

14

Introduction to Parallel Computing

Lab Objective: *Many modern problems involve so many computations that running them on a single processor is impractical or even impossible. There has been a consistent push in the past few decades to solve such problems with parallel computing, meaning computations are distributed to multiple processors. In this lab, we explore the basic principles of parallel computing by introducing the cluster setup, standard parallel commands, and code designs that fully utilize available resources.*

Parallel Architectures

A *serial* program is executed one line at a time in a single process. Since modern computers have multiple processor cores, serial programs only use a fraction of the computer's available resources. This can be beneficial for smooth multitasking on a personal computer because programs can run uninterrupted on their own core. However, to reduce the runtime of large computations, it is beneficial to devote all of a computer's resources (or the resources of many computers) to a single program. In theory, this parallelization strategy can allow programs to run N times faster where N is the number of processors or processor cores that are accessible. Communication and coordination overhead prevents the improvement from being quite that good, but the difference is still substantial.

A *supercomputer* or *computer cluster* is essentially a group of regular computers that share their processors and memory. There are several common architectures that combine computing resources for parallel processing, and each architecture has a different protocol for sharing memory and processors between *computing nodes*, the different simultaneous processing areas. Each architecture offers unique advantages and disadvantages, but the general commands used with each are very similar.

The iPyParallel Architecture

In most circumstances, processors communicate and coordinate with a message-passing system such as the standard *Message Passing Interface* (MPI). Many basic commands used for parallel programming with MPI are implemented by Python's `ipyparallel` package. There are three main parts of the iPyParallel architecture.

- *Client*: The main human-written program that is being run.

- *Controller*: Receives directions from the client and distributes instructions and data to the computing nodes. Consists of a *hub* to manage communications and *schedulers* to assign processes to the engines.
- *Engines*: The individual computing nodes. Each engine is like a separate Python process, each with its own namespace, and computing resources.

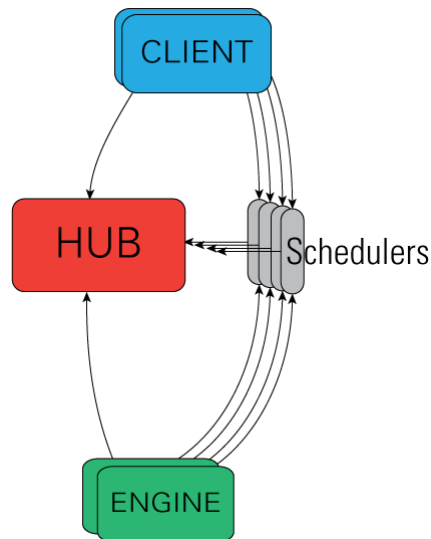


Figure 14.1: An outline of the iPyParallel architecture.

Setting up an iPyParallel Cluster

Anaconda includes iPyParallel, so it can be installed with `conda install ipyparallel`. Establishing a cluster on multiple machines requires a bit of extra setup, which is detailed in the Additional Material section. For now, we demonstrate how to use a single machine with multiple processor cores as a cluster. The following commands initialize parts or all of a cluster in a terminal window.

Command	Description
<code>ipcontroller start</code>	Initialize a controller process.
<code>ipengine start</code>	Initialize an engine process.
<code>ipcluster start</code>	Initialize a controller process and several engines simultaneously.

Each of these processes can be stopped with a keyboard interrupt (`Ctrl+C`). By default, the controller uses JSON files in `UserDirectory/.ipython/profile-default/security/` to determine its settings. Once a controller is running, it acts like a server listening for client connections from engine processes. Engines connect by default to a controller with the settings defined in the aforementioned JSON files. There is no limit to the number of engines that can be started in their own terminal windows and connected to the controller, but it is recommended to only use as many engines as there are cores to maximize efficiency. Once started, each engine has its own ID number on the controller that is used for communication.

ACHTUNG!

The directory that the controller and engines are started from matters. To facilitate connections, navigate to the same folder as your source code before using `ipcontroller`, `ipengine`, or `ipcluster`. Otherwise, the engines may not connect to the controller or may not be able to find auxiliary code as directed by the client.

