C.E.C.I

Consortium des Equipements
de Calcul Intensif
en Fédération Wallonie-Bruxelles

Introduction to Parallel Computing

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Why parallel?

Speed up – Solve a problem faster
→ more processing power
(a.k.a. strong scaling)

Scale up – Solve a larger problem
→ more memory and network capacity
(a.k.a. weak scaling)

Scale out – Solve many problems
→ more storage capacity

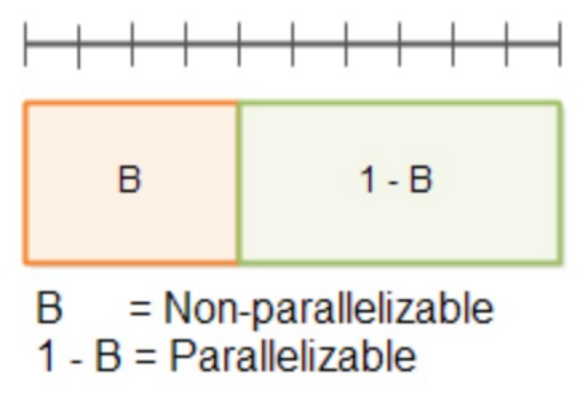
Agenda

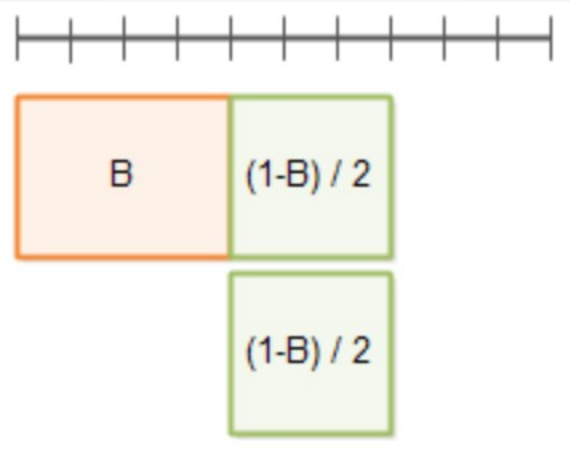
1. General concepts
2. Hardware
3. Programming models
4. User tools

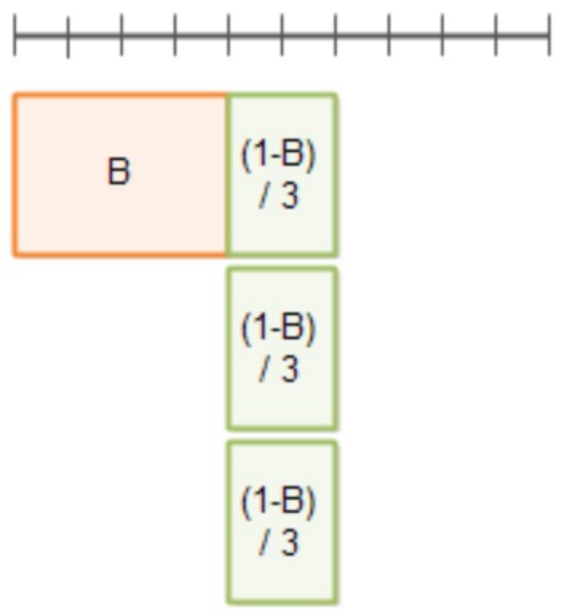
1.

General concepts

Amdahl's Law



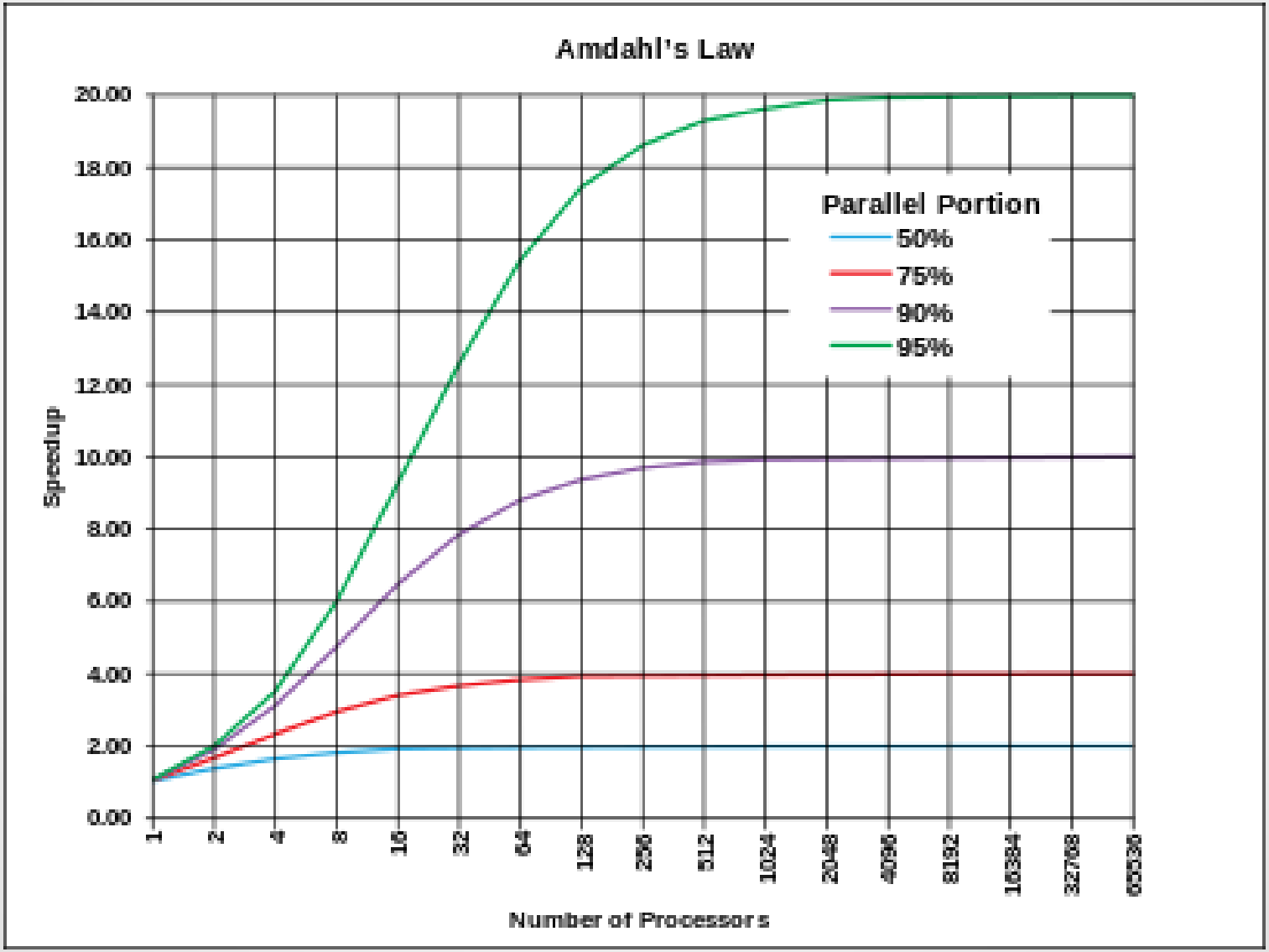




In parallel computing, Amdahl's law is mainly used to predict the theoretical maximum speedup for programs using multiple processors.

