JIT compilers for scientific computing in Python: Numba vs. JAX

A Case Study Evaluating Gravitational Lensing Likelihood

HTML presentation, PDF archive

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Abstract

Accelerating scientific Python with JITs. We share our journey migrating a gravitational lensing likelihood calculation from Numba to JAX. Learn about performance gains, automatic differentiation benefits, and practical lessons for high-performance scientific computing in Python.

Python is widely used in scientific research, but pure Python can sometimes be too slow for computationally intensive tasks. Just-In-Time (JIT) compilers are essential tools for boosting performance, allowing Python code to run closer to native speeds. While libraries like Numba have long been popular for accelerating numerical Python functions, JAX offers a new paradigm, combining JIT compilation with powerful features like automatic differentiation (auto-diff) and execution across different hardware (CPUs, GPUs, TPUs).

This talk will take you on a journey through our experience optimizing a critical component of an astrophysics analysis pipeline: the calculation of the likelihood function for gravitational lensing models, used with data from the James Webb Space Telescope. We initially used Numba to accelerate this calculation, but the need for performance portability across hardwares, and the potential speed up from gradient computation for model fitting led us to explore JAX's unique capabilities.

This session will walk through the practical steps, challenges, and insights gained from migrating this complex scientific code from its existing Numba implementation to a JAX-based one.

You will learn:

- Why leveraging performance tools like JITs is crucial for cutting-edge scientific analysis in Python.
- The practical considerations when migrating existing numerical code from Numba to JAX, including syntax changes and managing state.
- How JAX's auto-differentiation simplifies gradient calculations essential for scientific optimization and sampling tasks.
- The significant performance improvements achieved in our specific gravitational lensing case study by using JAX's compiled functions.
- Broader lessons learned about structuring scientific Python projects to effectively use modern JIT compilers and harness capabilities like auto-diff.

We'll conclude by comparing Numba and JAX in benchmark performance, developer ergonomics, and tradeoffs between the two, providing you with practical guidance for choosing the right tool for your scientific computing needs.

This case study offers a concrete example of how evolving Python libraries are enabling researchers to perform complex, high-performance computations directly within the Python ecosystem. Join us to see how tools like JAX are empowering scientific discoveries, one optimised function at a time.

This talk is suitable for intermediate Python programmers familiar with NumPy.

Contents

Context: Why Python in HPC?

Why do I use Python in HPC?

- Cosmologist
- PhD: CMB Data Analysis
  - processing $\sim O(10\ \mathrm{TiB}) \sim O(\mathrm{PiB})$ of data for cosmological inference
  - using scientific softwares in Python
  - running on NERSC (a top 10 HPC system)

I am a cosmologist. I did my PhD in UCBerkeley Physics department on the topic of Cosmic Microwave Background radiation. During my research, I use the NERSC HPC facility in the US, a top 10 supercomputing system, to perform CMB data analysis. Briefly speaking, as we cannot do an experiment cosmologically, we instead observe a huge amount of data and use statistical methods such as Bayesian inference to deduce information about our universe, such as deducing dark matter composition, finding evidence of inflation during the Big Bang. My main interst in Python is therefore primarily on its application of scientific computing on HPC.

Questions: which language can you use to write applications for HPC?

Languages that has demonstrated to scale to state-of-the-art, full system supercomputer

- Fortran
- C/C++
- Python
- Julia
- ~~matlab~~
- ~~rust~~

Questions: Why Python in HPC? What is its superpower in supercomputing?

- Because it is where the community is.
- Because we are the people who don't care what language our algorithm is implemented in.
  - C
  - C++
  - Fortran
  - Julia
  - Rust

  - …

The opening keynote resonates with me a lot. Python has superpowers. I recommend people watching that to see the history and the bigger picture. Here, I am more narrowly focused to tell you why, at this particular moment, Python is the language of choice to write and run scientific applications on supercomputers.

First of all, it is where the community is. Numpy, Scipy, Astropy, you name it.

Secondly, it is because we are the people who don't care what language our algorithm is implemented in. In order words, Python is the glue. If we look back to the list of languages that has demonstrate they can scale to the state-of-the-art supercomputer at a given era, there is not a lot on the list, and Python is one of them. You might call that cheating, because in this case Python is mostly just calling C modules or libraries written in Fortran. But we don't care. Python is the glue that successfully composed very complicated scientific workflow together.

Context: Why JIT?

Short introduction on aot/jit compilations & interpreter

- interpreters
  - CPython
  - bash
- compilers
  - AOT
    - `gcc` from GNU compilers, `clang` from LLVM compilers
      - CPython is AOT compiled by these compilers!
    - traditionally excels at HPC: C/C++, Fortran
  - JIT
    - `pypy`
    - Julia
    - Javascript has a JIT

Back to the languages, focusing on the aspect of how source code eventually runs, it falls into two categories, compilers and interpreters. And within compilers, there are also ahead-of-time (AOT) compilation and just-in-time (JIT) compilation.

Here we will name a few examples. The reference Python implementation, `CPython`, is an interpreter, which is AOT compiled by C compilers such as `gcc` and `clang`. Another well known Python implementation `pypy` is a jit compiler.

