Parallelism in Numerical Python Libraries

Welcome to the Design Document for CPU parallelism in NumPy, SciPy, scikit-learn, and pandas. Each library has varying levels of support for running parallel computation. This document details the current status of parallelism with shipping code on PyPI and possible paths for improvement.

# Current Landscape

Each library ships with an assortment of parallel interfaces on PyPi:

* NumPy’s linalg module and matrix multiplication utilize OpenBLAS, which is multi-threaded by default. NumPy ships with OpenBLAS built with pthreads.
* SciPy’s linalg module uses OpenBLAS, which is also multi-threaded by default and built with pthreads. SciPy also has a workers parameter that configures multiprocessing, multithreading, or pthreads.
* By default, most computation in Pandas runs in serial. The only parallel mechanism is enabled through Numba by setting passing parallel=True to engine\_kwargs.
* Scikit-learn uses the linalg module from NumPy and SciPy, which is multi-threaded by default. Scikit-learn ships with OpenMP and runs OpenMP accelerated code in parallel by default. The library also has a n\_jobs parameter that uses Python’s multithreading or [loky](https://github.com/joblib/loky), an improved Python-based Process Pool Executor.

On PyPi, if a library requires OpenMP or OpenBLAS, it bundles the shared library into the wheel:

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| Current PyPI landscape: [image source](https://www.slideshare.net/RalfGommers/parallelism-in-a-numpybased-program) |

# Issues with the Current Landscape

The current landscape has three broad categories of issues:

* APIs for controlling parallelism are not consistent between libraries.
* By default, BLAS and scikit-learn’s OpenMP are multi-threaded and can lead to unexpected problems.
* Interactions between different forms of parallelism may lead to slowdowns, crashes, or oversubscription.

## APIs for Configuring Parallelism

There are three ways to configure parallelism across the libraries: environment variables, [threadpoolctl](https://github.com/joblib/threadpoolctl), or library-specific Python API.

Examples of environment variables consist of:

* OPENBLAS\_NUM\_THREADS for OpenBLAS
* MKL\_NUM\_THREADS for MKL
* OMP\_NUM\_THREADS for OpenMP

These environment variables control how many threads a specific backend uses. These environment variables do not influence code that does not use a particular backend, like OpenMP. For example, SciPy’s fft module uses pthreads directly.

Threadpoolctl provides a Python interface for configuring the number of threads in OpenBLAS, MKL, and OpenMP. Linear algebra function calls from NumPy, SciPy, or scikit-learn can all be configured with threadpoolctl or an environment variable. These configuration options also control Scikit-learn’s OpenMP routines.

SciPy and scikit-learn have a library-specific Python API for controlling parallelism. SciPy’s workers can mean multithreading, multiprocessing, or pthreads. Scikit-learn’s n\_jobs is either multiprocessing or multithreading. Note that scikit-learn’s n\_jobs does not configure OpenMP or OpenBLAS parallelism.

### Proposal

Here is a two step proposal:

1. Document the functions or methods using OpenMP or BLAS and can be configured with an environment variable or threadpoolctl.
2. Adopt a consistent Python API for configuring parallelism. We use SciPy’s workers parameter because it is more consistent in controlling the number of cores used. workers denotes any form of parallelism such as: multi-threading, multiprocessing, OpenMP threads, or pthreads. Please see the [FAQ section](#X0a3467814b156e62b007955c9d0b302ea344c46) for more information.

## Multi-threaded by Default

BLAS implementations such as OpenBLAS are multi-threaded by default. Scikit-learn followed this convention with OpenMP, which is also multi-threaded by default. Using all the CPU cores by default is convenient for interactive use cases like in a Jupyter Notebook. The downside of using all CPU cores is during deployment to shared environments. The user needs to know which API to configure their program to become serial from the above section.

There can be oversubscription when multiprocessing or multi-thraeding is used together with OpenBLAS or OpenMP. Distributed Python libraries such as [Dask](https://docs.dask.org/en/stable/array-best-practices.html#avoid-oversubscribing-threads) and [Ray](https://docs.ray.io/en/latest/serve/scaling-and-resource-allocation.html#configuring-parallelism-with-omp-num-threads) recommend setting environment variables to configure OpenBLAS and OpenMP to run serially.

### Proposal

Here are some possible paths we can take:

1. Keep the status quo where BLAS is multi-threaded by default. SciPy’s linalg module or scikit-learn’s OpenMP accelerated routines will continue to be parallel as the default.
2. Libraries all have a serial fallback and we only ship the serial form on PyPi. We encourage OpenMP anywhere the whole stack is built in in a consistent fashion.
3. Migrate from multi-threaded to single-thread as the default. Each library has the option to include a global flag that configures all computations to be parallel.

Options 2 and 3 helps with oversubscription because the library is serial by default.

