An Efficient and Flexible Parallel FFT Implementation Based on FFTW

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Discrete 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

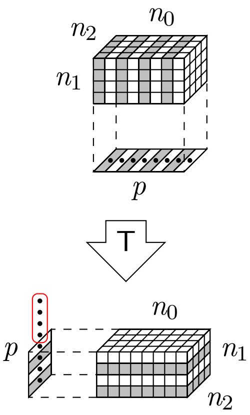
$$\begin{aligned} g_{l_0 l_1 l_2} &:= \sum_{k_0=0}^{n_0-1} \sum_{k_1=0}^{n_1-1} \sum_{k_2=0}^{n_2-1} \hat{g}_{k_0 k_1 k_2} \, \mathrm{e}^{-2\pi\mathrm{i}(k_2 \frac{l_2}{n_2} + k_1 \frac{l_1}{n_1} + k_0 \frac{l_0}{n_0})} \\ &= \sum_{k_0=0}^{n_0-1} \left(\sum_{k_1=0}^{n_1-1} \sum_{k_2=0}^{n_2-1} \hat{g}_{k_0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

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
- communicator
- arbitrary size
- d-dim. FFT
- in place FFT
- high performance
- many transforms
- adjust blocksize
- adjust planning
- collect wisdom

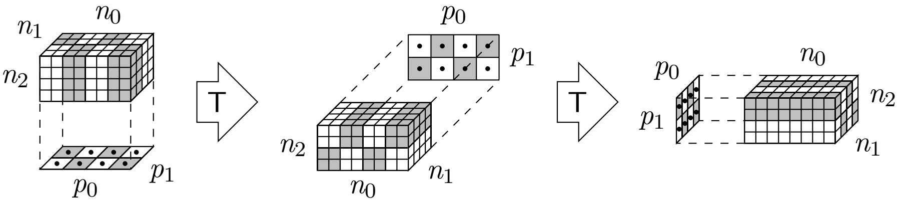
Maximum Number of Processors $p_{\max}^{1\mathrm{D}}$ $(n_0 = n_1 = n_2 = n)$

$$p_{\max}^{1\mathrm{D}} = n$$

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^{2D}_{max} $(n_0 = n_1 = n_2 = n)$

$$p^{2D}_{max} = n^2$$

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

Algorithms Supported by FFTW3.3alpha1

Aim

Implement a new parallel FFT sofware library (PFFT) based on FFTW and the highly scalable two-dimensional data distribution.

1d-FFT Combined with Local Transposition

$$
\begin{aligned}
\hat{n}_0 \times \hat{n}_1 \times \hat{n}_2 \quad &\underset{012}{\overset{\text{FFT2}}{\longrightarrow}} \quad \hat{n}_0 \times \hat{n}_1 \times n_2 \\
\hat{n}_0 \times \hat{n}_1 \times \hat{n}_2 \quad &\underset{102}{\overset{\text{FFT2}}{\longrightarrow}} \quad \hat{n}_1 \times \hat{n}_0 \times n_2 \\
\hat{n}_0 \times \hat{n}_1 \times \hat{n}_2 \quad &\underset{021}{\overset{\text{FFT2}}{\longrightarrow}} \quad \hat{n}_0 \times n_2 \times \hat{n}_1 \\
(\hat{n}_0 \times \hat{n}_1) \times \hat{n}_2 \quad &\underset{201}{\overset{\text{FFT2}}{\longrightarrow}} \quad n_2 \times (\hat{n}_0 \times \hat{n}_1)
\end{aligned}
$$

Algorithms Supported by FFTW3.3alpha1

Transposition of One-Dimensional Distributed Data

$$N_0 \times \frac{N_1}{P} \quad \xrightarrow{\mathsf{T}} \quad \frac{N_0}{P} \times N_1$$

Group two of the three dimensions to use FFTWs matrix transposition on two-dimensional decomposed data, e.g. $N_0 = n_2, N_1 = n_0 \times \frac{n_1}{p_1}, P = p_0$.

Transposition of Two-Dimensional Distributed Data

$$n_2 \times \left(\frac{n_0}{p_0} \times \frac{n_1}{p_1}\right) \quad \xrightarrow{\mathsf{T}} \quad \frac{n_2}{p_0} \times \left(n_0 \times \frac{n_1}{p_1}\right)$$

Two-Dimensional Distributed FFT Based on FFTW

PFFT Forward Transform

$$\frac{\hat{n}_0}{p_0} \times \frac{\hat{n}_1}{p_1} \times \hat{n}_2 \quad \underset{201}{\overset{\text{FFT2}}{\longrightarrow}} \quad n_2 \times \frac{\hat{n}_0}{p_0} \times \frac{\hat{n}_1}{p_1} \quad \overset{\text{T}}{\longrightarrow}$$

$$\frac{n_2}{p_1} \times \frac{\hat{n}_0}{p_0} \times \hat{n}_1 \quad \underset{201}{\overset{\text{FFT2}}{\longrightarrow}} \quad n_1 \times \frac{n_2}{p_1} \times \frac{\hat{n}_0}{p_0} \quad \overset{\text{T}}{\longrightarrow}$$

$$\frac{n_1}{p_0} \times \frac{n_2}{p_1} \times \hat{n}_0 \quad \underset{102}{\overset{\text{FFT2}}{\longrightarrow}} \quad \frac{n_2}{p_1} \times \frac{n_1}{p_0} \times n_0$$

