Fast Fourier transforms at nonequispaced nodes and applications

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"The FFT is, without doubt, one of the most important algorithm in applied mathematics and engineering." (V. Olshevsky)

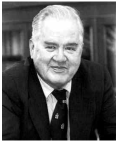
"The Fast Fourier transform (FFT) is one of the truly great computational developments of this century. It has changed the face of science and engineering so that it is not an exaggeration to say that life as we know it would be very different without FFT." (Charles Van Loan)

1805 Carl Friedrich Gauß used an algorithm similar to FFT.
1903 Runge
1942 Danielson and Lanczos
1965 Cooley and Tukey

Gauß

Runge

Lanczos



Tukey

Problem: fast computation of

$$f(x_j) = \sum_{k=-M/2}^{M/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k x_j} \qquad (j = -N/2, \ldots, N/2-1)$$

$$h(k) = \sum_{j=-N/2}^{N/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} k x_j} \qquad (k = -M/2, \ldots, M/2-1)$$

$$x_j \in \mathbb{T} := [-1/2, 1/2)$$

for equispaced nodes x_j and $M = N$

$$x_j := \frac{j}{M} \quad (j = -M/2, \ldots, M/2-1)$$

FFT in $\mathcal{O}(M \log M)$ instead of $\mathcal{O}(M^2)$ flops

NFFT

Problem: (NFFT) evaluation of the 1–periodic function

$$f(w) = \sum_{k=-M/2}^{M/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k w}$$

at arbitrary knots $w_j \in \mathbb{T}$ $(j = -N/2, \ldots, N/2-1)$

Idea:

1. approximate f by s_1: $m := \sigma M$ $(\sigma > 1)$, $\tilde{\varphi}(x) := \sum_{k \in \mathbb{Z}} \varphi(x+k)$

$$s_1(w) := \sum_{l=-m/2}^{m/2-1} g_l \, \tilde{\varphi}\left(w - \frac{l}{m}\right)$$

2. approximate s_1 by s: $p \ll m$, $\psi(x) := \varphi(x) \cdot \chi_{[-\frac{p}{m}, \frac{p}{m}]}(x)$

$$s(w) := \sum_{l=-m/2}^{m/2-1} g_l \tilde{\psi}\left(w - \frac{l}{m}\right) = \sum_{l=[wm]-p}^{[wm]+p} g_l \, \tilde{\psi}\left(w - \frac{l}{m}\right)$$

3. $f(w_j) \approx s_1(w_j) \approx s(w_j)$

Approximate

$$f(w) = \sum_{k=-M/2}^{M/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k w}$$

by

$$\begin{aligned} s_1(w) &= \sum_{l=-m/2}^{m/2-1} g_l \, \tilde{\varphi}\left(w - \frac{l}{m}\right) = \sum_{k=-\infty}^{\infty} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k w} \\ &\approx \sum_{k=-m/2}^{m/2-1} \hat{g}_k \, c_k(\tilde{\varphi}) \, \mathrm{e}^{-2\pi \mathrm{i} k w} \end{aligned}$$

1. set

$$\hat{g}_k := \begin{cases} \hat{f}_k / c_k(\tilde{\varphi}) & k = -M/2, \dots, M/2-1, \\ 0 & k = -m/2, \dots, -M/2-1, M/2, \dots, m/2-1 \end{cases}$$

2. by FFT(m):

$$g_l = \frac{1}{m} \sum_{k=-M/2}^{M/2-1} \hat{g}_k \mathrm{e}^{-2\pi \mathrm{i} k l / m}$$

NFFT

Algorithm-1D (NFFT)

1. For $k = -M/2, \ldots, M/2-1$ compute

$$\hat{g}_k := \hat{f}_k / c_k(\tilde{\varphi}).$$

2. For $l = -m/2, \ldots, m/2-1$ compute by FFT(m)

$$g_l := \frac{1}{m} \sum_{k=-M/2}^{M/2-1} \hat{g}_k \, \mathrm{e}^{-2\pi \mathrm{i} k l / m}.$$

