On the Relation of Ewald Summation and NFFT-Based Fast Summation

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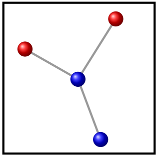
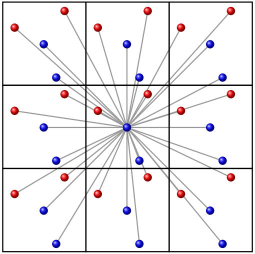
Motivation

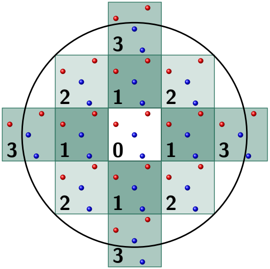
Coulomb Interaction in Particle Systems - $\mathcal{O}(M^2)$

$$\phi(\boldsymbol{x}_j) = \sum_{l=1}^{M}{}' \frac{q_l}{\|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2}, \qquad j = 1, \ldots, M$$

$$\widetilde{\phi}(\boldsymbol{x}_j) = \sum_{\boldsymbol{r} \in \mathbb{Z}^3} \sum_{l=1}^{M}{}' \frac{q_l}{\|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2}, \qquad j = 1, \ldots, M$$







Motivation

Coulomb Interaction in Particle Systems - $\mathcal{O}(M^2)$

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Fast Algorithms

Ewald Sum	P^3MG	Tree Codes	FMM	P^3M	Fast Sum
1921	1977	1986	1987	1988	2004
$\mathcal{O}(M^{3/2})$	$\mathcal{O}(M)$	$\mathcal{O}(M \log M)$	$\mathcal{O}(M)$	$\mathcal{O}(M \log M)$	$\mathcal{O}(M \log M)$
Ewald	Brandt	Barnes	Greengard	Hockney	Nieslony
	Hackbusch	Hut	Rokhlin	Eastwood	Potts
	Trottenberg				Steidl

Nonequispaced Discrete Fourier Transform

Task of 3d-DFT

For $\hat{f}_{k_0 k_1 k_2} \in \mathbb{C}$ compute

$$f_{l_0 l_1 l_2} = \sum_{k_0=0}^{N-1} \sum_{k_1=0}^{N-1} \sum_{k_2=0}^{N-1} \hat{f}_{k_0 k_1 k_2} \, \mathrm{e}^{-2\pi \mathrm{i} (k_0 \frac{l_0}{N} + k_1 \frac{l_1}{N} + k_2 \frac{l_2}{N})}$$

for all $l_0, l_1, l_2 \in \{0, \ldots, N-1\}$ $\left(\Rightarrow \frac{l_0}{N}, \frac{l_1}{N}, \frac{l_2}{N} \in [0,1)\right)$.

Task of 3d-NDFT

For $\hat{f}_{k_0 k_1 k_2} \in \mathbb{C}$ compute

$$f_j = \sum_{k_0=0}^{N-1} \sum_{k_1=0}^{N-1} \sum_{k_2=0}^{N-1} \hat{f}_{k_0 k_1 k_2} \, \mathrm{e}^{-2\pi \mathrm{i} (k_0 x_j + k_1 y_j + k_2 z_j)}$$

for $x_j, y_j, z_j \in [0,1)$, $j = 1, \ldots, M$.

Nonequispaced Fast Fourier Transforms

Matrix-Vector-Notation of NDFT and NDFT$^{\mathsf{H}}$

For $\hat{\boldsymbol{f}} \in \mathbb{C}^{N^3}$ and $\boldsymbol{h} \in \mathbb{C}^M$ compute

$$\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}} \in \mathbb{C}^M, \qquad \text{(NDFT)}$$

$$\hat{\boldsymbol{h}} = \boldsymbol{A}^{\mathsf{H}}\boldsymbol{h} \in \mathbb{C}^{N^3}, \qquad (\text{NDFT}^{\mathsf{H}})$$

where $\boldsymbol{A} = \left(\mathrm{e}^{-2\pi \mathrm{i}(k_0 x_j + k_1 y_j + k_2 z_j)}\right)_{j,(k_0,k_1,k_2)} \in \mathbb{C}^{M \times N^3}$.

