Build You a NumPy: From Dot-Products to Machine Code

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FASRC Training Course

In [1]:
```
%matplotlib notebook
```

In [2]:
```
import perfplot
import kuramoto as km
import numpy as np
import numpy.typing as npt
import matplotlib.pyplot as plt
```

Numerics 101: start with a PDE

Numerical optimization is best approached with a concrete problem. We will start with a 2-dimensional lattice variant of the Kuramoto model, a simple protoyipical model of synchronization in multi-oscillator systems.

Classically, it was formulated as the system of ordinary differential equations:

$$\frac{d\theta_i}{dt} = \omega_i + \frac{K}{N}\sum_{j=1}^{N} \sin(\theta_j - \theta_i)$$

where θ_i is the phase of oscillator i and ω_i is its *intrinsic frequency*.

This is a fully-connected model, and for visualization purposes we we will turn this into a two-dimensional PDE as follows. First, we consider $\theta_j \sim \theta_i$ only if j, i are "nearest-neighbors" on a two-dimensional lattice. Then, we will take the lattice spacing $\epsilon \to 0$, in which case $\theta_j - \theta_i$ becomes the gradient $\nabla\theta(x, y)$. Finally, the outer sum becomes a divergence operator, giving us:

$$\frac{\partial\theta}{\partial t} = \omega + K\nabla \cdot \sin(\nabla\theta)$$

where $\theta(x, y)$ and $\omega(x, y)$ are now fields which we define on the unit square $[0, 1] \times [0, 1]$. In addition, we'll impose the *zero-flux* boundary conditions:

$$\frac{\partial \theta}{\partial x}(0, y) = \frac{\partial \theta}{\partial x}(1, y) = \frac{\partial \theta}{\partial y}(x, 0) = \frac{\partial \theta}{\partial y}(x, 1) = 0$$

which just means that the difference $\theta_j - \theta_i$ is zero at the boundary, so the system is "insulated".

This looks like a diffusion equation (the $\nabla \cdot \nabla$), but the $\sin(\cdot)$ nonlinearity makes it impossible to express the operator $\nabla \cdot \sin \circ \nabla$ as a matrix. Surprisingly, this equation has an exact solution, but we're going to solve it numerically.

Starting with a naive implementation

In src/kuramoto/base.py, you'll find the `KuramotoSolver` class which implements most of the basic functionality we need:

- parameters (size of grid $N \times N$; coupling constant K)
- time-stepping (we will use Euler's method for simplicity with fixed Δt)

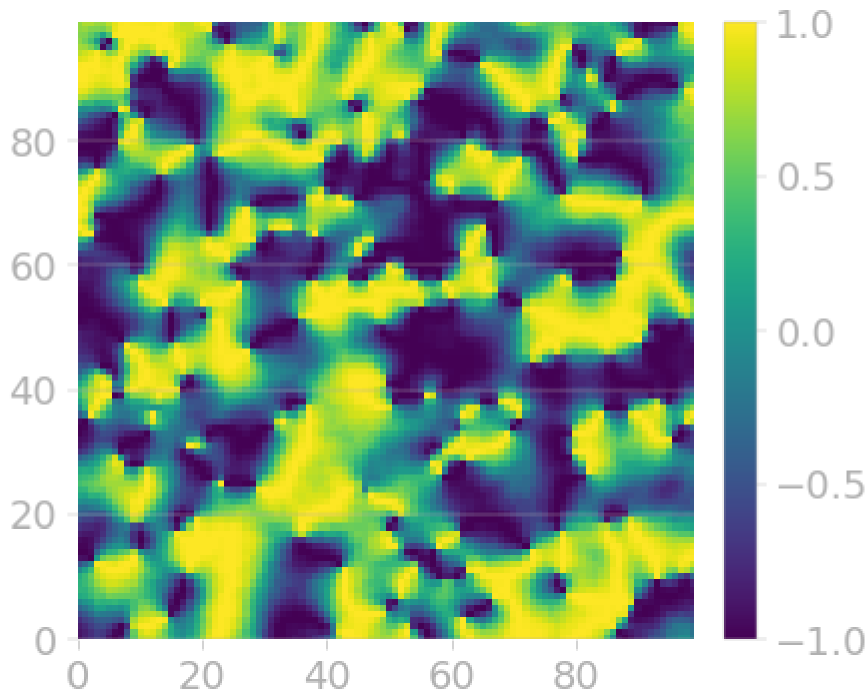
Our goal is to implement the right-hand side of $\frac{\partial \theta}{\partial t}$. Let's start with a naive implementation:

In [3]:
```
class NaiveSolver(km.KuramotoSolver):

    def dudt(self, u: npt.NDArray) -> npt.NDArray:
        ''' Centered-difference gradient with zero Neumann condition '''

        dudt = self.omega.copy()

        for row in range(self.N):
            for col in range(self.N):

                # Horizontal neighbors
                if row > 0:
                    dudt[row, col] += self.K * np.sin(u[row-1, col] - u[row, cc
                if row < self.N-1:
                    dudt[row, col] += self.K * np.sin(u[row+1, col] - u[row, cc

                # Vertical neighbors
                if col > 0:
                    dudt[row, col] += self.K * np.sin(u[row, col-1] - u[row, cc
                if col < self.N-1:
                    dudt[row, col] += self.K * np.sin(u[row, col+1] - u[row, cc

        return dudt
```

This is the simplest implementation we can imagine. Now let's visualize it!

In [4]:
```
solver = NaiveSolver(N=100, T=10, K=2.0, record=True)
solver.integrate()
anim = solver.play_video()
```

```
Using dtype: <class 'numpy.float64'>
Solving...
Finished.
```



Pro-tip: to turn the sequence of solutions into a video, we use matplotlib's FuncAnimation.

Benchmarking the naive solution

That took a few seconds (or more, depending on your machine). Not bad, but in realistic settings we might want to run with N or T very large. Let's see where time and memory are spent so we can think about optimizing it.

Time

To profile time line-by-line, we'll use the excellent line_profiler library. This can either be used as a decorator:

```
@profile
def my_expensive_func():
    do_something_real_difficult()
```

and then use the command-line utility `kernprof` to produce and visualize the benchmark:

```
kernprof -l script.py
python -m line_profiler script.py.lprof
```

However, we would like to avoid using the `kernprof` command and run our script natively (for benchmarking memory, hardware events, etc.). Thus, `KuramotoSolver` includes a profile implementation as part of the class:

```
import line_profiler
import atexit
```

```
# Import C++ shared object file -- this will appear in this directory at build-time
# import kuramoto._cpp

@dataclass
class KuramotoSolver:
    ...
    profile: bool = False               # Whether to run the line-profiler


    def __post_init__(self):
        ...
        if self.profile:
            print('Running profiler.')
            pf = line_profiler.LineProfiler()
            self.dudt = pf(self.dudt)    # Run the profiler on our implementation
            atexit.register(pf.print_stats)
    ...
```

This is automatically invoked on any subclasses too, like `NaiveSolver`. So let's pass the `profile` flag:

In [5]:
```
solver = NaiveSolver(N=100, T=10, K=2.0, profile=True)
solver.integrate()
```

```
Using dtype: <class 'numpy.float64'>
Running profiler.
Solving...
Finished.
Timer unit: 1e-06 s

Total time: 5.81919 s
File: /var/folders/bd/lpd6x9zs40g4bjb_14mp94rw0000gq/T/ipykernel_95579/2848623
984.py
Function: dudt at line 3

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     3                                           def dudt(self, u: npt.NDA
rray) -> npt.NDArray:
     4                                               ''' Centered-differen
ce gradient with zero Neumann condition '''
     5
     6       101        500.0      5.0      0.0          dudt = self.omega.cop
y()
     7
     8     10201       2001.0      0.2      0.0          for row in range(sel
f.N):
     9   1020100     189315.0      0.2      3.3              for col in range
(self.N):
    10
    11                                                           # Horizontal
neighbors
    12   1010000     191003.0      0.2      3.3                  if row > 0:
    13    999900    1198942.0      1.2     20.6                      dudt[row,
col] += self.K * np.sin(u[row-1, col] - u[row, col])
    14   1010000     234676.0      0.2      4.0                  if row < sel
f.N-1:
    15    999900    1172881.0      1.2     20.2                      dudt[row,
col] += self.K * np.sin(u[row+1, col] - u[row, col])
    16
    17                                                           # Vertical ne
ighbors
    18   1010000     212147.0      0.2      3.6                  if col > 0:
    19    999900    1183396.0      1.2     20.3                      dudt[row,
col] += self.K * np.sin(u[row, col-1] - u[row, col])
    20   1010000     242292.0      0.2      4.2                  if col < sel
f.N-1:
    21    999900    1191965.0      1.2     20.5                      dudt[row,
col] += self.K * np.sin(u[row, col+1] - u[row, col])
    22
    23       101         67.0      0.7      0.0          return dudt
```

This gives us a line-by-line printout of total time spent in `self.dudt` (computing the vector field). Time here is measured in microseconds.

