From built-in concurrency primitives to large scale distributed computing

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Content

1. Introduction to concurrency and parallelism
2. Python's built-in concurrency primitives
3. Scaling out: Distributed computing with Dask and Ray

1. Introduction to concurrency and parallelism

Concurrency lets you wait efficiently

- Concurrency enables you doing other things while waiting for results or other resources.
  - For example, you can wait for multiple calculations or API responds.
  - It’s like a superpower of **waiting** in multiple queues at once.
- You do not need to care how the work to clear a queue is done.

(Foto: Archiv Ladislava Růžičky)

- Would be great for (Czech socialist) queues
  - Sometimes people even did not know what they were waiting for.
  - Wait in multiple queues at once would help.

Concurrency lets you organise work efficiently

- You can respond to (accept) multiple requests even if there are still tasks to be done.
  - Requests can come, for example, from a queue or an API.
- You can dispatch queue requests to multiple workers.
  - … or just switch between tasks efficiently.
  - … although context switching is not free.

Parallelism lets you *execute* multiple things at once

- Parallelism is about executing multiple things simultaneously.
- Concurrency does not imply parallelism.
  - Although parallelism is typically desired in concurrent systems.
- Examples of parallel calculation:
  - GPU’s or vectorized CPU operations (SIMD - single instruction multiple data).
  - Multi-core machines with shared memory (MIMD - multiple instructions multiple data).
  - Distributed systems: clusters, clouds (MIMD).

Where do you need concurrency and parallellism?

- Web servers
- High-performance computing (HPC)
- Data engineering
- Machine learning
- … and many more

Data processing cares about both concurrency and parallelism

- In data processing, we often care about both concurrency and parallelism.
  - We need processes to be responsive → concurrency.
  - We need to execute processing tasks fast and efficiently → parallelism.

2. Python’s built-in concurrency primitives

Python defines built-in concurrency primitives

- `concurrent.futures`
  - > … provides a high-level interface for asynchronously executing callables.
  - Proposed in 2009: PEP-3148
  - We will focus on using and building on these primitives.
- Other standard lib modules for concurrent execution include:
  - `threading` and `multiprocessing`: parallelism, synchronisation primitives.
  - `subprocess`: subprocess management.
  - `asyncio`: cooperative multitasking.
  - `contextvars`: context-local state.

`from concurrent.futures import Executor`

> Executor is an abstract class that provides methods to execute calls asynchronously.

- This is indeed abstract 😅
- What does one need in particular?
  1. Create an executor: Choose type and parameters.
  2. Submit tasks to the executor.
  3. Collect results.
  4. Shutdown the executor.

1. Create an executor

```
from concurrent.futures import ThreadPoolExecutor, ProcessPoolExecutor

MAX_WORKERS = 4

thread_executor = ThreadPoolExecutor(max_workers=MAX_WORKERS)
process_executor = ProcessPoolExecutor(max_workers=MAX_WORKERS)
```

2. Submit tasks to the executor

```python
def do_some_math(x: float) -> float:
    return x * x
```

1. Single calculation via `submit`:

```python
result = thread_executor.submit(do_some_math, 5)
```

2. Multiple calculations via `map`:

```python
results = thread_executor.map(do_some_math, range(10))
```

3a. Collect result: single `Future`

- The output of `submit` is a `concurrent.futures.Future` object:

```
print(result)
```

```
<Future at 0x122921490 state=finished returned int>
```

- `Future` is a placeholder for the result of a computation that may not be completed yet.
- `Future` encapsulates the asynchronous execution.
- Most important `Future` methods are:
  - `result(timeout=None)`: Waits for the computation to complete and returns the result.
  - `done()`: Returns `True` if the call was successfully cancelled or finished running.
  - `cancel()`: Attempts to cancel the computation.

3b. Collect multiple results

- The output of `map` is a generator object:

```
print(results)
```

```
<generator object Executor.map.<locals>.result_iterator at 0x122a1f4d0>
```

- This generator yields results as they become available, *in the order* they were submitted.
- One would typically iterate over the generator:

```
for result in results:
    ...
```

- or collect all results into a list:

```
completed_results = list(results)
```

- Slow tasks may block the iteration (although do not block the execution in the workers).

