On the Equivalence of $\mathrm{P}^3\mathrm{M}$ and NFFT-Based Fast Summation

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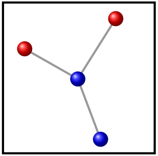
Motivation

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

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

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



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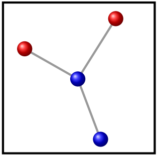

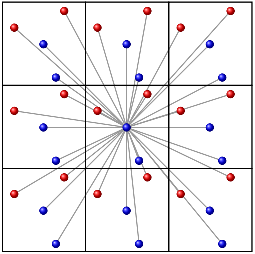

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Applications

- molecular dynamics
- astrophysics
- statistical physics
- plasma physics
- material sciences
- physical chemistry
- biophysics

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Fast Algorithms

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

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Fast Algorithms Based on Discrete Fourier Transforms

Ewald Sum	Multigrid	Tree Codes	FMM	$\mathrm{P}^3\mathrm{M}$	Fast Sum
1921	1977	1986	1987	1988	2004
$\mathcal{O}(N^{3/2})$	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$	$\mathcal{O}(N \log N)$
Ewald	Brandt	Barnes	Greengard	Hockney	Potts
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	Trottenberg				

Outline

Discrete Fourier Transforms

Task of 3d-DFT (Discrete Fourier Transform)

For $\hat{f}_{\boldsymbol{k}} \in \mathbb{C}$ compute

$$f_{\boldsymbol{l}} = \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{-2\pi \mathrm{i} (k_0 \frac{l_0}{M} + k_1 \frac{l_1}{M} + k_2 \frac{l_2}{M})}$$

for all $\boldsymbol{l} \in \mathcal{I}_M := \{0, \dots, M-1\}^3$ $\left(\Rightarrow \frac{l_0}{M}, \frac{l_1}{M}, \frac{l_2}{M} \in [0,1)\right)$.

Task of 3d-NDFT (Nonequispaced DFT)

For $\hat{f}_{\boldsymbol{k}} \in \mathbb{C}$ compute

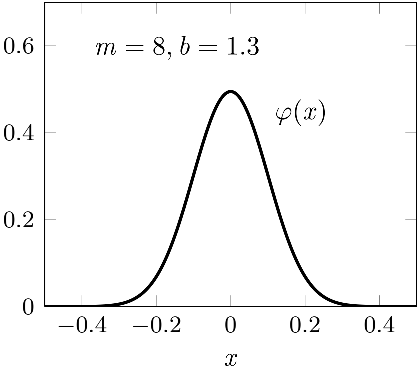
$$f_j = \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{-2\pi \mathrm{i} (k_0 x_j + k_1 y_j + k_2 z_j)}$$

for $x_j, y_j, z_j \in [0,1)$, $j = 1, \dots, N$.

Window Function

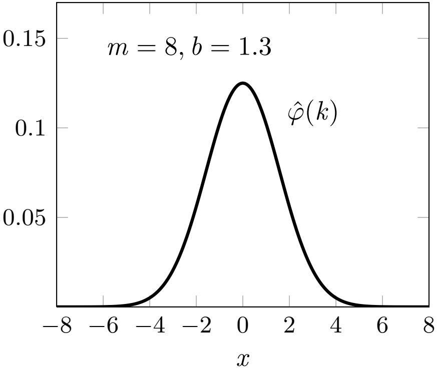
Real Space

$$\varphi(x) = \frac{1}{\sqrt{(\pi b)}} \mathrm{e}^{-\frac{(mx)^2}{b}}$$



Fourier Space

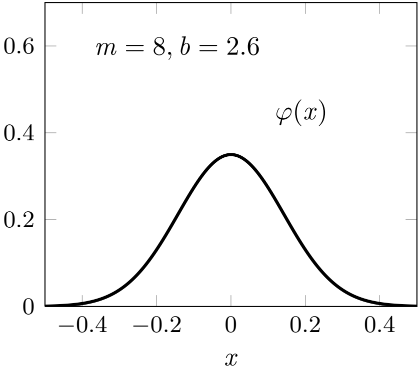
$$\hat{\varphi}(k) = \frac{1}{m} \mathrm{e}^{-b\left(\frac{\pi k}{m}\right)^2}$$



