A Superfast Direct Solver for Nonuniform Discrete Fourier Transform of Type III

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NUDFT

Nonuniform discrete Fourier transform (NUDFT):

$$f_j = \sum_{k=0}^{N-1} \mathrm{e}^{2\pi \mathrm{i} x_j \omega_k} u_k, \quad 0 \le j \le M-1.$$

- $M \ge N$.
- Sample points: $\{x_j\}_{j=0}^{M-1} \subset [0,1)$.
- Frequencies: $\{\omega_k\}_{k=0}^{N-1} \subset [-1/2, N-1/2)$.
- Coefficients: $\{u_k\}_{k=0}^{N-1} \subset \mathbb{C}$.
- Target values: $\{f_j\}_{j=0}^{M-1} \subset \mathbb{C}$.

NUFFT

Fast forward computation:

- Uniform case (FFT): $M = N$, $x_j = j/M$ and $\omega_k = k$.
  Complexity: $\mathscr{O}(N \log N)$ [Cooley and Tukey 1965]
- Nonuniform case (NUFFT)
  - Type I: Equispaced sample points, i.e., $x_j = j/M$;
  - Type II: Integer frequencies, i.e., $\omega_k = k$;
  - Type III: Nonequispaced sample points and noninteger frequencies.

  Complexity: $\mathscr{O}(M + N \log N)$
  - Local expansions: [Anderson and Dahleh 1996], [Ruiz-Antolín and Townsend 2018]
  - Gridding algorithms: [Dutt and Rokhlin 1993], [Greengard and Lee 2004], [A. Barnett, Magland, and Klinteberg 2019].

INUDFT

Problem (Inverse NUDFT Problem, INUDFT)

Given sample points $\{x_j\}$ *and frequencies* $\{\omega_k\}$, *determine the coefficients* $\{u_k\}$ *from the target values* $\{f_j\}$.

- Can be modeled as a least-squares problem associated with the NUDFT matrix $\mathbf{A} = \left(\mathrm{e}^{2\pi \mathrm{i} x_j \omega_k}\right)_{j,k}$.
- The pseudoinverse of a NUDFT matrix does not simpliy equal to its adjoint.
- Accuracy is heavily affected by the distribution of sample points and frequencies.

Existing methods:

- Iterative methods: CG + NUFFT.
- Direct methods: [Kircheis and Potts 2019], [Wilber, Epperly, and A. H. Barnett 2025]

Displacement Structure of NUDFT-II Matrix

Method in [Wilber, Epperly, and A. H. Barnett 2025]:
NUDFT-II matrix

$$\mathbf{A}(j,k) = \mathrm{e}^{2\pi \mathrm{i} x_j k} = \gamma_j^k$$

is a Vandermonde matrix and satisfies the following Sylvester equation:

$$\mathbf{\Gamma A} - \mathbf{AC} = \mathbf{a}\mathbf{e}_{N-1}^*,$$

where

- $\mathbf{\Gamma} = \mathrm{diag}(\gamma_0, \gamma_1, \ldots, \gamma_{M-1})$ is diagonal;
- $\mathbf{C} = [\mathbf{e}_1 \ \mathbf{e}_2 \ \cdots \ \mathbf{e}_0]$ is a circulant matrix;
- $a_j = \gamma_j^N - 1$.

Displacement Structure of NUDFT-II Matrix

Fact: $\mathbf{C} = \mathbf{F}^{-1}\mathbf{D}\mathbf{F}$, where $\mathbf{F}$ is the standard $N \times N$ DFT matrix and $\mathbf{D} = \operatorname{diag}(\mathbf{F}\mathbf{e}_1)$.
The Sylvester equation thus becomes

$$\mathbf{\Gamma}\mathbf{A} - \mathbf{A}\mathbf{F}^{-1}\mathbf{D}\mathbf{F} = \mathbf{a}\mathbf{e}_{N-1}^*.$$

Let $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{F}^{-1}$ and $\mathbf{b} = \mathbf{F}^{-*}\mathbf{e}_{N-1}$, then

$$\mathbf{\Gamma}\tilde{\mathbf{A}} - \tilde{\mathbf{A}}\mathbf{D} = \mathbf{a}\mathbf{b}^*,$$

where $b_k = \mathrm{e}^{-2\pi \mathrm{i} k/N}/N$.
[Beckermann and Townsend 2017]: Displacement structure $\Rightarrow$ Low-rankness.
Approximate $\tilde{\mathbf{A}}$ by a hierarchical semiseparable (HSS) matrix: Fast construction based on the factorized alternating direction implicit (fADI) method [Wilber 2021].