3c. Collect multiple results with `as_completed`

- We can submit multiple tasks without using executor's `map` method.
  - This will yield multiple `Future` objects.

```
futures = [executor.submit(do_some_math, x) for x in range(10)]
```

or using built-in `map`:

```
futures = map(functools.partial(executor.submit, do_some_math), range(10))
```

- `as_completed` iterates over a collection of futures as they complete:
  - Can specify waiting timeout.

```
from concurrent.futures import as_completed

for future in as_completed(futures):
    print(future.result())
```

3d. Collect multiple results with `wait`

- `wait` gives us more flexibility and control over the futures while waiting.
  - We can use waiting timeout.
  - Can wait for first completed, all completed, or first exception.
  - We can, e.g., cancel futures that have not started running.

```
done, not_done = wait(futures, timeout=1, return_when=FIRST_COMPLETED)
```

- `done` and `not_done` are sets of futures.

4. Shutdown the executor

- Executors should be shutdown to release resources.
    - This may be done automatically when the executor is garbage collected.
    - The type and released resources depend on the executor type.

```
executor.shutdown(wait=True, cancel_futures=False)
```

- `wait=True` blocks until all futures are completed and resources are freed.
- `cancel_futures=False` cancels pending futures tha have not started running.
- Lifetime can also be managed by a `with` block:

```
with ThreadPoolExecutor(max_workers=4) as executor:
    result = executor.submit(do_some_math, 5)
```

Gotcha example: A non-obvious random numbers stale state

```
list(process_executor.map(np.random.randint, 8*[100]))
```

```
[51, 51, 51, 51, 51, 51, 51, 51]
```

- Surprisingly, random generator state is shared and not mutated.
- 💡 `randint` is not a (pure) function, it's a `RandomState` instance's method.

`ThreadPoolExecutor` limitation: Global Interpreter Lock (GIL)

- Global Interpreter Lock (GIL) is probably the most (in)famous limitation of CPython.
- GIL prevents multiple threads from executing Python code simultaneously (in parallel).
- However, GIL can be released by:
  - I/O operations (file operations, network requests).
  - C extensions (NumPy, Pandas, TensorFlow).
- … thus enabling threads to run in parallel.

`ProcessPoolExecutor` limitation: Serialization

- Submitted tasks, i.e callables and data, are sent as pickles to the worker processes.
- Not all objects can be pickled.
  - E.g., lambda or nested functions.

```
process_executor.submit(lambda x: x * x, 5).result()
```

```
PicklingError: Can't pickle <function <lambda> ...
```

Resolving serialization issues

- Libraries like `cloudpickle` or `dill` resolve a lot of these limitations.
- Meet our first non-builtin executor: `joblib/loky`
    - > The aim of this project is to provide a robust, cross-platform and cross-version implementation of the `ProcessPoolExecutor` class of `concurrent.futures` .
    - Consistent and robust spawn behaviour
    - Reusable executor
    - Transparent cloudpickle integration

```
# Create an executor with 4 worker processes, that will
# automatically shutdown after idling for 2s
executor = loky.get_reusable_executor(max_workers=4, timeout=2)
```

- tldr; `loky` is a straightforward replacement for `ProcessPoolExecutor`.

`concurrent.futures` within `asyncio`

- `asyncio` cooperative multitasking enables concurrent code using the `async` / `await` syntax.
  - An internal event loop manages the execution of coroutines.
- `asyncio.Future` is similar to `concurrent.futures.Future`.
  - and can be created from `concurrent.futures.Future`:

```
concurrent_future = executor.submit(do_some_math, 5)
asyncio_future = asyncio.wrap_future(concurrent_future)
await asyncio_future
```

  - … or via `loop.run_in_executor`:

```
loop = asyncio.get_event_loop()
asyncio_future = loop.run_in_executor(executor, do_some_math, 5)
```

- This basically *removes the usual limitation of `asyncio` not supporting CPU-bound tasks.*

Practical data processing usecases with `concurrent.futures` examples

- Quick parallel batch processing, e.g.:
  - Run Pandas pipeline on multiple files.
  - Grid search hyperparameters.
- Non-blocking data processing in a web server or a streaming processor.
  - Even a single-worker executor can enable non-blocking processing.
  - Especially useful for `asyncio` applications.
- Must be careful with resource utilisation, in particular RAM.

3. Scaling out: Distributed computing with Dask and Ray

Scaling out: Distributed computing

- At some point, your calculation may not fit into a single machine.
    - Need to process huge datasets.
    - The calculation is too heavy.
    - We need too many repetitions, e.g. in a grid search.
- Sometimes, reasons for distributed computing are not resource-related.
    - Security or compliance can constrain local or ad-hoc processing.
    - You simply need to turn off your computer.

Resource drivers for scaling out: RAM and CPU

- Two main resource-type drivers exist for scaling out:
- Memory: "My data do not fit into my (computer’s) memory."
  - Symptoms: OOM (Out Of Memory) kills, swapping leading to system freeze.
- Processing power: "My calculation takes too long."
  - Symptoms: CPU, GPU, other PU’s at 100%, calculation time too long.