Starting a controller and engines in individual terminal windows with `ipcontroller` and `ipengine` is a little inconvenient, but having separate terminal windows for the engines allows the user to see individual errors in detail. It is also actually more convenient when starting a cluster of multiple computers. For now, we use `ipcluster` to get the entire cluster started quickly.

```
$ ipcluster start          # Assign an engine to each processor core.
$ ipcluster start --n 4    # Or, start a cluster with 4 engines.
```

NOTE

Jupyter notebooks also have a **Clusters** tab in which clusters can be initialized using an interactive GUI. To enable the tab, run the following command. This operation may require root permissions.

```
$ ipcluster nbextension enable
```

The iPyParallel Interface

Once a controller and its engines have been started and are connected, a cluster has successfully been established. The controller will then be able to distribute messages to each of the engines, which will compute with their own processor and memory space and return their results to the controller. The client uses the `ipyparallel` module to send instructions to the controller via a `Client` object.

```
>>> from ipyparallel import Client

>>> client = Client()          # Only works if a cluster is running.
>>> client.ids
[0, 1, 2, 3]                   # Indicates that there are four engines running.
```

Once the client object has been created, it can be used to create one of two classes: a `DirectView` or a `LoadBalancedView`. These views allow for messages to be sent to collections of engines simultaneously. A `DirectView` allows for total control of task distribution while a `LoadBalancedView` automatically tries to spread out the tasks equally on all engines. The remainder of the lab will be focused on the `DirectView` class.

```
>>> dview = client[:]          # Group all engines into a DirectView.
>>> dview2 = client[:2]        # Group engines 0,1, and 2 into a DirectView.
```

```
>>> dview2.targets      # See which engines are connected.
[0, 1, 2]
```

Since each engine has its own namespace, modules must be imported in every engine. There is more than one way to do this, but the easiest way is to use the `DirectView` object's `execute()` method, which accepts a string of code and executes it in each engine.

```
# Import NumPy in each engine.
>>> dview.execute("import numpy as np")
```

Problem 1. Write a function that initializes a `Client` object, creates a `DirectView` with all available engines, and imports `scipy.sparse` as `sparse` on all engines.

Managing Engine Namespaces

Push and Pull

The `push()` and `pull()` methods of a `DirectView` object manage variable values in the engines. Use `push()` to set variable values and `pull()` to get variables. Each method has an easy shortcut via indexing.

```
>>> dview.block = True      # IMPORTANT!! Blocking will be explained later.

# Initialize the variables 'a' and 'b' on each engine.
>>> dview.push({'a':10, 'b':5})      # OR dview['a'] = 10; dview['b'] = 5
[None, None, None, None]

# Check the value of 'a' on each engine.
>>> dview.pull('a')              # OR dview['a']
[10, 10, 10, 10]

# Put a new variable 'c' only on engines 0 and 2.
>>> dview.push({'c':12}, targets=[0, 2])
[None, None]
```

Problem 2. Write a function `variables(dx)` that accepts a dictionary of variables. Create a `Client` object and a `DirectView` and distribute the variables. Pull the variables back and make sure they haven't changed.

Scatter and Gather

Parallelization almost always involves splitting up collections and sending different pieces to each engine for processing. The process is called *scattering* and is usually used for dividing up arrays or

lists. The inverse process of pasting a collection back together is called *gathering*. This method of distributing and collecting a dataset is the foundation of the prominent MapReduce algorithm.

```
>>> import numpy as np

# Send parts of an array of 8 elements to each of the 4 engines.
>>> x = np.arange(1, 9)
>>> dview.scatter("nums", x)
>>> dview["nums"]
[array([1, 2]), array([3, 4]), array([5, 6]), array([7, 8])]

# Scatter the array to only the first two engines.
>>> dview.scatter("nums_big", x, targets=[0,1])
>>> dview.pull("nums_big", targets=[0,1])
[array([1, 2, 3, 4]), array([5, 6, 7, 8])]

# Gather the array again.
>>> dview.gather("nums")
array([1, 2, 3, 4, 5, 6, 7, 8])

>>> dview.gather("nums_big", targets=[0,1])
array([1, 2, 3, 4, 5, 6, 7, 8])
```

Executing Code on Engines

Execute

The `execute()` method is the simplest way to run commands on parallel engines. It accepts a string of code (with exact syntax) to be executed. Though simple, this method works well for small tasks.

```
# 'nums' is the scattered version of np.arange(1, 9).
>>> dview.execute("c = np.sum(nums)") # Sum each scattered component.
<AsyncResult: execute:finished>
>>> dview['c']
[3, 7, 11, 15]
```

Apply

The `apply()` method accepts a function and arguments to plug into it, and distributes them to the engines. Unlike `execute()`, `apply()` returns the output from the engines directly.

```
>>> dview.apply(lambda x: x**2, 3)
[9, 9, 9, 9]
>>> dview.apply(lambda x,y: 2*x + 3*y, 5, 2)
[16, 16, 16, 16]
```

Note that the engines can access their local variables in any of the execution methods.

