Parallel Fast Ewald Summation Based on Nonequispaced Fourier Transforms

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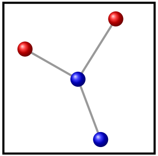
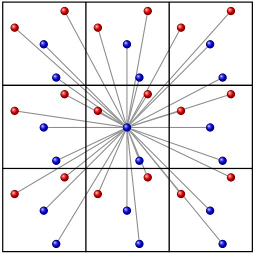
Motivation

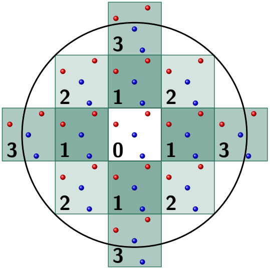
Coulomb Interaction in Particle Systems - $\mathcal{O}(M^2)$

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

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







Motivation

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

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

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Fast Algorithms

Ewald Sum	P^3MG	Tree Codes	FMM	P^3M	Fast Sum
1921	1977	1986	1987	1987	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

Outline

Fast Fourier Transform

Task of 3d-DFT

Consider a three-dimensional dataset of $n_0 \times n_1 \times n_2$ complex numbers $\hat{g}_{k_0 k_1 k_2} \in \mathbb{C}$. Compute

$$g_{l_0 l_1 l_2} := \sum_{k_0=0}^{n_0-1} \sum_{k_1=0}^{n_1-1} \sum_{k_2=0}^{n_2-1} \hat{g}_{k_0 k_1 k_2} \, \mathrm{e}^{-2\pi \mathrm{i} (k_2 \frac{l_2}{n_2} + k_1 \frac{l_1}{n_1} + k_0 \frac{l_0}{n_0})}$$

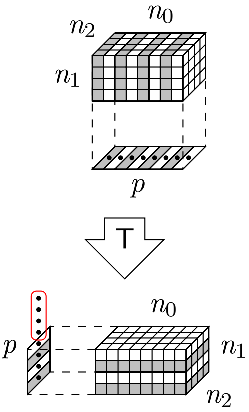
$$= \sum_{k_0=0}^{n_0-1} \left(\sum_{k_1=0}^{n_1-1} \sum_{k_2=0}^{n_2-1} \hat{g}_{k_0 k_1 k_2} \, \mathrm{e}^{-2\pi \mathrm{i} (k_2 \frac{l_2}{n_2} + k_1 \frac{l_1}{n_1})} \right) \mathrm{e}^{-2\pi \mathrm{i} k_0 \frac{l_0}{n_0}}$$

for all $l_t = 0, \ldots, n_t - 1$ $(t = 0, 1, 2)$.

Realized by 3d-FFT ($n_0 = n_1 = n_2 = n$)

$\Rightarrow \mathcal{O}(n^3 \log n)$ instead of $\mathcal{O}(n^6)$

One-Dimensional Data Distribution



p - number of processors

Features of FFTW [Frigo, Johnson]

- open source
- easy interface
- arbitrary size
- d-dim. FFT
- in place FFT
- high performance
- many transforms
- communicator
- adjust planning
- collect wisdom

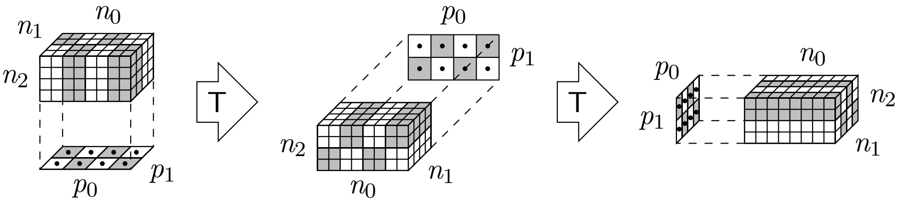
Maximum Number of Processors $p^{\mathrm{1D}}_{\max}$ $(n_0 = n_1 = n_2 = n)$

$$p^{\mathrm{1D}}_{\max} = n$$

FFTW combines portable performance and good usability, but is not scalable enough.