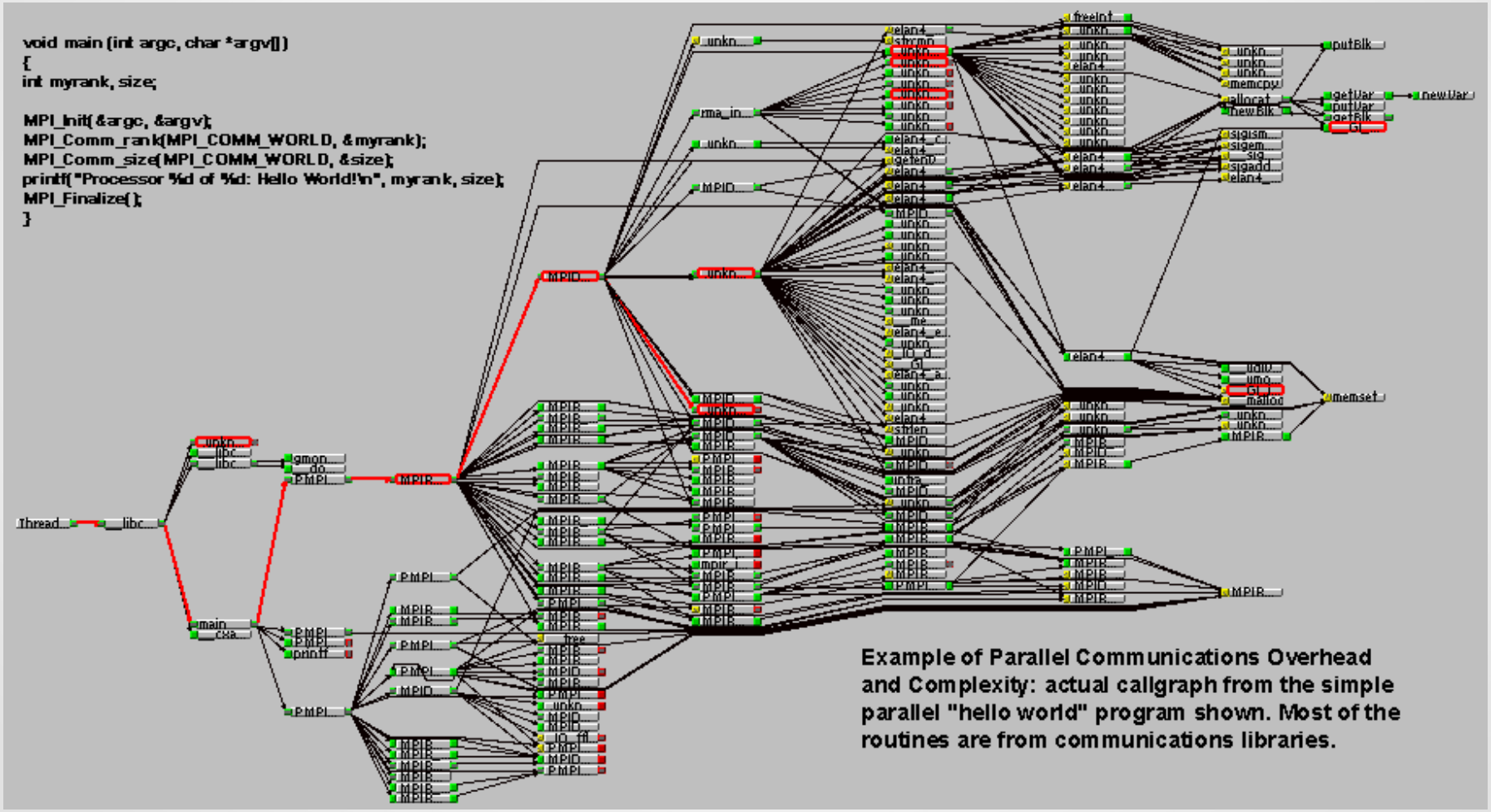
http://tutorials.jenkov.com/java-concurrency/amdahls-law.html

Amdahl's Law



https://en.wikipedia.org/wiki/Amdahl%27s_law

Parallel overhead



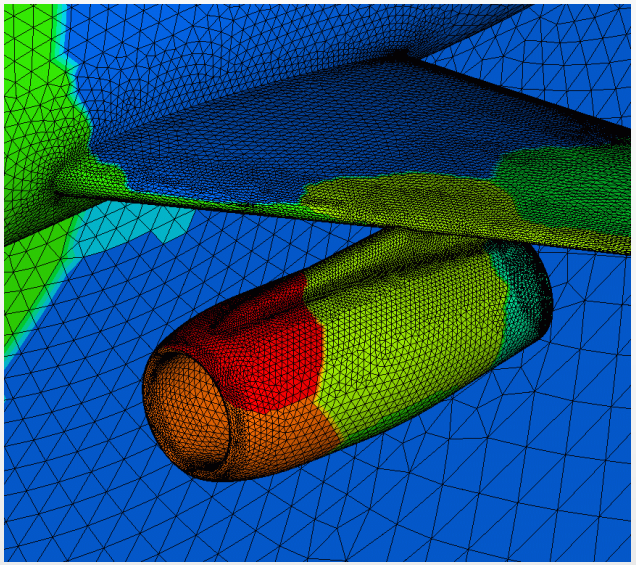
https://computing.llnl.gov/tutorials/parallel_comp/images/helloWorldParallelCallgraph.gif

Parallelization involves

- *decomposition* of the work
  - **distributing instructions** to processors
  - **distributing data** to memories
- *collaboration* of the workers
  - **synchronization** of the distributed work
  - **communication** of data

Decomposition

- **Work decomposition** : task-level parallelism
- **Data decomposition** : data-level parallelism
- **Domain decomposition** : decomposition of work and data is done in a higher model, e.g. in the reality



Collaboration

- **Synchronous** (SIMD) at the processor level
- **Fine-grained** parallelism if subtasks must communicate many times per second (instruction level); loosely synchronous
- **Coarse-grained** parallelism if they do not communicate many times per second (function-call level)
- **Embarrassingly parallel** if they rarely or never have to communicate (asynchronous)

Parallel programming paradigms

- **Task-farming** (master/slave or work stealing)
- **SPMD** (Single program multiple data)
- **Pipelining** (A->B->C, one process per task concurrently)
- **Divide and Conquer** (processes spawned at need and report their result to the parent)
- **Speculative parallelism** (processes spawned and result possibly discarded)

2.

Hardware

At the processor level

- Instruction-level parallelism (ILP)
  - Instruction pipelining
  - Superscalar execution
  - Out-of-order execution
  - Speculative execution
- Single Instruction Multiple Data (SIMD)

