Parallel Fast Computation of Coulomb Interactions Based on Nonequispaced Fourier Methods

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Motivation

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

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

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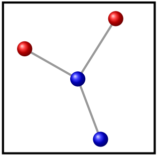

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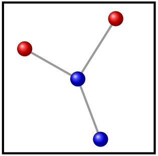

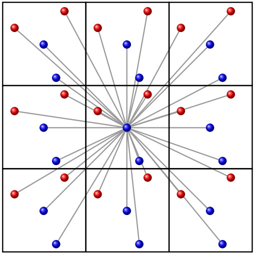

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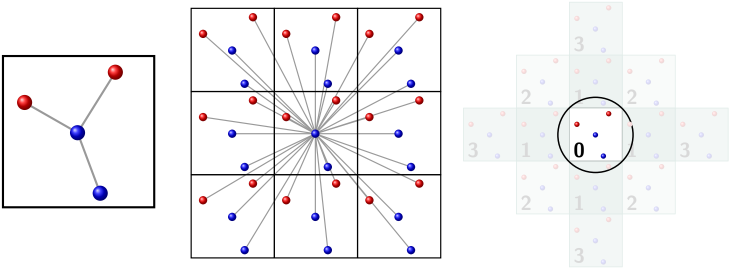

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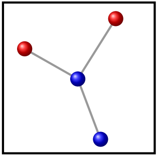

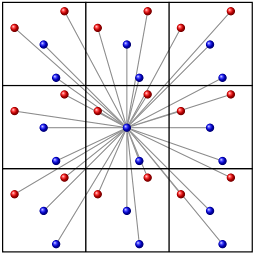

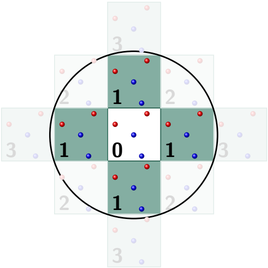

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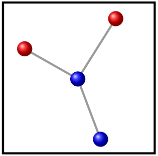

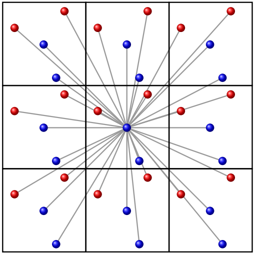

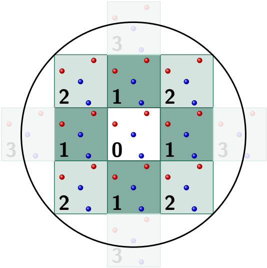

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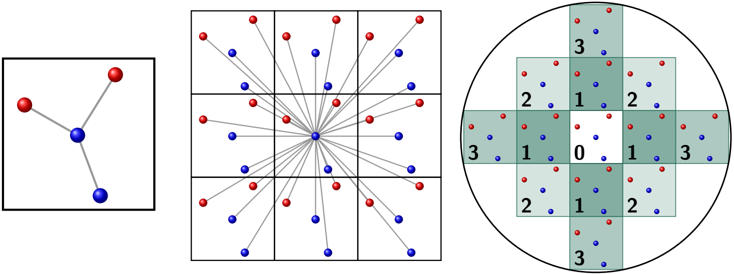

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Applications

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

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Fast Algorithms

Ewald Sum	Multigrid	Tree Codes	FMM	P^3M	Fast Sum
1921	1977	1986	1987	1988	2004
$\mathcal{O}(M^{3/2})$	$\mathcal{O}(M)$	$\mathcal{O}(M \log M)$	$\mathcal{O}(M)$	$\mathcal{O}(M \log M)$	$\mathcal{O}(M \log M)$
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	Trottenberg				Steidl

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Fast Algorithms Based on Discrete Fourier Transforms

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Outline

Discrete Fourier Transforms

Task of 3d-DFT (Discrete Fourier Transform)

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

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

for all $\boldsymbol{l} \in I_{\boldsymbol{N}} := \{0, \ldots, N-1\}^3 \ \left(\Rightarrow \frac{l_0}{N}, \frac{l_1}{N}, \frac{l_2}{N} \in [0,1)\right)$.