Two-Dimensional Data Distribution

[Ding, Eleftheriou et al. 03, Plimpton, Pekurovsky - P3DFFT]



$p_0 \times p_1$ - size of processor grid

Maximum Number of Processors $p_{\max}^{2D}$ ($n_0 = n_1 = n_2 = n$)

$$p_{\max}^{2D} = n^2$$

n	$p_{\max}^{1D} = n$	$p_{\max}^{2D} = n^2$
64	64	4096
128	128	16384
256	256	65536
512	512	262144
1024	1024	1048576

Comparison of PFFT and P3DFFT

P3DFFT Unique Features [Pekurovsky]

- r2c FFT

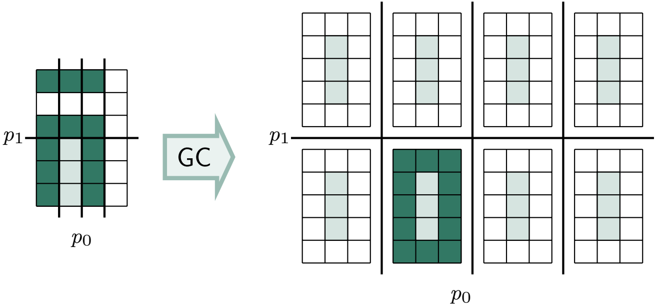
Common Features

- open source
- high scalability
- portability
- multiple precisions
- C interface
- Fortran interface
- ghost cell support

PFFT Unique Features

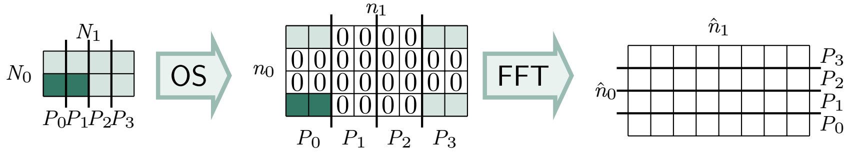
- c2c FFT
- completely in place FFT
- FFTW like interface (basic, advanced and guru)
- adjustable blocksize
- separate communicator
- accumulated wisdom
- change of planning effort without recompilation
- d-dimensional parallel FFT
- over- and downsampling

