finufft Documentation

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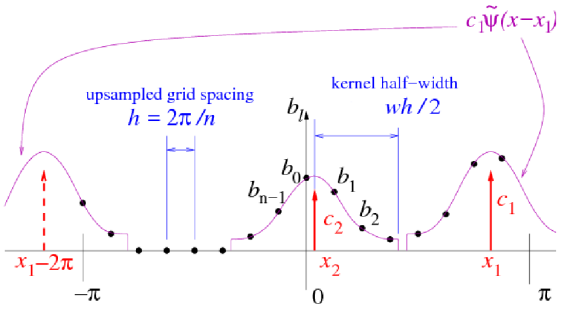

FINUFFT is a multi-threaded library to compute efficiently the three most common types of nonuniform fast Fourier transform (NUFFT) to a specified precision, in one, two, or three dimensions, on a multi-core shared-memory machine. It is extremely fast (typically achieving 10^6 to 10^8 points per second), 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. It is written in C++ (with limited use of ++ features), OpenMP, and uses FFTW. It has been developed at the Center for Computational Mathematics at the Flatiron Institute, by *Alex Barnett and others*, and is released under an Apache v2 license.

CHAPTER

ONE

WHAT DOES FINUFFT DO?

As an example, given M arbitrary real numbers x_j and complex numbers c_j, with $j = 1, \dots, M$, and a requested integer number of modes N, FINUFFT computes the 1D type 1 (aka "adjoint") transform, which means it evaluates the N numbers

$$f_k = \sum_{j=1}^{M} c_j e^{ikx_j} \ , \qquad \text{for } \ k \in \mathbb{Z}, \quad -N/2 \le k \le N/2 - 1 \ . \tag{1.1}$$

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 (1.1) to within the user's desired relative tolerance with only $O(N \log N + M)$ effort, ie, quasi-linear. Thus the speed-up is similar to that of the FFT. You may want to jump to *quickstart*, or see the *definitions* of the type 2 and 3 transforms, and 2D and 3D cases.

One interpretation of (1.1) is: the returned values f_k are the *Fourier series coefficients* of the 2π-periodic 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, including signal processing (scattered data interpolation, applying convolutional transforms, fast summation), imaging (cryo-EM, CT, MRI gridding, coherent diffraction, VLBI astronomy), and numerical analysis (computing Fourier *transforms* of functions, moving between non-conforming quadrature grids, solving partial differential equations). See our *tutorials and demos* pages and the *related works* for examples of how to use the NUFFT in applications. In fact, there are several application areas where it has been overlooked that the needed computation is simply a NUFFT (eg, particle-mesh Ewald in molecular dynamics).

CHAPTER

TWO

WHY FINUFFT? FEATURES AND COMPARISON AGAINST OTHER NUFFT LIBRARIES

The basic scheme used by FINUFFT is not new, but there are many mathematical and software engineering improvements over other libraries. As is common in NUFFT algorithms, under the hood is an FFT on a regular "fine" (upsampled) grid—the user has no need to access this directly. Nonuniform points are either spread to, or interpolated from, this fine grid, using a specially designed kernel (see right figure above). Our main features are:

- **High speed**. For instance, at similar accuracy, FINUFFT is up to 10x faster than the multi-threaded Chemnitz NFFT3 library, and (in single-thread mode) up to 50x faster than the CMCL NUFFT library. This is achieved via:
  1. a simple new "exponential of semicircle" kernel that is provably close to optimal
  2. quadrature approximation for this kernel's Fourier transform
  3. load-balanced multithreaded spreading/interpolation (see left figure above)
  4. bin-sorting of points to improve cache reuse
  5. a low upsampling option for smaller FFTs, especially in type 3 transforms
  6. piecewise polynomial kernel evaluation (additions and multiplications only) that SIMD-vectorizes reliably on open-source compilers
- **Less RAM**. Our kernel is so fast that there is no point in precomputation; it is always evaluated on the fly. Thus our memory footprint is often an order of magnitude less than the fastest (precomputed) modes of competitors such as NFFT3 and MIRT, especially at high accuracy.
- **Automated kernel parameters**. Unlike many competitors, we do not force the user to worry about kernel choice or parameters. The user simply requests a desired relative accuracy, then FINUFFT chooses parameters that achieve this accuracy as fast as possible.
- **Simplicity**. We provide interfaces that perform a NUFFT with a single command—just like an FFT—from seven common languages/environments. For advanced users we also have "many vector" interfaces that can be much faster than repeated calls to the simple interface with the same points. Finally (like NFFT3) we have a "guru" interface for maximum flexibility, in all of these languages.

For technical details on much of the above see our *papers*. Note that there are other tasks (eg, transforms on spheres, inverse NUFFTs) provided by other libraries, such as NFFT3, that FINUFFT does not provide.

CHAPTER

THREE

DO I EVEN NEED A NUFFT?

A user's need for a nonuniform fast Fourier transform is often obscured by the lack of mathematical description in science application areas. Therefore, read our *tutorials and demos* to try and match to your task. Write the task in terms of one of the *three transform types*. If both M and N are larger than of order 10^2, FINUFFT should be the ticket. However, if M and/or N is small (of order 10 or less), there is no need for a "fast" algorithm: simply evaluate the sums directly.

If you need to fit off-grid data to a Fourier representation (eg, if you have off-grid $\mathbf{k}$-space samples of an unknown image) but you do not have *quadrature weights* for the off-grid points, you may need to *invert* the NUFFT, which actually means solving a large linear system; see the *tutorials and demos* and *references* [GLI] [KKP]. Poor coverage of the nonuniform point set leads to ill-conditioning and a heavy reliance on regularization.

Another scenario is that you wish to evaluate a forward transform such as (1.1) repeatedly with the same set of nonuniform points x_j, but *fresh* strength vectors $\{c_j\}_{j=1}^M$, as in the "many vectors" interface mentioned above. For small such problems it may be even faster to fill an N-by-M matrix A with entries $a_{kj} = e^{ikx_j}$, then use BLAS3 (eg `ZGEMM`) to compute $F = AC$, where each column of F and C is a new instance of (1.1). If you have very many columns this can be competitive with a NUFFT even for M and N up to 10^4, because BLAS3 is so fast.

CHAPTER

FOUR

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4.1 Installation

4.1.1 Quick linux install instructions

In brief, go to the github page https://github.com/flatironinstitute/finufft and follow instructions to download the source (eg see the green button). Make sure you have packages `fftw3` and `fftw3-devel` installed. Then `cd` into your FINUFFT directory and `make test`, or `make test -j8` for a faster build. This should compile the static library in `lib-static/`, some C++ test drivers in `test/`, then run them, printing some terminal output ending in:

```
0 fails out of 8 tests done
```

If this fails see the more detailed instructions below. If it succeeds, run `make lib` and proceed to link to the library. Alternatively, try one of our precompiled linux and OSX binaries. Type `make` to see a list of other aspects to build (examples, language interfaces, etc). Please read Usage and look in `examples/` and `test/` for other usage examples.

4.1.2 Dependencies

This library is fully supported for unix/linux and almost fully on Mac OSX. We have also heard that it can be compiled under Windows using MinGW; we also suggest trying within the Windows Subsystem for Linux (WSL).

For the basic libraries you need

- C++ compiler, such as `g++` packaged with GCC, or `clang` with OSX
- FFTW3 including its development libraries
- GNU `make` and other standard unix/POSIX tools such as `bash`

Optional:

- for Fortran wrappers: compiler such as `gfortran`
- for MATLAB/octave wrappers: MATLAB, or octave and its development libraries
- for the python wrappers you will need `python` (it is assumed you have python v3; v2 is unsupported). You will also need the python module `pybind11`
- for rebuilding new matlab/octave wrappers (experts only): `mwrap` version>=0.33.10

4.1.3 Tips for installing dependencies on linux

On a Fedora/CentOS linux system, dependencies can be installed as follows:

```
sudo yum install make gcc gcc-c++ gcc-gfortran fftw3 fftw3-devel libgomp octave␣
↪octave-devel
```

Note: we are not exactly sure how to install python3 and pip3 using yum

Alternatively, on Ubuntu linux:

```
sudo apt-get install make build-essential libfftw3-dev gfortran python3 python3-pip␣
↪octave liboctave-dev
```

You should then compile via the various `make` tasks, eg `make test -j8` then checking you got `0 fails`.

Note: GCC versions on linux. Rather than using the default GCC which may be as old as 4.8 or 5.4 on current linux systems, we **strongly** recommend you compile with a recent GCC version such as GCC 7.3 (which we used benchmarks in our SISC paper), or GCC 9+. We do not recommend GCC versions prior to 7. We also **do not recommend GCC8** since its auto vectorization has worsened, and its kernel evaluation rate using the default looped piecewise-polynomial Horner code drops to less than 150 Meval/s/core on an i7. This contrasts 400-700 Meval/s/core achievable with GCC7 or GCC9 on i7. If you wish to test these raw kernel evaluation rates, do into `devel/`, compile `test_ker_ppval.cpp` and run `fig_speed_ker_ppval.m` in MATLAB. We are unsure if GCC8 is poor in Mac OSX (see below).

4.1.4 Tips for installing dependencies and compiling on Mac OSX

Note: Improved Mac OSX instructions, and possibly a brew package, will come shortly. Stay tuned. The below has been tested on 10.14 (Mojave) with both clang and gcc-8.

First you'll want to set up Homebrew, as follows. If you don't have Xcode, install Command Line Tools (this is only around 130 MB in contrast to the full 6 GB size of Xcode), by opening a terminal (from `/Applications/Utilities/`) and typing:

```
xcode-select --install
```

You will be asked for an administrator password. Then, also as an administrator, install Homebrew by pasting the installation command from https://brew.sh

Then do:

```
brew install libomp fftw
```

This happens to also install the latest GCC, which is 8.2.0 in our tests.

Note: There are two options for compilers: 1) the native `clang` which works with octave but will *not* so far allow you to link against fortran applications, or 2) GCC, which will allow fortran linking with `gfortran`, but currently fails with octave.

First the **clang route**, which is the default. Once you have downloaded FINUFFT, to set up for this, do:

```
cp make.inc.macosx_clang make.inc
```

This gives you compile flags that should work with `make test` and other tasks. Please try `make test` at this point, and check for `0 fails`. Then for python (note that pip is not installed with the default python v2):

```
brew install python3
pip3 install numpy pybind11
make python
```

This should generate the `finufft` module. However, we have found that it may fail with an error about `-lstdc++`, in which case you should try setting an environment variable:

```
export MACOSX_DEPLOYMENT_TARGET=10.14
```

We have also found that running:

```
pip3 install .
```

in the command line can work even when `make python` does not (probably to do with environment variables). Octave interfaces work out of the box:

```
brew install octave
make octave
```

Look in `make.inc.macosx_*`, and see below, for ideas for building MATLAB MEX interfaces.

Alternatively, here's the **GCC route**, which we have also tested on Movaje:

```
cp make.inc.macosx_gcc-8 make.inc
```

You must now by hand edit `python/setup.py`, changing `gcc` to `gcc-8` and `g++` to `g++-8`. Then proceed as above with python3. `make fortran` in addition to the above (apart from octave) should now work.

Note: Choosing GCC-8 in OSX there is a problem with octave MEX compilation. Please help if you can!

4.1.5 Details about compilation and tests

The make tasks (eg `make lib`) compiles double and single precision functions, which live simultaneously in `libfinufft`, with distinct function names.

The only selectable option at compile time is multithreaded (default, using OpenMP) vs single-threaded (to achieve this append `OMP=OFF` to the make tasks). Since you may always set `opts.nthreads=1` when calling the multithreaded library, the point of having a single-threaded library is mostly for small repeated problems to avoid any OpenMP overhead, or for debugging purposes. You *must* do at least `make objclean` before changing this threading option.

Note: By default, neither the multithreaded or single-threaded library (e.g. made by `make lib OMP=OFF`) are thread-safe, due to the FFTW3 plan stage. However, see below for the compiler option to fix this if you have a recent FFTW3 version.

If you have a nonstandard unix environment (eg a Mac) or want to change the compiler or its flags, then place your compiler and linking options in a new file `make.inc`. For example such files see `make.inc.*`. See the text of `makefile` for discussion of what can be overridden.

Compile and do a rapid (few seconds duration) test of FINUFFT via:

```
make test
```

This should compile the main libraries then run double- and single-precision tests which should report zero segfaults and zero fails. Its initial test is `test/basicpassfail` which is the most basic smoke test, producing the exit code 0 if success, nonzero if fail. You can check the exit code thus:

```
test/basicpassfail; echo $?
```

The make task also runs `(cd test; ./check_finufft.sh)` which is the main validation of the library in double precision, and `(cd test; ./check_finufft.sh SINGLE)` which does it in single precision. Text (and stderr) outputs are written into `test/results/*.out`.

Use `make perftest` for larger spread/interpolation and NUFFT tests taking 10-20 seconds. This writes log files into `test/results/` where you will be able to compare to results from standard CPUs.

Run `make` without arguments for full list of possible make tasks.

`make examples` to compile and run the examples for calling from C++ and from C.

`make fortran` to compile and run the fortran wrappers and examples.

Here are all the **compile flags** that the FINUFFT source responds to. Active them by adding a line of the form `CFLAGS+=-DMYFLAG` in your `make.inc`:

- `-DFFTW_PLAN_SAFE`: This makes FINUFFT call `fftw_make_planner_thread_safe()` as part of its FFTW3 planner stage; see http://www.fftw.org/fftw3_doc/Thread-safety.html. This makes FINUFFT thread-safe. This is only available in FFTW version >=3.3.5; for this reason it is not the default.
- `-DSINGLE`: This is internally used by our build process to switch (via preprocessor macros) the source from double to single precision. You should not need to use this flag yourself.

If there is an error in testing on a standard set-up, please file a bug report as a New Issue at https://github.com/flatironinstitute/finufft/issues

4.1.6 Building MATLAB/octave wrappers, including in Mac OSX

`make matlab` to build the MEX interface to matlab.

`make octave` to build the MEX-like interface to octave.

We have had success in Mac OSX Mojave compiling the octave wrapper out of the box. For MATLAB, the MEX settings may need to be overridden: edit the file `mex_C++_maci64.xml` in the MATLAB distro, to read, for instance:

```
CC="gcc-8"
CXX="g++-8"
CFLAGS="-ansi -D_GNU_SOURCE -fexceptions -fPIC -fno-omit-frame-pointer -pthread"
CXXFLAGS="-ansi -D_GNU_SOURCE -fPIC -fno-omit-frame-pointer -pthread"
```

These settings are copied from the `glnxa64` case. Here you will want to replace the compilers by whatever version of GCC you
or the default gcc/g++ that are aliased to clang.

For pre-2016 MATLAB Mac OSX versions you'll instead want to edit the `maci64` section of `mexopts.sh`.

4.1.7 Building the python wrappers

First make sure you have python3 and pip3 (or python and pip) installed, and that you can already compile the C++ library (eg via `make test`). Next make sure you have NumPy and pybind11 installed:

```
pip install numpy pybind11
```

You may then do `make python` which calls `pip` for the install then runs some tests and examples. An additional performance test you could then do is:

```
python python/test/run_speed_tests.py
```

Note our new (v2.0) python interface is now quite different from the Dan Foreman-Mackey's original repo that wrapped finufft: python-finufft

A few words about python environments

There can be confusion and conflicts between various versions of python and installed packages. It is therefore a very good idea to use virtual environments. Here's a simple way to do it (after installing python-virtualenv):

```
Open a terminal
virtualenv -p /usr/bin/python3 env1
. env1/bin/activate
```

Now you are in a virtual environment that starts from scratch. All pip installed packages will go inside the env1 directory. (You can get out of the environment by typing `deactivate`). Also see documentation for `conda`. In both cases `python` will call the version of python you set up, which these days should be v3.

4.2 Directories in this package

When you `git clone https://github.com/flatironinstitute/finufft`, or unpack a tar ball, you will get the following. (Please see *installation* instructions)

Main library source:

- `makefile` : the single GNU makefile (there are no makefiles in subdirectories)
- `make.inc.*` : system-specific example overrides to use as your `make.inc`
- `src` : main library C++ sources
- `include` : header files, including those for users to compile against
- `contrib` : 3rd-party codes in the main library
- `lib` : dynamic (`.so`) library will be built here
- `lib-static` : static (`.a`) library will be built here

Examples, tutorials, and docs:

- `examples` : simple example codes for calling the library from C++ and C
- `tutorial` : application demo codes (various languages), supporting `docs/tutorial/`
- `finufft-manual.pdf` : the manual (auto-generated by sphinx, eg via `make docs`)
- `docs` : source files for documentation (`.rst` files are human-readable, kinda)
- `README.md` : github-facing (and human text-only reader) welcome

- `LICENSE` : how you may use this software
- `CHANGELOG` : list of changes, release notes
- `TODO` : list of things needed to fix or extend (also see git Issues)

Testing:

- `test` : main validation tests (C++/bash), including:
  - `test/basicpassfail{f}` simple smoke test with exit code
  - `test/check_finufft.sh` is the main pass-fail validation bash script
  - `test/results` has validation comparison outputs (`\*.refout`; do not remove these), and local test outputs (`\*.out`; you may remove these)
- `perftest` : main performance and developer tests (C++/bash), including:
  - `test/spreadtestnd.sh` spread/interp performance test bash script
  - `test/nuffttestnd.sh` NUFFT performance test bash script

Other language interfaces, further testing:

- `fortran` : wrappers and example drivers for Fortran (see `fortran/README`)
- `matlab` : MATLAB/octave wrappers, tests, and examples
- `python` : python wrappers, examples, and tests
  - `python/ci` continuous integration tests
- `julia` : (not yet functional; for now see FINUFFT.jl)

4.3 Mathematical definitions of transforms

We use notation with a general space dimensionality d, which will be 1, 2, or 3, in our library. The arbitrary (ie nonuniform) points in space are denoted $\mathbf{x}_j \in \mathbb{R}^d$, $j = 1, \dots, M$. We will see that for type 1 and type 2, without loss of generality one could restrict to the periodic box $[-\pi, \pi)^d$. For type 1 and type 3, each such NU point carries a given associated strength $c_j \in \mathbb{C}$. Type 1 and type 2 involve the Fourier "modes" (Fourier series coefficients) with integer indices lying in the set

$$K = K_{N_1,\dots,N_d} := K_{N_1} K_{N_2} \dots K_{N_d} \ ,$$

where

$$K_{N_i} := \begin{cases} \{-N_i/2, \dots, N_i/2 - 1\}, & N_i \text{ even}, \\ \{-(N_i-1)/2, \dots, (N_i-1)/2\}, & N_i \text{ odd}. \end{cases}$$

For instance, $K_{10} = \{-5, -4, \dots, 4\}$, whereas $K_{11} = \{-5, -4, \dots, 5\}$. Thus, in the 1D case K is an interval containing N_1 integer indices, in 2D it is a rectangle of $N_1 N_2$ index pairs, and in 3D it is a cuboid of $N_1 N_2 N_3$ index triplets.

Then the type 1 (nonuniform to uniform, aka "adjoint") NUFFT evaluates

$$f_{\mathbf{k}} := \sum_{j=1}^{M} c_j e^{\pm i \mathbf{k} \cdot \mathbf{x}_j} \qquad \text{for } \mathbf{k} \in K \tag{4.1}$$

This can be viewed as evaluating a set of Fourier series coefficients due to sources with strengths c_j at the arbitrary locations $\mathbf{x}_j$. Either sign of the imaginary unit in the exponential can be chosen in the interface. Note that our normalization differs from that of references [DR,GL].

The type 2 (U to NU, aka "forward") NUFFT evaluates

$$c_j := \sum_{\mathbf{k}\in K} f_{\mathbf{k}} e^{\pm i \mathbf{k}\cdot\mathbf{x}_j} \qquad \text{for } j = 1,\dots,M \tag{4.2}$$

This is the adjoint of the type 1, ie the evaluation of a given Fourier series at a set of arbitrary points. Both type 1 and type 2 transforms are invariant under translations of the NU points by multiples of 2π, thus one could require that all NU points live in the origin-centered box $[-\pi,\pi)^d$. In fact, as a compromise between library speed, and flexibility for the user (for instance, to avoid boundary points being flagged as outside of this box due to round-off error), our library only requires that the NU points lie in the three-times-bigger box $\mathbf{x}_j \in [-3\pi, 3\pi]^d$. This allows the user to choose a convenient periodic domain that does not touch this three-times-bigger box. However, there may be a slight speed increase if most points fall in $[-\pi,\pi)^d$.

Finally, the type 3 (NU to NU) transform does not have restrictions on the NU points, and there is no periodicity. Let $\mathbf{x}_j \in \mathbb{R}^d$, $j = 1,\dots,M$, be NU locations, with strengths $c_j \in \mathbb{C}$, and let $\mathbf{s}_k$, $k = 1,\dots,N$ be NU frequencies. Then the type 3 transform evaluates:

$$f_{\mathbf{k}} := \sum_{j=1}^{M} c_j e^{\pm i \mathbf{s}_k\cdot\mathbf{x}_j} \qquad \text{for } k = 1,\dots,N \tag{4.3}$$

For all three transforms, the computational effort scales like the product of the space-bandwidth products (real-space width times frequency-space width) in each dimension. For type 1 and type 2 this means near-linear scaling in the total number of modes $N := N_1 \dots N_d$. However, be warned that for type 3 this means that, even if N and M are small, if the product of the tightest intervals enclosing the coordinates of $\mathbf{x}_j$ and $\mathbf{s}_k$ is large, the algorithm will be inefficient. For such NU points, a direct sum should be used instead.