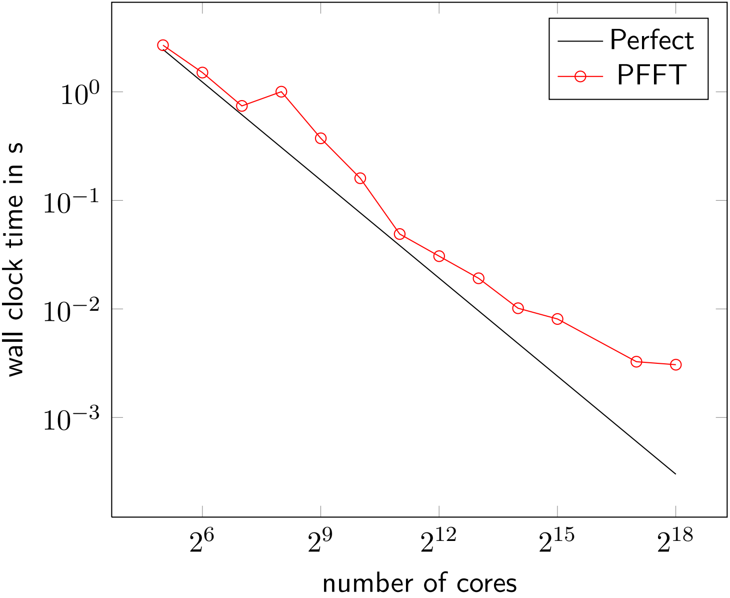
NFFT [Dutt, Rohklin 93, Beylkin 95, Steidl 96, ...]

$$\boldsymbol{A} \approx \boldsymbol{BFD}, \qquad \boldsymbol{A}^{\mathsf{H}} \approx \boldsymbol{DF}^{\mathsf{H}}\boldsymbol{B}^{\top}$$

- $\boldsymbol{D} \in \mathbb{R}^{N^3 \times N^3}$ diagonal matrix
- $\boldsymbol{F} \in \mathbb{C}^{n^3 \times N^3}$ truncated Fourier matrix ($n \geq N$)
- $\boldsymbol{B} \in \mathbb{R}^{M \times n^3}$ sparse matrix

$\Rightarrow \mathcal{O}(N^3 \log N + \log^3(\frac{1}{\varepsilon})M)$ instead of $\mathcal{O}(N^3 M)$

Scaling Parallel FFT of Size 512^3 on BlueGene/P



Coulomb Interaction in Open Particle Systems

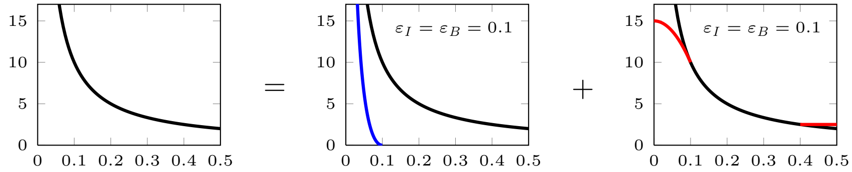
Calculation of the Potential

$$\phi(\boldsymbol{x}_j) = \sum_{l=1}^{M}{}' \frac{q_l}{\|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2}, \quad j = 1, \dots, M$$

Split Kernel into Nearfield and Farfield

$$\tfrac{1}{r} = \left(\tfrac{1}{r} - R(r)\right) + R(r) \quad \Rightarrow \quad R(\|\boldsymbol{x}\|_2) \approx \sum_{k \in I_{\boldsymbol{N}}} \hat{b}_{\boldsymbol{k}} \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{x}}$$

$$\frac{1}{r} \quad = \quad \frac{1}{r} - R(r) \quad + \quad R(r)$$



Fast Summation [Nieslony, Potts, Steidl 2004]

Nearfield Approximation - $\mathcal{O}(\nu M)$

$$\phi^{\text{near}}(\boldsymbol{x}_j) = -q_j P_I(0) + \sum_{l \in I_j}{}' q_l \left(\frac{1}{\|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2} - R(\|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2) \right)$$

$$I_j = \left\{ l = 1, \ldots, M : \|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2 < \varepsilon_I \right\}, \quad \nu := \max_j |I_j|$$

