C.E.C.I

Consortium des Equipements
de Calcul Intensif
en Fédération Wallonie-Bruxelles

Introduction to Parallel Computing

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UCL Université catholique de Louvain

INSTITUT DE CALCUL INTENSIF ET DE STOCKAGE DE MASSE

Agenda

1. General concepts, definitions, blockers
2. Hardware for parallel computing
3. Programming models
4. User tools

1.

General concepts

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)

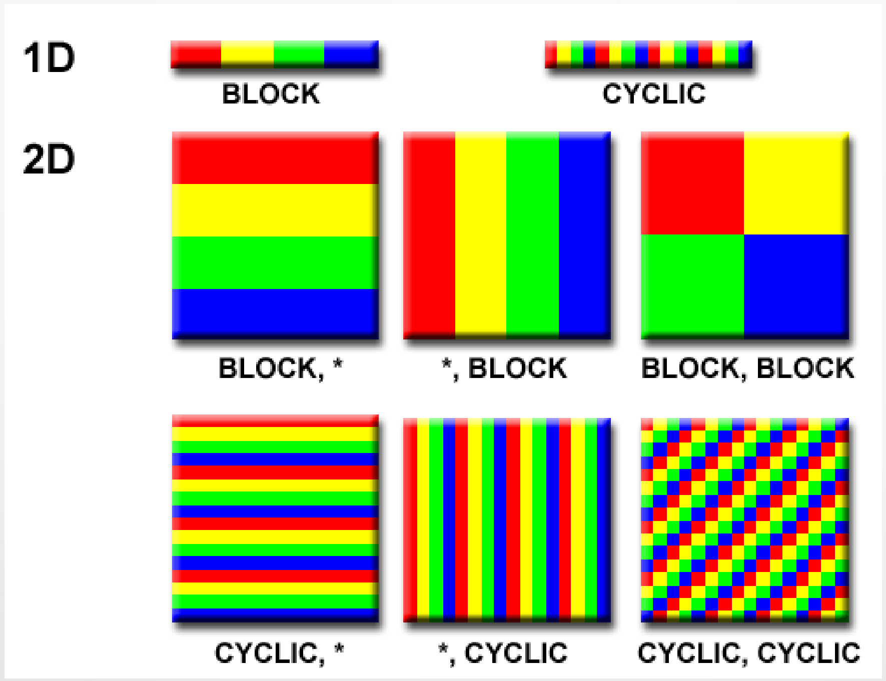
Scale out – Solve many problems
→ more storage capacity

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

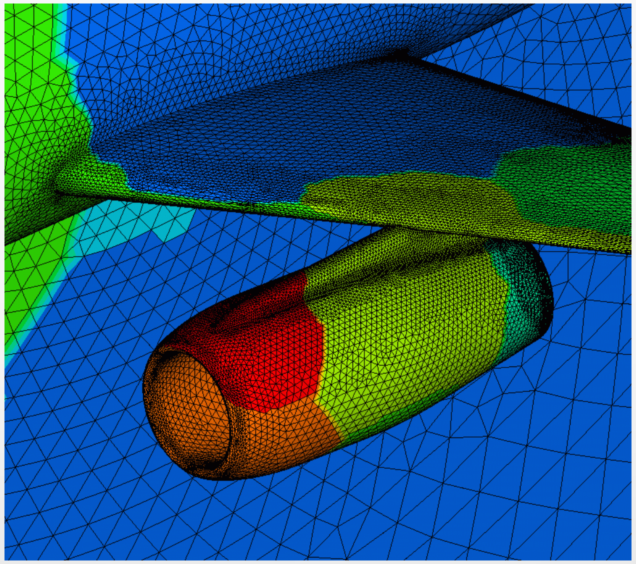
- **Work decomposition** : task-level parallelism
- **Data decomposition** : data-level parallelism
  - **Block, cyclic**



https://nyu-cds.github.io/python-mpi/04-decomposition/

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



https://fun3d.larc.nasa.gov/example-54.html

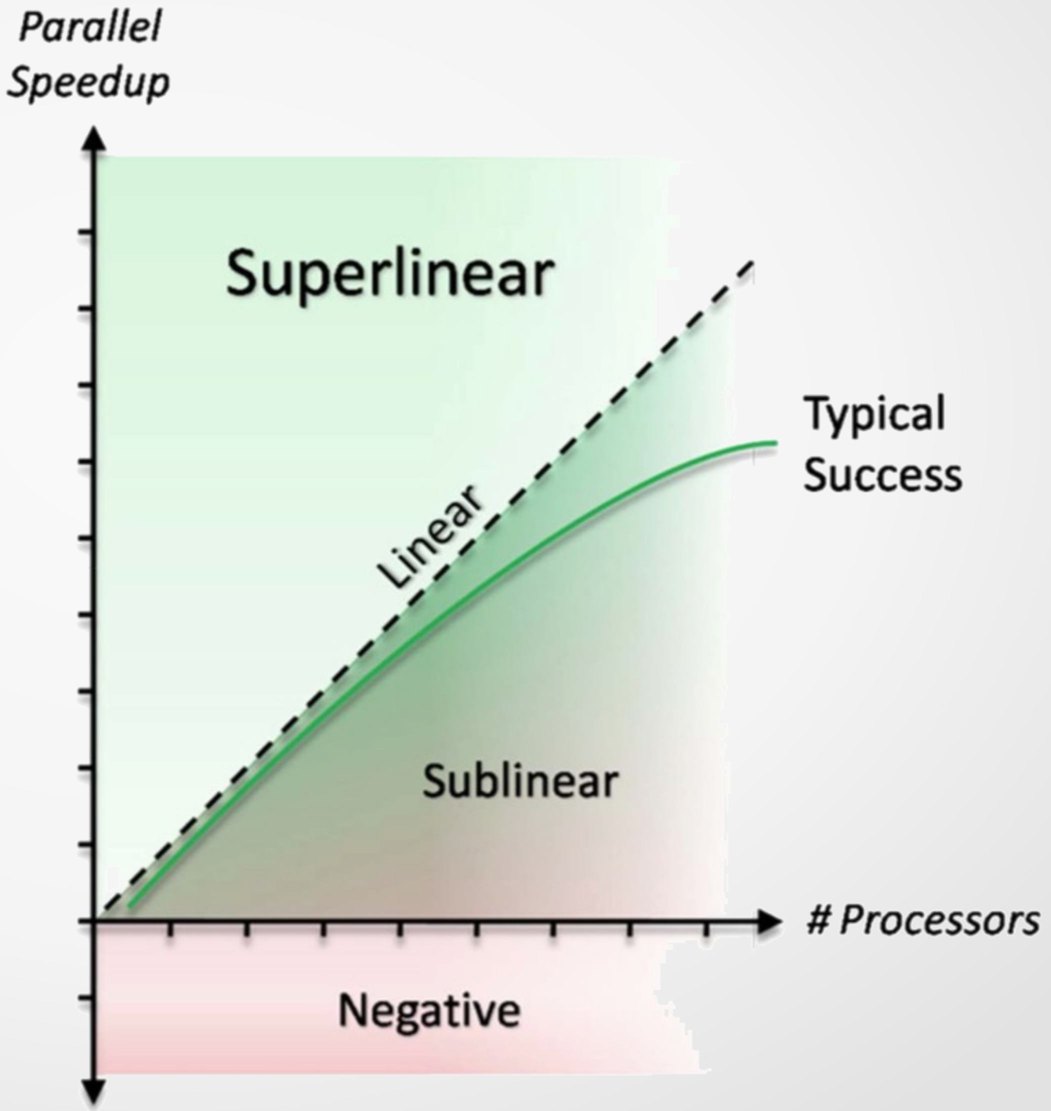
Collaboration

- **Synchronous** (SIMD) at the processor level ; the same processor instruction for each worker at any time ; e.g. linear algebrae
- **Fine-grained** parallelism if subtasks must communicate many times per second (typically at the loop level)
- **Coarse-grained** parallelism if they do not communicate many times per second (typically function-call level) e.g. global parameter optimisation
- **Embarrassingly parallel** if they rarely or never have to communicate (asynchronous) – e.g. identical processing of multiple files

