Software Libraries for Fast Fourier Transforms and Applications

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September 11, 2013

supported by the German Ministery of Science and Education (BMBF)
under grant 01IH08001

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2. Parallel FFT Algorithms
3. Particle-Particle–NFFT

Discrete Fast Fourier Transform

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

Realized by 3d-FFT

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

FFT Software Libraries

Popular FFT Implementations

- IBM ESSL
- Intel MKL
- FFTW

Features of FFTW [Frigo, Johnson 2005]

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

Available at
`http://www.fftw.org`

Using FFTW

FFTW workflow

Plan - only once

- hardware adaptive
- time consuming

Execute - several times

- fast transform

Finalize - only once

- free memory

FFTW_ESTIMATE

- heuristic choice of algorithm

FFTW_MEASURE

- compare different algorithms

FFTW_PATIENT

- compare more algorithms

FFTW_EXHAUSTIVE

- compare all available algorithms

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

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

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

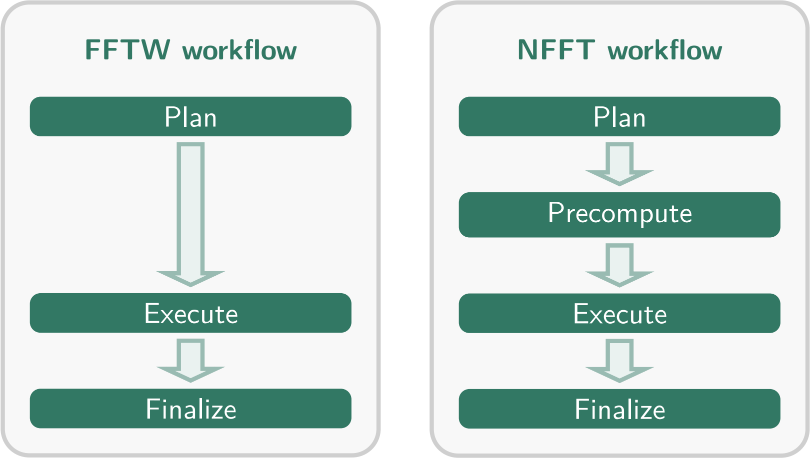
$$g_{\boldsymbol{l}} = \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{g}_{\boldsymbol{k}}\, \mathrm{e}^{-2\pi \mathrm{i}(k_0 \frac{l_0}{m} + k_1 \frac{l_1}{m} + k_2 \frac{l_2}{m})}\,, \quad \boldsymbol{l} \in \mathcal{I}_m, \quad M \le m$$

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 $\mathcal{O}(M^3 N)$

NFFT Software Library [Keiner, Kunis, Potts 06]



FFTW workflow

Plan

Execute

Finalize

NFFT workflow

Plan

Precompute

Execute

Finalize

Download NFFT Software Library at

`http://www.tu-chemnitz.de/~potts/nfft`

NFFT Precompute

PRE_FULL_PSI

- fully precomputed window function
- Storage: $(2p+2)^d N$, Computation: None

PRE_PSI

- tensor product based precomputation
- Storage: $d(2p+2)N$, Computation: $(2p+2)^d N$

PRE_LIN_PSI

- linear interpolation from lookup table
- Storage: dK, Computation: $2(2p+2)^d M$

PRE_FG_PSI

- fast Gaussian gridding
- Storage: $2dN$, Computation: $(2p+2)^d N$

Outline

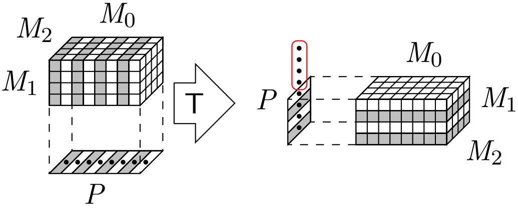
1. Serial FFT Algorithms
2. **Parallel FFT Algorithms**
3. Particle-Particle–NFFT

Highly Scalable Parallel FFT

FFTW

[Frigo, Johnson 05]

