# jaxDecomp: JAX Library for 3D Domain Decomposition and Parallel FFTs

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Summary

JAX (Bradbury et al., 2018) has become a popular framework for machine learning and scientific computing, offering high performance, composability, and distributed computing. However, its use as a full HPC framework has been limited by partial native support for key distributed operations. Libraries like MPI4JAX (Häfner & Vicentini, 2021) enable large-scale parallelism but face limitations, notably buffer size constraints and incompatibility with native JAX distribution, making it hard to use with the JAX ecosystem.

The introduction of JAX's unified array API and tools like pjit and custom_partitioning has made SPMD-style programming more accessible. However, many HPC workflows require specialized operations such as optimized distributed Fast Fourier Transforms (FFTs) or halo exchange operations.

To fill this gap, we present jaxDecomp, a fully differentiable JAX library for distributed 3D FFTs and halo exchanges. It wraps NVIDIA's cuDecomp library (Romero et al., 2022), exposing its functionality as JAX primitives while maintaining compatibility with JAX transformations like jit and grad. Beyond basic distributed FFTs, jaxDecomp provides halo exchange operations and automatic optimization of communication backends (NCCL, MPI, NVSHMEM) based on the target hardware. Benchmarks show competitive performance with native JAX while adding HPC-specific features.

Statement of Need

For numerical simulations on HPC systems, a distributed, easy-to-use, and differentiable FFT is essential for achieving peak performance and scalability. While JAX now provides native distributed FFT support, this was introduced only very recently and lacks the specialized HPC features required by many applications. There is a pressing need for a solution that provides not only distributed FFTs but also halo exchanges, optimized communication backends, and seamless integration with existing cluster infrastructure.

In scientific applications such as cosmological particle mesh (PM) simulations, specialized frameworks like FlowPM (Modi et al., 2020) built on mesh-TensorFlow (Shazeer et al., 2018) or JAX-based codes like pmwd (Li et al., 2022) often struggle to scale beyond single-node memory limits or rely on manual distribution strategies. These challenges highlight the need for a scalable, high-performance approach to distributed FFTs that remains differentiable for advanced algorithms (like Hamiltonian Monte Carlo (Brooks et al., 2011) or the No-U-Turn Sampler (NUTS) (Hoffman & Gelman, 2011)).

Implementation

Distributed FFT Algorithm

jaxDecomp performs 3D FFTs by applying 1D FFTs along the Z, Y, and X axes, with global transpositions between steps to ensure each axis is locally accessible. This enables fully local computation while distributing the workload across devices.

The table below summarizes the FFT-transpose sequence:

Steps	Operation Description
FFT along Z	Batched 1D FFT along the Z-axis.
Transpose Z to Y	Transpose to $Z \times X \times Y$. Partition the Y-axis
FFT along Y	Batched 1D FFT along the Y-axis.
Transpose Y to X	Transpose to $Y \times Z \times X$. Partition the X-axis
FFT along X	Batched 1D FFT along the X-axis.

jaxDecomp uses pencil and slab decomposition schemes to distribute 3D data across GPUs. Each FFT step is followed by a transposition that reshapes and rebalances the array to align the next axis for local computation. More technical details, including decomposition strategies and axis layouts, are available in the documentation.

Distributed Halo Exchange

jaxDecomp includes efficient halo exchange operations required in stencil computations and PDE solvers. It supports multiple backends—NCCL, MPI, and NVSHMEM—to adapt to different cluster architectures and communication patterns. Details and visuals of the halo exchange logic are available in the documentation.

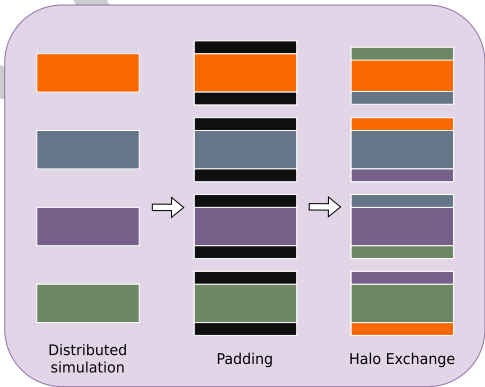**Figure 1:** Visualization of the distributed halo exchange process in jaxDecomp

Benchmarks

Benchmarks were run on the Jean Zay supercomputer using NVIDIA A100 GPUs to evaluate strong and weak scaling of large 3D FFTs across nodes.