Task of 3d-NDFT (Nonequispaced DFT)

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

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

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

Nonequispaced Fast Fourier Transforms

Matrix-Vector-Notation of NDFT and adjont NDFT

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

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

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, ...]

$$\boldsymbol{A} \approx \boldsymbol{C}\boldsymbol{F}\boldsymbol{D}, \qquad \boldsymbol{A}^{\mathsf{H}} \approx \boldsymbol{D}\boldsymbol{F}^{\mathsf{H}}\boldsymbol{C}^{\top}$$

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

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

Highly Scalable Parallel FFT

FFTW

[Frigo, Johnson 2005]

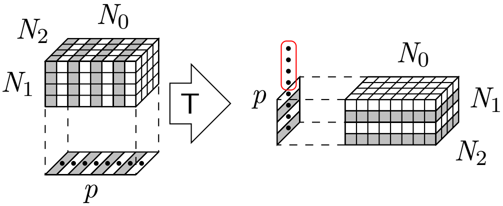
Highly Scalable Parallel FFT

FFTW

[Frigo, Johnson 2005]

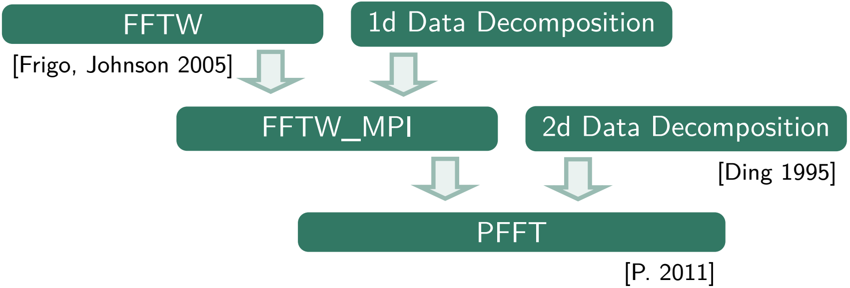
1d Data Decomposition

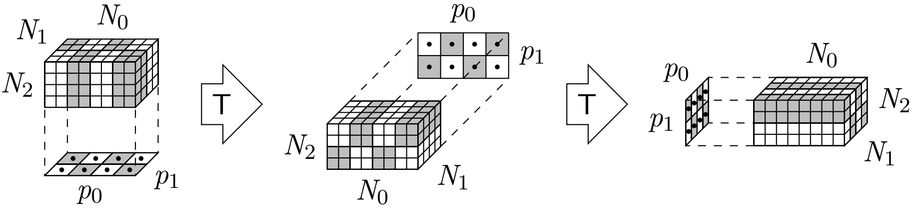
FFTW_MPI



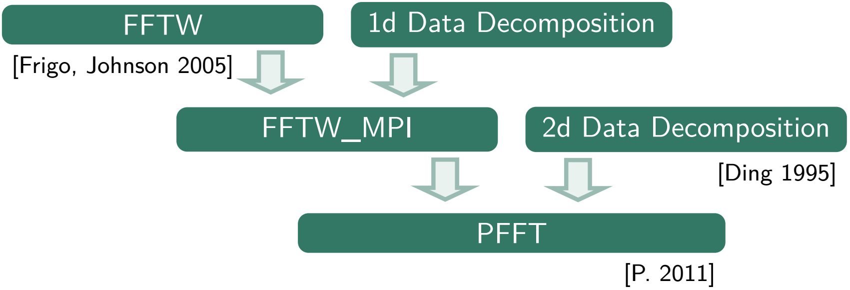
N	N^2
64	4096
128	16384
256	65536
512	262144
1024	1048576