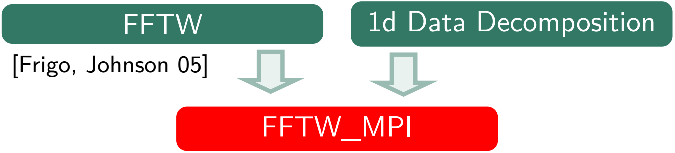
1d Data Decomposition



Maximum Number of Processes $P^{\mathrm{1D}}_{\max}$
$(M_0 = M_1 = M_2 = M)$

$$P^{\mathrm{1D}}_{\max} = M$$

Highly Scalable Parallel FFT

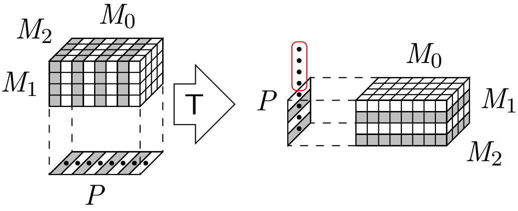


FFTW

[Frigo, Johnson 05]

1d Data Decomposition

FFTW_MPI



Maximum Number of Processes $P^{\mathrm{1D}}_{\max}$
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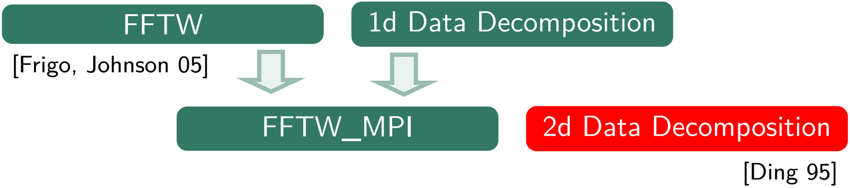
Highly Scalable Parallel FFT



FFTW

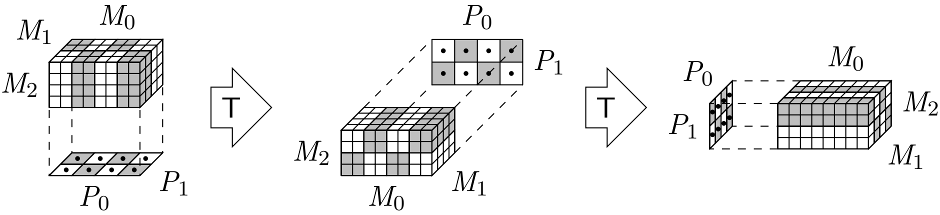
[Frigo, Johnson 05]

1d Data Decomposition

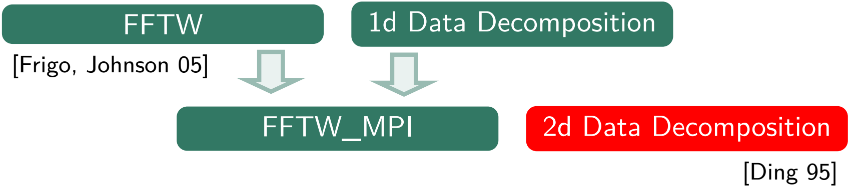
FFTW_MPI

2d Data Decomposition

[Ding 95]



Highly Scalable Parallel FFT



FFTW

[Frigo, Johnson 05]

1d Data Decomposition

FFTW_MPI

2d Data Decomposition

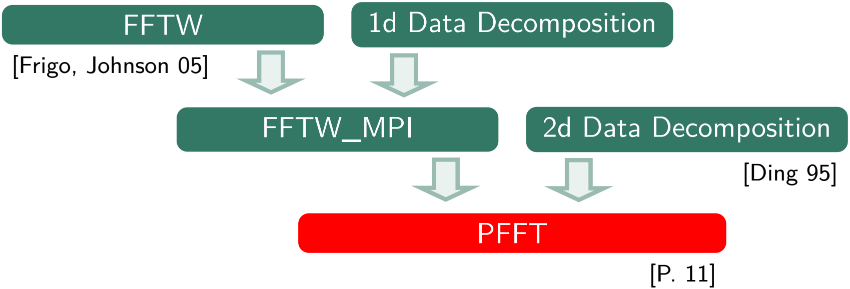
[Ding 95]

