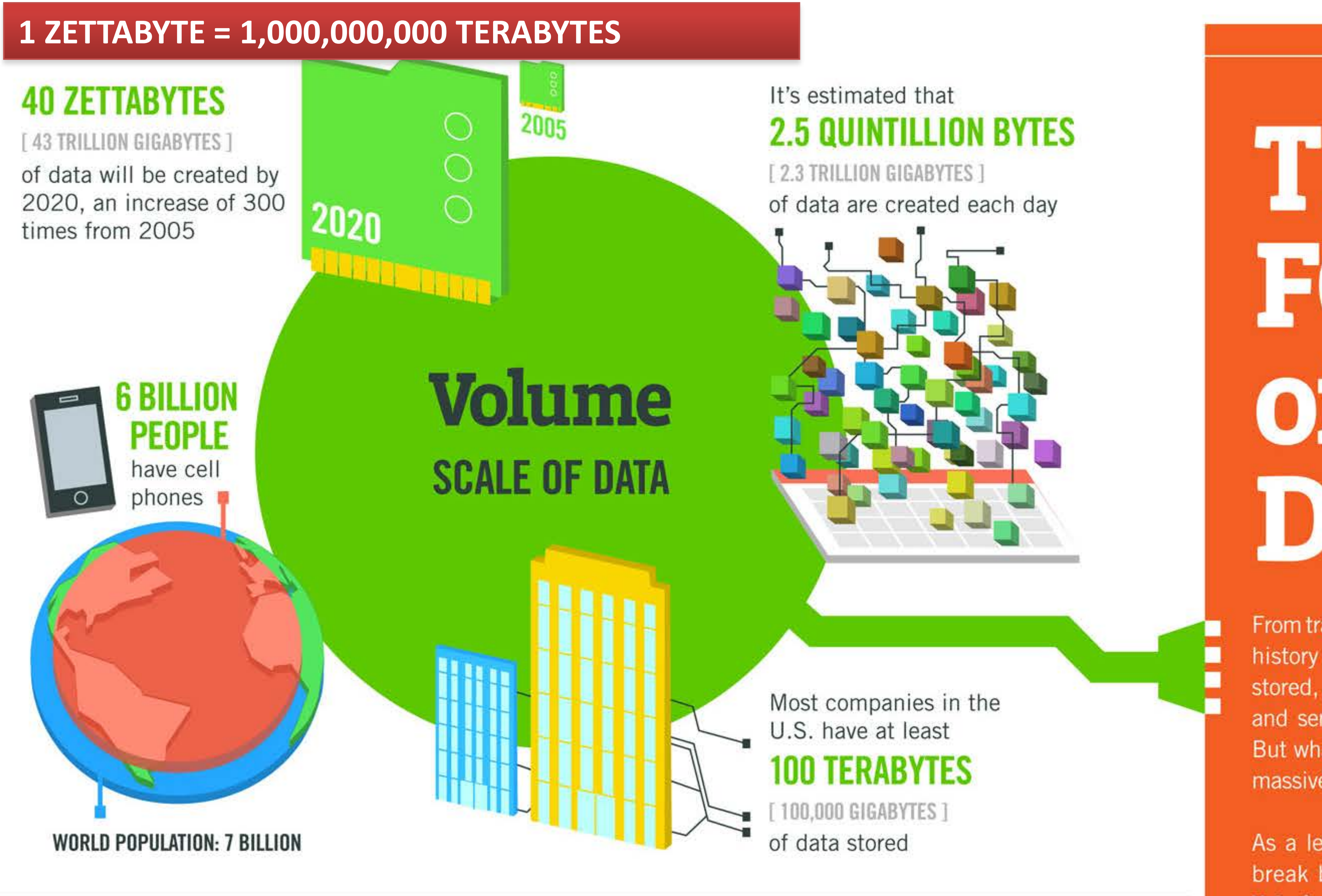
Parallel processing of large datasets

What are Big Data?