Window Function

Real Space

$$\varphi(x) = \frac{1}{\sqrt{(\pi b)}} \mathrm{e}^{-\frac{(mx)^2}{b}}$$



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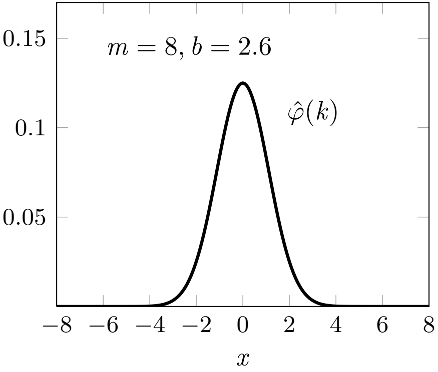

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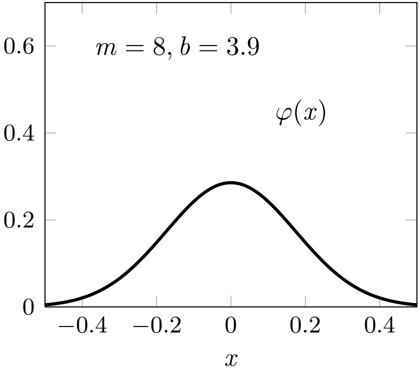
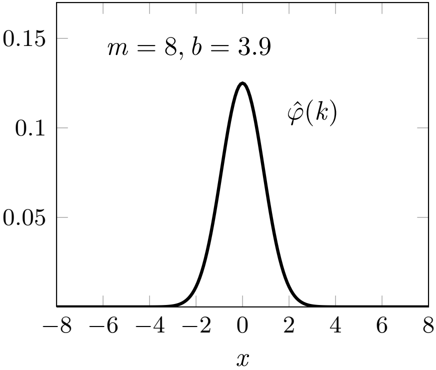




NFFT [Dutt, Rohklin 93, Beylkin 95, Steidl 96, Greengard, Lee 04, ...]

1. Deconvolution Step, $\boldsymbol{D}_\varphi \in \mathbb{R}^{M^3 \times M^3}$ $\mathcal{O}(M^3)$

$$\hat{g}_{\boldsymbol{k}} = \frac{1}{|\mathcal{I}_m|} \cdot \frac{\hat{f}_{\boldsymbol{k}}}{\hat{\varphi}(k_0)\hat{\varphi}(k_1)\hat{\varphi}(k_2)}, \quad \boldsymbol{k} \in \mathcal{I}_M$$

2. Oversampled FFT, $\boldsymbol{F} \in \mathbb{C}^{m^3 \times M^3}$ $\mathcal{O}(M^3 \log M)$

$$g_{\boldsymbol{l}} = \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{g}_{\boldsymbol{k}} \, \mathrm{e}^{-2\pi \mathrm{i}(k_0 \frac{l_0}{m} + k_1 \frac{l_1}{m} + k_2 \frac{l_2}{m})}, \quad \boldsymbol{l} \in \mathcal{I}_m, \quad M \le m$$

3. Convolution Step, $\boldsymbol{C}_\varphi \in \mathbb{R}^{N \times m^3}$ $\mathcal{O}(|\log \varepsilon|^3 N)$

$$f_j \approx \sum_{\boldsymbol{l} \in \mathcal{I}_m} \varphi\left(x_j - \tfrac{l_0}{m}\right) \varphi\left(y_j - \tfrac{l_1}{m}\right) \varphi\left(z_j - \tfrac{l_2}{m}\right) g_{\boldsymbol{l}}, \quad j = 1, \dots, N$$