Immediately, we can see that most of the time is spend in adding the contributions of nearest-neighbors, lines 13, 15, 19, and 21. What can we do to improve the performance?

Here we have two nested for-loops, running inside a third one which performs the time-stepping. You may have heard that "for-loops in Python are slow." This is certainly an overgeneralization, but let's follow this intuition and implement our solver using NumPy operations.

Writing a solution in NumPy

The heuristic for writing fast code in NumPy is *vectorization*. That is, express your operations in terms of NumPy functions (which themselves contain loops in C -- except for SIMD, everything ultimately becomes loops), instead of writing your loops manually.

Here's what a simple but effective NumPy version of the above looks like:

In [6]:
```
class NumpySolver(km.KuramotoSolver):

    def dudt(self, u: npt.NDArray) -> npt.NDArray:
        dudt = self.omega.copy()

        # Horizontal gradient in the direction of +infinity
        dudx_right = u[:, 1:] - u[:, :-1]

        # Vertical gradient in the direction of -infinity
        dudy_down = u[1:, :] - u[:-1, :]

        # Apply contribution from horizontal neighbors
        dudt[:, :-1] += self.K * np.sin(dudx_right)
        dudt[:, 1:] += self.K * np.sin(-dudx_right)

        # Apply contribution from vertical neighbors
        dudt[:-1, :] += self.K * np.sin(dudy_down)
        dudt[1:, :] += self.K * np.sin(-dudy_down)

        return dudt
```

Let's unpack this operation.

1. First, we compute two intermediate arrays, which give us the finite-differences between any node and its *right neighbors* (`dudx_right`), as well as any node and its *below neighbors* (`dudy_down`). If you have numerically solved PDEs before, you may recognize the indexing as a simple kind of *stencil*.

2. Next, note that, by not computing any differences at the boundaries, we are *implicitly* enforcing the zero-flux condition. (This is also why we chose that boundary condition).

3. Finally, we make use of the fact that the gradient is *symmetric*. That is, the differences between any nodes and their right neighbors is also the negative of the differences between any nodes and their left neighbors, shifted one element to the right. This is why we only need to compute two gradient matrices (for two spatial dimensions).

Once we have this vectorized gradient, the remaining operations look identical to the naive solver, except now we have no need for for-loops, since NumPy will *broadcast* $\sin(\cdot)$ over the matrices. This is because `np.sin` is what is referred to as a ufunc, or an automatically vectorizable function. One can define custom `ufunc` s in this manner.

Now, let's benchmark the NumPy implementation.

In [7]:
```
solver = NumpySolver(N=100, T=10, K=2.0, profile=True)
solver.integrate()
```

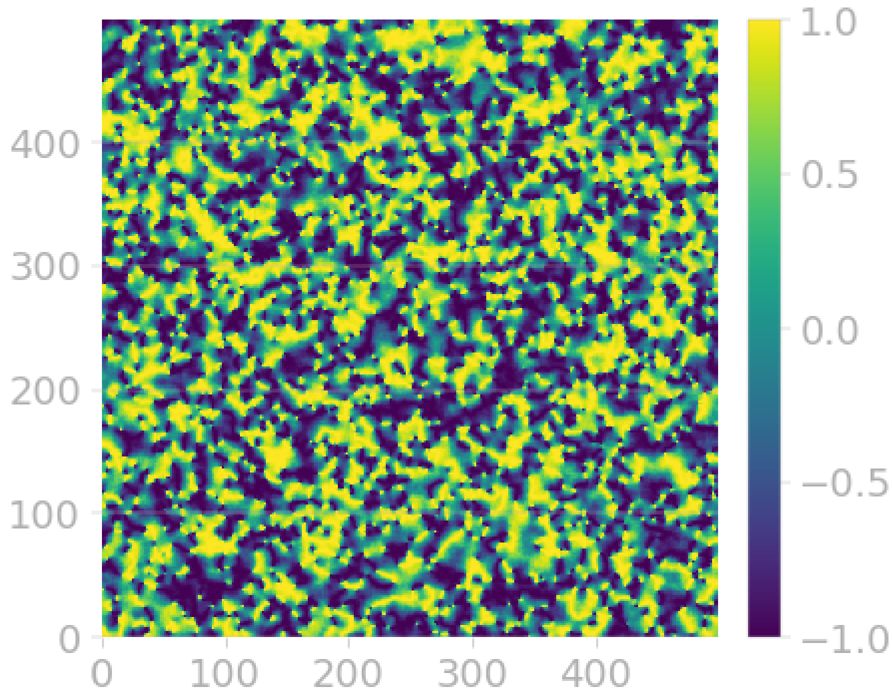
```
Using dtype: <class 'numpy.float64'>
Running profiler.
Solving...
Finished.
Timer unit: 1e-06 s

Total time: 0.032684 s
File: /var/folders/bd/lpd6x9zs40g4bjb_14mp94rw0000gq/T/ipykernel_95579/1312998
327.py
Function: dudt at line 3

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     3                                           def dudt(self, u: npt.NDA
rray) -> npt.NDArray:
     4       101        329.0      3.3      1.0          dudt = self.omega.cop
y()
     5
     6                                                   # Horizontal gradient
in the direction of +infinity
     7       101       1009.0     10.0      3.1          dudx_right = u[:, 1:]
- u[:, :-1]
     8
     9                                                   # Vertical gradient i
n the direction of -infinity
    10       101        340.0      3.4      1.0          dudy_down = u[1:, :]
- u[:-1, :]
    11
    12                                                   # Apply contribution
from horizontal neighbors
    13       101       7878.0     78.0     24.1          dudt[:, :-1] += self.
K * np.sin(dudx_right)
    14       101       7749.0     76.7     23.7          dudt[:, 1:] += self.K
* np.sin(-dudx_right)
    15
    16                                                   # Apply contribution
from vertical neighbors
    17       101       7456.0     73.8     22.8          dudt[:-1, :] += self.
K * np.sin(dudy_down)
    18       101       7894.0     78.2     24.2          dudt[1:, :] += self.K
* np.sin(-dudy_down)
    19
    20       101         29.0      0.3      0.1          return dudt
```

The time cost goes from ~5 seconds to ~0.3 seconds -- a more than 100x speedup! If you take nothing else away from this tutorial, try to express your math in a vectorized form whenever possible. This may involve slightly difficult indexing (as we saw above), but you will see dramatic gains. NumPy is *fast*.

Note that the time savings per-computation are *linear* in time, but *quadratic* in the size (N) of the problem. This means we can solve much larger problems easily:

In [8]:
```
solver = NumpySolver(N=500, T=10, K=2.0, record=True)
solver.integrate()
solver.play_video()
```

```
Using dtype: <class 'numpy.float64'>
Solving...
Finished.
```



Out[8]: `<matplotlib.animation.FuncAnimation at 0x115c007c0>`

Now, suppose we need to get things even faster. (PI says I need to run a 10,000 x 10,000 simulation by tomorrow.) That means we're going to take on the difficult task of beating NumPy -- but in order to do so, we have to understand why the NumPy implementation is faster.

Again, remember that the two implementations are functionally identical -- both *abstractly* perform the same mathematical operations. In fact, the NumPy implementation constructs two additional intermediate arrays.

Quiz: how many loops are in this code?

```
# Horizontal gradient in the direction of +infinity
dudx_right = u[:, 1:] - u[:, :-1]

# Vertical gradient in the direction of -infinity
dudy_down = u[1:, :] - u[:-1, :]

# Apply contribution from horizontal neighbors
dudt[:, :-1] += self.K * np.sin(dudx_right)
dudt[:, 1:] += self.K * np.sin(-dudx_right)
```

```
# Apply contribution from vertical neighbors
dudt[:-1, :] += self.K * np.sin(dudy_down)
dudt[1:, :] += self.K * np.sin(-dudy_down)
```

We'll come back to this later.