Ghost Cell Support

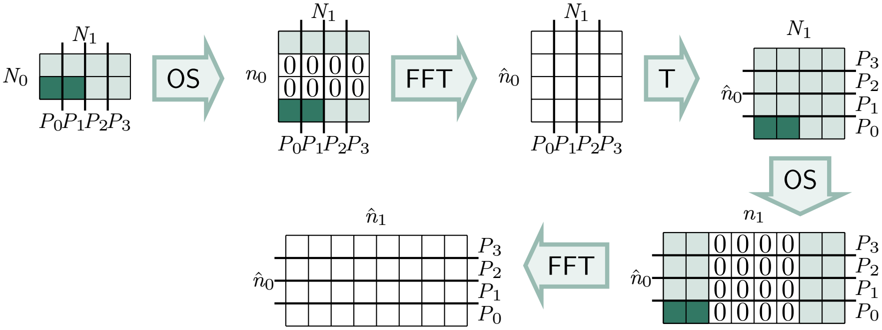


Oversampled & Downsampled FFT

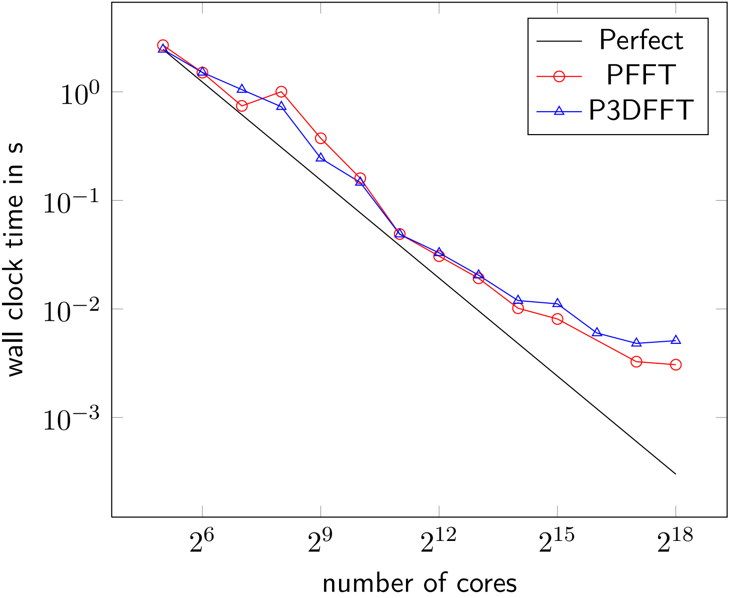
Without Library Support



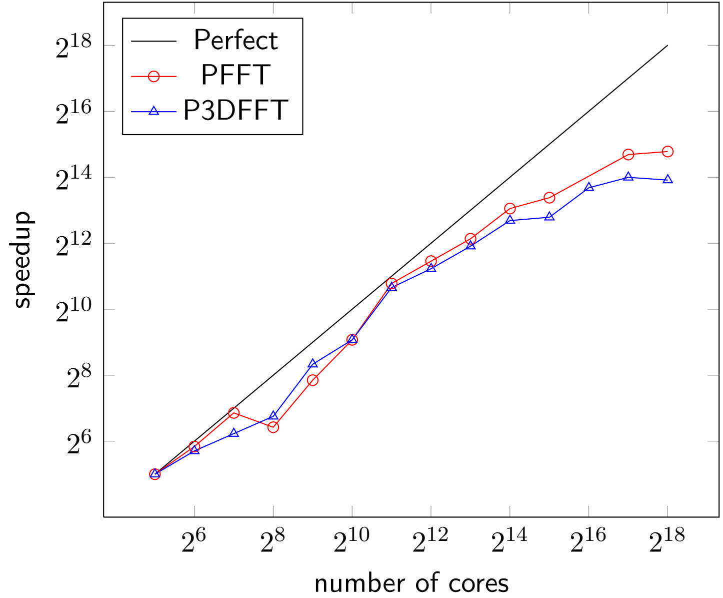
PFFT Library Support



Scaling PFFT of Size 512^3 on BlueGene/P



Scaling PFFT of Size 512^3 on BlueGene/P



Outline

Nonequispaced Discrete Fourier Transform

Task of 3d-DFT and 3d-NDFT

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

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

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

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

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

Nonequispaced Discrete Fourier Transforms

Task of 3d-NDFT and 3d-NDFT$^{\mathsf{H}}$

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

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

for $x_j, y_j, z_j \in [0, 1)$, $j = 1, \ldots, M$, and for $h_j \in \mathbb{C}$ compute

$$\hat{h}_{k_0 k_1 k_2} = \sum_{j=1}^{M} h_j \, \mathrm{e}^{+2\pi \mathrm{i}(k_2 z_j + k_1 y_j + k_0 x_j)} \qquad (\text{NDFT}^{\mathsf{H}})$$

for $z_j, y_j, x_j \in [0, 1)$, $k_0, k_1, k_2 \in \{0, \ldots, N-1\}$.

