Sparse Spectral Methods for Solving High-Dimensional and Multiscale Elliptic PDEs

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January 30$^{\mathrm{th}}$, 2026

Joint work with: **Craig Gross** (former Ph. D. student)

Sparse Fourier Transforms for Functions of Many Variables

Theorem (High Dim. SFT [Gross, M.I., Kämmerer, Volkmer, 2022])

Choose any finite $\mathcal{I} \subseteq \mathbb{Z}^d \cap [-K/2, K/2]^d$ you like. There exist Sparse Fourier Transform (SFT) algorithms that use samples from $g : \mathbb{T}^d \to \mathbb{C}$ (corrupted by errors at most $e_\infty > 0$ in absolute magnitude) to produce a sparse approximation $\hat{g}^s$ to $\hat{g}$ satisfying the error bounds

$$\|\hat{g}^s - \hat{g}\|_2 \lesssim K \left[\frac{\left\| \hat{g}|_{\mathcal{I}} - (\hat{g}|_{\mathcal{I}})_s^{\mathrm{opt}} \right\|_1}{\sqrt{s}} + \sqrt{s}(\|\hat{g} - \hat{g}|_{\mathcal{I}}\|_1 + e_\infty) \right]$$

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- *deterministically with complexity $\mathcal{O}(ds^2 \operatorname{polylog}(d, |\mathcal{I}|, K))$,*
- *and with high probability with complexity $\mathcal{O}(ds \operatorname{polylog}(d, |\mathcal{I}|, K))$.*

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Model periodic diffusion equation

- Consider the *stationary diffusion equation*

$$\mathcal{L}[a]u := -\nabla \cdot (a\nabla u) = f.$$

- There are three functions (assuming periodicity $\mathbb{T} := \mathbb{R}/\mathbb{Z}$):
  - $a : \mathbb{T}^d \to \mathbb{R}$ is the diffusion coefficient,
  - $f : \mathbb{T}^d \to \mathbb{R}$ is the forcing function,
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Fourier spectral methods in 3 minutes

- Substitute Fourier series for data and solution:

$$-\nabla \cdot (a(\mathrm{x}) \nabla u(\mathrm{x})) = f(\mathrm{x})$$

$$-\nabla \cdot \left(\sum_{\mathrm{l} \in \mathbb{Z}^d} \hat{a}_{\mathrm{l}} \mathrm{e}^{2\pi i \mathrm{l} \cdot \mathrm{x}} \nabla \sum_{\mathrm{k} \in \mathbb{Z}^d} \hat{u}_{\mathrm{k}} \mathrm{e}^{2\pi i \mathrm{k} \cdot \mathrm{x}} \right) = \sum_{\mathrm{j} \in \mathbb{Z}^d} \hat{f}_{\mathrm{j}} \mathrm{e}^{2\pi i \mathrm{j} \cdot \mathrm{x}}$$

$$\sum_{\mathrm{l},\mathrm{k} \in \mathbb{Z}^d} (2\pi)^2 (\mathrm{l} + \mathrm{k}) \cdot \mathrm{k}\, \hat{a}_{\mathrm{l}} \hat{u}_{\mathrm{k}} \mathrm{e}^{2\pi i (\mathrm{l}+\mathrm{k}) \cdot \mathrm{x}} = \sum_{j \in \mathbb{Z}^d} \hat{f}_{\mathrm{j}} \mathrm{e}^{2\pi i \mathrm{j} \cdot \mathrm{x}}.$$

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- Except d is huge... (1) need a subset of $\mathbb{Z}^d$... & (2) need $\hat{f}$ and $\hat{a}$
- FFTs save the day?!? They
  - enforce a basis truncation,
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Lemma (Special case of Céa/Strang's lemma [Canuto et al., 2006])

Let $\tilde{}$ denote an approximate Fourier transform algorithm, and let v have Fourier coefficients solving the matrix equation

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Then $$\|u-v\|_{H^1} \lesssim_{a,f} \|u-u|_{\mathcal{I}}\|_{H^1} + \|\hat{f}-\tilde{f}\|_2 + \|\hat{a}-\tilde{a}\|_1.$$

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1. Use an SFT to compute $\tilde{a}_{\mathrm{k}} \approx \hat{a}_{\mathrm{k}}$ on $\forall \mathrm{k}\in \mathrm{supp}(\hat{a})$.
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1. Use an SFT to compute $\tilde{a}_{\mathrm{k}} \approx \hat{a}_{\mathrm{k}}$ on $\forall \mathrm{k} \in \mathrm{supp}(\hat{a})$.
2. Use an SFT to compute $\tilde{f}_{\mathrm{k}} \approx \hat{f}_{\mathrm{k}}$ on $\forall \mathrm{k} \in \mathrm{supp}(\hat{f})$.
3. Use discovered $\mathrm{supp}(\hat{a})$ and $\mathrm{supp}(\hat{f})$ to construct a "good" set $\mathcal{I} \subset \mathbb{Z}^d$.
4. Solve (1) to find the $\hat{v}_{\mathrm{k}}$ $\forall \mathrm{k} \in \mathcal{I}$.