Speedup, Efficiency, Scalability

$$S = \frac{T_S}{T_P}$$

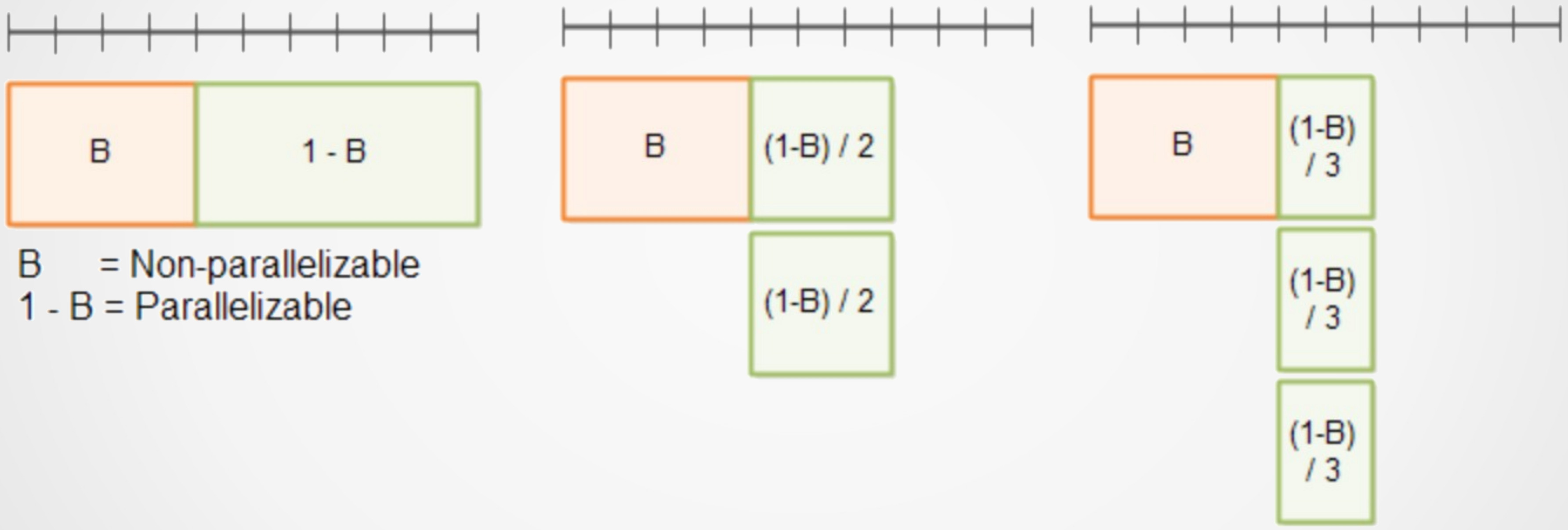
$$E = \frac{S}{p} = \frac{T_S}{pT_p}$$



https://www.cs.uky.edu/~jzhang/CS621/chapter7.pdf

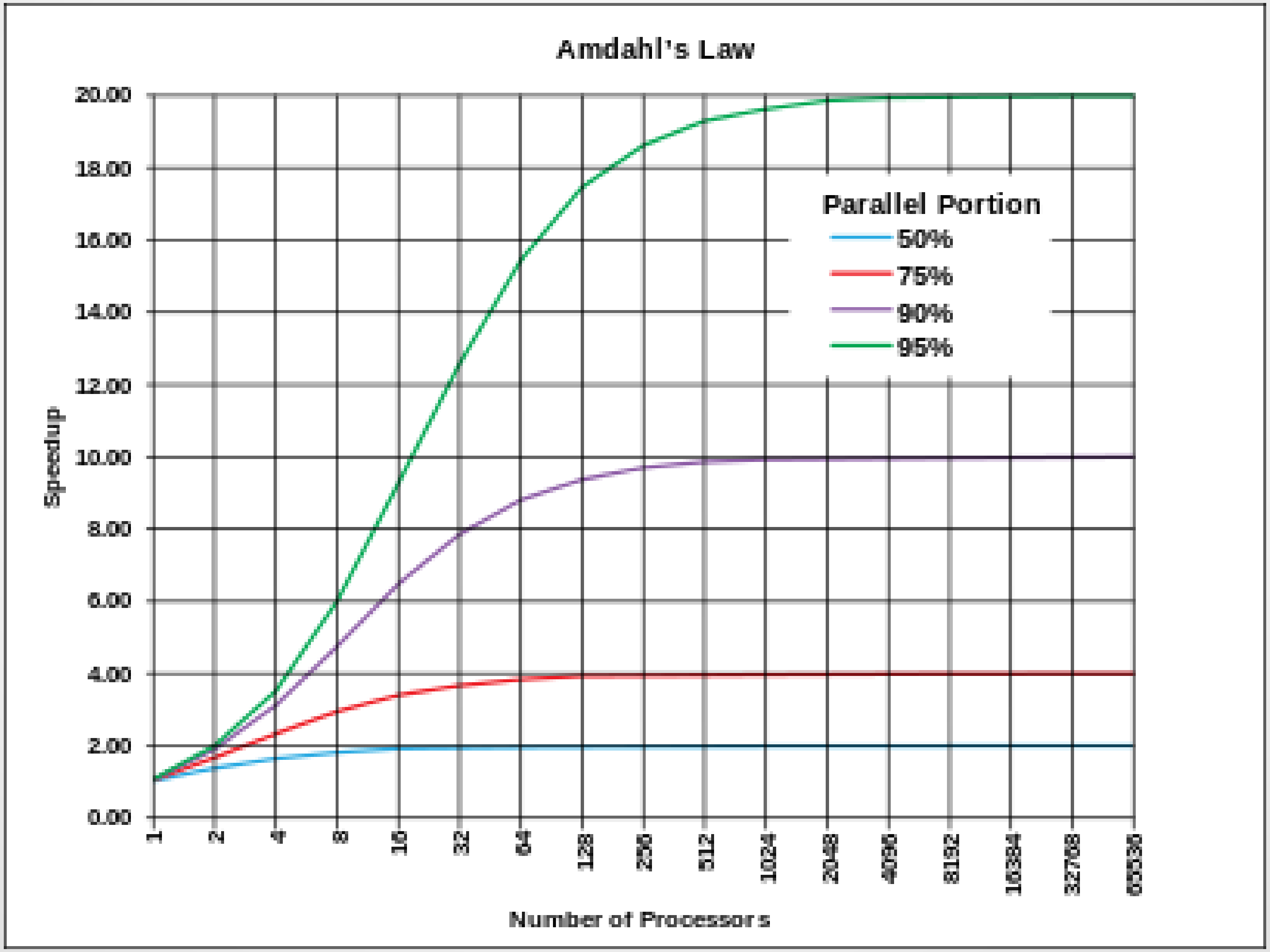
Issue 1: Amdahl's Law

Often, not all the work can be decomposed



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

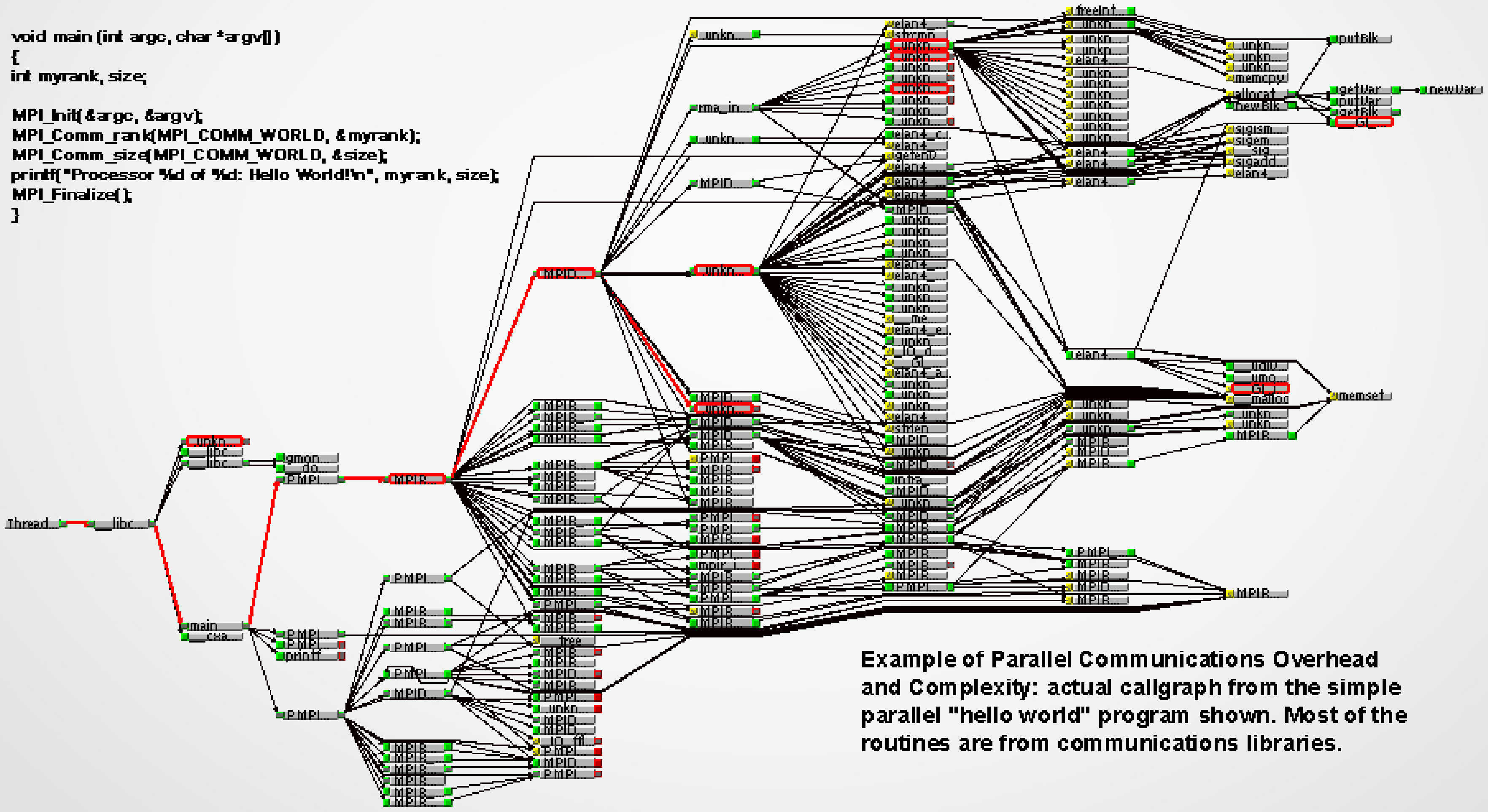
Issue 1: Amdahl's Law



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

Issue 2: Parallel overhead

Collaboration means communication and a lot of extra work



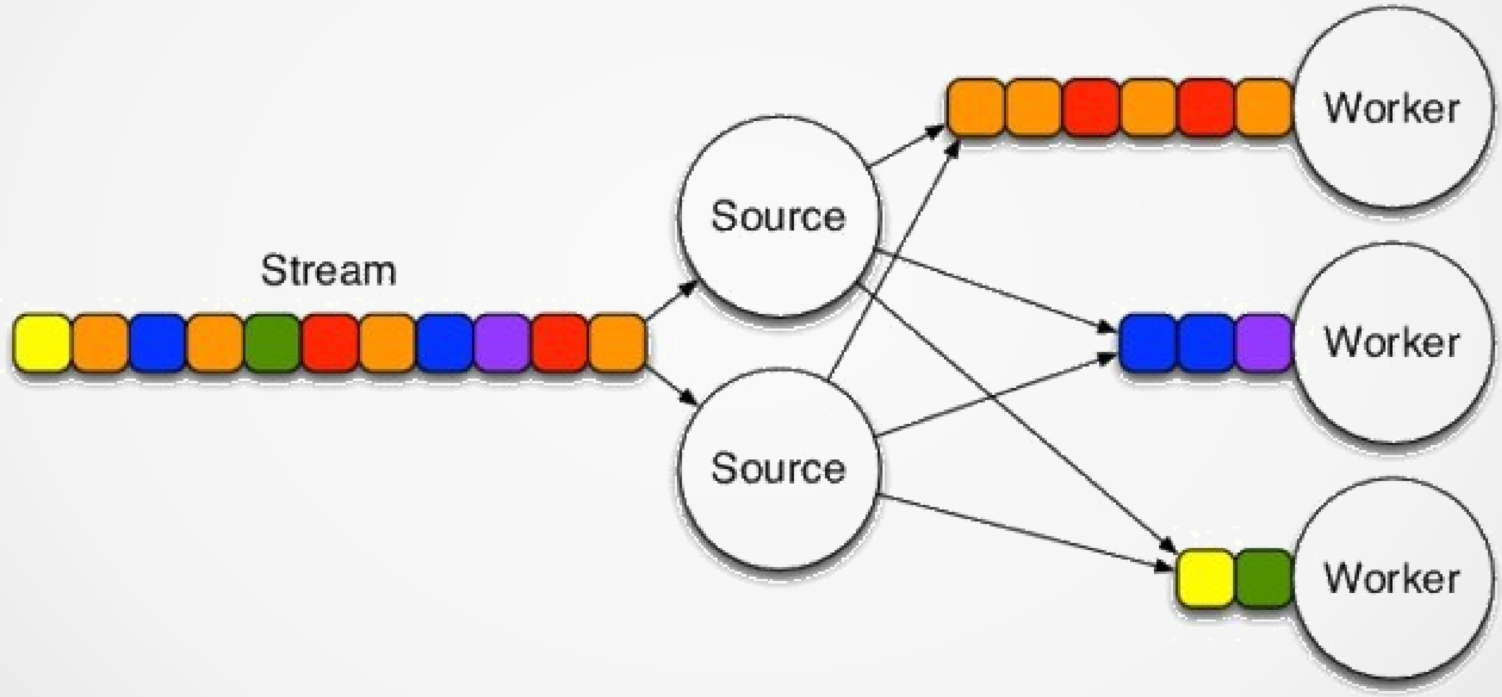
```
void main (int argc, char *argv[])
{
int myrank, size;

MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
printf("Processor %d of %d: Hello World!\n", myrank, size);
MPI_Finalize();
}
```

Example of Parallel Communications Overhead and Complexity: actual callgraph from the simple parallel "hello world" program shown. Most of the routines are from communications libraries.

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

Issue 2: Parallel overhead

Load imbalance



2.

Hardware for parallel computing

At the core level

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

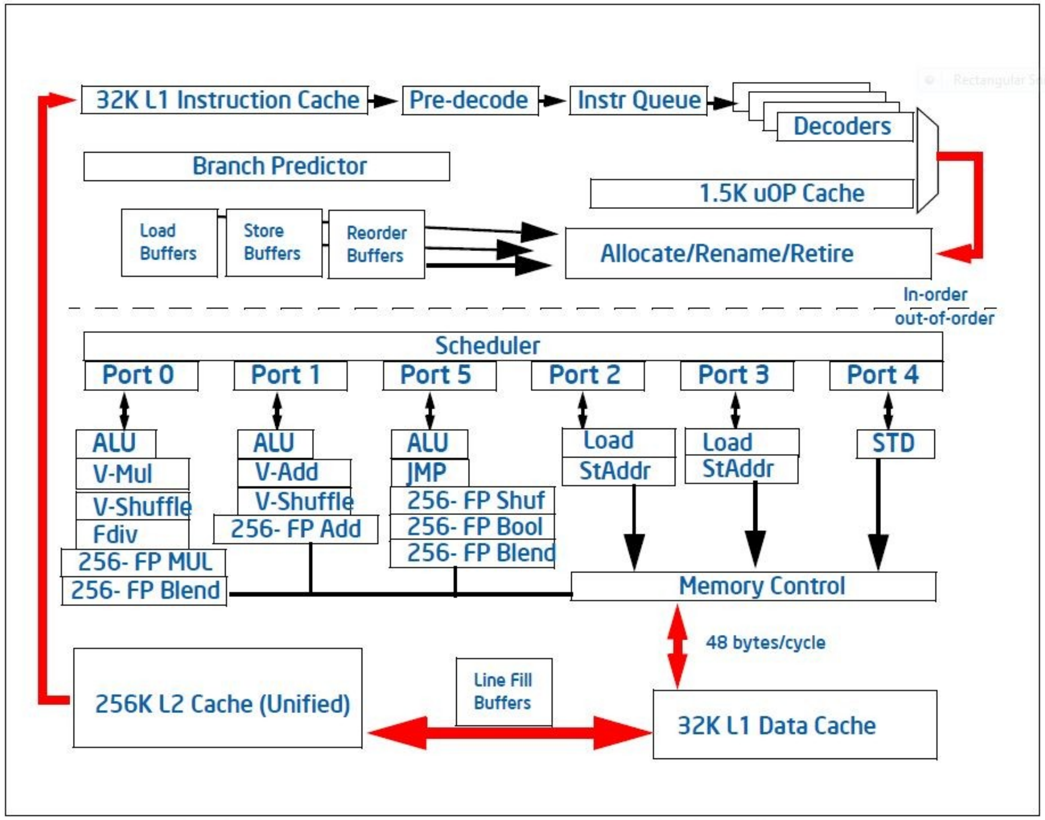
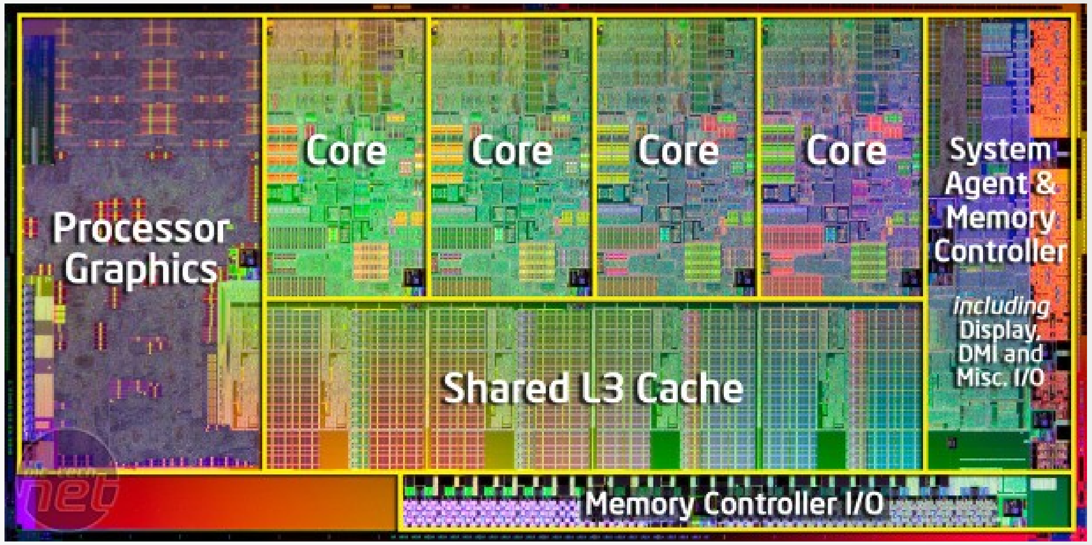


Figure 2-1. Intel microarchitecture code name Sandy Bridge Pipeline Functionality