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

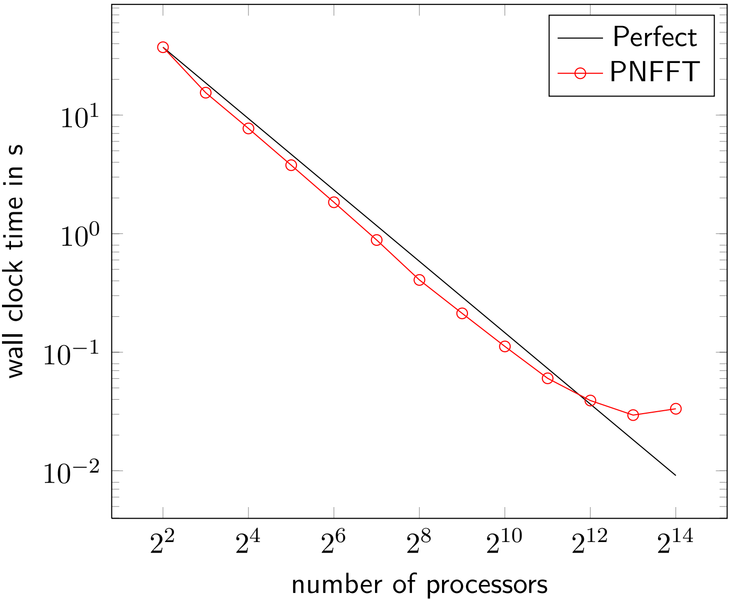
NFFT [Dutt, Rohklin 93, Beylkin 95, Steidl 96, . . .]

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

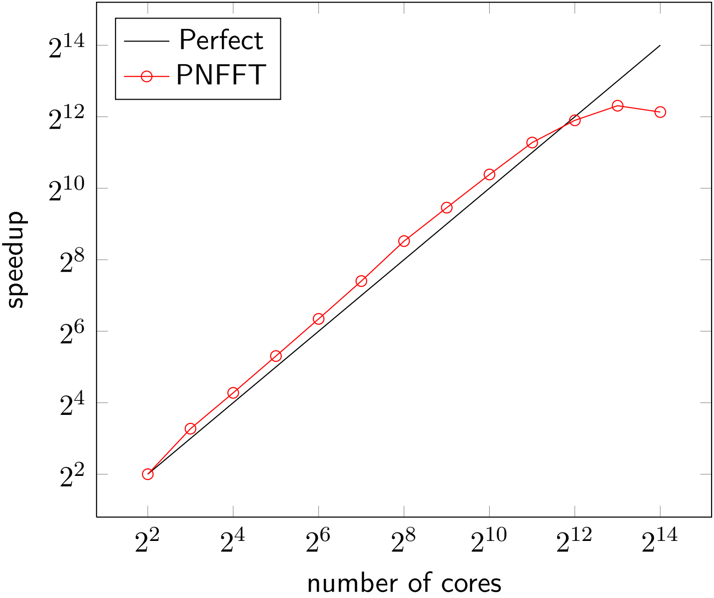
- $\boldsymbol{D} \in \mathbb{R}^{N^3 \times N^3}$ diagonal matrix
- $\boldsymbol{F} \in \mathbb{C}^{n^3 \times N^3}$ truncated Fourier matrix ($n \geq N$)
- $\boldsymbol{B} \in \mathbb{R}^{M \times n^3}$ sparse matrix

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

Scaling PNFFT of Size 128^3 on BlueGene/P



Scaling PNFFT of Size 128^3 on BlueGene/P



Outline

Coulomb Interaction in Periodic Particle Systems

Calculation of the Potential

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

- conditionally convergent
- computational work is $\mathcal{O}(M^2)$

Ewald Splitting

$$\frac{1}{r} = \frac{1 - f(r)}{r} + \frac{f(r)}{r} \quad \Rightarrow \quad \widetilde{\phi} = \widetilde{\phi}^{\text{real}} + \widetilde{\phi}^{\text{reci}}$$

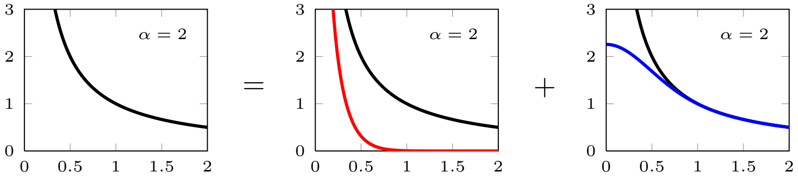
- $\frac{1-f(r)}{r}$ converges fast in real space
- $\frac{f(r)}{r}$ converges fast in reciprocal space and $\lim_{r\to 0} \frac{f(r)}{r}$ exists