1 ZETTABYTE = 1,000,000,000 TERABYTES



40 ZETTABYTES
[43 TRILLION GIGABYTES]
of data will be created by 2020, an increase of 300 times from 2005

It's estimated that
2.5 QUINTILLION BYTES
[2.3 TRILLION GIGABYTES]
of data are created each day

6 BILLION PEOPLE
have cell phones

Volume
SCALE OF DATA

WORLD POPULATION: 7 BILLION

Most companies in the U.S. have at least
100 TERABYTES
[100,000 GIGABYTES]
of data stored

Processing big data: the issues

- Parallel processing in the Environmental Sciences has historically focussed on running highly-parallelised models.
- Data analysis was typically run sequentially because:
  - It was a smaller problem
  - It didn’t have parallel resources available
  - The software/scientists were not equipped to work in parallel
- The generation of enormous datasets (e.g. UPSCALE – around 300Tb) means that:
  - Processing big data **requires** a parallel approach
  - Fortunately, platforms, tools, and programmers are becoming better equipped

Some Terminology

Concurrency: A property of a system in which multiple tasks that comprise the system remain active and make progress at the same time.

Parallelism: Exploiting concurrency in a programme with the goal of solving a problem in less time.

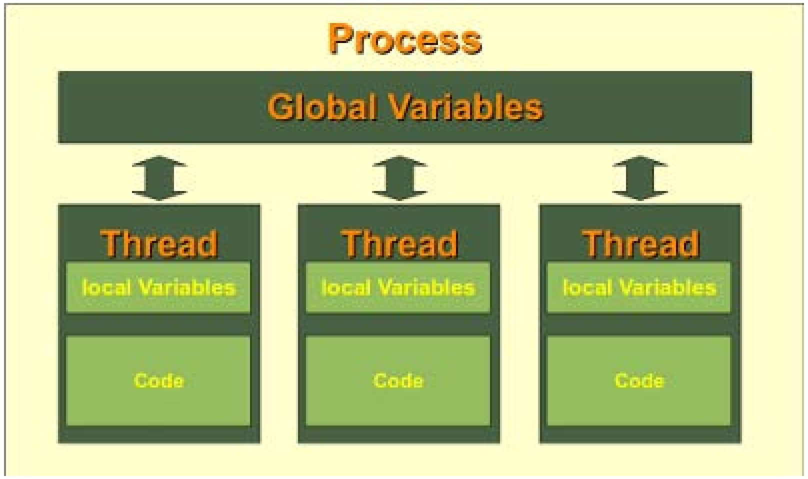
Race condition: A race condition occurs within concurrent environments. It is when a piece of code prevents code that is running elsewhere from accessing a shared resource, e.g., memory, and thus delays the other process.

How does my computer do so many things at once?

These days most computers, and even phones, have multiple processors.

However, even on a single processor modern operating systems can give the illusion that multiple tasks are running at the same time by rapidly switching between many active threads.

This is because the modern CPU clock is measuring time at the nanosecond scale where we humans can only keep track of milliseconds.



Picture: http://www.python-course.eu/threads.php

Parallel processing for data analysis

- Data analysis tools do not (typically) do parallelisation automatically.
- But parallelisation is normally achievable at a small price.
- A lot can be done with:
  - Decomposition of large jobs into smaller jobs
  - Batch processing
  - Understanding tools and schedulers

We will look at these and show examples

(Almost) everything is parallel these days

YOUR DESKTOP MACHINE IS A PARALLEL COMPUTER!

It runs a multi-core processor...