HSS Tree

Definition (HSS Tree)

A tree T is called an HSS tree if

- T is a full binary tree with root node 1.
- There are two index sets I_τ and J_τ associated with each node τ of T, satisfying
  - $I_1 = [0, \dots, M-1]$, $J_1 = [0, \dots, N-1]$.
  - For a non-leaf node τ with children α_1 and α_2, $I_\tau = I_{\alpha_1} \sqcup I_{\alpha_2}$ and $J_\tau = J_{\alpha_1} \sqcup J_{\alpha_2}$.

Level 0: 1 — $J_1 = [0, ..., 255]$

Level 1: 2, 3 — $J_2 = [0, ..., 127]$, $J_3 = [128, ..., 255]$

Level 2: 4, 5, 6, 7 — $J_4 = [0, ..., 63]$, $J_5 = [64, ..., 127]$, ...

HSS Matrix

Definition (HSS Matrix)

A matrix $\mathbf{H}$ is said to be an HSS matrix with respect to an HSS tree T if there are matrices $\mathbf{D}_\tau$, $\mathbf{U}_\tau$, $\mathbf{V}_\tau$, $\mathbf{R}_\tau$, $\mathbf{W}_\tau$, $\mathbf{B}_{\tau,\sigma}$ (called HSS generators) associated with each node τ and its silbing σ, satisfying the following recursion:

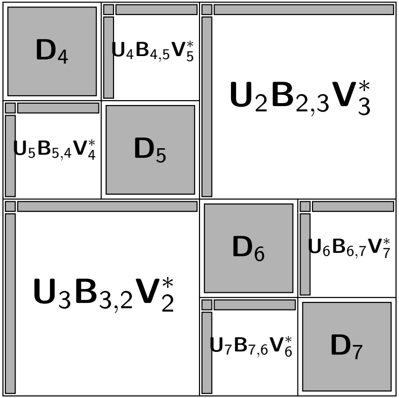
1. For a non-leaf node τ with children α_1 and α_2,

$$\mathbf{D}_\tau = \mathbf{H}(I_\tau, J_\tau) = \begin{bmatrix} \mathbf{D}_{\alpha_1} & \mathbf{U}_{\alpha_1}\mathbf{B}_{\alpha_1,\alpha_2}\mathbf{V}^*_{\alpha_2} \\ \mathbf{U}_{\alpha_2}\mathbf{B}_{\alpha_2,\alpha_1}\mathbf{V}^*_{\alpha_1} & \mathbf{D}_{\alpha_2} \end{bmatrix}.$$

2. For a non-leaf and non-root node τ with children α_1 and α_2,

$$\mathbf{U}_\tau = \begin{bmatrix} \mathbf{U}_{\alpha_1}\mathbf{R}_{\alpha_1} \\ \mathbf{U}_{\alpha_2}\mathbf{R}_{\alpha_2} \end{bmatrix}, \quad \mathbf{V}_\tau = \begin{bmatrix} \mathbf{V}_{\alpha_1}\mathbf{W}_{\alpha_1} \\ \mathbf{V}_{\alpha_2}\mathbf{W}_{\alpha_2} \end{bmatrix}.$$

An Example of the HSS Matrix



$$\mathbf{U}_2 = \begin{bmatrix} \mathbf{U}_4\mathbf{R}_4 \\ \mathbf{U}_5\mathbf{R}_5 \end{bmatrix}, \quad \mathbf{V}_2 = \begin{bmatrix} \mathbf{V}_4\mathbf{W}_4 \\ \mathbf{V}_5\mathbf{W}_5 \end{bmatrix},$$

$$\mathbf{U}_3 = \begin{bmatrix} \mathbf{U}_6\mathbf{R}_7 \\ \mathbf{U}_6\mathbf{R}_7 \end{bmatrix}, \quad \mathbf{V}_3 = \begin{bmatrix} \mathbf{V}_6\mathbf{W}_6 \\ \mathbf{V}_7\mathbf{W}_7 \end{bmatrix}.$$

Shared basis (nested basis) property: $\mathbf{U}_\tau$ is the column basis of $\mathbf{A}(I_\tau, J_\tau^c)$.