Short introduction on the landscape of acceleration framework of numeric code in Python

- AOT
  - C with CPython API
    - e.g. Numpy, which is a framework in itself
  - Cython: superset of the Python language, compiled to C modules, handle CPython API and Python interface automatically
  - pybind11: C++ 11+, handle CPython API and Python interface semi-automatically
- JIT
  - `pypy`: general purpose Python implementation (any valid Python should runs)
  - CPython 3.13+ experimental JIT: only a subset of Python code will be jit compiled (and is not clear on when and where), not focused on numerical
  - Numba, JAX: DSL, jit-compile a subset of Python, focused on numerical

I hope we all agree the CPython interpreter is slow, right? To accelerate applications running in CPython, there are multiple frameworks to do it. The traditional model is C modules: write your performance critical part of the code in C and use the CPython API to expose a Python interface to the users. A prominent example of that is `numpy`, which defines an interface often used in high performance numerical operations, and is architected in C with a pythontic interface. This is still one of the fastest and pythonic way to write numerical code in Python without introducing further compliation to the users. Other examples on AOT are cython and C++ with pybind11, which I won't go into details.

Turning our attention to the spotlight of the day: JIT. `pypy` is a general purpose Python jit compiled runtime for a long time. There is also an experimental JIT compiler in CPython 3.13+, which would jit compiled a subset of hot code.

The remaining JIT compilers are the one we are focusing on today. Numba and JAX can both be regarded as Domain Specfic Languages that will jit compiled a subset of the Python language, focused on numerical compuations.

Why jit: solving the 2 language problem

To replace this single function from Numba to C++ with pybind11,

```
@numba.jit(parallel=True)
def _fma(out, weights, *arrays):
    for weight, array in zip(weights, arrays):
        out += weight * array
```

hpc4cmb/toast#a38d1d6:

```
14 files changed
+230 -36 lines changed
```

… and 30% faster!

- Python gives you velocity: rapid prototyping science code is a path dependent evolution
- Numba jit gives you speed (SIMD + multi-threading): C++ with SIMD and OpenMP multi-threading is only 30% faster in this case. The single `@jit` decorator gives you 3 times speed up comparing to pure Numpy implementation.
- JIT sometimes has advantage over AOT because it can see the data
- JIT obviously has overhead, but if you are processing "big data", that amount of time usually is much shorter than it takes to run the calculation itself.

To briefly give an idea why JIT may be useful, we can look at this function as an example. If you are familiar with Numba enough, as soon as you write down this simple function with Numpy, adding the jit decorator there is a no-brainer. You would be able to immediately predict that it will be faster, and memory allocation is simpler, and hence lesser memory pressure and lesser chance of getting killed by out-of-memory (OOM) error.

However, when I ported this to C++ with pybind11, 14 files are changed, 230 lines are added. If you look into the commit change, for sure a lot of them are boilerplates. But that is exactly the point. It went from using Numba as a 10s decision to being 30% faster after a ton of work.

This sort of things happens all the time when writing science code. How your program eventually got there is often not obvious in the beginning. It involves repid prototyping and sometimes solving complicated mathematical or algorithmic problems. Having a DSL within Python that can be jitted is a superpower Python given us to move fast and run fast at the same time.

Concrete example of Numba vs. JAX

$\tilde{w}$

$$\tilde{w}_{ij} = \sum_{k=1}^{K} \frac{1}{n_k^2} \cos\left(2\pi \left[\left(\vec{g}_i - \vec{g}_j\right) \cdot \vec{u}_k\right]\right), \quad 1 \le i,j \le M$$

Now it all makes sense, kind of. Let us do an actual example to see how JIT works.

I call this a slow track. It is a live demo without being live. I hope it will gives you a feel of the languages and gain intuitions yourself. Later on, we will have a fast track and you just have to believe the high level summaries I am going to give you.

Let's stare at this equation and see how you would implement it.

Numpy

$$\tilde{w}_{ij} = \sum_{k=1}^{K} \frac{1}{n_k^2} \cos\left(2\pi \left[\left(\vec{g}_i - \vec{g}_j\right) \cdot \vec{u}_k\right]\right), \quad 1 \le i,j \le M$$

As usual in Numpy, we vectorize everything:

```python
import numpy as np


def w_mm_np(
    n_k: np.ndarray[tuple[int], np.float64],
    u_k_vec: np.ndarray[tuple[int, int], np.float64],
    g_m_vec: np.ndarray[tuple[int, int], np.float64],
) -> np.ndarray[tuple[int, int], np.float64]:
    # (M, M, 1, 2)
    δg_mm1_vec =  g_m_vec.reshape(-1, 1, 1, 2) - g_m_vec.reshape(1, -1, 1, 2)
    # (1, 1, K, 2)
    u_11k_vec = u_k_vec.reshape(1, 1, -1, 2)
    return (
        np.cos(
            (2.0 * np.pi) *
            # (M, M, K)
            (
                δg_mm1_vec[:, :, :, 0] * u_11k_vec[:, :, :, 1] +
                δg_mm1_vec[:, :, :, 1] * u_11k_vec[:, :, :, 0]
            )
        ) /
        # (1, 1, K)
        np.square(n_k).reshape(1, 1, -1)
    ).sum(2)  # sum over k
```

```
898 ms ± 9.62 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Ignore the tiny little details there where the order of the dimensions in $\vec{g}$ and $\vec{u}$ are opposite to each other.

Numba

How would you implement it in Numba? Just add the jit decorator:

```python
import numba


@numba.jit("f8[:, ::1](f8[::1], f8[:, ::1], f8[:, ::1])", nopython=True, nogil=True, parallel=True)
def w_mm_numba(
    ...
```

