Nonuniform FFTs at Flatiron

— $\sim *$ *OR* $* \sim$ —

Lessons from developing a small numerical library

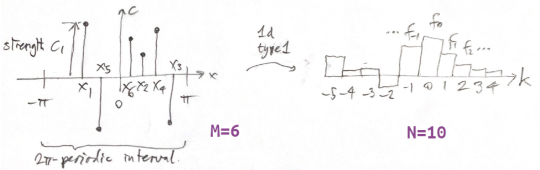
Alex Barnett[1], with much help from: Jeremy Magland[1], Ludvig af Klinteberg (Mälardalen U.), Melody Shih (NVidia), Joakim Andén (KTH), Libin Lu[1], Robert Blackwell (SCC), Andrea Malleo (Bloomberg), and many others...

FWAM5 Friday, October 20, 2023

[1]Center for Computational Mathematics, Flatiron Institute

What is this non-uniform fast Fourier transform? (NUFFT)

1D case, "type 1" transform:



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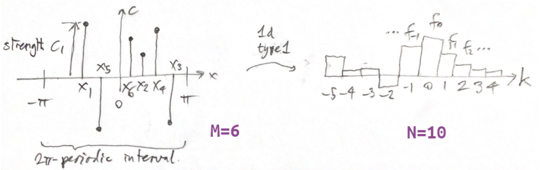

Given locations $x_1, \ldots, x_M$, and their “strengths” $c_1, \ldots, c_M$, return

$$f_k = \sum_{j=1}^{M} e^{ikx_j} c_j, \quad \text{for } k = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-2, \frac{N}{2}-1$$

- Has N outputs, each a sum of M terms: naively $\mathcal{O}(NM)$ cost (flops)
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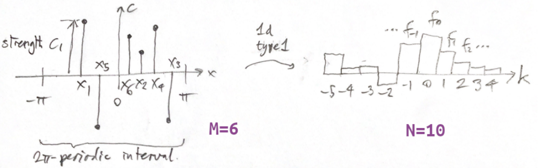

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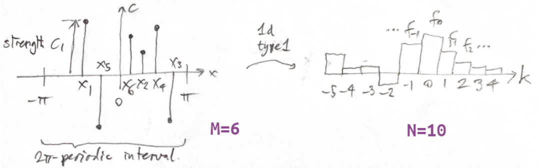

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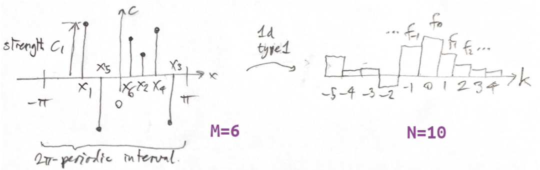

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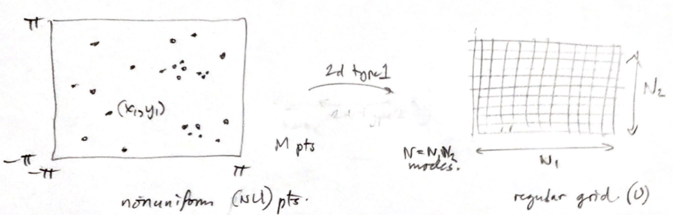
"Type 3" as type 1 but arbitrary target freqs. $\{s_k\}_{k=1}^{N}$: $f_k = \sum_{j=1}^{M} e^{is_k x_j} c_j$

NU $\to$ NU

Higher dimensions also needed

2D type 1: $f_{k,\ell} = \sum_{j=1}^{M} e^{i(kx_j + \ell y_j)} c_j$ for k, ℓ in a rectangle of modes



3D type 1: $f_{k,\ell,m} = \sum_{j=1}^{M} e^{i(kx_j + \ell y_j + mz_j)} c_j$

etc

- dimensions $\{1, 2, 3\}$ $\times$ types $\{1, 2, 3\}$ $=$ 9 transforms

  Software design: how to avoid code repetition?