Maximum Number of Processes $P^{\mathbf{2D}}_{\max}$
$(M_0 = M_1 = M_2 = M)$

$$P^{\mathrm{2D}}_{\max} = M^2$$

M	$P^{\mathrm{1D}}_{\max} = M$	$P^{\mathrm{2D}}_{\max} = M^2$
64	64	4096
128	128	16384
256	256	65536
512	512	262144
1024	1024	1048576

Highly Scalable Parallel FFT



FFTW

[Frigo, Johnson 05]

1d Data Decomposition

FFTW_MPI

2d Data Decomposition

[Ding 95]

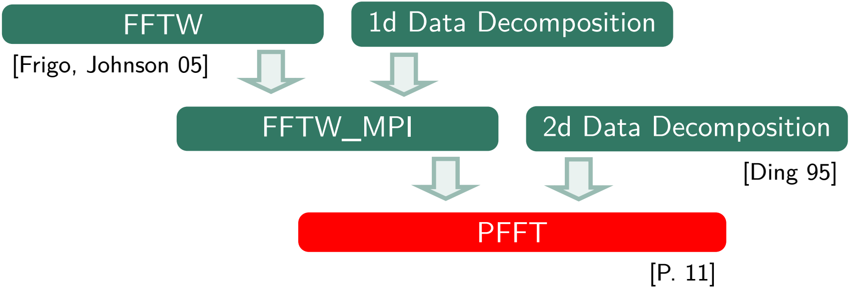
PFFT

[P. 11]

Selected PFFT Features

- open source
- high scalability
- portability
- c2c, r2c, r2r FFT
- pruned FFT
- FFTW like interface
- completely in place FFT
- d-dim. parallel FFT
- r-dim. data decomposition
- ghost cell support

Highly Scalable Parallel FFT



FFTW

[Frigo, Johnson 05]

1d Data Decomposition

FFTW_MPI

2d Data Decomposition

[Ding 95]

PFFT

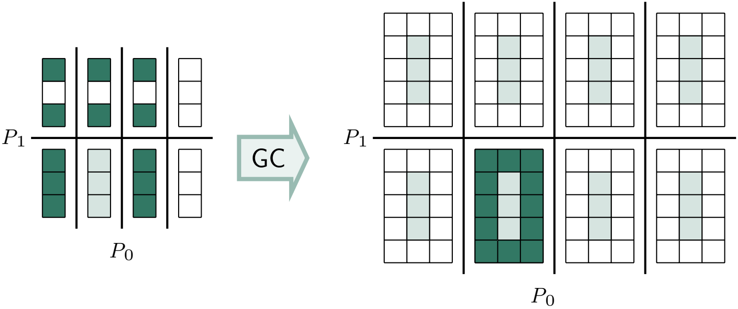
[P. 11]

Download PFFT Software Library at

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

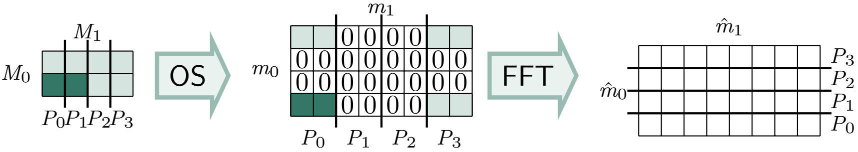
M. Pippig, *PFFT - An Extension of FFTW to Massively Parallel Architectures*, SIAM J. Sci. Comput., 35(3), C213-C236, 2013.

