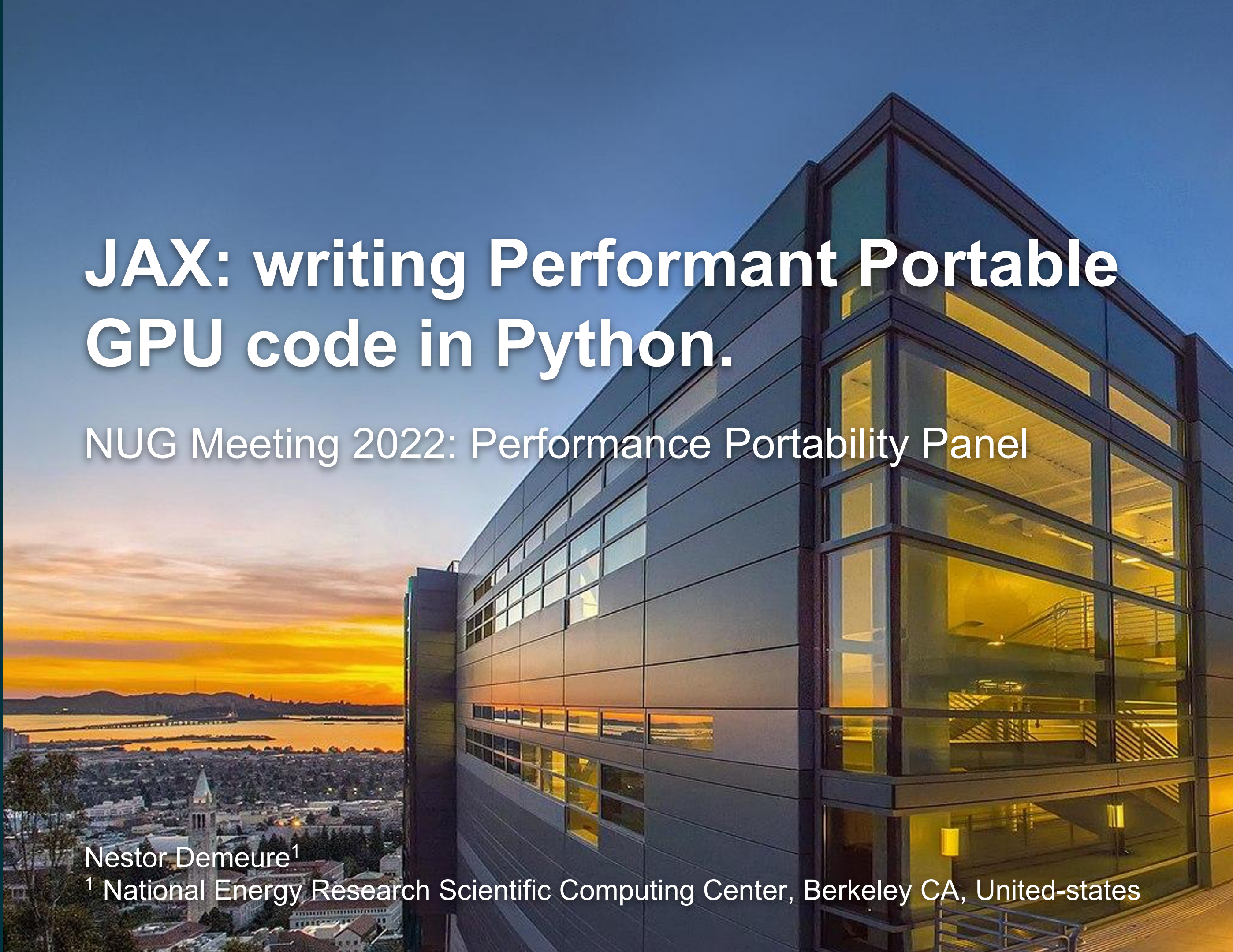

JAX: writing Performant Portable GPU code in Python.

NUG Meeting 2022: Performance Portability Panel

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Who am I?

I am a **NESAP Postdoctoral Researcher at NERSC** with a focus on high performance computing, numerical accuracy and artificial intelligence.

I specialize in helping teams of researchers make use of high performance computing environments.

I am currently working to help port the TOAST software framework to the new Perlmutter supercomputer and, in particular, port it to graphic processors (GPU).

Can we have good GPU performance, portability and *productivity*?

Introducing JAX

High-level introduction to JAX

What is JAX?

JAX is a Python library to write code that can run in parallel on:

- CPU,
- GPU (Nvidia and AMD),
- TPU,
- etc.

Developed by Google as a building block for deep-learning frameworks. Seeing wider use in numerical applications including:

- Molecular dynamics,
- computational fluid dynamics,
- ocean simulation.

What does JAX look like?