We emphasise that the NUFFT tasks that this library performs should not be confused with either the discrete Fourier transform (DFT), the (continuous) Fourier transform (although it may be used to approximate this via a quadrature rule), or the inverse NUFFT (the iterative solution of the linear system arising from nonuniform Fourier sampling, as in, eg, MRI). It is also important to know that, for NU points, *the type 1 is not the inverse of the type 2*. See the references for clarification.

4.4 Example usage from C++ and C

4.4.1 Quick-start example in C++

Here's how to perform a 1D type-1 transform in double precision from C++, using STL complex vectors. First include our header, and some others needed for the demo:

```
#include "finufft.h"
#include <vector>
#include <complex>
#include <stdlib.h>
```

We need nonuniform points `x` and complex strengths `c`. Let's create random ones for now:

```
int M = 1e7;                                    // number of nonuniform points
vector<double> x(M);
vector<complex<double> > c(M);
complex<double> I = complex<double>(0.0,1.0);   // the imaginary unit
for (int j=0; j<M; ++j) {
  x[j] = M_PI*(2*((double)rand()/RAND_MAX)-1); // uniform random in [-pi,pi)
  c[j] = 2*((double)rand()/RAND_MAX)-1 + I*(2*((double)rand()/RAND_MAX)-1);
}
```

With N as the desired number of Fourier mode coefficients, allocate their output array:

```
int N = 1e6;                                    // number of output modes
vector<complex<double> > F(N);
```

Now do the NUFFT (with default options, indicated by the NULL in the following call). Since the interface is C-compatible, we pass pointers to the start of the arrays (rather than C++-style vector objects), and also pass N:

```
int ier = finufft1d1(M,&x[0],&c[0],+1,1e-9,N,&F[0],NULL);
```

This fills F with the output modes, in increasing ordering with the integer frequency indices from -N/2 up to N/2-1 (since N is even; for odd is would be -(N-1)/2 up to (N-1)/2). The transform (10^7 points to 10^6 modes) takes 0.4 seconds on a laptop. The index is thus offset by N/2 (this is integer division in the odd case), so that frequency k is output in F[N/2 + k]. Here +1 sets the sign of i in the exponentials (see *definitions*), 1e-9 requests 9-digit relative tolerance, and ier is a status output which is zero if successful (otherwise see *error codes*).

Note: FINUFFT works with a periodicity of 2π for type 1 and 2 transforms; see *definitions*. For example, nonuniform points $x = \pm\pi$ are equivalent. Points must lie in the input domain $[-3\pi, 3\pi)$, which allows the user to assume a convenient periodic domain such as $[-\pi, \pi)$ or $[0, 2\pi)$. To handle points outside of $[-3\pi, 3\pi)$ the user must fold them back into this domain before passing to FINUFFT. FINUFFT does not handle this case, for speed reasons. To use a different periodicity, linearly rescale your coordinates.

If instead you want to change some options, first put default values in a nufft_opts struct, make your changes, then pass the pointer to FINUFFT:

```
nufft_opts* opts = new nufft_opts;
finufft_default_opts(opts);
opts->debug = 1;                                // prints timing/debug info
int ier = finufft1d1(M,&x[0],&c[0],+1,tol,N,&F[0],opts);
```

Warning:

- Without the finufft_default_opts call, options may take on arbitrary values which may cause a crash.
- Note that, as of version 2.0, opts is passed as a pointer in both places.

See examples/simple1d1.cpp for a simple full working demo of the above, including a test of the math. If you instead use single-precision arrays, replace the tag finufft by finufftf in each command; see examples/simple1d1f.cpp.

Then to compile on a linux/GCC system, linking to the double-precision static library, use eg:

```
g++ simple1d1.cpp -o simple1d1 -I$FINUFFT/include $FINUFFT/lib-static/libfinufft.a -
↪fopenmp -lfftw3_omp -lfftw3 -lm
```

where $FINUFFT denotes the absolute path of your FINUFFT installation. Better is instead link to the dynamic shared (.so) library, via eg:

```
g++ simple1d1.cpp -o simple1d1 -I$FINUFFT/include -L$FINUFFT/lib -lfinufft -lm
```

The examples and test directories are good places to see further usage examples. The documentation for all 18 simple interfaces, and the more flexible guru interface, follows below.

4.4.2 Quick-start example in C

The FINUFFT C++ interface is intentionally also C-compatible, for simplity. Thus, to use from C, the above example only needs to replace the C++ `vector` with C-style array creation. Using C99 style, the above code, with options setting, becomes:

```
#include <finufft.h>
#include <stdlib.h>
#include <complex.h>

int M = 1e7;            // number of nonuniform points
double* x = (double *)malloc(sizeof(double)*M);
double complex* c = (double complex*)malloc(sizeof(double complex)*M);
for (int j=0; j<M; ++j) {
  x[j] = M_PI*(2*((double)rand()/RAND_MAX)-1);  // uniform random in [-pi,pi)
  c[j] = 2*((double)rand()/RAND_MAX)-1 + I*(2*((double)rand()/RAND_MAX)-1);
}
int N = 1e6;            // number of modes
double complex* F = (double complex*)malloc(sizeof(double complex)*N);
nufft_opts opts;                      // make an opts struct
finufft_default_opts(&opts);          // set default opts (must do this)
opts.debug = 2;                       // more debug/timing to stdout
int ier = finufft1d1(M,x,c,+1,1e-9,N,F,&opts);

// (now do something with F here!...)

free(x); free(c); free(F);
```

See `examples/simple1d1c.c` and `examples/simple1d1cf.c` for double- and single-precision C examples, including the math check to insure the correct indexing of output modes.

4.4.3 2D example in C++

We assume Fortran-style contiguous multidimensional arrays, as opposed to C-style arrays of pointers; this allows the widest compatibility with other languages. Assuming the same headers as above, we first create points (x_j, y_j) in the square $[-\pi, \pi)^2$, and strengths as before:

```
int M = 1e7;                                    // number of nonuniform points
vector<double> x(M), y(M);
vector<complex<double> > c(M);
for (int j=0; j<M; ++j) {
  x[j] = M_PI*(2*((double)rand()/RAND_MAX)-1);
  y[j] = M_PI*(2*((double)rand()/RAND_MAX)-1);
  c[j] = 2*((double)rand()/RAND_MAX)-1 + I*(2*((double)rand()/RAND_MAX)-1);
}
```

Let's say we want `N1=1000` by `N2=2000` 2D Fourier coefficients. We allocate and do the (default options) transform thus:

```
int N1=1000, N2=2000;
vector<complex<double> > F(N1*N2);
int ier = finufft2d1(M,&x[0],&y[0], &c[0], +1, 1e-6, N1, N2, &F[0], NULL);
```

This transform takes 0.6 seconds on a laptop. The modes have increasing ordering of integer frequency indices from `-N1/2` up to `N1/2-1` in the fast (`x`) dimension, then indices from `-N2/2` up to `N2/2-1` in the slow (`y`) dimension

(since both `N1` and `N2` are even). So, the output frequency `(k1,k2)` is found in `F[N1/2 + k1 + (N2/2 + k2)*N1]`.

See `opts.modeord` in *Options* to instead use FFT-style mode ordering, which simply differs by an "fftshift" (as it is commonly called).

See `examples/simple2d1.cpp` for an example with a math check, to insure that the mode indexing is correctly understood.

4.4.4 Vectorized interface example

A common use case is to perform a stack of identical transforms with the same size and nonuniform points, but for new strength vectors. (Applications include interpolating vector-valued data, or processing MRI images collected with a fixed set of k-space sample points.) Because it amortizes sorting, FFTW planning, and FFTW plan lookup, it can be faster to use a "vectorized" interface (which does the entire stack in one call) than to repeatedly call the above "simple" interfaces. This is especially true for many small problems. Here we show how to do a stack of `ntrans=10` 1D type 1 NUFFT transforms, in C++, assuming the same headers as in the first example above. The strength data vectors are taken to be contiguous (the whole first vector, followed by the second, etc, rather than interleaved.) Ie, viewed as a matrix in Fortran storage, each column is a strength vector.

```
int ntrans = 10;                                // how many transforms
int M = 1e7;                                    // number of nonuniform points
vector<double> x(M);
vector<complex<double> > c(M*ntrans);           // ntrans strength vectors
complex<double> I = complex<double>(0.0,1.0);   // the imaginary unit
for (int j=0; j<M; ++j)
  x[j] = M_PI*(2*((double)rand()/RAND_MAX)-1);
for (int j=0; j<M*ntrans; ++j)                  // fill all ntrans vectors...
  c[j] = 2*((double)rand()/RAND_MAX)-1 + I*(2*((double)rand()/RAND_MAX)-1);
int N = 1e6;                                    // number of output modes
vector<complex<double> > F(N*trans);            // ntrans output vectors
int ier = finufft1d1(M,&x[0],&c[0],+1,1e-9,N,&F[0],NULL);     // default opts
```

This takes 2.6 seconds on a laptop, around 1.4x faster than making 10 separate "simple" calls. The frequency index `k` in transform number `t` (zero-indexing the transforms) is in `F[k + (int)N/2 + N*t]`.

See `examples/many1d1.cpp` and `test/finufft?dmany_test.cpp` for more examples.

4.4.5 Guru interface example

If you want more flexibility than the above, use the "guru" interface: this is similar to that of FFTW3, and to the main interface of NFFT3. It lets you change the nonuniform points while keeping the same pointer to an FFTW plan for a particular number of stacked transforms with a certain number of modes. This avoids the overhead (typically 0.1 ms per thread) of FFTW checking for previous wisdom which would be significant when doing many small transforms. You may also send in a new set of stacked strength data (for type 1 and 3, or coefficients for type 2), reusing the existing FFTW plan and sorted points. Now we redo the above 2D type 1 C++ example with the guru interface.

One first makes a plan giving transform parameters, but no data:

```
// (assume x, y, c are filled, and F allocated, as in the 2D code above...)
int type=1, dim=2, ntrans=1;
int64_t Ns[] = {1000,2000};                     // N1,N2 as 64-bit int array
// step 1: make a plan...
finufft_plan plan;
int ier = finufft_makeplan(type, dim, Ns, +1, ntrans, 1e-6, &plan, NULL);
```

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```
// step 2: send in M nonuniform points (just x, y in this case)...
finufft_setpts(plan, M, &x[0], &y[0], NULL, 0, NULL, NULL, NULL);
// step 3: do the planned transform to the c strength data, output to F...
finufft_execute(plan, &c[0], &F[0]);
// ... you could now send in new points, and/or do transforms with new c data
// ...
// step 4: when done, free the memory used by the plan...
finufft_destroy(plan);
```

This writes the Fourier coefficients to `F` just as in the earlier 2D example. One difference from the above simple and vectorized interfaces is that the `int64_t` type (aka `long long int`) is needed since the Fourier coefficient dimensions are passed as an array.

> You must destroy a plan before making a new plan using the same plan object, otherwise a memory leak results.

The complete code with a math test is in `examples/guru2d1.cpp`, and for more examples see `examples/guru1d1*.c*`

4.5 Documentation of all C++ functions

All functions have double-precision (`finufft`) and single-precision (`finufftf`) versions. Do not forget this `f` suffix in the latter case. We group the simple and vectorized interfaces together, by each of the nine transform types (dimensions 1,2,3, and types 1,2,3). The guru interface functions are defined at the end. You will also want to refer to the *options* and *error codes* which apply to all 46 routines.

A reminder on Fourier mode ordering; see *modeord*. For example, if `N1=8` in a 1D type 1 or type 2 transform:

- if `opts.modeord=0`: frequency indices are ordered `-4,-3,-2,-1,0,1,2,3` (CMCL ordering)
- if `opts.modeord=1`: frequency indices are ordered `0,1,2,3,-4,-3,-2,-1` (FFT ordering)

The orderings are related by a "fftshift". This holds for each dimension. Multidimensional arrays are passed by a pointer to a contiguous Fortran-style array, with the "fastest" dimension x, then y (if present), then z (if present), then transform number (if `ntr>1`). We do not use C/C++-style multidimensional arrays; this gives us the most flexibility from several languages without loss of speed or memory due to unnecessary array copying.

In all of the simple, vectorized, and plan functions below you may either pass `NULL` as the last options argument to use default options, or a pointer to a valid `nufft_opts` struct. In this latter case you will first need to create an options struct then set default values by passing a pointer (here `opts`) to the following:

```
void finufft_default_opts(nufft_opts* opts)
void finufftf_default_opts(nufft_opts* opts)

 Set values in a NUFFT options struct to their default values.
```

Be sure to use the first version for double-precision and the second for single-precision. You may then change options with, for example, `opts->debug=1;` and then pass `opts` to the below routines.

4.5.1 Simple and vectorized interfaces

The "simple" interfaces (the first two listed in each block) perform a single transform, whereas the "vectorized" (the last two listed in each block, with the word "many" in the function name) perform `ntr` transforms with the same set of nonuniform points but stacked complex strengths or coefficients vectors.

Note: The motivations for the vectorized interface (and guru interface, see below) are as follows. 1) It is more efficient to bin-sort the nonuniform points only once if there are not to change between transforms. 2) For small problems, certain start-up costs cause repeated calls to the simple interface to be slower than necessary. In particular, we note that FFTW takes around 0.1 ms per thread to look up stored wisdom, which for small problems (of order 10000 or less input and output data) can, sadly, dominate the runtime.

1D transforms

```
int finufft1d1(int64_t M, double* x, complex<double>* c, int iflag, double eps, int64_
↪t
N1, complex<double>* f, nufft_opts* opts)
int finufftf1d1(int64_t M, float* x, complex<float>* c, int iflag, float eps, int64_t␣
↪N1,
complex<float>* f, nufft_opts* opts)

int finufft1d1many(int ntr, int64_t M, double* x, complex<double>* c, int iflag,␣
↪double
eps, int64_t N1, complex<double>* f, nufft_opts* opts)
int finufftf1d1many(int ntr, int64_t M, float* x, complex<float>* c, int iflag, float
eps, int64_t N1, complex<float>* f, nufft_opts* opts)

  1D complex nonuniform FFT of type 1 (nonuniform to uniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

              M-1
     f[k1] =  SUM c[j] exp(+/-i k1 x(j))  for -N1/2 <= k1 <= (N1-1)/2
              j=0

  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x      nonuniform points in [-3pi,3pi) (length M real array)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of output Fourier modes to be computed
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f      Fourier mode coefficients (size N1*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
```

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```
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft1d2(int64_t M, double* x, complex<double>* c, int iflag, double eps, int64_
↪t
N1, complex<double>* f, nufft_opts* opts)
int finufftf1d2(int64_t M, float* x, complex<float>* c, int iflag, float eps, int64_t␣
↪N1,
complex<float>* f, nufft_opts* opts)

int finufft1d2many(int ntr, int64_t M, double* x, complex<double>* c, int iflag,␣
↪double
eps, int64_t N1, complex<double>* f, nufft_opts* opts)
int finufftf1d2many(int ntr, int64_t M, float* x, complex<float>* c, int iflag, float
eps, int64_t N1, complex<float>* f, nufft_opts* opts)

  1D complex nonuniform FFT of type 2 (uniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

     c[j] = SUM   f[k1] exp(+/-i k1 x[j])      for j = 0,...,M-1
             k1
     where the sum is over integers -N1/2 <= k1 <= (N1-1)/2.

  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point targets
    x      nonuniform points in [-3pi,3pi) (length M real array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of input Fourier modes
    f      Fourier mode coefficients (size N1*ntr complex array)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    c      values at nonuniform point targets (size M*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft1d3(int64_t M, double* x, complex<double>* c, int iflag, double eps, int64_
↪t
N, double* s, complex<double>* f, nufft_opts* opts)
int finufftf1d3(int64_t M, float* x, complex<float>* c, int iflag, float eps, int64_t␣
↪N,
float* s, complex<float>* f, nufft_opts* opts)

int finufft1d3many(int ntr, int64_t M, double* x, complex<double>* c, int iflag,␣
↪double
eps, int64_t N, double* s, complex<double>* f, nufft_opts* opts)
int finufftf1d3many(int ntr, int64_t M, float* x, complex<float>* c, int iflag, float
```

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```
eps, int64_t N, float* s, complex<float>* f, nufft_opts* opts)

  1D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

              M-1
     f[k]  =  SUM   c[j] exp(+-i s[k] x[j]),      for k = 0,...,N-1
              j=0

  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x      nonuniform points in R (length M real array)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N      number of nonuniform frequency targets
    s      nonuniform frequency targets in R (length N real array)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f     Fourier transform values at targets (size N*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
```

2D transforms

```
int finufft2d1(int64_t M, double* x, double* y, complex<double>* c, int iflag, double
eps, int64_t N1, int64_t N2, complex<double>* f, nufft_opts* opts)
int finufftf2d1(int64_t M, float* x, float* y, complex<float>* c, int iflag, float␣
↪eps,
int64_t N1, int64_t N2, complex<float>* f, nufft_opts* opts)

int finufft2d1many(int ntr, int64_t M, double* x, double* y, complex<double>* c, int
iflag, double eps, int64_t N1, int64_t N2, complex<double>* f, nufft_opts* opts)
int finufftf2d1many(int ntr, int64_t M, float* x, float* y, complex<float>* c, int␣
↪iflag,
float eps, int64_t N1, int64_t N2, complex<float>* f, nufft_opts* opts)

  2D complex nonuniform FFT of type 1 (nonuniform to uniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

                 M-1
     f[k1,k2] =  SUM c[j] exp(+/-i (k1 x[j] + k2 y[j]))
                 j=0

              for -N1/2 <= k1 <= (N1-1)/2,      -N2/2 <= k2 <= (N2-1)/2.

  Inputs:
```

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```
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x,y    nonuniform point coordinates in [-3pi,3pi)^2 (length M real arrays)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of output Fourier modes to be computed (x direction)
    N2     number of output Fourier modes to be computed (y direction)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f      Fourier mode coefficients (size N1*N2*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft2d2(int64_t M, double* x, double* y, complex<double>* c, int iflag, double
eps, int64_t N1, int64_t N2, complex<double>* f, nufft_opts* opts)
int finufftf2d2(int64_t M, float* x, float* y, complex<float>* c, int iflag, float␣
↪eps,
int64_t N1, int64_t N2, complex<float>* f, nufft_opts* opts)

int finufft2d2many(int ntr, int64_t M, double* x, double* y, complex<double>* c, int
iflag, double eps, int64_t N1, int64_t N2, complex<double>* f, nufft_opts* opts)
int finufftf2d2many(int ntr, int64_t M, float* x, float* y, complex<float>* c, int␣
↪iflag,
float eps, int64_t N1, int64_t N2, complex<float>* f, nufft_opts* opts)

  2D complex nonuniform FFT of type 2 (uniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

     c[j] =   SUM   f[k1,k2] exp(+/-i (k1 x[j] + k2 y[j]))    for j = 0,...,M-1
            k1,k2
     where the sum is over integers -N1/2 <= k1 <= (N1-1)/2,
                                    -N2/2 <= k2 <= (N2-1)/2.
  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point targets
    x,y    nonuniform point coordinates in [-3pi,3pi)^2 (length M real arrays)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of input Fourier modes (x direction)
    N2     number of input Fourier modes (y direction)
    f      Fourier mode coefficients (size N1*N2*ntr complex array)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    c      values at nonuniform point targets (size M*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)
```

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```
  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft2d3(int64_t M, double* x, double* y, complex<double>* c, int iflag, double
eps, int64_t N, double* s, double* t, complex<double>* f, nufft_opts* opts)
int finufftf2d3(int64_t M, float* x, float* y, complex<float>* c, int iflag, float␣
↪eps,
int64_t N, float* s, float* t, complex<float>* f, nufft_opts* opts)

int finufft2d3many(int ntr, int64_t M, double* x, double* y, complex<double>* c, int
iflag, double eps, int64_t N, double* s, double* t, complex<double>* f, nufft_opts*␣
↪opts)
int finufftf2d3many(int ntr, int64_t M, float* x, float* y, complex<float>* c, int␣
↪iflag,
float eps, int64_t N, float* s, float* t, complex<float>* f, nufft_opts* opts)

  2D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

              M-1
     f[k]  =  SUM  c[j] exp(+-i (s[k] x[j] + t[k] y[j])),   for k = 0,...,N-1
              j=0

  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x,y    nonuniform point coordinates in R^2 (length M real arrays)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N      number of nonuniform frequency targets
    s,t    nonuniform frequency target coordinates in R^2 (length N real arrays)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f     Fourier transform values at targets (size N*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
```

3D transforms

```
int finufft3d1(int64_t M, double* x, double* y, double* z, complex<double>* c, int␣
↪iflag,
double eps, int64_t N1, int64_t N2, int64_t N3, complex<double>* f, nufft_opts* opts)
int finufftf3d1(int64_t M, float* x, float* y, float* z, complex<float>* c, int iflag,
float eps, int64_t N1, int64_t N2, int64_t N3, complex<float>* f, nufft_opts* opts)

int finufft3d1many(int ntr, int64_t M, double* x, double* y, double* z, complex
↪<double>*
c, int iflag, double eps, int64_t N1, int64_t N2, int64_t N3, complex<double>* f,
nufft_opts* opts)
int finufftf3d1many(int ntr, int64_t M, float* x, float* y, float* z, complex<float>*␣
↪c,
int iflag, float eps, int64_t N1, int64_t N2, int64_t N3, complex<float>* f, nufft_
↪opts*
opts)

  3D complex nonuniform FFT of type 1 (nonuniform to uniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