3. For $j = -N/2, \ldots, N/2-1$ compute

$$f(w_j) \approx s(w_j) := \sum_{l=[w_j m]-p}^{[w_j m]+p} g_l \, \tilde{\psi}\left(w_j - \frac{l}{m}\right).$$

arithmetic operations:

$$\mathcal{O}(M + m\log m + (2p+1)N) = \mathcal{O}(M \log M + pN)$$

Matrix-vector notation:

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

where $\boldsymbol{A}$ may be factorised approximately as follows:

$$\boldsymbol{A} \approx \boldsymbol{C}\boldsymbol{F}\boldsymbol{D}.$$

Each of the three matrices corresponds to a step in the NFFT algorithm:

1. $\boldsymbol{D} \in \mathbb{R}^{M \times M}$ is a diagonal matrix:

$$\boldsymbol{D} := \operatorname{diag}\left(\frac{1}{m\, c_k(\tilde{\varphi})}\right)_{k=-M/2}^{M/2-1}$$

2. $\boldsymbol{F} \in \mathbb{R}^{m \times M}$ is a truncated Fourier matrix:

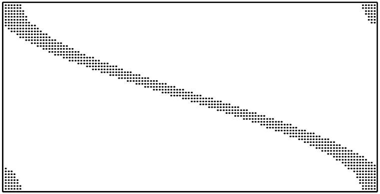
$$\boldsymbol{F} := \left(\mathrm{e}^{-2\pi \mathrm{i} kl/m}\right)_{l=-m/2,\; k=-M/2}^{m/2-1 \quad M/2-1}$$

3. $\boldsymbol{C} \in \mathbb{R}^{N \times m}$ is a sparse band matrix with $2p+1$ non-zero entries per row:

$$\boldsymbol{C} := \left(c_{j,l}\right)_{j=-N/2,\; l=-m/2}^{N/2-1 \quad m/2-1}$$

where

$$c_{j,l} = \begin{cases} \tilde{\psi}\left(x_j - \frac{l}{m}\right) & \text{if } l \in \{\lfloor x_j m \rfloor - p, \dots, \lceil x_j m \rceil + p\} \\ 0 & \text{otherwise.} \end{cases}$$



Structure of the matrix $\boldsymbol{C}$. Non-zero entries are indicated by dots. The row index j runs from $-N/2$ to $N/2-1$, the column index l runs from $-m/2$ to $m/2-1$. Parameters used were $N = M = 64$, $m = 128$ and $p = 5$; Legendre nodes were used for the x_j.

Error estimates:

$$|f(w_j) - s(w_j)| \le E_{\mathrm{a}}(w_j) + E_{\mathrm{t}}(w_j)$$

aliasing error $\quad E_{\mathrm{a}}(w_j) := |f(w_j) - s_1(w_j)|$

truncation error $\quad E_{\mathrm{t}}(w_j) := |s_1(w_j) - s(w_j)|$

$$E_{\mathrm{a}}(w_j) \le \|\hat{\boldsymbol{f}}\|_1 \max_{-M/2 \le k < M/2} \sum_{\substack{r=-\infty \\ r \neq 0}}^{\infty} \left| \frac{c_{k+mr}(\tilde{\varphi})}{c_k(\tilde{\varphi})} \right|$$

$$E_{\mathrm{t}}(w_j) \le \frac{\|\hat{\boldsymbol{f}}\|_1}{m} \max_{-M/2 \le k < M/2} \frac{1}{|c_k(\tilde{\varphi})|} \sum_{l=-m/2}^{m/2-1} \left| \tilde{\varphi}\left(w_j - \frac{l}{m}\right) - \tilde{\psi}\left(w_j - \frac{l}{m}\right) \right|$$

Window functions $\tilde{\varphi}(w) = \sum_{k\in\mathbb{Z}} \varphi(w+k)$:

- Gaussian (Dutt, Rokhlin 1993; Steidl 1998)

$$\varphi(w) = (\pi b)^{-1/2}\, \mathrm{e}^{-(mw)^2/b} \qquad \left(b := \frac{2\sigma}{2\sigma-1}\frac{p}{\pi}\right)$$

- B-splines (Beylkin 1995; Potts, Steidl, Tasche 1998)

$$\varphi(w) = B_{2p}(mw)$$

- Sinc–function (Potts 2001)

$$\varphi(w) = \frac{(2\sigma-1)M}{2p}\left(\operatorname{sinc}\left(\frac{\pi(2\sigma-1)Mw}{2p}\right)\right)^{2p}$$

- Kaiser–Bessel function (Fourmont 2001, Jackson 1991)

$$|w| \le \frac{p}{m}: \quad \varphi(w) = \frac{1}{\pi}\frac{\sinh(b\sqrt{p^2-m^2w^2})}{\sqrt{p^2-m^2w^2}} \qquad \left(b := \pi\left(2-\frac{1}{\sigma}\right)\right)$$

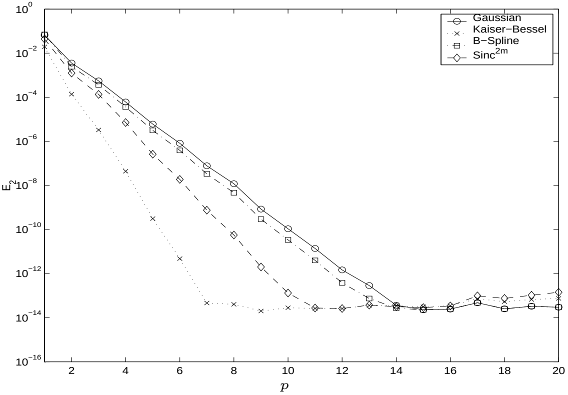
Error estimates for special window functions φ:

$$|f(w_j) - s(w_j)| \le C(\sigma, p)\, \|\hat{\boldsymbol{f}}\|_1$$

with

$$C(\sigma,p) := \begin{cases} 4\,\mathrm{e}^{-p\pi(1-1/(2\sigma-1))} & \text{for Gaussian} \\ 4\left(\frac{1}{2\sigma-1}\right)^{2p} & \text{for B-Splines} \\ \frac{1}{p-1}\left(\frac{2}{\sigma^{2p}} + \left(\frac{\sigma}{2\sigma-1}\right)^{2p}\right) & \text{for sinc} \\ 4\pi(\sqrt{p}+p)\sqrt[4]{1-\frac{1}{\sigma}}\,\mathrm{e}^{-p2\pi\sqrt{1-1/\sigma}} & \text{for Kaiser-Bessel} \end{cases}$$

For fixed $\sigma > 1$, the error decays exponentially with p.



The error with options double precision, $d = 1$, parameters $M = 1024$, $N = 2000$, $\sigma = 2$ for E_2

$$E_2 = \frac{\|\boldsymbol{f} - \boldsymbol{s}\|_2}{\|\boldsymbol{f}\|_2} = \left(\sum_{j=-N/2}^{N/2-1} |f_j - s(w_j)|^2 \right)^{\frac{1}{2}} \cdot \left(\sum_{j=-N/2}^{N/2-1} |f_j|^2 \right)^{-\frac{1}{2}}$$

NFFT – fast computation of

$$f(w_j) = \sum_{k=-M/2}^{M/2-1} \hat{f}_k \, \mathrm{e}^{-2\pi \mathrm{i} k w_j} \qquad (j = -N/2, \ldots, N/2-1)$$

matrix–vector form

$$\hat{\boldsymbol{f}} := (\hat{f}_k)_{k=-M/2}^{M/2}, \; \boldsymbol{f} := (f(w_j))_{j=-N/2}^{N/2}, \; \boldsymbol{A} := \left(\mathrm{e}^{-2\pi \mathrm{i} k w_j}\right)_{j=-N/2,k=-M/2}^{N/2-1,M/2-1}$$