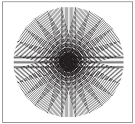
- 9 transforms $\times$ {float,double} $=$ 18 functions

  How reduce number of functions to write and maintain?

Who uses such transforms?

1) Fourier image reconstruction: $f_{k,\ell}$ is unknown pixel intensities
apparatus measures strengths c_j at nonuniform frequency points (x_j, y_j)

- MRI (either 2D slice, or 3D)
- coherent diffraction/powder imaging (X-ray)
- very long baseline interferometry (VLBI)
- cryo electron microscopy



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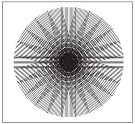

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2) Numerical forward solvers, simulation

- electrostatics or fluid problems in periodic box
  spectral Ewald method: Poisson solve trivial in Fourier space
- numerical PDE eg, interpolating between overlapping grids
- eval Fourier *transform* by numerical quadrature (type 1)
- Fresnel diffraction (optics)

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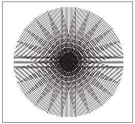

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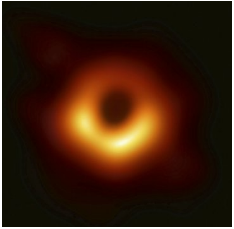
3) Spatial/temporal statistics

- power-spectrum of NU time-series, or point-masses galaxies
- fast kernel apply in Gaussian process regression

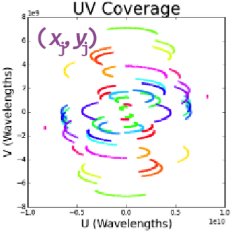
Fourier imaging example: black hole by VLBI

Probably the most famous astro image of 2019: 10^{-10} radian resolution!

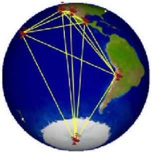


uniform image grid $f_{k,\ell}$

2D type 2 $\longrightarrow$



predicted signals $\{g_j\}$ at NU pts



Telescope Locations

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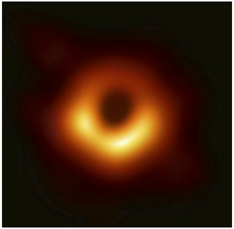

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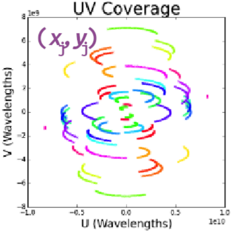

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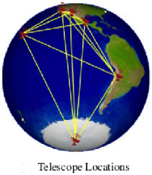

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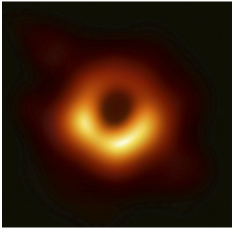

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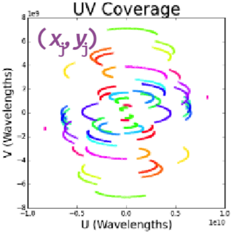

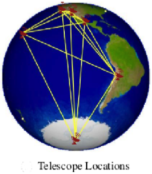

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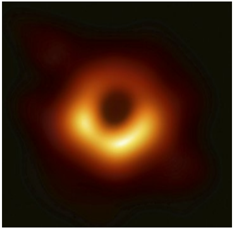

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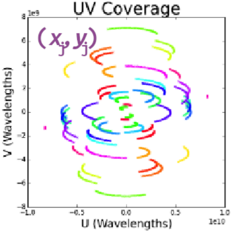

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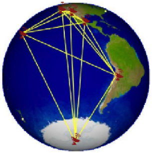

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Iterative optimization of $\boldsymbol{f}$ until it best fits the detected signal:

$$\boldsymbol{f}_{\text{recon}} = \arg\min_{\boldsymbol{f}} \|A\boldsymbol{f} - \boldsymbol{g}_{\text{detected}}\|_2^2 + \lambda_1 \|\boldsymbol{f}\|_1 + \lambda_{\text{TV}} \|\boldsymbol{f}\|_{\text{TV}}$$

- each iteration, A and A^* applied fast by NUFFTs dominant cost, I think
- same idea in other 2D or 3D Fourier imaging (MRI, cryo-EM, etc)

The most common NUFFT algorithm—and ours

(Dutt–Rokhlin '93, Steidl '98, Greengard–Lee '04, Potts et al, . . .)