                  M-1
     f[k1,k2] =   SUM c[j] exp(+/-i (k1 x[j] + k2 y[j] + k3 z[j]))
                  j=0

 for -N1/2 <= k1 <= (N1-1)/2,  -N2/2 <= k2 <= (N2-1)/2,  -N3/2 <= k3 <= (N3-1)/2

  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x,y,z  nonuniform point coordinates in [-3pi,3pi)^3 (length M real arrays)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of output Fourier modes to be computed (x direction)
    N2     number of output Fourier modes to be computed (y direction)
    N3     number of output Fourier modes to be computed (z direction)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f      Fourier mode coefficients (size N1*N2*N3*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft3d2(int64_t M, double* x, double* y, double* z, complex<double>* c, int␣
↪iflag,
double eps, int64_t N1, int64_t N2, int64_t N3, complex<double>* f, nufft_opts* opts)
int finufftf3d2(int64_t M, float* x, float* y, float* z, complex<float>* c, int iflag,
float eps, int64_t N1, int64_t N2, int64_t N3, complex<float>* f, nufft_opts* opts)
```

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```
int finufft3d2many(int ntr, int64_t M, double* x, double* y, double* z, complex
↪<double>*
c, int iflag, double eps, int64_t N1, int64_t N2, int64_t N3, complex<double>* f,
nufft_opts* opts)
int finufftf3d2many(int ntr, int64_t M, float* x, float* y, float* z, complex<float>*␣
↪c,
int iflag, float eps, int64_t N1, int64_t N2, int64_t N3, complex<float>* f, nufft_
↪opts*
opts)

  3D complex nonuniform FFT of type 2 (uniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

     c[j] =   SUM    f[k1,k2,k3] exp(+/-i (k1 x[j] + k2 y[j] + k3 z[j]))
            k1,k2,k3

     for j = 0,...,M-1,
     where the sum is over integers -N1/2 <= k1 <= (N1-1)/2,
                                    -N2/2 <= k2 <= (N2-1)/2,
                                    -N3/2 <= k3 <= (N3-1)/2.
  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point targets
    x,y,z  nonuniform point coordinates in [-3pi,3pi)^3 (length M real arrays)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N1     number of input Fourier modes (x direction)
    N2     number of input Fourier modes (y direction)
    N3     number of input Fourier modes (z direction)
    f      Fourier mode coefficients (size N1*N2*N3*ntr complex array)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    c      values at nonuniform point targets (size M*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * complex arrays interleave Re, Im values, and their size is stated with
      dimensions ordered fastest to slowest.
    * Fourier frequency indices in each dimension i are the integers lying
      in [-Ni/2, (Ni-1)/2]. See above, and modeord in opts.rst for possible orderings.
```

```
int finufft3d3(int64_t M, double* x, double* y, double* z, complex<double>* c, int␣
↪iflag,
double eps, int64_t N, double* s, double* t, double* u, complex<double>* f, nufft_
↪opts*
opts)
int finufftf3d3(int64_t M, float* x, float* y, float* z, complex<float>* c, int iflag,
float eps, int64_t N, float* s, float* t, float* u, complex<float>* f, nufft_opts*␣
↪opts)

int finufft3d3many(int ntr, int64_t M, double* x, double* y, double* z, complex
↪<double>*
c, int iflag, double eps, int64_t N, double* s, double* t, double* u, complex<double>
↪* f,
```

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```
nufft_opts* opts)
int finufftf3d3many(int ntr, int64_t M, float* x, float* y, float* z, complex<float>*␣
↪c,
int iflag, float eps, int64_t N, float* s, float* t, float* u, complex<float>* f,
nufft_opts* opts)

  3D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

  Computes to precision eps, via a fast algorithm, one or more transforms of the form:

              M-1
     f[k]  =  SUM  c[j] exp(+-i (s[k] x[j] + t[k] y[j] + u[k] z[j])),
              j=0
                          for k = 0,...,N-1.
  Inputs:
    ntr    how many transforms (only for vectorized "many" functions, else ntr=1)
    M      number of nonuniform point sources
    x,y,z  nonuniform point coordinates in R^3 (length M real arrays)
    c      source strengths (size M*ntr complex array)
    iflag  if >=0, uses +i in complex exponential, otherwise -i
    eps    desired relative precision; smaller is slower. This can be chosen
           from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    N      number of nonuniform frequency targets
    s,t,u  nonuniform frequency target coordinates in R^3 (length N real arrays)
    opts   pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
    f     Fourier transform values at targets (size N*ntr complex array)
    return value  0: success, 1: success but warning, >1: error (see error.rst)
```

4.5.2 Guru plan interface

This provides more flexibility than the simple or vectorized interfaces. Any transform requires (at least) calling the following four functions in order. However, within this sequence one may insert repeated `execute` calls, or another `setpts` followed by more `execute` calls, as long as the transform sizes (and number of transforms `ntr`) are consistent with those that have been set in the `plan` and in `setpts`.

```
int finufft_makeplan(int type, int dim, int64_t* nmodes, int iflag, int ntr, double␣
↪eps,
finufft_plan* plan, nufft_opts* opts)
int finufftf_makeplan(int type, int dim, int64_t* nmodes, int iflag, int ntr, float␣
↪eps,
finufftf_plan* plan, nufft_opts* opts)

  Make a plan to perform one or more general transforms.

  Under the hood, for type 1 and 2, this does FFTW planning and kernel Fourier
  transform precomputation. For type 3, this does very little, since the FFT
  sizes are not yet known.

Inputs:
     type   type of transform (1,2, or 3)
     dim    spatial dimension (1,2, or 3)
     nmodes if type is 1 or 2, numbers of Fourier modes (length dim array),
            ie, {N1} in 1D, {N1,N2} in 2D, or {N1,N2,N3} in 3D.
```

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```
            If type is 3, it is unused.
    iflag   if >=0, uses +i in complex exponential, otherwise -i
    ntr     how many transforms (only for vectorized "many" functions, else ntr=1)
    eps     desired relative precision; smaller is slower. This can be chosen
            from 1e-1 down to ~ 1e-14 (in double precision) or 1e-6 (in single)
    opts    pointer to options struct (see opts.rst), or NULL for defaults

  Outputs:
     plan   plan object (under the hood this is a pointer to another struct)
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
     * All available threads are planned by default (but see opts.nthreads)
     * The vectorized (many vector) plan, ie ntrans>1, can be much faster
       than repeated calls with the same nonuniform points.
       Note that here the I/O data ordering is stacked rather than interleaved.
     * For more details about the fields in the opts pointer, see opts.rst
```

```
int finufft_setpts(finufft_plan plan, int64_t M, double* x, double* y, double* z,␣
↪int64_t
N, double* s, double* t, double* z)
int finufftf_setpts(finufftf_plan plan, int64_t M, float* x, float* y, float* z,␣
↪int64_t
N, float* s, float* t, float* z)

  Input nonuniform points with coordinates x (and possibly y, and possibly z),
  and, if type 3, nonuniform frequency target coordinates s (and possibly t,
  and possibly u), into an existing plan. If type is 1 or 2 then the last four
  arguments are ignored. Unused dimensions are ignored.

  Under the hood, for type 1 or 2, this routine bin-sorts the points (storing
  just the permutation rather than new copies of the coordinates). For type
  3 it also bin-sorts the frequencies, chooses two levels of grid sizes, then
  plans the inner type 2 call (interpolation and FFTW).

  Inputs:
     M      number of nonuniform spatial points (used by all types)
     x      nonuniform point x-coordinates (length M real array)
     y      if dim>1, nonuniform point y-coordinates (length M real array),
            ignored otherwise
     z      if dim>2, nonuniform point z-coordinates (length M real array),
            ignored otherwise
     N      number of nonuniform frequency targets (type 3 only, ignored
            otherwise)
     s      nonuniform frequency x-coordinates (length N real array)
     t      if dim>1, nonuniform frequency y-coordinates (length N real array),
            ignored otherwise
     u      if dim>2, nonuniform frequency z-coordinates (length N real array),
            ignored otherwise

  Input/Outputs:
     plan   plan object

  Outputs:
    return value  0: success, 1: success but warning, >1: error (see error.rst)
```

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```
  Notes:
    * For type 1 and 2, the values in x (and if nonempty, y and z) must
      lie in the interval [-3pi,3pi). For type 1 they are "sources", but for
      type 2, "targets". In contrast, for type 3 there are no restrictions on
      them, or on s, t, u, other than the resulting size of the internal fine
      grids fitting in memory.
    * The coordinates pointed to by any used arrays x, y, z, s, t, u must
      not be changed between this call and the below execute call!
```

```
int finufft_execute(finufft_plan plan, complex<double>* c, complex<double>* f)
int finufftf_execute(finufftf_plan plan, complex<float>* c, complex<float>* f)

  Perform one or more NUFFT transforms using previously entered nonuniform
  points and an existing plan. To summarize, this maps
    type 1: c -> f
    type 2: f -> c
    type 3: c -> f

  Inputs:
       plan   plan object

  Input/Outputs:
       c      for types 1 and 3, the input strengths (size N1*ntr or N1*N2*ntr
              or N1*N2*N3*ntr complex array, when dim = 1, 2, or 3 respectively)
              For type 2, the output values at the nonuniform points (size
              M*ntr complex array).
       f      for type 1, the output Fourier mode coefficients (size N1*ntr or
              N1*N2*ntr or N1*N2*N3*ntr complex array, when dim = 1, 2, or 3
              respectively). For type 2, the input Fourier mode coefficients
              (of the same size as for type 1). For type 3, the output values
              at the nonuniform frequency targets (size N*ntr complex array).

  Outputs:
    return value  0: success, 1: success but warning, >1: error (see error.rst)

  Notes:
    * The coordinates pointed to by any used arrays x, y, z, s, t, u must
      not have changed since the finufft_setpts call that inputted them.
```

```
int finufft_destroy(finufft_plan plan)
int finufftf_destroy(finufftf_plan plan)

  Deallocate a plan object. This must be used upon clean-up, or before reusing
  a plan in another call to finufft_makeplan.

  Inputs/Outputs:
       plan   plan object

  Outputs:
    return value  0: success, 1: success but warning, >1: error (see error.rst)
```

4.6 Options parameters

Aside from the mandatory inputs (dimension, type, nonuniform points, strengths or coefficients, and, in C++/C/Fortran/MATLAB, sign of the imaginary unit and tolerance) FINUFFT has optional parameters. These adjust the workings of the algorithm, change the output format, or provide debug/timing text to stdout. Sensible default options are chosen, so that the new user need not worry about changing them. However, users wanting to try to increase speed or see more timing breakdowns will want to change options from their defaults. See each language doc page for how this is done, but is generally by creating an options structure, changing fields from their defaults, then passing this (or a pointer to it) to the simple, vectorized, or guru makeplan routines. Recall how to do this from C++:

```
// (... set up M,x,c,tol,N, and allocate F here...)
nufft_opts* opts;
finufft_default_opts(opts);
opts->debug = 1;
int ier = finufft1d1(M,x,c,+1,tol,N,F,opts);
```

This setting produces more timing output to `stdout`.

Warning: In C/C++ and Fortran, don't forget to call the command which sets default options (`finufft_default_opts` or `finufftf_default_opts`) before you start changing them and passing them to FINUFFT.

4.6.1 Summary and quick advice

Here is a 1-line summary of each option, taken from the code (the header `include/nufft_opts.h`):

```
  // FINUFFT options:
  // data handling opts...
  int modeord;            // (type 1,2 only): 0 CMCL-style increasing mode order
                          //                  1 FFT-style mode order
  int chkbnds;            // 0 don't check NU pts in [-3pi,3pi), 1 do (<few % slower)

  // diagnostic opts...
  int debug;              // 0 silent, 1 some timing/debug, or 2 more
  int spread_debug;       // spreader: 0 silent, 1 some timing/debug, or 2 tonnes
  int showwarn;           // 0 don't print warnings to stderr, 1 do

  // algorithm performance opts...
  int nthreads;           // number of threads to use, or 0 uses all available
  int fftw;               // plan flags to FFTW (FFTW_ESTIMATE=64, FFTW_MEASURE=0,...)
  int spread_sort;        // spreader: 0 don't sort, 1 do, or 2 heuristic choice
  int spread_kerevalmeth; // spreader: 0 exp(sqrt()), 1 Horner piecewise poly (faster)
  int spread_kerpad;      // (exp(sqrt()) only): 0 don't pad kernel to 4n, 1 do
  double upsampfac;       // upsampling ratio sigma: 2.0 std, 1.25 small FFT, 0.0 auto
  int spread_thread;      // (vectorized ntr>1 only): 0 auto, 1 seq multithreaded,
                          //                          2 parallel single-thread spread
  int maxbatchsize;       // (vectorized ntr>1 only): max transform batch, 0 auto
```

Here are their default settings (from `src/finufft.cpp:finufft_default_opts`):

```
  o->modeord = 0;
  o->chkbnds = 1;
```

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```
o->debug = 0;
o->spread_debug = 0;
o->showwarn = 1;

o->nthreads = 0;
o->fftw = FFTW_ESTIMATE;
o->spread_sort = 2;
o->spread_kerevalmeth = 1;
o->spread_kerpad = 1;
o->upsampfac = 0.0;
o->spread_thread = 0;
o->maxbatchsize = 0;
```

As for quick advice, the main options you'll want to play with are:

- `modeord` to flip ("fftshift") the Fourier mode ordering
- `debug` to look at timing output (to determine if your problem is spread/interpolation dominated, vs FFT dominated)
- `nthreads` to run with a different number of threads than the current maximum available through OpenMP (a large number can sometimes be detrimental, and very small problems can sometimes run faster on 1 thread)
- `fftw` to try slower plan modes which give faster transforms. The next natural one to try is `FFTW_MEASURE` (look at the FFTW3 docs)

See *Troubleshooting* for good advice on trying options, and read the full options descriptions below.

Some of the options are for experts only, and will result in slow or incorrect results. Please test options in a small known test case so that you understand their effect.

4.6.2 Documentation of all options

Data handling options

modeord: Fourier coefficient frequency index ordering in every dimension. For type 1, this is for the output; for type 2 the input. It has no effect in type 3. Here we use `N` to denote the size in any of the relevant dimensions:

- if `modeord=0`: frequency indices are in increasing ordering, namely $\{-N/2, -N/2+1, \dots, N/2-1\}$ if N is even, or $\{-(N-1)/2, \dots, (N-1)/2\}$ if N is odd. For example, if `N=6` the indices are `-3,-2,-1,0,1,2`, whereas if `N=7` they are `-3,-2,-1,0,1,2,3`. This is called "CMCL ordering" since it is that of the CMCL NUFFT.
- if `modeord=1`: frequency indices are ordered as in the usual FFT, increasing from zero then jumping to negative indices half way along, namely $\{0, 1, \dots, N/2-1, -N/2, -N/2+1, \dots, -1\}$ if N is even, or $\{0, 1, \dots, (N-1)/2, -(N-1)/2, \dots, -1\}$ if N is odd. For example, if `N=6` the indices are `0,1,2,-3,-2,-1`, whereas if `N=7` they are `0,1,2,3,-3,-2,-1`.

Note: The index *sets* are the same in the two `modeord` choices; their ordering differs only by a cyclic shift. The FFT ordering cyclically shifts the CMCL indices floor$(N/2)$ to the left (often called an "fftshift").

---

chkbnds: whether to check the nonuniform points lie in the correct bounds.

- `chkbnds=0`: input nonuniform points in the arrays `x`, `y`, `z`, are fed straight into the spreader which assumes (for speed) that they lie in $[-3\pi, 3\pi)$. Points outside of this will then cause a segfault.

- `chkbnds=1`: the nonuniform points are checked to lie in this interval, and if any are found not to, the library exits with an error code and message to stderr. The trade-off is that simply doing this checking can lose several % in overall speed, especially in low-precision 3D transforms.

Diagnostic options

debug: Controls the amount of overall debug/timing output to stdout.

- `debug=0` : silent
- `debug=1` : print some information
- `debug=2` : prints more information

spread_debug: Controls the amount of debug/timing output from the spreader/interpolator.

- `spread_debug=0` : silent
  - `spread_debug=1` : prints some timing information
  - `spread_debug=1` : prints lots. This can print thousands of lines since it includes one line per *subproblem*.

showwarn: Whether to print warnings (these go to stderr).

- `showwarn=0` : suppresses such warnings
- `showwarn=1` : prints warnings

Algorithm performance options

nthreads: Number of threads to use. This sets the number of threads FINUFFT will use in FFTW, bin-sorting, and spreading/interpolation steps. This number of threads also controls the batch size for vectorized transforms (ie `ntr>1` *here*). Setting `nthreads=0` uses all threads available (up to an internal maximum that has been chosen based on performance; see `MAX_USEFUL_NTHREADS` in `include/defs.h`). For repeated small problems it can be advantageous to use a small number, such as 1.

fftw: FFTW planner flags. This number is simply passed to FFTW's planner; the flags are documented here. A good first choice is `FFTW_ESTIMATE`; however if you will be making multiple calls, consider `FFTW_MEASURE`, which could spend many seconds planning, but will give a faster run-time when called again from the same process. These macros are bit-wise flags defined in `/usr/include/fftw3.h` on a linux system; they currently have the values `FFTW_ESTIMATE=64` and `FFTW_MEASURE=0`. Note that FFTW plans are saved (by FFTW's library) automatically from call to call in the same executable (incidentally, also in the same MATLAB/octave or python session); there is a small overhead for lookup of such plans, which with many repeated small problems can motivate use of the *guru interface*.

spread_sort: Sorting mode within the spreader/interpolator.

- `spread_sort=0` : never sorts
- `spread_sort=1` : always sorts
- `spread_sort=2` : uses a heuristic to decide whether to sort or not.

The heuristic bakes in empirical findings such as: generally it is not worth sorting in 1D type 2 transforms, or when the number of nonuniform points is small. Do not change this from its default unless you obsever.

spread_kerevalmeth: Kernel evaluation method in spreader/interpolator. This should not be changed from its default value, unless you are an expert wanting to compare against outdated

- `spread_kerevalmeth=0` : direct evaluation of `sqrt(exp(beta(1-x*x)))` in the ES kernel.

This is outdated, and it's only possible use could be in exploring upsampling factors σ different from standard (see below).

- `spread_kerevalmeth=1` : use Horner's rule applied to piecewise polynomials with precomputed

coefficients. This is faster, less brittle to compiler/glibc/CPU variations, and is the recommended approach. It only works for the standard upsampling factors listed below.

spread_kerpad: whether to pad the number of direct kernel evaluations per dimension and per nonuniform point to a multiple of four; this can help SIMD vectorization. It only applies to the (outdated) `spread_kerevalmeth=0` choice. There is thus little reason for the nonexpert to mess with this option.

- `spread_kerpad=0` : do not pad
- `spread_kerpad=0` : pad to next multiple of four

upsampfac: This is the internal real factor by which the FFT (fine grid) is chosen larger than the number of requested modes in each dimension, for type 1 and 2 transforms. We have built efficient kernels for only two settings, as follows. Otherwise, setting it to zero chooses a good heuristic:

- `upsampfac=0.0` : use heuristics to choose `upsampfac` as one of the below values, and use this value internally. The value chosen is visible in the text output via setting `debug>=2`. This setting is recommended for basic users; however, if you seek more performance it is quick to try the other of the below.
- `upsampfac=2.0` : standard setting of upsampling. This is necessary if you need to exceed 9 digits of accuracy.
- `upsampfac=1.25` : low-upsampling option, with lower RAM, smaller FFTs, but wider spreading kernel.

The latter can be much faster than the standard when the number of nonuniform points is similar or smaller to the number of modes, and/or if low accuracy is required. It is especially much (2 to 3 times) faster for type 3 transforms. However, the kernel widths w are about 50% larger in each dimension, which can lead to slower spreading (it can also be faster due to the smaller size of the fine grid). Because the kernel width is limited to 16, currently, thus only 9-digit accuracy can currently be reached when using `upsampfac=1.25`.

spread_thread: in the case of multiple transforms per call (`ntr>1`, or the "many" interfaces), controls how multi-threading is used to spread/interpolate each batch of data.

- `spread_thread=0` : makes an automatic choice between the below. Recommended.
- `spread_thread=1` : acts on each vector in the batch in sequence, using multithreaded spread/interpolate on that vector. It can be slightly better than `2` for large problems.
- `spread_thread=2` : acts on all vectors in a batch (of size chosen typically to be the number of threads) simultaneously, assigning each a thread which performs a single-threaded spread/interpolate. It is much better than `1` for all but large problems. (Historical note: this was used by Melody Shih for the original "2dmany" interface in 2018.)

Note: Historical note: A former option `3` has been removed. This was like `2` except allowing nested OMP parallelism, so multi-threaded spread-interpolate was used for each of the vectors in a batch in parallel. This was used by Andrea Malleo in 2019. We have not yet found a case where this beats both `1` and `2`, hence removed it due to complications with changing the OMP nesting state in both old and new OMP versions.

---

maxbatchsize: in the case of multiple transforms per call (`ntr>1`, or the "many" interfaces), set the largest batch size of data vectors. Here `0` makes an automatic choice. If you are unhappy with this, then for small problems it should equal the number of threads, while for large problems it appears that `1` often better (since otherwise too much simultaneous RAM movement occurs). Some further work is needed to optimize this parameter.