It has a Numpy-like interface:

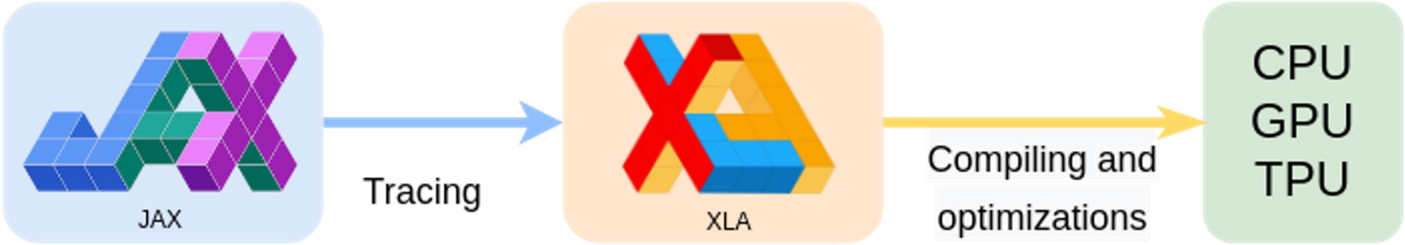
```python
from jax import random
from jax import numpy as jnp

key = random.PRNGKey(0)
x = random.normal(key, shape=(3000, 3000), dtype=jnp.float32)

y = jnp.dot(x, x.T) # runs on GPU if available
```

How does JAX work?

Calls a ***just-in-time compiler*** when you execute your function with a ***new problem size***:



JAX’s limitations

- Compilation happens just-in-time, at runtime,
  easily amortized on a long running computation
- input sizes must be known to the tracer,
  padding, masking and recompiling for various sizes
- loops and tests are limited inside JIT sections,
  JAX provides replacement functions
- no side effects and no in-place modifications,
  one gets used to it, it actually helps with correctness
- focus on GPU optimizations rather than CPU.
  there is growing attention to the problem

Is it worth it?

Case study

Porting the TOAST codebase to GPU

TOAST

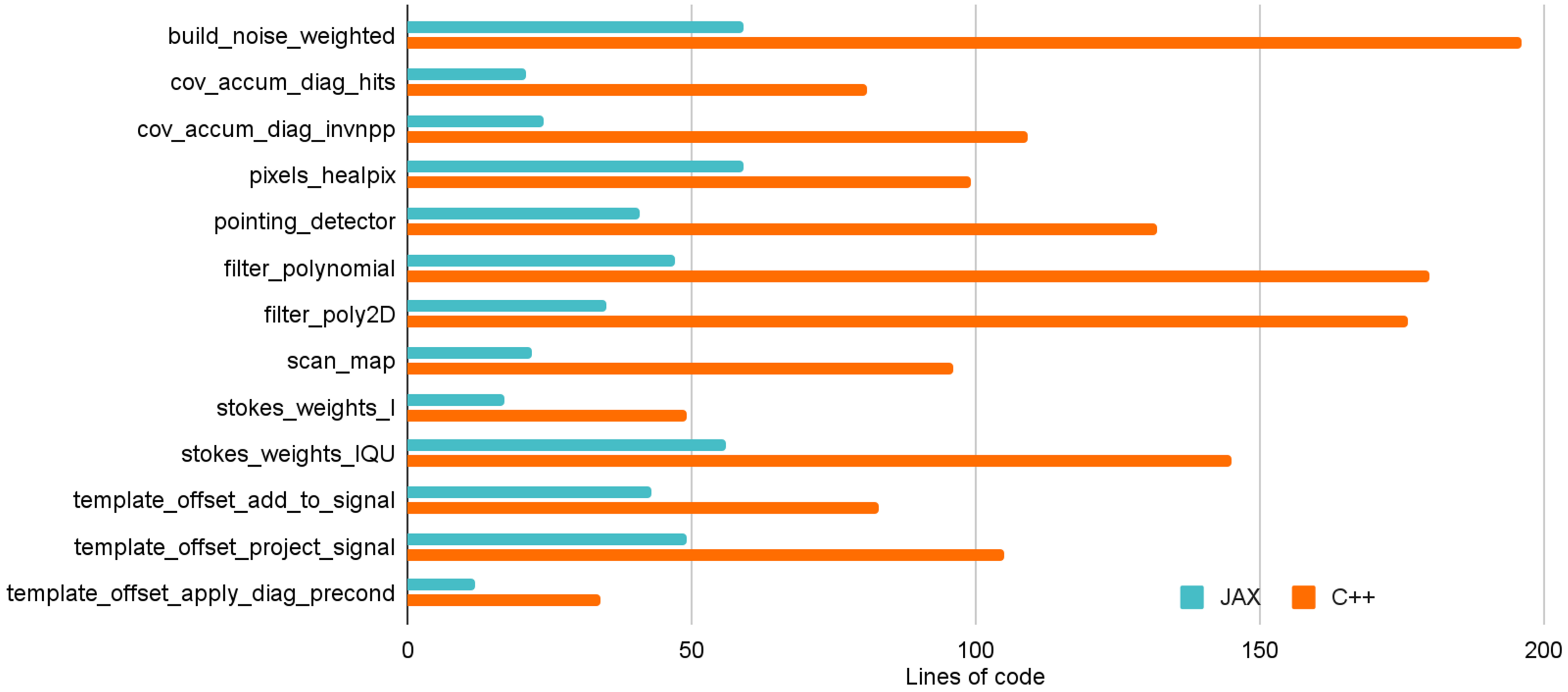
TOAST is a large Python application used to study the **cosmic microwave background**.