A Least-Squares Solver for the HSS Matrix

URV factorization [Xi et al. 2014]:

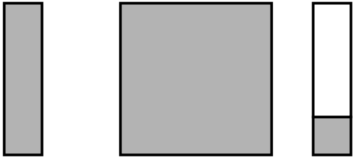
$$\mathbf{H} = \mathbf{Z}^{(L)} \cdots \mathbf{Z}^{(1)} \mathbf{Z}^{(0)} \mathbf{T}^{(0)} \mathbf{T}^{(1)} \mathbf{W}^{(1)*} \cdots \mathbf{T}^{(L)} \mathbf{W}^{(L)*},$$

where

- $\{\mathbf{Z}^{(\ell)}\}$, $\{\mathbf{W}^{(\ell)}\}$ are block unitary matrices;
- $\{\mathbf{T}^{(\ell)}\}$ are block upper-triangular matrices;
- Each block contains at most $\mathscr{O}(1)$ nonzeros.

Idea: Introduce zeros by a reverse QR factorization.

$$\mathbf{V}_4 = \mathbf{Q}_4 \begin{bmatrix} \mathbf{0} \\ \hat{\mathbf{V}}_4 \end{bmatrix}$$



URV Factorization: Process

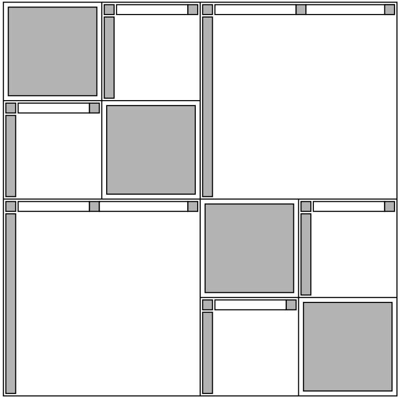


Figure: Introducing zeros into off-diagonal columns.

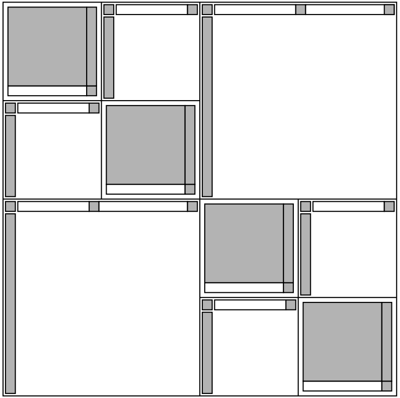


Figure: QR factorization on diagonal blocks.

Algorithm 1: A direct solver for INUDFT-II

Input: Samples $\{x_j\}_{j=0}^{M-1}$ and target values $\{f_j\}_{j=0}^{M-1}$.

Output: Coefficients $\{u_k\}_{k=0}^{N-1}$.

`/* Construction. */`

Approximate $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{F}^{-1}$ by an HSS matrix $\tilde{\mathbf{A}}_{\mathrm{HSS}}$;

`/* Factorization. */`

Compute the URV factorization of $\tilde{\mathbf{A}}_{\mathrm{HSS}}$;

`/* Solution. */`

Solve $\mathbf{v} = \arg\min_{\mathbf{w}} \|\tilde{\mathbf{A}}_{\mathrm{HSS}}\mathbf{w} - \mathbf{f}\|_2$;

Compute $\mathbf{u} = \mathbf{F}\mathbf{v}$ using FFT;

Fast structure in INUDFT-II:

$$\mathbf{A}_{\mathrm{fast}} = \tilde{\mathbf{A}}_{\mathrm{HSS}}\mathbf{F} \quad \text{and} \quad \mathbf{A}_{\mathrm{fast}}^{\dagger} = \mathbf{F}^{-1}\tilde{\mathbf{A}}_{\mathrm{HSS}}^{\dagger}.$$

Complexity

Stage	Operation	Complexity	Total
Construction	Construct $\tilde{\mathbf{A}}_{\mathrm{HSS}}$	$k^2 M$	$k^2 M$
Factorization	Factorize $\tilde{\mathbf{A}}_{\mathrm{HSS}}$	$k^2 M$	$k^2 M$
Solution	Apply $\tilde{\mathbf{A}}_{\mathrm{HSS}}^{\dagger}$ Apply $\mathbf{F}$	kM $N \log N$	$kM + N \log N$

Table: Complexities in the INUDFT–2 algorithm ($\mathscr{O}$ omitted).