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

Outline

Coulomb Interaction in Periodic Particle Systems

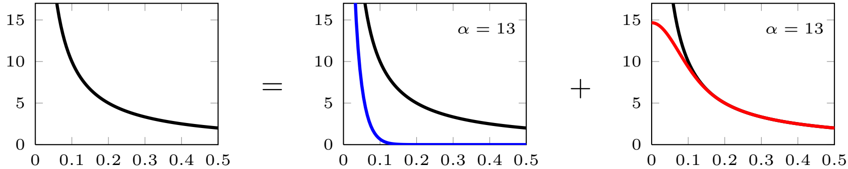
Calculation of the Potential

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

Ewald Splitting with Error Function

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

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



Ewald Summation

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

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

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

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

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

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

$$\approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \left(\sum_{l=1}^{N} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l} \right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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

$$I_j(\boldsymbol{r}) := \{l=1,\dots,N : \|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2 < R\}, \quad \nu := \max_{j,\boldsymbol{r}} |I_j(\boldsymbol{r})|$$

Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$$\widetilde{\phi}^{\text{far}}(\boldsymbol{x}_j) \approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \sum_{l=1}^{N} q_l \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}(\boldsymbol{x}_j-\boldsymbol{x}_l)}$$

$$= \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \left(\sum_{l=1}^{N} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l} \right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomp.: $\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \boldsymbol{F} \boldsymbol{D}_\varphi \boldsymbol{D}_G \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \boldsymbol{C}_\varphi^\top$ Nearfield

Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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$$= \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \left(\sum_{l=1}^{N} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l} \right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomp.: $\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \boldsymbol{F} \boldsymbol{D}_\varphi \boldsymbol{D}_G \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \boldsymbol{C}_\varphi^\top$ NFFT$^{\mathsf{H}}$

Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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

$$I_j(\boldsymbol{r}) := \{l = 1,\dots,N : \|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2 < R\}, \quad \nu := \max_{j,\boldsymbol{r}} |I_j(\boldsymbol{r})|$$

Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3\log M)$

$$\widetilde{\phi}^{\text{far}}(\boldsymbol{x}_j) \approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \sum_{l=1}^{N} q_l \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}(\boldsymbol{x}_j-\boldsymbol{x}_l)}$$

$$= \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \left(\sum_{l=1}^{N} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomp.: $\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \boldsymbol{F} \boldsymbol{D}_\varphi \boldsymbol{D}_G \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \boldsymbol{C}_\varphi^{\top}$ convolution

Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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

$$I_j(\boldsymbol{r}) := \{l=1,\dots,N : \|\boldsymbol{x}_j-\boldsymbol{x}_l+\boldsymbol{r}\|_2 < R\}, \quad \nu := \max_{j,\boldsymbol{r}} |I_j(\boldsymbol{r})|$$

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$$\widetilde{\phi}^{\text{far}}(\boldsymbol{x}_j) \approx \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \sum_{l=1}^{N} q_l \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}(\boldsymbol{x}_j-\boldsymbol{x}_l)}$$

$$= \frac{1}{\pi} \sum_{\boldsymbol{k}\in\mathcal{I}_M\setminus\{\boldsymbol{0}\}} \hat{G}(\boldsymbol{k}) \left(\sum_{l=1}^{N} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomp.: $\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \boldsymbol{F} \boldsymbol{D}_\varphi \boldsymbol{D}_G \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \boldsymbol{C}_\varphi^\top$ NFFT

P^{3}M [Hockney, Eastwood 1988]

P^{3}M Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$\boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_G^{\text{opt}}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$ Smear charges on grid

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\text{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

P^{3}M becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\text{opt}} = \operatorname{diag}\left(\hat{G}^{\text{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

P^{3}M [Hockney, Eastwood 1988]

P^{3}M Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$\boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_G^{\text{opt}}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$ Shift to Fourier space

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\text{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

P^{3}M becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\text{opt}} = \operatorname{diag}\left(\hat{G}^{\text{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

P^3M [Hockney, Eastwood 1988]

P^3M Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_G^{\mathsf{opt}} \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top$ Apply modified Green's fct.