4.7 Error (status) codes

In all FINUFFT interfaces, the returned value `ier` is a status indicator. It is `0` if successful, otherwise the error code has the following meanings (see `include/defs.h`):

```
1  requested tolerance epsilon too small to achieve (warning only)
2  attemped to allocate internal array larger than MAX_NF (defined in defs.h)
3  spreader: fine grid too small compared to spread (kernel) width
4  spreader: if chkbnds=1, a nonuniform point coordinate is out of input range [-3pi,
↪3pi]^d
5  spreader: array allocation error
6  spreader: illegal direction (should be 1 or 2)
7  upsampfac too small (should be >1.0)
8  upsampfac not a value with known Horner poly eval rule (currently 2.0 or 1.25 only)
9  ntrans not valid in "many" (vectorized) or guru interface (should be >= 1)
10 transform type invalid
11 general allocation failure
12 dimension invalid
13 spread_thread option invalid
```

When `ier=1` (warning only) the transform(s) is/are still completed, at the smallest epsilon achievable, so, with that caveat, the answer should still be usable.

For any other nonzero values of `ier` the transform may not have been performed and the output should not be trusted. However, we hope that the value of `ier` will help to narrow down the problem.

FINUFFT sometimes also sends error text to `stderr` if it detects faulty input parameters.

If you are getting error codes, please reread the documentation for your language, then see our *troubleshooting advice*.

4.7.1 Large internal arrays

In case your input parameters demand the allocation of very large arrays, an internal check is done to see if their size exceeds a rather generous internal limit, set in `defs.h` as `MAX_NF`. The current value in the source code is `1e11`, which corresponds to about 1TB for double precision. Allocations beyond this cause a graceful exit with error code `2` as above. Such a large allocation can be due to enormous `N` (in types 1 or 2), or `M`, but also large values of the space-bandwidth product (loosely, range of $\mathbf{x}_j$ points times range of $\mathbf{k}_j$ points) for type 3 transforms; see Remark 5 in *reference FIN*. Note that mallocs smaller than this, but which still exceed available RAM, may cause segfaults as usual. For simplicity of code, we do not do error checking on every malloc or STL vector creation in the code, and neither is this recommended in modern style guides. If you have a large-RAM machine and want to exceed the above hard-coded limit, you will need to edit `defs.h` and recompile.

4.8 Troubleshooting

If you are having issues (segfaults, slowness, "wrong" answers, etc), there is a high probability it is something we already know about, so please first read all of the advice below in the section relevant to your problem: math, speed, or segfaults.

4.8.1 Mathematical "issues" and advice

- When requested tolerance is around 10^{-14} or less in double-precision, or 10^{-6} or less in single-precision, it will most likely be impossible for FINUFFT (or any other NUFFT library) to achieve this, due to inevitable round-off error. Here, "error" is to be understood relative to the norm of the returned vector of values. This is especially true when there is a large number of modes in any single dimension (N_1, N_2 or N_3), since this empirically scales the round-off error (fortunately, round-off does not appear to scale with the total N or M). Such round-off error is analysed and measured in Section 4.2 of our SISC paper.
- If you request a tolerance that FINUFFT knows it cannot achieve, it will return `ier=1` after performing transforms as accurately as it can. However, the status `ier=0` does not imply that the requested accuracy *was* achieved, merely that parameters were chosen to give this estimated accuracy, if possible. As our SISC paper shows, for typical situations, relative ℓ_2 errors match the requested tolerances over a wide range. Users should always check *convergence* (by, for instance, varying `tol` and measuring any changes in their results); this is generally true in scientific computing.
- The type 1 and type 2 transforms are adjoints but **not inverses of each other** (unlike in the plain FFT case, where, up to a constant N, the adjoint is the inverse). Therefore, if you are not getting the expected answers, please check that you have not made this assumption. In the *tutorials* we will add examples showing how to invert the NUFFT; also see NFFT3 inverse transforms.

4.8.2 Speed issues and advice

If FINUFFT is slow (eg, less than 10^6 nonuniform points per second), here is some advice:

- Try printing debug output to see step-by-step progress by FINUFFT. Do this by setting `opts.debug` to 1 or 2 then looking at the timing information.
- Try reducing the number of threads either externally or via `opts.nthreads`, perhaps down to 1 thread, to make sure you are not having collisions between threads, or slowdown due to thread overheads. The former is possible if large problems are run with a large number of (say more than 30) threads. We added the constant `MAX_USEFUL_NTHREADS` in `include/defs.h` to catch this case. Another corner case causing slowness is very many repetitions of small problems; see `test/manysmallprobs` which exceeds 10^7 points/sec with one thread via the guru interface, but can get ridiculously slower with many threads; see https://github.com/flatironinstitute/finufft/issues/86
- Try setting a crude tolerance, eg `tol=1e-3`. How many digits do you actually need? This has a big effect in higher dimensions, since the number of flops scales like $(\log 1/\epsilon)^d$, but not quite as big an effect as this scaling would suggest, because in higher dimensions the flops/RAM ratio is higher.
- If type 3, make sure your choice of points does not have a massive *space-bandwidth product* (ie, product of the volumes of the smallest d-dimension axes-aligned cuboids enclosing the nonuniform source and the target points); see Remark 5 of our SISC paper. In short, if the spreads of $\mathbf{x}_j$ and of $\mathbf{s}_k$ are both big, you may be in trouble. This can lead to enormous fine grids and hence slow FFTs. Set `opts.debug=1` to examine the `nf1`, etc, fine grid sizes being chosen, and the array allocation sizes. If they are huge, consider direct summation, as discussed *here*.
- The timing of the first FFTW call is complicated, depending on the FFTW flags (plan mode) used. This is really an FFTW planner flag usage question. Such issues are known, and modes benchmarked in other documentation, eg for 2D in poppy. In short, using more expensive FFTW planning modes like `FFTW_MEASURE` can give better performance for repeated FFTW calls, but be **much** more expensive in the first (planning) call. This is why we choose `FFTW_ESTIMATE` as our default `opts.fftw` option.
- Make sure you did not override `opts.spread_sort`, which if set to zero does no sorting, which can give very slow RAM access if the nonuniform points are ordered poorly (eg randomly) in larger 2D or 3D problems.

- Are you calling the simple interface a huge number of times for small problems, but these tasks have something in common (number of modes, or locations of nonuniform points)? If so, try the "many vector" or guru interface, which removes overheads in repeated FFTW plan look-up, and in bin-sorting. They can be 10-100x faster.

4.8.3 Crash (segfault) issues and advice

- The most common problem is passing in pointers to the wrong size of object,

eg, single vs double precision, or int32 vs int64. The library includes both precisions, so make sure you are calling the correct one (commands begin `finufft` for double, `finufftf` for single).

- If you use C++/C/Fortran and tried to change options, did you forget to call `finufft_default_opts` first?
- Maybe you have switched off nonuniform point bounds checking (`opts.chkbnds=0`) for a little extra speed? Try switching it on again to catch illegal coordinates.
- To isolate where a crash is occurring, set `opts.debug` to 1 or 2, and check the text output of the various stages. With a debug setting of 2 or above, when `ntrans>1` a large amount of text can be generated.
- To diagnose problems with the spread/interpolation stage, similarly setting `opts.spread_debug` to 1 or 2 will print even more output. Here the setting 2 generates a large amount of output even for a single transform.

4.8.4 Other known issues with library and interfaces

The master list is the github issues for the project page, https://github.com/flatironinstitute/finufft/issues

A secondary and more speculative list is in the `TODO` text file.

Please look through those issue topics, since sometimes workarounds are discussed before the problem is fixed in a release.

4.8.5 Bug reports

If you think you have found a new bug, and have read the above, please file a new issue on the github project page, https://github.com/flatironinstitute/finufft/issues . Include a minimal code which reproduces the bug, along with details about your machine, operating system, compiler, version of FINUFFT, and output with `opts.debug` at least 1. If you have a known bug and have ideas, please add to the comments for that issue.

You may also contact Alex Barnett (`abarnett` at-sign `flatironinstitute.org`) with FINUFFT in the subject line.

4.9 Tutorials and application demos

The following are instructive demos of using FINUFFT for a variety of spectrally-related tasks arising in scientific computing and signal/image processing. We will slowly grow the list (contact us to add one). For conciseness of code, and ease of writing, they are currently in MATLAB (they should work on versions at least back to R2017a).

4.9.1 Fast evaluation of Fourier series at arbitrary points

This is a simple demo of using type 2 NUFFTs to evaluate a given 1D and then 2D Fourier series rapidly (close to optimal scaling) at arbitrary points. For conciseness of code, we use the MATLAB interface. The series we use are vaguely boring random ones relating to Gaussian random fields—please insert Fourier series coefficient vectors you care about.

1D Fourier series

Let our periodic domain be $[0, L)$, so that we get to see how to rescale from the fixed period of 2π in FINUFFT. We set up a random Fourier series with Gaussian decaying coefficients (this in fact is a sample from a stationary *Gaussian random field*, or *Gaussian process* with covariance kernel itself a periodized Gaussian):

```
L = 10;              % period
kmax = 500;          % bandlimit
k = -kmax:kmax-1;    % freq indices (negative up through positive mode ordering)
N = 2*kmax;          % # modes
rng(0);              % make some convenient Fourier coefficients...
fk = randn(N,1)+1i*randn(N,1);       % iid random complex data, column vec
k0 = 100;            % a freq scale parameter
fk = fk .* exp(-(k/k0).^2).';        % scale the amplitudes, kills high freqs
```

Now we use a 1D type 2 to evaluate this series at a large number of points very quickly:

```
M = 1e6; x = L*rand(1,M);         % make random target points in [0,L)
tol = 1e-12;
x_scaled = x * (2*pi/L);          % don't forget to scale to 2pi-periodic!
tic; c = finufft1d2(x_scaled,+1,tol,fk); toc   % evaluate Fourier series at x
```

```
Elapsed time is 0.026038 seconds.
```

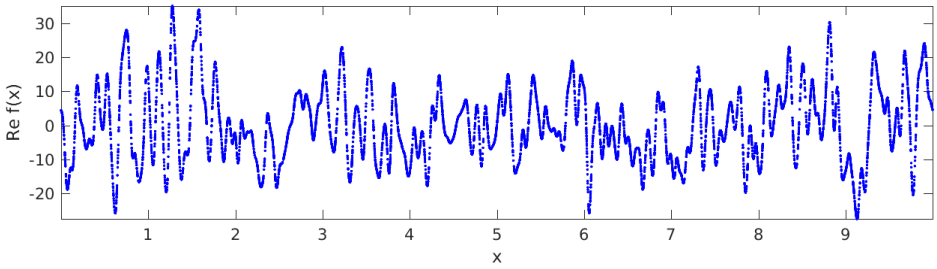
Compare this to a naive calculation (which serves to remind us exactly what sum FINUFFT approximates):

```
tic; cn = 0*c; for m=k, cn = cn + fk(m+N/2+1)*exp(1i*m*x_scaled.'); end, toc
norm(c-cn,inf)
```

```
Elapsed time is 11.679265 seconds.
ans =
      1.76508266507874e-11
```

Thus, with only 10^3 modes, FINUFFT is 500 times faster than naive multithreaded summation. (Naive summation with reversed loop order is even worse, taking 29 seconds.) We plot 1% of the resulting values and get the smooth but randomly-sampled graph below:

```
Mp = 1e4;                % how many pts to plot
jplot = 1:Mp;            % indices to plot
plot(x(jplot),real(c(jplot)),'b.'); axis tight; xlabel('x'); ylabel('Re f(x)');
```



See the full code tutorial/serieseval1d.m which also shows how to evaluate the same series on a uniform grid via the plain FFT.

2D Fourier series

Since we already know how to rescale to periodicity L, let's revert to the natural period and work in the square $[0, 2\pi)^2$. We create a random 2D Fourier series, which happens to be for a Gaussian random field with (doubly periodized) isotropic Matérn kernel of arbitrary power:

```
kmax = 500;                     % bandlimit per dim
k = -kmax:kmax-1;               % freq indices in each dim
N1 = 2*kmax; N2 = N1;           % # modes in each dim
[k1 k2] = ndgrid(k,k);          % grid of freq indices
rng(0); fk =  randn(N1,N2)+1i*randn(N1,N2);          % iid random complex modes
k0 = 30;                       % freq scale parameter
alpha = 3.7;                   % power; alpha>2 to converge in L^2
fk = fk .* ((k1.^2+k2.^2)/k0^2 + 1).^(-alpha/2);     % sqrt of spectral density
```

We then simply call a 2D type 2 to evaluate this double series at whatever target points you like:

```
M = 1e6; x = 2*pi*rand(1,M); y = 2*pi*rand(1,M);    % random targets in square
tol = 1e-9;
tic; c = finufft2d2(x,y,+1,tol,fk); toc   % evaluate Fourier series at (x,y)'s
```

```
Elapsed time is 0.092743 seconds.
```

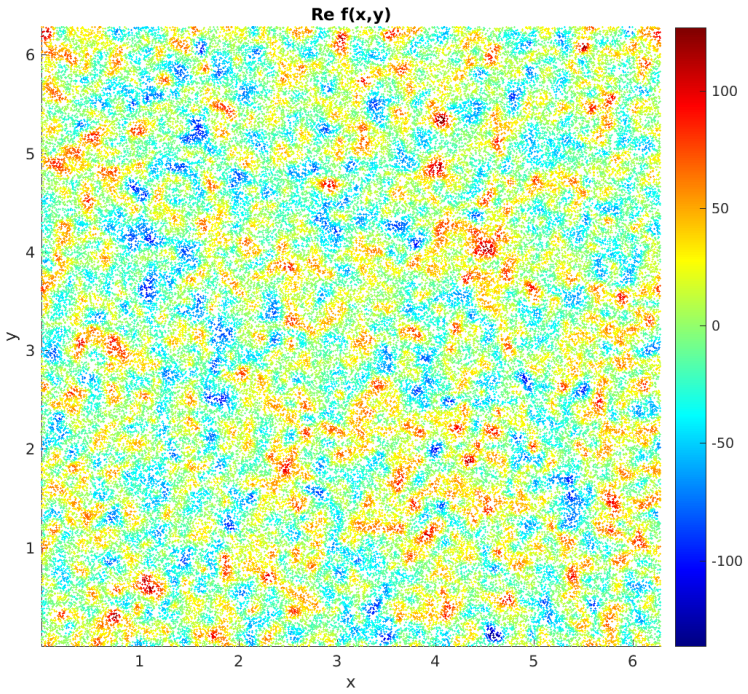
1 million modes to 1 million points in 92 milliseconds on a laptop is decent. We check the math (using a relative error measure) at just one (generic) point:

```
j = 1;                          % do math check on 1st target...
c1 = sum(sum(fk.*exp(1i*(k1*x(j)+k2*y(j)))));
abs(c1-c(j)) / norm(c,inf)
```

```
ans =
      2.30520830208365e-10
```

Finally we use a colored scatter plot to show the first 10% of the points in the square, and see samples of the underlying random field (reminiscent of WMAP microwave background data):

```
jplot = 1:1e5;            % indices to plot
scatter(x(jplot),y(jplot),1.0,real(c(jplot)),'filled'); axis tight equal
xlabel('x'); ylabel('y'); colorbar; title('Re f(x,y)');
```



See the full code tutorial/serieseval2d.m.

For background on Gaussian random fields, aka, Gaussian processes, see, eg, C. E. Rasmussen & C. K. I. Williams, *Gaussian Processes for Machine Learning*, the MIT Press, 2006. http://www.GaussianProcess.org/gpml

4.9.2 Efficient evaluation of (continuous) Fourier transforms

Say you want to evaluate the continous (as opposed to discrete) Fourier *transform* (FT) of a given function, but you do not know the analytic formula for the FT. You need a numerical method. It is common to assume that the FFT is the right tool to do this, but this rarely so ... unless you are content with very poor accuracy! The reason is that the FFT applies only to equispaced data samples, which enforces the use of N equispaced nodes in any quadrature scheme for the Fourier integral. Thus, unless you apply endpoint weight corrections (which are available only in 1D, and stable only up to around 8th order; see references at the bottom of this page), you are generally stuck with 1st or 2nd order (the standard trapezoid rule) convergence with respect to N. And there are many situations where a FFT-based scheme would be even worse: this includes nonsmooth or singular functions (which demand custom quadrature rules even in 1D), smooth functions with varying scales (demanding *adaptive* quadrature for efficiency), and possibly nonsmooth functions on complicated domains in higher dimensions.

Here we show that the NUFFT is often the right tool for efficient and accurate Fourier tranform evaluation, since it allows the user to apply their favorite quadrature scheme as appropriate for whatever nasty function they desire. As long as N is bigger than around 10, the NUFFT becomes more efficient than direct evaluation of exponential sums; as we know, most quadrature rules, especially in 2D or 3D, involve many more points than this.

1D FTs evaluated at arbitrary frequencies

Given a function f, we'll need a single quadrature scheme with nodes x_j and weights w_j, $j = 1, \ldots, N$, that allows *accurate* approximation of its Fourier integral

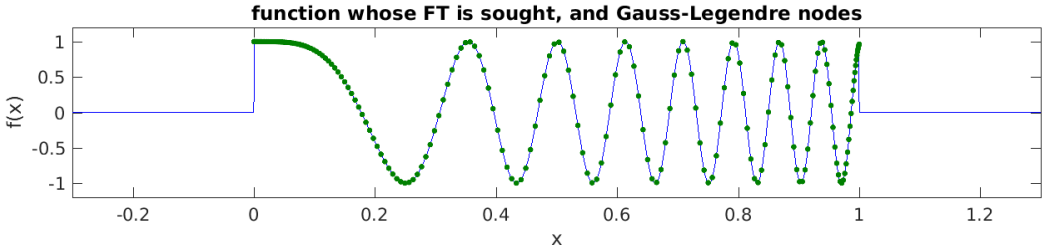
$$\hat{f}(k) = \int f(x) e^{ikx} dx \approx \sum_{j=1}^{N} f(x_j) e^{ikx_j} w_j \tag{4.4}$$

for all "target" frequencies k in some domain of interest. You can apply the below to any f for which you have such a rule.

For simplicity let's take f a smooth (somewhat oscillatory) function on (a, b), choose a million random frequency targets out to some `kmax`, then pick Gauss-Legendre quadrature for (a, b):

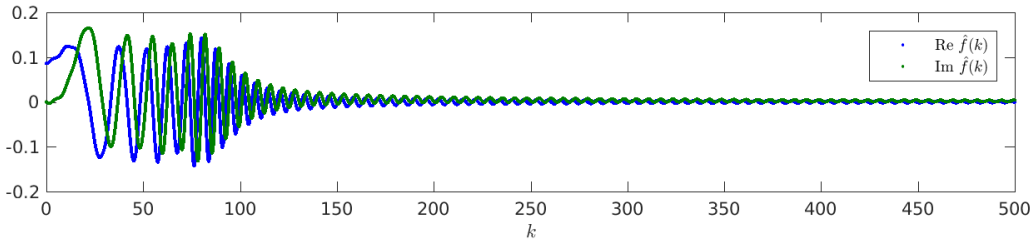
```
a=0; b=1;                          % interval
f = @(x) cos(50*x.^2);             % our smooth function defined on (a,b), zero elsewhere
M = 1e6;                           % # targets we want to compute the FT at
kmax = 500;
k = kmax * (2*rand(1,M)-1);        % desired target frequencies
N = 200;                           % how many quadrature nodes
[xj,wj] = lgwt(N,a,b);             % quadrature rule for smooth funcs on (a,b)
```

Below is f with the 200-node rule overlayed on it. You'll notice that the rule seems to be excessively fine (over-resolving $f(x)$), but that's because it actually needs to be able to resolve $f(x)e^{ikx}$ for all of our k values:



Notice (4.4) is simply a type 3 NUFFT with strengths $c_j = f(x_j)w_j$, so we evaluate it by calling FINUFFT (this takes 0.1 sec) then plot the resulting FT at its target k points:

```
tol = 1e-10;
fhat = finufft1d3(xj, f(xj).*wj, +1, tol, k);
plot(k, [real(fhat),imag(fhat)], '.');
```



This looks like a continuous curve, but is actually (half a) million discrete points. Notice that because f was discontinuous on $\mathbb{R}$, $\hat{f}(k)$ decays slowly like $|k|^{-1}$. How do we know to trust the answer? A convergence study in `N` shows that 200 nodes was indeed enough to reduce the quadrature error to below the 10^{-10} NUFFT tolerance:

```
Ns = 100:10:220;                   % N values to check convergence
for i=1:numel(Ns), N=Ns(i);
  [xj,wj] = lgwt(N,a,b);           % N-node quadrature scheme for smooth funcs on (a,b)
```

(continues on next page)

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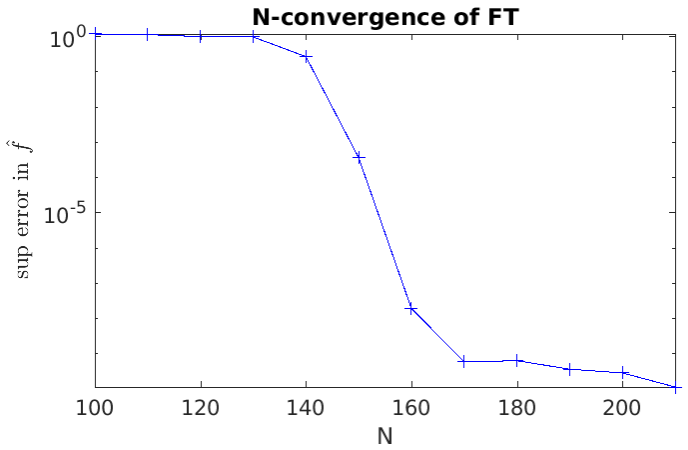
```
  fhats{i} = finufft1d3(xj, f(xj).*wj, +1, tol, k);
end
f0 = norm(fhats{end},inf);    % compute rel sup norm of fhat vs highest-N case
for i=1:numel(Ns)-1, errsup(i) = norm(fhats{i}-fhats{end},inf)/f0; end
semilogy(Ns(1:end-1),errsup,'+-');
```



Remember: always do a convergence study! We see rapid spectral convergence as the quadrature rule resolves the oscillations in e^{ikx} at $|k| = k_{\max}$. See tutorial/contft1d.m for the full code.