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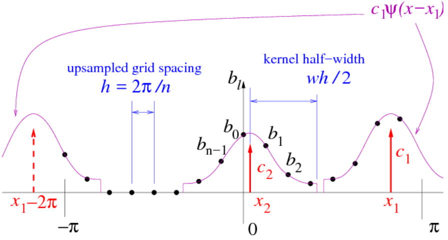

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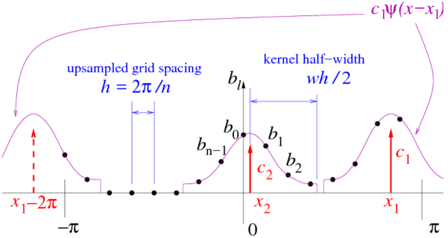

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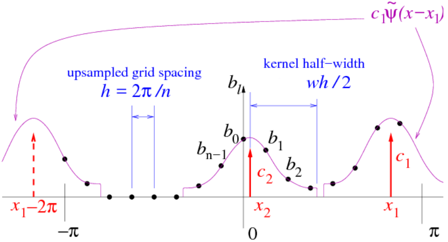

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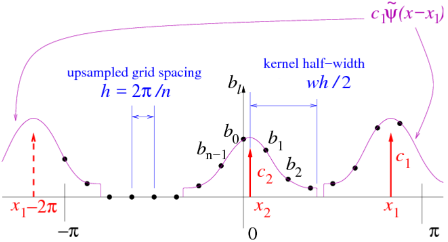

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- Type 2 reverses the steps; Type 3 is "Type 2 wrapped inside a Type 1"

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Prehistory (2015): Leslie Greengard, Jeremy Magland, Marina Spivak, myself, at SCDA

NUFFT needed for imaging (cryo-EM, etc)

had: NYU single-threaded Fortran, Gaussian kernel $\psi(x)$ too wide (Greengard–Lee '09)

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Lesson: keep a `CHANGELOG` in your repo commit messages not enough ☺

"Small" (lib = 3k lines of C++) Dive into some aspects...

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Fix: piecewise polynomial approx + Horner's rule   C gen. by MATLAB!