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\mathsf{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

P^3M becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\mathsf{opt}} = \operatorname{diag}\left(\hat{G}^{\mathsf{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi$$

P^{3}M [Hockney, Eastwood 1988]

P^{3}M Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$\boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_G^{\mathsf{opt}}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$ Shift to real space

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\mathsf{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

P^{3}M becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\mathsf{opt}} = \operatorname{diag}\left(\hat{G}^{\mathsf{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

P^{3}M [Hockney, Eastwood 1988]

P^{3}M Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3\log M)$

$\boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_G^{\mathsf{opt}}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$ Interpolate from grid

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\mathsf{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k}+\frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

P^{3}M becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\mathsf{opt}} = \operatorname{diag}\left(\hat{G}^{\mathsf{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi\,\boldsymbol{D}_G\,\boldsymbol{D}_\varphi$$

$\mathrm{P}^3\mathrm{M}$ [Hockney, Eastwood 1988]

$\mathrm{P}^3\mathrm{M}$ Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$$\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_G^{\mathsf{opt}} \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top$$

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\mathsf{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a}) \hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a}) \hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

$\mathrm{P}^3\mathrm{M}$ becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\mathsf{opt}} = \operatorname{diag}\left(\hat{G}^{\mathsf{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})} \hat{G}(\boldsymbol{k}) \frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi$$

$\mathrm{P}^3\mathrm{M}$ [Hockney, Eastwood 1988]

$\mathrm{P}^3\mathrm{M}$ Farfield Approximation - $\mathcal{O}(|\log\varepsilon|^3 N + M^3 \log M)$

$$\boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_G^{\mathsf{opt}}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^{\top}$$

Optimal Green's function minimizes RMS potential error

$$\hat{G}^{\mathsf{opt}}(\boldsymbol{k}) = \frac{\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}\in\mathbb{Z}^3} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2}$$

$$\approx \frac{\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\,\hat{G}(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})}{\left[\sum_{\boldsymbol{a}=\boldsymbol{0}} \hat{\varphi}^2(\boldsymbol{k} + \frac{2\pi}{h}\boldsymbol{a})\right]^2} = \frac{\hat{G}(\boldsymbol{k})}{\hat{\varphi}^2(\boldsymbol{k})}$$

$\mathrm{P}^3\mathrm{M}$ becomes NFFT based Ewald

$$\boldsymbol{D}_G^{\mathsf{opt}} = \operatorname{diag}\left(\hat{G}^{\mathsf{opt}}(\boldsymbol{k})\right) \approx \operatorname{diag}\left(\frac{1}{\hat{\varphi}(\boldsymbol{k})}\hat{G}(\boldsymbol{k})\frac{1}{\hat{\varphi}(\boldsymbol{k})}\right) = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

Structure of P^{3}M and NFFT-Based Ewald

Different Viewpoints on the Same Algorithm

P^{3}M:

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \, \boldsymbol{F} \, \overbrace{\boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi}^{\boldsymbol{D}_G^{\text{opt}}} \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^{\top}$$

NFFT-based:

$$\boldsymbol{C}^{\text{near}} + \underbrace{\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi}_{\text{NFFT}} \, \boldsymbol{D}_G \, \underbrace{\boldsymbol{D}_\varphi \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^{\top}}_{\text{NFFT}^{\mathsf{H}}}$$

P^{3}M is a NFFT-Based Ewald Method with

- φ - B-spline window
- no oversampling, i.e., $M = m$

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_{\varphi}\,\boldsymbol{F}\,\boldsymbol{D}_{\varphi}\,\boldsymbol{D}_{G}\,\boldsymbol{D}_{\varphi}\,\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{C}_{\varphi}^{\top}$$

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
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