```
522 ms ± 9.01 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

JAX

How would you implement it in JAX? By add the jit decorator, and replacing `numpy` with `jax.numpy`:

```python
import jax
import jax.numpy as jnp

@jax.jit
def w_mm_jax(
    n_k: np.ndarray[tuple[int], np.float64],
    u_k_vec: np.ndarray[tuple[int, int], np.float64],
    g_m_vec: np.ndarray[tuple[int, int], np.float64],
) -> np.ndarray[tuple[int, int], np.float64]:
    # (M, M, 1, 2)
    δg_mm1_vec =  g_m_vec.reshape(-1, 1, 1, 2) - g_m_vec.reshape(1, -1, 1, 2)
    # (1, 1, K, 2)
    u_11k_vec = u_k_vec.reshape(1, 1, -1, 2)
    return (
        jnp.cos(
            (2.0 * jnp.pi) *
            # (M, M, K)
            (
                δg_mm1_vec[:, :, :, 0] * u_11k_vec[:, :, :, 1] +
                δg_mm1_vec[:, :, :, 1] * u_11k_vec[:, :, :, 0]
```

```
            )
        ) /
        # (1, 1, K)
        jnp.square(n_k).reshape(1, 1, -1)
    ).sum(2)  # sum over k
```

```
144 ms ± 1.53 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

You would notice the speed up from Numpy to Numba to JAX, in this order, which is often the case.

Ok, case closed, right?

Hold on, not so fast. Does anyone spot any potential problem with this implementation?

Case closed?

```
import numpy as np


def w_mm_np(
    n_k: np.ndarray[tuple[int], np.float64],
    u_k_vec: np.ndarray[tuple[int, int], np.float64],
    g_m_vec: np.ndarray[tuple[int, int], np.float64],
) -> np.ndarray[tuple[int, int], np.float64]:
    # (M, M, 1, 2)
    δg_mm1_vec =  g_m_vec.reshape(-1, 1, 1, 2) - g_m_vec.reshape(1, -1, 1, 2)
    # (1, 1, K, 2)
    u_11k_vec = u_k_vec.reshape(1, 1, -1, 2)
    return (
        np.cos(
            (2.0 * np.pi) *
            # (M, M, K)
            (
                δg_mm1_vec[:, :, :, 0] * u_11k_vec[:, :, :, 1] +
                δg_mm1_vec[:, :, :, 1] * u_11k_vec[:, :, :, 0]
            )
        ) /
        # (1, 1, K)
        np.square(n_k).reshape(1, 1, -1)
    ).sum(2)  # sum over k
```

Digression in problem sizes

$$\tilde{w}_{ij} = \sum_{k=1}^{K} \frac{1}{n_k^2} \cos\left(2\pi \left[\left(\vec{g}_i - \vec{g}_j\right) \cdot \vec{u}_k\right]\right), \quad 1 \le i,j \le M$$

Number of image pixels $M \sim 70,000 \Rightarrow M^2 \sim 5 \times 10^9, \quad 0 \le i,j < M$
Number of visibilities $K \sim 10^7, \quad 0 \le k < K$

$(M, M, K, 2)$ of 64-bit array would be $\sim$ 700 PiB!

While (M, M) of 64-bit array would be $\sim$ 40 GiB only.

To put that into perspective, whole system aggregated memory of NERSC is $\sim$ 2 PiB.

Numpy—low memory version

- avoid expanding K

The solution is simple, we do not want to expand the K-dimension fully in memory. We want to evaluate that lazily and accumulate it over k.

There is no efficient solution in numpy however without using Python loops.

Numba—low memory version

```
@numba.jit("f8[:, ::1](f8[::1], f8[:, ::1], f8[:, ::1])", nopython=True, nogil=True, parallel=True)
def w_mm_numba_iterative(
```

```
    n_k: np.ndarray[tuple[int], np.float64],
    u_k_vec: np.ndarray[tuple[int, int], np.float64],
    g_m_vec: np.ndarray[tuple[int, int], np.float64],
) -> np.ndarray[tuple[int, int], np.float64]:
    M = g_m_vec.shape[0]
    K = u_k_vec.shape[0]
    δg_mm_vec = g_m_vec.reshape(-1, 1, 2) - g_m_vec.reshape(1, -1, 2)

    w_mm = np.zeros((M, M))
    for k in numba.prange(K):
        w_mm += np.cos((2.0 * np.pi) * (δg_mm_vec[:, :, 1] * u_k_vec[k, 0] + δg_mm_vec[:, :, 0] *
↪   u_k_vec[k, 1])) / np.square(n_k[k])
    return w_mm
```

```
55 ms ± 1.59 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

In Numba, however, we can have efficient loops, we can even do it in parallel. It will handles the reduced sum there in parallel correctly for you. It actually maps very nicely to C with SIMD and OpenMP parallel-for there. In fact, OpenMP is one of the threading layer backend in Numba.