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Fix: piecewise polynomial approx + Horner's rule C gen. by MATLAB!

```
// Code generated by gen_all_horner_C_code.m in finufft/devel
// Authors: Alex Barnett & Ludvig af Klinteberg.
// (C) The Simons Foundation, Inc.
  if (w==2) {
    FLT c0[] = {4.5147043243215315E+01, 4.5147043243215300E+01, 0.0000000000000000E+00, 0.0000000000000000E+00};
    FLT c1[] = {5.7408070938221300E+01, -5.7408070938221293E+01, 0.0000000000000000E+00, 0.0000000000000000E+00};
    FLT c2[] = {-1.8395117920046484E+00, -1.8395117920046560E+00, 0.0000000000000000E+00, 0.0000000000000000E+00};
    FLT c3[] = {-2.0382426253182082E+01, 2.0382426253182086E+01, 0.0000000000000000E+00, 0.0000000000000000E+00};
    FLT c4[] = {-2.0940804433577420E+00, -2.0940804433577389E+00, 0.0000000000000000E+00, 0.0000000000000000E+00};
    for (int i=0; i<4; i++) ker[i] = c0[i] + z*(c1[i] + z*(c2[i] + z*(c3[i] + z*(c4[i]))));
  } else if (w==3) {
    FLT c0[] = {1.5653991189315119E+02, 8.8006872410780295E+02, 1.5653991189967152E+02, 0.0000000000000000E+00};
    FLT c1[] = {3.1653018869611077E+02, 7.4325702843759617E-14, -3.1653018868907071E+02, 0.0000000000000000E+00};
    FLT c2[] = {1.7742692790454484E+02, -3.3149255274727801E+02, 1.7742692791117119E+02, 0.0000000000000000E+00};
    FLT c3[] = {-1.5357716116473156E+01, 9.5071486252033243E-15, 1.5357716122720193E+01, 0.0000000000000000E+00};
    FLT c4[] = {-3.7757583061523668E+01, 5.3222970968867315E+01, -3.7757583054647384E+01, 0.0000000000000000E+00};
    FLT c5[] = {-3.9654011076088804E+00, 1.8062124448285358E-13, 3.9654011139270540E+00, 0.0000000000000000E+00};
    for (int i=0; i<4; i++) ker[i] = c0[i] + z*(c1[i] + z*(c2[i] + z*(c3[i] + z*(c4[i] + z*(c5[i])))));
  } else if (w==4) {
    FLT c0[] = {5.4284366850213200E+02, 1.0073871433088398E+04, 1.0073871433088396E+04, 5.4284366850213223E+02};
    FLT c1[] = {1.4650917259256939E+03, 6.1905285583602863E+03, -6.1905285583602881E+03, -1.4650917259256937E+03};
    FLT c2[] = {1.4186910680718345E+03, -1.3995339862725591E+03, -1.3995339862725598E+03, 1.4186910680718347E+03};
    FLT c3[] = {5.1133995502497419E+02, -1.4191608683682996E+03, 1.4191608683682998E+03, -5.1133995502497424E+02};
    FLT c4[] = {-4.8293622641174039E+01, 3.9393732546135226E+01, 3.9393732546135816E+01, -4.8293622641174061E+01};
    FLT c5[] = {-7.8386867802392288E+01, 1.4918904800408930E+02, -1.4918904800408751E+02, 7.8386867802392359E+01};
    FLT c6[] = {-1.0039212571700894E+01, 5.0626747735616746E+00, 5.0626747735625512E+00, -1.0039212571700640E+01};
    for (int i=0; i<4; i++) ker[i] = c0[i] + z*(c1[i] + z*(c2[i] + z*(c3[i] + z*(c4[i] + z*(c5[i] + z*(c6[i]))))));
  } else if (w==5) {
    FLT c0[] = {9.9223677575398392E+02, 3.7794697666613320E+04, 9.8715771010760494E+04, 3.7794697666613283E+04, 9.9223
677575398403E+02, 0.0000000000000000E+00, 0.0000000000000000E+00, 0.0000000000000000E+00};
-:---  ker_horner_allw_loop.c   Top L1   Git-master  (C/*l WS Abbrev)
```

- GCC/ICC compilers SIMD-vectorize this; get 400-700 M evals/sec/core
- think hard re SIMD, but avoid maintaining intrinsics `immintrin.h`
- are exploring custom AVX512 (Wenda Zhou + R. Blackwell)

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Performance: spreading

The *order* in which NU points spread to grid has big effect on speed!

- bin-sort NU pts (into $16 \times 4 \times 4$ cuboids of grid)
- process all pts in bin 1, then bin 2, ... good for keeping grid in cache (J. Magland)
- multithreaded the bin-sort (2023: M. Reinecke speeds it up!)

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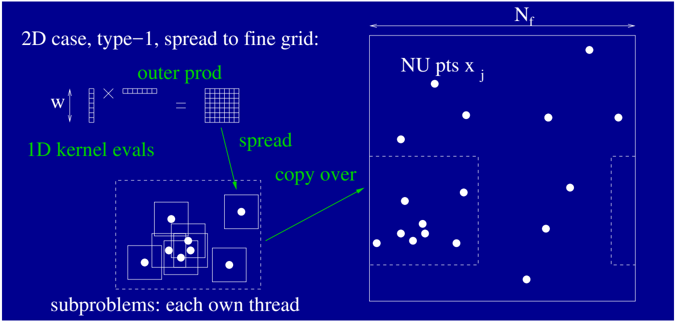
Load-balanced multithreading (also collab with J. Magland)