Ghost Cell Support

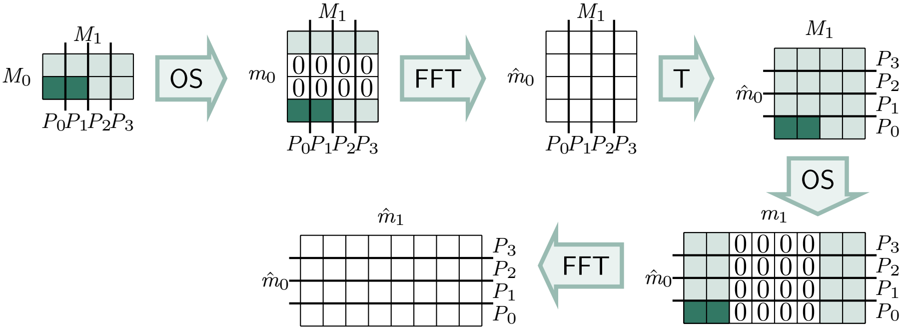


Parallel Pruned FFT

Without Library Support



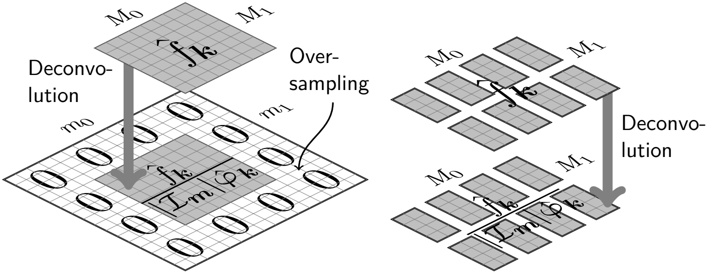
PFFT Library Support



Parallel NFFT [P., Potts 13]

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

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



Deconvolution

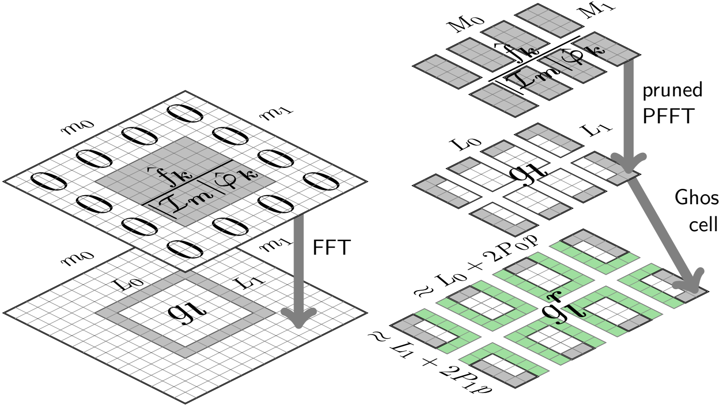
Oversampling

Deconvolution

Parallel NFFT [P., Potts 13]

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

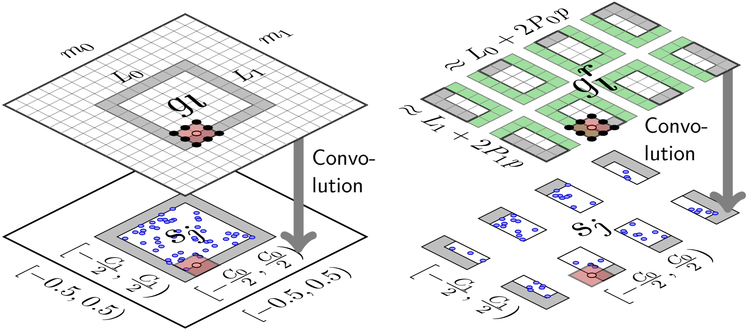
$$g_{\boldsymbol{l}} = \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{g}_{\boldsymbol{k}} \, \mathrm{e}^{-2\pi \mathrm{i} (k_0 \frac{l_0}{m} + k_1 \frac{l_1}{m} + k_2 \frac{l_2}{m})}, \quad \boldsymbol{l} \in \mathcal{I}_L, \quad M, L \leq m$$



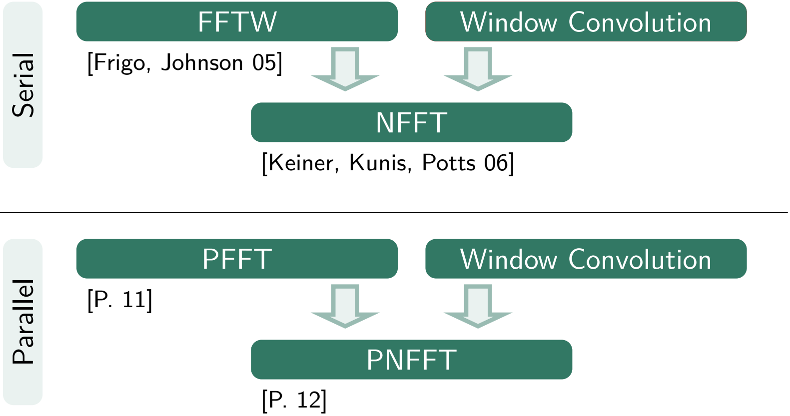
Parallel NFFT [P., Potts 13]