Farfield Approximation - $\mathcal{O}(MN^3) \to \mathcal{O}(\log^3(\frac{1}{\varepsilon})M + N^3 \log N)$

$$\phi^{\text{far}}(\boldsymbol{x}_j) = \sum_{l=1}^{M} q_l R(\|\boldsymbol{x}_j - \boldsymbol{x}_l\|_2) \approx \sum_{l=1}^{M} q_l \sum_{\boldsymbol{k} \in I_{\boldsymbol{N}}} \hat{b}_{\boldsymbol{k}} \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}(\boldsymbol{x}_j - \boldsymbol{x}_l)}$$

$$= \sum_{\boldsymbol{k} \in I_{\boldsymbol{N}}} \hat{b}_{\boldsymbol{k}} \left(\sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_l} \right) \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j}$$

Matrix decomposition: $\boldsymbol{C}^{\text{near}} + \boldsymbol{A} \boldsymbol{D}_R \boldsymbol{A}^{\mathsf{H}}$

Coulomb Interaction in Periodic Particle Systems

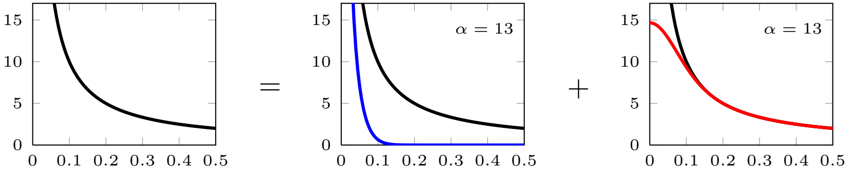
Calculation of the Potential

$$\widetilde{\phi}(\boldsymbol{x}_j) = \sum_{\boldsymbol{r}\in\mathbb{Z}^3} \sum_{l=1}^{M}{}' \frac{q_l}{\|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2}, \quad j = 1, \dots, M$$

Ewald Splitting with Error Function

$$\frac{1}{r} = \frac{1-\operatorname{erf}(\alpha r)}{r} + \frac{\operatorname{erf}(\alpha r)}{r} \quad \Rightarrow \quad \hat{b}_{\boldsymbol{k}} = \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|_2^2/\alpha^2}}{\|\boldsymbol{k}\|_2^2}$$

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



Ewald Summation

Nearfield Approximation - $\mathcal{O}(M\varepsilon_I^3) \xrightarrow{\alpha_{\text{opt}}} \mathcal{O}(M^{3/2})$

$$\widetilde{\phi}^{\text{near}}(\boldsymbol{x}_j) = -q_j \frac{2\alpha}{\sqrt{\pi}} + \sum_{\boldsymbol{r}\in\mathbb{Z}^3} \sum_{l=1}^{M}{}' q_l \frac{1-\operatorname{erf}(\alpha\|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2)}{\|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2}$$

$$\approx -q_j \frac{2\alpha}{\sqrt{\pi}} + \sum_{\boldsymbol{r}\in\mathbb{Z}^3} \sum_{l\in I_j(\boldsymbol{r})}{}' q_l \frac{1-\operatorname{erf}(\alpha\|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2)}{\|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2}$$

$$I_j(\boldsymbol{r}) := \{l = 1,\dots,M : \|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2 < \varepsilon_I\}$$

Farfield Approximation - $\mathcal{O}(MN^3) \xrightarrow{\alpha_{\text{opt}}} \mathcal{O}(M^{3/2})$

$$\widetilde{\phi}^{\text{far}}(\boldsymbol{x}_j) = \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathbb{Z}^3\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|_2^2/\alpha^2}}{\|\boldsymbol{k}\|_2^2} \sum_{l=1}^{M} q_l \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}(\boldsymbol{x}_j-\boldsymbol{x}_l)}$$

$$\approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in I_{\boldsymbol{N}}\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|_2^2/\alpha^2}}{\|\boldsymbol{k}\|_2^2} \left(\sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Fast Ewald Summation [Hedman, Laaksonen 2006]

Farfield Approximation - $\mathcal{O}(MN^3)$

$$\widetilde{\phi}^{\text{far}}(\boldsymbol{x}_j) \approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in I_{\boldsymbol{N}}\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|_2^2/\alpha^2}}{\|\boldsymbol{k}\|_2^2} \left(\sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Calculate by NFFT$^{\mathsf{H}}$ - $\mathcal{O}(\log^3(\frac{1}{\varepsilon})M + N^3 \log N)$

$$S(\boldsymbol{k}) = \sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}$$

Calculate by NFFT - $\mathcal{O}(\log^3(\frac{1}{\varepsilon})M + N^3 \log N)$

$$\sum_{\boldsymbol{k}\in I_{\boldsymbol{N}}\setminus\{\boldsymbol{0}\}} \left(\frac{1}{\pi} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|_2^2/\alpha^2}}{\|\boldsymbol{k}\|_2^2} S(\boldsymbol{k})\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomposition: $\boldsymbol{C}^{\text{near}} + \boldsymbol{A}\boldsymbol{D}_R\boldsymbol{A}^{\mathsf{H}}$