Error analysis

Lemma (Special case of Céa/Strang's lemma [Canuto et al., 2006])

Let $\tilde{}$ *denote an approximate Fourier transform algorithm, and let* v *have Fourier coefficients solving the matrix equation*

$$\sum_{\mathrm{k} \in \mathcal{I}} L[\tilde{a}]_{\mathrm{j},\mathrm{k}} \hat{v}_{\mathrm{k}} = \tilde{f}_{\mathrm{j}} \quad \forall \mathrm{j} \in \mathcal{I}. \tag{1}$$

Then $$\|u - v\|_{H^1} \lesssim_{a,f} \|u - u|_{\mathcal{I}}\|_{H^1} + \|\hat{f} - \tilde{f}\|_2 + \|\hat{a} - \tilde{a}\|_1.$$

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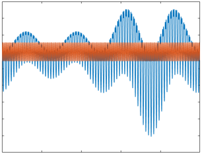
Swapping out FFTs for SFTs when $d = 1$

Choose trigonometric polynomials for data

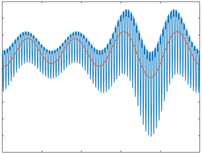
$$a(x) = 2 + \sin(2\pi x),$$
$$f(x) = \cos(2\pi 4x) - 500\cos(2\pi 75x) + 1000\cos(2\pi 150x).$$

SFT spectral method



- Each frame increases s by 1.
- Takes $s = 3$ to resolve the full solution.

DFT spectral method



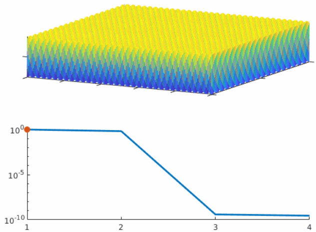
- Only parameter is bandwidth K. Increases by 2 each frame.
- Takes $K \approx 400$ to resolve the full solution.

Swapping out FFTs for SFTs when $d = 2$

Choose trigonometric polynomials for data

$$\begin{aligned} a(x, y) &= 2 + \sin(2\pi(x + 2y)), \\ f(x, y) &= \cos(2\pi(5x + 3y)) - 500\cos(2\pi(74x + 76y)) + \\ &\qquad 1000\cos(2\pi(151x + 149y)). \end{aligned}$$

SFT spectral method



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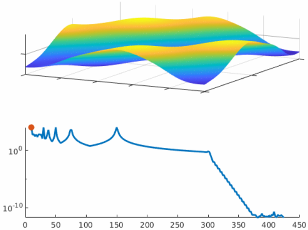


The error in the computed solutions is shown as s and K increase each frame of the respective animations. Note that each FFT requires $\mathcal{O}(K^d \log^d(K))$ operations compared to $\mathcal{O}(ds\,\text{polylog}(d, |\mathcal{I}|, K))$ for an SFT.

But How Should we Choose $\mathcal{I}$?

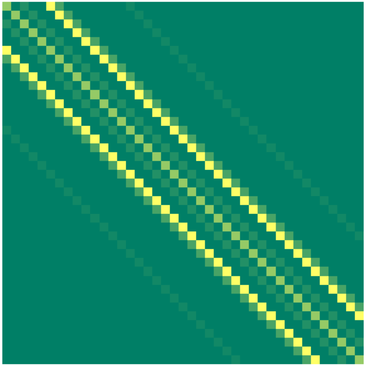
SFTs Control Last Two Terms in Céa's Lemma... & for the First...???

$$\|u - v\|_{H^1} \lesssim_{a,f} \|u - u|_{\mathcal{I}}\|_{H^1} + \|\hat{f} - \tilde{f}\|_2 + \|\hat{a} - \tilde{a}\|_1$$

- Assume data is Fourier sparse.
- Let's take a closer look at our Galerkin operator

$$L[\hat{a}] = \left((2\pi)^2 \mathrm{j} \cdot \mathrm{k} \hat{a}_{\mathrm{j}-\mathrm{k}}\right)_{\mathrm{j},\mathrm{k} \in \mathbb{Z}^d}.$$

- Only elements of $\hat{u}$ spaced out according to $\mathrm{supp}(\hat{a})$ will interact in $L[\hat{a}]\hat{u}$.