Note: If you cared about only a few very high k values, numerical steepest descent applied at the endpoints a and b would eventually beat the above.

Faster FTs when frequencies lie on a grid

When the target frequencies lie on a uniform grid, the above type 3 NUFFT can be replaced by a type 1, which is faster, by a simple rescaling. Say that we replace the random targets in the above example by this uniform grid with spacing `dk`:

```
dk = 2*kmax/M;               % spacing of target k grid
k = dk * (-M/2:(M/2-1));     % a particular uniform M-grid of this spacing
```

Reusing our quadrature `xj`, `wj` from above, we wish to stretch the frequency grid from spacing `dk` to have unit spacing, which is the integer (Fourier mode) grid implied by (1.1), the definition of the type 1. This is equivalent to squeezing the inputs x_j by the same factor, which we do as we send them in:

```
cj = f(xj).*wj;              % strengths (same as before)
fhat = finufft1d1(dk*xj, cj, +1, tol, M);    % type 1, requesting M modes
```

This took only 0.05 sec, around twice as fast as before. We must check it is giving what we want:

```
fhat3 = finufft1d3(xj, cj, +1, tol, k);      % old type 3 method
norm(fhat-fhat3,inf)
```

which reports around `3e-11`, so it worked. Note the specific offset of the `k` grid matched that of the Fourier mode indices; if you want a different offset, you will have to shift (by it to this specific offset, then post-multiply `fhat` with a corresponding phase.

1D FTs of singular functions

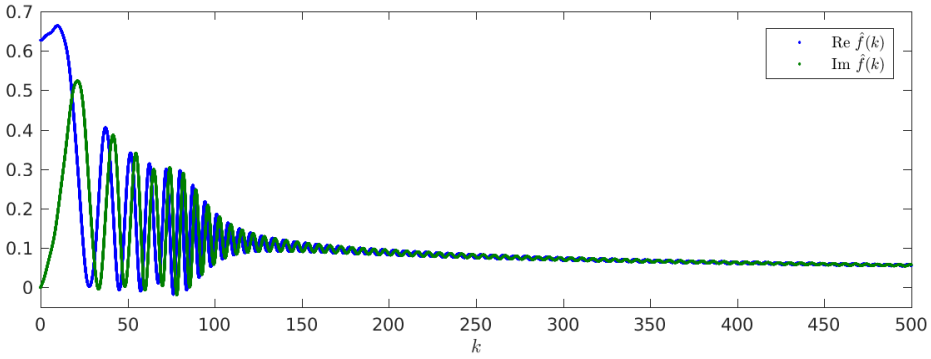
The above f was merely discontinuous. But you can now go further and easily replace (x_j, w_j) by a rule that is accurate for a function with known singularities. Eg, say $f(x) = x^{-1/2}g(x)$ where g is smooth on $[0,1]$, then the change of variable $x = y^2$ means that $\int_0^1 f(x)dx = \int_0^1 2yf(y)dy$, the latter having a smooth integrand to which plain Gauss-Legendre can be applied, giving a new rule $x'_j = x_j^2$ and $w'_j = 2x_j w_j$. Notice how this bypassed the pain of building a $(\alpha = 0, \beta = -1/2)$ Gauss-Jacobi quadrature!

Let's try out this new rule on a suitably singular function, keeping other aspects the same as the above type 1 method:

```
f = @(x) cos(50*x.^2)./sqrt(x);     % singular function defined on (0,1), zero␣
↪elsewhere
Ns = 180:20:240;                    % N values to check convergence
for i=1:numel(Ns), N=Ns(i);
  [xj,wj] = lgwt(N,a,b);            % N-node scheme for smooth funcs on (0,1)
  wj = 2*xj.*wj; xj = xj.*xj;       % convert to rule for -1/2 power singularity @ 0
  fhats{i} = finufft1d1(dk*xj, f(xj).*wj, +1, tol, M);          % type 1 as above
end
f0 = norm(fhats{end},inf);          % compute rel sup norm of fhat vs highest-N case
for i=1:numel(Ns)-1, errsup(i) = norm(fhats{i}-fhats{end},inf)/f0; end
disp([Ns(1:3); errsup(1:3)]')
fhat = fhats{end}; plot(k, [real(fhats),imag(fhat)], '.');
```

This exhibits rapid convergence kinking in at a slightly higher N, while $\hat{f}(k)$ now has even slower decay (which one can check is $|k|^{-1/2}$):

```
180         0.208975054515039
200      3.04233050928417e-05
220       1.9202016281569e-10
```



Neither f nor $\hat{f}$ is in $L^2(\mathbb{R})$. Other rules (adaptive, etc) can be designed to efficiently handle various other features of even nastier f choices.

2D FTs

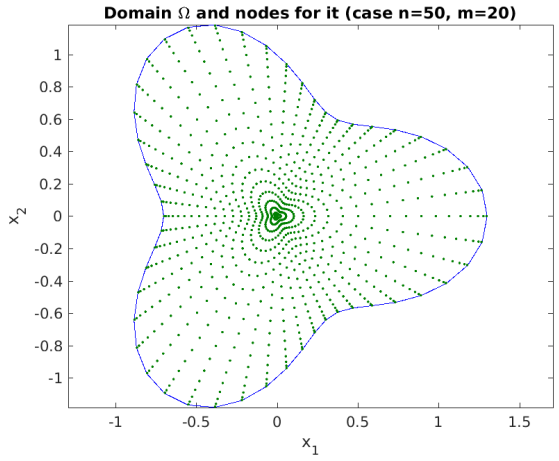
In higher dimensions, the idea is the same: set up a good quadrature rule for your function f, then apply it to the Fourier integral

$$\hat{f}(\mathbf{k}) = \int f(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x} \approx \sum_{j=1}^{N} f(\mathbf{x}_j)e^{i\mathbf{k}\cdot\mathbf{x}_j}w_j \tag{4.5}$$

for all "target" frequencies $\mathbf{k}$ in your domain of interest. We demo the case of $f = \chi_\Omega$, the characteristic function of a bounde domain $\Omega \subset \mathbb{R}^2$, that is, $f(\mathbf{x}) = 1$ for $x \in \Omega$, and 0 otherwise. For simplicity, let's take Ω with boundary

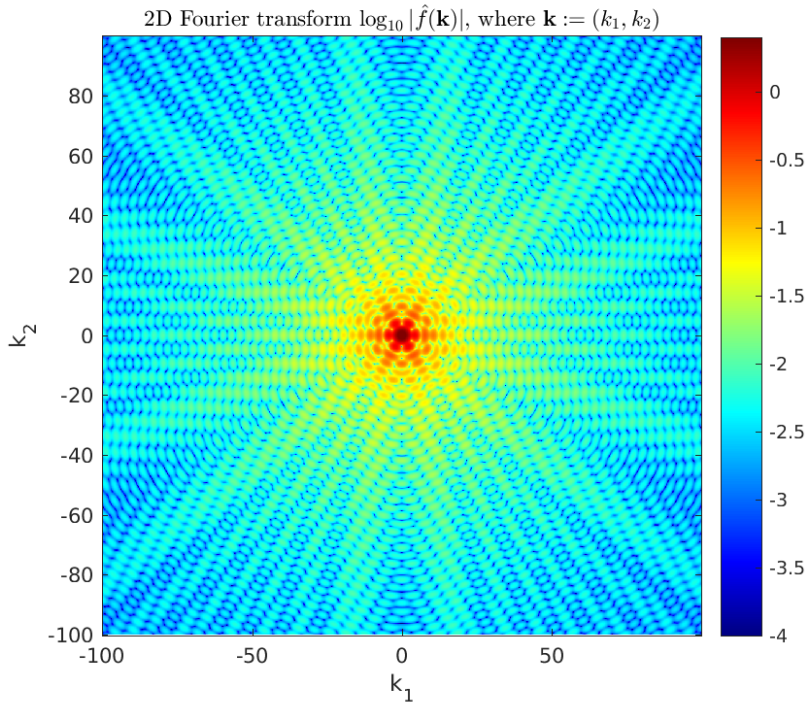
described in polar coordinates by $g(\theta) = 1 + 0.3\cos 5\theta$. This enables a simple two-level quadrature scheme, namely an outer n-node periodic trapezoid rule in θ, whose integrand is an inner m-node Gauss-Legendre rule applied to the radial integral. Since g is smooth, this will have spectral convergence in n and m. Here is a fresh code to make this quadrature over Ω:

```
g = @(t) 1 + 0.3*cos(3*t);                              % boundary shape
n = 280;                                                % # theta nodes
t = 2*pi*(1:n)/n; wt = (2*pi/n);                        % theta nodes, const weights
bx = cos(t).*g(t); by = sin(t).*g(t);                   % boundary points
m = 70;                                                 % # r nodes
[xr,wr] = lgwt(m,0,1);                                  % rule for (0,1)
xj = nan(n*m,1); yj = xj; wj = xj;
for i=1:n                                               % loop over angles
  r = g(t(i)); jj = (1:m) + (i-1)*m;                    % this radius; index list
  xj(jj) = cos(t(i))*r*xr; yj(jj) = sin(t(i))*r*xr;     % line of nodes
  wj(jj) = wt*r^2*xr.*wr;             % theta weight times rule for r.dr on (0,r)
end
plot([bx bx(1)],[by by(1)],'-'); hold on; plot(xj,yj,'.');
```



Note that we reduced the numbers of nodes in the plot for clarity. Say we want $\hat{f}$ on a 2D square grid of frequency targets. We apply the 2D version of the above type 1 scheme. The function is identically 1 in the domain, so the weights simply become the source strengths. We also image the result on a log scale:

```
kmax = 100;                                             % half the side length in k
M1 = 1e3;                                               % target grid will be M1-by-M1
dk = 2*kmax/M1;
k1 = dk * (-M1/2:(M1/2-1));                             % same 1D freq grid as before
tol = 1e-9;
fhat = finufft2d1(dk*xj, dk*yj, wj, +1, tol, M1, M1);   % M1^2 output nodes
imagesc(k1,k1,log10(abs(fhat))'); axis xy equal tight; colorbar
```



Thus we have computed the 2D FT of a discontinous function on a million-point grid to around 10-digit accuracy in 0.05 sec (the FINUFFT transform time). Note that, as with 1D discontinuous functions, the decay with $k := |\mathbf{k}|$ is slow (it is like $1/k$). See the full code tutorial/contft2d.m also for the study that shows that, for the above `kmax`, convergence to the tolerance has occurred by `n=280` and `m=70`, needing $N = 19600$ nodes. A more efficient set would vary `m` with θ.

Note: An application of the above to optics is that Ω is a planar scatterer (or its complement, an aperture, via Babinet's principle) upon which a monochromatic plane wave is incident. The wavelength is small compared to the size of Ω, so that a scalar Kirchhoff diffraction model is a good one. If a downstream planar detector is very distant (the Fraunhofer diffraction limit), and the angles of scattering are small, then $|\hat{f}|^2$ is a good model for the detected scattered intensity.

Further reading

Higher-order end corrections to the trapezoid rule in 1D settings can allow all but $\mathcal{O}(1)$ of the nodes to be on a regular grid. They also can be useful for known singularities (log, 1/sqrt, etc):

- Kapur, S., Rokhlin, V. High-order corrected trapezoidal quadrature rules for singular functions. SIAM J. Numer. Anal. 34(4), 1331–1356 (1997)
- Alpert, B. K. Hybrid Gauss-Trapezoidal Quadrature Rules, SIAM J. Sci. Comput. 20(5), 1551–1584 (1999)

Kirchhoff approximation and Fraunhofer diffraction in optics:

- M. Born and E. Wolf, *Principles of Optics*, 6th edition. Section 8.3.

4.9.3 Periodic Poisson solve on non-Cartesian quadrature grid

It is standard to use the FFT as a fast solver for the Poisson equation on a periodic domain, say $[0,2\pi)^d$. Namely, given f, find u satisfying

$$-\Delta u = f\ , \qquad \text{where } \int_{[0,2\pi)^d} f\,dx = 0\ ,$$

which has a unique solution up to constants. When f and u live on a regular Cartesian mesh, three steps are needed. The first takes an FFT to approximate the Fourier series coefficient array of f, the second divides by $\|k\|^2$, and the third uses another FFT to evaluate the Fourier series for u back on the original grid. Here is a MATLAB demo in $d=2$ dimensions. Firstly we set up a smooth function, periodic up to machine precision:

```
w0 = 0.1;  % width of bumps
src = @(x,y) exp(-0.5*((x-1).^2+(y-2).^2)/w0^2)-exp(-0.5*((x-3).^2+(y-5).^2)/w0^2);
```

Now we do the FFT solve, using a loop to check convergence with respect to `n` the number of grid points in each dimension:

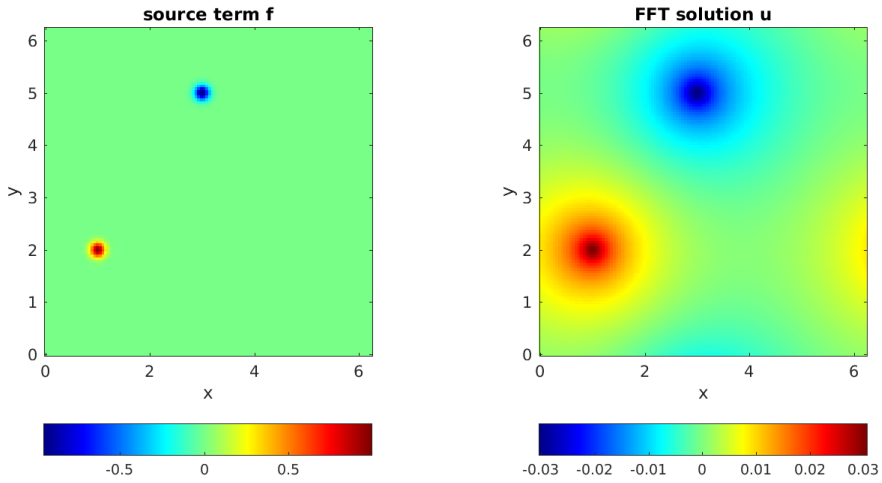
```
ns = 40:20:120;               % convergence study of grid points per side
for i=1:numel(ns), n = ns(i);
  x = 2*pi*(0:n-1)/n;         % grid
  [xx yy] = ndgrid(x,x);      % ordering: x fast, y slow
  f = src(xx,yy);             % eval source on grid
  fhat = ifft2(f);            % step 1: Fourier coeffs by Euler-F projection
  k = [0:n/2-1 -n/2:-1];      % Fourier mode grid
  [kx ky] = ndgrid(k,k);
  kfilter = 1./(kx.^2+ky.^2);     % -(Laplacian)^{-1} in Fourier space
  kfilter(1,1) = 0;           % kill the zero mode (even if inconsistent)
  kfilter(n/2+1,:) = 0; kfilter(:,n/2+1) = 0;  % kill n/2 modes since non-symm
  u = fft2(kfilter.*fhat);    % steps 2 and 3
  u = real(u);
  fprintf('n=%d:\t\tu(0,0) = %.15e\n',n,u(1,1))    % check conv at a point
end
```

We observe spectral convergence to 14 digits:

```
n=40:         u(0,0) = 1.551906153625019e-03
n=60:         u(0,0) = 1.549852227637310e-03
n=80:         u(0,0) = 1.549852190998224e-03
n=100:        u(0,0) = 1.549852191075839e-03
n=120:        u(0,0) = 1.549852191075828e-03
```

Here we plot the FFT solution:

```
figure; subplot(1,2,1); imagesc(x,x,f'); colorbar('southoutside');
axis xy equal tight; title('source term f'); xlabel('x'); ylabel('y');
subplot(1,2,2); imagesc(x,x,u'); colorbar('southoutside');
axis xy equal tight; title('FFT solution u'); xlabel('x'); ylabel('y');
```



Now let's say you wish to do a similar Poisson solve on a **non-Cartesian grid** covering the same domain. There are two cases: a) the grid is unstructured and you do not know the weights of a quadrature scheme, or b) you do know the weights of a quadrature scheme (which ususally implies that the grid is structured, such as arising from a different coordinate system or an adaptive subdivision). By *quadrature scheme* we mean nodes $x_j \in \mathbb{R}^d$, $j = 1, \dots, M$, and weights w_j such that, for all smooth functions f,

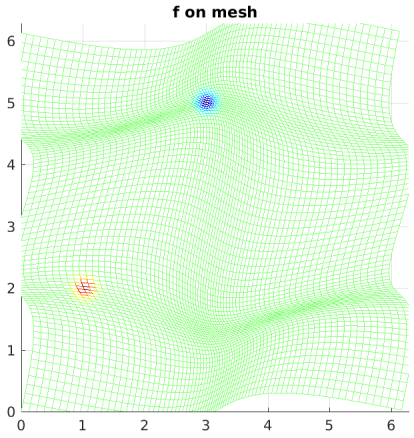
$$\int_{[0,2\pi)^d} f(x)dx \approx \sum_{j=1}^{M} f(x_j)w_j$$

holds to sufficient accuracy. We consider case b) only. For demo purposes, we use a simple smooth diffeomorphism from $[0, 2\pi)^2$ to itself to define a distorted mesh (the associated quadrature weights will come from the determinant of the Jacobian):

```
map = @(t,s) [t + 0.5*sin(t) + 0.2*sin(2*s); s + 0.3*sin(2*s) + 0.3*sin(s-t)];
mapJ = @(t,s) [1 + 0.5*cos(t), 0.4*cos(2*s); ...
               -0.3*cos(s-t),  1+0.6*cos(2*s)+0.3*cos(s-t)]; % its 2x2 Jacobian
```

For convenience of checking the solution against the above one, we chose the map to take the origin to itself. To visualize the grid, we plot f on it, noting that it covers the domain when periodically extended:

```
t = 2*pi*(0:n-1)/n;              % 1d unif grid
[tt ss] = ndgrid(t,t);
xxx = map(tt(:)',ss(:)');
xx = reshape(xxx(1,:),[n n]); yy = reshape(xxx(2,:),[n n]);   % 2D NU pts
f = src(xx,yy);
figure; mesh(xx,yy,f); view(2); axis equal; axis([0 2*pi 0 2*pi]); title('f on mesh');
```

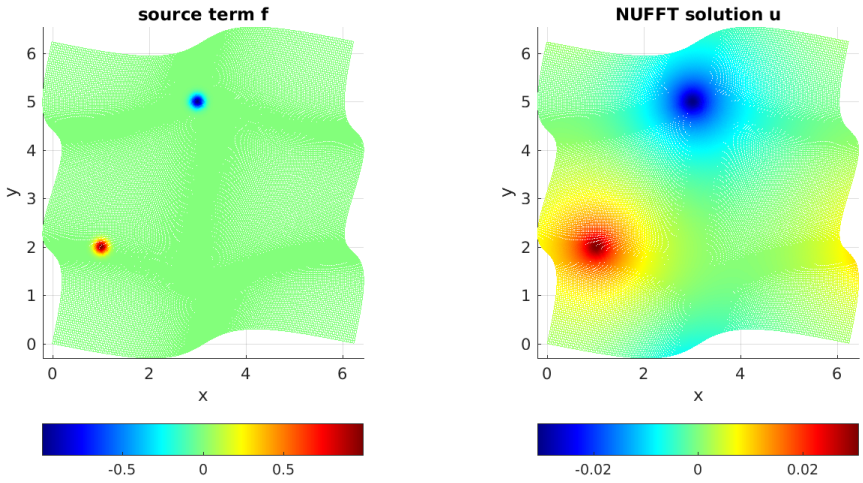


To solve on this grid, replace step 1 above by evaluating the Euler-Fourier formula using the quadrature scheme, which needs a type-1 NUFFT, and step 3 (evaluation on the nonuniform grid) by a type-2 NUFFT. Step 2 (the frequency filter) remains the same. Here is the demo code:

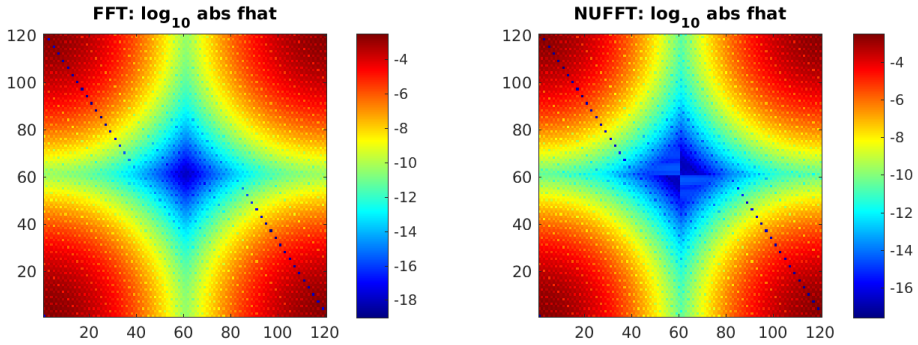
```
tol = 1e-12;            % NUFFT precision
ns = 80:40:240;         % convergence study of grid points per side
for i=1:numel(ns), n = ns(i);
  t = 2*pi*(0:n-1)/n;   % 1d unif grid
  [tt ss] = ndgrid(t,t);
  xxx = map(tt(:)',ss(:)');
  xx = reshape(xxx(1,:),[n n]); yy = reshape(xxx(2,:),[n n]);  % 2d NU pts
  J = mapJ(tt(:)',ss(:)');
  detJ = J(1,1:n^2).*J(2,n^2+1:end) - J(2,1:n^2).*J(1,n^2+1:end);
  ww = detJ / n^2;      % 2d quadr weights, including 1/(2pi)^2 in E-F integr
  f = src(xx,yy);
  Nk = 0.5*n; Nk = 2*ceil(Nk/2);  % modes to trust due to quadr err
  o.modeord = 1;        % use fft output mode ordering
  fhat = finufft2d1(xx(:),yy(:),f(:).*ww(:),1,tol,Nk,Nk,o);  % do E-F
  k = [0:Nk/2-1 -Nk/2:-1];   % Fourier mode grid
  [kx ky] = ndgrid(k,k);
  kfilter = 1./(kx.^2+ky.^2);  % inverse -Laplacian in k-space (as above)
  kfilter(1,1) = 0; kfilter(Nk/2+1,:) = 0; kfilter(:,Nk/2+1) = 0;
  u = finufft2d2(xx(:),yy(:),-1,tol,kfilter.*fhat,o);  % eval filt F series @ NU
  u = reshape(real(u),[n n]);
  fprintf('n=%d:\tNk=%d\tu(0,0) = %.15e\n',n,Nk,u(1,1))  % check conv at same pt
end
```

Here a convergence parameter (`Nk = 0.5*n`) had to be set to choose how many modes to trust with the quadrature. Thus `n` is about twice what it needed to be in the uniform case, accounting for the stretching of the grid. The convergence is again spectral, down to at least `tol`, and matches the FFT solution at the test point to 12 relative digits:

```
n=80:           Nk=40   u(0,0) = 1.549914931081811e-03
n=120:          Nk=60   u(0,0) = 1.549851996895389e-03
n=160:          Nk=80   u(0,0) = 1.549852191032026e-03
n=200:          Nk=100  u(0,0) = 1.549852191076891e-03
n=240:          Nk=120  u(0,0) = 1.549852191077001e-03
```



Finally, here is the decay of the modes $\hat{f}_k$ on a log plot, for the FFT and NUFFT versions. They are identical down to the level `tol`:



The full code is at tutorial/poisson2dnuquad.m.