Optimization 0: Data locality

It may seem like the following two are the same:

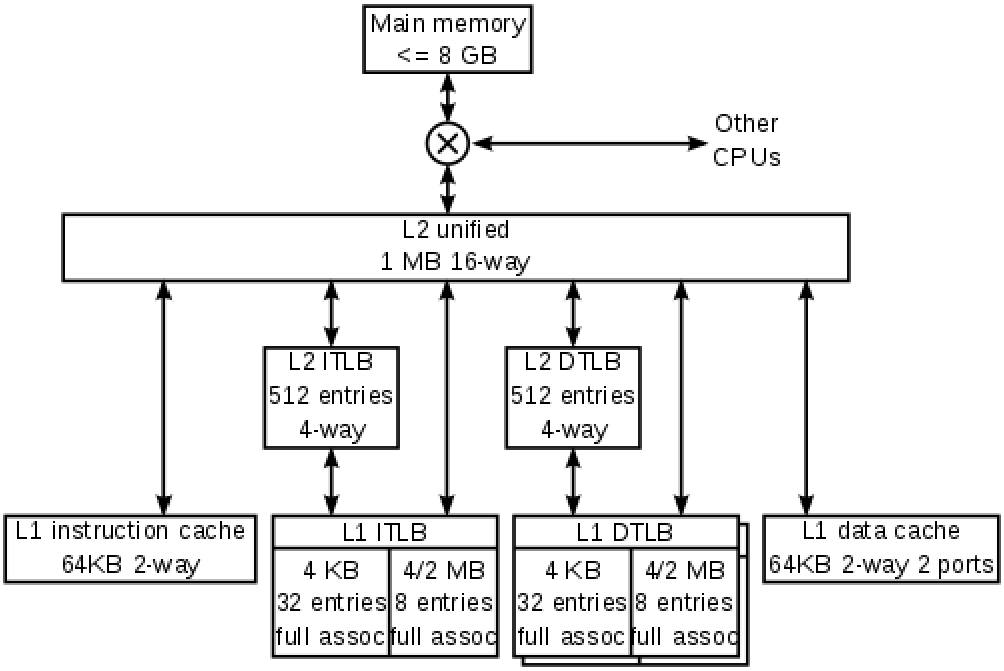
```
x = np.zeros(10)

# For-loop version
for i in range(10):
    x[i] = 1

# Numpy version
x[:] = 1
```

But they're not. In fact, we can time it:

In [9]:
```
N = 1000
x = np.zeros(N)

def set_ones(x):
    for i in range(N):
        x[i] = 1

%timeit set_ones(x)
%timeit x[:] = 1
```

```
53.4 µs ± 279 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
332 ns ± 7.6 ns per loop (mean ± std. dev. of 7 runs, 1,000,000 loops each)
```

The reason why has to do with the way Python interprets these two statements, and something called the CPU cache:



Wikipedia

All modern processors (even Apple M1) do not have direct access to the entire region of memory in your computer. Rather, data is stored in a hierarchy of increasingly large caches (typically, L1, L2, and main memory). Any data which is not in one of these caches when requested by an instruction results in a *cache miss*, in which case the missing data must be fetched from a lower-level cache or the main memory. Moving all this data around costs time.

This brings us back to why dynamic languages like Python are so easy to use, but can incur costs which seem invisible. Let's see what's happening in this loop:

```
for i in range(N):
    x[i] = 1
```

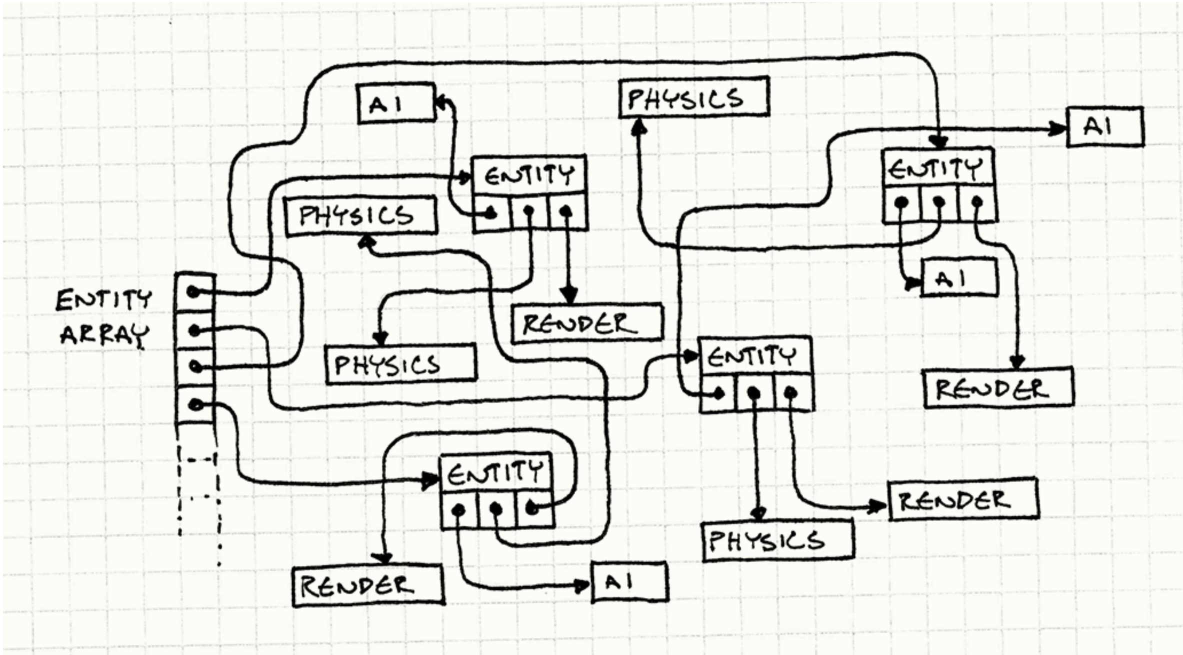
If you're familiar with Python's duck typing, you'll recognize what happens in each loop:

```
class ndarray:
    ...
    def __setitem__(self, idx: slice, value: Any):
        ...
```

Every time we make the innocuous call `x[i]`, we have to:

1. Look up the method `__getitem__` of `ndarray` (resolving any polymorphism due to inheritance, if it exists)
2. Reference the indices inside the `slice` object which tells us how to do slicing
3. Finally, dereference the value inside of the array data itself.

Step (1) requires loading the class definition into memory, if not already. Step (2) involves the construction of another intermediate slice object. Finally, step (3) loads the actual data. What this means is that our data is laid out in memory something like this:



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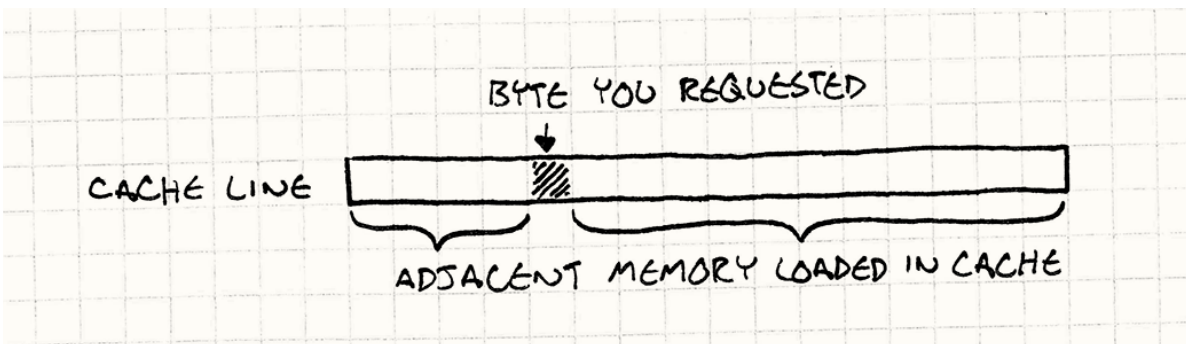
Meanwhile, our L1/L2 cache is constantly loading chunks of data which are irrelevant:



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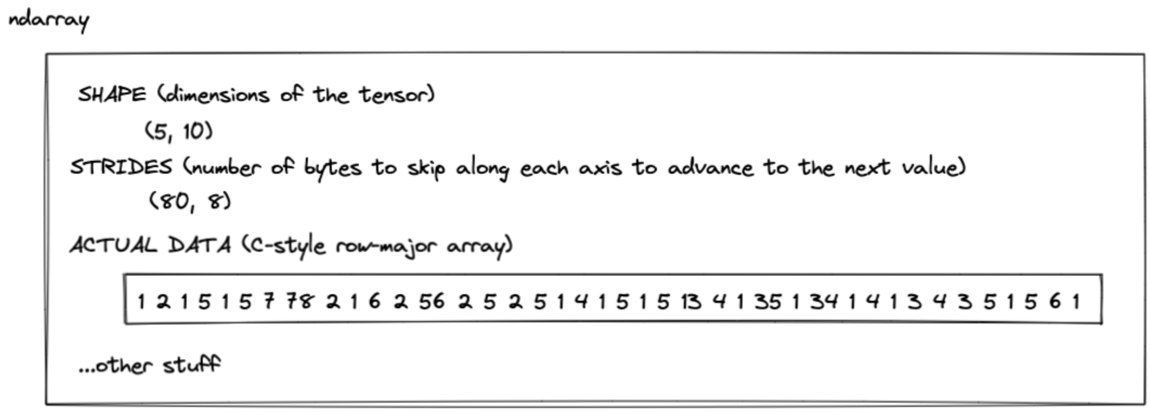
On the other hand, the second approach:

```
x[:] = 1
```

does all of the fancy Python-duck typing exactly once. We pass one `slice(None, None, None)` indicating we want the whole array to be set, and then all other data is referenced *contiguously*. The iteration is done in C on a C-style contiguous array of `int64`, and thus we incur fewer cache misses because the next referenced piece of data is *already in the cache*.