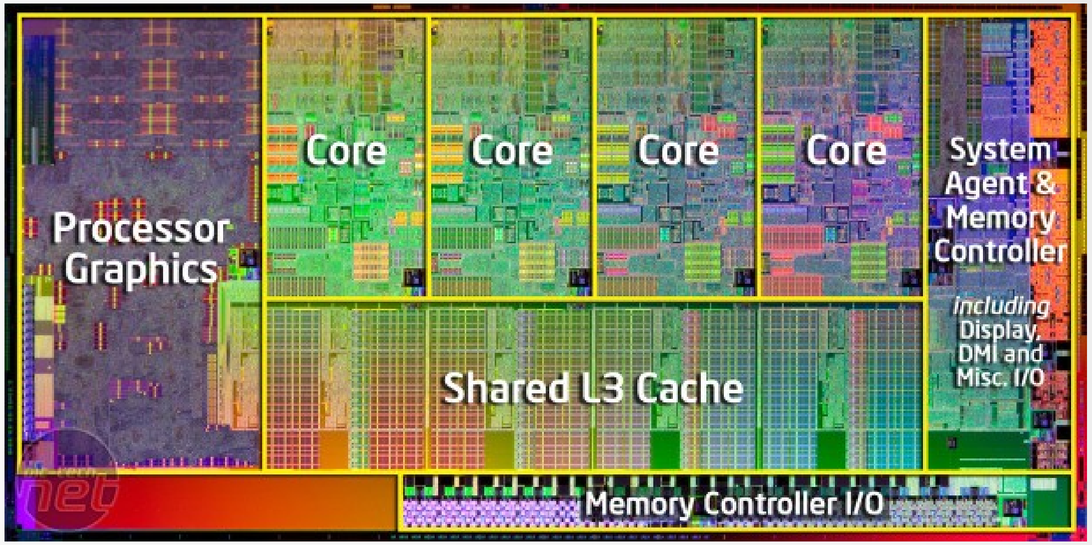
At the CPU (socket) level

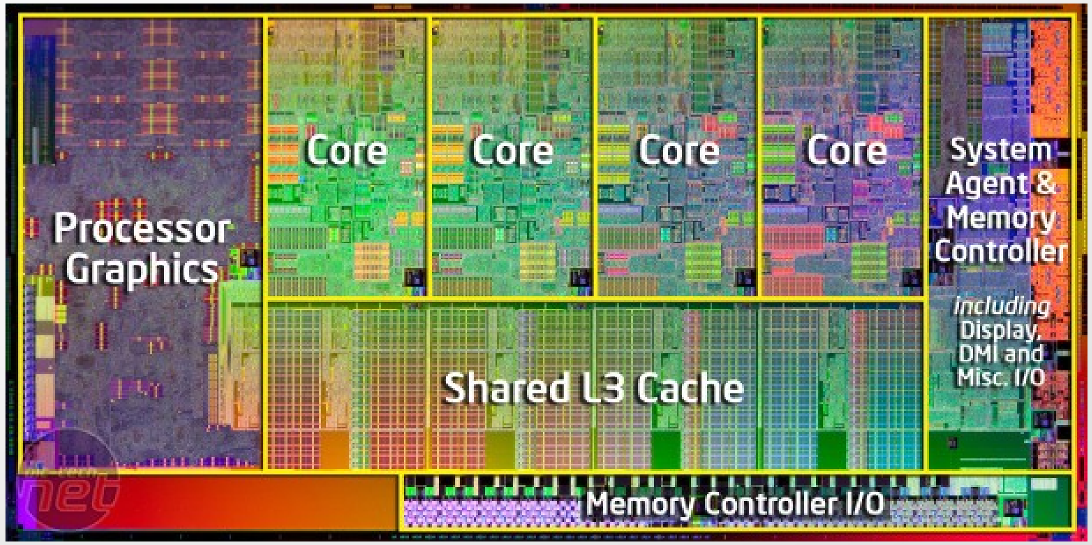
- Multicore parallelism



At the computer level

- Multi-socket parallelism
  - SMP
  - NUMA
- Accelerators





At the data center level

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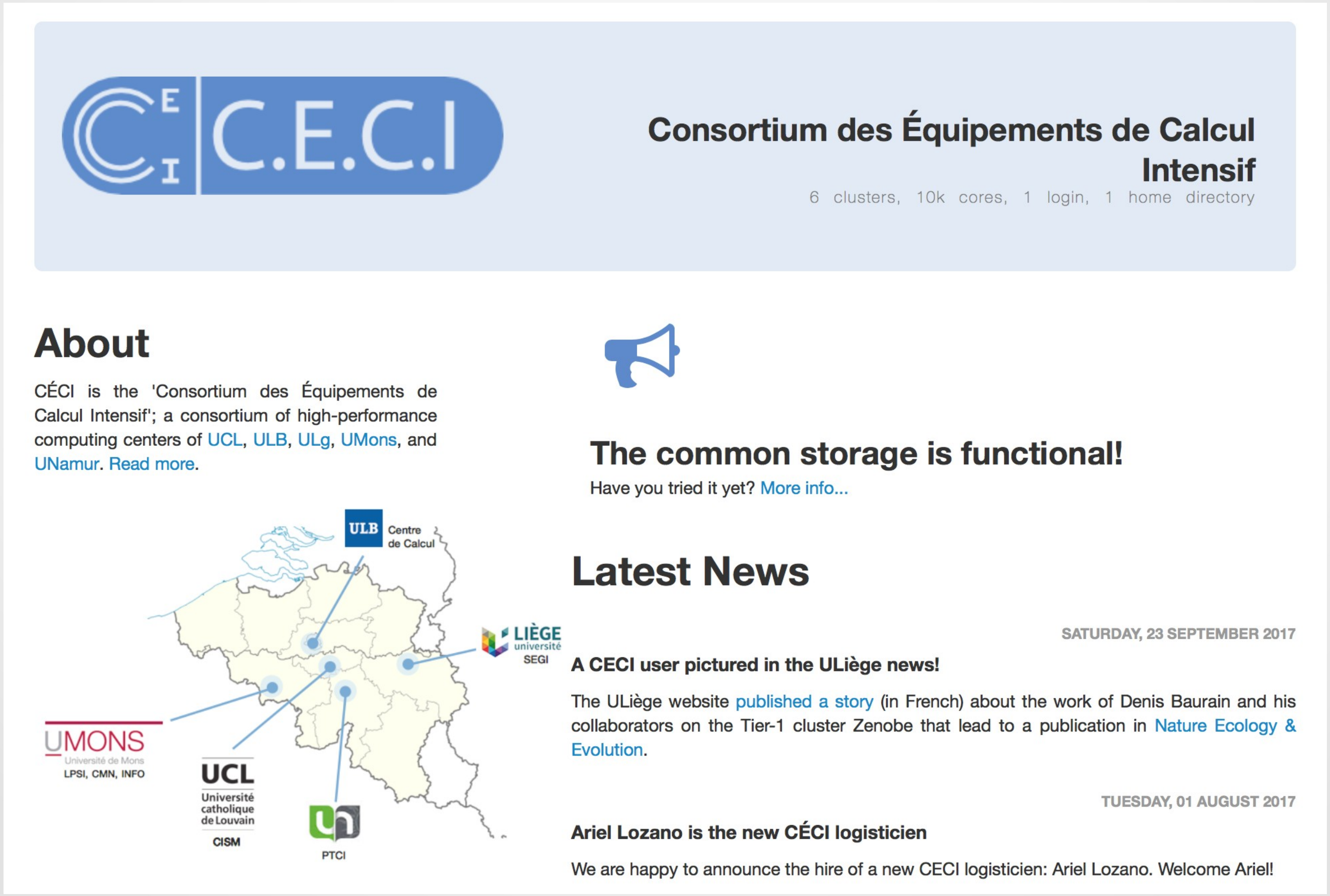
At the data center level

Cluster computing

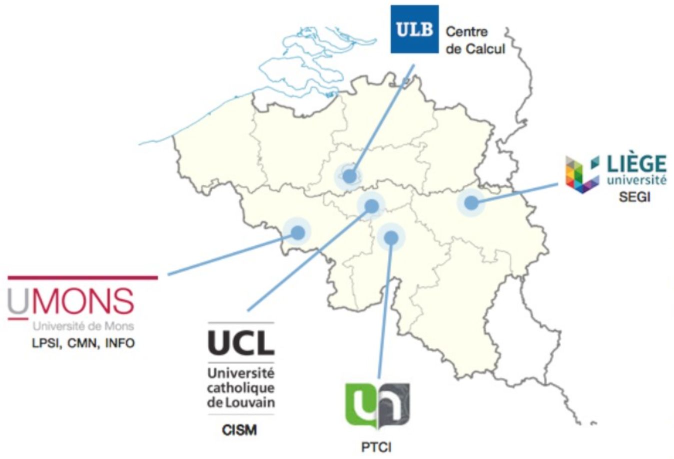


Consortium des Équipements de Calcul Intensif

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.


ULB Centre de Calcul
LIÈGE université SEGI
UMONS Université de Mons LPSI, CMN, INFO
UCL Université catholique de Louvain CISM
PTCI

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.