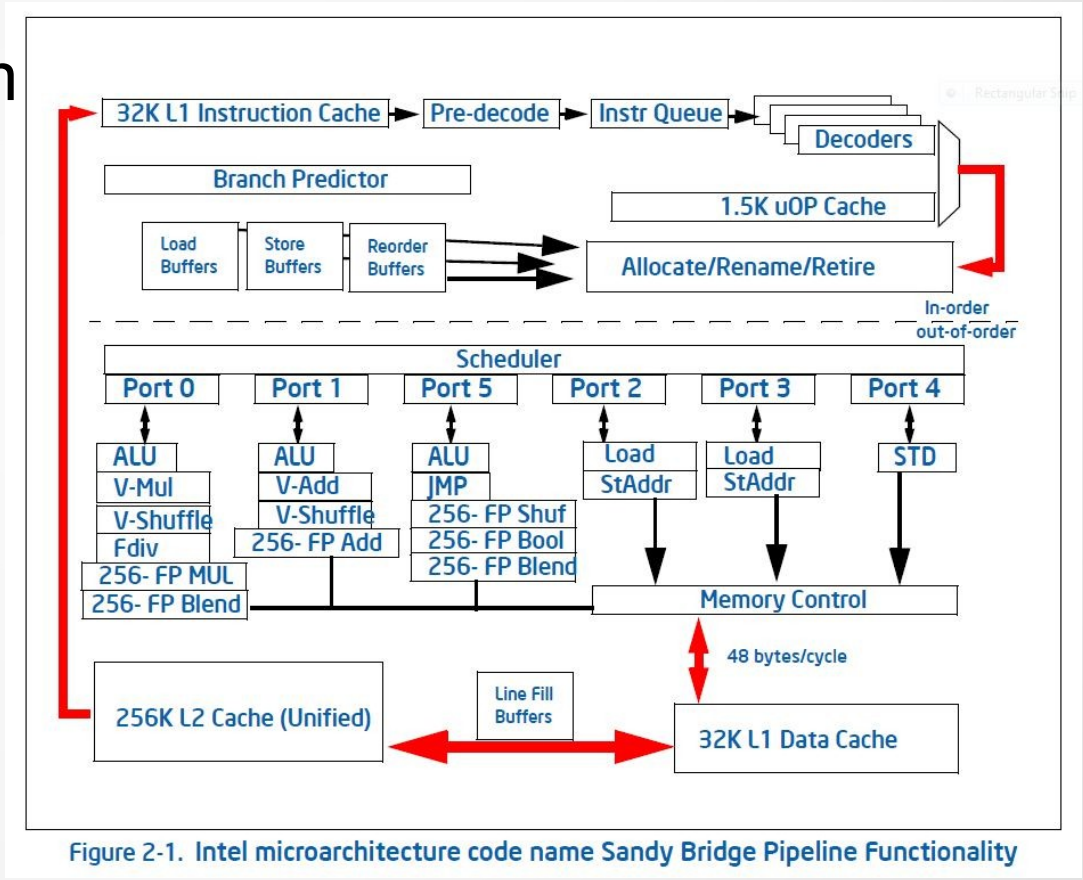
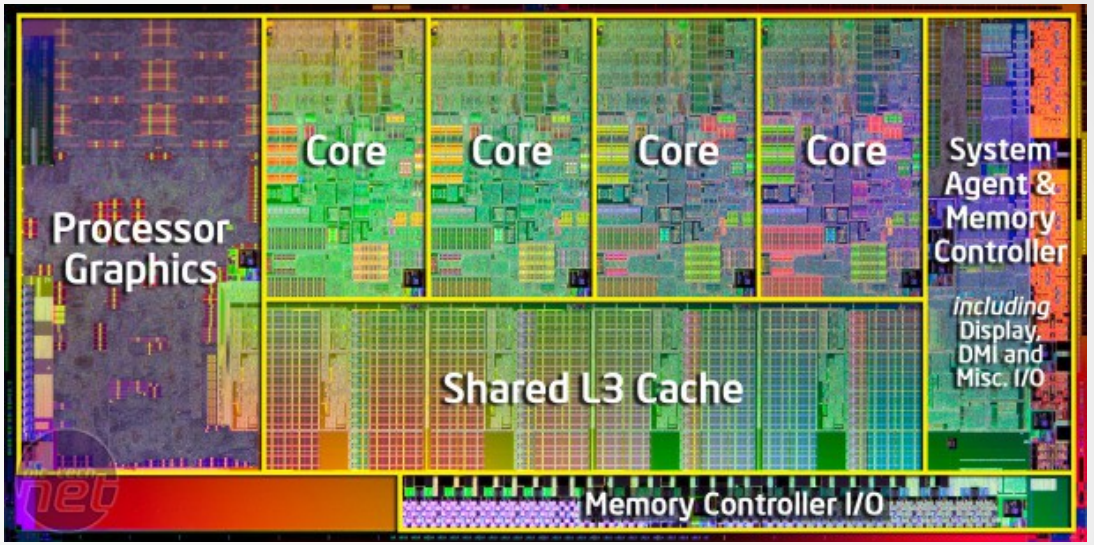
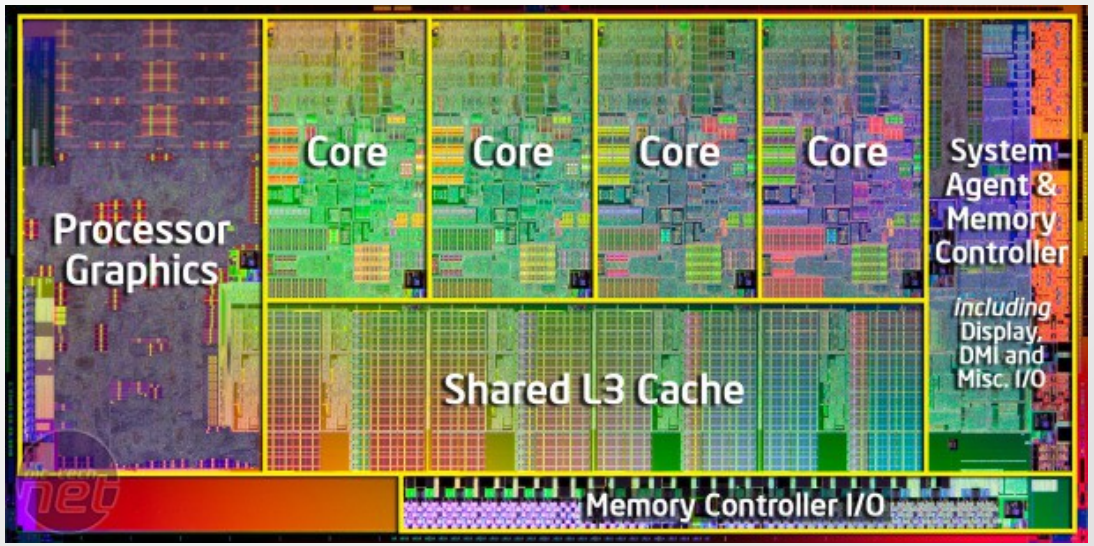


Figure 2-1. Intel microarchitecture code name Sandy Bridge Pipeline Functionality

At the computer level

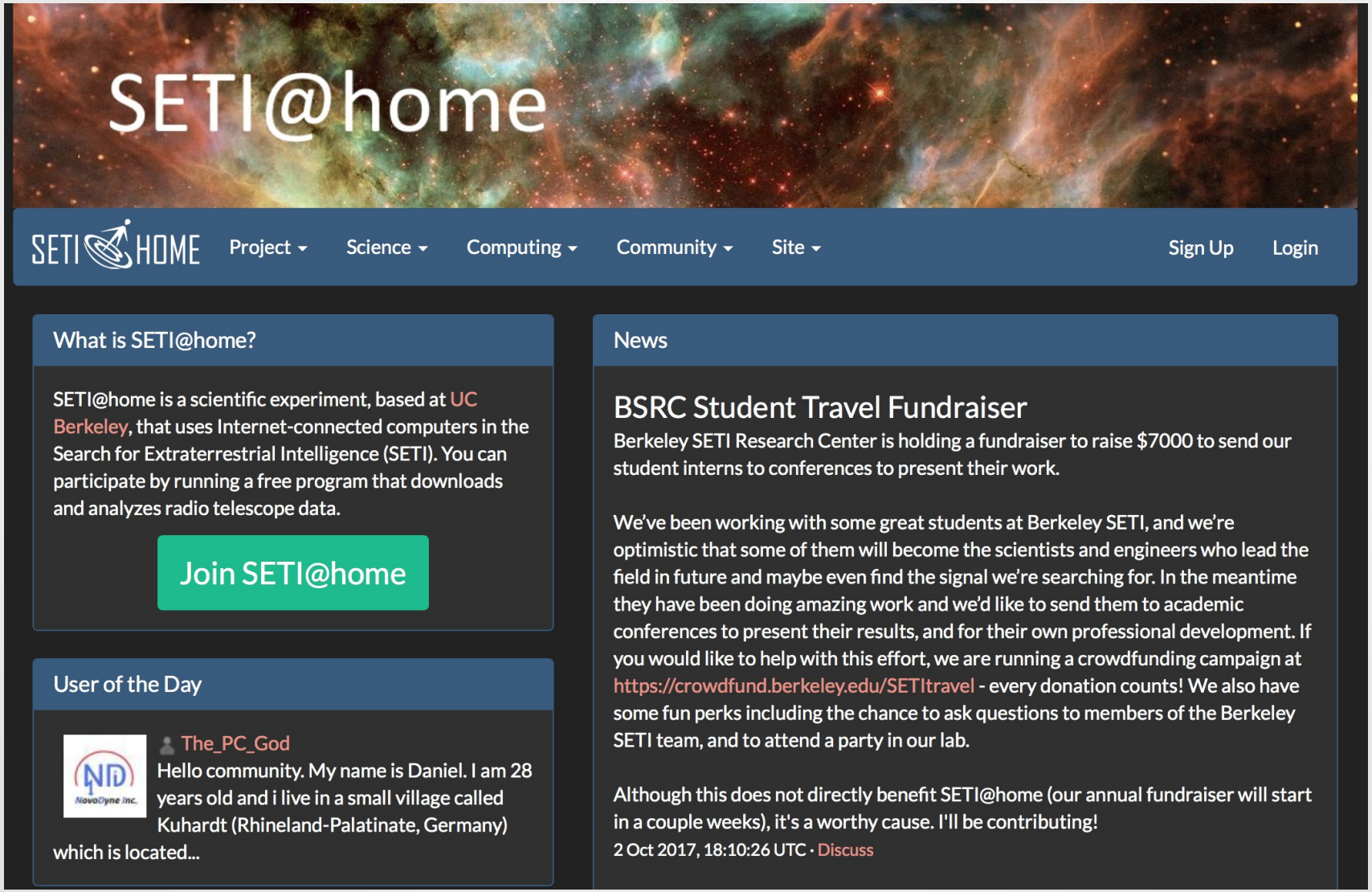
- Multithreading
  - SMP
  - NUMA
- Accelerators