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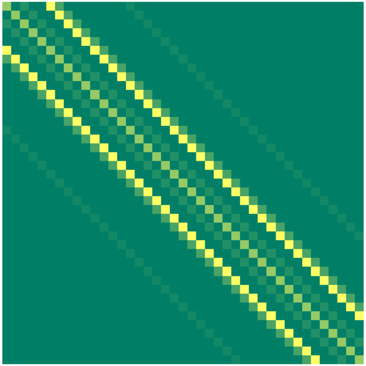

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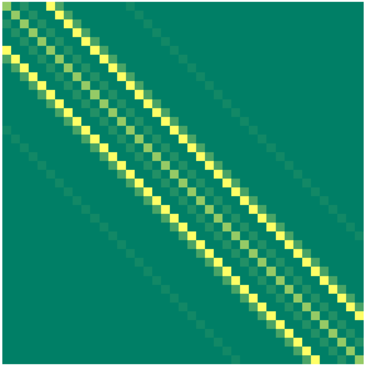
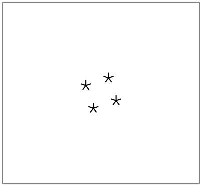


"Stamp" sets

- Consider supp($\hat{a}$).
- Now supp($\hat{f}$).
- Let

$$\mathcal{S}^N := \begin{cases} \mathrm{supp}(\hat{f}) & N = 0 \\ \mathcal{S}^{N-1} + \mathrm{supp}(\hat{a}) & N > 0. \end{cases}$$

supp($\hat{a}$)



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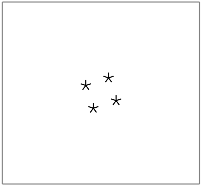

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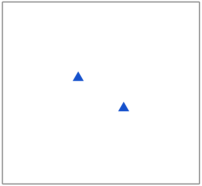

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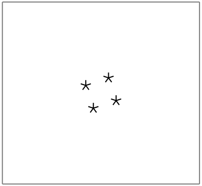

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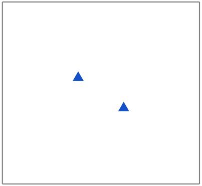

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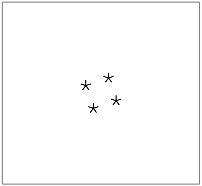

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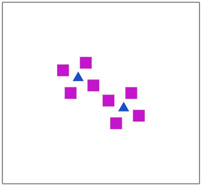

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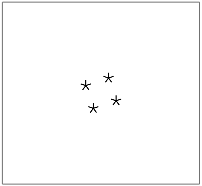
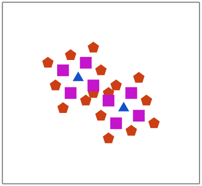


$\mathcal{S}^2$



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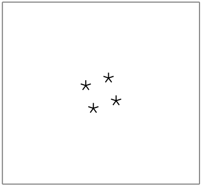

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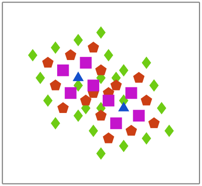

Error analysis of spectral method

Theorem (Sparse spectral algorithm [Gross, M.I., 2023])

Let a^s, f^s *be from high-dimensional SFT previously discussed, and let* $u^{s,N}$ *have Fourier coefficients solving the matrix equation*

$$\sum_{\mathrm{k}\in\mathcal{S}^N} L[\hat{a}^s]_{\mathrm{j},\mathrm{k}}\hat{u}^{s,N}_{\mathrm{k}} = \hat{f}^s_{\mathrm{j}} \quad \forall \mathrm{j}\in\mathcal{S}^N.$$

Then for a decay rate $A < 1$ *characterized by the ellipticity of* a*,*

$$\|u - u^{s,N}\|_{H^1} \lesssim_{a,f} A^{N+1} + \|\hat{f} - \hat{f}^s\|_2 + \|\hat{a} - \hat{a}^s\|_1.$$

With a randomly chosen rank-1 lattice w.h.p. we have

$$\left\|\hat{f} - \hat{f}^s\right\|_2 \lesssim K\sqrt{s}\left\|\hat{f} - \left(\hat{f}|_{[-K/2,K/2]^d}\right)^{\mathrm{opt}}_s\right\|_1$$

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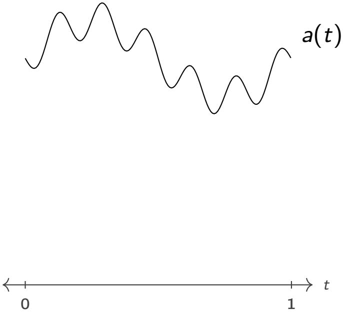
More on stamping factor



Two quantities of diffusion coefficient, a, determine exponential decay:

- Minimum: $a_{\min}$.
- Deviation from mean: $\|a - \hat{a}_0\|_{L^\infty}$.