JAX—low memory version

```
@jax.jit
def w_mm_jax_iterative(
    n_k: np.ndarray[tuple[int], np.float64],
    u_k_vec: np.ndarray[tuple[int, int], np.float64],
    g_m_vec: np.ndarray[tuple[int, int], np.float64],
) -> np.ndarray[tuple[int, int], np.float64]:
    M = g_m_vec.shape[0]
    δg_mm_vec = g_m_vec.reshape(M, 1, 2) - g_m_vec.reshape(1, M, 2)
    δg_mm_y = δg_mm_vec[:, :, 0]
    δg_mm_x = δg_mm_vec[:, :, 1]

    def _w_mm_k(
        n: float,
        u_vec: np.ndarray[tuple[int], np.float64],
    ) -> np.ndarray[tuple[int, int], np.float64]:
        return jnp.cos((2.0 * jnp.pi) * (δg_mm_x * u_vec[0] + δg_mm_y * u_vec[1])) / (n * n)

    def _accumulate_w_mm(
        sum_: np.ndarray[tuple[int, int], np.float64],
        args: tuple[float, np.ndarray[tuple[int], np.float64]],
    ) -> tuple[np.ndarray[tuple[int, int], np.float64], None]:
        n, u_vec = args
        return sum_ + _w_mm_k(n, u_vec), None

    res, _ = jax.lax.scan(
        _accumulate_w_mm,
        jnp.zeros((M, M)),
        (
            n_k,
            u_k_vec,
        ),
    )
    return res
```

```
86.6 ms ± 102 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

This means we can does the same in JAX, right? Wrong.

This is where one of the core design of JAX matters. JAX is essentially designed with pure functional programming paradigm in mind. It enforces immutable data, where the in-place reduced sum there is prohibited.

It does not mean it does not have semantics for looping. Here, I choose `scan`. What it does basically is to focus on each term for a dixed k, and then accumulate the sum over different values of k.

See python-autojax/experiments/reduced_sum at main · ickc/python-autojax for more details on how this can be expressed in JAX.

Numba vs. JAX on paper

What is Numba / JAX

- Numba
  - jit compiler powered by LLVM compiler
  - CPU only
    - `numba.cuda` is an entirely different interface
- JAX
  - tracing, jit compiler powered by XLA compiler
  - designed for machine learning workflow
  - no side effects → functional paradiagm
  - targets CPU, GPU (NVidia, AMD, Intel, Apple), TPU simultaneously
  - solving 2 language problem
  - solving "3 implementations problem"
- Better think of them as language + compiler + library

Now that we have seen some examples on how jit works, we will introduce them once more in details.

Numba is a jit compiler supporting a subset of Python and NumPy operations, powered by LLVM. While it is possible to target the GPU via CUDA, it requires rewriting the function using different APIs and paradigms, not to mention it is CUDA (i.e. NVidia) only.

JAX is a jit compiler, tracing compiler by Google, powered by XLA compiler, originated from Google. JAX is designed primarily for machine learning workloads but is suitable for scientific computing as well. It is a tracing compiler removing side-effects of function. I.e. effectively it encourages functional programming paradigm and thinking. It automatically targets multiple hardware architectures including CPU, GPU, TPU, without requiring rewriting. I.e. it solves the "two-language problem", or more accurately, "three-implementation problem": prototype/API, CPU, GPU.

This is where JAX shines over other solutions to develop for the GPU. In principle, one single implementation is all you need. You do not need to optimize a function for the CPU, optimize another for the GPU.

Numba vs. JAX

Table 1: Numba vs. JAX

Numba	JAX
C-like mini language	Smaller language (JAX $\subset$ Numba): restrictions on control flow, mutation, and dynamic shapes
Implements a subset of Python+NumPy, with a parallelization model similar to a mini-"OpenMP"	Implements a subset of Python+NumPy+SciPy exposed via duck-typing.
NumPy implementations are dropped in replacement but only a subset is implemented. Calling NumPy within jitted function is completely hijacked. Documentation is minimal.	`jax.numpy` and `jax.scipy` have similar API comparing to NumPy and SciPy, but has its own documentation. This facilitates deviations in behaviors.
Functions "recompile" whenever input type changes.	Functions "recompile" whenever input type **and shape** changes.
No automatic compiling & offloading to accelerator. No autograd/autodiff.	Going through FFI is more costly: memory transfer from and to device, losing autograd/autodiff.

Characteristics of JAX

- tracing compiler & recompile per shape change ⇒ `static_argnums`