At the system level

Distributed computing



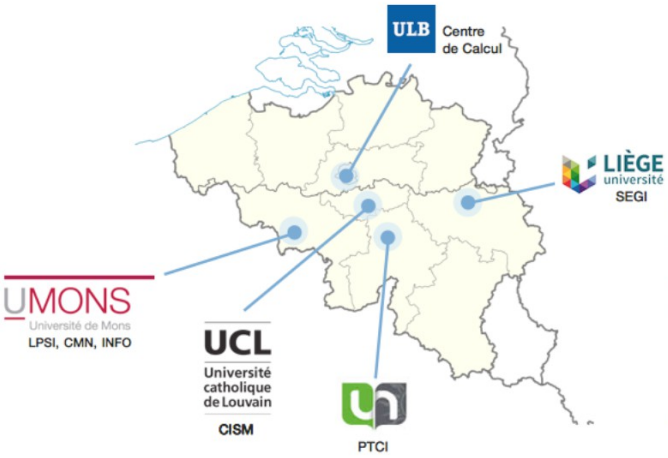
Cluster computing

Consortium des Équipements de Calcul Intensif

6 clusters, 10k cores, 1 login, 1 home directory

About

CÉCI is the 'Consortium des Équipements de Calcul Intensif'; a consortium of high-performance computing centers of UCL, ULB, ULg, UMons, and UNamur. Read more.



The common storage is functional!

Have you tried it yet? More info...

Latest News

SATURDAY, 23 SEPTEMBER 2017

A CECI user pictured in the ULiège news!

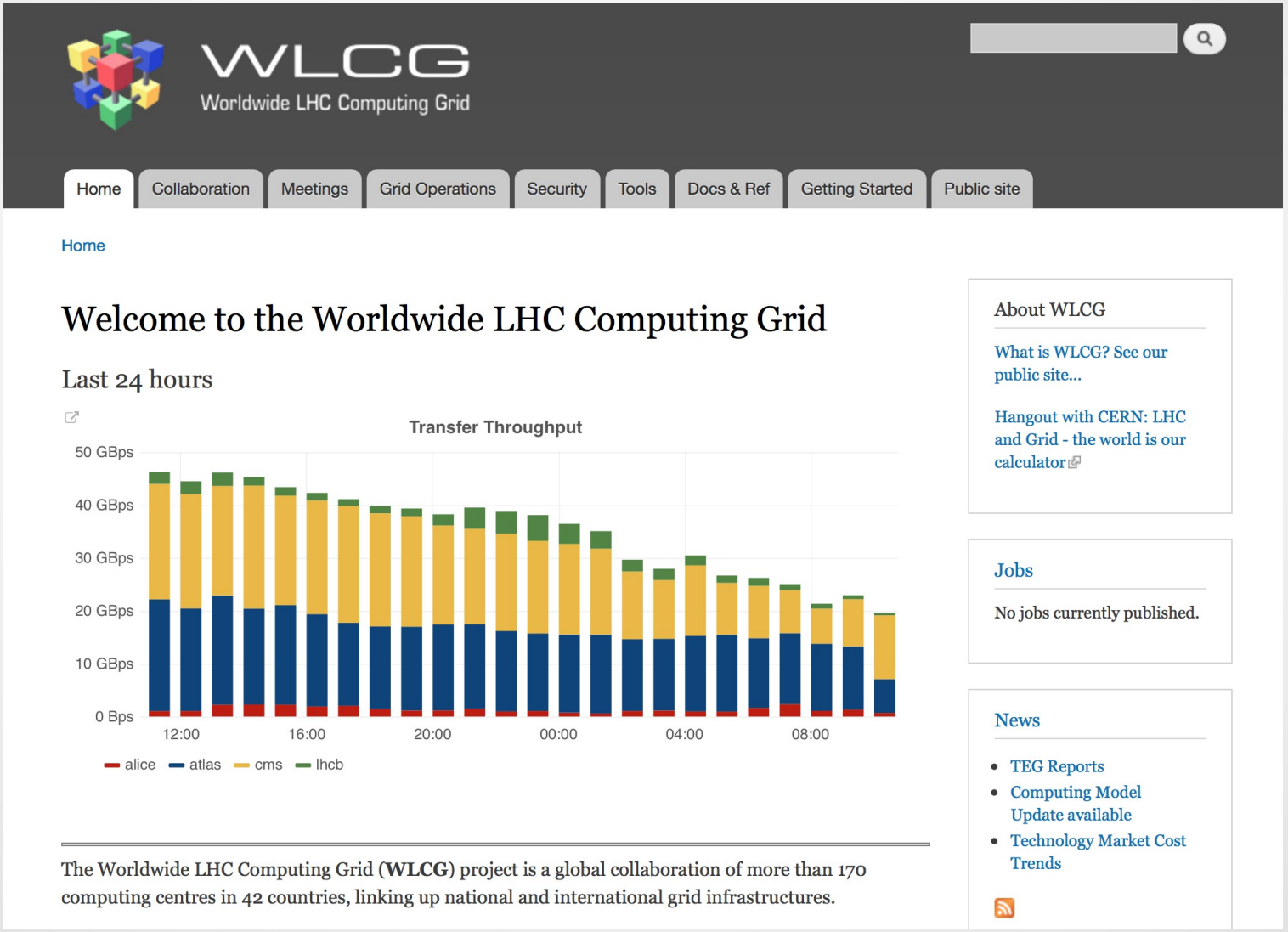
The ULiège website published a story (in French) about the work of Denis Baurain and his collaborators on the Tier-1 cluster Zenobe that lead to a publication in Nature Ecology & Evolution.

TUESDAY, 01 AUGUST 2017

Ariel Lozano is the new CÉCI logisticien

We are happy to announce the hire of a new CECI logisticien: Ariel Lozano. Welcome Ariel!

Grid computing



Cloud computing

3.