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

$\mathrm{NFFT}^{\mathrm{H}}$ (adjoint, not inverse!) – fast computation of

$$h(k) = \sum_{j=-N/2}^{N/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} k w_j} \qquad (j = -M/2, \ldots, M/2-1)$$

The factorisation that was derived for $\boldsymbol{A}$ allows us to derive an $\mathrm{NFFT}^{\mathrm{H}}$ algorithm simply by transposing $\boldsymbol{A}$:

$$\boldsymbol{h} = \boldsymbol{A}^{\mathrm{H}}\boldsymbol{f} \approx \boldsymbol{D}^{\mathrm{H}}\boldsymbol{F}^{\mathrm{H}}\boldsymbol{C}^{\mathrm{H}}\boldsymbol{f}.$$

NFFT (multivariate case)

fast computation of the sums

$$f(\boldsymbol{w}_j) = \sum_{k_1=-M/2}^{M/2-1} \dots \sum_{k_d=-M/2}^{M/2-1} f_{\boldsymbol{k}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{w}_j} \qquad (j = -N/2, \dots, N/2-1)$$

$$h(\boldsymbol{k}) = \sum_{j=-N/2}^{N/2-1} f_j \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{w}_j} \qquad \left(\boldsymbol{k} \in \{-M/2, \dots, M/2-1\}^d =: \mathcal{I}_M^d\right)$$

for equispaced nodes $\boldsymbol{w}_j := \frac{\boldsymbol{j}}{M}$ $(N = M^d)$

FFT (*fast Fourier transform*) in $\mathcal{O}(M^d \log M)$

for arbitrary nodes $\boldsymbol{w}_j \in [-1/2, 1/2)^d$

NFFT (*nonequispaced FFT*) in $\mathcal{O}(M^d \log M + p^d N)$

NFFT

Software available:

NFFT – C subroutine library (Keiner, Kunis, Potts 2002–2013)

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

Generalization:
Nonequispaced in time and frequency (NNFFT), nonequispaced DCT/DST, hyperbolic cross, NFFT on the sphere, iterative solution of the inverse transforms

Applications:
fast summation, fast Gauss transform, summation on the sphere, MRI, polar FFT, Radon transform, CT, ridgelet transform

Documentation:

NFFT3 Tutorial (Keiner, Kunis, Potts)

Fast summation algorithms of radial functions

$\sum$

Problem: fast computation of

$$f(\boldsymbol{x}_j) := \sum_{k=1}^{N} \alpha_k \mathcal{K}(\boldsymbol{x}_j - \boldsymbol{x}_k) \qquad (j = 1, \ldots, N)$$

nodes $\boldsymbol{x}_j \in \mathbb{R}^d$, $\mathcal{K}(\boldsymbol{x}) = K(\|\boldsymbol{x}\|)$ radial functions

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

K are special kernels, e.g.

singular kernels: $\frac{1}{|x|}$, $\frac{1}{x^2}$, $\log|x|$, $x^2 \log|x|$

nonsingular kernels: $(x^2 + c^2)^{\pm 1/2}$, $\mathrm{e}^{-\delta x^2}$

Applications: integral equations, scattered data approximation, image processing, discrete Gauss transform, ...