Problem 3. Write a function that accepts an integer n . Instruct each engine to make n draws from the standard normal distribution, then hand back the minimum, maximum, and mean draw to the client. Print the results. If you have four engines running, your output should resemble the following:

```
means = [0.0031776784, -0.0058112042, 0.0012574772, -0.0059655951]
maxs = [4.0388107, 4.3664958, 4.2060184, 4.3391623]
mins = [-4.1508589, -4.3848019, -4.1313324, -4.2826519]
```

Problem 4. Use your function from Problem 3 to compare serial and parallel execution times. For $n = 1000000, 5000000, 10000000, 15000000$,

1. Time how long it takes to run your function.
2. Time how long it takes to do the same process (make n draws and calculate and record the statistics) in a for loop with N iterations, where N is the number of engines running.

Plot the execution times against n . You should notice an increase in efficiency in the parallel version as the problem size increases.

Map

The built-in `map()` function applies a function to each element of an iterable. The `iPyParallel` equivalent, the `map()` method of the `DirectView` class, combines `apply()` with `scatter()` and `gather()`. Simply put, it accepts a dataset, splits it between the engines, executes a function on the given elements, returns the results, and combines them into one object. This function also represents a key component in the MapReduce algorithm.

```
>>> num_list = [1, 2, 3, 4, 5, 6, 7, 8]
>>> def triple(x):
...     return 3*x
...
>>> dview.map(triple, num_list)
[3, 6, 9, 12, 15, 18, 21, 24]

>>> def add_three(x, y, z):
...     return x+y+z
...
>>> x_list = [1, 2, 3, 4]
>>> y_list = [2, 3, 4, 5]
>>> z_list = [3, 4, 5, 6]
>>> dview.map(add_three, x_list, y_list, z_list)
[6, 9, 12, 15]
```

Blocking vs. Non-Blocking

Parallel commands can be implemented two ways. The difference is subtle but extremely important.

- *Blocking*: The controller places commands on the specified engines' execution queues, then "blocks" execution until every engine finishes its task. The main program halts until the answer is received from the controller. This mode is usually best for problems in which each node is performing the same task.
- *Non-Blocking*: The controller places commands on the specified engines' execution queues, then immediately returns an `AsyncResult` object that can be used to check the execution status and eventually retrieve the actual result. The main program continues without waiting for responses.

The execution methods `execute()`, `apply()`, and `map()`, as well as `push()`, `pull()`, `scatter()`, and `gather()`, each have a keyword argument `block` that specifies whether or not to using blocking. If not specified, the argument defaults to the `block` attribute of the `DirectView`. Alternatively, the methods `apply_sync()` and `map_sync()` always use blocking, and `apply_async()` and `map_async()` always use non-blocking.

```
>>> f = lambda n: np.sum(np.random.random(n))

# Evaluate f(n) for n=0,1,...,999 with blocking.
>>> %time block_results = [dview.apply_sync(f, n) for n in range(1000)]
CPU times: user 9.64 s, sys: 879 ms, total: 10.5 s
Wall time: 13.9 s

# Evaluate f(n) for n=0,1,...,999 with non-blocking.
>>> %time responses = [dview.apply_async(f, n) for n in range(1000)]
CPU times: user 4.19 s, sys: 294 ms, total: 4.48 s
Wall time: 7.08 s

# The non-blocking method is faster, but we still need to get its results.
>>> block_results[1]          # This list holds actual result values.
[5.9734047365913572,
 5.1895936886345959,
 4.9088268102823909,
 4.8920224621657855]
>>> responses[10]            # This list holds AsyncResult objects.
<AsyncResult: <lambda>:finished>
>>> %time nonblock_results = [r.get() for r in responses]
CPU times: user 3.52 ms, sys: 11 µs, total: 3.53 ms
Wall time: 3.54 ms          # Getting the responses takes little time.
```

As was demonstrated above, when non-blocking is used, commands can be continuously sent to engines before they have finished their previous task. This allows them to begin their next task without waiting to send their calculated answer and receive a new command. However, this requires a design that incorporates check points to retrieve answers and enough memory to store response objects.

Table 14.1 details the methods of the `AsyncResult` object.