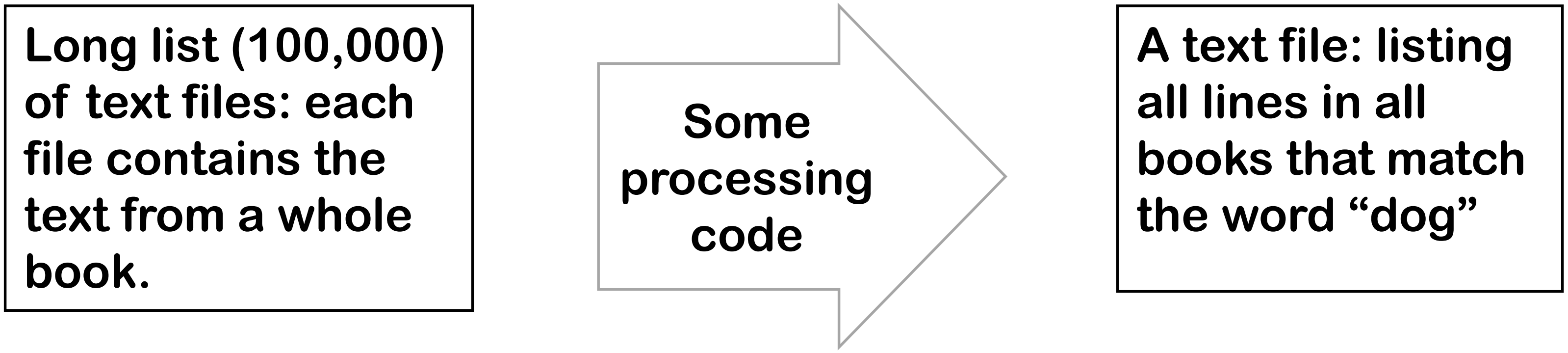
...which means you can speed up processing by asking different parts of your programme to run on different cores.

*"But what about **race conditions**?"...*

...True: you still need to design your approach to avoid things getting out of hand!

Simple parallelism by hand (1)

- Running on a multi-core machine you can exploit local processes, e.g.:



Long list (100,000) of text files: each file contains the text from a whole book.

Some processing code

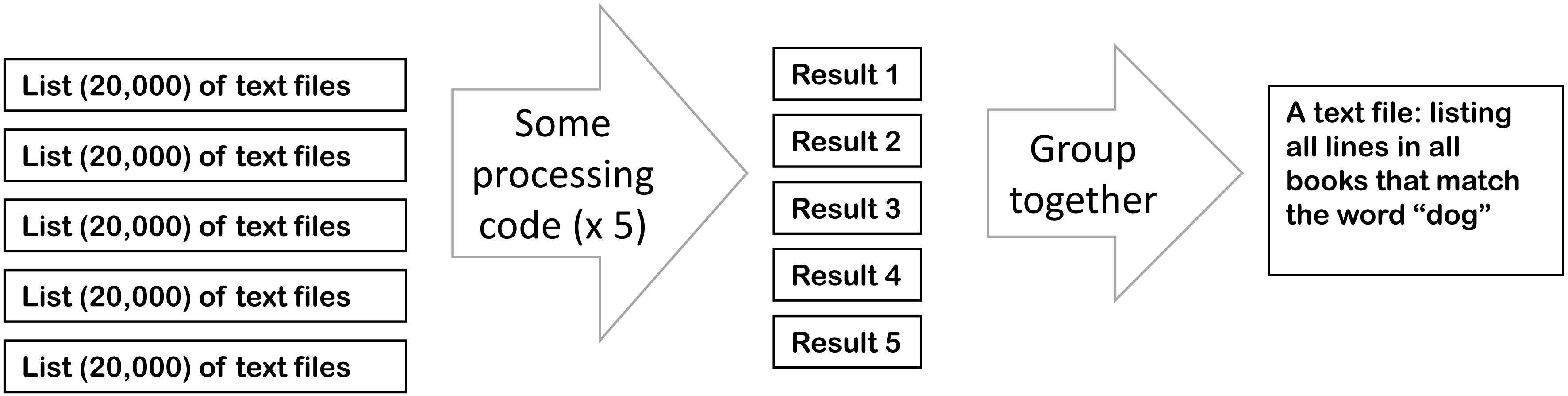
A text file: listing all lines in all books that match the word “dog”

grep_for_dog.sh

```
#!/bin/bash
input_file=$1
while read FILENAME; do
      grep dog $FILENAME >>
${input_file}_result.txt
done <  $input_file
```

Simple parallelism by hand (2)

- A simple re-factoring splits the job into five parts:



List (20,000) of text files

List (20,000) of text files

List (20,000) of text files

List (20,000) of text files

List (20,000) of text files

Some processing code (x 5)