Programming models

Programming models

- Single computer:
  - multicore: PThreads, OpenMP, TBB, OpenCL
  - GPUs: CUDA, OpenCL, OpenAcc
- Multi-computer:
  - Distributed memory:
    - Shared storage: MPI (clusters)
    - Distributed storage: MapReduce (clouds)
    - No storage: BOINC (distributed computing)
  - Shared memory: CoArray, UPC

User tools

that GNU/Linux offers

Parallel processes in Bash

dfr@hmem00 — bash

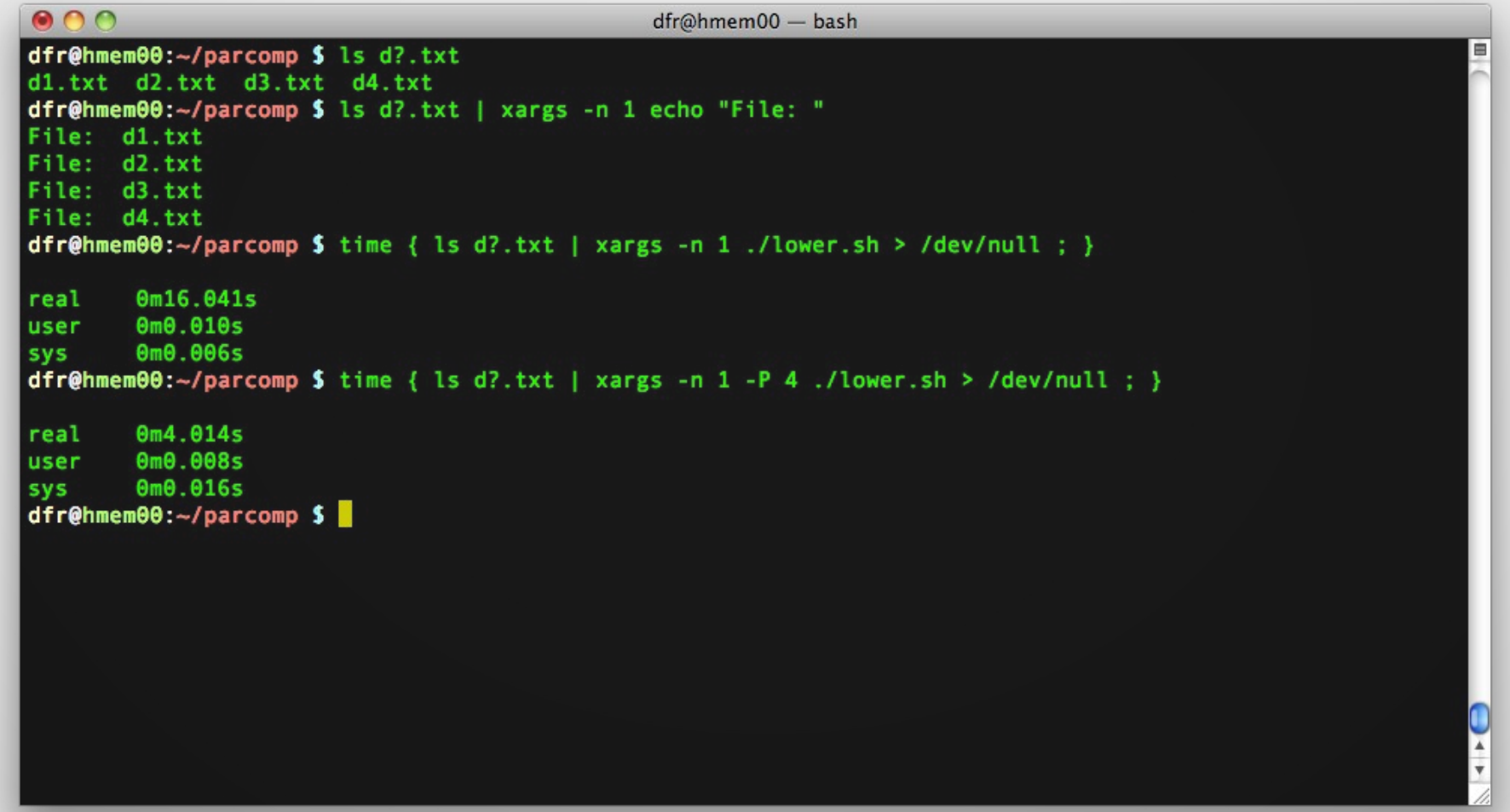
```
dfr@hmem00:~/parcomp $ cat lower.sh
#!/bin/bash
#
# Usage:
#    ./lower.sh [input_file [output_file]]
#
# Make ACTG chars lower case with extra processing.
#
# If output_file is not defined, stdout is used
# If input_file and output_file are not defined, stdin and stdout are used.

while read line; do
sleep 1
echo $line | tr ACTG actg >> ${2-/dev/stdout}
done < ${1-/dev/stdin}

dfr@hmem00:~/parcomp $ cat d.txt
G
C
A
G
dfr@hmem00:~/parcomp $ ./lower.sh d.txt
g
c
a
g
dfr@hmem00:~/parcomp $
```

Parallel processes in Bash

dfr@hmem00 — bash

```
dfr@hmem00:~/parcomp $ # Foreground: commands end with ';'
dfr@hmem00:~/parcomp $ time { ./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt ; };

real    0m8.033s
user    0m0.004s
sys     0m0.019s
dfr@hmem00:~/parcomp $ # Background, in parallel: commands end with '&' and 'wait' necessary
dfr@hmem00:~/parcomp $ time { ./lower.sh d2.txt r1.txt & ./lower.sh d2.txt r2.txt & wait ; };
[1] 49722
[2] 49723
[1]-  Done                    ./lower.sh d2.txt r1.txt
[2]+  Done                    ./lower.sh d2.txt r2.txt

real    0m4.011s
user    0m0.004s
sys     0m0.005s
dfr@hmem00:~/parcomp $
```