The decay factor has the form

$$A := \frac{\|a - \hat{a}_0\|_{L^\infty}}{a_{\min} - 2\|a - \hat{a}_0\|_{L^\infty}}.$$

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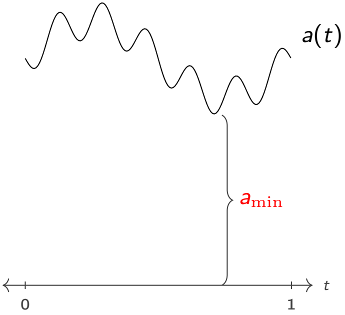

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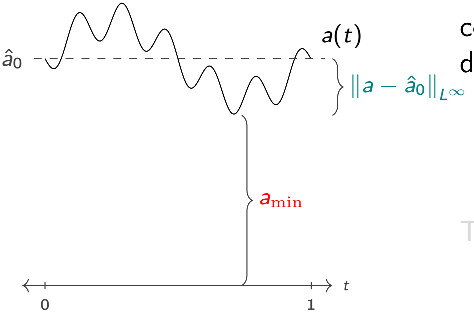

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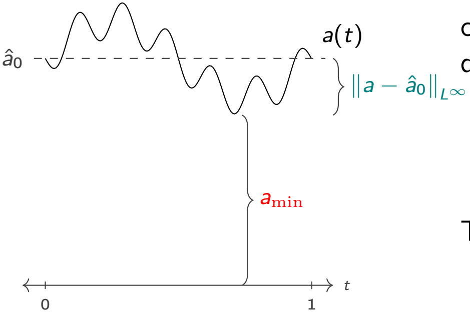

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Complexity analysis of spectral method

- The algorithm uses two SFTs and a $|\mathcal{S}^N| \times |\mathcal{S}^N|$ (sparse) matrix system solve.
- Each SFT succeeds with high probability with complexity $\mathcal{O}(ds \operatorname{polylog}(d, s, K))$.
- $|\mathcal{S}^N|$ can be upper bounded by

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- So dependence on ambient dimension is linear.
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High-dimensional example

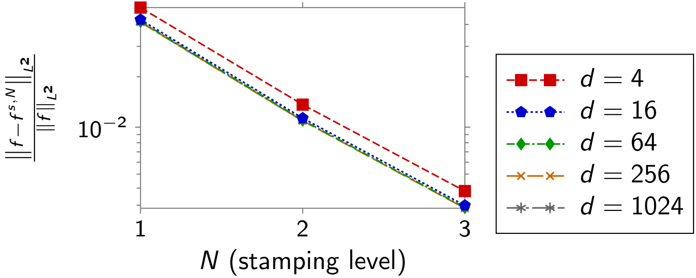


Figure: Proxy error solving $\nabla \cdot (a\nabla u) = f$

- a sparsity is 51.
- f sparsity is 2.
- Frequencies are chosen randomly in bandwidth of 1000 in each dimension.

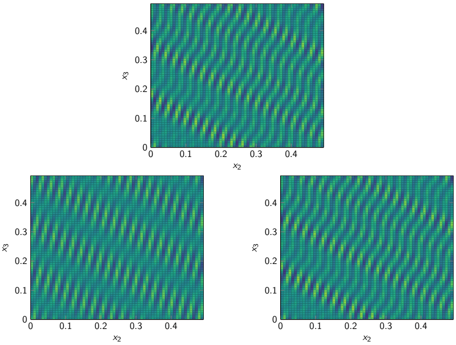
3D advection-diffusion-reaction example

$$-\nabla \cdot (a(\mathrm{x})\nabla u(\mathrm{x})) + \mathrm{b}(\mathrm{x}) \cdot \nabla u(\mathrm{x}) + c(\mathrm{x})u(\mathrm{x}) = f(\mathrm{x}).$$

Each term is $\approx$ 20 sparse for 90 total operator terms and 10 forcing terms.

s	N	$\left\|f - f^{s,N}\right\|_{L^2} / \left\|f\right\|_{L^2}$
8	1	0.518
	2	0.518
20	1	0.054
	2	0.031

Table: Error in approximating ADR solution.



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