiy: $\mathcal{O}(|\mathcal{M}| \log |\mathcal{M}| + N)$

Hessian NFFT

Approximate the Hessians

$$\nabla\nabla^\top f(\boldsymbol{r}_j) := -4\pi^2 \sum_{\boldsymbol{k}\in\mathcal{M}} \boldsymbol{k}\boldsymbol{k}^\top \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{r}_j}$$

for arbitrary $\boldsymbol{r}_j \in \mathbb{T}^3$, $j = 1, \ldots, N$.
Complextiy: $\mathcal{O}(|\mathcal{M}| \log |\mathcal{M}| + N)$

Adjoint NFFT

Approximate the sums

$$h(\boldsymbol{k}) := \sum_{j=1}^{N} f_j\, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{r}_j}, \ \boldsymbol{k} \in \mathcal{M},$$

for arbitrary $\boldsymbol{r}_j \in \mathbb{T}^3$, $j = 1, \ldots, N$.
Complextiy: $\mathcal{O}(|\mathcal{M}| \log |\mathcal{M}| + N)$

Adjoint gradient NFFT

Approximate the sums

$$h(\boldsymbol{k}) := \sum_{j=1}^{N} \boldsymbol{f}_j^\top \nabla_{\boldsymbol{r}_j} \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}^\top\boldsymbol{r}_j}, \ \boldsymbol{k} \in \mathcal{M},$$

for arbitrary $\boldsymbol{r}_j \in \mathbb{T}^3$, $j = 1, \ldots, N$.
Complextiy: $\mathcal{O}(|\mathcal{M}| \log |\mathcal{M}| + N)$

Method

P²NFFT algorithm

1. **Precomputations:** Compute the Fourier coefficients $\hat{b}_{\boldsymbol{\kappa}}$, $\boldsymbol{\kappa} \in \mathcal{M}$.
2. **Direct computations:** $\mathcal{O}(N)$
   Short range interactions (via truncation) and self interactions.
3. **Approximate long range interactions:** $\mathcal{O}(N \log N)$

$$\phi^{\mathrm{L}}(j) \approx \underbrace{\sum_{\boldsymbol{\kappa}\in\mathcal{M}} \hat{b}_{\boldsymbol{\kappa}} \Big(\underbrace{\sum_{i\in\mathcal{C}} q_i\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_i}}_{\text{adj. NFFT}} + \underbrace{\sum_{i\in\mathcal{D}} \boldsymbol{\mu}_i^\top \nabla_{\boldsymbol{r}_i} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_i}}_{\text{adj. grad. NFFT}} \Big) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{\kappa}^\top\check{\boldsymbol{r}}_j}}_{\text{NFFT}}$$

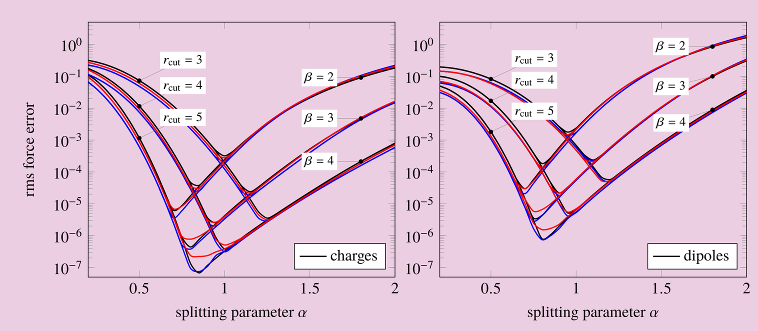
Analogously: $\boldsymbol{E}^{\mathrm{L}}(j) = -\nabla_{\boldsymbol{r}_j}\phi^{\mathrm{L}}(j)$ via gradient NFFT and
$\boldsymbol{G}^{\mathrm{L}}(j) = -\nabla_{\boldsymbol{r}_j}\nabla_{\boldsymbol{r}_j}^\top\phi^{\mathrm{L}}(j)$ via Hessian NFFT

Features

- ✓ Complexity $\mathcal{O}(N \log N)$
- ✓ Full periodicity
- ✓ Mixed periodicity (1d and 2d)
- ✓ Open boundary conditions
- ✓ Pure charge systems
- ✓ Pure dipole systems
- ✓ Mixed charge-dipole systems
- ✓ Error estimates (3d-periodic)
- ✓ High accuracy
- ✓ Massively parallel
- ✓ Publicly available

Numerical results

Example: Particle system with 100 charges and 100 dipoles in a box of size $8 \times 10 \times 12$.
→ fully periodic, 1d-periodic and open b.c.
→ different near field cutoff radii r_{cut}
→ different grids $\mathcal{M}$ of size $8\beta \times 10\beta \times 12\beta$,
$8\beta \times h\beta \times h\beta$ and $h\beta \times h\beta \times h\beta$



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