One program and many files

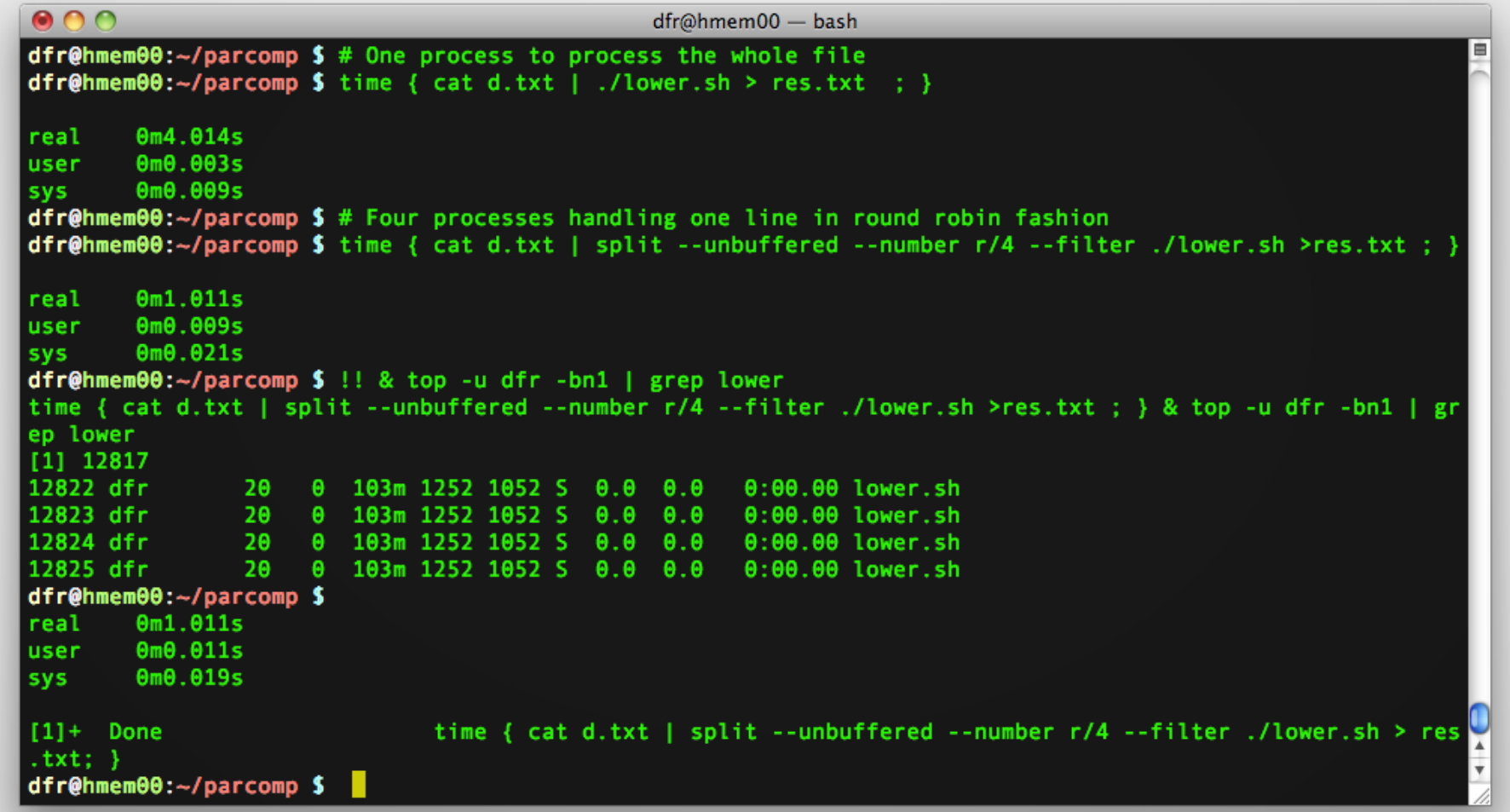


Several programs and one file

dfr@hmem00 — bash

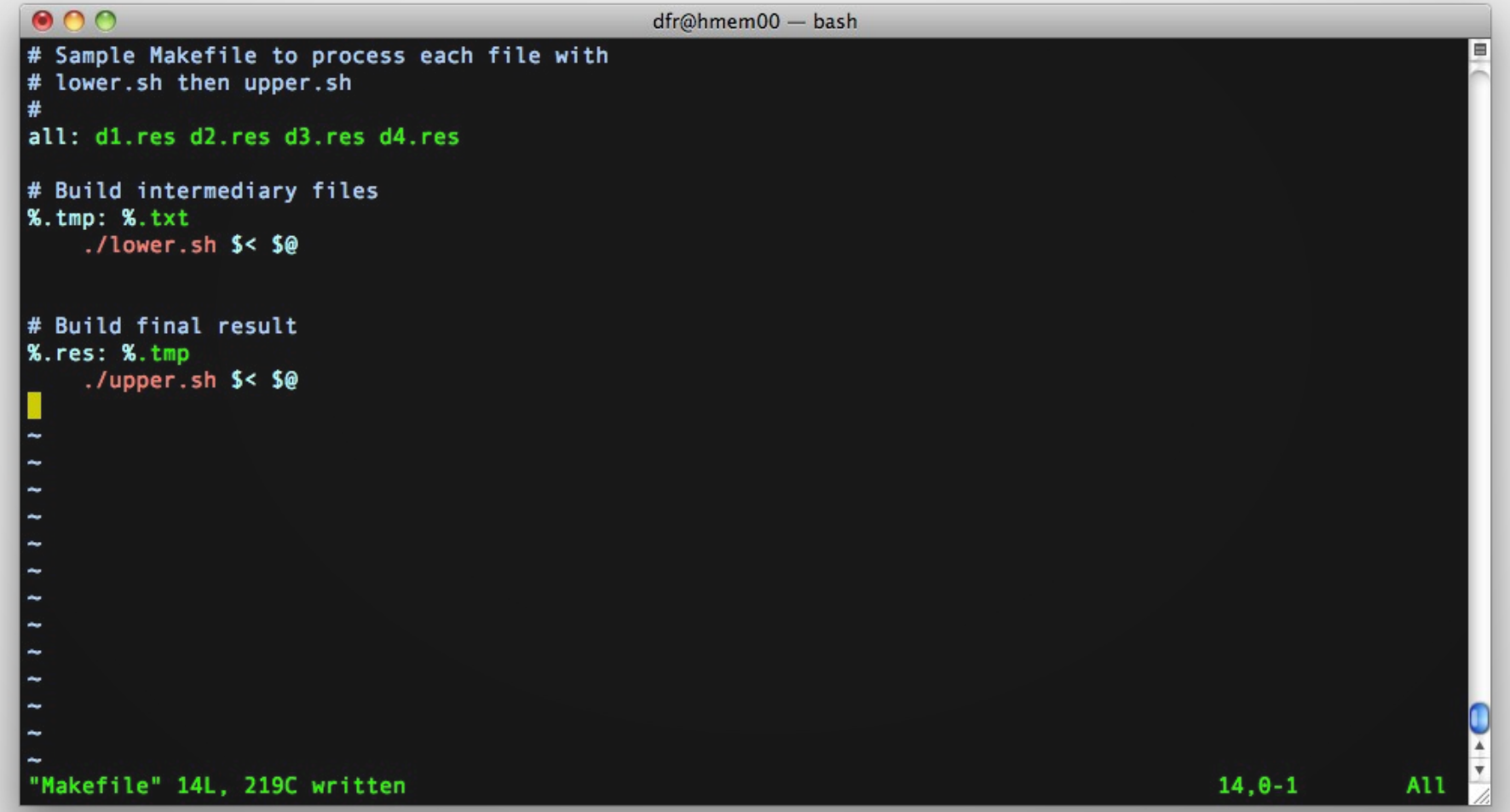
```
dfr@hmem00:~/parcomp $ # Using an intermediay file
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }

real    0m8.033s
user    0m0.005s
sys     0m0.017s
dfr@hmem00:~/parcomp $ # Using pipes (as our programs can handle stdin and stdout)
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt | ./upper.sh > res.txt ; }

real    0m5.014s
user    0m0.006s
sys     0m0.009s
dfr@hmem00:~/parcomp $ mkfifo tmpfifo
dfr@hmem00:~/parcomp $ ls -l tmpfifo
prw-rw-r-- 1 dfr dfr 0 Oct  7 10:27 tmpfifo
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt tmpfifo & ./upper.sh tmpfifo res.txt ; }
[1] 65343
[1]+  Done                    ./lower.sh d.txt tmpfifo

real    0m5.013s
user    0m0.002s
sys     0m0.007s
dfr@hmem00:~/parcomp $
```

One program and one large file



Need recent version of Coreutils/8.22-goolf-1.4.10

Several programs and many files



Several programs and many files

dfr@hmem00 — bash

```
dfr@hmem00:~/parcomp $ time make
./lower.sh d1.txt d1.tmp
./upper.sh d1.tmp d1.res
./lower.sh d2.txt d2.tmp
./upper.sh d2.tmp d2.res
./lower.sh d3.txt d3.tmp
./upper.sh d3.tmp d3.res
./lower.sh d4.txt d4.tmp
./upper.sh d4.tmp d4.res
rm d1.tmp d2.tmp d4.tmp d3.tmp

real    0m32.260s
user    0m0.028s
sys     0m0.099s
dfr@hmem00:~/parcomp $ rm *res
dfr@hmem00:~/parcomp $ time make -j 4
./lower.sh d1.txt d1.tmp
./lower.sh d2.txt d2.tmp
./lower.sh d3.txt d3.tmp
./lower.sh d4.txt d4.tmp
./upper.sh d1.tmp d1.res
./upper.sh d2.tmp d2.res
./upper.sh d4.tmp d4.res
./upper.sh d3.tmp d3.res
rm d1.tmp d2.tmp d4.tmp d3.tmp

real    0m8.163s
user    0m0.025s
```

Summary

- You have either
  - one very large file to process
    - with one program: split
    - with several programs: pipes, fifo
  - many files to process
    - with one program xargs
    - with many programs make

GNU Parallel

GNU Parallel

GNU **parallel** is a shell tool for executing jobs in parallel using one or more computers. A job can be a single command or a small script that has to be run for each of the lines in the input. The typical input is a list of files, a list of hosts, a list of users, a list of URLs, or a list of tables. A job can also be a command that reads from a pipe. GNU **parallel** can then split the input and pipe it into commands in parallel.