Note: If the non-Cartesian grids were of *tensor product* form, one could instead exploit 1D NUFFTs for the above, and, most likely the use of BLAS3 (`ZGEMM` with an order-`n` dense NUDFT matrix) would be optimal.

Note: Using the NUFFT as above does *not* give an optimal scaling scheme in the case of a **fully adaptive grid**, because all frequencies must be handled up to the highest one needed. The latter is controlled by the smallest spatial scale, so that the number of modes needed, N, is no smaller than the number in a *uniform* spatial discretization of the original domain at resolution needed to capture the smallest features. In other words, the advantage of full adaptivity is lost when using the NUFFT, and one may as well have used the FFT with a uniform Cartesian grid. To remedy this and recover linear complexity in the fully adaptive case, an FMM could be used to convolve f with the (periodized) Laplace fundamental solution to obtain u, or a multigrid or direct solver used on the discretization of the Laplacian on

the adaptive grid.

For further applications, see *references*, and:

- The numerical sampling of random plane waves.
- These seminar PDF slides.

4.10 Usage from Fortran

We provide Fortran interfaces that are very similar to those in C/C++. We deliberately use "legacy" Fortran style (in the terminology of FFTW), enabling the widest applicability and avoiding the complexity of later Fortran features. Namely, we use f77, with two features from f90: dynamic allocation and derived types. The latter is only needed if options must be changed from default values.

4.10.1 Quick-start example

To perform a double-precision 1D type 1 transform from `M` nonuniform points `xj` with strengths `cj`, to `N` output modes whose coefficients will be written into the `fk` array, using 9-digit tolerance, the $+i$ imaginary sign, and default options, the declarations and call are

```
      integer ier,iflag
      integer*8 N,M
      real*8, allocatable :: xj(:)
      real*8 tol
      complex*16, allocatable :: cj(:),fk(:)
      integer*8, allocatable :: null

!     (...allocate xj, cj, and fk, and fill xj and cj here...)

      tol = 1.0D-9
      iflag = +1
      call finufft1d1(M,xj,cj,iflag,tol,N,fk,null,ier)
```

which writes the output to `fk`, and the status to the integer `ier`. Since the default is CMCL mode ordering, the output for frequency index `k` is found in `fk(k+N/2+1)`. `ier=0` indicates success, otherwise error codes are as in *here*. All available OMP threads are used, unless FINUFFT was built single-threaded. (Note that here the unallocated `null` is simply a way to pass a NULL pointer to our C++ wrapper; another would be `%val(0_8)`.) For a minimally complete test code demonstrating the above see `fortran/examples/simple1d1.f`.

Note: Higher-dimensional arrays are stored in Fortran ordering with x (`N1`) the fastest direction, and, in the vectorized ("many") calls, the transform number is slowest (transforms are stacked not interleaved). For instance, for the 2D type 1 vectorized transform `finufft2d1many(ntrans,M,xj,yj,cj,iflag,tol,N1,N2,fk,opts, ier)` with CMCL mode-ordering, the `(k1,k2)` frequency coefficient from transform number `t` is to be found at `fk(k1+N1/2+1 + (k2+N2/2)*N1 + t*N1*N2)`.

To compile (eg using GCC/linux) and link such a program against the FINUFFT dynamic (`.so`) library (which links all dependent libraries):

```
gfortran -I $(FINUFFT)/include simple1d1.f -o simple1d1 -L$(FINUFFT)/lib -lfinufft
```

where `$(FINUFFT)` indicates the top-level FINUFFT directory. Or, using the static library, one must list dependent libraries:

```
gfortran -I $(FINUFFT)/include simple1d1.f -o simple1d1 $(FINUFFT)/lib-static/
↪libfinufft.a -lfftw3 -lfftw3_omp -lgomp -lstdc++
```

Alternatively you may want to compile with `g++` and use `-lgfortran` at the end of the compile statement instead of `-lstdc++`. In Mac OSX, replace `fftw3_omp` by `fftw3_threads`, and if you use clang, `-lgomp` by `-lomp`. See `makefile` and `make.inc.*`.

Note: Our simple interface is designed to be a near drop-in replacement for the native f90 CMCL libraries of Greengard-Lee. The differences are: i) we added a penultimate argument in the list which allows options to be changed, and ii) our normalization differs for type 1 transforms (divide FINUFFT output by M to match CMCL output).

4.10.2 Changing options

To choose non-default options in the above example, create an options derived type, set it to default values, change whichever you wish, and pass it to FINUFFT, for instance

```
      include 'finufft.fh'
      type(nufft_opts) opts

!     (...declare, allocate, and fill stuff as above...)

      call finufft_default_opts(opts)
      opts%debug = 2
      opts%upsampfac = 1.25d0
      call finufft1d1(M,xj,cj,iflag,tol,N,fk,opts,ier)
```

See `fortran/examples/simple1d1.f` for the complete code, and below for the complete list of Fortran subroutines available, and more complicated examples.

See `modeord` in *Options* to instead use FFT-style mode ordering, which simply differs by an `fftshift` (as it is commonly called).

4.10.3 Summary of Fortran interface

The names of routines and the meanings of all arguments is identical to the *C/C++ routines*. Eg, `finufft2d3` means double-precision 2D transform of type 3. `finufft2d3many` means applying double-precision 2D transforms of type 3 to a stack of many strength vectors (vectorized interface). `finufft2d3f` means single-precision 2D type 3. The guru interface has very similar arguments to its C/C++ version. Compared to C/C++, all argument lists have `ier` appended at the end, to which the status is written; this is the same as the return value in the C/C++ interfaces. These routines and arguments are, in double-precision:

```
      include 'finufft.fh'

      integer ier,iflag,ntrans,type,dim
      integer*8 M,N1,N2,N3,Nk
      integer*8 plan,n_modes(3)
      real*8, allocatable :: xj(:),yj(:),zj(:), sk(:),tk(:),uk(:)
      real*8 tol
      complex*16, allocatable :: cj(:), fk(:)
      type(nufft_opts) opts
```

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```
!     simple interface
      call finufft1d1(M,xj,cj,iflag,tol,N1,fk,opts,ier)
      call finufft1d2(M,xj,cj,iflag,tol,N1,fk,opts,ier)
      call finufft1d3(M,xj,cj,iflag,tol,Nk,sk,fk,opts,ier)
      call finufft2d1(M,xj,yj,cj,iflag,tol,N1,N2,fk,opts,ier)
      call finufft2d2(M,xj,yj,cj,iflag,tol,N1,N2,fk,opts,ier)
      call finufft2d3(M,xj,yj,cj,iflag,tol,Nk,sk,tk,fk,opts,ier)
      call finufft3d1(M,xj,yj,zj,cj,iflag,tol,N1,N2,N3,fk,opts,ier)
      call finufft3d2(M,xj,yj,zj,cj,iflag,tol,N1,N2,N3,fk,opts,ier)
      call finufft3d3(M,xj,yj,zj,cj,iflag,tol,Nk,sk,tk,uk,fk,opts,ier)

!     vectorized interface
      call finufft1d1many(ntrans,M,xj,cj,iflag,tol,N1,fk,opts,ier)
      call finufft1d2many(ntrans,M,xj,cj,iflag,tol,N1,fk,opts,ier)
      call finufft1d3many(ntrans,M,xj,cj,iflag,tol,Nk,sk,fk,opts,ier)
      call finufft2d1many(ntrans,M,xj,yj,cj,iflag,tol,N1,N2,fk,opts,ier)
      call finufft2d2many(ntrans,M,xj,yj,cj,iflag,tol,N1,N2,fk,opts,ier)
      call finufft2d3many(ntrans,M,xj,yj,cj,iflag,tol,Nk,sk,tk,fk,opts,ier)
      call finufft3d1many(ntrans,M,xj,yj,zj,cj,iflag,tol,N1,N2,N3,fk,opts,ier)
      call finufft3d2many(ntrans,M,xj,yj,zj,cj,iflag,tol,N1,N2,N3,fk,opts,ier)
      call finufft3d3many(ntrans,M,xj,yj,zj,cj,iflag,tol,Nk,sk,tk,uk,fk,opts,ier)

!     guru interface
      call finufft_makeplan(type,dim,n_modes,iflag,ntrans,tol,plan,opts,ier)
      call finufft_setpts(plan,M,xj,yj,zj,Nk,sk,yk,uk,ier)
      call finufft_execute(plan,cj,fk,ier)
      call finufft_destroy(plan,ier)
```

The single-precision (ie, `real*4` and `complex*8`) functions are identical except with the replacement of `finufft` with `finufftf` in each function name. All are defined (from the C++ side) in `fortran/finufftfort.cpp`.

4.10.4 Code examples

The `fortran/examples` directory contains the following demos, in both precisions. Each has a math test to check the correctness of some or all outputs:

```
simple1d1.f        - 1D type 1, simple interface, default and various opts
guru1d1.f          - 1D type 1, guru interface, default and various opts
nufft1d_demo.f     - 1D types 1,2,3, minimally changed from CMCL demo codes
nufft2d_demo.f     - 2D "
nufft3d_demo.f     - 3D "
nufft2dmany_demo.f - 2D types 1,2,3, vectorized (many strengths) interface
```

These are the double-precision file names; the single precision have a suffix `f` before the `.f`. The last four here are modified from demos in the CMCL NUFFT libraries. The first three of these have been changed only to use FINUFFT. The final tolerance they request is `tol=1d-16`. For this case FINUFFT will report a warning that it cannot achieve it, and gets merely around 10^{-14}. The last four demos require direct summation (slow) reference implementations of the transforms in `fortran/directft`, modified from their CMCL counterparts only to remove the $1/M$ prefactor for type 1 transforms.

All demos have self-contained example GCC compilation/linking commands in their comment headers. For dynamic linking so that execution works from any directory, bake in an absolute path via the compile flag `-Wl,-rpath,$(FINUFFT)/lib`.

For authorship and licensing of the Fortran wrappers, see the README in the fortran directory.

4.11 MATLAB/octave interfaces

4.11.1 Quick-start examples

To demo a single 1D transform of type 1 (nonuniform points to uniform Fourier coefficients), we set up random data then do the transform as follows:

```
M = 1e5;                                % number of NU source points
x = 2*pi*rand(M,1);                     % points in a 2pi-periodic domain
c = randn(M,1)+1i*randn(M,1);           % iid random complex data (row or col vec)
N = 2e5;                                % how many desired Fourier modes?
f = finufft1d1(x,c,+1,1e-12,N);         % do it (takes around 0.02 sec)
```

The column vector output `f` should be interpreted as the Fourier coefficients with frequency indices `k = -N/2:N/2-1`. (This is because `N` is even; otherwise `k = -(N-1)/2:(N-1)/2`.) The values in `f` are accurate (relative to this vector's 2-norm) to roughly 12 digits, as requested by the tolerance argument `1e-12`. Choosing a larger (ie, worse) tolerance leads to faster transforms. The `+1` controls the sign in the exponential; recall equation (1) on the *front page*. All *options* maybe be changed from their defaults, for instance:

```
o.modeord = 1;                          % choose FFT-style output mode ordering
f = finufft1d1(x,c,+1,1e-12,N,o);       % do it
```

The above usage we call the "simple" interface. There is also a "vectorized" interface which does the transform for multiple stacked strength vectors, using the same nonuniform points each time. We demo this, reusing `x` and `N` from above:

```
ntr = 1e2;                              % number of vectors (transforms to do)
C = randn(M,ntr)+1i*randn(M,ntr);       % iid random complex data (matrix)
F = finufft1d1(x,C,+1,1e-12,N);         % do them (takes around 1.2 sec)
```

Here this is nearly twice as fast as doing 100 separate calls to the simple interface. For smaller transform sizes the acceleration factor of this vectorized call can be much higher.

If you want yet more control, consider using the "guru" interface. This can be faster than fresh calls to the simple or vectorized interfaces for the same number of transforms, for reasons such as this: the nonuniform points can be changed between transforms, without forcing FFTW to look up a previously stored plan. Usually, such an acceleration is only important when doing repeated small transforms, where "small" means each transform takes of order 0.01 sec or less. Here we use the guru interface to repeat the first demo above:

```
type = 1; ntr = 1; o.modeord = 1;       % transform type, #transforms, opts
N = 2e5;                                % how many desired Fourier modes?
plan = finufft_plan(1,N,+1,ntr,1e-12,o);      % plan for N output modes
M = 1e5;                                % number of NU source points
plan.setpts(2*pi*rand(M,1),[],[]);      % set some nonuniform points
c = randn(M,1)+1i*randn(M,1);           % iid random complex data (row or col vec)
f = plan.execute(c);                    % do the transform (0.008 sec)
% ...one could now change the points with setpts, and/or do new transforms
% with new c data...
delete(plan);                           % don't forget to clean up
```

Finally, we demo a 2D type 1 transform using the simple interface. Let's request a rectangular Fourier mode array of 1000 modes in the x direction but 500 in the y direction. The source points are in the square of side length 2π:

```
M = 1e6; x = 2*pi*rand(1,M); y = 2*pi*rand(1,M);     % points in [0,2pi]^2
c = randn(M,1)+1i*randn(M,1);           % iid random complex data (row or col vec)
```

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```
N1 = 1000; N2 = 500;                % desired Fourier mode array sizes
f = finufft2d1(x,y,c,+1,1e-9,N1,N2);          % do it (takes around 0.08 sec)
```

The resulting output `f` is indeed size 1000 by 500. The first dimension (number of rows) corresponds to the x input coordinate, and the second to y.

If you need to change the definition of the period from 2π, simply linearly rescale your points before sending them to FINUFFT.

Note: Under the hood FINUFFT has double- and single-precision libraries. The simple and vectorized MATLAB/octave interfaces infer which to call by checking the class of its input arrays, which must all match (ie, all must be `double` or all must be `single`). Since by default MATLAB arrays are double-precision, this is the precision that all of the above examples run in. To perform single-precision transforms, send in single-precision data. In contrast, precision in the guru interface is set with the `finufft_plan` option string `o.floatprec`, either `'double'` (the default), or `'single'`.

See tests and examples in the repo and *tutorials and demos* for plenty more MATLAB examples.

4.11.2 Full documentation

Here are the help documentation strings for all MATLAB/octave interfaces. They only abbreviate the options (for full documentation see *Options parameters*). Informative warnings and errors are raised in MATLAB style with unique codes (see `../matlab/errhandler.m`, `../matlab/finufft.mw`, and `../valid_*.m`). The low-level error number codes are not used.

If you have added the `matlab` directory of FINUFFT correctly to your MATLAB path via something like `addpath FINUFFT/matlab`, then `help finufft/matlab` will give the summary of all commands:

```
% FINUFFT: Flatiron Institute Nonuniform Fast Fourier Transform
% Version 1.2.0 23-Jul-2020
%
% Basic and many-vector interfaces
%   finufft1d1 - 1D complex nonuniform FFT of type 1 (nonuniform to uniform).
%   finufft1d2 - 1D complex nonuniform FFT of type 2 (uniform to nonuniform).
%   finufft1d3 - 1D complex nonuniform FFT of type 3 (nonuniform to nonuniform).
%   finufft2d1 - 2D complex nonuniform FFT of type 1 (nonuniform to uniform).
%   finufft2d2 - 2D complex nonuniform FFT of type 2 (uniform to nonuniform).
%   finufft2d3 - 2D complex nonuniform FFT of type 3 (nonuniform to nonuniform).
%   finufft3d1 - 3D complex nonuniform FFT of type 1 (nonuniform to uniform).
%   finufft3d2 - 3D complex nonuniform FFT of type 2 (uniform to nonuniform).
%   finufft3d3 - 3D complex nonuniform FFT of type 3 (nonuniform to nonuniform).
%
% Guru interface
%   finufft_plan - create guru plan object for one/many general nonuniform FFTs.
%   setpts       - process nonuniform points for general FINUFFT transform(s).
%   execute      - do a single or many-vector FINUFFT transform in a plan.
```

The individual commands have the following help documentation:

```
FINUFFT1D1   1D complex nonuniform FFT of type 1 (nonuniform to uniform).

f = finufft1d1(x,c,isign,eps,ms)
f = finufft1d1(x,c,isign,eps,ms,opts)
```

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```
This computes, to relative precision eps, via a fast algorithm:

              nj
    f(k1) =  SUM c[j] exp(+/-i k1 x(j))  for -ms/2 <= k1 <= (ms-1)/2
             j=1
  Inputs:
    x     locations of nonuniform sources on interval [-3pi,3pi), length nj
    c     length-nj complex vector of source strengths. If numel(c)>nj,
          expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
          transformed with the same source locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    ms    number of Fourier modes computed, may be even or odd;
          in either case, mode range is integers lying in [-ms/2, (ms-1)/2]
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
  Outputs:
    f     size-ms complex column vector of Fourier coefficients, or, if
          ntrans>1, a matrix of size (ms,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT1D2   1D complex nonuniform FFT of type 2 (uniform to nonuniform).

c = finufft1d2(x,isign,eps,f)
c = finufft1d2(x,isign,eps,f,opts)

This computes, to relative precision eps, via a fast algorithm:

   c[j] = SUM   f[k1] exp(+/-i k1 x[j])      for j = 1,...,nj
           k1
    where sum is over -ms/2 <= k1 <= (ms-1)/2.

 Inputs:
    x     location of nonuniform targets on interval [-3pi,3pi), length nj
```

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```
    f     complex Fourier coefficients. If a vector, length sets ms
          (with mode ordering given by opts.modeord). If a matrix, each
          of ntrans columns is transformed with the same nonuniform targets.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
 Outputs:
    c     complex column vector of nj answers at targets, or,
          if ntrans>1, matrix of size (nj,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT1D3   1D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

f = finufft1d3(x,c,isign,eps,s)
f = finufft1d3(x,c,isign,eps,s,opts)

This computes, to relative precision eps, via a fast algorithm:

             nj
    f[k]  =  SUM   c[j] exp(+-i s[k] x[j]),      for k = 1, ..., nk
             j=1
  Inputs:
    x     locations of nonuniform sources on R (real line), length-nj vector.
    c     length-nj complex vector of source strengths. If numel(c)>nj,
          expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
          transformed with the same source and target locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    s     frequency locations of nonuniform targets on R, length-nk vector.
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
```

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```
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
  Outputs:
    f     length-nk complex vector of values at targets, or, if ntrans>1,
          a matrix of size (nk,ntrans)

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT2D1   2D complex nonuniform FFT of type 1 (nonuniform to uniform).

f = finufft2d1(x,y,c,isign,eps,ms,mt)
f = finufft2d1(x,y,c,isign,eps,ms,mt,opts)

This computes, to relative precision eps, via a fast algorithm:

                  nj
    f[k1,k2] =   SUM  c[j] exp(+-i (k1 x[j] + k2 y[j]))
                 j=1

    for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2.

