From built-in concurrency primitives to large scale distributed computing

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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

```
\begin{array}{c} \text{def do\_some\_math}(x\colon \text{float}) \, \to \, \text{float} \colon \\ \text{return } x \, \star \, x \end{array}
```

1. Single calculation via submit:

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

2. Multiple calculations via 'map':

```
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 0×122921490 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 0×122a1f4d0>
```

- 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 that 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]
```

- 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 \S \S \S), 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.

```
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:

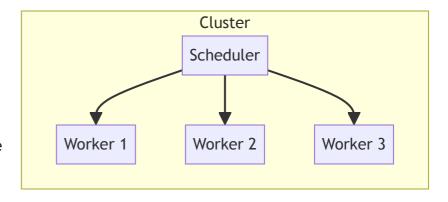
```
async_task = asyncio.ensure_future(ref)
async_future = asyncio.wrap_future(ref.future())
```

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</pre>
```

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) acannot "run out of CPU".
 - Memory: Finite capacity acan 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.
- Slides available at https://github.com/coobas/europython-24.