```
@partial(jax.jit, static_argnums=0)
def this_recompile_everytime(shape):
    return jax.numpy.zeros(shape)
```

- Compiler Driven Design

  - Especially in JAX, partly because of its functional paradigm, framing your problem in JAX idiomatic expressions results in great speed up, sometimes more than you could do otherwise in Numba because of its design (recompile per shape, fusion/fusing compatible operations, etc.), but you'll hit a wall if you want more low-level optimizations.
  - It can also means performance improvements can come for free through compiler improvements, as long as your code is written in JAX idiomatic way.
- Easy to port to GPU without setting one up.
- JAX vs numba-cuda: The XLA compiler handles device-specific optimization automatically.
- As a functional language, JAX nudges you to write correct code, and performance comes as a bonus.

When not to JIT in Python?

- Don't wrestle with languages, choose something else
  - AOT: C++ + pybind11
  - JIT: Julia

If you find yourself wrestling against the language, deviating from idioms and best practices, time to choose something else!

Numba vs. JAX: case study of PyAutoLens

Benchmark: Numba vs JAX with 1 CPU core

$$\tilde{w}_{ij} = \sum_{k=1}^{K} \frac{1}{n_k^2} \cos\left(2\pi \left[\left(\vec{g}_i - \vec{g}_j\right) \cdot \vec{u}_k\right]\right), \quad 1 \le i,j \le M$$

Table 2: $N = 64, \quad K = 32768, \quad M \sim N^2 \approx 4000$

Implementation	s	σ
`jax_compact`	2.5543 (1.00)	0.0050
`numba_compact`	2.8768 (1.13)	0.0012
`jax`	3,368.6229 (>1000.0)	1.6803
`numba`	3,702.7006 (>1000.0)	0.7385

We previously have seen different implementations of $\tilde{w}$ and some informal benchmarks.

Here we are seeing the benchmark generated using the actual library I wrote.

The `numba` and `jax` in this table corresponds to the low memory implementation we've shown previously. We see that given 1 single CPU core, the JAX version is slightly faster than the Numba version.

But more importantly, we see that there is a `_compact` version that I have not shown before. This is 3 orders of magnitude faster. This is done by taking advantage of the fact that δg there has a lot of repeatitive values. The algorithm that I shown to you is $O(M^2)$ while the compact version is $O(M)$.

This also illustrates that sometimes you can focus on low level optimization and have 30% speed up. Or you could spend your time instead on the mathematics behind it and find a better algorithm that can achieves unlimited amount of speed up.