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{B}\,\boldsymbol{F}\,\boldsymbol{D}\,\boldsymbol{D}_R\,\boldsymbol{D}\,\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{B}^{\top}$$

Particle-Mesh Algorithms

- P3M [Hockney, Eastwood 1988] - periodic
- PME [Darden et al. 1993] - periodic
- SPME [Essmann et al. 1995] - periodic
- GSE [Shan et. al 2004] - periodic
- Fastsum [Nieslony, Potts, Steidl 2004] - nonperiodic
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Special Setting

$$\boldsymbol{D}_{\mathbf{opt}} = \boldsymbol{D}\,\boldsymbol{D}_R\,\boldsymbol{D}$$ Bspline window function

The Structure of Particle-Mesh Algorithms

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Special Setting

Lagrangian interpolation

The Structure of Particle-Mesh Algorithms

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$$C^{\text{near}} + B\,F\,\not{D}\,D_R\,\not{D}\,F^{\mathsf{H}}\,B^{\top}$$

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Special Setting

Bspline window function

The Structure of Particle-Mesh Algorithms

Building Blocks

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Special Setting

Gaussian window function

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\mathrm{near}} + \boldsymbol{B}\,\boldsymbol{F}\,\boldsymbol{D}\,\boldsymbol{D}_R\,\boldsymbol{D}\,\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{B}^{\top}$$

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Special Setting

$$\boldsymbol{A} = \boldsymbol{B}\,\boldsymbol{F}\,\boldsymbol{D}$$

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{B}\,\boldsymbol{F}\,\boldsymbol{D}\,\boldsymbol{D}_R\,\boldsymbol{D}\,\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{B}^{\top}$$

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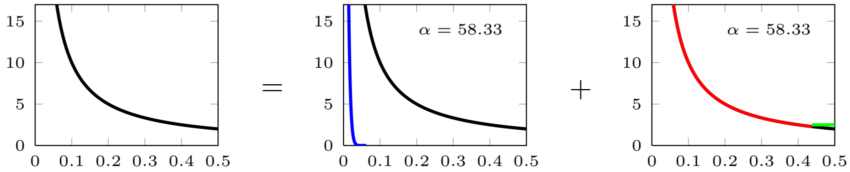
Special Setting

$$\boldsymbol{A} = \boldsymbol{B}\,\boldsymbol{F}\,\boldsymbol{D}$$

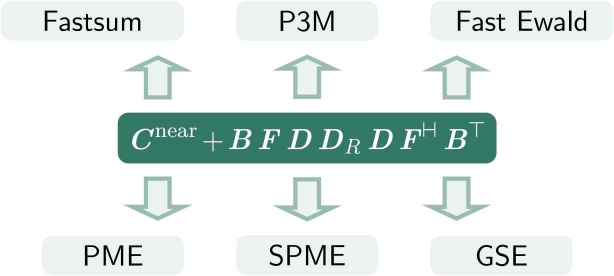
Nonperiodic Fast Ewald Summation

$$\frac{1}{r} = \color{blue}{\frac{1-\mathrm{erf}(\alpha r)}{r}} + \color{red}{\frac{\mathrm{erf}(\alpha r)}{r}}$$



		Taylor		Error function		
$\varepsilon_I = \varepsilon_B$	FFT size	p	$\lVert e \rVert_\infty$	p	α	$\lVert e \rVert_\infty$
$2/128$	128	5	$2.96 \cdot 10^{-1}$	13	124.34	$3.84 \cdot 10^{-1}$
$4/128$	128	5	$5.21 \cdot 10^{-3}$	5	85.02	$5.49 \cdot 10^{-3}$
$8/128$	128	12	$7.57 \cdot 10^{-6}$	6	58.33	$5.03 \cdot 10^{-6}$
$4/64$	64	5	$2.55 \cdot 10^{-3}$	3	42.55	$2.71 \cdot 10^{-3}$
$2/32$	32	8	$0.99 \cdot 10^{-3}$	3	21.37	$1.26 \cdot 10^{-3}$

Summary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PME
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