We benchmarked both backends in jaxDecomp; cuDecomp was slightly faster than native JAX, especially on large, multi-node workloads.

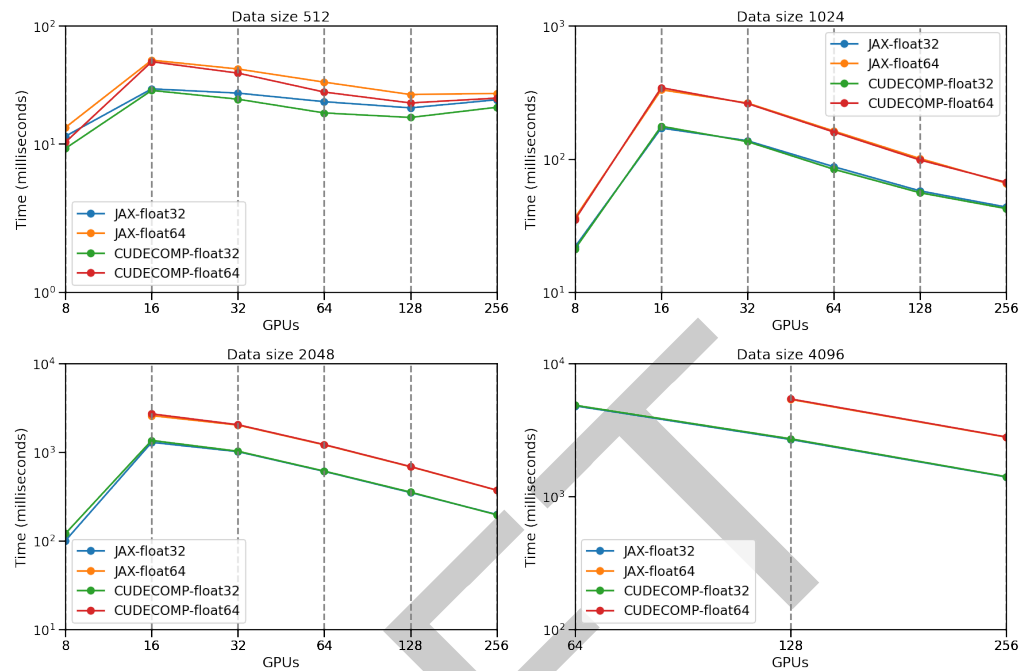**Figure 2:** Strong scaling results on the Jean Zay supercomputer using A100 GPUs.
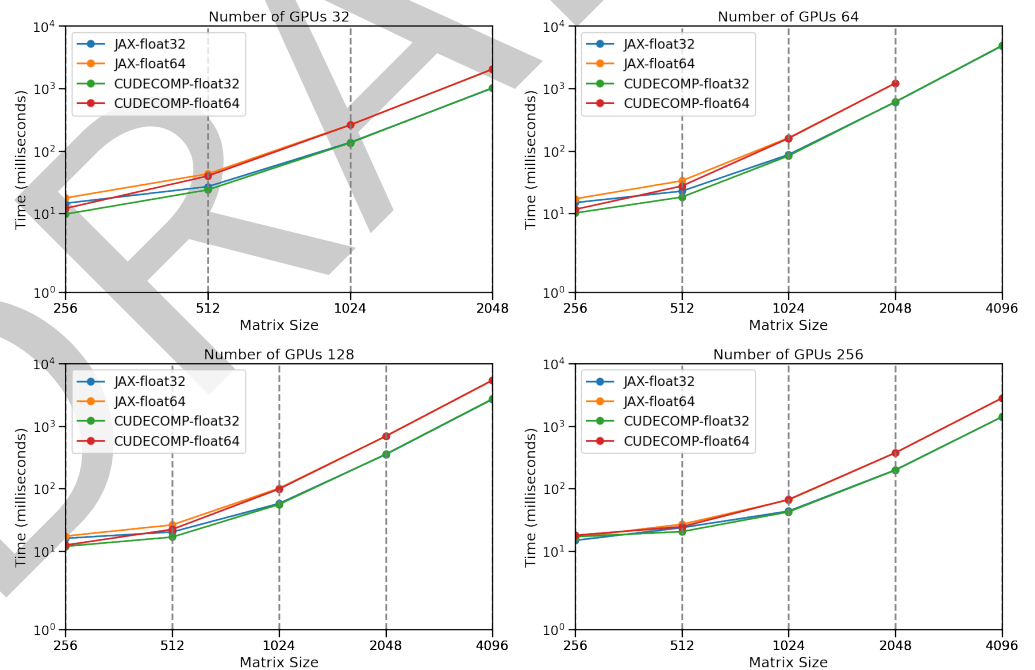