Type-2 easy: OpenMP parallel over NU pts no collisons reading from U blocks

Type-1 not so: writes collide! load-balance via "subproblems" each of 10^4 NU pts



Interface—how it evolved

2017: I wanted simple, familiar to users in C/Fortran   and match NYU code

C-compatible: pass pointers, explicit array sizes, return value is error code...

```
int M = 1e8;                                        // number of nonuniform points
vector<double>           x(M);                      // NU pts
vector<complex<double> > c(M);                      // NU strengths
// (here user fills x and c as they like)
int N = 1e7;                                        // number of output modes
vector<complex<double> > f(N);                      // allocate output array
int status = finufft1d1(M, &x[0], &c[0], +1, 1e-9, N, &f[0], NULL);   // do it
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4-function pattern: Create plan, Set the NU pts, Execute transform(s), Destroy plan.

`finufft_plan`: "opaque" pointer to (private) C++ struct. (as in Brian's talk)

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Lesson: learn about public vs private headers, namespacing (as I had to)

Lesson: think hard about interface, break it VERY rarely!

help users: preserve all simple and batch interfaces (they call guru)

Wrappers to other languages: expands user base

Guru interface made wrapping easier: just wrap 4 funcs, pass opaque ptr

write the simple and batched functions via a few lines *in each high-level language*

MATLAB/Octave (Libin Lu)

simple for users `f = finufft1d1(x,c,+1,1e-9,N);`

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- served well for a while. But eg forced recompile of `libfinufft.so`

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Others have wrapped (cu)FINUFFT in autodiff frameworks:
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Julia wrapper is separate repo: helps separate concerns (L. af Klinteberg)

Lessons: each new language brings installation troubles linux/OSX/Windows

Testing

Need tests that check accuracy for all transforms   fail if measured error $\geq 10\varepsilon$?

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> make test              [includes bunch of edge cases M=0, N=0, eps=0.0, etc...]
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Such speed and accuracy testers are crucial for progress

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thus: each C++ test driver now uses exit code 0 for success, 1 for fail

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Continuous Integration (CI)   each GitHub push reruns tests: C++ Build passing

Jenkins (was using makefile, now uses CMake)

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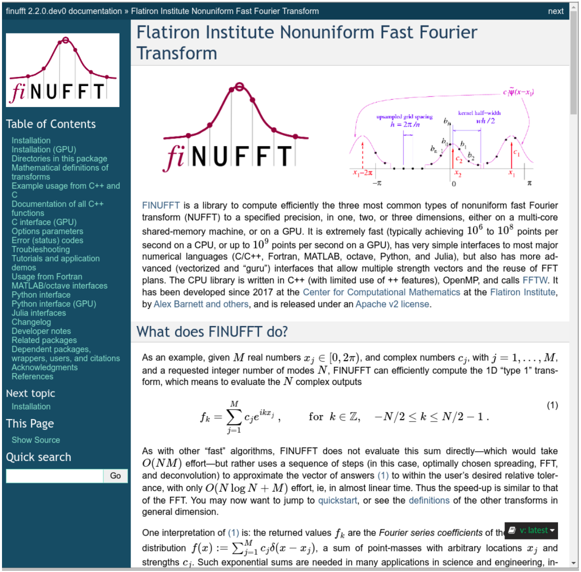
Documentation

`README.md`, or a `.tex` file to PDF, fine for small project, but:



finufft 2.2.0.dev0 documentation » Flatiron Institute Nonuniform Fast Fourier Transform next

fiNUFFT

Table of Contents

Next topic

Installation

This Page

Show Source

Quick search

Go

Flatiron Institute Nonuniform Fast Fourier Transform