Window Function φ

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^{\top}$$

Particle-Mesh Algorithms

- P3M [Hockney, Eastwood 1988] - periodic
- PME [Darden et al. 1993] - periodic
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- GSE [Shan et. al 2004] - periodic
- Fastsum [Nieslony, Potts, Steidl 2004] - nonperiodic
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

$$\boldsymbol{D}_G^{\text{opt}} = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

Window Function φ

B-spline

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \cancel{\boldsymbol{D}_\varphi}\, \boldsymbol{D}_G\, \cancel{\boldsymbol{D}_\varphi}\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$$

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
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

cancel $\boldsymbol{D}_\varphi$

Window Function φ

Lagrangian interpolation

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \, \boldsymbol{F} \, \cancel{\boldsymbol{D}_\varphi} \, \boldsymbol{D}_G \, \cancel{\boldsymbol{D}_\varphi} \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top$$

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
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

cancel $\boldsymbol{D}_\varphi$

Window Function φ

B-spline

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$$

Particle-Mesh Algorithms

- P3M [Hockney, Eastwood 1988] - periodic
- PME [Darden et al. 1993] - periodic
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- GSE [Shan et. al 2004] - periodic
- Fastsum [Nieslony, Potts, Steidl 2004] - nonperiodic
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

$$\boldsymbol{D}_{G/\varphi^2} = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

Window Function φ

Gaussian

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi \, \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top$$

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
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

NFFT: $\boldsymbol{A} = \boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi$

Window Function φ

arbitrary

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\text{near}} + \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^{\top}$$

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
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

NFFT: $\boldsymbol{A} = \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_\varphi$

Window Function φ

arbitrary

The Structure of Particle-Mesh Algorithms

Building Blocks

$$\boldsymbol{C}^{\mathrm{near}} + \boldsymbol{C}_\varphi\, \boldsymbol{F}\, \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi\, \boldsymbol{F}^{\mathsf{H}}\, \boldsymbol{C}_\varphi^\top$$

Particle-Mesh Algorithms

- P3M [Hockney, Eastwood 1988] - periodic
- PME [Darden et al. 1993] - periodic
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- Fastsum [Nieslony, Potts, Steidl 2004] - nonperiodic
- NFFT-Ewald [Hedman, Laaksonen 2006] - periodic
- Spectral Ewald [Lindbo, Tornberg 2011] - periodic

Special Setting

$$\boldsymbol{D}_{G/\varphi^2} = \boldsymbol{D}_\varphi\, \boldsymbol{D}_G\, \boldsymbol{D}_\varphi$$

Window Function φ

Gaussian

Advantages of the Modularized Approach

Features of NFFT-based PM methods

- easy to use
- periodic and non-periodic boundary conditions
- arbitrary window functions
- optimal window parameters
- parallelization

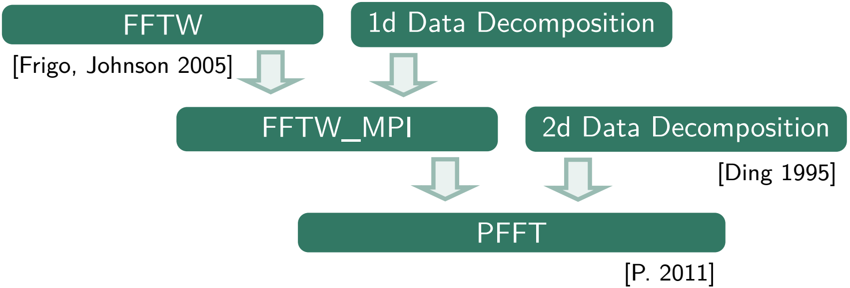
All presented (and even more) PM methods benefit from