How does NumPy make this possible? Because..

Anatomy of a NumPy array: contiguous vs. non-contiguous data



NumPy data is arranged in a *contiguous* array. Meaning, the actual values are stored literally adjacent in memory, which means that loading data into cache in blocks results in infrequent misses if iterating *in order*. (You'll see different performance if you index the array in an arbitrary unsorted order.) This is one of the major benefits of vectorization: moving for-loops from Python to C avoids referencing data in memory *out of order*. This optimization is known as *data locality*.

Ultimately, what this means from a programmer's perspective is that structuring *data dependencies* in our program in a manner which is friendly to the processor (and its linear memory layout) will improve performance.

Extending Python with C++ using Pybind11

As mentioned earlier, NumPy gets a speed boost largely by moving its iteration to a lower-level language, avoiding referencing unnecessary data and creating short-lived data structures. Fortunately, the most commonly used implementation of Python is actually called `CPython` and is implemented in `C`. It has a very well-documented C API:

```
PyMODINIT_FUNC
PyInit_spam(void)
{
    PyObject *m;

    m = PyModule_Create(&spammodule);
    if (m == NULL)
        return NULL;

    SpamError = PyErr_NewException("spam.error", NULL, NULL);
    Py_XINCREF(SpamError);
    if (PyModule_AddObject(m, "error", SpamError) < 0) {
        Py_XDECREF(SpamError);
        Py_CLEAR(SpamError);
        Py_DECREF(m);
        return NULL;
    }
```

```
    return m;
}
```

This creates a Python module in C. If you want to get the absolute fastest performance out of your code and love tuning C or including custom assembly, you can immediately get started building C extensions for Python. However, this API can be a little intimidating, and it can also be confusing where and when to release the Global Interpreter Lock.

Another approach we can take is to use Cython, a Python-like language that compiles to C:

```
def primes(int nb_primes):
    cdef int n, i, len_p
    cdef int p[1000]

    if nb_primes > 1000:
        nb_primes = 1000

    len_p = 0  # The current number of elements in p.
    n = 2
    while len_p < nb_primes:
        # Is n prime?
        for i in p[:len_p]:
            if n % i == 0:
                break

        # If no break occurred in the loop, we have a prime.
        else:
            p[len_p] = n
            len_p += 1
        n += 1

    # Let's copy the result into a Python list:
    result_as_list = [prime for prime in p[:len_p]]
    return result_as_list
```

this is the approach taken by some popular libraries such as scikit-learn. It's great for writing one-off functions with speed.

However, organizing a larger or existing C/C++ codebase this way can get difficult, and many of the difficulties of C (manual memory management) are still there, just slightly hidden. Instead, we can use C++ and its RAII philosophy (Resource Acquisition Is Initialization) to use object-oriented programming to abstract away many of the complexities of the Python C API as well as manual memory management, while making use of excellent C++ libraries such as Eigen or the PyTorch C++ frontend -- imagine embedded neural networks in numerical computations!

To get started, we'll need to move to a Python package rather than a one-off script. While researchers are used to hacking scripts together for one-off purposes, this is a case where building a package is not only needed to link Python and C++, but will also greatly organize the codebase as it grows. You'll find a simple package setup in setup.py:

```python
import sys
from glob import glob
from setuptools import setup, find_packages
from pybind11.setup_helpers import Pybind11Extension, build_ext
import platform

compile_args = ['-O3', '-Wall']
link_args = []
if sys.platform in ['linux', 'linux2']:
    compile_args.append('-fopenmp') # Link OpenMP
    link_args.append('-fopenmp')

ext = Pybind11Extension(
    'kuramoto._cpp',
    include_dirs=['./cpp'],
    sources=sorted(glob('cpp/*.c*')),
    define_macros = [('EXTENSION_NAME', '_cpp')],
    extra_compile_args = compile_args,
    extra_link_args = link_args
)

setup(
    name='kuramoto',
    version="0.0.1",
    author='Anand Srinivasan',
    author_email='asrinivasan@fas.harvard.edu',
    description='Kuramoto model using NumPy + PyBind11',
    url='https://github.com/asrvsn/numpy-talk',
    package_dir={'': 'src'},
    packages=find_packages(where="src"),
    python_requires='>=3.9',
    install_requires=[
        'numpy>=1.21',
        'matplotlib',
        'line_profiler',
        'perfplot',
    ],
    include_package_data=True,
    cmdclass={"build_ext": build_ext},
    ext_modules=[ext],
)
```

The main part is `Pybind11Extension`, which will automate the process of compiling our C++ sources, linking against any necessary libraries (`OpenMP`, which we'll come to later), and producing a shared object `.so` file which can be imported in Python using

```python
from kuramoto import _cpp
```

Don't forget `-O3`!

Now the big question: how do we pass NumPy arrays to C++?

In cpp/operators.cpp you'll see how we use the C++ pybind11 library to accomplish this. As a simple example, let's compute the sum of a matrix M.

```
#include <pybind11/pybind11.h>
#include <pybind11/numpy.h>

namespace py = pybind11;

float matrix_sum(py::array_t<float> M)
{
  auto M_data = M.unchecked<2>();
  const int m = M.shape(0);
  const int n = M.shape(1);

  float sum = 0;
  for (int i = 0; i < m; i++) {
    for (int j = 0; j < n; j++) {
      sum += M_data(i, j);
    }
  }

  return sum;
}

PYBIND11_MODULE(_cpp, m) {
    m.def("matrix_sum", &matrix_sum, "Compute the sum of a matrix",
      py::arg("M").noconvert()
  );
}
```

Let's break this down:

Include the `pybind11` libraries and use the shorthand `py`:

```
#include <pybind11/pybind11.h>
#include <pybind11/numpy.h>

namespace py = pybind11;
```

Declare a function which takes a NumPy array of type `float32` and returns a `float32` value:

```
float matrix_sum(py::array_t<float> M)
{
    ...
```

Get access to the raw data (a C array) as a utility function which accepts coordinates and automatically indexes the array according to the stride:

```
auto M_data = M.unchecked<2>();
...
    sum += M_data(i, j);
```

Declare a Python module and bind the function with one argument, `M` -- also, make sure not to automatically type-cast this argument, which could lead to unwanted array copies:

```
PYBIND11_MODULE(_cpp, m) {
    m.def("matrix_sum", &matrix_sum, "Compute the sum of a matrix",
      py::arg("M").noconvert()
  );
}
```

`.noconvert()` is something you'll generally want to use, since if we accidentally pass a `float64` array instead, we could end up copying the result and down-casting to `float32`, which would eliminate some of our performance gains. More importantly, a use of C++ will be to operate on NumPy arrays *in-place*; making a copy would throw away the result.

There are important subtleties in Pybind11 about **memory ownership**. In this case, we returned a simple `float32` which is passed by value to Python. However, we could create arbitrary C++ structures and new NumPy arrays, and passing them to Python requires that we hand over memory ownership too -- otherwise the data could be freed and result in an invalid memory access in Python.

We will sidestep these issues by simply creating all necessary data structures from the Python-side first (meaning that Python always owns the data), but further discussion of this can be found in pybind11 return value policies.

Lastly, a good C++ programmer will organize their code into `.h` / `.cpp` files -- here we have used a single `.cpp` file containing all the functions for simplicity, but a more principled approach is to use `CMake` to build and organize your code. That way, you can define tests and executables for your C++ code independent of your Python code, and even build libraries which aren't tied to the Python package. For an example, see the scikit-build pybind11 project.

Now we have 3 simple files:

1. Our python script
2. A `setup.py` script specifying how to build the package
3. Our C++ "fast" code

With the build system out of the way, let's get back to optimizing our code!