Benchmark: Numba with 128 CPU cores and JAX with CUDA on GPU (A100)

Table 3: $N = 32, \quad K = 8192, \quad M \sim N^2 \approx 1000$

Implementation	ms	σ
`numba_compact`	2.5029 (1.0)	0.0520
`jax_compact`	61.5560 (24.59)	6.8555
`jax`	143.2451 (57.23)	0.0749
`numba`	1,794.1949 (716.83)	14.9648

Now how about the million dollar question, how would JAX perform on the GPU? Since the Numba implementation cannot run on the GPU, let us give it a boost to have some resembance of fair fight, 128 CPU cores, vs. JAX on the NVidia A100.

(Notice the slight change of problem size here.)

What we see is the Numba version scales almost perfectly with 128 CPU cores. The JAX implementation is however another order of magnitude faster.

What happens for the `compact` case though? I think it is because they are so efficient so that the problem size is not big enough to "warm up" the GPU. But note that it is not a fair fight anyway, as we can talking about comparing benchmark from different hardware.

Bonus round 1: Numba vs JAX with 1 CPU core (F)

$$F = T^T \tilde{w} T$$

Table 4: $N = 64, \quad B = 3, \quad K = 32768, \quad P = 32, \quad S = 256,$ `curvature_matrix`

Implementation	ms	σ
`numba_sparse`	8.0733 (1.0)	0.0501
`jax`	19.7302 (2.44)	1.6986
`jax_sparse`	25.0091 (3.10)	0.1484
`jax_BCOO`	48.5340 (6.01)	0.1571
`numba_compact_sparse`	49.8400 (6.17)	0.0794
`original_preload_direct`	99.2061 (12.29)	0.3163
`numba`	125.3019 (15.52)	0.1143
`original`	132.4863 (16.41)	0.1376
`numba_compact_sparse_direct`	139.9244 (17.33)	0.1562
`jax_compact_sparse_BCOO`	379.7214 (47.03)	1.4144
`jax_compact_sparse`	380.8865 (47.18)	2.4322

Just to give you one more benchmark to look at, here is another complicated example I have done in the project. You are already familar with $\tilde{w}$, where as T here can be a sparse matrix.

While I am not going into details here, but there is a bunch of combinatorics here. Should we calculate $\tilde{w}$ directly, or go through the `compact` version? Should we use the sparse structure of matrix T, or expand that in memory first?

My claim is that this depends on the size of input data, and which is the fastest to choose from depends on your data which can be informed by benchmark like this.

Bonus round 2: Numba with 128 CPU cores and JAX with CUDA on GPU (A100) (F)

Table 5: $N = 32, \quad B = 300, \quad K = 8192, \quad P = 32, \quad S = 256,$ `curvature_matrix`