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

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



Highly Scalable Parallel NFFT



Serial

FFTW

[Frigo, Johnson 05]

Window Convolution

NFFT

[Keiner, Kunis, Potts 06]

Parallel

PFFT

[P. 11]

Window Convolution

PNFFT

[P. 12]

M. Pippig, D. Potts, *Parallel Three-Dimensional Nonequispaced Fast Fourier Transforms and Their Application to Particle Simulation*, SIAM J. Sci. Comput., 35(4), C411–C437, 2013.

Outline

1. Serial FFT Algorithms

2. Parallel FFT Algorithms

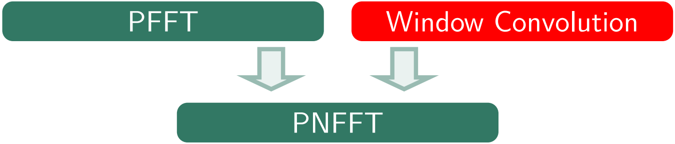
3. **Particle-Particle–NFFT**

The P^{2}NFFT Framework

PFFT

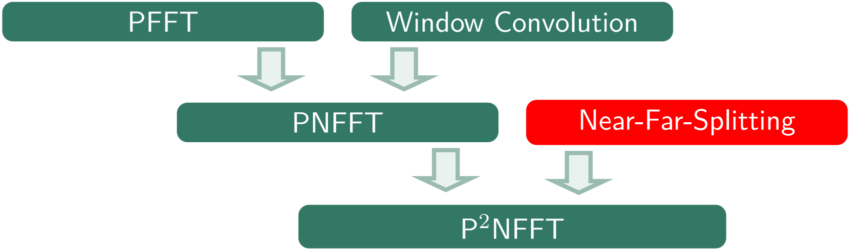
$\boldsymbol{F}$ $\boldsymbol{F}^{\mathsf{H}}$

The P^{2}NFFT Framework



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

The P^{2}NFFT Framework



PFFT

Window Convolution

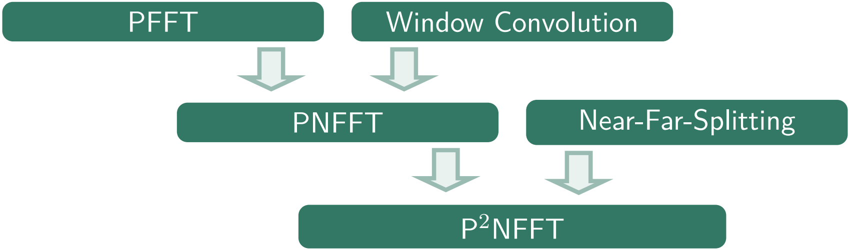
PNFFT

Near-Far-Splitting

P^{2}NFFT

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

The P^{2}NFFT Framework



PFFT

Window Convolution

PNFFT

Near-Far-Splitting

P^{2}NFFT

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

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] - 3dp
- PME [Darden et al. 1993] - 3dp
- SPME [Essmann et al. 1995] - 3dp
- GSE [Shan et. al 2004] - 3dp
- Fastsum [Nieslony, Potts, Steidl 2004] - 0dp
- NFFT-Ewald [Hedman, Laaksonen 2006] - 3dp
- Spectral Ewald [Lindbo, Tornberg 2011, 2012] - 3dp, 2dp
- 1dp/2dp NFFT-Ewald [N., P., Potts 2013] - 1dp, 2dp