Class Method	Description
<code>wait(timeout)</code>	Wait until the result is available or until <code>timeout</code> seconds pass. This method always returns <code>None</code> .
<code>ready()</code>	Return whether the call has completed.
<code>successful()</code>	Return whether the call completed without raising an exception. Will raise <code>AssertionError</code> if the result is not ready.
<code>get(timeout)</code>	Return the result when it arrives. If <code>timeout</code> is not <code>None</code> and the result does not arrive within <code>timeout</code> seconds then <code>TimeoutError</code> is raised.

Table 14.1: All information from <https://ipyparallel.readthedocs.io/en/latest/details.html#AsyncResult>.

There are additional magic methods supplied by `iPyParallel` that make some of these operations easier. These methods are contained in the Additional Material section. More information on `iPyParallel` architecture, interface, and methods at <https://ipyparallel.readthedocs.io/en/latest/index.html>.

Applications

Parallel computing, when used correctly, is one of the best ways to speed up the run time of an algorithm. As a result, it is very commonly used today and has many applications, such as the following:

- Graphic rendering
- Facial recognition with large databases
- Numerical integration
- Calculating Discrete Fourier Transforms
- Simulation of various natural processes (weather, genetics, etc.)
- Natural language processing

In fact, there are many problems that are only possible to solve through parallel computing because solving them serially would take too long. In these types of problems, even the parallel solution could take years. Some brute-force algorithms, like those used to crack simple encryptions, are examples of this type of problem.

The problems mentioned above are well suited to parallel computing because they can be manipulated in such a way that running them on multiple processors results in a significant run time improvement. Manipulating an algorithm to be run with parallel computing is called *parallelizing* the algorithm. When a problem only requires very minor manipulations to parallelize, it is often called *embarrassingly parallel*. Typically, an algorithm is embarrassingly parallel when there is little to no dependency between results. Algorithms that do not meet this criteria can still be parallelized, but there is not always a significant enough improvement in run time to make it worthwhile. For example, calculating the Fibonacci sequence using the usual formula, $F(n) = F(n-1) + F(n-2)$, is poorly suited to parallel computing because each element of the sequence is dependent on the previous two elements.

Problem 5. The *trapezoid rule* is a simple technique for numerical integration:

$$\int_a^b f(x)dx \approx \frac{h}{2} \sum_{k=1}^N (f(x_k) + f(x_{k+1})),$$

where $a = x_1 < x_2 < \dots < x_N = b$ and $h = x_{n+1} - x_n$ for each n . See Figure 14.2.

Note that estimation of the area of each interval is independent of all other intervals. As a result, this problem is considered embarrassingly parallel.

Write a function that accepts a function handle to integrate, bounds of integration, and the number of points to use for the approximation. Parallelize the trapezoid rule in order to estimate the integral of f . That is, evenly divide the points among all available processors and run the trapezoid rule on each portion simultaneously. The sum of the results of all the processors will be the estimation of the integral over the entire interval of integration. Return this sum.

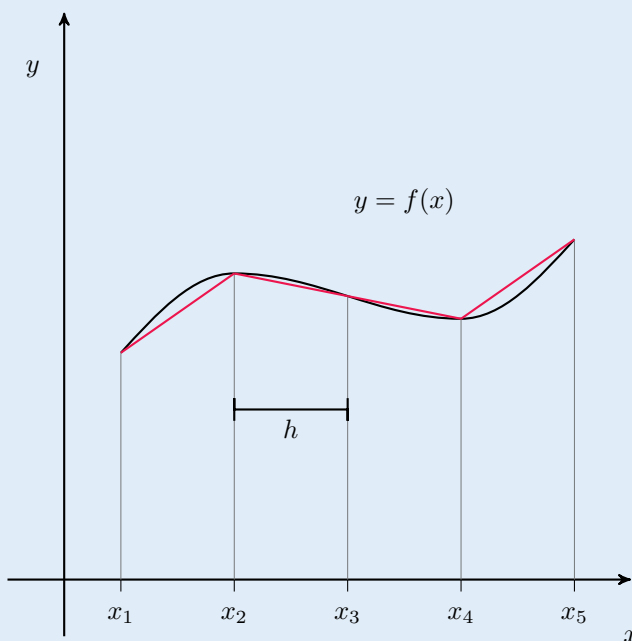


Figure 14.2: A depiction of the trapezoid rule with uniform partitioning.

Intercommunication

The phrase *parallel computing* refers to designing an architecture and code that makes the best use of computing resources for a problem. Occasionally, this will require nodes to be interdependent on each other for previous results. This contributes to a slower result because it requires a great deal of communication latency, but is sometimes the only method to parallelize a function. Although important, the ability to effectively communicate between engines has not been added to `iPyParallel`. It is, however, possible in an MPI framework and will be covered in a later lab.