If you use xargs and tee today you will find GNU **parallel** very easy to use as GNU **parallel** is written to have the same options as xargs. If you write loops in shell, you will find GNU **parallel** may be able to replace most of the loops and make them run faster by running several jobs in parallel.

GNU **parallel** makes sure output from the commands is the same output as you would get had you run the commands sequentially. This makes it possible to use output from GNU **parallel** as input for other programs.

For people who live life in the parallel lane.

For each line of input GNU **parallel** will execute *command* with the line as arguments. If no *command* is given, the line of input is executed. Several lines will be run in parallel. GNU **parallel** can often be used as a substitute for **xargs** or **cat | bash**.

More complicated to use but very powerful

GNU Parallel

- Syntax: parallel *command* ::: *argument list*

```
dfr@hmem00 — bash
dfr@hmem00:~/parcomp $ parallel echo ::: 1 2 3 4
1
2
3
4
dfr@hmem00:~/parcomp $ parallel echo ::: {1..10}
1
2
3
4
5
6
7
8
9
10
dfr@hmem00:~/parcomp $ time parallel sleep ::: {1..10}

real    0m11.200s
user    0m0.206s
sys     0m0.129s
dfr@hmem00:~/parcomp $ parallel echo ::: d?.txt
d1.txt
d2.txt
d3.txt
d4.txt
dfr@hmem00:~/parcomp $
```

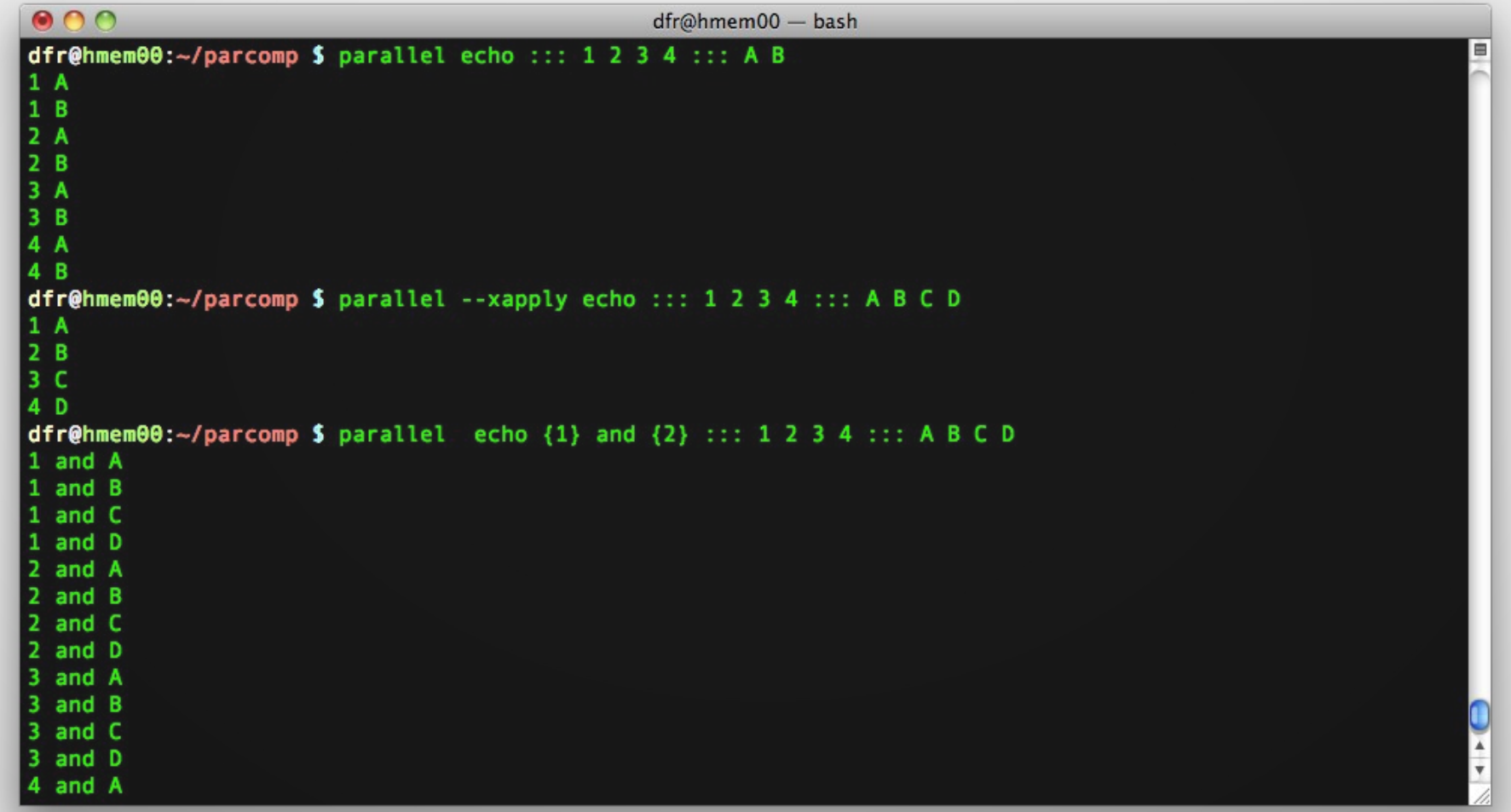
GNU Parallel

- Syntax: {} as argument placeholder. Can be modified

```
dfr@hmem00:~/parcomp $ parallel echo {} ::: d?.txt
d1.txt
d2.txt
d3.txt
d4.txt
dfr@hmem00:~/parcomp $ parallel echo {} {.}.res ::: d?.txt
d1.txt d1.res
d2.txt d2.res
d3.txt d3.res
d4.txt d4.res
dfr@hmem00:~/parcomp $ parallel echo {} ::: ../parcomp/d?.txt
../parcomp/d1.txt
../parcomp/d2.txt
../parcomp/d3.txt
../parcomp/d4.txt
dfr@hmem00:~/parcomp $ parallel echo {/} ::: ../parcomp/d?.txt
d1.txt
d2.txt
d3.txt
d4.txt
dfr@hmem00:~/parcomp $
dfr@hmem00:~/parcomp $
dfr@hmem00:~/parcomp $
```