Special Setting

Window Function φ

The Structure of Particle-Mesh Algorithms

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

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

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Special Setting

cancel $\boldsymbol{D}_\varphi$

Window Function φ

Lagrangian interpolation

The Structure of Particle-Mesh Algorithms

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

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Special Setting

cancel $\boldsymbol{D}_\varphi$

Window Function φ

B-spline

The Structure of Particle-Mesh Algorithms

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

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

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

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Special Setting

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Window Function φ

Gaussian

The Structure of Particle-Mesh Algorithms

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Window Function φ

arbitrary

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- NFFT-Ewald [Hedman, Laaksonen 2006] - 3dp
- Spectral Ewald [Lindbo, Tornberg 2011, 2012] - 3dp, 2dp
- 1dp/2dp NFFT-Ewald [N., P., Potts 2013] - 1dp, 2dp

Special Setting

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

Window Function φ

arbitrary

Advantages of the Modularized Approach

Features of the P^{2}NFFT Framework

- one implementation includes all particle-mesh methods
- mixed periodic boundary conditions

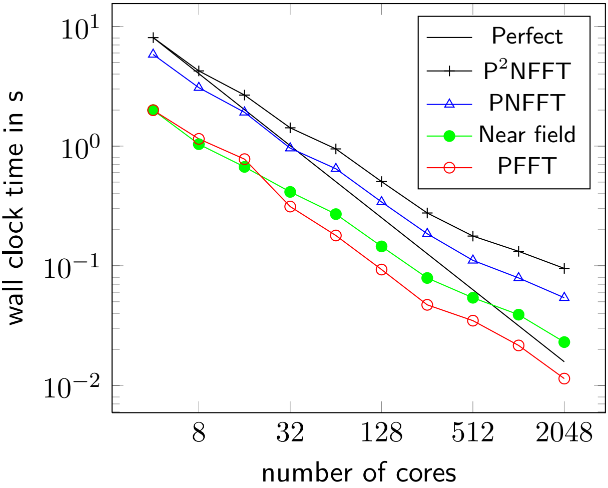
All Presented (and even more) PM Methods Benefit from

- parallelization
- arbitrary window functions
- $\mathrm{i}\boldsymbol{k}$ and analytic differentiation
- interlaced NFFT
- precomputed window functions
- ongoing NFFT optimizations and improvements

Easy and fair comparison of particle-mesh methods

Scaling Parallel 0dp-P^2NFFT on BlueGene/P

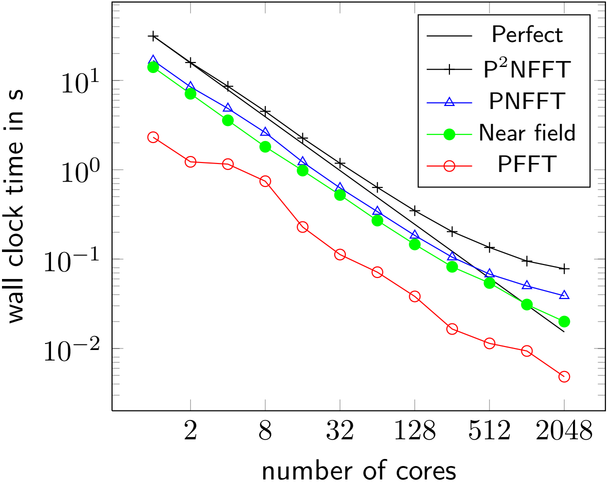
silica melt with $N = 103680$ particles: RMS-force error 2.03×10^{-5}



Parameters: $M = 256, m = 288, p = 4, \varepsilon_I = \varepsilon_B = 0.016$

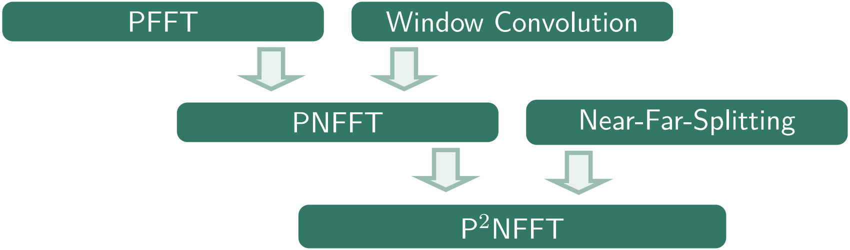
Scaling Parallel 3dp-P^{2}NFFT on BlueGene/P

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



Parameters: $M = 128, m = 128, p = 4, \varepsilon_I = 0.068, \alpha = 0.396$

Summary



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

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