Motivation

Fact: $\{e^{2\pi i \ell x}\}_{\ell \in \mathbb{Z}}$ forms an orthogonal basis of $L^2[0, 1]$.
From direct calculation,

$$e^{2\pi i \omega_k x} = \sum_{\ell \in \mathbb{Z}} Q_{\ell,k} e^{2\pi i \ell x},$$

where

$$Q_{\ell,k} = \int_0^1 e^{2\pi i(\omega_k - \ell)x} dx = e^{\pi i(\omega_k - \ell)} \frac{\sin(\pi(\omega_k - \ell))}{\pi(\omega_k - \ell)} = G(\ell - \omega_k).$$

By truncating both sides to the R-th term,

$$e^{2\pi i \omega_k x} = \underbrace{\sum_{|\ell - \omega_k| \le R} Q_{\ell,k} e^{2\pi i \ell x}}_{\text{Approximation}} + \underbrace{\sum_{|\ell - \omega_k| > R} Q_{\ell,k} e^{2\pi i \ell x}}_{\text{Error}}.$$

The error term has the estimate: $\|\mathrm{err}_k\|_{L^2}^2 \le \mathscr{O}(1/R)$.

Error Bound When Sample Points Are Uniform Random Variables

For the NUDFT-III matrix:

$$\mathbf{A}(j,k) = \mathrm{e}^{2\pi\mathrm{i}x_j\omega_k} \approx \sum_{-R\le\ell\le N-1+R} \mathrm{e}^{2\pi\mathrm{i}x_j\ell} Q_{\ell,k}.$$

Or, in matrix form,

$$\mathbf{A} = \mathbf{B}\mathbf{Q} + \mathbf{E}.$$

Proposition

Suppose $\{x_j\}$ are i.i.d. uniform random variables in $[0,1)$ and $R \ge 2$, then $\mathbf{E}$ is a random matrix satisfying $\mathbb{E}\mathbf{E} = \mathbf{0}$ and

$$\mathbb{E}\|\mathbf{E}\|_{\mathrm{F}}^2 \le \|\mathbf{A}\|_{\mathrm{F}}^2 \frac{2}{\pi^2} \frac{1}{R-3/2}.$$

Practical Algorithm

Denoting $\mathbf{H} = \mathbf{B}^{\dagger}\mathbf{A}$, we have

$$\mathbf{H} = \mathbf{Q} + \mathbf{B}^{\dagger}\mathbf{E},$$

$$\mathbf{A} = \mathbf{B}\mathbf{H} + \left(\mathbf{I} - \mathbf{B}\mathbf{B}^{\dagger}\right)\mathbf{E}.$$

- $\mathbf{B}$ is a NUDFT-II matrix having a fast structure;
- $\mathbf{Q}$ is a kernel matrix, can be compressed into an HSS matrix;
- $\mathbf{H}$ can be empirically compressed into an HSS matrix;
- $\mathbf{I} - \mathbf{B}\mathbf{B}^{\dagger}$ is a projection matrix.

The Construction of the Direct Solver

Construction on $\mathbf{B}_{\mathrm{fast}}$: Type II direct solver.

Goal: Find an efficient way to construct $\mathbf{H} = \mathbf{B}_{\mathrm{fast}}^{\dagger}\mathbf{A}$.

- Fast forward computation on $\mathbf{A}$: NUFFT.
- Fast forward computation on $\mathbf{B}_{\mathrm{fast}}^{\dagger}$: URV factorization and FFT.

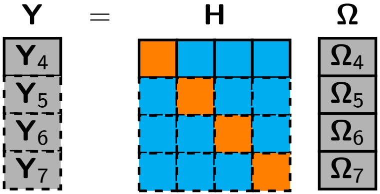
Black-box setting: Compress a matrix into its HSS form through matrix-vector multiplication.

Black-Box Construction of the HSS Matrix

Method in [Levitt and Martinsson 2024]: Recover the HSS structure using random samplings.

- Target rank: r.
- Sample number: $s \geq \max\{m + r, 3r\}$ where m is maximum size of the leaf node.

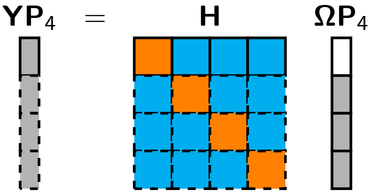
Their algorithm constructs an HSS matrix using $\{\mathbf{\Omega}, \mathbf{H\Omega}, \mathbf{\Psi}, \mathbf{H}^*\mathbf{\Psi}\}$ where $\mathbf{\Omega}$ and $\mathbf{\Psi}$ are Gaussian random matrices of size $N \times s$.