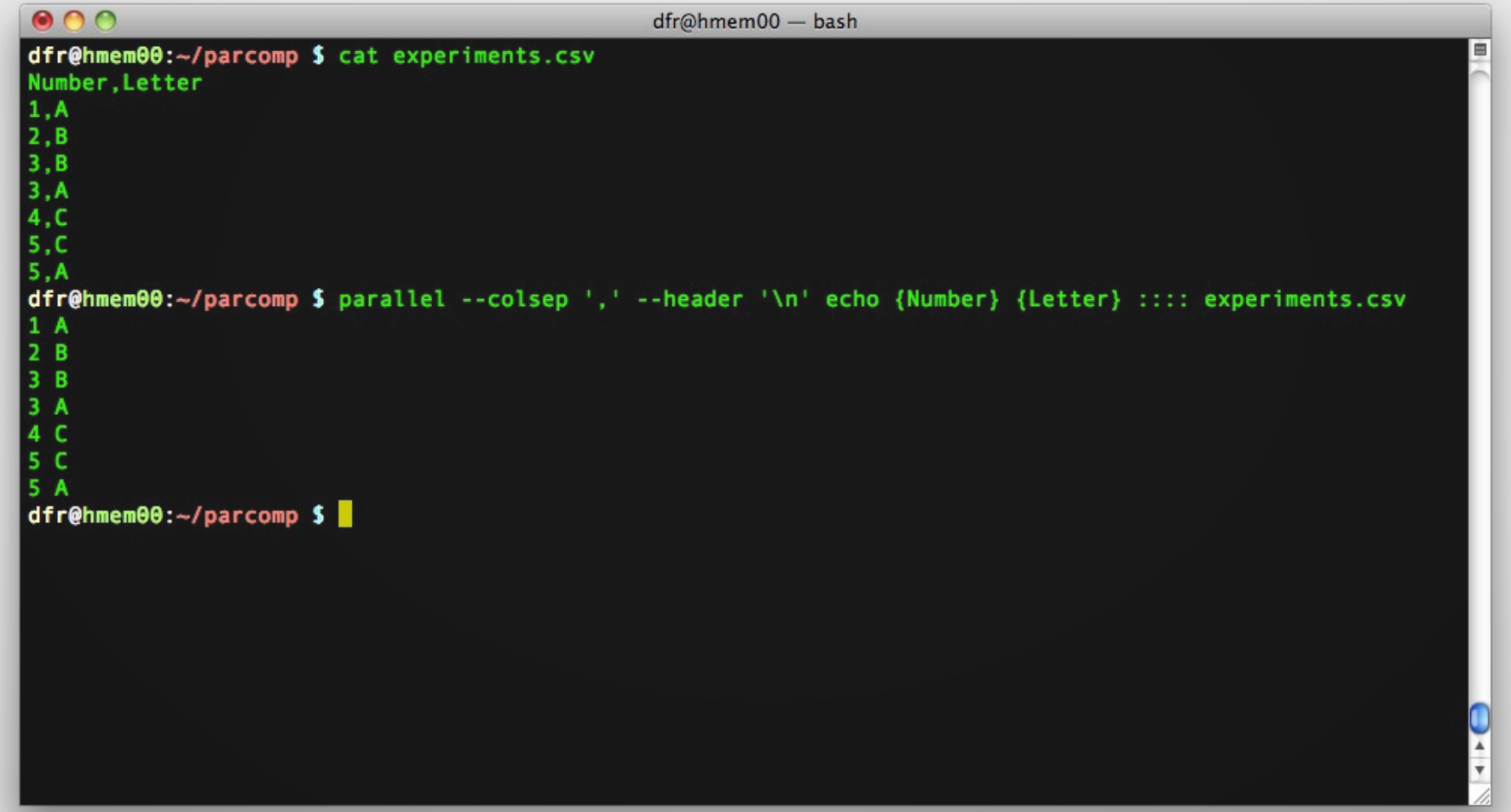
GNU Parallel

- Syntax: --xapply



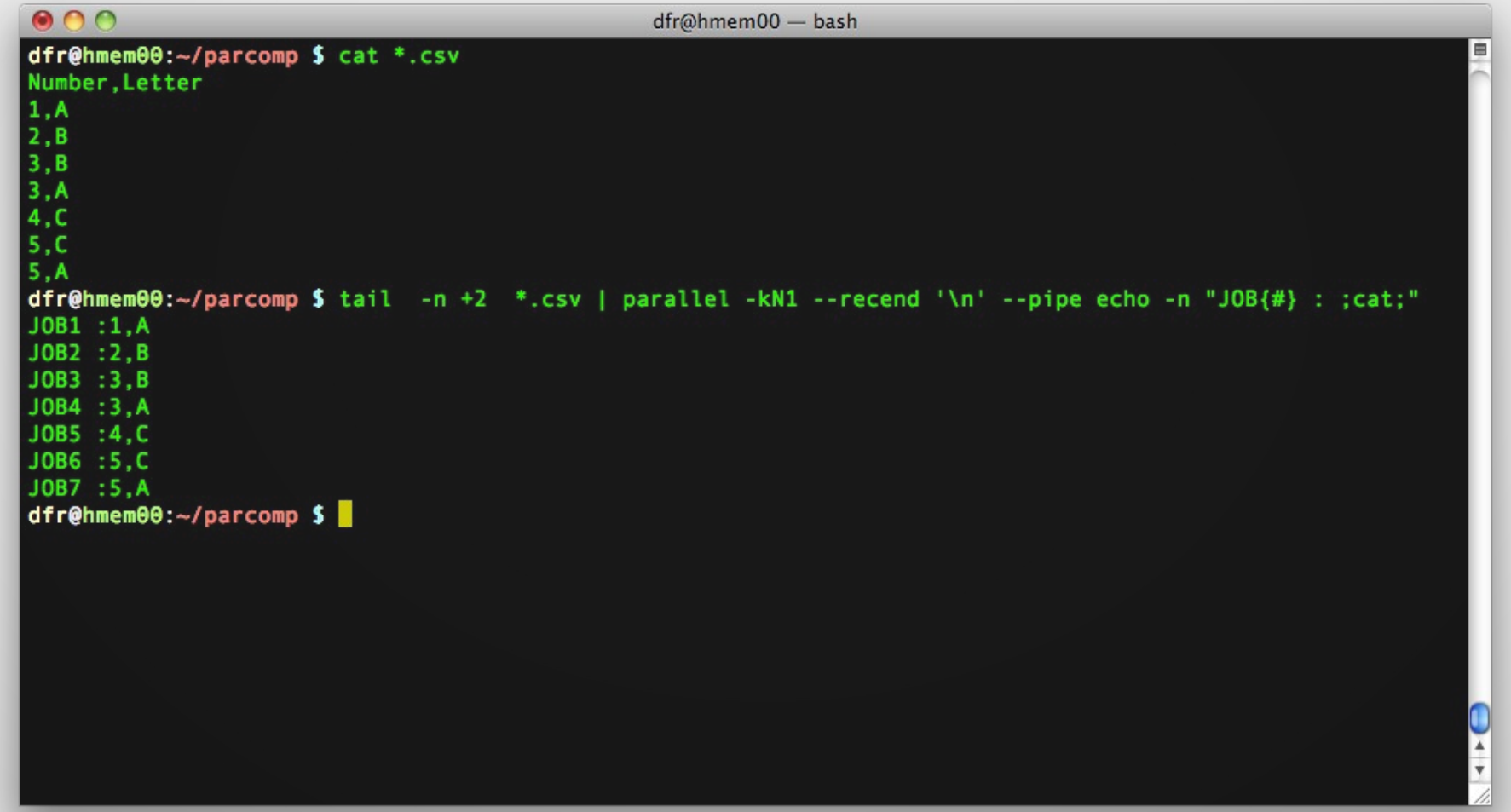
GNU Parallel

- Syntax: :::: arguments in file



GNU Parallel

- Syntax: --pipe



Other interesting options

`-S`	Use remote servers through SSH
`-j n`	Run n jobs in parallel
`-k`	Keep same order
`--delay n`	Ensure there are n seconds between each start
`--timeout n`	Kill task after n seconds if still running

Author asks to be cited: O. Tange (2011): *GNU Parallel - The Command-Line Power Tool*, The USENIX Magazine, February 2011:42-47.

Exercise

Reproduce the examples with ./lower and ./upper.sh using GNU Parallel

Solutions

- One program and many files

```
$ time parallel -k ./lower.sh {} > res.txt  ::: d?.txt
```

- One program and one large file

```
$ time cat d.txt | parallel -k -N1 --pipe ./lower.sh {} > res.txt
```

- Several programs and several files

```
$ time { parallel ./lower.sh {} {.}.tmp ::: d?.txt ; \
> parallel  ./upper.sh {} {.}.res ::: d?.tmp ; }
```