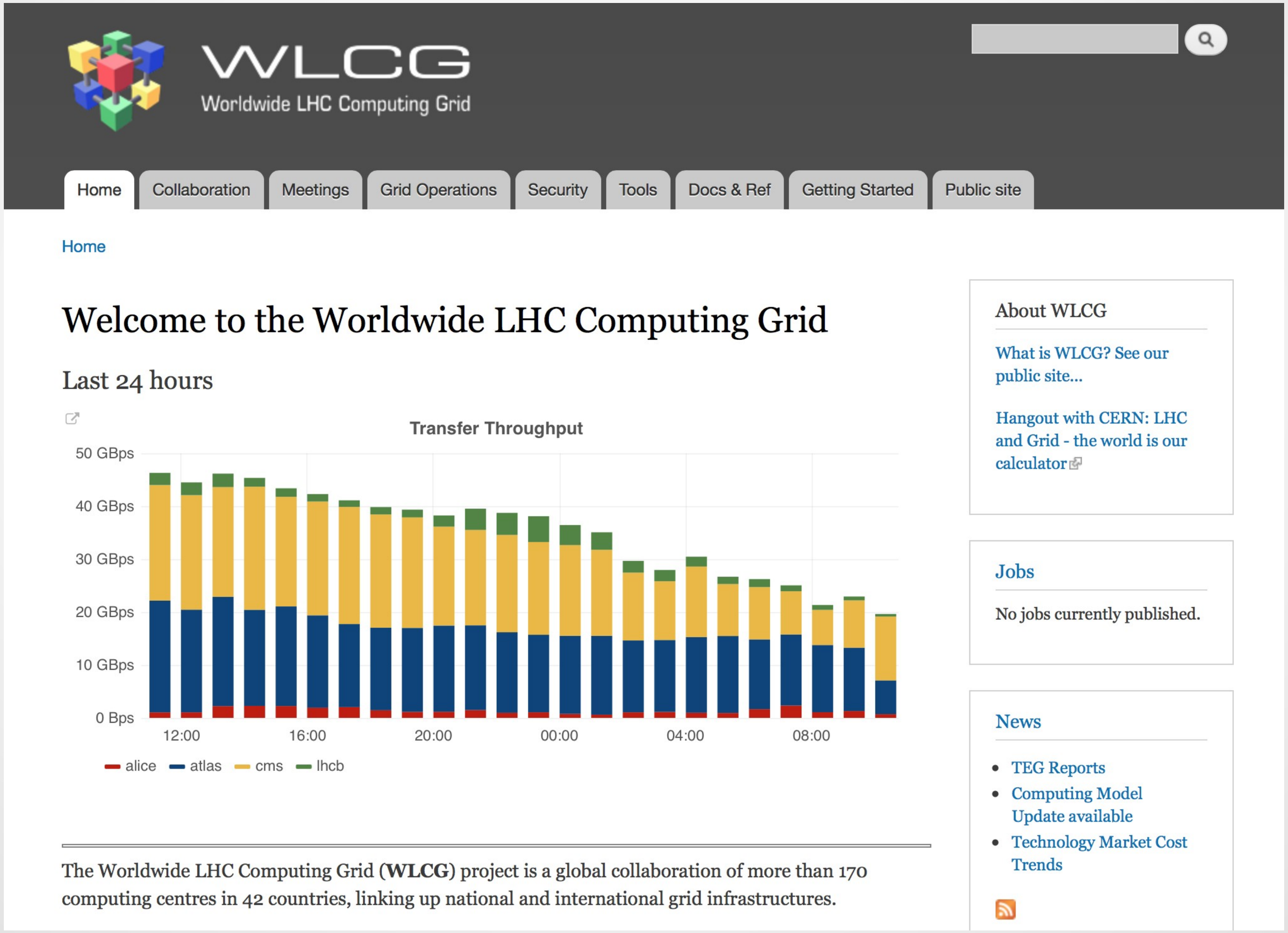
TUESDAY, 01 AUGUST 2017

Ariel Lozano is the new CÉCI logisticien

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

At the world level

Grid computing



Welcome to the Worldwide LHC Computing Grid

Last 24 hours

The Worldwide LHC Computing Grid (**WLCG**) project is a global collaboration of more than 170 computing centres in 42 countries, linking up national and international grid infrastructures.

About WLCG

What is WLCG? See our public site...

Hangout with CERN: LHC and Grid - the world is our calculator

Jobs

No jobs currently published.

News

- TEG Reports
- Computing Model Update available
- Technology Market Cost Trends

At the data center level

C.E.C.I

Cloud computing

amazon web services

Google Cloud Platform

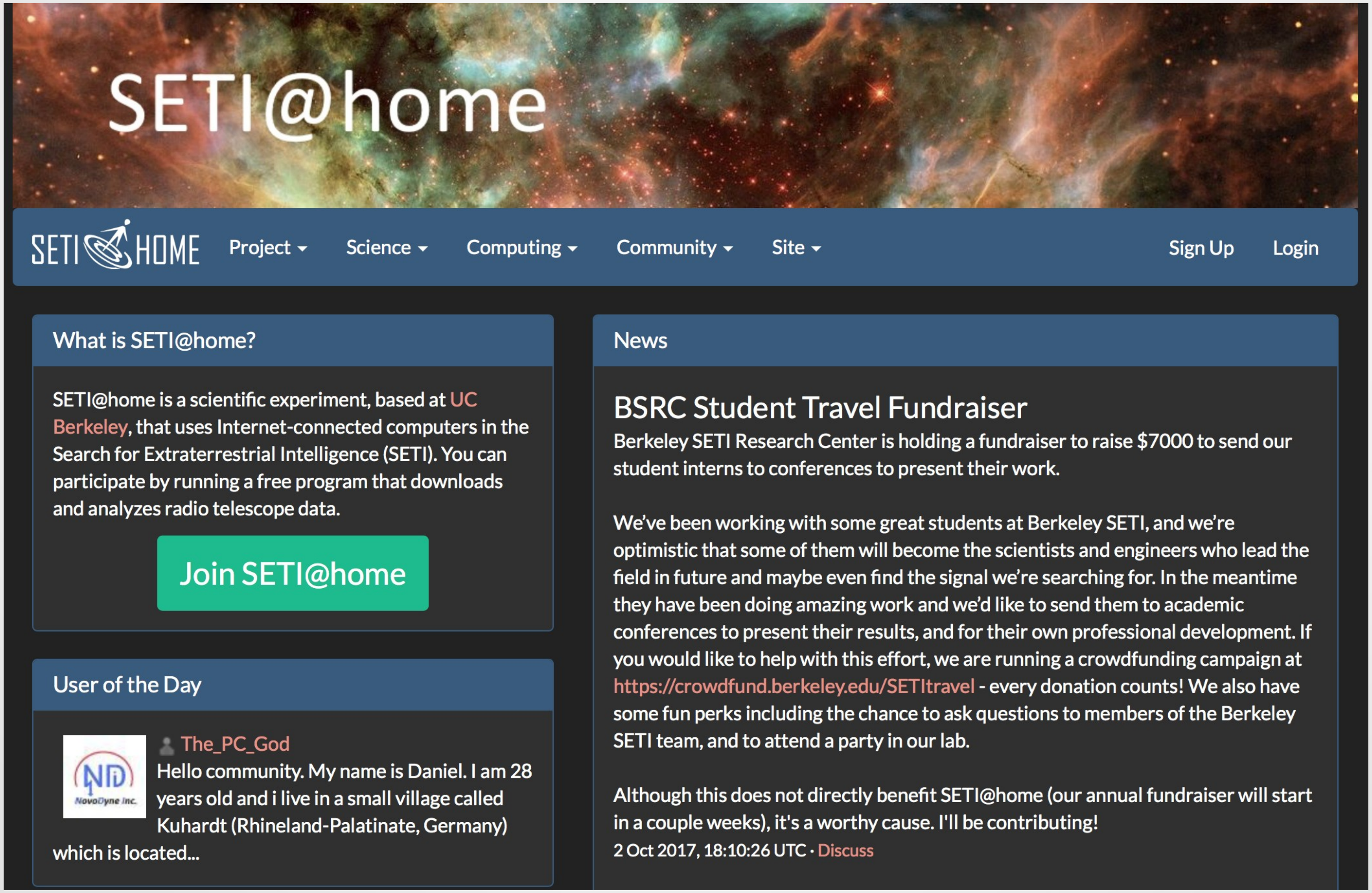
Microsoft Azure

OpenNebula

openstack™

At the world level

Distributed computing



What is SETI@home?

SETI@home is a scientific experiment, based at UC Berkeley, that uses Internet-connected computers in the Search for Extraterrestrial Intelligence (SETI). You can participate by running a free program that downloads and analyzes radio telescope data.

Join SETI@home

User of the Day

The_PC_God
Hello community. My name is Daniel. I am 28 years old and i live in a small village called Kuhardt (Rhineland-Palatinate, Germany) which is located...

News

BSRC Student Travel Fundraiser

Berkeley SETI Research Center is holding a fundraiser to raise $7000 to send our student interns to conferences to present their work.

We've been working with some great students at Berkeley SETI, and we're optimistic that some of them will become the scientists and engineers who lead the field in future and maybe even find the signal we're searching for. In the meantime they have been doing amazing work and we'd like to send them to academic conferences to present their results, and for their own professional development. If you would like to help with this effort, we are running a crowdfunding campaign at https://crowdfund.berkeley.edu/SETItravel - every donation counts! We also have some fun perks including the chance to ask questions to members of the Berkeley SETI team, and to attend a party in our lab.

Although this does not directly benefit SETI@home (our annual fundraiser will start in a couple weeks), it's a worthy cause. I'll be contributing!
2 Oct 2017, 18:10:26 UTC · Discuss

3.

Programming models

Parallel programming paradigms

How is work organized?

- **Task-farming:** no communication among workers
  - Master distribute work to workers (leader/follower); or
  - Workers pick up tasks from pool (work stealing).
- **SPMD** (Single program multiple data)

  A single program that contains both the logic for distributing work (master) and the computing part (workers) of which many instances are started and linked together at the same time
- **MPMD** (Multiple programs multiple data)

Parallel programming paradigms

How is work organized?

- **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)

Programming models

What programming libraries/syntax constructs, etc. exist?