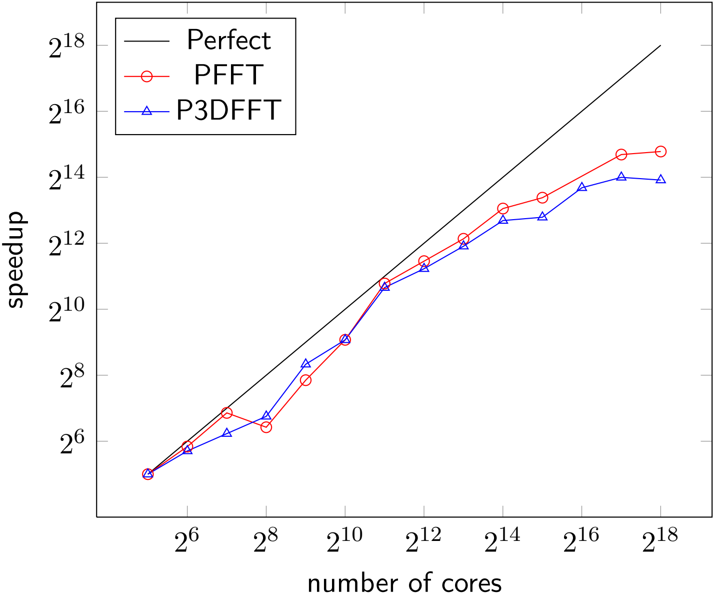
PFFT Backward Transform

$$\frac{n_2}{p_1} \times \frac{n_1}{p_0} \times n_0 \quad \underset{201}{\overset{\text{FFT2}}{\longrightarrow}} \quad \hat{n}_0 \times \frac{n_2}{p_1} \times \frac{n_1}{p_0} \quad \overset{\text{T}}{\longrightarrow}$$

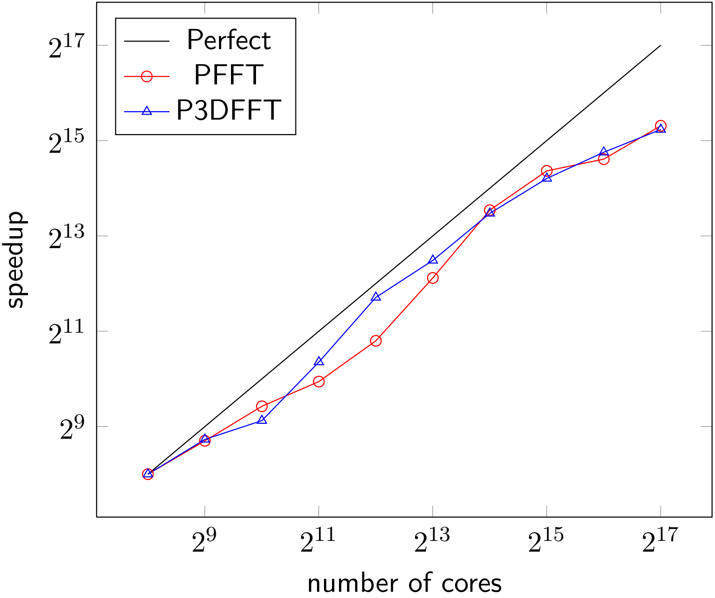
$$\frac{\hat{n}_0}{p_0} \times \frac{n_2}{p_1} \times n_1 \quad \underset{201}{\overset{\text{FFT2}}{\longrightarrow}} \quad \hat{n}_1 \times \frac{\hat{n}_0}{p_0} \times \frac{n_2}{p_1} \quad \overset{\text{T}}{\longrightarrow}$$

$$\frac{\hat{n}_1}{p_1} \times \frac{\hat{n}_0}{p_0} \times n_2 \quad \underset{102}{\overset{\text{FFT2}}{\longrightarrow}} \quad \frac{\hat{n}_0}{p_0} \times \frac{\hat{n}_1}{p_1} \times \hat{n}_2$$

Scaling FFT of Size 512^3 on BlueGene/P



Scaling FFT of Size 1024^3 on BlueGene/P



Comparison of PFFT and P3DFFT

P3DFFT Unique Features [Pekurovsky]

- r2c FFT
- Fortran interface

Common Features

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

PFFT Unique Features

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

Non-Equispaced Discrete Fourier Transform

Task of 3d-DFT and 3d-NDFT

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

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

for all $0 \leq l_t < N$ ($\Rightarrow 0 \leq \frac{l_t}{N} < 1$), $t = 0, 1, 2$, and compute

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

for $x_j^{(t)} \in [0, 1)$ $(t = 0, 1, 2)$, $j = 1, \ldots, M$.

Realized by 3d-NFFT [NFFT software library]

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

Parallel NFFT

Matrix-Vector-Notation

$$\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}},$$

where $\boldsymbol{f} = (f_j)_j$, $\boldsymbol{A} = (\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j})_{\boldsymbol{k},j}$, $\hat{\boldsymbol{f}} = (\hat{f}_{k_0 k_1 k_2})_{\boldsymbol{k}}$

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

$$\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}} \approx \boldsymbol{B}\boldsymbol{F}\boldsymbol{D}\hat{\boldsymbol{f}},$$

where

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

Summary

High Scalability

- 2d data distribution

FFTW Features

- performance
- interface
- portability

Additional Features

- truncated FFT
- ghost cells

PFFT

PNFFT