Additional Material

Installation and Initialization

If you have not already installed `ipyparallel`, you may do so using the conda package manager.

```
$ conda update conda
$ conda update anaconda
$ conda install ipyparallel
```

Clusters of Multiple Machines

Though setting up a computing cluster with `iPyParallel` on multiple machines is similar to a cluster on a single computer, there are a couple of extra considerations to make. The majority of these considerations have to do with the network setup of your machines, which is unique to each situation. However, some basic steps have been taken from <https://ipyparallel.readthedocs.io/en/latest/process.html> and are outlined below.

SSH Connection

When using engines and controllers that are on separate machines, their communication will most likely be using an SSH tunnel. This *Secure Shell* allows messages to be passed over the network.

In order to enable this, an SSH user and IP address must be established when starting the controller. An example of this follows.

```
$ ipcontroller --ip=<controller IP> --user=<user of controller> --enginessh=<↔
  user of controller>@<controller IP>
```

Engines started on remote machines then follow a similar format.

```
$ ipengine --location=<controller IP> --ssh=<user of controller>@<controller IP>↔
>
```

Another way of affecting this is to alter the configuration file in `UserDirectory/.ipython/profile-default/security/ipcontroller-engine.json`. This can be modified to contain the controller IP address and SSH information.

All of this is dependent on the network feasibility of SSH connections. If there are a great deal of remote engines, this method will also require the SSH password to be entered many times. In order to avoid this, the use of SSH Keys from computer to computer is recommended.

Magic Methods & Decorators

To be more usable, the `iPyParallel` module has incorporated a few magic methods and decorators for use in an interactive iPython or Python terminal.

Magic Methods

The `iPyParallel` module has a few magic methods that are very useful for quick commands in `iPython` or in a Jupyter Notebook. The most important are as follows. Additional methods are found at <https://ipyparallel.readthedocs.io/en/latest/magics.html>.

%px - This magic method runs the corresponding Python command on the engines specified in `dview.targets`.

%autopx - This magic method enables a boolean that runs any code run on every engine until `%autopx` is run again.

Examples of these magic methods with a client and four engines are as follows.

```
# %px
In [4]: with dview.sync_imports():
...:     import numpy
...:
importing numpy on engine(s)
In [5]: \%px a = numpy.random.random(2)

In [6]: dview['a']
Out[6]:
[array([ 0.30390162,  0.14667075]),
 array([ 0.95797678,  0.59487915]),
 array([ 0.20123566,  0.57919846]),
 array([ 0.87991814,  0.31579495])]

# %autopx
In [7]: %autopx
%autopx enabled
In [8]: max_draw = numpy.max(a)

In [9]: print('Max_Draw: {}'.format(max_draw))
[stdout:0] Max_Draw: 0.30390161663280246
[stdout:1] Max_Draw: 0.957976784975849
[stdout:2] Max_Draw: 0.5791984571339429
[stdout:3] Max_Draw: 0.8799181411958089

In [10]: %autopx
%autopx disabled
```

Decorators

The `iPyParallel` module also has a few decorators that are very useful for quick commands. The two most important are as follows:

@remote - This decorator creates methods on the remote engines.

@parallel - This decorator creates methods on remote engines that break up element wise operations and recombine results.

Examples of these decorators are as follows.

```
# Remote decorator
>>> @dview.remote(block=True)
>>> def plusone():
...     return a+1
>>> dview['a'] = 5
>>> plusone()
[6, 6, 6, 6,]

# Parallel decorator
>>> import numpy as np

>>> @dview.parallel(block=True)
>>> def combine(A,B):
...     return A+B
>>> ex1 = np.random.random((3,3))
>>> ex2 = np.random.random((3,3))
>>> print(ex1+ex2)
[[ 0.87361929  1.41110357  0.77616724]
 [ 1.32206426  1.48864976  1.07324298]
 [ 0.6510846   0.45323311  0.71139272]]
>>> print(combine(ex1,ex2))
[[ 0.87361929  1.41110357  0.77616724]
 [ 1.32206426  1.48864976  1.07324298]
 [ 0.6510846   0.45323311  0.71139272]]
```

Connecting iPyParallel with MPI

The iPyParallel cluster can be imbued with the ability to interpret MPI commands. More information on making this connection can be found at <https://ipyparallel.readthedocs.io/en/latest/mpi.html>.