Result 1

Result 2

Result 3

Result 4

Result 5

Group together

A text file: listing all lines in all books that match the word “dog”

```
$ split –l 20000 -d list_of_files.txt   # Writes to “x00”, “x01”, …
$ for i in x??; do grep_for_dog.sh $i & done
$ cat *_result.txt > output.txt
```

Simple parallelism by hand (3)

```
$ for i in x??; do grep_for_dog.sh $i & done
[2] 3325
[3] 3326
[4] 3327
[5] 3328
[6] 3329
```

```
$ ps -ef | grep grep_for_dog
alison   3325   2669   0 00:40 pts/1   00:00:00 /bin/bash   ./grep_for_dog.sh   x00
alison   3326   2669   0 00:40 pts/1   00:00:00 /bin/bash   ./grep_for_dog.sh   x01
alison   3327   2669   0 00:40 pts/1   00:00:00 /bin/bash   ./grep_for_dog.sh   x02
alison   3328   2669   0 00:40 pts/1   00:00:00 /bin/bash   ./grep_for_dog.sh   x03
alison   3329   2669   0 00:40 pts/1   00:00:00 /bin/bash   ./grep_for_dog.sh   x04
```

Simple parallelism by hand (4)

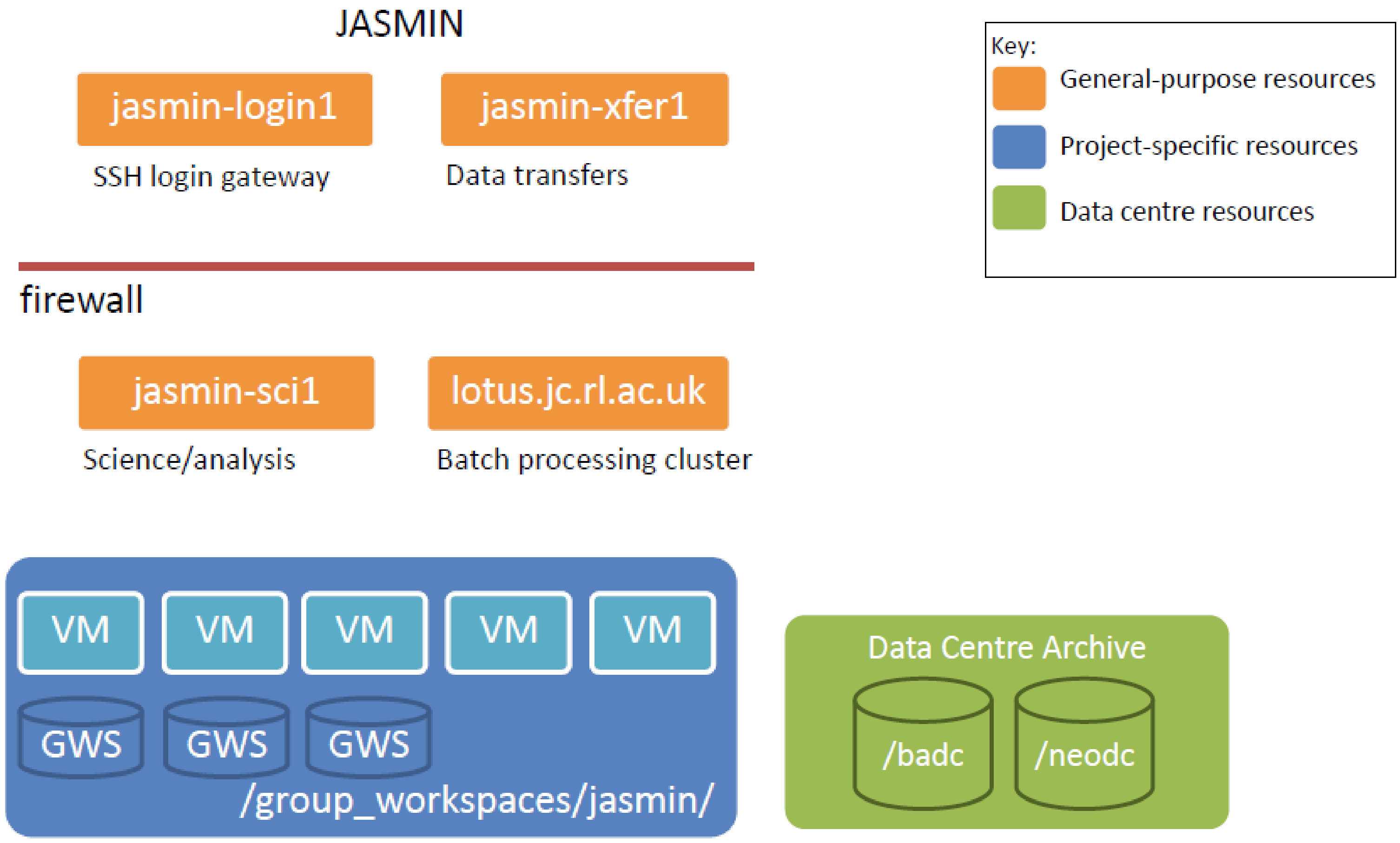
Some time later…

```
$ ps –ef  | grep grep_for_dog
```

```
[2]   Done                    ./grep_for_dog.sh $i
[3]   Done                    ./grep_for_dog.sh $i
[4]   Done                    ./grep_for_dog.sh $i
[5]-  Done                    ./grep_for_dog.sh $i
[6]+  Done                    ./grep_for_dog.sh $i
```