Known methods for products of vectors with specially structured dense matrices

$$\boldsymbol{f} = \boldsymbol{K}\boldsymbol{\alpha}$$

panel clustering, fast multipole method, wavelet methods

Standard algorithm for equispaced nodes: $\boldsymbol{K}$ – Toeplitz matrix

$$\boldsymbol{f} = \mathrm{FFT}(\,\mathrm{diag}(\boldsymbol{b})\,\mathrm{FFT}^{\mathrm{H}}(\boldsymbol{\alpha}))$$

Known methods for products of vectors with specially structured dense matrices

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$$\boldsymbol{f} = \mathrm{FFT}(\,\mathrm{diag}(\boldsymbol{b})\,\mathrm{FFT}^{\mathrm{H}}(\boldsymbol{\alpha}))$$

Idea for nonequispaced nodes: replace FFT by NFFT

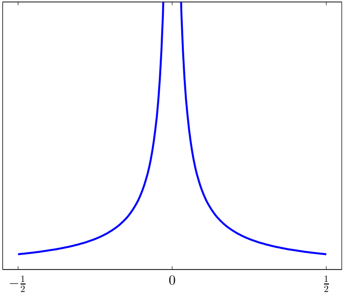
$$\boldsymbol{f} = \mathrm{NFFT}(\,\mathrm{diag}(\tilde{\boldsymbol{b}})\,\mathrm{NFFT}^{\mathrm{H}}(\boldsymbol{\alpha})) + \text{near field}$$

Problem: fast evaluation of

$$f(\boldsymbol{x}) := \sum_{k=1}^{N} \alpha_k \mathcal{K}(\boldsymbol{x} - \boldsymbol{x}_k) = \sum_{k=1}^{N} \alpha_k K(\|\boldsymbol{x} - \boldsymbol{x}_k\|),$$

at the N given nodes $\boldsymbol{x} = \boldsymbol{x}_j \in \mathbb{R}^d$

Singular kernels: $\frac{1}{|x|}, \ \frac{1}{x^2}, \ \log|x|, \ x^2 \log|x|$



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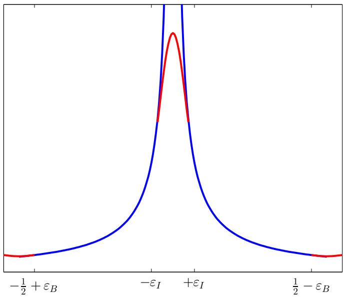
Singular kernels: $\frac{1}{|x|}$, $\frac{1}{x^2}$, $\log|x|$, $x^2 \log|x|$

Regularize $\mathcal{K}$:

- near $\mathbf{0}$, $\|\boldsymbol{x}\| \le \varepsilon_{\mathrm{I}}$
- at boundary, $\frac{1}{2} - \varepsilon_{\mathrm{B}} \le \|\boldsymbol{x}\| \le \frac{1}{2}$ (assume $\|\boldsymbol{x}_j - \boldsymbol{x}_k\| \le \frac{1}{2} - \varepsilon_{\mathrm{B}}$)



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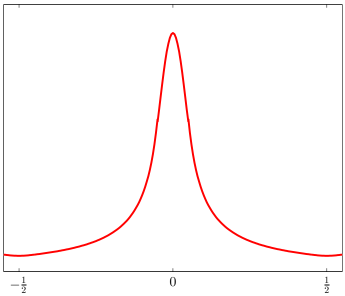
Regularize $\mathcal{K}$:

- near $\mathbf{0}$, $\|\boldsymbol{x}\| \le \varepsilon_{\mathrm{I}}$
- at boundary, $\frac{1}{2} - \varepsilon_{\mathrm{B}} \le \|\boldsymbol{x}\| \le \frac{1}{2}$ (assume $\|\boldsymbol{x}_j - \boldsymbol{x}_k\| \le \frac{1}{2} - \varepsilon_{\mathrm{B}}$)
- smooth and periodic function $\mathcal{K}_{\mathrm{R}}$

Approximation:

$$\mathcal{K}_{\mathrm{R}}(\boldsymbol{x}) \approx \mathcal{K}_{\mathrm{RF}}(\boldsymbol{x}) := \sum_{\boldsymbol{l} \in \mathcal{I}_m^d} b_{\boldsymbol{l}} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{l} \boldsymbol{x}}$$