Highly Scalable Parallel FFT





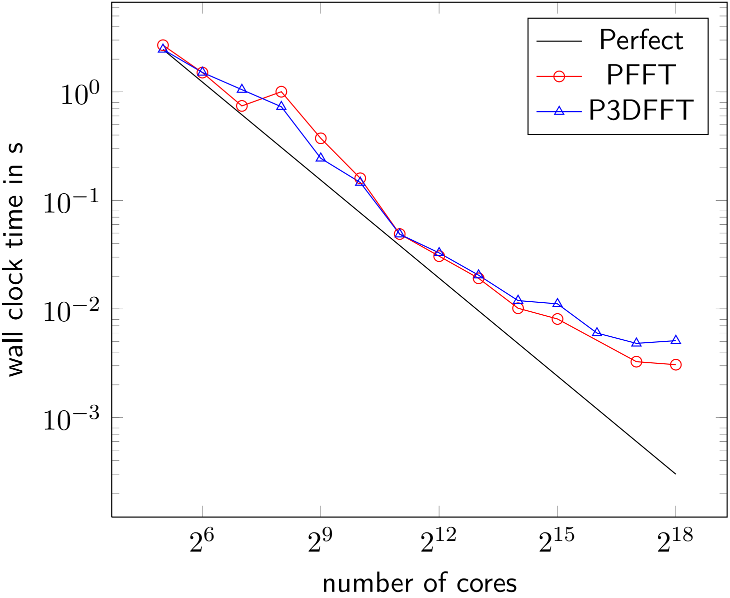
Highly Scalable Parallel FFT



PFFT Features

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

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



Highly Scalable Parallel NFFT

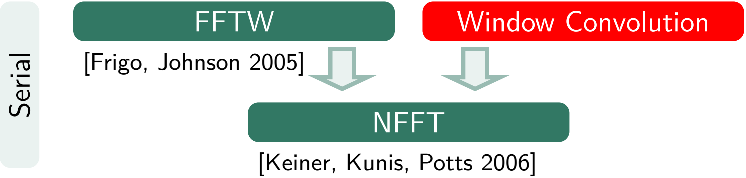
Serial

FFTW

[Frigo, Johnson 2005]

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

Highly Scalable Parallel NFFT



$$\boldsymbol{A} = \boldsymbol{C}\,\boldsymbol{F}\,\boldsymbol{D}, \quad \boldsymbol{A}^{\mathsf{H}} = \boldsymbol{D}\,\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{C}^{\top}$$

Highly Scalable Parallel NFFT

Serial

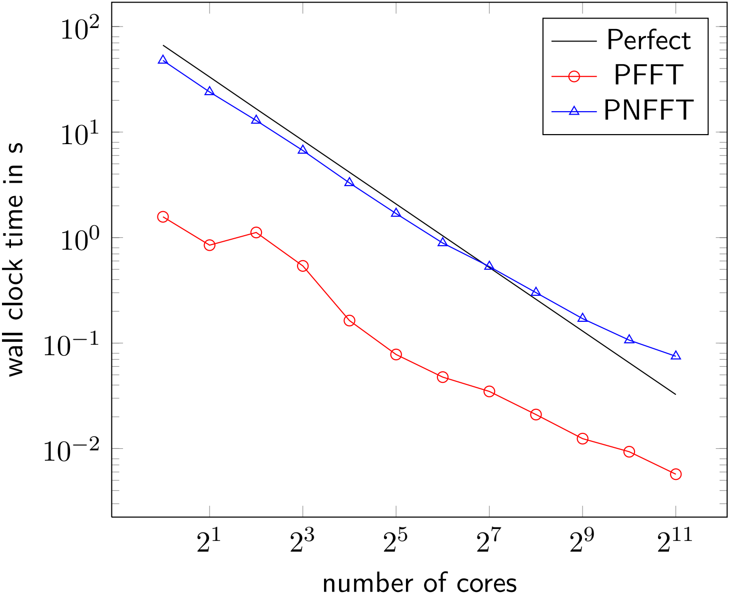
FFTW [Frigo, Johnson 2005] + Window Convolution → NFFT [Keiner, Kunis, Potts 2006]

$$A = C\,F\,D, \quad A^{\mathsf{H}} = D\,F^{\mathsf{H}}\,C^{\top}$$

Parallel

PFFT [P. 2011] + Window Convolution → PNFFT [P. 2012]

Scaling PNFFT of Size 128^3 on BlueGene/P



Outline

Coulomb Interaction in Open Particle Systems

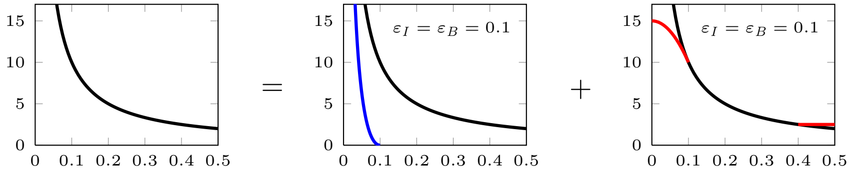
Calculation of the Potential

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

Split Kernel into Nearfield and Farfield

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

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



Fast Summation [Nieslony, Potts, Steidl 2004]

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

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

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

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

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

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

Matrix decomposition: $\boldsymbol{C}^{\text{near}} + \boldsymbol{A} \,\mathrm{diag}(\hat{R}_{\boldsymbol{k}})\, \boldsymbol{A}^{\mathsf{H}}$

Outline

Coulomb Interaction in Periodic Particle Systems

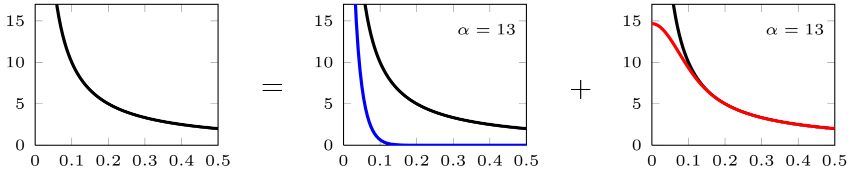
Calculation of the Potential

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

Ewald Splitting with Error Function

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

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



Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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