Implementation	μs	σ
`jax`	260.5957 (1.0)	29.3714
`jax_BCOO`	3,078.2068 (11.81)	35.9463
`jax_compact_sparse_BCOO`	3,207.3388 (12.31)	107.0798
`numba_sparse`	5,548.5175 (21.29)	64.3711
`jax_compact_sparse`	7,190.9015 (27.59)	35.7355
`numba`	18,187.5003 (69.79)	5,603.6081
`original`	18,279.9851 (70.15)	6,052.1386
`jax_sparse`	19,786.7200 (75.93)	42.9344
`numba_compact_sparse`	32,605.2243 (125.12)	248.8764
`numba_compact_sparse_direct`	1,362,329.9249 (>1000.0)	1,366.9112
`original_preload_direct`	25,218,633.7856 (>1000.0)	8,722.4870

Looking at how JAX runs on the GPU, surprisingly the simplest implementation is fastest. Again I suspect there is not enough data for those faster algorithm to flex its muscle.

Flow chart

If either Numba or JAX have enough feature to acommplish what you need, performance-wise, here's a flowchart:

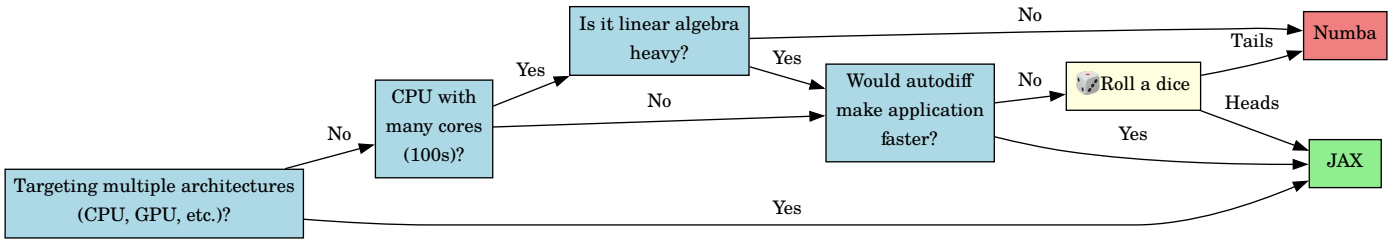


Figure 1: Numba or JAX flowchart

What JIT has enabled in scientific computing?

Context: Maximal Likelihood Estimation (MLE)

- $\tilde{w}, T, F$, etc. are part of a likelihood function
- Aim: seek the input parameters corresponding to maximum likelihood
  - $\Rightarrow$ peak finding
  - Gradient information is going to be useful here.
- JAX another secret weapon: autodiff / autograd (`jax.grad`)
  - compilers can transform code
  - transform function to find its gradient automatically

Now, let's see what JIT has enabled our science.

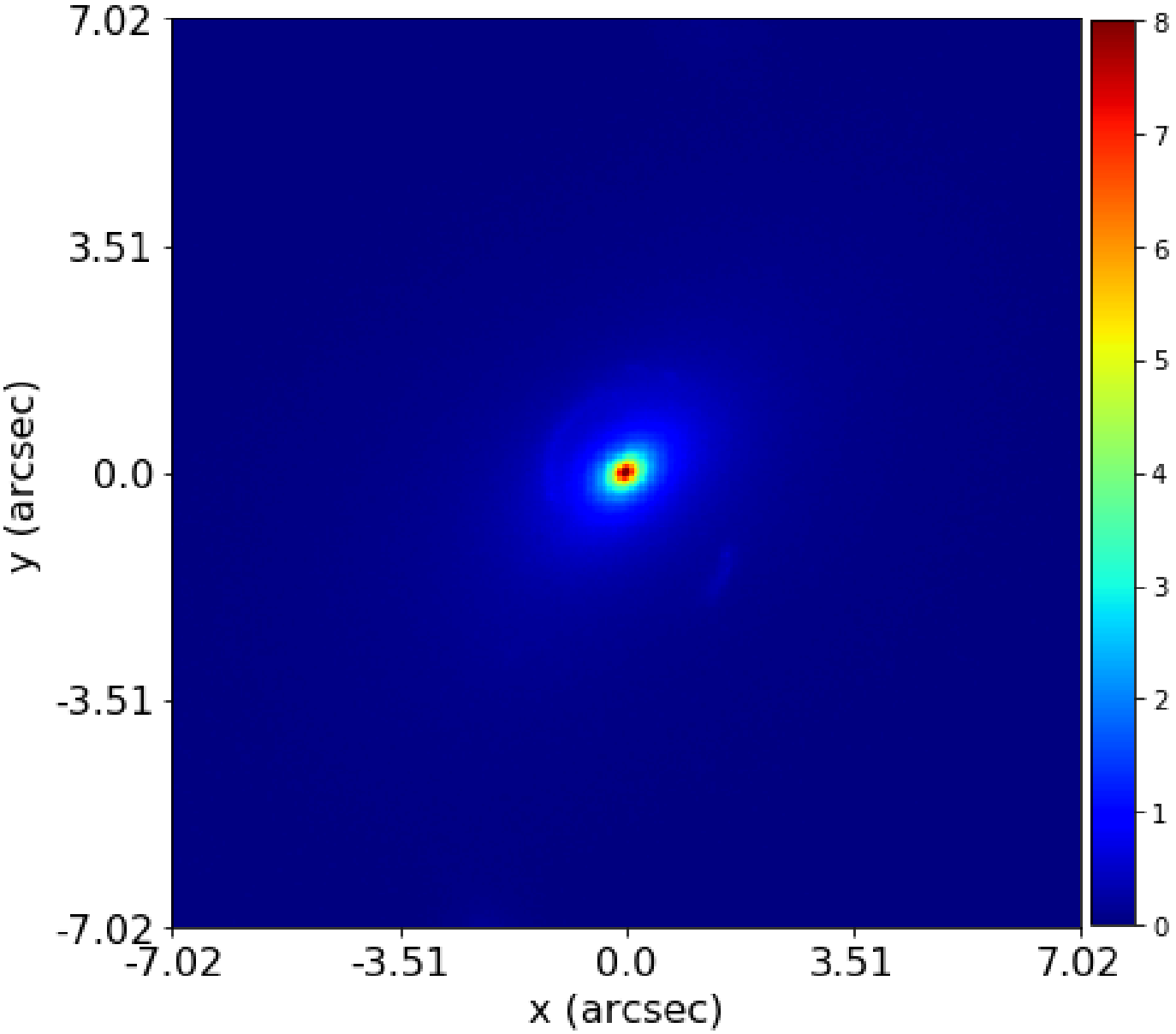
I am not going to give these graphs a justice. But, I am going to have a crash course here and jump to conclusion. The $\tilde{w}, T, F$, etc. you have seen before is part of a calculation known as the likelihood function. The $\tilde{w}$ is a big part of turning the observed data into a likelihood function. Now you can make predictions from models given some parameters. and the likelihood function is going to tell you how likely those parameters are. Using different kinds of samplers, which all involve running the likelihood functions repeatedly, often with $O(100,000)$ of iterations. And the parameters that corresponds to the maximum likelihood is simply called the maximal likelihood estmator (MLE).

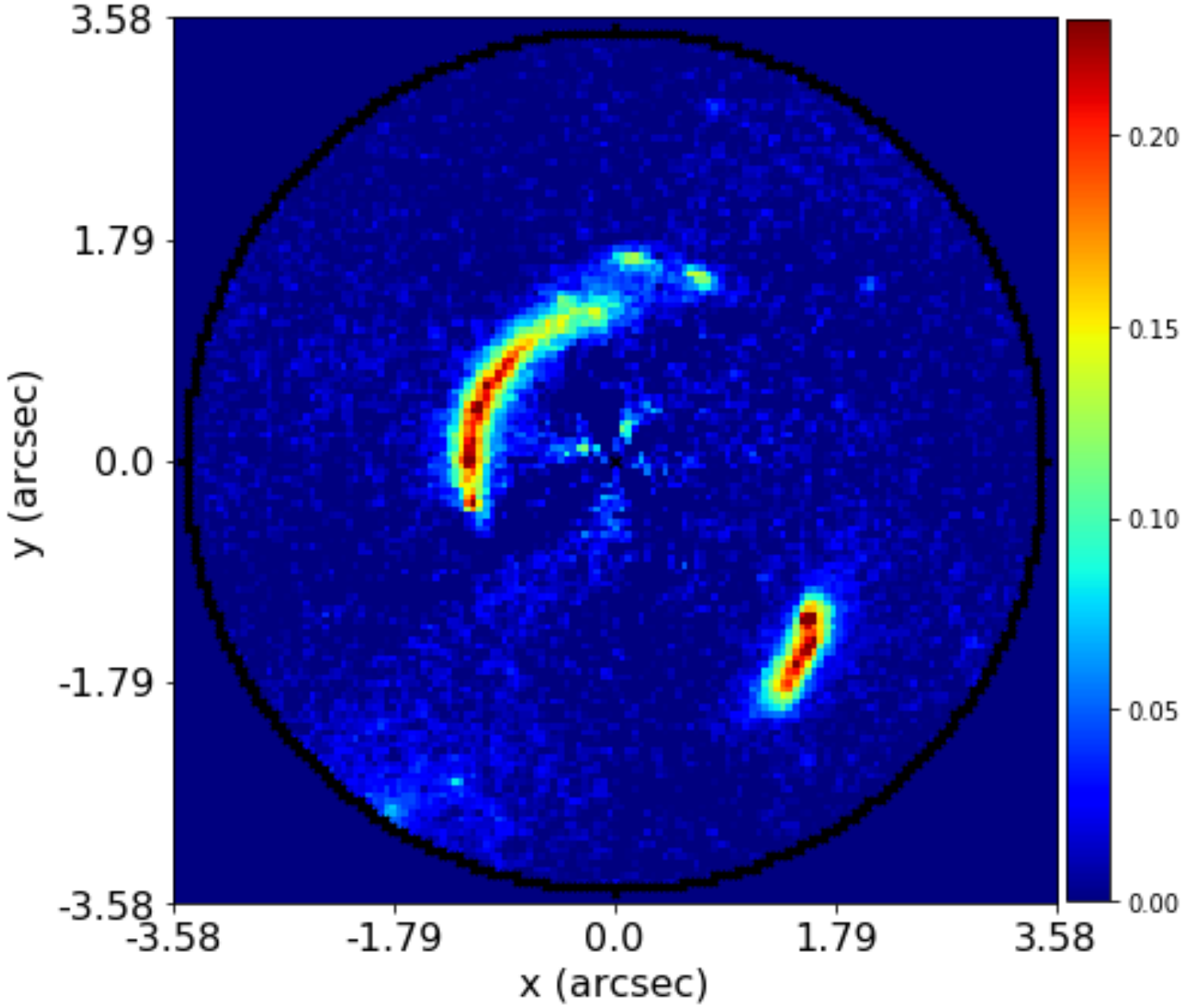
This is basically how we do inverse problem statistically. And obviously it is some kind of maximization problem.

MLE in action

- 25 free parameters
  - Lens Light (11): Sersic + Exponential
  - Lens Mass (7): SIE + Shear