Optimization 1: Loop fusion

Coming back to the quiz: how many loops are in this code?

```
dudx_right = u[:, 1:] - u[:, :-1]
dudy_down = u[1:, :] - u[:-1, :]

# Horizontal gradient
```

```
dudt[:, :-1] += self.K * np.sin(dudx_right)
dudt[:, 1:] += self.K * np.sin(-dudx_right)

# Vertical gradient
dudt[:-1, :] += self.K * np.sin(dudy_down)
dudt[1:, :] += self.K * np.sin(-dudy_down)
```

There are 6 loops in this code, one for each line. We create and assign the gradients `dudx_right`, `dudy_down` and the accumulate their values into `dudt`. This means we fetch all of the blocks of each array into cache 6 times instead of once. Can we merge all the loops into one?

Due to the indexing, the only way we can reduce the number of loops is by doing a subexpression substitution:

```
dudt[:, :-1] += self.K * np.sin(u[:, 1:] - u[:, :-1])
dudt[:, 1:] += self.K * np.sin(u[:, :-1] - u[:, 1:])

# Vertical gradient
dudt[:-1, :] += self.K * np.sin(u[1:, :] - u[:-1, :])
dudt[1:, :] += self.K * np.sin(u[:-1, :] - u[1:, :])
```

which still only gets us down to 4 loops, and now looks uglier (and does redundant computations). This is where we run into the limits of the NumPy vectorized API.

Simple idea: what if we write out our original naive solution, but in C++? This merges all the above loops in an optimization known as loop fusion. Note that, in the Python case, it cannot be referred to as a true loop fusion since we are frequently referencing data other than the array we're operating on.

In src/cpp/operators.cpp, you'll find the following `km_laplace` operator:

```
template <typename T>
void km_laplace(
  py::array_t<T> X,
  py::array_t<T> Y,
  float K
  )
// Kuramoto Laplacian
{
  auto X_data = X.template unchecked<2>();
  auto Y_data = Y.template mutable_unchecked<2>();
  const int m = X.shape(0);
  const int n = X.shape(1);

  int i = 0, j = 0;
  for (i = 0; i < m; i++) {
    for (j = 0; j < n; j++) {
      auto x = X_data(i, j);

      if (i > 0) Y_data(i, j) += K * sin(X_data(i-1, j) - x);
      if (j > 0) Y_data(i, j) += K * sin(X_data(i, j-1) - x);
      if (i < m-1) Y_data(i, j) += K * sin(X_data(i+1, j) - x);
```

```
        if (j < n-1) Y_data(i, j) += K * sin(X_data(i, j+1) - x);
      }
    }
  }
```

This implements the nonlinear differential operator $K\nabla \cdot \sin(\nabla\theta)$. Notice how all of the loops from NumPy have been flattened into one.

You'll notice two new things:

```
template <typename T>
void km_laplace(
  py::array_t<T> X,
  py::array_t<T> Y,
  float K
  )
...
    auto Y_data = Y.template mutable_unchecked<2>();
    ...
```

The first is a use of template metaprogramming, which allows us to declare one function taking NumPy arrays of multiple types (in our case, `float` and `double`.

The second is the polymorphic method call `Y.template mutable_unchecked<2>()`, which gets us the raw data in a mutable form. In this function, we are reading from the matrix `X`, and operating in-place on the matrix `Y`.

Here's how we'll call this code in Python (see src/kuramoto/solvers.py):

```python
import kuramoto._cpp as _cpp

class CppSolver(KuramotoSolver):

    def dudt(self, u: npt.NDArray) -> npt.NDArray:
        dudt = self.omega.copy()
        _cpp.km_laplace(u, dudt, self.K)
        return dudt
```

Where did `kuramoto._cpp` come from? It doesn't exist as a file until you build the package using `pip install .`, at which point your C++ sources will be compiled into a single `_cpp.so` file which can be imported in Python at runtime.

So, let's compare our two methods! We're going to benchmark the C++ solver as defined in the package, instead of defining it here, for the above reason. First, let's increase the size of the problem to get some decently large numbers:

In [10]:
```python
solver = NumpySolver(N=200, T=100, K=2.0, profile=True)
solver.integrate()
```

```
Using dtype: <class 'numpy.float64'>
Running profiler.
Solving...
Finished.
Timer unit: 1e-06 s

Total time: 0.99851 s
File: /var/folders/bd/lpd6x9zs40g4bjb_14mp94rw0000gq/T/ipykernel_95579/1312998
327.py
Function: dudt at line 3

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     3                                           def dudt(self, u: npt.NDA
rray) -> npt.NDArray:
     4      1001       6211.0      6.2      0.6      dudt = self.omega.cop
y()
     5
     6                                               # Horizontal gradient
in the direction of +infinity
     7      1001      25226.0     25.2      2.5      dudx_right = u[:, 1:]
- u[:, :-1]
     8
     9                                               # Vertical gradient i
n the direction of -infinity
    10      1001       8321.0      8.3      0.8      dudy_down = u[1:, :]
- u[:-1, :]
    11
    12                                               # Apply contribution
from horizontal neighbors
    13      1001     240925.0    240.7     24.1      dudt[:, :-1] += self.
K * np.sin(dudx_right)
    14      1001     253593.0    253.3     25.4      dudt[:, 1:] += self.K
* np.sin(-dudx_right)
    15
    16                                               # Apply contribution
from vertical neighbors
    17      1001     225065.0    224.8     22.5      dudt[:-1, :] += self.
K * np.sin(dudy_down)
    18      1001     238964.0    238.7     23.9      dudt[1:, :] += self.K
* np.sin(-dudy_down)
    19
    20      1001        205.0      0.2      0.0      return dudt
```

In [11]:

```
solver = km.CppSolver(N=200, T=100, K=2.0, profile=True)
solver.integrate()
```

```
Using dtype: <class 'numpy.float64'>
Running profiler.
Solving...
Finished.
Timer unit: 1e-06 s

Total time: 0.739681 s
File: /Users/anandsrinivasan/mambaforge/lib/python3.9/site-packages/kuramoto/s
olvers.py
Function: dudt at line 68

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
    68                                           def dudt(self, u: npt.
NDArray) -> npt.NDArray:
    69      1001       6480.0      6.5      0.9                  dudt = self.om
ega.copy()
    70      1001     732965.0    732.2     99.1                  _cpp.km_laplac
e(u, dudt, self.K)
    71      1001        236.0      0.2      0.0                  return dudt
```

There we have it, we have beat the NumPy implementation by about 40% with a simple translation of our naive Python solution to C++!

Let's use perfplot to compare our solvers across a range of problem sizes:

In [12]:
```
bench = perfplot.bench(
    setup = lambda T: T,
    n_range = np.logspace(1, 3, 10).astype(int),
    kernels = [
        lambda T: NumpySolver(N=100, T=T, K=2.0).integrate(),
        lambda T: km.CppSolver(N=100, T=T, K=2.0).integrate()
    ],
    xlabel = 'T',
    labels = ['NumPy', 'C++'],
    equality_check = None
)
bench
```

```
Output()
```

n	NumPy	C++
10	0.02746575	0.020586417000000003
16	0.042880833	0.031450416
27	0.070274	0.052022541000000005
46	0.1183555	0.08680775
77	0.19243175	0.14756054200000002
129	0.32970408300000004	0.24507104100000002
215	0.5549328330000001	0.40751020800000004
359	0.9120682080000001	0.682745375
599	1.5216791250000001	1.128388334
1000	2.54043725	1.886987208

Out[12]:

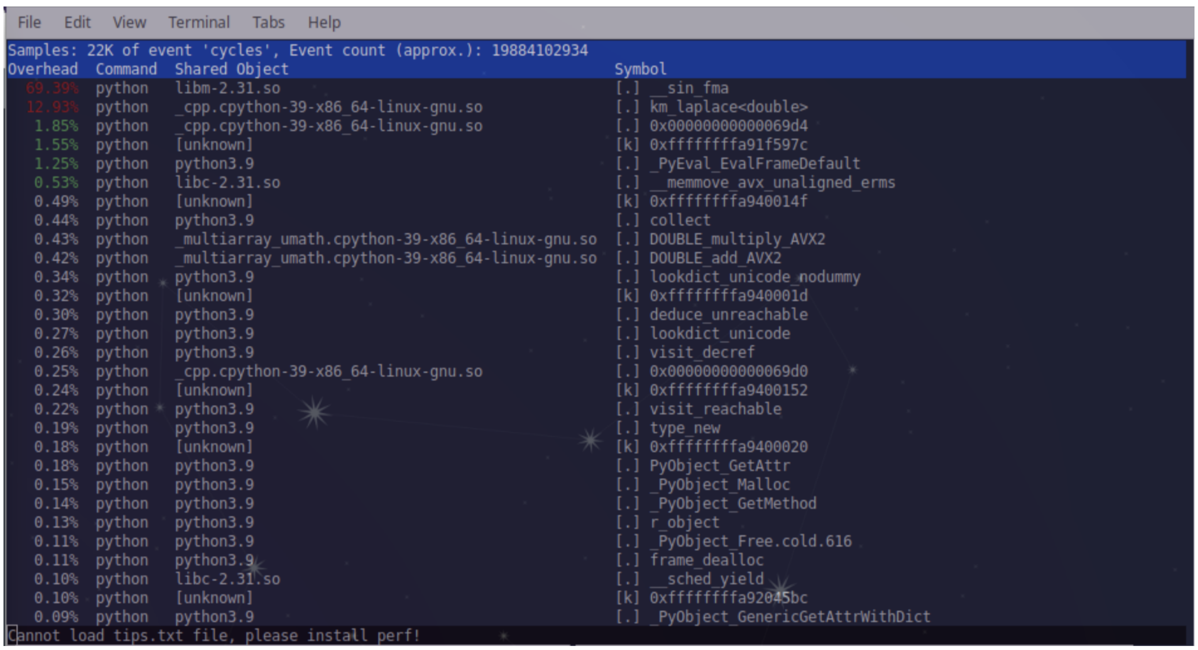
Can we go even faster?

One of the downsides of moving our numerical code to C++ is that we no longer get line-by-line profiles. But this is where we can use the linux perf tool to get detailed information about hardware events, arithmetic operations, and which functions we're spending time in.

Unfortunately, `perf` is available only on linux-based OSes, and in particular cannot be used inside of containers (due to security reasons). Therefore, we will describe the steps for running it:

```
sudo sh -c 'echo 1 > /proc/sys/kernel/perf_event_paranoid' # Suppress some kernel warnings
perf record ./bin/main -N 100 -K 2 -T 1000
perf report
```

Upon running it on our C++ solver, we will see a detailed output like this:



```
File  Edit  View  Terminal  Tabs  Help
Samples: 22K of event 'cycles', Event count (approx.): 19884102934
Overhead  Command  Shared Object                                       Symbol
  69.39%  python   libm-2.31.so                                        [.] __sin_fma
  12.93%  python   _cpp.cpython-39-x86_64-linux-gnu.so                 [.] km_laplace<double>
   1.85%  python   _cpp.cpython-39-x86_64-linux-gnu.so                 [.] 0x00000000000069d4
   1.55%  python   [unknown]                                           [k] 0xffffffffa91f597c
   1.25%  python   python3.9                                           [.] _PyEval_EvalFrameDefault
   0.53%  python   libc-2.31.so                                        [.] __memmove_avx_unaligned_erms
   0.49%  python   [unknown]                                           [k] 0xffffffffa940014f
   0.44%  python   python3.9                                           [.] collect
   0.43%  python   _multiarray_umath.cpython-39-x86_64-linux-gnu.so    [.] DOUBLE_multiply_AVX2
   0.42%  python   _multiarray_umath.cpython-39-x86_64-linux-gnu.so    [.] DOUBLE_add_AVX2
   0.34%  python   python3.9                                           [.] lookdict_unicode_nodummy
   0.32%  python   [unknown]                                           [k] 0xffffffffa940001d
   0.30%  python   python3.9                                           [.] deduce_unreachable
   0.27%  python   python3.9                                           [.] lookdict_unicode
   0.26%  python   python3.9                                           [.] visit_decref
   0.25%  python   _cpp.cpython-39-x86_64-linux-gnu.so                 [.] 0x00000000000069d0
   0.24%  python   [unknown]                                           [k] 0xffffffffa9400152
   0.22%  python   python3.9                                           [.] visit_reachable
   0.19%  python   python3.9                                           [.] type_new
   0.18%  python   [unknown]                                           [k] 0xffffffffa9400020
   0.18%  python   python3.9                                           [.] PyObject_GetAttr
   0.15%  python   python3.9                                           [.] _PyObject_Malloc
   0.14%  python   python3.9                                           [.] _PyObject_GetMethod
   0.13%  python   python3.9                                           [.] r_object
   0.11%  python   python3.9                                           [.] _PyObject_Free.cold.616
   0.11%  python   python3.9                                           [.] frame_dealloc
   0.10%  python   libc-2.31.so                                        [.] __sched_yield
   0.10%  python   [unknown]                                           [k] 0xffffffffa92045bc
   0.09%  python   python3.9                                           [.] _PyObject_GenericGetAttrWithDict
Cannot load tips.txt file, please install perf!
```

Immediately we will see that calls to the `sin()` functions dominate the runtime. This brings up a numerical question -- can we approximate the sin function faster? It depends on the use-case. In our case, the non-linearity is fundamental to the problem; if we instead approximate $\sin(x) \approx x$ (which is valid as $x \to 0$) then we get the very different *diffusion* problem:

$$\partial_t \theta = \omega + K \nabla \cdot \nabla \theta = \omega + K \Delta \theta$$

Just for fun, let's use the result of `perf` to replace $\sin(x)$ with x to see how the performance changes:

In [13]:
```
bench = perfplot.bench(
    setup = lambda T: T,
    n_range = np.logspace(1, 3, 10).astype(int),
    kernels = [
        lambda T: NumpySolver(N=100, T=T, K=2.0).integrate(),
        lambda T: km.CppSolver(N=100, T=T, K=2.0).integrate(),
```

```
        lambda T: km.ApproximateCppSolver(N=100, T=T, K=2.0).integrate(),
    ],
    xlabel = 'T',
    labels = ['NumPy', 'C++', 'C++ (Approximate)'],
    equality_check = None
)
bench
```

Output()

n	NumPy	C++	C++ (Approximate)
10	0.027816583000000002	0.020439416000000002	0.00217066600000000
16	0.042787250000000006	0.031778917000000004	0.003408041
27	0.069460834	0.051697042000000006	0.00567612500000000
46	0.11842862500000001	0.08735050000000001	0.009680917
77	0.19733629100000002	0.14758341600000002	0.016015833
129	0.330488542	0.24360441700000002	0.02698237500000000
215	0.553858417	0.411211042	0.04531454200000000
359	0.91181075	0.680809958	0.07624
599	1.5310652500000002	1.133345625	0.128187666
1000	2.587857209	1.888907542	0.21488616700000002

Out[13]:

The results are pretty dramatic, and the lesson is that some of the best optimizations are done mathematically. (For example, if we can take a change of coordinates in which the system becomes linear).

Optimization 2: Floating-point precision

Now we'll make a rather simple optimization: what if we don't need 64-bit precision?

One of the gotchas with using NumPy is that, unless you're very careful, it's easy to "accidentally" up-cast your data from `float32` to `float64`. (This is one of the reasons that major ML frameworks like PyTorch, TensorFlow, etc. don't simply re-use the NumPy library for their CPU implementations).

In our C++ code, we declared a polymorphic function using templates:

```
template <typename T>
void km_laplace(
  py::array_t<T> X,
  py::array_t<T> Y,
  float K
  )
```

Therefore we simply need to initialize our state with the correct precision in NumPy (see src/kuramoto/base.py):

```
self.initial_state = np.random.uniform(0, 2*np.pi, size=(self.N,
self.N)).astype(self.dtype)
```

Now we'll run the benchmarks:

In [14]:
```
bench = perfplot.bench(
    setup = lambda T: T,
    n_range = np.logspace(1, 3, 10).astype(int),
    kernels = [
        lambda T: NumpySolver(N=100, T=T, K=2.0).integrate(),
        lambda T: km.CppSolver(N=100, T=T, K=2.0).integrate(),
         lambda T: km.CppSolver(N=100, T=T, K=2.0, dtype=np.float32).integrate(
    ],
    xlabel = 'T',
    labels = ['NumPy', 'C++', 'C++ (float32)'],
    equality_check = None
)
bench
```

Output()

n	NumPy	C++	C++ (float32)
10	0.027747916	0.020581125000000002	0.01785112500000000
16	0.042494750000000005	0.031845917	0.02742300000000000
27	0.070070792	0.052133083000000004	0.04497983300000000
46	0.11901012500000001	0.087882417	0.076164541
77	0.197727709	0.14770945800000002	0.128133208
129	0.332191917	0.24621183300000002	0.21597475000000002
215	0.551235333	0.408076292	0.357413083
359	0.956002459	0.6813559170000001	0.600566
599	1.6130757500000001	1.1404556670000001	1.001856667
1000	2.6288705830000003	1.8875962080000002	1.6619633340000002

Out[14]:

A moderate improvement, but certainly noticeable at large scales.