JASMIN & LOTUS

JASMIN in pictures



JASMIN

jasmin-login1

SSH login gateway

jasmin-xfer1

Data transfers

firewall

jasmin-sci1

Science/analysis

lotus.jc.rl.ac.uk

Batch processing cluster

VM VM VM VM VM

GWS GWS GWS

/group_workspaces/jasmin/

Data Centre Archive

/badc

/neodc

Key:

🟧 General-purpose resources

🟦 Project-specific resources

🟩 Data centre resources

The LOTUS cluster on JASMIN

- The **LOTUS cluster is a far bigger resource** for running compute intensive jobs than the JASMIN Scientific Analysis Servers.

- Having the same software installed on the JASMIN-Sci machines and LOTUS means you can:
  1. develop code on the generic Analysis Servers
  2. run in batch mode via LOTUS

What is a batch job?

- “Interactive processing” is when a user enters individual commands to be processed immediately by the computer.

- A “batch job” is a program or a sequence of commands that are executed without user interaction.

LOTUS: Job Control

Submitting a job (you must SSH to **lotus.jc.rl.ac.uk**):

```
$ bsub [options] <command>
```

View the status of jobs:

```
$ bjobs
JOBID USER STAT QUEUE FROM_HOST   EXEC_HOST JOB_NAME SUBMIT_TIME
71880 fred PEND lotus lotus.jc.rl */hostname        Mar 18 16:26
```

Cancel a job with:

```
$ bkill <job_id>
```

http://www.ceda.ac.uk/help/users-guide/lotus/

Batch job example: extract spatial subsets from CMIP5 experiments (1)

Processing requirement:

For each model:

For each variable (hus, ps, ta, ua & va):

- Extract a spatial subset
  - (80° to 140° Longitude; -30° to 40° Latitude)

Where:

- Frequency: 6hr
- Ensemble: r1i1p1
- Realm: atmosphere

Batch job example:
extract spatial subsets from CMIP5 experiments (2)

Basic (Sequential) Implementation:

Script 1 (bash):

- For each variable (hus, ps, ta, ua & va):
  - Make output directory
  - Find all relevant input NetCDF files
  - Loop through list of input files and for each one call Python script

Extract from: **extract_cmip5_subset.py**

```
import cf
f = cf.read(infile)
subset = f[2].subspace(latitude=cf.wi(bb.south, bb.north),
longitude=cf.wi(bb.west, bb.east))
cf.write(subset, outfile)
```

Batch job example:
extract spatial subsets from CMIP5 experiments (3)

Parallel Implementation using LOTUS:

Script 1 (bash):