- all NFFT features
- ongoing NFFT optimizations and improvements

Easy and fair comparison of particle-mesh methods

Outline

Highly Scalable Parallel FFT

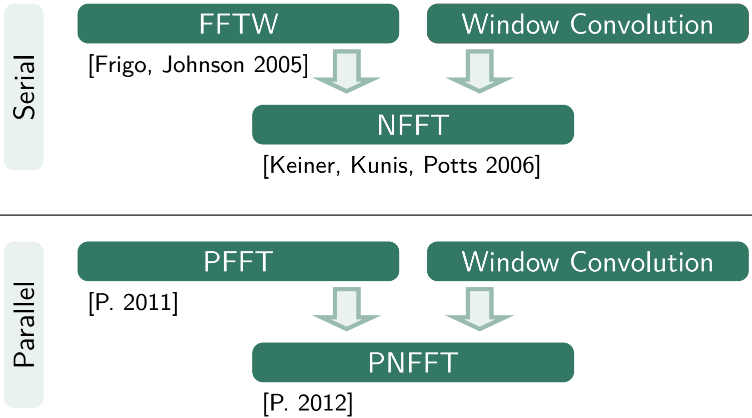


Selected PFFT Features

- open source
- high scalability
- portability
- c2c, r2c, r2r FFT
- FFTW like interface
- completely in place FFT
- d-dimensional parallel FFT
- ghost cell support

M. Pippig, *PFFT - An Extension of FFTW to Massively Parallel Architectures*,
SIAM J. Sci. Comput., 2013 (accepted)

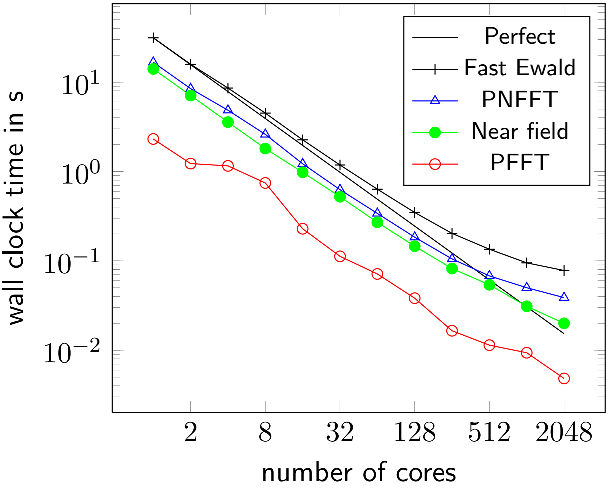
Highly Scalable Parallel NFFT



M. Pippig, D. Potts, *Parallel Three-Dimensional Nonequispaced Fast Fourier Transforms and Their Application to Particle Simulation*, Preprint Chemnitz UT, Preprint 8, 2012 (submitted to SIAM J. Sci. Comput.)

Scaling Parallel Fast Ewald on BlueGene/P

silica melt with 103680 particles: RMS-force error 1.08×10^{-5}



Parameters: $N = 128, n = 128, m = 4, R = 0.068, \alpha = 0.396$

Summary

FFT

$\boldsymbol{F}$ $\boldsymbol{F}^{\mathsf{H}}$

Summary

FFT

Window Convolution

NFFT

$$\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi \qquad \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top$$

Summary

FFT

Window Convolution

NFFT

Near-Far-Splitting

Various Particle Mesh Methods

$$\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^\top + \boldsymbol{C}^{\mathrm{near}}$$

Summary

FFT ⇩ Window Convolution ⇩

NFFT ⇩ Near-Far-Splitting ⇩

Various Particle Mesh Methods

$$\boldsymbol{C}_\varphi \, \boldsymbol{F} \, \boldsymbol{D}_\varphi \, \boldsymbol{D}_G \, \boldsymbol{D}_\varphi \boldsymbol{F}^{\mathsf{H}} \, \boldsymbol{C}_\varphi^{\top} + \boldsymbol{C}^{\mathrm{near}}$$

PFFT & PNFFT Software Library and Papers

Available at

`http://www.nfft.org`

`http://www.tu-chemnitz.de/~mpip`