FINUFFT is a library to compute efficiently the three most common types of nonuniform fast Fourier transform (NUFFT) to a specified precision, in one, two, or three dimensions, either on a multi-core shared-memory machine, or on a GPU. It is extremely fast (typically achieving 10^6 to 10^8 points per second on a CPU, or up to 10^9 points per second on a GPU), has very simple interfaces to most major numerical languages (C/C++, Fortran, MATLAB, octave, Python, and Julia), but also has more advanced (vectorized and "guru") interfaces that allow multiple strength vectors and the reuse of FFT plans. The CPU library is written in C++ (with limited use of ++ features), OpenMP, and calls FFTW. It has been developed since 2017 at the Center for Computational Mathematics at the Flatiron Institute, by Alex Barnett and others, and is released under an Apache v2 license.

What does FINUFFT do?

As an example, given M real numbers $x_j \in [0, 2\pi)$, and complex numbers c_j, with $j = 1, \ldots, M$, and a requested integer number of modes N, FINUFFT can efficiently compute the 1D "type 1" transform, which means to evaluate the N complex outputs

$$f_k = \sum_{j=1}^{M} c_j e^{ikx_j}\,, \qquad \text{for } k \in \mathbb{Z}, \quad -N/2 \le k \le N/2 - 1\,. \qquad (1)$$

As with other "fast" algorithms, FINUFFT does not evaluate this sum directly—which would take $O(NM)$ effort—but rather uses a sequence of steps (in this case, optimally chosen spreading, FFT, and deconvolution) to approximate the vector of answers (1) to within the user's desired relative tolerance, with only $O(N \log N + M)$ effort, ie, in almost linear time. Thus the speed-up is similar to that of the FFT. You may now want to jump to quickstart, or see the definitions of the other transforms in general dimension.

One interpretation of (1) is: the returned values f_k are the *Fourier series coefficients* of th[...] v: latest distribution $f(x) := \sum_{j=1}^{M} c_j \delta(x - x_j)$, a sum of point-masses with arbitrary locations x_j and strengths c_j. Such exponential sums are needed in many applications in science and engineering, in-

Web-facing essential for professionalism

- math definitions
- installation
- examples
- tutorial cases
- troubleshooting
- devnotes

. . .

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Documentation: lessons

- Decent solution I recommend: sphinx, host at `readthedocs.io`

  `docs/*.rst` ReStructuredText, in master branch (unlike GHpages)

  LaTeX math pretty good via `mathjax`, `texext`

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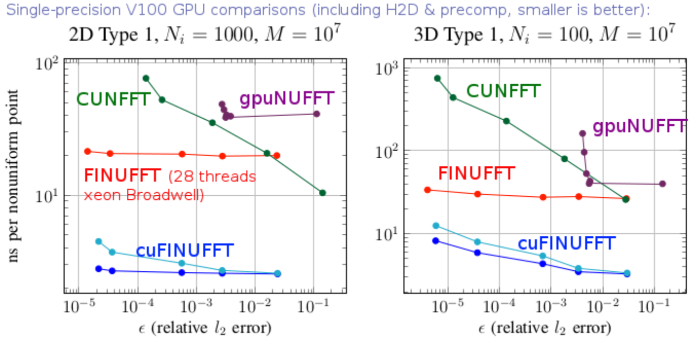
- Always update docs *at the time you change the source*

GPU version

`cuFINUFFT`: CUDA called from C++ (Melody Shih, intern '18, '19 [NYU→NVidia])



- spreading done in shared memory (subproblems), not global memory

(Shih et al, PDSEC 2021, best paper prize)

2023: cleaned up GPU lib (+tests,...) into `FINUFFT` repo (R. Blackwell)

Future: language interfaces auto-detect GPU arrays?

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Conclusions: developing a small(ish) library

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Installation, dependencies & language wrappers takes much of our time!
- helps users, but needs a team (linux,OSX,Windows). Your choice.

  Eg: guess which language wrapper SMILI black hole astro code uses?
- still plenty of fun with math & floating-point speed hacking!

Thank-you!

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