- For each variable (hus, ps, ta, ua & va):
    - Make output directory
    - Find all relevant input NetCDF files
    - Loop through list of files and for each one submit a batch job to LOTUS to call the Python script using **bsub**

```
bsub –q par–single –o $outdir/`date +%s`.txt
~/extract_cmip5_subset.py $nc_file $this_dir $var
```

Batch job example: extract spatial subsets from CMIP5 experiments (4)

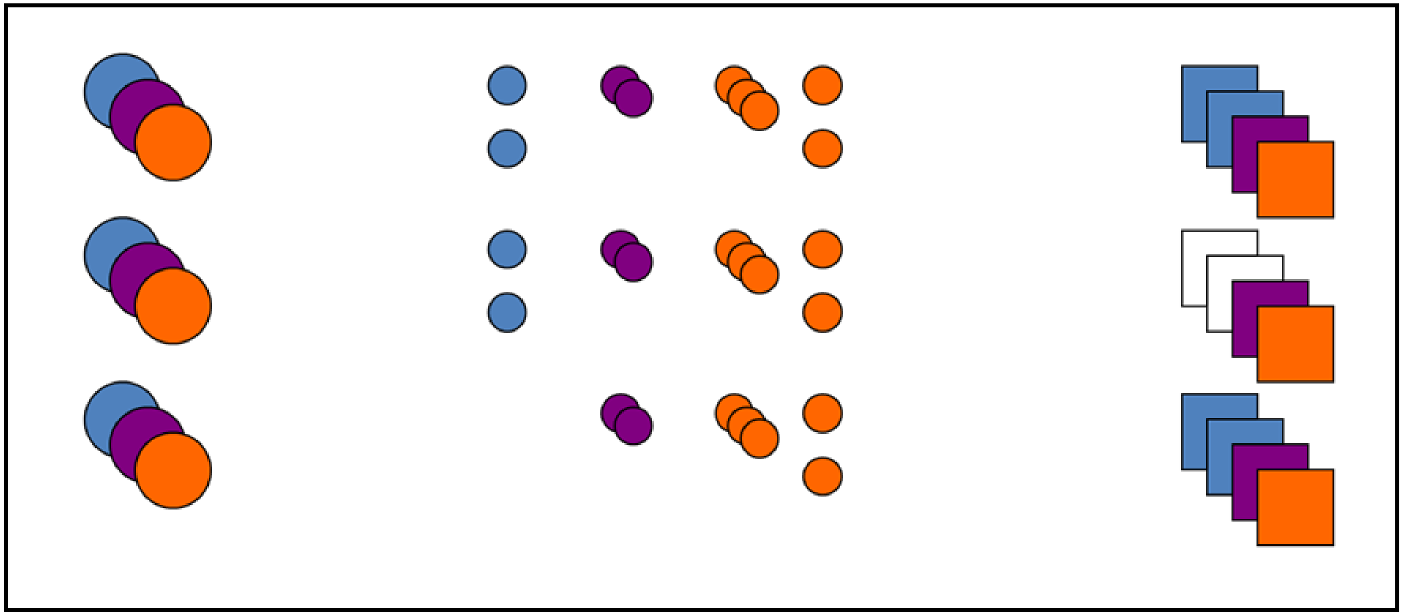
Why use this approach?

- Because you can submit 200 jobs in one go.
- Lotus executes jobs when resource becomes available
- They will all run and complete in parallel

```
bsub –q par–single –o $outdir/`date +%s`.txt
~/extract_cmip5_subset.py $nc_file $this_dir $var
```

Job Submission

- Jobs are submitted using the LSF scheduler
- Resources are allocated as they become available
- Fair share of resources between users



Efficiency gains through re-factoring (1)

Major gains can be made by changing the order and structure of your code. Issues might be:

1. Code runs sequentially and takes a long time
2. Code runs slowly because processing order leads to inefficient I/O
3. Code will not run because of memory requirements

In some cases you can create loops that can be scripted as separate processes allowing you to submit them in parallel.

Efficiency gains through re-factoring (2)

Here is a real-world example:

The Problem: Trying to run the NCO tool **ncea** to calculate an average from a large dataset. It will not run!