## Interactions Between Different Forms of Parallelism

When different parallelism interfaces are running concurrently, it is possible to run into crashes or oversubscription. The following is a list of known issues:

* libgomp (OpenMP for GCC) is not fork-safe while libomp (OpenMP for Clang) is fork-safe. Scikit-learn’s community developed [loky](https://github.com/joblib/loky) as a workaround. There is a [patch to GCC OpenMP](https://gcc.gnu.org/bugzilla/show_bug.cgi?id=60035) to make it fork safe, but it has not progressed. For details, see [scikit-learn’s FAQ entry](https://scikit-learn.org/stable/faq.html#why-do-i-sometime-get-a-crash-freeze-with-n-jobs-1-under-osx-or-linux).
* libomp (OpenMP for Clang) not compatible with libiomp (OpenMP for Intel Complier). The workaround is to set MKL\_THREADING\_LAYER=GNU. See [this link for details](https://github.com/joblib/threadpoolctl/blob/master/multiple_openmp.md).
* libgomp (OpenMP for GCC) is also not compatible with libiomp (OpenMP for Intel Complier): [pytorch#37377](https://github.com/pytorch/pytorch/issues/37377)
* There are performance issues when OpenBLAS (built with pthreads) and OpenMP have separate thread pools: [OpenBLAS#3187](https://github.com/xianyi/OpenBLAS/issues/3187). A workaround is to share the same thread pool by building OpenBLAS with OpenMP.
* There are performance issues when two OpenBLAS are present, such as in NumPy and SciPy: [scipy#15129](https://github.com/scipy/scipy/issues/15129). The current workaround is to set OPENBLAS\_THREAD\_TIMEOUT=1 on the affected platforms.

### Proposal

The following are feasible steps we can take to improve the issues listed above:

1. The library sends a warning or error to notify the user when a known issue is detected. For example, [Numba detects](https://github.com/numba/numba/blob/2e9b58cfce0391b968ab8c7c84393cc12c4d1bfb/numba/np/ufunc/omppool.cpp#L107-L124) when libgomp and fork are used together, raising an error.
2. The library detects and raises a warning recommending MKL\_THREADING\_LAYER when LLVM OpenMP and Intel OpenMP are loaded together. For example, threadpoolctl [has such a warning](https://github.com/joblib/threadpoolctl/blob/a39c6a49a297d0ef941269fc655670b63edab84c/threadpoolctl.py#L750-L762).
3. Move towards a single OpenMP and OpenBLAS on PyPI by shipping an OpenMP and OpenBLAS wheel. NumPy, SciPy, and Scikit-learn will link to those libraries during runtime. Please see the [FAQ section](#how-to-ship-openmp-and-openblas-on-pypi) for more information.

# FAQ

## How to ship OpenMP and OpenBLAS on PyPI?

OpenMP and OpenBLAS are shipped with their header files. When building an upstream library such as NumPy, extensions will use RPATH to link to the OpenMP and OpenBLAS wheels. auditwheel repair needs a patch so that it does not copy PyPi libraries into the wheel: [auditwheel#392](https://github.com/pypa/auditwheel/pull/392). Note that [PEP513](https://peps.python.org/pep-0513/#auditwheel) explicitly allows for shared libraries to be distributed as separate packages on PyPI.

## Which compiler to use for OpenMP?

There are two options: libgomp (OpenMP for GCC) or libomp (Clang for GCC).

* libgomp is not fork safe, but uses the GCC and shipped with all Linux distros. We advocate for the [patch in GCC](https://gcc.gnu.org/bugzilla/show_bug.cgi?id=60035) to make it fork safe.
* libomp is fork safe, but it is an implementation detail and not part of the OpenMP specification.

On PyPI, I propose we go with libomp, because it has the same symbols as libgomp and is fork safe. Upstream libraries such as NumPy or SciPy can still use GCC as their compiler. Package managers can still ship libraries linked with libgomp. SciPy has an existing discussion regarding OpenMP adoption and the compiler choice: [scipy#10239](https://github.com/scipy/scipy/issues/10239).

## With a OpenMP wheel, can workers configure and use another threading API like pthreads?

Yes, this design documentation does **not** restrict the usage of other API for parallelism. The only requirement is to link the library to the OpenMP wheel if it uses OpenMP. This way, all libraries can share the same OpenMP thread pool.

## Can the multiprocessing and multithreading modules still be used?

Yes, this design documentation does **not** restrict the usage of other APIs for parallelism. If Python’s multithreading or multiprocessing fits your library’s use case, you are welcome to use them.

## What to do with nested parallel calls?

Libraries will do their best to account for over-subscription from nested parallelism. For example, if multiple OpenMP threads call a BLAS routine, then the BLAS routine is configured to run serially. On the other hand, a library can have an API to perform multiprocessing on a user-defined function. If the user-defined function is also parallelized, then there is nested parallelism. The best a library can do is to document how its parallelism interacts with user-defined functions.

## How does conda-forge work?

For BLAS, conda-forge builds with netlib. During installation time, BLAS can be switched to other implementations such as MKL, BLIS, OpenBLAS. See [this link for details](https://conda-forge.org/docs/maintainer/knowledge_base.html#switching-blas-implementation).

For OpenMP, conda-forge builds with libgomp, the GNU build of OpenMP. During installation time, OpenMP can be switched to libomp, the LLVM build of OpenMP. Recall that the LLVM implementation is fork-safe. Note, that the GNU implementation has target offloading symbols, while LLVM does not. See this [link for details](https://conda-forge.org/docs/maintainer/knowledge_base.html#openmp).

Conda-forge has a mutex package ensuring that a single OpenMP or BLAS library is installed and loaded.