Checklist before scaling out

- Before spinning up a cluster (and spending 💰 💰 💰), there are possibilities:
- Profile and possibly optimise your code.
  - Remember the 80:20 Pareto rule.
  - Save either RAM or CPU.
- Data can (sometimes) be memory-mapped.
- Large data can be processed in chunks.
  - This is where executors can help.
- Frameworks like Dask or Ray can help even when running on a single machine.

Scaling out with Dask (Distributed)

- `Dask` may be better known for its `DataFrame` pandas-like API. However,

> `Dask` is a Python library for parallel and distributed computing.
>
> - Easy to use and set up (it's just a Python library)
> - Powerful at providing scale, and unlocking complex algorithms
> - and Fun 🎉

https://docs.dask.org

- I.e., Dask is a *generic* parallel computing framework.
    - We can submit tasks to a Dask cluster using `concurrent.futures`-like API.
    - Dask can operate and scale efficiently from a single machine to a (big) cluster.

`Dask` Futures API is like `concurrent.futures`

- `Dask` supports a `concurrent.futures`-like interface in its Futures API.
- This is the foundation for other APIs like Dask arrays and dataframes.

```
from dask.distributed import Client, as_completed, wait
dask_client = Client()
```

- `dask.Client` API is similar to `concurrent.futures.Executor`.

```
dask_future = dask_client.submit(do_some_math, 10)
```

- There are substantial differences, e.g. `map` yields a list of futures, not a generator.
  - Hence, `as_completed` or `wait` should be used to iterate over futures as they complete.
  - This is probably more useful than `concurrent.futures`'s `map`.

Dask provides `concurrent.futures` compatibility

- `distributed.client.Future` is *not* compatible with `concurrent.futures.Future`.
    - This will raise an exception:

    ```
    concurrent.futures.wait([dask_future])
    ```

- A fully compatible `concurrent.futures` executor can be obtained from `Dask`:

```
executor = dask_client.get_executor()
```

- Need to decide whether to work with `Dask`,
    - and profit from its specific features,
- or with `concurrent.futures` and `Dask` as a backend,
    - and profit from the `concurrent.futures` full compatibility, e.g. within `asyncio`.

Scaling out with Ray

Ray Overview

- Ray is an open-source unified framework for scaling AI and Python applications like machine learning.
- It provides the compute layer for parallel processing so that you don't need to be a distributed systems expert.
- Ray minimizes the complexity of running your distributed individual and end-to-end machine learning workflows ...

- Ray focuses on machine learning and AI workloads.
- Ray Core provides core primitives for distributed computing, similarly to Dask Future API.

```python
import ray
ray.init()

@ray.remote
def f(x):
    return x * x

references = [f.remote(i) for i in range(4)]
results = ray.get(references)
```

Ray `concurrent.futures` interface

- Ray `ObjectRef`'s can return `concurrent.futures.Future` object:

```
ref = ray.remote(do_some_math).remote(5)
future = ref.future()
```

- A pull request is open to add `RayExecutor` as a drop-in replacement for `concurrent.futures.Executor`.

Both Ray and Dask integrate well with `asyncio`

- Very conveniently, Ray's `ObjectRef` can be directly `await` ed:

```
reference = ray.remote(do_some_math).remote(5)
result = await reference
```

- Alternatively, `wrap_future` or `ensure_future` can be used:

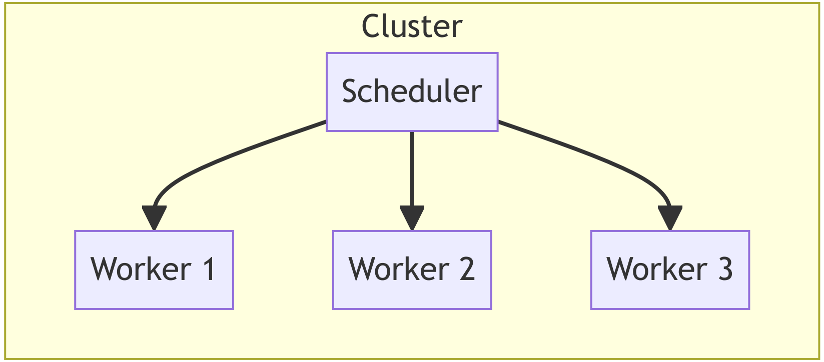
```
async_task = asyncio.ensure_future(ref)
async_future = asyncio.wrap_future(ref.future())
```

- Dask can operate in `asyncio` mode by using the `asynchronous=True` parameter.

```
client = await Client(asynchronous=True)
future = client.submit(do_some_math, 5)
result = await future
```