Why? The **ncea** command reports this:

```
unable to allocate 7932598800 bytes
```

(which is about 8 Gbytes) ...and then exits.

Possible solutions:

1. Data files hold multiple variables: Operate on one at a time:

```
ea -v vosaline means/199[45678]/*y01T.nc -o test.nc
```

2. ncReduce the number of files (i.e. years) processed each time:

```
ncea means/199[45]/*y01T.nc -o test.nc
```

Many Python-based Parallel tools

The following page brings together details of many different parallel tools available for python users:

https://wiki.python.org/moin/ParallelProcessing

The future of parallel data analysis (1)

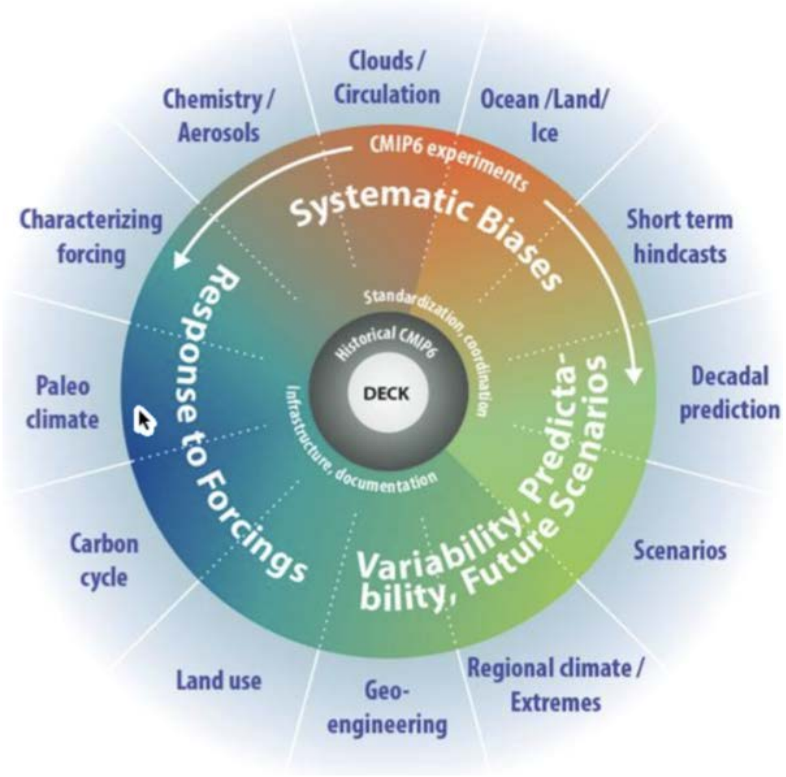
- Analysing Big Data is a challenge! Software needs to adapt and scientists need to be able to adapt their code to keep up!

CMIP5 Status (early 2013)	
Number of files	3,222,967
Number of datasets	54,274
Archive Volume (TB)	1,483
Models with data published	64
Models with documentation published in archive	38
Experiments	108
Modelling centres	32
Data Nodes	22

The future of parallel data analysis (2)

CMIP6: 6th Coupled Model Intercomparison Project

Global community activity under the World Meteorological Organisation (WMO) via the World Climate Research Programme (WCRP)



- 33 institutions
- 75 models
- 248 experiments
- Approximately 20-30PB

CEDA are currently preparing for ~13PB to be archived

The future of parallel data analysis (2)

We are likely to see more:

- Web processing services that do the parallel analysis remotely;
- Analysis Platforms (like JASMIN) that allow scientists to run code next to the data;
- Parallel I/O in software libraries.

Learning to write parallel code now is likely to be of great benefit in future

Further information

JASMIN Analysis Platform (software packages):

jasmin.ac.uk/services/jasmin-analysis-platform/

LOTUS Overview:

help.ceda.ac.uk/article/110-lotus-overview

LOTUS User Guide

help.ceda.ac.uk/category/107-batch-computing-on-lotus

Jug:

jug.readthedocs.io/en/latest/

Parallel processing:

https://computing.llnl.gov/tutorials/parallel_comp/