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

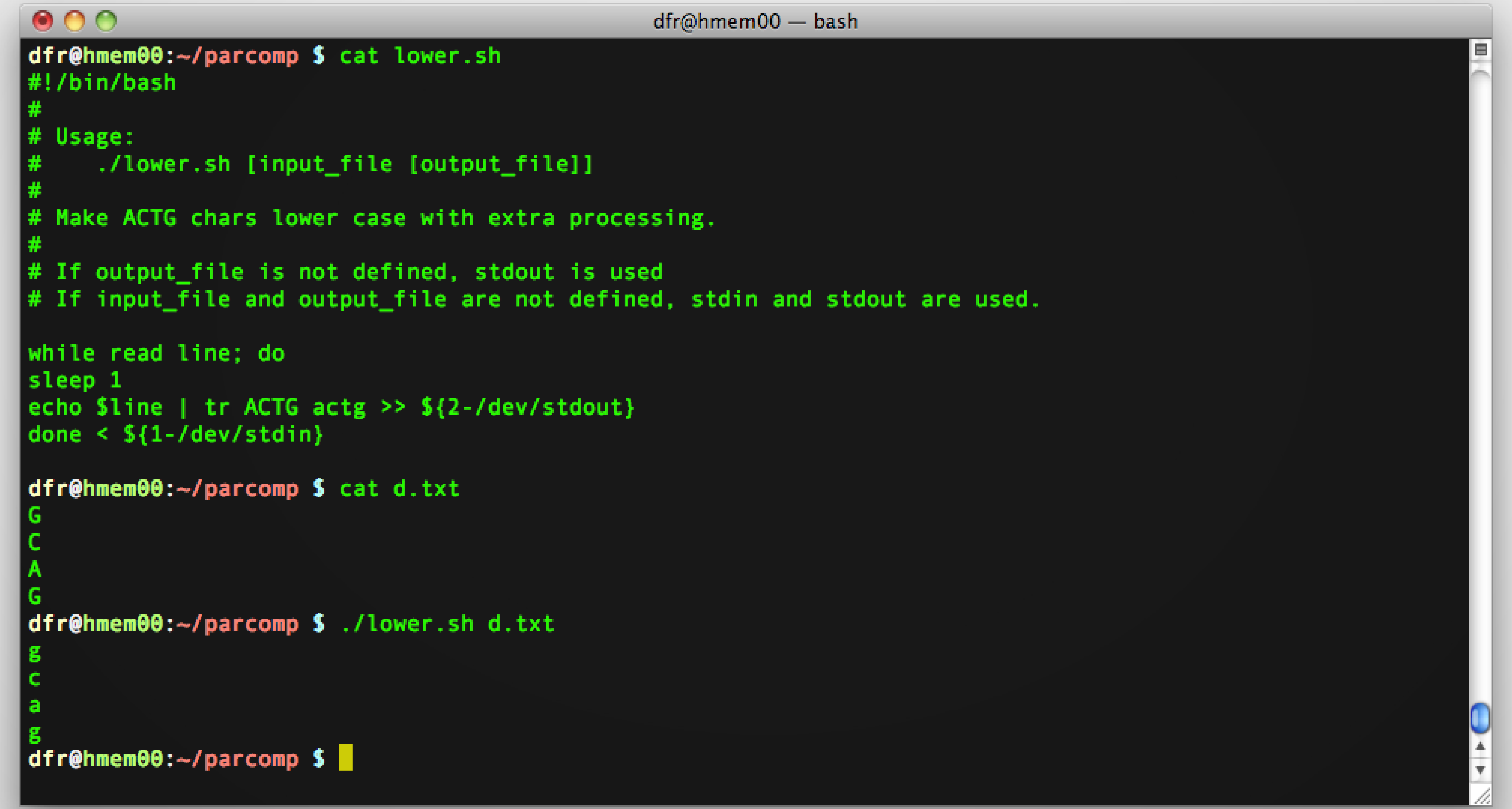
4.

User tools

that GNU/Linux offers

Parallel processes in Bash

Consider the following example program

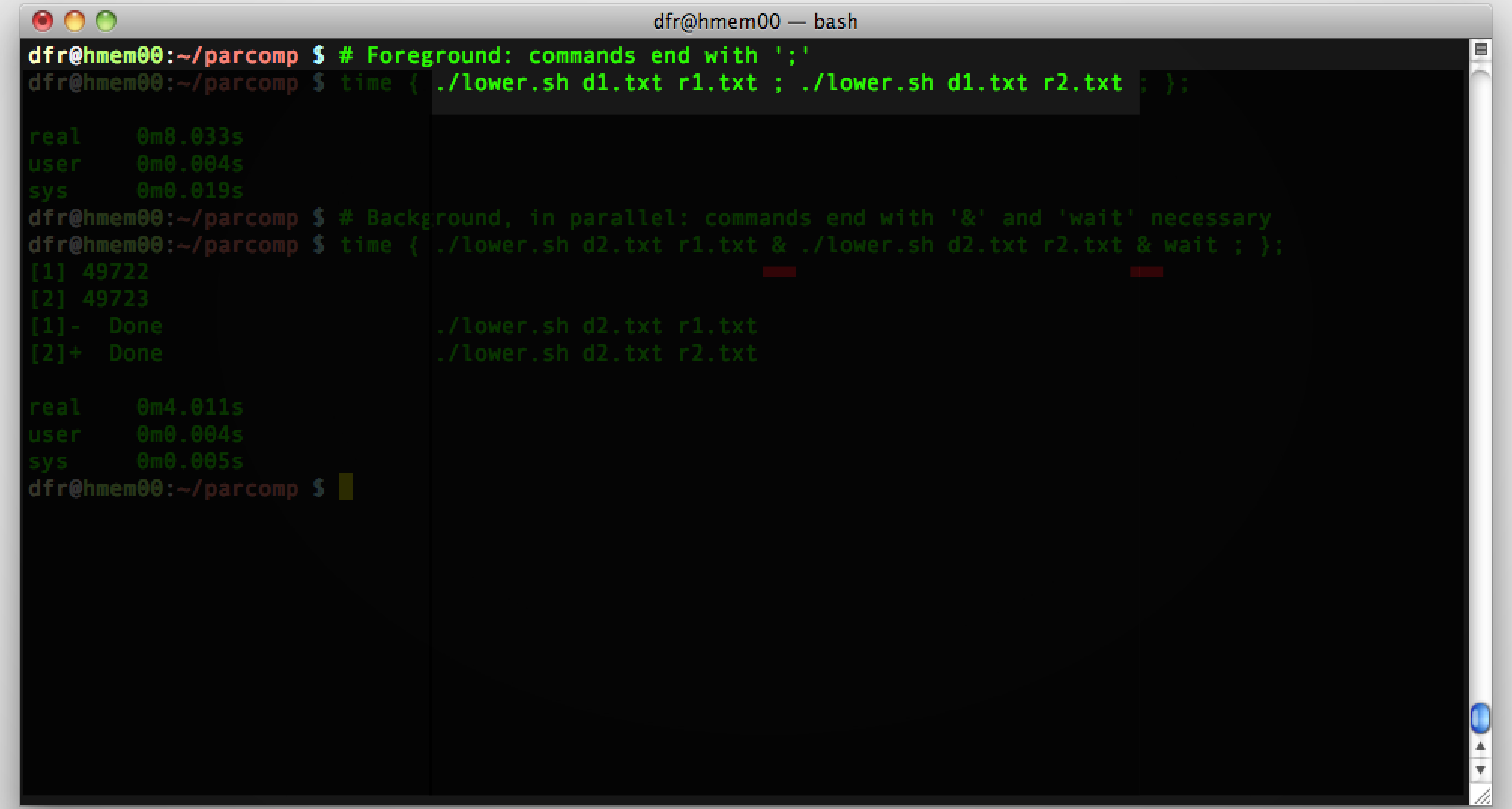


```
dfr@hmem00:~/parcomp $ cat lower.sh
#!/bin/bash
#
# Usage:
#    ./lower.sh [input_file [output_file]]
#
# Make ACTG chars lower case with extra processing.
#
# If output_file is not defined, stdout is used
# If input_file and output_file are not defined, stdin and stdout are used.

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 $
```

It is written in Bash and just transforms some upper case letters to lower case

Parallel processes in Bash

Run the program twice

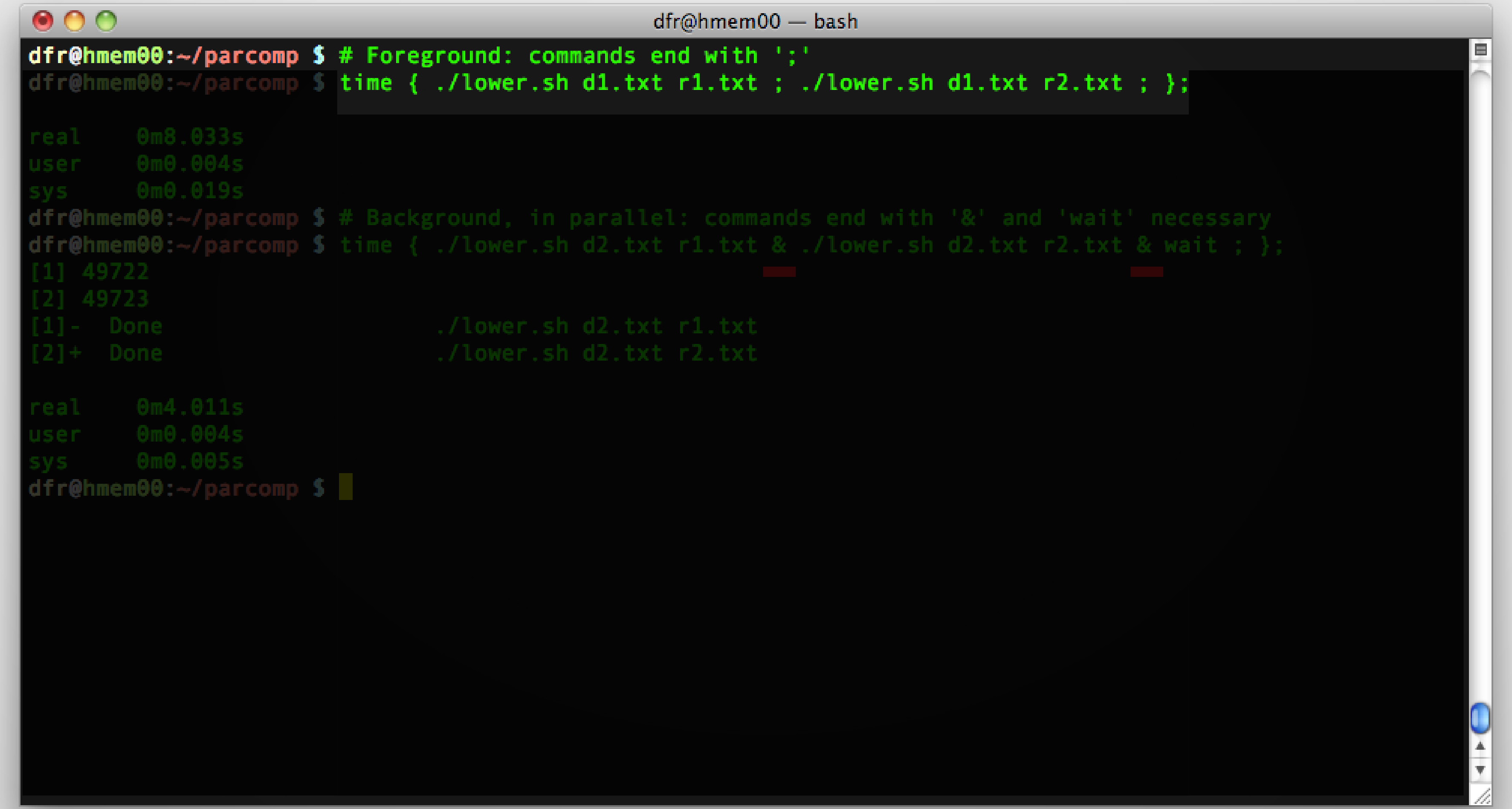


```
dfr@hmem00:~/parcomp $ # Foreground: commands end with ';'
dfr@hmem00:~/parcomp $ time { ./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt ; };

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 $ 
```