Regularization by algebraic polynomials

Given: a_j, b_j, $j = 0, \ldots, q-1$
Compute: polynomial P with

$$P^{(j)}(c-r) = a_j \quad (j = 0, \ldots, q-1) \qquad (1)$$

$$P^{(j)}(c+r) = b_j \quad (j = 0, \ldots, q-1) \qquad (2)$$

Theorem (Two point Taylor interpolation):
For given a_j, b_j $(j = 0, \ldots, q-1)$ there exists a unique polynomial P of degree $2q-1$ which satisfies the conditions (1) and (2):

$$P(x) = \frac{1}{2^q} \sum_{j=0}^{q-1} \sum_{k=0}^{q-1-j} \frac{r^j}{j!2^k} \binom{q-1+k}{k} \left[(1+y)^{j+k} (1-y)^q a_j + (-1)^j (1-y)^{j+k} (1+y)^q b_j \right],$$

where $y := \frac{x-c}{r}$. For symmetric functions: $(-1)^j b_j = a_j$.

Σ Around **0**: $a_j = K^{(j)}(-\varepsilon_{\mathrm{I}}), b_j = K^{(j)}(\varepsilon_{\mathrm{I}})$

At the boundary: $a_j = K^{(j)}(1/2 - \varepsilon_{\mathrm{B}}), b_j = K^{(j)}(-1/2 + \varepsilon_{\mathrm{B}})$

Splitting: $\mathcal{K}(x) = [\mathcal{K}(\boldsymbol{x}) - \mathcal{K}_{\mathrm{R}}(\boldsymbol{x})] + \mathcal{K}_{\mathrm{R}}(\boldsymbol{x}) =: \mathcal{K}_{\mathrm{NE}}(\boldsymbol{x}) + \mathcal{K}_{\mathrm{R}}(\boldsymbol{x})$

Approximation $\mathcal{K}_{\mathrm{R}}(\boldsymbol{x}) \approx \mathcal{K}_{\mathrm{RF}}(\boldsymbol{x})$: $f(\boldsymbol{x}) \approx \tilde{f}(\boldsymbol{x}) := f_{\mathrm{NE}}(\boldsymbol{x}) + f_{\mathrm{RF}}(\boldsymbol{x})$

Near field ($\|\boldsymbol{x} - \boldsymbol{x}_k\| \leq \varepsilon_{\mathrm{I}}$, direct):

$$f_{\mathrm{NE}}(\boldsymbol{x}) := \sum_{k=1}^{N} \alpha_k \mathcal{K}_{\mathrm{NE}}(\boldsymbol{x} - \boldsymbol{x}_k)$$

Fourier method

$$f_{\mathrm{RF}}(\boldsymbol{x}) := \sum_{k=1}^{N} \alpha_k \mathcal{K}_{\mathrm{RF}}(\boldsymbol{x} - \boldsymbol{x}_k)$$

$$f_{\mathrm{RF}}(\boldsymbol{x}_j) = \sum_{k=1}^{N} \alpha_k \sum_{\boldsymbol{l} \in \mathcal{I}_m^d} b_{\boldsymbol{l}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{l}(\boldsymbol{x}_j - \boldsymbol{x}_k)} = \underbrace{\sum_{\boldsymbol{l} \in \mathcal{I}_m^d} b_{\boldsymbol{l}} \underbrace{\left(\sum_{k=1}^{N} \alpha_k \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}_k} \right)}_{\mathrm{NFFT}^{\mathrm{H}}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}_j}}_{\mathrm{NFFT}}$$

Complexity: $\mathcal{O}(M^d \log M + p^d N)$

Particle-particle NFFT (P^{2}NFFT)

Coulomb potential in charged particle systems:

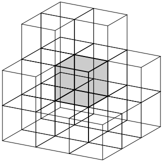
$$\phi(\boldsymbol{x}_j) := \sum_{i=1, i\neq j}^{N} \frac{q_i}{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|}$$

Approach:

- set $K(\|\boldsymbol{x}\|) := \|\boldsymbol{x}\|^{-1}$
- let $\|\boldsymbol{x}_i - \boldsymbol{x}_j\| \leq h(1/2 - \varepsilon_{\mathrm{B}})$
- construct h-periodic regularization
- fast computation of the far field by NFFT based fast summation

$$\phi_{\mathrm{RF}}(\boldsymbol{x}_j) = \underbrace{\sum_{\boldsymbol{l}\in\mathcal{I}_m^3} b_{\boldsymbol{l}} \underbrace{\left(\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}_i/h}\right)}_{\text{NFFT}^{\text{H}}} \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{l}\boldsymbol{x}_j/h}}_{\text{NFFT}}$$

Coulomb potential in charged particle systems:



$$\phi(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N}{}' \frac{q_i}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|}$$

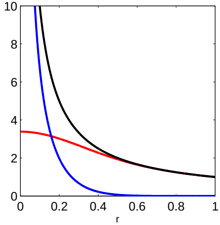
s.t. periodic boundary conditions
$\boldsymbol{x}_j \in B_1\mathbb{T} \times B_2\mathbb{T} \times B_3\mathbb{T}$

fully periodic: $\mathcal{S} = B_1\mathbb{Z} \times B_2\mathbb{Z} \times B_3\mathbb{Z}$

- Ewald summation

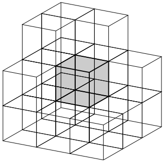
Ewald splitting

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



- $\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t$ (error function)
- $\operatorname{erfc}(x) := 1 - \operatorname{erf}(x)$ (complementary error function)
- $\alpha > 0$ (splitting parameter)

Coulomb potential in charged particle systems:



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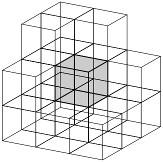
- Ewald summation

$$\sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N}{}' \frac{q_i}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|} = \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N}{}' q_i \frac{\operatorname{erfc}(\alpha\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|)}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|} + \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N} q_i \frac{\operatorname{erf}(\alpha\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|)}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|} - \frac{2\alpha}{\sqrt{\pi}} q_j$$

- short range part: direct evaluation after truncation
- $\lim_{r\to 0} \frac{\operatorname{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}} \Rightarrow$ substract self potential
- transform long range part into a sum in Fourier space

Coulomb potential in charged particle systems:



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fully periodic: $\mathcal{S} = B_1\mathbb{Z} \times B_2\mathbb{Z} \times B_3\mathbb{Z}$

- Ewald summation
- compute long range part using NFFTs (Hedman, Laaksonen 2006)

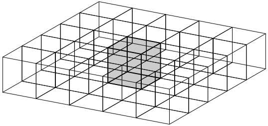
$$\phi^{\mathrm{L}}(\boldsymbol{x}_j) = \frac{4\pi}{B_1 B_2 B_3} \underbrace{\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\mathrm{e}^{-\|\boldsymbol{k}\|^2/(4\alpha^2)}}{\|\boldsymbol{k}\|^2} \underbrace{\left(\sum_{i=1}^{N} q_i \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}_i}\right)}_{\text{NFFT}^{\mathrm{H}}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}}_{\text{NFFT}}$$

$\boldsymbol{k} \in \frac{2\pi}{B_1}\mathbb{Z} \times \frac{2\pi}{B_2}\mathbb{Z} \times \frac{2\pi}{B_3}\mathbb{Z}$

- $\hat{=}$ P^3M if $\varphi =$ B-Spline

Coulomb potential in charged particle systems:

$$\phi(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N}{}' \frac{q_i}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|}$$



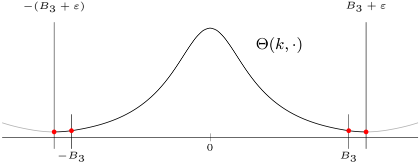
s.t. periodic boundary conditions
$\boldsymbol{x}_j \in B_1\mathbb{T} \times B_2\mathbb{T} \times B_3\mathbb{T}$