It is made of pipelines distributed with MPI and composed of **C++ kernels parallelized with OpenMP**.

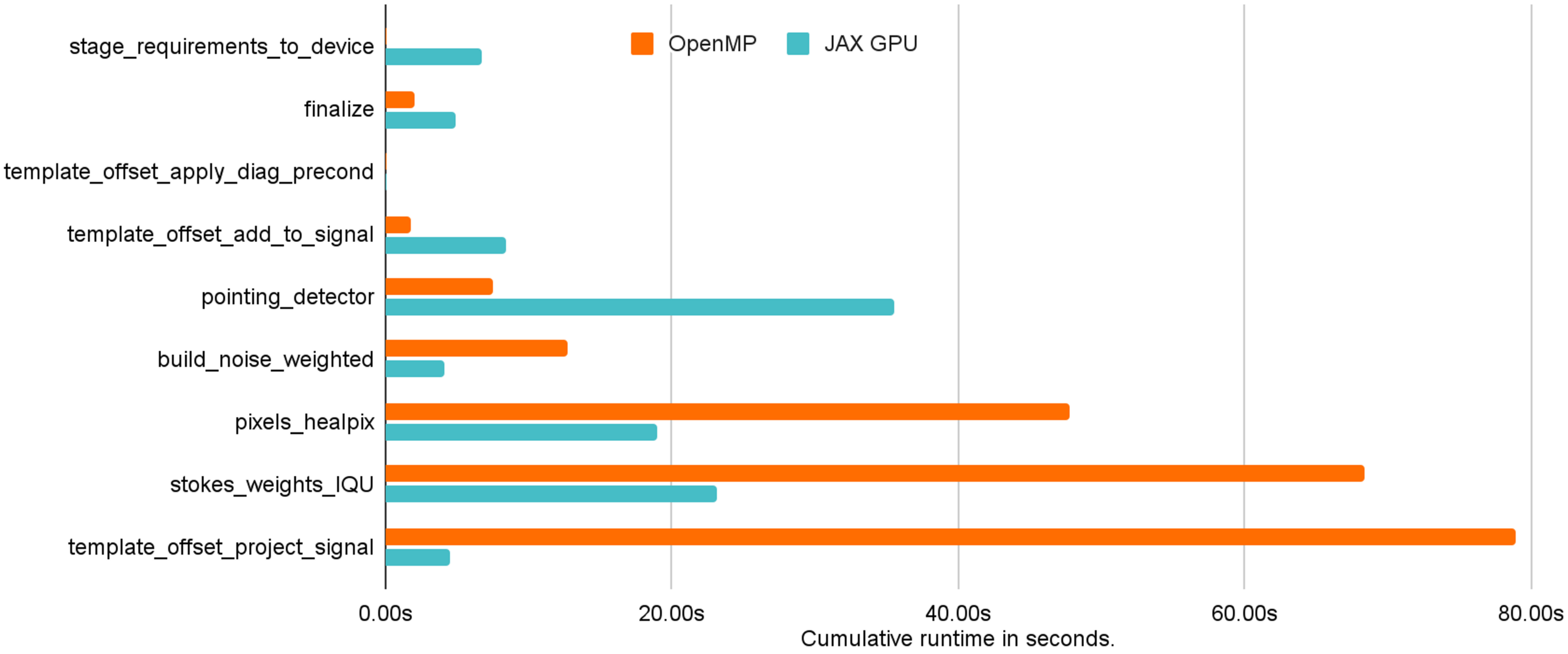
Kernels use a **wide variety of numerical methods** including random number generation, linear algebra and fast fourier transforms.

We ported **one pipeline to GPU**, from **C++ to Numpy to JAX**.

Porting the code (x7 reduction in lines of code)



Performance per kernel (up to x17 speed-up)



Overview

Should you use JAX in your project?

JAX’s strengths

I believe JAX is in a **sweet spot for research and complex numerical codes**:

- Focus on the semantic, leaves optimization to the compiler,
- single code base to deal with CPU and GPUs,
- immutable design is actually *nice* for correctness,
- easy to use numerical building blocks inside kernels.

Should you use JAX?

- Your code is written in **Python**,
- your code can be written with **Numpy**,
- your array sizes are **not too dynamic**,
- single-thread CPU is an **acceptable fallback** in the absence of GPU.

Thank you!

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