Ewald Splitting with Error Function

Error Function

$$f(r) = \mathrm{erf}(\alpha r) = \frac{2}{\sqrt{\pi}} \int_0^r \mathrm{e}^{-t^2} \mathrm{d}t, \qquad \lim_{r \to 0} \frac{\mathrm{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}}$$

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



Ewald Summation

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

$$\begin{aligned}
\widetilde{\phi}^{\text{real}}(\boldsymbol{x}_j) &= -2q_j \frac{\alpha}{\sqrt{\pi}} + \sum_{\boldsymbol{r} \in \mathbb{Z}^3} {\sum_{l=1}^{M}}' q_l \frac{\operatorname{erfc}(\alpha \|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2)}{\|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2} \\
&\approx -2q_j \frac{\alpha}{\sqrt{\pi}} + \sum_{\boldsymbol{r} \in I_{\boldsymbol{R}}} \sum_{l=1}^{M} q_l \frac{\operatorname{erfc}(\alpha \|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2)}{\|\boldsymbol{x}_j - \boldsymbol{x}_l + \boldsymbol{r}\|_2}
\end{aligned}$$

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

$$\begin{aligned}
\widetilde{\phi}^{\text{reci}}(\boldsymbol{x}_j) &= \frac{1}{\pi} \sum_{\boldsymbol{k} \in \mathbb{Z}^3 \setminus \{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2 \|\boldsymbol{k}\|_2^2 / \alpha^2}}{\|\boldsymbol{k}\|_2^2} \sum_{l=1}^{M} q_l \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}(\boldsymbol{x}_j - \boldsymbol{x}_l)} \\
&\approx \frac{1}{\pi} \sum_{\boldsymbol{k} \in I_{\boldsymbol{N}} \setminus \{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2 \|\boldsymbol{k}\|_2^2 / \alpha^2}}{\|\boldsymbol{k}\|_2^2} \left(\sum_{l=1}^{M} q_l \mathrm{e}^{+2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_l} \right) \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j}
\end{aligned}$$

Fast Ewald Summation [Hedman, Laaksonen 2006]

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

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

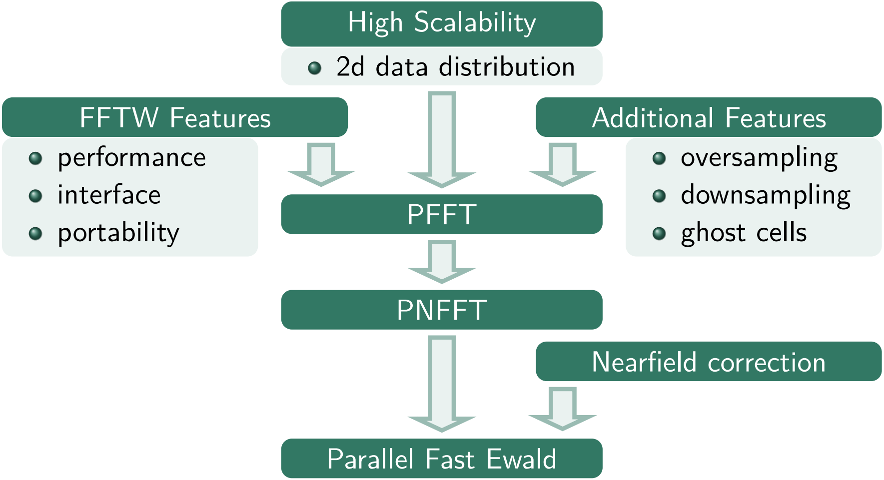
Calculate by NFFT$^{\mathsf{H}}$ - $\mathcal{O}(\log^3(\frac{1}{\varepsilon})M + N^3 \log N)$

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

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

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

Summary



PFFT & PNFFT Software Library and Papers

Available at

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