2d-periodic: $\mathcal{S} = B_1\mathbb{Z} \times B_2\mathbb{Z} \times \{0\}$

- Ewald summation, long range part: $\boldsymbol{k} \in \frac{2\pi}{B_1}\mathbb{Z} \times \frac{2\pi}{B_2}\mathbb{Z}$

$$\phi^{\mathrm{L}}(\boldsymbol{x}_j) = \frac{\pi}{B_1 B_2} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\Theta(\|\boldsymbol{k}\|, x_{ij,3})}{\|\boldsymbol{k}\|} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(x_{ij,1}, x_{ij,2})}$$

- Idea: regularize the functions $\Theta(k,\cdot)$ (N., Potts 2013)



$$\approx \sum_{l=-M/2}^{M/2-1} b_{k,l} \mathrm{e}^{\pi \mathrm{i} l x/(B_3+\varepsilon)}$$

Coulomb potential in charged particle systems:

$$\phi(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{i=1}^{N}{}' \frac{q_i}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + \boldsymbol{n}\|}$$

s.t. periodic boundary conditions
$\boldsymbol{x}_j \in B_1\mathbb{T} \times B_2\mathbb{T} \times B_3\mathbb{T}$

summary:

- $\mathcal{S} = \{0\}^3$: NFFT based fast summation in 3d
- fully periodic: Ewald + NFFT
- 2d-periodic: Ewald + NFFT based fast summation in 1d
- 1d-periodic: Ewald + NFFT based fast summation in 2d

Structure

$$\text{Near field} + \underbrace{\boldsymbol{C}\boldsymbol{F}\boldsymbol{D}}_{\text{NFFT}}\ \underbrace{\tilde{\boldsymbol{D}}}_{\text{diag}}\ \underbrace{\boldsymbol{D}^{\mathrm{H}}\boldsymbol{F}^{\mathrm{H}}\boldsymbol{C}^{\mathrm{H}}}_{\text{NFFT}^{\mathrm{H}}}$$

Calculation of the fields

$$\boldsymbol{E}_j := -\nabla\phi(\boldsymbol{y})\Big|_{\boldsymbol{y}=\boldsymbol{x}_j}$$

Long range part for fully p.b.c.:

two possibilies:

1. i$\boldsymbol{k}$ differentation (apply ∇ to Fourier series)

$$\boldsymbol{E}_j^{\mathrm{L}} = \frac{4\mathrm{i}\pi}{B_1 B_2 B_3} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\mathrm{e}^{\|\boldsymbol{k}\|^2/(4\alpha^2)}}{\|\boldsymbol{k}\|^2} \boldsymbol{k} S(\boldsymbol{k}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j} \quad \text{with} \quad S(\boldsymbol{k}) := \sum_{i=1}^{N} q_i \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}_i}$$

2. analytic differentation (apply ∇ to NFFT window function)

$$\nabla\phi^{\mathrm{L}}(\boldsymbol{x}_j) = \frac{4\pi}{B_1 B_2 B_3} \nabla \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\mathrm{e}^{-\|\boldsymbol{k}\|^2/(4\alpha^2)}}{\|\boldsymbol{k}\|^2} S(\boldsymbol{k}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}$$

$$\approx \frac{4\pi}{B_1 B_2 B_3} \sum_{\boldsymbol{l}\in\mathcal{I}_n^3} g_{\boldsymbol{l}} \nabla\tilde{\varphi}\left(\boldsymbol{x}_j - \tfrac{1}{m}\boldsymbol{l}\right)$$

Analog for other types of boundary conditions

Conclusions

- **NFFT**: fast evaluation of trigonometric sums for nonequispaced data
- software available
- important: NFFT based fast summation
- application to particle simulation: methods for all types of boundary conditions

http://www.tu-chemnitz.de/∼potts/nfft
http://www.tu-chemnitz.de/∼nesfr