Main step: Find a basis $\mathbf{U}_4$ of $\mathbf{H}(I_4, J_4^c)$.

Black-Box Construction of the HSS Matrix

Idea: Eliminate the contribution of diagonal blocks.
Suppose $\mathbf{P}_4 = \mathrm{null}(\mathbf{\Omega}_4, r)$, then



Therefore, we have

$$\underbrace{\mathbf{Y}_4\mathbf{P}_4}_{\text{sample matrix}} = \sum_{\sigma=5}^{7} \mathbf{H}_{4,\sigma} \underbrace{\mathbf{\Omega}_\sigma \mathbf{P}_4}_{\text{test matrix}} .$$

Then construct $\mathbf{U}_4$ using $\mathbf{Y}_4\mathbf{P}_4$.
Complexity: $\mathscr{O}(k^2 N + k T_{\mathrm{mult}})$.

A Superfast Direct Solver of INUDFT-III

Algorithm 2: A direct solver for INUDFT-III.

Input: Sample points $\{x_j\}_{j=0}^{M-1}$, frequencies $\{\omega_k\}_{k=0}^{N-1}$, target values $\{f_j\}_{j=0}^{M-1}$.

Output: Coefficients $\{u_k\}_{k=0}^{N-1}$.

`/* Construction. */`

Construct a superfast direct solver $\mathbf{B}_{\text{fast}}$ for the NUDFT-II matrix $\mathbf{B} \in \mathbb{C}^{M\times N}$;

Compress $\mathbf{B}_{\text{fast}}^{\dagger}\mathbf{A}$ into an HSS matrix $\mathbf{H}_{\text{HSS}}$ using the black-box method;

`/* Factorization. */`

Compute the URV factorization of $\mathbf{H}_{\text{HSS}}$;

`/* Solution. */`

Calculate $\mathbf{u} = \mathbf{H}_{\text{HSS}}^{-1}\mathbf{B}_{\text{fast}}^{\dagger}\mathbf{f}$;

Fast structure in INUDFT-III:

$$\mathbf{A}_{\text{fast}} = \mathbf{B}_{\text{fast}}\mathbf{H}_{\text{HSS}} \quad \text{and} \quad \mathbf{A}_{\text{fast}}^{\dagger} = \mathbf{H}_{\text{HSS}}^{-1}\mathbf{B}_{\text{fast}}^{\dagger}.$$

Complexity

Stage	Operation	Complexity	Total
Construction	Construct $\mathbf{B}_{\text{fast}}$	$k^2 M$	$k^2 M + kN \log N$
	Apply $\mathbf{A}$	$M + N \log N$	
	Apply $\mathbf{B}_{\text{fast}}^{\dagger}$	kM	
	Compress $\mathbf{H}_{\text{HSS}}$	$k^2 N$	
Factorization	Factorize $\mathbf{H}_{\text{HSS}}$	$k^2 N$	$k^2 N$
Solution	Apply $\mathbf{B}_{\text{fast}}^{\dagger}$	$kM + N \log N$	$kM + N \log N$
	Apply $\mathbf{H}_{\text{HSS}}^{\dagger}$	kN	

Table: Complexities in the INUDFT-III algorithm ($\mathscr{O}$ omitted).

Experiment Setting

- $M = 4N$.
- Samples are i.i.d. uniform random variables in $[0, 1)$.
- Frequencies are perturbed integers given by

$$\omega_k = k + \alpha\psi_k, \quad 0 \leq k \leq N - 1,$$

where $\{\psi_k\}$ are IID uniform random variables on $[-1, 1]$ and $0 \leq \alpha < 1/2$ controls the non-uniformity.