Figure 3: Weak scaling results showing that `jaxDecomp` maintains high efficiency as both problem size and GPU count increase.

Stability and releases

We aim for 100% test coverage across all core functionalities: FFT, halo exchange, and transposition. The code has been tested on the Jean Zay supercomputer, with simulations

63 distributed on 64 GPUs. The package is available on PyPI and can be installed via `pip`
64 `install jaxDecomp`.

Contributing and Community

66 Contributions are welcome. The project follows clear guidelines and uses `yapf` and `pre-commit`
67 for formatting. A full guide is available in the repository's CONTRIBUTING.md. Users and
68 developers are invited to participate by opening issues, submitting pull requests, or joining
69 discussions via GitHub.

Acknowledgements

Appendix

79 Particle-Mesh Example (PM Forces)

80 The following example computes gravitational forces using a Particle-Mesh (PM) scheme in a
81 JAX-based setup, running on multiple GPUs with `jaxDecomp`.while remaining fully differentiable.

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

def pm_forces(density):
    # `density` is a 3D distributed array of shape (Nx, Ny, Nz) is defined over the simu
    delta_k = jaxdecomp.fft.pfft3d(density)
    ky, kz, kx = jaxdecomp.fft.fftfreq3d(delta_k)
    kk = kx**2 + ky**2 + kz**2
    laplace_kernel = jnp.where(kk == 0, 1.0, -1.0 / kk)
    pot_k = delta_k * laplace_kernel
    forces = [-jaxdecomp.fft.pifft3d(1j * k * pot_k) for k in [kx, ky, kz]]
    return jnp.stack(forces, axis=-1)
```

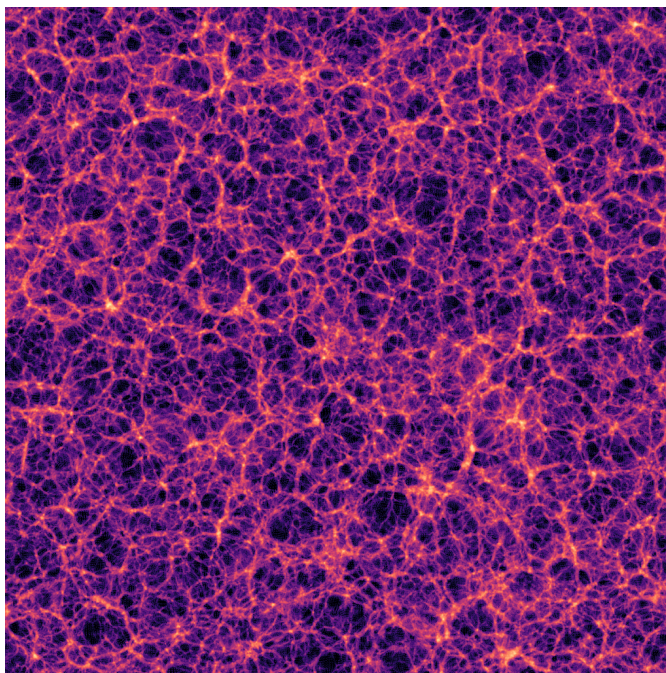82 A more detailed example of an LPT simulation can be found in the jaxdecomp_lpt example.

Figure 4: Visualization of an LPT density field at z=0 for a 2048³ grid generated using `jaxDecomp`.

I refer the reader to the full API description in the jaxDecomp documentation.

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