https://www.gnu.org/software/bash/manual/html_node/Job-Control-Basics.html

Parallel processes in Bash

Run the program twice and measure the time it takes



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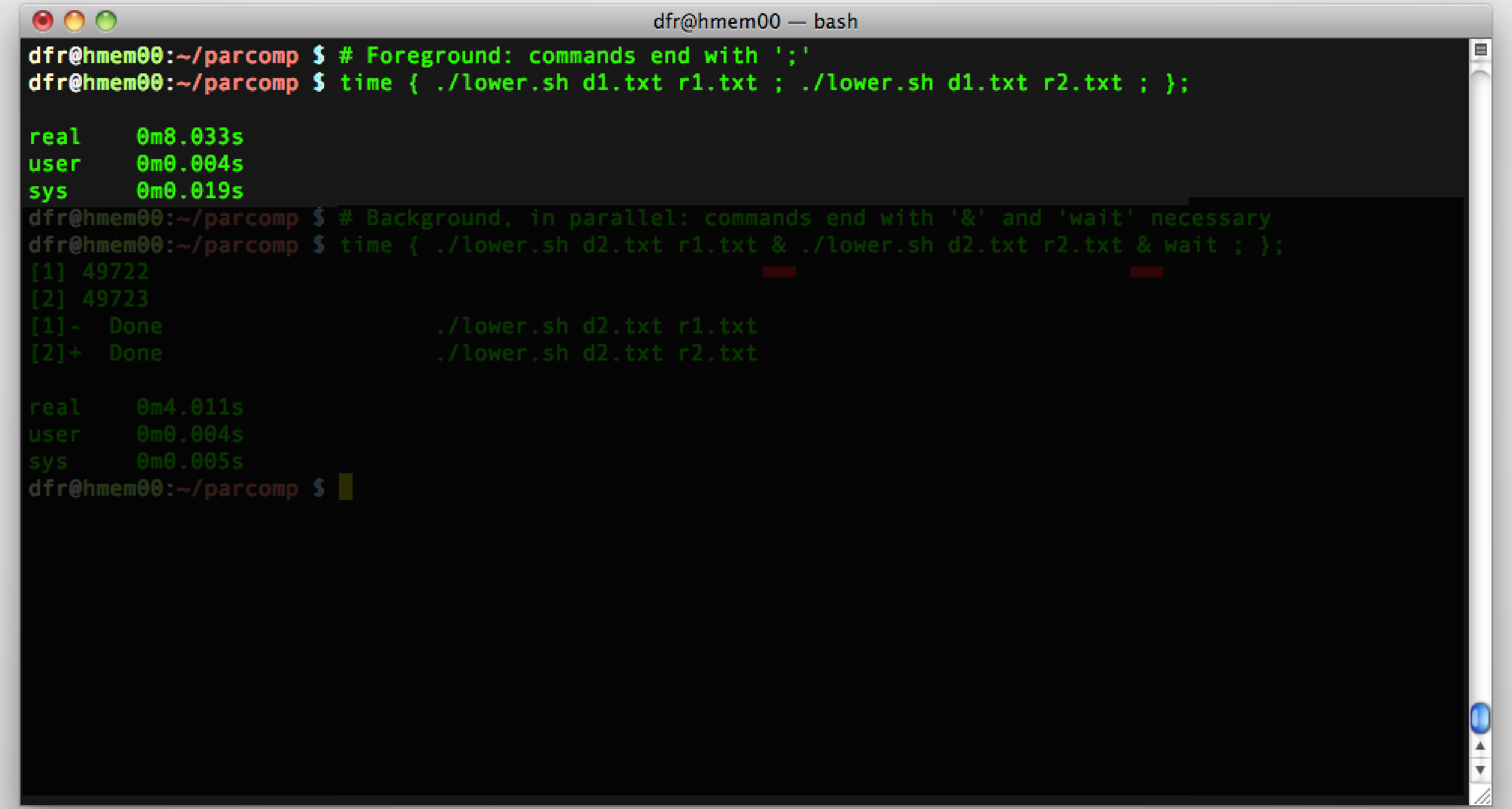

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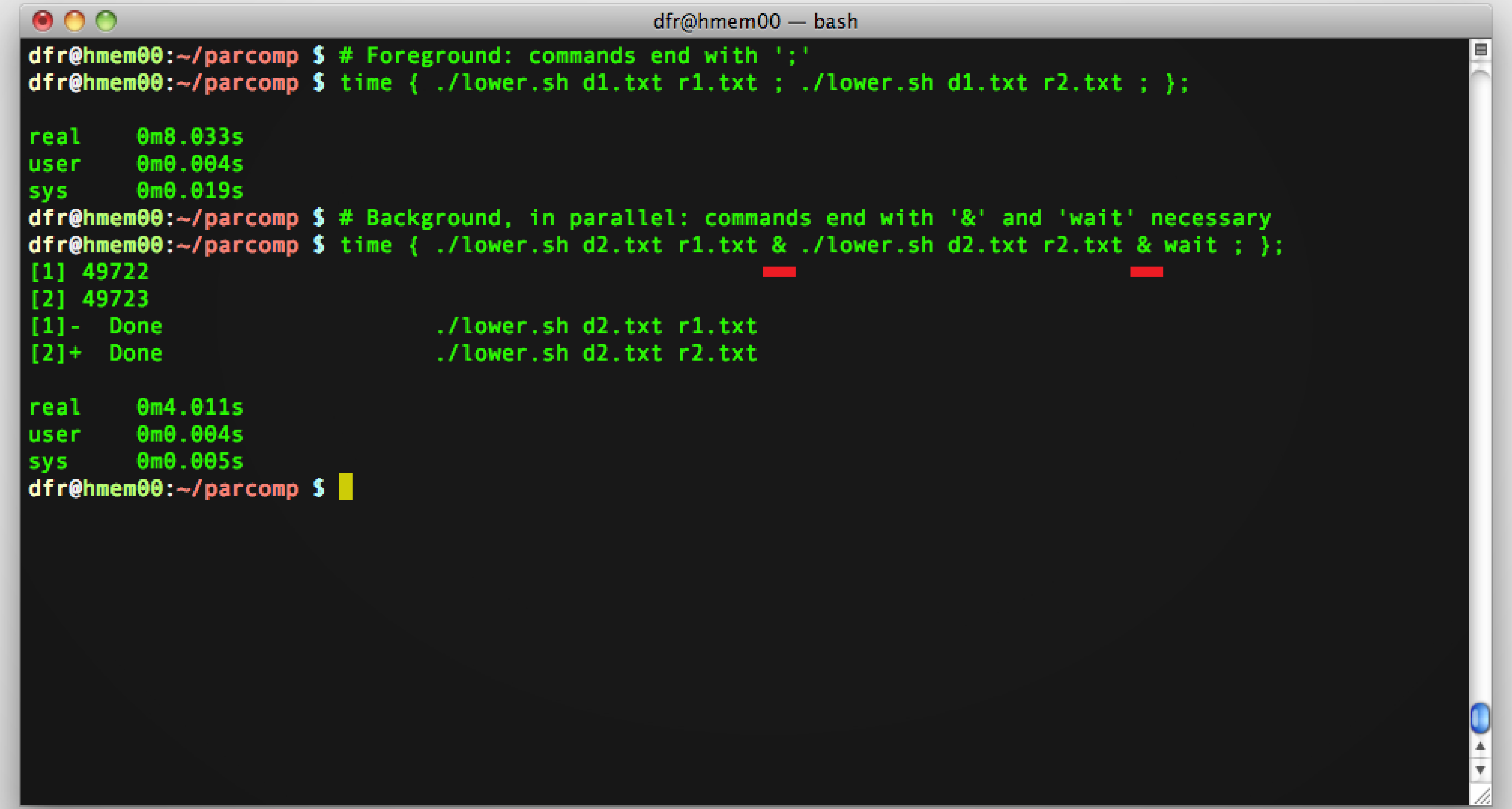
dfr@hmem00:~/parcomp $ time { ./lower.sh d2.txt r1.txt & ./lower.sh d2.txt r2.txt & wait ; };
[1] 49722
[2] 49723
[1]-  Done                    ./lower.sh d2.txt r1.txt
[2]+  Done                    ./lower.sh d2.txt r2.txt