Optimization 3: Multithreading

Lastly, we arrive at the most "fun" optimization, and one that cannot be done by NumPy or within Python: **multi-threading**.

If you've used Python long enough, you've heard of the Global Interpreter Lock. This is a mutex which prevents access to any Python object by more than one thread at a time.

By breaking out to C++, we are no longer operating on Python objects (only on the C data structures underlying them, as specified in the C API), and thus we are free to open multiple threads to operate on a NumPy array without fear of the dreaded GIL.

Here, we will use OpenMP, a library and set of compiler directives for C/C++ which enable shared-memory parallelism. This is in contrast to other tools you may have used in cluster (or *multi-node*) environments such as MPI, which enables multi-process applications by using explicit message passing. In OpenMP, all threads will have access to any data which we *share* among them, and any other data will be *copied* or *private*. Let's see how this works:

```
#include <omp.h>

...

template <typename T>
void km_laplace_parallel(
  py::array_t<T> X,
  py::array_t<T> Y,
  float K
  )
// Parallel Kuramoto Laplacian
{
  auto X_data = X.template unchecked<2>();
  auto Y_data = Y.template mutable_unchecked<2>();
  const int m = X.shape(0);
  const int n = X.shape(1);

  #pragma omp parallel for collapse(2) shared(X_data, Y_data, m, n)
  for (int i = 0; i < m; i++) {
    for (int j = 0; j < n; j++) {
      auto x = X_data(i, j);

      if (i > 0) Y_data(i, j) += K * sin(X_data(i-1, j) - x);
      if (j > 0) Y_data(i, j) += K * sin(X_data(i, j-1) - x);
      if (i < m-1) Y_data(i, j) += K * sin(X_data(i+1, j) - x);
      if (j < n-1) Y_data(i, j) += K * sin(X_data(i, j+1) - x);
    }
  }
}
```

In cpp/operators.cpp, you'll find the above definition for `km_laplace_parallel`. Using OpenMP is surprisingly simple. First, you'll need the OpenMP headers, which you can install e.g. on Ubuntu using

```
sudo apt-get install libomp-dev
```

On Mac, unfortunately, OpenMP is not supported out-of-the-box because the Apple Clang compiler disables OpenMP support. This is also why we run this notebook in Docker.

Unpacking the above, the main and only difference from our previous C++ code is this pragma:

```
...
    #pragma omp parallel for collapse(2) shared(X_data, Y_data, m, n)
...
```

- `#pragma omp parallel for` is a compiler directive telling `gcc` to automatically parallelize the following for-loop; if your system doesn't have OpenMP, this will simply be ignored and your program will run in serial.

- Next, `collapse(2)` says there are two nested for loops, and we'd like to parallelize them both.
- Finally, `shared(X_data, Y_data, m, n)` declares that the variables `X_data, Y_data, m, n` must be shared across threads (this is necessary to store the results computed by each thread).

That's it! You can learn more about OpenMP pragmas here.

Finally let's benchmark our program. Your performance will vary depending on the number of physical cores you have, and what other work they're doing (such as running a Chrome browser and jupyter server). On my Thinkpad with 2 cores and 4 threads, we see:

In [20]:
```
bench = perfplot.bench(
    setup = lambda T: T,
    n_range = np.logspace(1, 3, 10).astype(int),
    kernels = [
        lambda T: NumpySolver(N=100, T=T, K=2.0).integrate(),
        lambda T: km.CppSolver(N=100, T=T, K=2.0).integrate(),
        lambda T: km.ParallelCppSolver(N=100, T=T, K=2.0).integrate(),
    ],
    xlabel = 'T',
    labels = ['NumPy', 'C++', 'C++ (OpenMP)'],
    equality_check = None
)
bench
```

```
Output()
```

n	NumPy	C++	C++ (OpenMP)
10	0.07222010400000001	0.062612728	0.028162174
16	0.114900677	0.09735291400000001	0.042832618
27	0.18380621400000002	0.16061488000000002	0.07338643
46	0.31400441700000004	0.263809821	0.137620654
77	0.521157893	0.43166795500000005	0.23442024600000003
129	0.8408792270000001	0.7032517660000001	0.400003792
215	1.406836685	1.170835802	0.6509469
359	2.314015564	1.9234021860000001	1.098779761
599	3.8883694500000003	3.2234017820000003	1.818755922
1000	6.466532826000001	5.356450026	3.1089954680000003

Out[20]:

Note that hyperthreading doesn't help much if the cores are busy all the time (as opposed to being I/O-bound). This is also why cluster setups typically disable hyper-threading.

Parting thoughts

The optimizations we covered here:

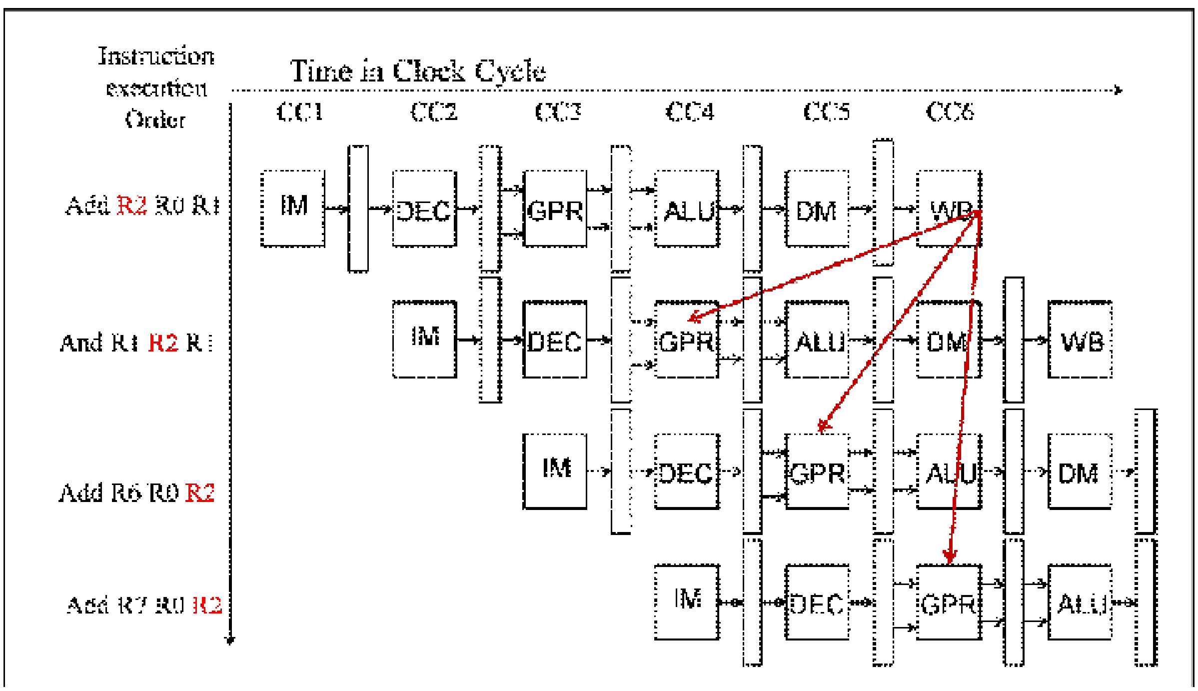
1. Improving data locality

2. Loop fusion
3. Floating-point precision
4. Shared-memory parallelism

are only the tip of the iceberg. To push your Python/C++ code further, you'll need to understand how modern processors work in a bit more detail and, most importantly, the actual code (Assembly) that is being sent to it. To optimize your C++ code further, check out this O'Reilly book.

Projects such as LLVM aim to make many of the optimizations we made above automatically; but note that the compiler can only go so far. If the program does extra work at a high-level, low-level compilers will find it difficult if not impossible to optimize this away.

Thus, if you take one thing away, the key idea is to **have the computer do as little work as possible.** This is easier said than done, but another way to think of this is to **reduce the data dependencies** on the way to obtaining a result as far as possible. Complex data dependences in your code lead to cache misses, inability to parallelize, and difficult to debug logic:



Kumar et al

Lazy functional languages such as Haskell can help automate the discovery and elimination of redundant data dependencies to some extent, but come with their own caveats and are certainly not the lingua franca of scientific programming (compared to imperative languages such as C / Python).