Dask and Ray Cluster architecture

- Dask and Rays clusters basically consists of
  - scheduler
  - workers
- Dashboard is available for observability.
- Deployment options scales from local use to large scale infrastructures like
  - Kubernetes (using operators)
  - Cloud, including managed SaaS solutions
  - High Performance Computing job queues (PBS, Slurm, …)



Dask and Ray manage distributed data

- With `concurrent.futures`, data is pickled and sent to workers.
  - This means data has to pass from / to the orchestrator.
  - … unless you use a distributed storage explicitly.
- Ray uses a shared-memory object store called Plasma.
- Dask primarily stores data in memory and schedules tasks close to data.
  - Dask can also use distributed storage like HDFS, S3, or GCS.
- Both Ray and Dask can explicitly send and persist data on workers.
  - `scatter` or `persist` in Dask `Client`.
  - `put` in Ray.
- *References to data can be used as arguments to tasks*.

Example with Ray put

1. Persist some data on workers:

```
data_ref = ray.put(np.random.sample((1000, 1000)))
```

2. Use the reference in a task:

```
@ray.remote
def process_data(data):
    return np.linalg.norm(data)

result_ref = process_data.remote(data_ref)
```

- No communication happens in step 2.
- The task is likely scheduled on a worker with the data.

Task dependencies - call graphs

- Imagine a simple case of two dependent tasks:

```
data = load_data()
result = process_data(data)
```

- Passing references (`Future` 's) directly would not work with a `concurrent.futures` executor:

```
data_ref = executor.submit(load_data)
result = executor.submit(process_data, data_ref)
```

- Raises a `TypeError` as `process_data` expects data, not a `Future` (which cannot be pickled).
- **Sending futures / references as task argument works directly using Dask or Ray.**
  - It's a very powerful feature for building complex task graphs.
  - The data persistence described above is in fact just a special case of this feature.

Nested tasks - avoiding locking

- Tasks in Dask and Ray can submit other tasks.
- There are specific solutions in both Dask and Ray for avoiding dead-locking.
  - Can happen when a task submits another task but scheduler does not have any free worker slots.
- Dask provides a context manager for nested tasks:

```
def fib(n):
    if n < 2:
        return n
    with dask.distributed.worker_client() as client:
        a_future = client.submit(fib, n - 1)
        b_future = client.submit(fib, n - 2)
        a, b = client.gather([a_future, b_future])
    return a + b
```

- Ray releases the lock on `ray.get` :

```
@ray.remote(num_cpus=1, num_gpus=1)
def g():
    return ray.get(f.remote())
```

Resource requests for task execution

- Resource management is crucial in distributed computing.
  - Not available in `concurrent.futures`.
- Both Dask and Ray support requesting resources for tasks.
  - Resources can be CPU, GPU, memory, or custom (abstract) resources.
- Resource requests *do not* impose limits on actual physical resource usage.
  - Scheduler uses requests for admission control and efficient scheduling.
  - It's up to the task to not use more resources than requested.
- CPU and memory are two fundamentally different types of resources:
  - CPU: Can be "shared" (throttled) ➡️ cannot "run out of CPU".
  - Memory: Finite capacity ➡️ can run out of memory ➡️ process OOM kill.
- A Ray example:

```
ref = process_data.options(num_cpus=2, memory=1024*1024*1024).remote(data_ref)
```

Fault tolerance

- Software fails, hardware fails, networks fail, user (codes) fail.
- Dask and Ray can recover from (some) failures.
- Tasks can be retried automatically.
  - With maximum number of retries explicitly specified.

Main challenges in distributed computing with Dask and Ray

- Communication overhead
- Consistent software environments (Python packages)
- Observability, logging
- Authentication and authorisation
- Costs monitoring and control

Choose between Dask and Ray?

- Architecture and features for asynchronous computing are very similar.
  - There are implementation differences we have not covered.
- The choice is more likely to be made by other features, or ecosystems.
  - Dask provides a pandas-like API for data processing.
  - Ray focuses more on ML end-to-end workflows.
  - Integrations with other frameworks differ so you may pick the one that fits your stack.
- Dask and Ray can interoperate so you may not need to choose 😌

Summary

- Python provides powerful built-in concurrency abstraction and implementation.
  - `concurrent.futures` is a high-level interface for asynchronous execution.
  - `Executor` and `Future` are the main abstractions that other frameworks build upon.
  - can be seamlessly employed within `asyncio`
- Dask, Ray and similar provide enhanced features and scaling to distributed computing.
  - Improve pickling, data communication, task dependencies, resilience, resource management, and more.
  - Scale from single machine to large clusters.
  - Integrate well with `asyncio`.