  - Source Light (7): Sersic

PyAutoLens (via PyAutoFit) supports Nested sampling (**Dynesty**), MCMC (emcee), particle swarm optimization (PySwarms)


7.02
3.51
0.0
-3.51
-7.02
y (arcsec)
-7.02
-3.51
0.0
3.51
7.02
x (arcsec)
8
7
6
5
4
3
2
1
0



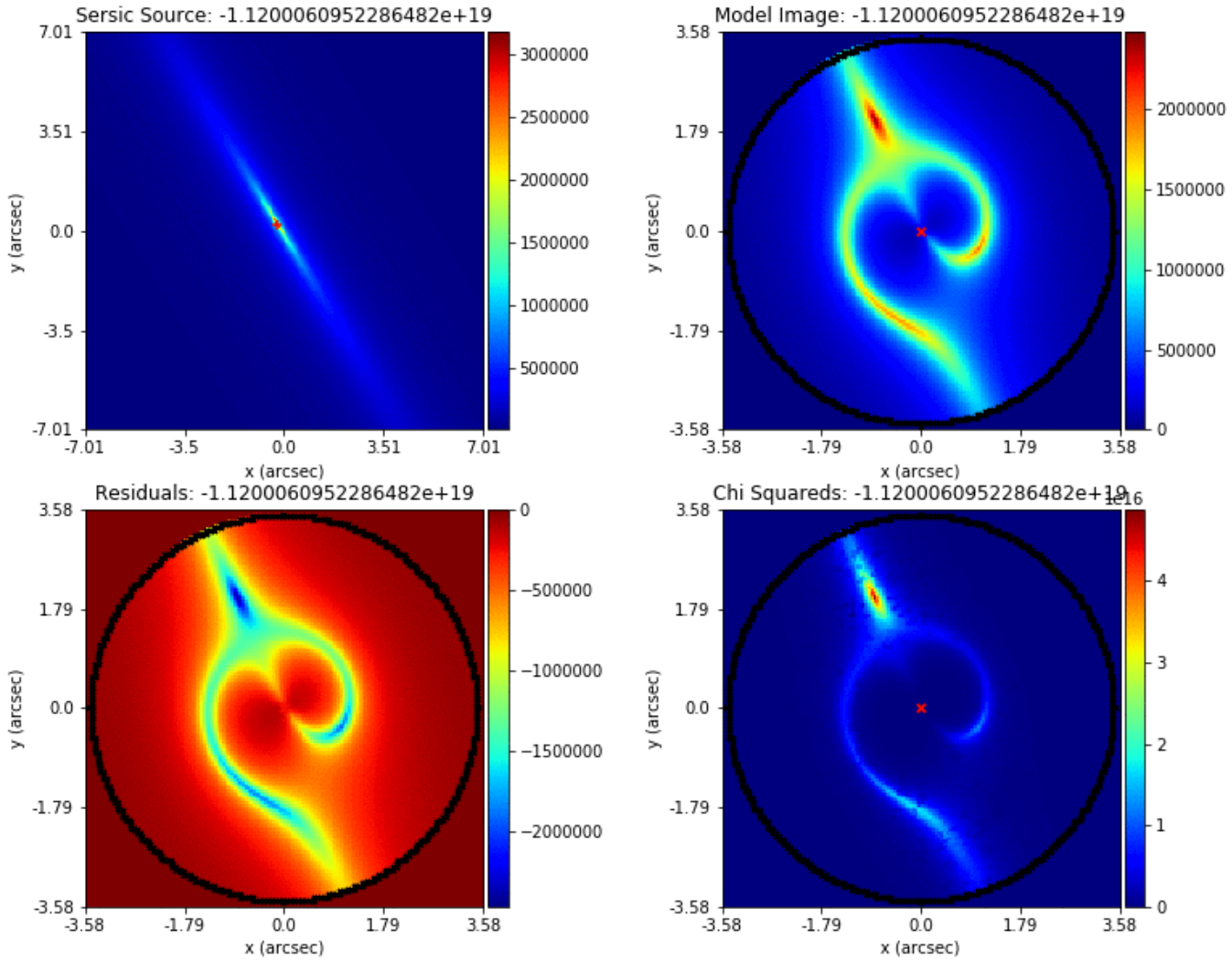
Here, we will see a concrete example of how PyAutoLens does it. Focusing on the image on the right, this is your observed data, and in fact is an image of a strong gravitational lensing.

In the next slide, we are going to see how iterations of different parameters would predict this pattern.

MLE in action

- 25 free parameters
  - Lens Light (11): Sersic + Exponential
  - Lens Mass (7): SIE + Shear
  - Source Light (7): Sersic

PyAutoLens (via PyAutoFit) supports Nested sampling (**Dynesty**), MCMC (emcee), particle swarm optimization (PySwarms)



Eventually, if we compare the image on the top right hand corner, we can see the modeled image pretty much ressemble the data in the previous slide.

Here is how we can infer on the mass of the dark matter we cannot see.

One more thing you can notice here is, while probably I can implement the likelihood function in any language I want, eventually I need to expose it in a Python interface because I need to pass it to these libraries: Nested sampling (**Dynesty**), MCMC (emcee), particle swarm optimization (PySwarms).

This is what I mean when I say the superpowers of Python is it is where the community is, and why which language we implement it does not matter. Python is still our favorite glue. With JIT in Python like Numba and JAX, we can stick to the glue a bit longer.

So, who won?

- In this particular case, who won the battle of JIT?
- JAX! By how much?
- 50x
  - accordingly to preliminary results

Team, Links, & References

- PyAutoLens Team
  - James W. Nightingale
  - Richard G. Hayes
  - Aristeidis Amvrosiadis
  - Coleman Krawczyk
  - Gokmen Kilic
  - …

- Link of this project: https://ickc.github.io/python-autojax/. This is a standalone framework to compare different implementations of functions. Functions are being upstreamed to PyAutoLens.
  - Link to example used today
  - For different ways to do reduced sum efficiently in JAX, see python-autojax/experiments/reduced_sum at main · ickc/python-autojax for more.
  - Scientific Computing with JAX | Durham HPC Days

Lastly, I just want to point you to the team of people working on this and some links to share.