Most people have heard of parallelizing serial code, but “serial” vs. “parallel” are two simplifications in the more complex world of data dependencies. Our PDE for-loop was fast due to **locality** of the operators (by contrast, imagine an integral operator, which is **nonlocal**):

$$\frac{\partial \theta}{\partial t}(t,x) = \omega + K \int_{[0,1]^2} \sin(\theta(t,y) - \theta(t,x))dy$$

This is a continuum limit of the original (non-lattice) Kuramoto model, which had all-all connections. Notice the data dependence on the entire domain.

Some of the most famous algorithms in use today are popular because of their simple and cheaply implementable data dependencies.

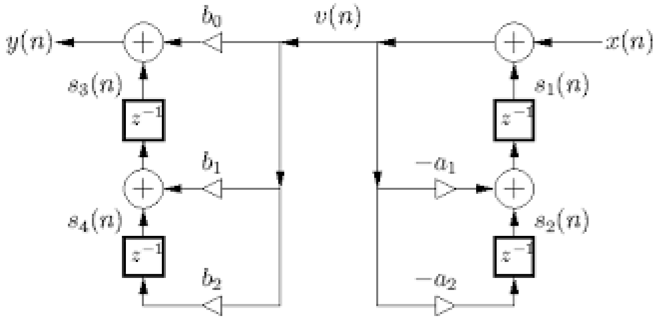
Reinforcement learning / Dynamic programming

$$\begin{aligned}
c_T(k) &= Ak^a \\
c_{T-1}(k) &= \frac{Ak^a}{1+ab} \\
c_{T-2}(k) &= \frac{Ak^a}{1+ab+a^2b^2} \\
&\dots \\
c_2(k) &= \frac{Ak^a}{1+ab+a^2b^2+\ldots+a^{T-2}b^{T-2}} \\
c_1(k) &= \frac{Ak^a}{1+ab+a^2b^2+\ldots+a^{T-2}b^{T-2}+a^{T-1}b^{T-1}} \\
c_0(k) &= \frac{Ak^a}{1+ab+a^2b^2+\ldots+a^{T-2}b^{T-2}+a^{T-1}b^{T-1}+a^Tb^T}
\end{aligned}$$

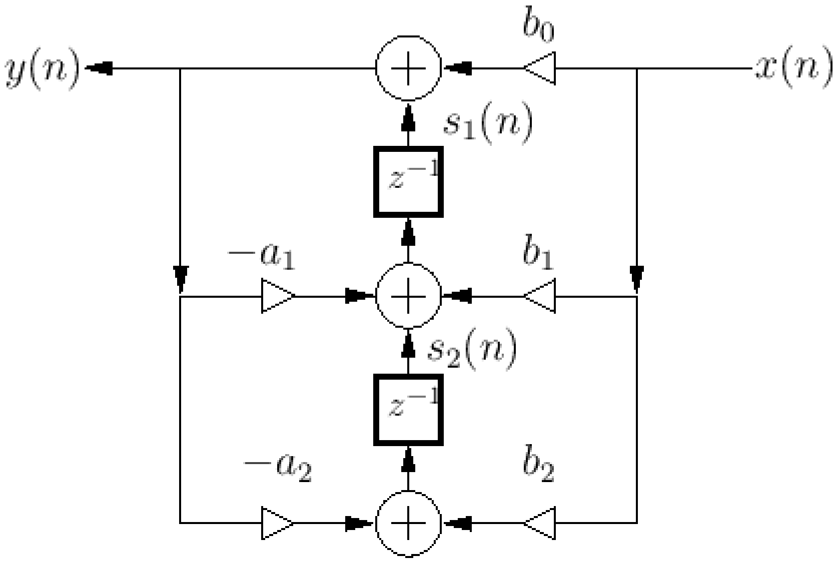
Optimal substructure: If I know the optimal solution in time $[t,T]$, it is a subsolution of the optimal solution $[t-\Delta t, T]$.

Digital signal processing

Direct I form:



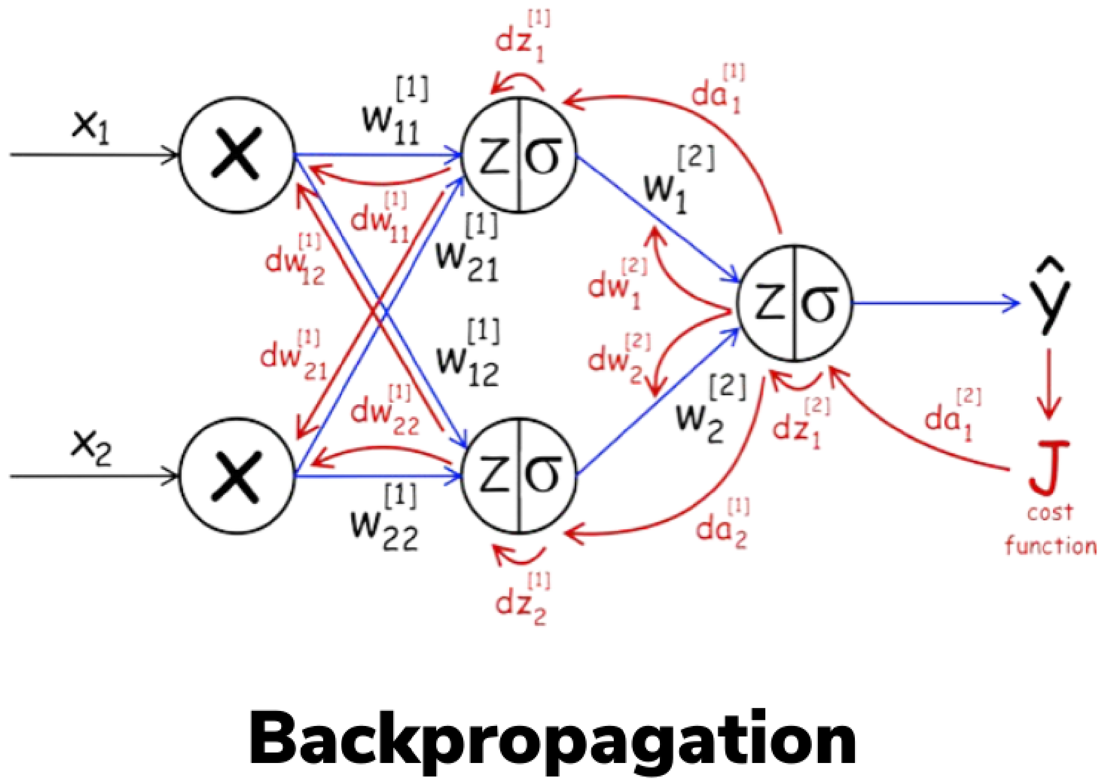
vs. **Direct II form**:



stanford.edu

Two different implementations of a transfer function with different data dependencies.

Backpropagation



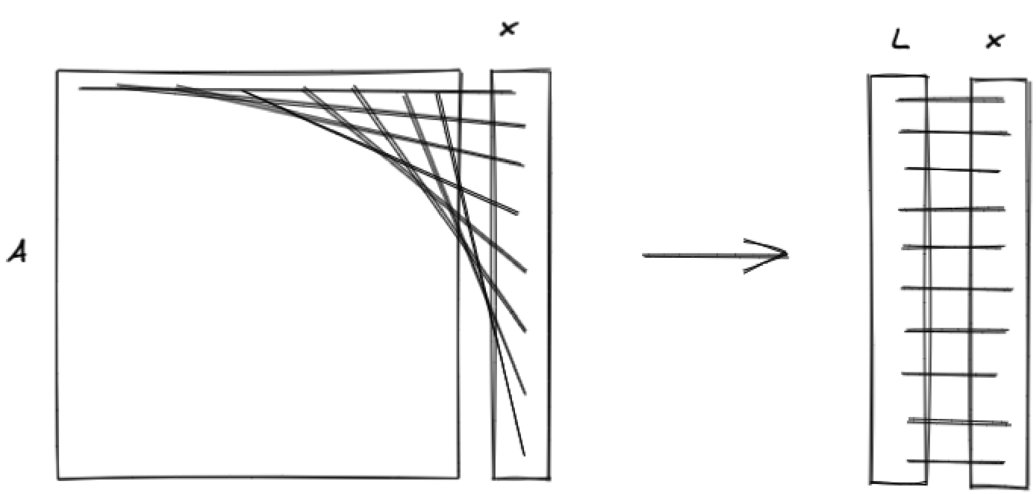
[analyticsarora]

Local data dependencies in the graph, as opposed to global optimization.

Undergraduate ODEs

Diagonalizing the fundamental matrix:

$$\dot{x} = Ax \mapsto \dot{z} = \Lambda z, z = Px$$



From a **matrix-vector product** to a **decoupled elementwise multiplication**. We just rotate the coordinates.

In [ ]:

```

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