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

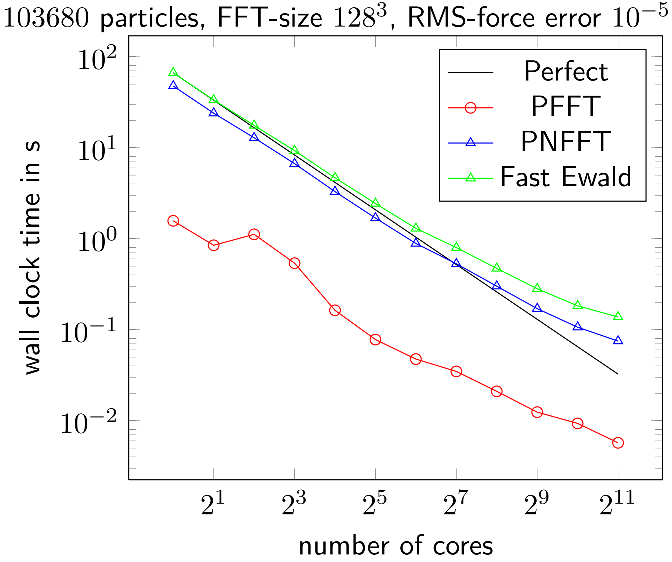
Farfield Approximation - $\mathcal{O}(\log^3(\frac{1}{\varepsilon})M + N^3\log N)$

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

$$= \frac{1}{\pi} \sum_{\boldsymbol{k}\in I_N\setminus\{\boldsymbol{0}\}} \hat{R}_{\boldsymbol{k}} \left(\sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_l}\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

Matrix decomposition: $\boldsymbol{C}^{\text{near}} + \boldsymbol{A}\,\operatorname{diag}(\hat{R}_{\boldsymbol{k}})\,\boldsymbol{A}^{\mathsf{H}}$

Scaling Parallel Fast Ewald on BlueGene/P



Summary

Parallel FFT

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

Summary

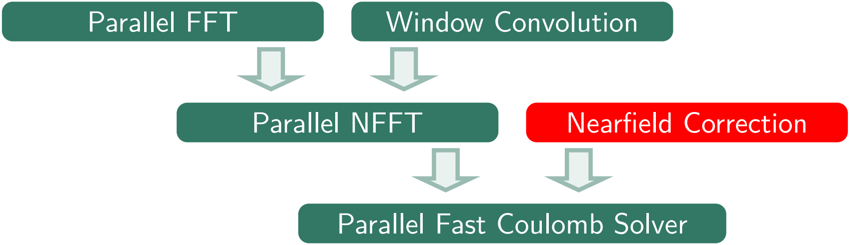
Parallel FFT

Window Convolution

Parallel NFFT

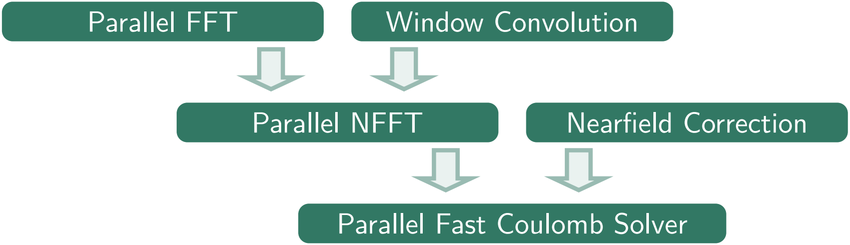
$$\boldsymbol{C}\,\boldsymbol{F}\,\boldsymbol{D} \qquad \boldsymbol{D}\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{C}^{\top}$$

Summary



$$\boldsymbol{C}\,\boldsymbol{F}\,\boldsymbol{D}\,\mathrm{diag}(\hat{R}_{\boldsymbol{k}})\;\boldsymbol{D}\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{C}^{\top} + \boldsymbol{C}^{\mathrm{near}}$$

Summary



$$\boldsymbol{C}\,\boldsymbol{F}\,\boldsymbol{D}\,\mathrm{diag}(\hat{R}_{\boldsymbol{k}})\;\boldsymbol{D}\boldsymbol{F}^{\mathsf{H}}\,\boldsymbol{C}^{\top} + \boldsymbol{C}^{\mathrm{near}}$$

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