  Inputs:
    x,y   coordinates of nonuniform sources on the square [-3pi,3pi)^2,
          each a length-nj vector
    c     length-nj complex vector of source strengths. If numel(c)>nj,
          expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
          transformed with the same source locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    ms,mt  number of Fourier modes requested in x & y; each may be even or odd.
           In either case the mode range is integers lying in [-m/2, (m-1)/2]
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
```

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```
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
  Outputs:
    f     size (ms,mt) complex matrix of Fourier coefficients
          (ordering given by opts.modeord in each dimension; ms fast, mt slow),
          or, if ntrans>1, a 3D array of size (ms,mt,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT2D2   2D complex nonuniform FFT of type 2 (uniform to nonuniform).

c = finufft2d2(x,y,isign,eps,f)
c = finufft2d2(x,y,isign,eps,f,opts)

This computes, to relative precision eps, via a fast algorithm:

   c[j] =  SUM   f[k1,k2] exp(+/-i (k1 x[j] + k2 y[j]))  for j = 1,..,nj
           k1,k2
    where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,

 Inputs:
    x,y   coordinates of nonuniform targets on the square [-3pi,3pi)^2,
          each a vector of length nj
    f     complex Fourier coefficient matrix, whose size determines (ms,mt).
          (Mode ordering given by opts.modeord, in each dimension.)
          If a 3D array, 3rd dimension sets ntrans, and each of ntrans
          matrices is transformed with the same nonuniform targets.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
 Outputs:
    c     complex column vector of nj answers at targets, or,
          if ntrans>1, matrix of size (nj,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
```

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```
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT2D3   2D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

f = finufft2d3(x,y,c,isign,eps,s,t)
f = finufft2d3(x,y,c,isign,eps,s,t,opts)

This computes, to relative precision eps, via a fast algorithm:

             nj
    f[k]  =  SUM   c[j] exp(+-i (s[k] x[j] + t[k] y[j])),  for k = 1, ..., nk
             j=1
  Inputs:
    x,y   coordinates of nonuniform sources in R^2, each a length-nj vector.
    c     length-nj complex vector of source strengths. If numel(c)>nj,
          expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
          transformed with the same source and target locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    s,t   frequency coordinates of nonuniform targets in R^2,
          each a length-nk vector.
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
  Outputs:
    f     length-nk complex vector of values at targets, or, if ntrans>1,
          a matrix of size (nk,ntrans)

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT3D1   3D complex nonuniform FFT of type 1 (nonuniform to uniform).
```

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```
f = finufft3d1(x,y,z,c,isign,eps,ms,mt,mu)
f = finufft3d1(x,y,z,c,isign,eps,ms,mt,mu,opts)

This computes, to relative precision eps, via a fast algorithm:

                     nj
    f[k1,k2,k3] =    SUM  c[j] exp(+-i (k1 x[j] + k2 y[j] + k3 z[j]))
                     j=1

    for -ms/2 <= k1 <= (ms-1)/2,  -mt/2 <= k2 <= (mt-1)/2,
        -mu/2 <= k3 <= (mu-1)/2.

  Inputs:
    x,y,z  coordinates of nonuniform sources on the cube [-3pi,3pi)^3,
           each a length-nj vector
    c      length-nj complex vector of source strengths. If numel(c)>nj,
           expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
           transformed with the same source locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps    relative precision requested (generally between 1e-15 and 1e-1)
    ms,mt,mu  number of Fourier modes requested in x,y and z; each may be
           even or odd.
           In either case the mode range is integers lying in [-m/2, (m-1)/2]
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
  Outputs:
    f      size (ms,mt,mu) complex array of Fourier coefficients
           (ordering given by opts.modeord in each dimension; ms fastest, mu
           slowest), or, if ntrans>1, a 4D array of size (ms,mt,mu,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT3D2   3D complex nonuniform FFT of type 2 (uniform to nonuniform).

c = finufft3d2(x,y,z,isign,eps,f)
c = finufft3d2(x,y,z,isign,eps,f,opts)
```

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```
This computes, to relative precision eps, via a fast algorithm:

   c[j] =   SUM   f[k1,k2,k3] exp(+/-i (k1 x[j] + k2 y[j] + k3 z[j]))
          k1,k2,k3
                           for j = 1,..,nj
    where sum is over -ms/2 <= k1 <= (ms-1)/2, -mt/2 <= k2 <= (mt-1)/2,
                      -mu/2 <= k3 <= (mu-1)/2.

 Inputs:
    x,y,z coordinates of nonuniform targets on the cube [-3pi,3pi)^3,
          each a vector of length nj
    f     complex Fourier coefficient array, whose size sets (ms,mt,mu).
          (Mode ordering given by opts.modeord, in each dimension.)
          If a 4D array, 4th dimension sets ntrans, and each of ntrans
          3D arrays is transformed with the same nonuniform targets.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
 Outputs:
    c     complex column vector of nj answers at targets, or,
          if ntrans>1, matrix of size (nj,ntrans).

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT3D3   3D complex nonuniform FFT of type 3 (nonuniform to nonuniform).

f = finufft3d3(x,y,z,c,isign,eps,s,t,u)
f = finufft3d3(x,y,z,c,isign,eps,s,t,u,opts)

This computes, to relative precision eps, via a fast algorithm:

             nj
    f[k]  =  SUM   c[j] exp(+-i (s[k] x[j] + t[k] y[j] + u[k] z[j])),
             j=1
```

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```
                            for k = 1, ..., nk
  Inputs:
    x,y,z  coordinates of nonuniform sources in R^3, each a length-nj vector.
    c      length-nj complex vector of source strengths. If numel(c)>nj,
           expects a stack of vectors (eg, a nj*ntrans matrix) each of which is
           transformed with the same source and target locations.
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps    relative precision requested (generally between 1e-15 and 1e-1)
    s,t,u  frequency coordinates of nonuniform targets in R^3,
           each a length-nk vector.
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
  Outputs:
    f      length-nk complex vector of values at targets, or, if ntrans>1,
           a matrix of size (nk,ntrans)

Notes:
 * The vectorized (many vector) interface, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * The class of input x (double vs single) controls whether the double or
   single precision library are called; precisions of all data should match.
 * For more details about the opts fields, see ../docs/opts.rst
 * See ERRHANDLER, VALID_* and FINUFFT_PLAN for possible warning/error IDs.
 * Full documentation is given in ../finufft-manual.pdf and online at
   http://finufft.readthedocs.io
```

```
FINUFFT_PLAN   is a class which wraps the guru interface to FINUFFT.

 Full documentation is given in ../finufft-manual.pdf and online at
 http://finufft.readthedocs.io
 Also see examples in the matlab/examples and matlab/test directories.

PROPERTIES
  mwptr - opaque pointer to a C++ finufft_plan object (see MWrap manual),
          whose properties cannot be accessed directly
  floatprec - either 'double' or 'single', tracks what precision of C++
          library is being called
  type, dim, n_modes, n_trans, nj, nk - other plan parameters
 Note: the user should never alter these plan properties directly! Rather,
 the below methods should be used to create, use, and destroy plans.

METHODS
  finufft_plan - create guru plan object for one/many general nonuniform FFTs.
  setpts       - process nonuniform points for general FINUFFT transform(s).
  execute      - execute single or many-vector FINUFFT transforms in a plan.
```

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```
General notes:
 * use delete(plan) to remove a plan after use.
 * See ERRHANDLER, VALID_*, and this code for warning/error IDs.



========== Detailed description of guru methods ========================

1) FINUFFT_PLAN create guru plan object for one/many general nonuniform FFTs.

plan = finufft_plan(type, n_modes_or_dim, isign, ntrans, eps)
plan = finufft_plan(type, n_modes_or_dim, isign, ntrans, eps, opts)

Creates a finufft_plan MATLAB object in the guru interface to FINUFFT, of
 type 1, 2 or 3, and with given numbers of Fourier modes (unless type 3).

Inputs:
    type            transform type: 1, 2, or 3
    n_modes_or_dim  if type is 1 or 2, the number of Fourier modes in each
                    dimension: [ms] in 1D, [ms mt] in 2D, or [ms mt mu] in 3D.
                    Its length sets the dimension, which must be 1, 2 or 3.
                    If type is 3, in contrast, its *value* fixes the dimension
    isign if >=0, uses + sign in exponential, otherwise - sign.
    eps   relative precision requested (generally between 1e-15 and 1e-1)
    opts   optional struct with optional fields controlling the following:
    opts.debug:   0 (silent, default), 1 (timing breakdown), 2 (debug info).
    opts.spread_debug: spreader: 0 (no text, default), 1 (some), or 2 (lots)
    opts.spread_sort:  0 (don't sort NU pts), 1 (do), 2 (auto, default)
    opts.spread_kerevalmeth:  0: exp(sqrt()), 1: Horner ppval (faster)
    opts.spread_kerpad: (iff kerevalmeth=0)  0: don't pad to mult of 4, 1: do
    opts.fftw: FFTW plan mode, 64=FFTW_ESTIMATE (default), 0=FFTW_MEASURE, etc
    opts.upsampfac:   sigma.  2.0 (default), or 1.25 (low RAM, smaller FFT)
    opts.spread_thread:   for ntrans>1 only. 0:auto, 1:seq multi, 2:par, etc
    opts.maxbatchsize:  for ntrans>1 only. max blocking size, or 0 for auto.
    opts.nthreads:   number of threads, or 0: use all available (default)
    opts.floatprec: library precision to use, 'double' (default) or 'single'.
    for type 1 and 2 only, the following opts fields are also relevant:
    opts.modeord: 0 (CMCL increasing mode ordering, default), 1 (FFT ordering)
    opts.chkbnds: 0 (don't check NU points valid), 1 (do, default)
Outputs:
    plan            finufft_plan object (opaque pointer)

Notes:
 * For type 1 and 2, this does the FFTW planning and kernel-FT precomputation.
 * For type 3, this does very little, since the FFT sizes are not yet known.
 * Be default all threads are planned; control how many with opts.nthreads.
 * The vectorized (many vector) plan, ie ntrans>1, can be much faster
   than repeated calls with the same nonuniform points. Note that here the I/O
   data ordering is stacked rather than interleaved. See ../docs/matlab.rst
 * For more details about the opts fields, see ../docs/opts.rst


2) SETPTS   process nonuniform points for general FINUFFT transform(s).

plan.setpts(xj)
plan.setpts(xj, yj)
plan.setpts(xj, yj, zj)
```

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```
plan.setpts(xj, [], [], s)
plan.setpts(xj, yj, [], s, t)
plan.setpts(xj, yj, zj, s, t, u)

 When plan is a finufft_plan MATLAB object, brings in nonuniform point
 coordinates (xj,yj,zj), and additionally in the type 3 case, nonuniform
 frequency target points (s,t,u). Empty arrays may be passed in the case of
 unused dimensions. For all types, sorting is done to internally store a
 reindexing of points, and for type 3 the spreading and FFTs are planned.
 The nonuniform points may be used for multiple transforms.

Inputs:
    xj     vector of x-coords of all nonuniform points
    yj     empty (if dim<2), or vector of y-coords of all nonuniform points
    zj     empty (if dim<3), or vector of z-coords of all nonuniform points
    s      vector of x-coords of all nonuniform frequency targets
    t      empty (if dim<2), or vector of y-coords of all frequency targets
    u      empty (if dim<3), or vector of z-coords of all frequency targets
Input/Outputs:
    plan   finufft_plan object

Notes:
 * For type 1 and 2, the values in xj (and if nonempty, yj and zj) must
   lie in the interval [-3pi,3pi). For type 1 they are "sources", but for
   type 2, "targets". In contrast, for type 3 there are no restrictions other
   than the resulting size of the internal fine grids.
 * s (and t and u) are only relevant for type 3, and may be omitted otherwise
 * The matlab vectors xj,... and s,... should not be changed before calling
   future execute calls, because the plan stores only pointers to the
   arrays (they are not duplicated internally).
 * The precision (double/single) of all inputs must match that chosen at the
   plan stage using opts.floatprec, otherwise an error is raised.


3) EXECUTE   execute single or many-vector FINUFFT transforms in a plan.

result = plan.execute(data_in);

 For plan a previously created finufft_plan object also containing all
 needed nonuniform point coordinates, do a single (or if ntrans>1 in the
 plan stage, multiple) NUFFT transform(s), with the strengths or Fourier
 coefficient inputs vector(s) from data_in. The result of the transform(s)
 is returned as a (possibly multidimensional) array.

Inputs:
    plan     finufft_plan object
    data_in  strengths (types 1 or 3) or Fourier coefficients (type 2)
             vector, matrix, or array of appropriate size. For type 1 and 3,
             this is either a length-M vector (where M is the length of xj),
             or an (M,ntrans) matrix when ntrans>1. For type 2, in 1D this is
             length-ms, in 2D size (ms,mt), or in 3D size (ms,mt,mu), or
             each of these with an extra last dimension ntrans if ntrans>1.
Outputs:
    result   vector of output strengths at targets (types 2 or 3), or array
             of Fourier coefficients (type 1), or, if ntrans>1, a stack of
             such vectors or arrays, of appropriate size.
             Specifically, if ntrans=1, for type 1, in 1D
```

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```
              this is a length-ms column vector, in 2D a matrix of size
              (ms,mt), or in 3D an array of size (ms,mt,mu); for types 2 and 3
              it is a column vector of length M (the length of xj in type 2),
              or nk (the length of s in type 3). If ntrans>1 its is a stack
              of such objects, ie, it has an extra last dimension ntrans.

Notes:
 * The precision (double/single) of all inputs must match that chosen at the
   plan stage using opts.floatprec, otherwise an error is raised.


4) To deallocate (delete) a nonuniform FFT plan, use delete(plan)

This deallocates all stored FFTW plans, nonuniform point sorting arrays,
 kernel Fourier transforms arrays, etc.
```

4.12 Python interface

4.12.1 Quick-start examples

The easiest way to install is to run `pip install finufft`, which downloads and installs the latest precompiled binaries from PyPI. If you would like to compile from source, see *the Python installation instructions*.

To calculate a 1D type 1 transform, from nonuniform to uniform points, we import `finufft`, specify the nonuniform points `x`, their strengths `c`, and call `nufft1d1`:

```
import numpy as np
import finufft

# number of nonuniform points
M = 100000

# the nonuniform points
x = 2 * np.pi * np.random.uniform(size=M)

# their complex strengths
c = (np.random.standard_normal(size=M)
    + 1J * np.random.standard_normal(size=M))

# desired number of Fourier modes (uniform outputs)
N = 200000

# calculate the transform
f = finufft.nufft1d1(x, c, N)
```

The input here is a set of complex strengths `c`, which are used to approximate (1) in *Mathematical definitions of transforms*. That approximation is stored in `f`, which is indexed from `-N // 2` up to `N // 2 - 1` (since `N` is even; if odd it would be `-(N - 1) // 2` up to `(N - 1) // 2`). The approximation is accurate to a tolerance of `1e-6`, which is the default tolerance of `nufft1d1`. It can be modified using the `eps` argument:

```
# calculate the transform to higher accuracy
f = finufft.nufft1d1(x, c, N, eps=1e-12)
```

Note, however, that a lower tolerance (that is, a higher accuracy) results in a slower transform. See `python/examples/simple1d1.py` for the demo code that includes a basic math test (useful to check both the math and the indexing).

For higher dimensions, we would specify point locations in more than one dimension:

```
# 2D nonuniform points (x,y coords)
x = 2 * np.pi * np.random.uniform(size=M)
y = 2 * np.pi * np.random.uniform(size=M)

# desired number of Fourier modes (in x, y directions respectively)
N1 = 1000
N2 = 2000

# the 2D transform outputs f array of shape (N1, N2)
f = finufft.nufft2d1(x, y, c, (N1, N2))
```

See `python/examples/simple2d1.py` for the demo code that includes a basic math test (useful to check both the math and the indexing).

We can also go the other way, from uniform to non-uniform points, using a type 2 transform:

```
# input Fourier coefficients
f = (np.random.standard_normal(size=(N1, N2))
     + 1J * np.random.standard_normal(size=(N1, N2)))

# calculate the 2D type 2 transform
c = finufft.nufft2d2(x, y, f)
```

Now the output is a complex vector of length `M` approximating (2) in *Mathematical definitions of transforms*, that is the adjoint (but not inverse) of (1). (Note that the default sign in the exponential is negative for type 2 in the Python interface.)

In addition to tolerance `eps`, we can adjust other options for the transform. These are listed in *Options parameters* and are specified as keyword arguments in the Python interface. For example, to change the mode ordering to FFT style (that is, in each dimension `Ni = N1` or `N2`, the indices go from `0` to `Ni // 2 - 1`, then from `-Ni // 2` to `-1`, since each `Ni` is even), we call

```
f = finufft.nufft2d1(x, y, c, (N1, N2), modeord=1)
```

We can also specify a preallocated output array using the `out` keyword argument. This would be done by

```
# allocate the output array
f = np.empty((N1, N2), dtype='complex128')

# calculate the transform
finufft.nufft2d1(x, y, c, out=f)
```

In this case, we do not need to specify the output shape since it can be inferred from `f`.

Note that the above functions are all vectorized, which means that they can take multiple inputs stacked along the first dimension (that is, in row-major order) and process them simultaneously. This can bring significant speedups for small inputs by avoiding multiple short calls to FINUFFT. For the 2D type 1 vectorized interface, we would call

```
# number of transforms
K = 4

# generate K stacked coefficient arrays
```

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```
c = (np.random.standard_normal(size=(K, M))
     + 1J * np.random.standard_normal(size=(K, M)))

# calculate the K transforms simultaneously (K is inferred from c.shape)
f = finufft.nufft2d1(x, y, c, (N1, N2))
```

The output array `f` would then have the shape `(K, N1, N2)`. See the complete demo in `python/examples/many2d1.py`.

More fine-grained control can be obtained using the plan (or *guru*) interface. Instead of preparing the transform, setting the nonuniform points, and executing the transform all at once, these steps are seperated into different function calls. This can speed up calculations if multiple transforms are executed for the same grid size, since the same FFTW plan can be reused between calls. Additionally, if the same nonuniform points are reused between calls, we gain an extra speedup since the points only have to be sorted once. To perform the call above using the plan interface, we would write

```
# specify type 1 transform
nufft_type = 1

# instantiate the plan (note ntrans must be set here)
plan = finufft.Plan(nufft_type, (N1, N2), n_trans=K)

# set the nonuniform points
plan.setpts(x, y)

# execute the plan
f = plan.execute(c)
```

See the complete demo in `python/examples/guru2d1.py`. All interfaces support both single and double precision, but for the plan, this must be specified at initialization time using the `dtype` argument

```
# convert input data to single precision
x = x.astype('float32')
y = y.astype('float32')
c = c.astype('complex64')

# instantiate the plan and set the points
plan = finufft.Plan(nufft_type, (N1, N2), n_trans=K, dtype='float32')
plan.setpts(x, y)

# execute the plan, giving single-precision output
f = plan.execute(c)
```

See the complete demo, with math test, in `python/examples/guru2d1f.py`.

4.12.2 Full documentation

The Python interface to FINUFFT is divided into two parts: the simple interface (through the `nufft*` functions) and the more advanced plan interface (through the `Plan` class). The former allows the user to perform an NUFFT in a single call while the latter allows for more efficient reuse of resources when the same NUFFT is applied several times to different data by saving FFTW plans, sorting the nonuniform points, and so on.

`finufft.`**`nufft1d1`**(*x*, *c*, *n_modes=None*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

1D type-1 (nonuniform to uniform) complex NUFFT

```
        M-1
f[k1] = SUM c[j] exp(+/-i k1 x(j))
        j=0

    for -N1/2 <= k1 <= (N1-1)/2
```

Parameters

- **x** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **c** (*complex[M] or complex[ntransf, M]*) – source strengths.
- **n_modes** (*integer or integer tuple of length 1, optional*) – number of uniform Fourier modes requested (N1,). May be even or odd; in either case, modes k1 are integers satisfying -N1/2 <= k1 <= (N1-1)/2. Must be specified if `out` is not given.
- **out** (*complex[N1] or complex[ntransf, N1], optional*) – output array for Fourier mode values. If `n_modes` is specifed, the shape must match, otherwise `n_modes` is inferred from `out`.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[N1] or complex[ntransf, N1]

Example

See `python/examples/simple1d1.py, python/examples/simpleopts1d1.py`.

`finufft.`**`nufft1d2`**(*x*, *f*, *out=None*, *eps=1e-06*, *isign=- 1*, ***kwargs*)

1D type-2 (uniform to nonuniform) complex NUFFT

```
c[j] = SUM f[k1] exp(+/-i k1 x(j))       for j = 0, ..., M-1
       k1

    where the sum is over -N1/2 <= k1 <= (N1-1)/2
```

Parameters

- **x** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **f** (*complex[N1] or complex[ntransf, N1]*) – Fourier mode coefficients, where N1 may be even or odd. In either case the mode indices k1 satisfy -N1/2 <= k1 <= (N1-1)/2.
- **out** (*complex[M] or complex[ntransf, M], optional*) – output array at targets.
- **eps** (*float, optional*) – precision requested (>1e-16).

- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.`**nufft1d3**(*x*, *c*, *s*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

1D type-3 (nonuniform to nonuniform) complex NUFFT

```
          M-1
f[k]   =  SUM   c[j] exp(+/-i s[k] x[j]),      for k = 0, ..., N-1
          j=0
```

Parameters

- **x** (*float[M]*) – nonuniform source points.
- **c** (*complex[M] or complex[ntransf, M]*) – source strengths.
- **s** (*float[N]*) – nonuniform target points.
- **out** (*complex[N] or complex[ntransf, N]*) – output values at target frequencies.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.`**`nufft2d1`**(*x*, *y*, *c*, *n_modes=None*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

2D type-1 (nonuniform to uniform) complex NUFFT

```
            M-1
f[k1, k2] = SUM c[j] exp(+/-i (k1 x(j) + k2 y(j)))
            j=0

    for -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2
```

Parameters

- **`x`** (*`float[M]`*) – nonuniform points, valid only in [-3pi, 3pi].
- **`y`** (*`float[M]`*) – nonuniform points, valid only in [-3pi, 3pi].
- **`c`** (*`complex[M] or complex[ntransf, M]`*) – source strengths.
- **`n_modes`** (*`integer or integer tuple of length 2, optional`*) – number of uniform Fourier modes requested (N1, N2). May be even or odd; in either case, modes k1, k2 are integers satisfying -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2. Must be specified if `out` is not given.
- **`out`** (*`complex[N1, N2] or complex[ntransf, N1, N2], optional`*) – output array for Fourier mode values. If `n_modes` is specifed, the shape must match, otherwise `n_modes` is inferred from `out`.
- **`eps`** (*`float, optional`*) – precision requested (>1e-16).
- **`isign`** (*`int, optional`*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- **`**kwargs`** (*`optional`*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[N1, N2] or complex[ntransf, N1, N2]

Example

See `python/examples/simple2d1.py, python/examples/many2d1.py`.