The Low-Rank Property of $\mathbf{H}$

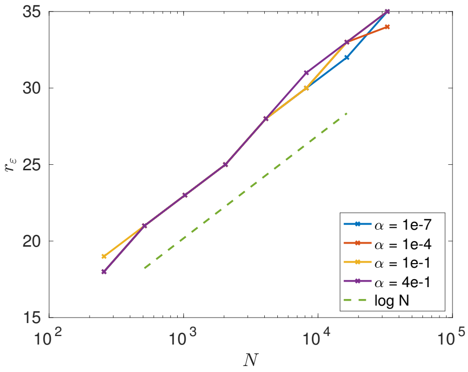
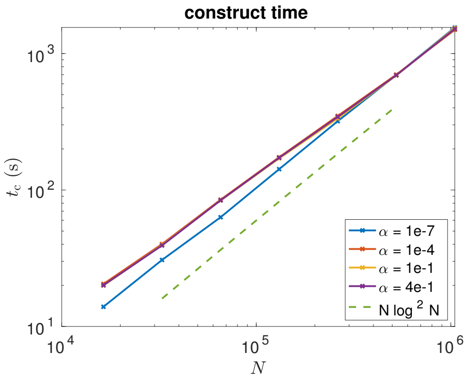
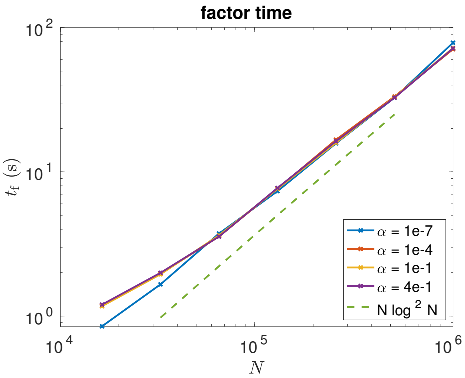


Figure: ε-rank of the top-right submatrix in $\mathbf{B}_{\text{fast}}^{\dagger}\mathbf{A}$ for $\varepsilon = 10^{-7}$. The size of the submatrix is $N/2$ where $N = 2^n$ for $n = 8 : 15$.

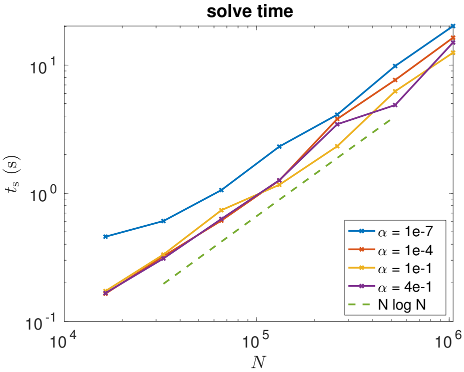


(a) Construction time.

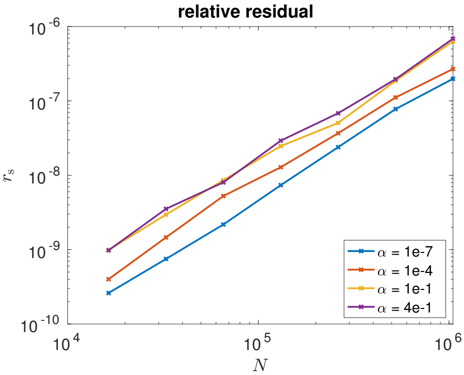


(b) Factorization time.

Direct Solver



(a) Solution time.



(b) Relative residual.

N	method	$\alpha = 1\text{e-}1$			
		t_{pre}	t_{iter}	n_{iter}	r_{s}
131072	CG	-	$\times$	$\times$	$\times$
	PCG	1.7e+02	1.4e+01	5	4.6e-13
262144	CG	-	$\times$	$\times$	$\times$
	PCG	3.4e+02	3.0e+01	5	7.4e-14
524288	CG	-	$\times$	$\times$	$\times$
	PCG	7.0e+02	5.6e+01	5	1.5e-13
1048576	CG	-	$\times$	$\times$	$\times$
	PCG	1.5e+03	1.4e+02	5	5.6e-14

Table: Time cost, iteration number and relative residual of CG and PCG when $\alpha = 0.1$. The marker "x" means iterative method does not converge in 500 steps.

Preconditioner

N	method	$\alpha = 4\text{e-}1$			
		t_{pre}	t_{iter}	n_{iter}	r_{s}
131072	CG	-	x	x	x
	PCG	1.7e+02	2.4e+01	9	1.0e-14
262144	CG	-	x	x	x
	PCG	3.4e+02	4.6e+01	8	7.1e-15
524288	CG	-	x	x	x
	PCG	7.0e+02	1.0e+02	9	4.1e-14
1048576	CG	-	x	x	x
	PCG	1.5e+03	2.1e+02	8	7.7e-13

Table: Time cost, iteration number and relative residual of CG and PCG when $\alpha = 0.4$. The marker "x" means iterative method does not converge in 500 steps.

Conclusions and Future Work

Conclusions:

- A superfast direct solver for INUDFT-III;
- The direct solver could also be used as an efficient preconditioner;
- Error bound of the forward approximation.

Future work:

- Extension to 2D and 3D problems;
- A method on regularized least-squares problem.

Thanks for listening!