`finufft.`**`nufft2d2`**(*x*, *y*, *f*, *out=None*, *eps=1e-06*, *isign=- 1*, ***kwargs*)

2D type-2 (uniform to nonuniform) complex NUFFT

```
c[j] = SUM f[k1, k2] exp(+/-i (k1 x(j) + k2 y(j)))       for j = 0, ..., M-1
       k1, k2

    where the sum is over -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2
```

Parameters

- **x** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **y** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **f** (*complex[N1, N2] or complex[ntransf, N1, N2]*) – Fourier mode coefficients, where N1, N2 may be even or odd. In either case the mode indices k1, k2 satisfy -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2.
- **out** (*complex[M] or complex[ntransf, M], optional*) – output array at targets.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.`**`nufft2d3`**(*x*, *y*, *c*, *s*, *t*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

2D type-3 (nonuniform to nonuniform) complex NUFFT

```
          M-1
f[k]   =  SUM   c[j] exp(+/-i (s[k] x[j] + t[k] y[j])),      for k = 0, ..., N-1
          j=0
```

Parameters

- **x** (*float[M]*) – nonuniform source points.
- **y** (*float[M]*) – nonuniform source points.
- **c** (*complex[M] or complex[ntransf, M]*) – source strengths.
- **s** (*float[N]*) – nonuniform target points.
- **t** (*float[N]*) – nonuniform target points.
- **out** (*complex[N] or complex[ntransf, N]*) – output values at target frequencies.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.nufft3d1` (*x*, *y*, *z*, *c*, *n_modes=None*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

3D type-1 (nonuniform to uniform) complex NUFFT

```
                 M-1
f[k1, k2, k3] = SUM c[j] exp(+/-i (k1 x(j) + k2 y(j) + k3 z(j)))
                 j=0

    for -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2, -N3/2 <= k3 <= (N3-1)/2
```

Parameters

- **x** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **y** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **z** (*float[M]*) – nonuniform points, valid only in [-3pi, 3pi].
- **c** (*complex[M] or complex[ntransf, M]*) – source strengths.
- **n_modes** (*integer or integer tuple of length 3, optional*) – number of uniform Fourier modes requested (N1, N2, N3). May be even or odd; in either case, modes k1, k2, k3 are integers satisfying -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2, -N3/2 <= k3 <= (N3-1)/2. Must be specified if `out` is not given.
- **out** (*complex[N1, N2, N3] or complex[ntransf, N1, N2, N3], optional*) – output array for Fourier mode values. If `n_modes` is specifed, the shape must match, otherwise `n_modes` is inferred from `out`.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[N1, N2, N3] or complex[ntransf, N1, N2, N3]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.`**`nufft3d2`**(*x*, *y*, *z*, *f*, *out=None*, *eps=1e-06*, *isign=- 1*, ***kwargs*)

3D type-2 (uniform to nonuniform) complex NUFFT

```
c[j] = SUM f[k1, k2, k3] exp(+/-i (k1 x(j) + k2 y(j) + k3 z(j)))        for j = 0,␣
↪..., M-1
       k1, k2, k3

    where the sum is over -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2, -N3/2
↪<= k3 <= (N3-1)/2
```

Parameters

- **`x`** (*`float[M]`*) – nonuniform points, valid only in [-3pi, 3pi].
- **`y`** (*`float[M]`*) – nonuniform points, valid only in [-3pi, 3pi].
- **`z`** (*`float[M]`*) – nonuniform points, valid only in [-3pi, 3pi].
- **`f`** (*`complex[N1, N2, N3] or complex[ntransf, N1, N2, N3]`*) – Fourier mode coefficients, where N1, N2, N3 may be even or odd. In either case the mode indices k1, k2, k3 satisfy -N1/2 <= k1 <= (N1-1)/2, -N2/2 <= k2 <= (N2-1)/2, -N3/2 <= k3 <= (N3-1)/2.
- **`out`** (*`complex[M] or complex[ntransf, M], optional`*) – output array at targets.
- **`eps`** (*`float, optional`*) – precision requested (>1e-16).
- **`isign`** (*`int, optional`*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- **`**kwargs`** (*`optional`*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

`finufft.`**`nufft3d3`**(*x*, *y*, *z*, *c*, *s*, *t*, *u*, *out=None*, *eps=1e-06*, *isign=1*, ***kwargs*)

3D type-3 (nonuniform to nonuniform) complex NUFFT

```
          M-1
f[k]   =  SUM   c[j] exp(+/-i (s[k] x[j] + t[k] y[j] + u[k] z[j])),      for k = 0,
↪ ..., N-1
          j=0
```

Parameters

- **x** (*float[M]*) – nonuniform source points.
- **y** (*float[M]*) – nonuniform source points.
- **z** (*float[M]*) – nonuniform source points.
- **c** (*complex[M] or complex[ntransf, M]*) – source strengths.
- **s** (*float[N]*) – nonuniform target points.
- **t** (*float[N]*) – nonuniform target points.
- **u** (*float[N]*) – nonuniform target points.
- **out** (*complex[N] or complex[ntransf, N]*) – output values at target frequencies.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign in exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

Note: The output is written into the `out` array if supplied.

Returns The resulting array.

Return type complex[M] or complex[ntransf, M]

Example

See `python/test/accuracy_speed_tests.py`.

class finufft.**Plan**(*nufft_type*, *n_modes_or_dim*, *n_trans=1*, *eps=1e-06*, *isign=None*, ***kwargs*)

A non-uniform fast Fourier transform (NUFFT) plan

The `Plan` class lets the user exercise more fine-grained control over the execution of an NUFFT. First, the plan is created with a certain set of parameters (type, mode configuration, tolerance, sign, number of simultaneous transforms, and so on). Then the nonuniform points are set (source or target depending on the type). Finally, the plan is executed on some data, yielding the desired output.

In the simple interface, all these steps are executed in a single call to the `nufft*` functions. The benefit of separating plan creation from execution is that it allows for plan reuse when certain parameters (like mode configuration) or nonuniform points remain the same between different NUFFT calls. This becomes especially important for small inputs, where execution time may be dominated by initialization steps such as allocating and FFTW plan and sorting the nonuniform points.

Example:

```
import numpy as np
import finufft

# set up parameters
n_modes = (1000, 2000)
n_pts = 100000
nufft_type = 1
n_trans = 4

```

(continues on next page)

(continued from previous page)

```
# generate nonuniform points
x = 2 * np.pi * np.random.uniform(size=n_pts)
y = 2 * np.pi * np.random.uniform(size=n_pts)

# generate source strengths
c = (np.random.standard_normal(size=(n_trans, n_pts)),
     + 1J * np.random.standard_normal(size=(n_trans, n_pts)))

# initialize the plan
plan = finufft.Plan(nufft_type, n_modes, n_trans)

# set the nonuniform points
plan.setpts(x, y)

# execute the plan
f = plan.execute(c)
```

Also see `python/examples/guru1d1.py` and `python/examples/guru2d1.py`.

Parameters

- **nufft_type** (*int*) – type of NUFFT (1, 2, or 3).
- **n_modes_or_dim** (*int or tuple of ints*) – if `nufft_type` is 1 or 2, this should be a tuple specifying the number of modes in each dimension (for example, `(50, 100)`), otherwise, if *nufft_type`* is 3, this should be the number of dimensions (between 1 and 3).
- **n_trans** (*int, optional*) – number of transforms to compute simultaneously.
- **eps** (*float, optional*) – precision requested (>1e-16).
- **isign** (*int, optional*) – if non-negative, uses positive sign exponential, otherwise negative sign.
- ****kwargs** (*optional*) – for more options, see *Options parameters*.

setpts (*x=None*, *y=None*, *z=None*, *s=None*, *t=None*, *u=None*)

Set the nonuniform points

For type 1, this sets the coordinates of the `M` nonuniform source points, for type 2, it sets the coordinates of the `M` target points, and for type 3 it sets both the `M` source points and the `N` target points.

The dimension of the plan determines the number of arguments supplied. For example, if `dim == 2`, we provide `x` and `y` (as well as `s` and `t` for a type-3 transform).

Parameters

- **x** (*float[M]*) – first coordinate of the nonuniform points (source for type 1 and 3, target for type 2).
- **y** (*float[M], optional*) – second coordinate of the nonuniform points (source for type 1 and 3, target for type 2).
- **z** (*float[M], optional*) – third coordinate of the nonuniform points (source for type 1 and 3, target for type 2).
- **s** (*float[N], optional*) – first coordinate of the nonuniform points (target for type 3).
- **t** (*float[N], optional*) – second coordinate of the nonuniform points (target for type 3).

- **u** (*float[N], optional*) – third coordinate of the nonuniform points (target for type 3).

execute(*data*, *out=None*)

Execute the plan

Performs the NUFFT specified at plan instantiation with the points set by `setpts`. For type-1 and type-3 transforms, the input is a set of source strengths, while for a type-2 transform, it consists of an array of size `n_modes`. If `n_transf` is greater than one, `n_transf` inputs are expected, stacked along the first axis.

Parameters

- **data** (*complex[M], complex[n_transf, M], complex[n_modes], or complex[n_transf, n_modes]*) – The input source strengths (type 1 and 3) or source modes (type 2).
- **out** (*complex[n_modes], complex[n_transf, n_modes], complex[M], or complex[n_transf, M], optional*) – The array where the output is stored. Must be of the right size.

Returns The output array of the transform(s).

Return type complex[n_modes], complex[n_transf, n_modes], complex[M], or complex[n_transf, M]

4.13 Julia interface

Ludvig af Klinteberg has built FINUFFT.jl, an interface from the Julia language. This package will automatically download and build FINUFFT at installation, as long as GCC is available. It has been tested on Linux and Mac OS X (the latter with GCC 8).

4.14 Developer notes

- To update the version number, this needs to be done by hand in the following places:
  - `docs/conf.py` for sphinx
  - `python/setup.py` for the python pkg version
  - `include/defs.h`
  - `CHANGELOG`: don't forget to describe the new features and changes.
- There are some sphinx tags in the source code, indicated by @ in comments. Please leave these alone since they are needed by the doc generation.
- Developers changing MATLAB/octave interfaces or docs, see `matlab/README`
- Developers changing overall web docs, see `docs/README`
- If you change any of the doc sources, which includes any of the above four items, the easiest way to regenerate everything needed is via `make docs`. See `makefile` for what's going on here. Also, do not edit files `docs/*.doc` since these are machine-generated; your changes will be overwritten. Instead edit files `*.docsrc` once you have understood how the bash scripts act on them.
- For testing and performance measuring routines see `test/REAME` and `perftest/README`. We need more of the latter, eg, something making performance graphs that enable rapid eyeball comparison of various settings/machines.

- **Installing MWrap**. This is needed to rebuild the matlab/octave interfaces. MWrap is a very useful MEX interface generator by Dave Bindel, now maintained and expanded by Zydrunas Gimbutas. Make sure you have `flex` and `bison` installed to build it. As of FINUFFT v.2.0 you will need a recent (>=0.33.10) version of MWrap. Make sure to override the location of MWrap by adding a line such as:

```
MWRAP = your-path-to-mwrap-executable
```

  to your `make.inc`, and then you can use the `make mex` task.

4.15 Related packages

4.15.1 Other recommended NUFFT libraries

- cuFINUFFT: Our GPU version of FINUFFT, for single precision in 2D and 3D, type 1 and 2. Still under development by Melody Shih (NYU) and others. Often achieves speeds around 10x the CPU version.
- NFFT3: well-supported and multi-featured C++ library using FFTW. Has MATLAB MEX interface. However, significantly slower and/or more memory-intensive than FINUFFT (see reference [FIN]). Has many more general abilities, eg, inverse NUFFT. We are working on this too.
- CMCL NUFFT: NYU single-threaded Fortran library using self-contained FFT, fast Gaussian gridding kernel. Has MATLAB MEX interface. Much (up to 50x even for one thread) slower than FINUFFT, but is very easy to compile.
- MIRT Michigan Image Reconstruction Toolbox. Native MATLAB, single-threaded sparse mat-vec, prestores all kernel evaluations, thus is memory-intensive but surprisingly fast for a single-threaded implementation. However, slower than FINUFFT for all tolerances smaller than 10^{-1}.
- PyNUFFT Python code supporting CPU and GPU operation. We have not compared against FINUFFT yet.

Also see the summary of library performances in our paper [FIN] in the *references*.

4.16 Dependent packages, users, and citations

Here we list packages that depend on FINUFFT, and papers or groups using it. Papers that merely cite our work are listed separately at the bottom. Please let us know (and use github's dependent package link) if you are a user or package maintainer but not listed.

4.16.1 Packages relying on FINUFFT

Here are some packages dependent on FINUFFT (please let us know of others, and also add them to github's Used By feature):

1. SMILI, very long baseline interferometry reconstruction code by Kazu Akiyama and others, uses FINUFFT (2d1, 2d2, Fortran interfaces) as a key library. Akiyama used SMILI to reconstruct the famous black hole image in 2019 from the Event Horizon Telescope.
2. ASPIRE: software for cryo-EM, based at Amit Singer's group at Princeton. github
3. sinctransform: C++ and MATLAB codes to evaluate sums of the sinc and sinc^2 kernels between arbitrary nonuniform points in 1,2, or 3 dimensions, by Hannah Lawrence (2017 summer intern at Flatiron).
4. fsinc: Gaute Hope's fast sinc transform and interpolation python package.

5. FTK: Factorization of the translation kernel for fast rigid image alignment, by Rangan, Spivak, Andén, and Barnett.
6. FINUFFT.jl: a julia language wrapper by Ludvig af Klinteberg (SFU), now using pure julia rather than python.
7. Vineet Bansal's pypi package https://pypi.org/project/finufftpy/. This will be updated soon.

4.16.2 Research output using FINUFFT

1. "Cryo-EM reconstruction of continuous heterogeneity by Laplacian spectral volumes", Amit Moscovich, Amit Halevi, Joakim Andén, and Amit Singer. To appear, Inv. Prob. (2020), https://arxiv.org/abs/1907.01898
2. "A Fast Integral Equation Method for the Two-Dimensional Navier-Stokes Equations", Ludvig af Klinteberg, Travis Askham, and Mary Catherine Kropinski (2019), use FINUFFT 2D type 2. https://arxiv.org/abs/1908.07392
3. "MR-MOTUS: model-based non-rigid motion estimation for MR-guided radiotherapy using a reference image and minimal k-space data", Niek R F Huttinga, Cornelis A T van den Berg, Peter R Luijten and Alessandro Sbrizzi, Phys. Med. Biol. 65(1), 015004. https://arxiv.org/abs/1902.05776
4. Koga, K. "Signal processing approach to mesh refinement in simulations of axisymmetric droplet dynamics", https://arxiv.org/abs/1909.09553 Koga uses 1D FINUFFT to generate a "guideline function" for reparameterizing 1D curves.
5. L. Wang and Z. Zhao, "Two-dimensional tomography from noisy projection tilt series taken at unknown view angles with non-uniform distribution", International Conference on Image Processing (ICIP), (2019).
6. "Factorization of the translation kernel for fast rigid image alignment," Aaditya Rangan, Marina Spivak, Joakim Andén, and Alex Barnett. Inverse Problems 36 (2), 024001 (2020). https://arxiv.org/abs/1905.12317
7. Aleks Donev's group at NYU; ongoing

Papers or codes using our new ES window (spreading) function but not the whole FINUFFT package:

1. Davood Shamshirgar and Anna-Karin Tornberg, "Fast Ewald summation for electrostatic potentials with arbitrary periodicity", exploit our "Barnett-Magland" (BM), aka exp-sqrt (ES) window function. https://arxiv.org/abs/1712.04732
2. Martin Reinecke, codes for radio astronomy reconstruction including https://gitlab.mpcdf.mpg.de/ift/nifty_gridder

4.16.3 Citations to FINUFFT that do not appear to be actual users

1. https://arxiv.org/abs/1903.08365
2. https://arxiv.org/abs/1908.00041
3. https://arxiv.org/abs/1908.00574
4. https://arxiv.org/abs/1912.09746

4.17 Acknowledgments

FINUFFT was initiated by Jeremy Magland and Alex Barnett at the Center for Computational Mathematics, Flatiron Institute in early 2017. The main developer and maintainer is:

- Alex Barnett

Major code contributions by:

- Jeremy Magland - early multithreaded spreader, benchmark vs other libraries, py wrapper
- Ludvig af Klinteberg - SIMD vectorization/acceleration of spreader, julia wrapper
- Yu-Hsuan ("Melody") Shih - 2d1many, 2d2many vectorized interface, GPU version
- Andrea Malleo - guru interface prototype and tests
- Libin Lu - guru Fortran, python, MATLAB/octave, julia interfaces
- Joakim Andén - python, MATLAB/FFTW issues, dual-precision, performance tests

Other significant code contributions by:

- Leslie Greengard and June-Yub Lee - CMCL Fortran test drivers
- Dan Foreman-Mackey - early python wrappers
- David Stein - python wrappers
- Vineet Bansal - py packaging
- Garrett Wright - dual-precision build, py packaging

Testing, bug reports, helpful discussions:

- Hannah Lawrence - user testing and finding bugs
- Marina Spivak - Fortran testing
- Hugo Strand - python bugs
- Amit Moscovich - Mac OSX build
- Dylan Simon - sphinx help
- Zydrunas Gimbutas - MWrap extension, explanation that NFFT uses Kaiser-Bessel backwards
- Charlie Epstein - help with analysis of kernel Fourier transform sums
- Christian Muller - optimization (CMA-ES) for early kernel design
- Andras Pataki - complex number speed in C++
- Timo Heister - pass/fail numdiff testing ideas
- Vladimir Rokhlin - piecewise polynomial approximation on complex boxes

We are also indebted to the authors of other NUFFT codes such as NFFT3, CMCL NUFFT, MIRT, BART, etc, upon whose interfaces, code, and algorithms we have built.

4.18 References

Please cite the following two papers if you use this software:

[FIN] A parallel non-uniform fast Fourier transform library based on an ``exponential of semicircle" kernel. A. H. Barnett, J. F. Magland, and L. af Klinteberg. SIAM J. Sci. Comput. 41(5), C479-C504 (2019). arxiv version

[B20] Aliasing error of the $\exp(\beta\sqrt{1-z^2})$ kernel in the nonuniform fast Fourier transform. A. H. Barnett. submitted, Appl. Comput. Harmon. Anal. (2020). arxiv version

4.18.1 Background references

For the Kaiser–Bessel kernel and the related PSWF, see:

[KK] Chapter 7. System Analysis By Digital Computer. F. Kuo and J. F. Kaiser. Wiley (1967).

[FT] K. Fourmont. Schnelle Fourier-Transformation bei nichtäquidistanten Gittern und tomographische Anwendungen. PhD thesis, Univ. Münster, 1999.

[F] Non-equispaced fast Fourier transforms with applications to tomography. K. Fourmont. J. Fourier Anal. Appl. 9(5) 431-450 (2003).

[FS] Nonuniform fast Fourier transforms using min-max interpolation. J. A. Fessler and B. P. Sutton. IEEE Trans. Sig. Proc., 51(2):560-74, (Feb. 2003)

[ORZ] Prolate Spheroidal Wave Functions of Order Zero: Mathematical Tools for Bandlimited Approximation. A. Osipov, V. Rokhlin, and H. Xiao. Springer (2013).

[KKP] Using NFFT3—a software library for various nonequispaced fast Fourier transforms. J. Keiner, S. Kunis and D. Potts. Trans. Math. Software 36(4) (2009).

[DFT] How exponentially ill-conditioned are contiguous submatrices of the Fourier matrix? A. H. Barnett, submitted, SIAM Rev. (2020). arxiv version

The appendix of the last of the above contains the first known published proof of the Kaiser–Bessel Fourier transform pair.

FINUFFT builds upon the CMCL NUFFT, and the Fortran wrappers are very similar to its interfaces. For that, the following are references:

[GL] Accelerating the Nonuniform Fast Fourier Transform. L. Greengard and J.-Y. Lee. SIAM Review 46, 443 (2004).

[LG] The type 3 nonuniform FFT and its applications. J.-Y. Lee and L. Greengard. J. Comput. Phys. 206, 1 (2005).

Inversion of the NUFFT is covered in [KKP] above and in:

[GLI] The fast sinc transform and image reconstruction from nonuniform samples in $\mathbf{k}$-space. L. Greengard, J.-Y. Lee and S. Inati, Commun. Appl. Math. Comput. Sci (CAMCOS) 1(1) 121-131 (2006).

The original NUFFT analysis using truncated Gaussians is (the second improving upon the first):

[DR] Fast Fourier Transforms for Nonequispaced data. A. Dutt and V. Rokhlin. SIAM J. Sci. Comput. 14, 1368 (1993).

[S] A note on fast Fourier transforms for nonequispaced grids. G. Steidl, Adv. Comput. Math. 9, 337-352 (1998).

4.18.2 Talk slides

These PDF slides may be a useful introduction.

PYTHON MODULE INDEX

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