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

Parallel processes in Bash

Run the program twice “in the background” and measure the time



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dfr@hmem00:~/parcomp $
```
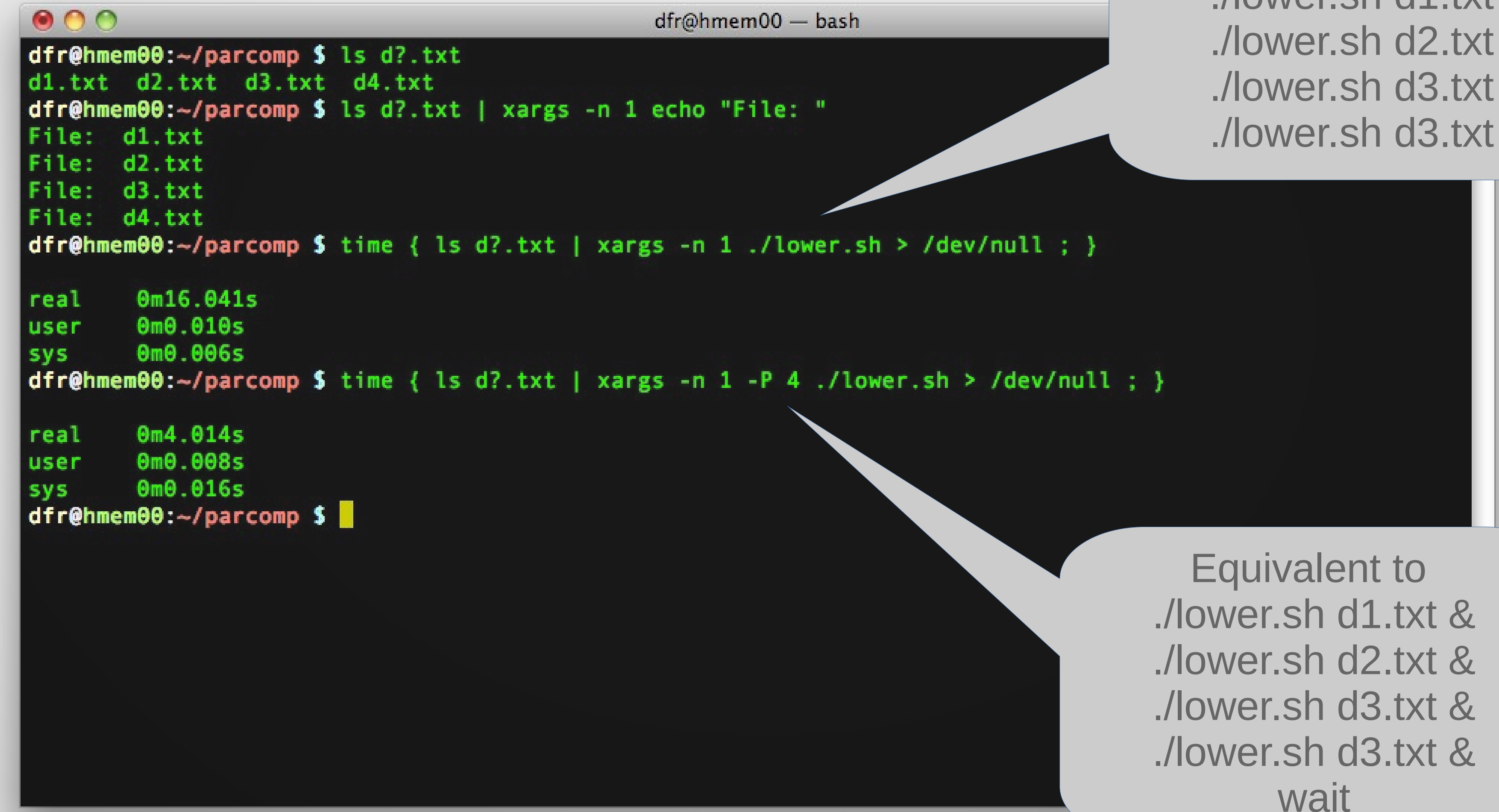

https://www.gnu.org/software/bash/manual/html_node/Job-Control-Basics.html

One program and many files

The xargs command distributes data from stdin to program



```
dfr@hmem00:~/parcomp $ ls d?.txt
d1.txt  d2.txt  d3.txt  d4.txt
dfr@hmem00:~/parcomp $ ls d?.txt | xargs -n 1 echo "File: "
File:  d1.txt
File:  d2.txt
File:  d3.txt
File:  d4.txt
dfr@hmem00:~/parcomp $ time { ls d?.txt | xargs -n 1 ./lower.sh > /dev/null ; }

real    0m16.041s
user    0m0.010s
sys     0m0.006s
dfr@hmem00:~/parcomp $ time { ls d?.txt | xargs -n 1 -P 4 ./lower.sh > /dev/null ; }

real    0m4.014s
user    0m0.008s
sys     0m0.016s
dfr@hmem00:~/parcomp $
```

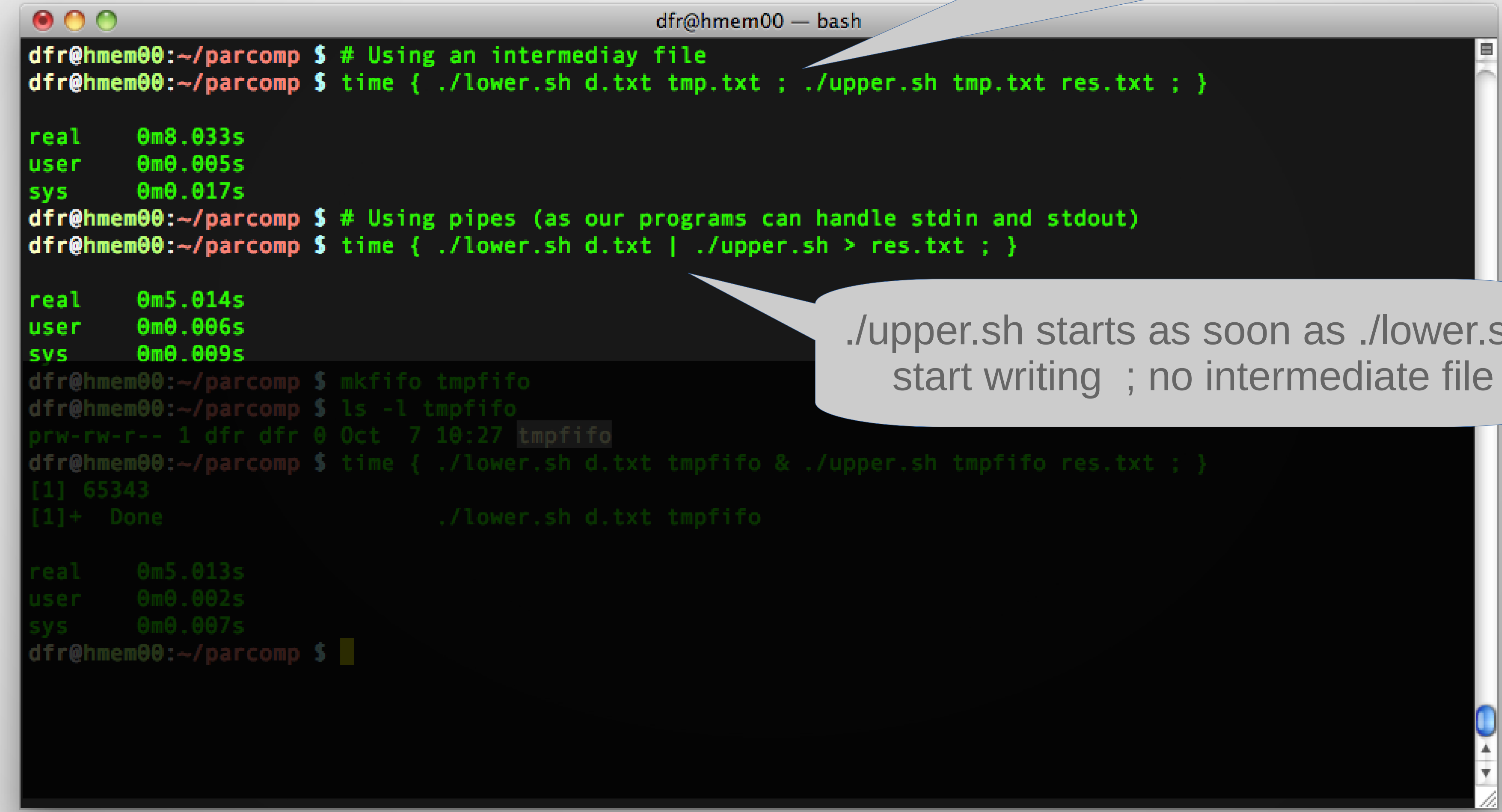
Equivalent to
./lower.sh d1.txt ;
./lower.sh d2.txt ;
./lower.sh d3.txt ;
./lower.sh d3.txt ;

Equivalent to
./lower.sh d1.txt &
./lower.sh d2.txt &
./lower.sh d3.txt &
./lower.sh d3.txt &
wait

Several programs and one file

Using UNIX pipes for pipelining operations

./upper.sh waits for ./lower.sh to finish
Note the intermediate file

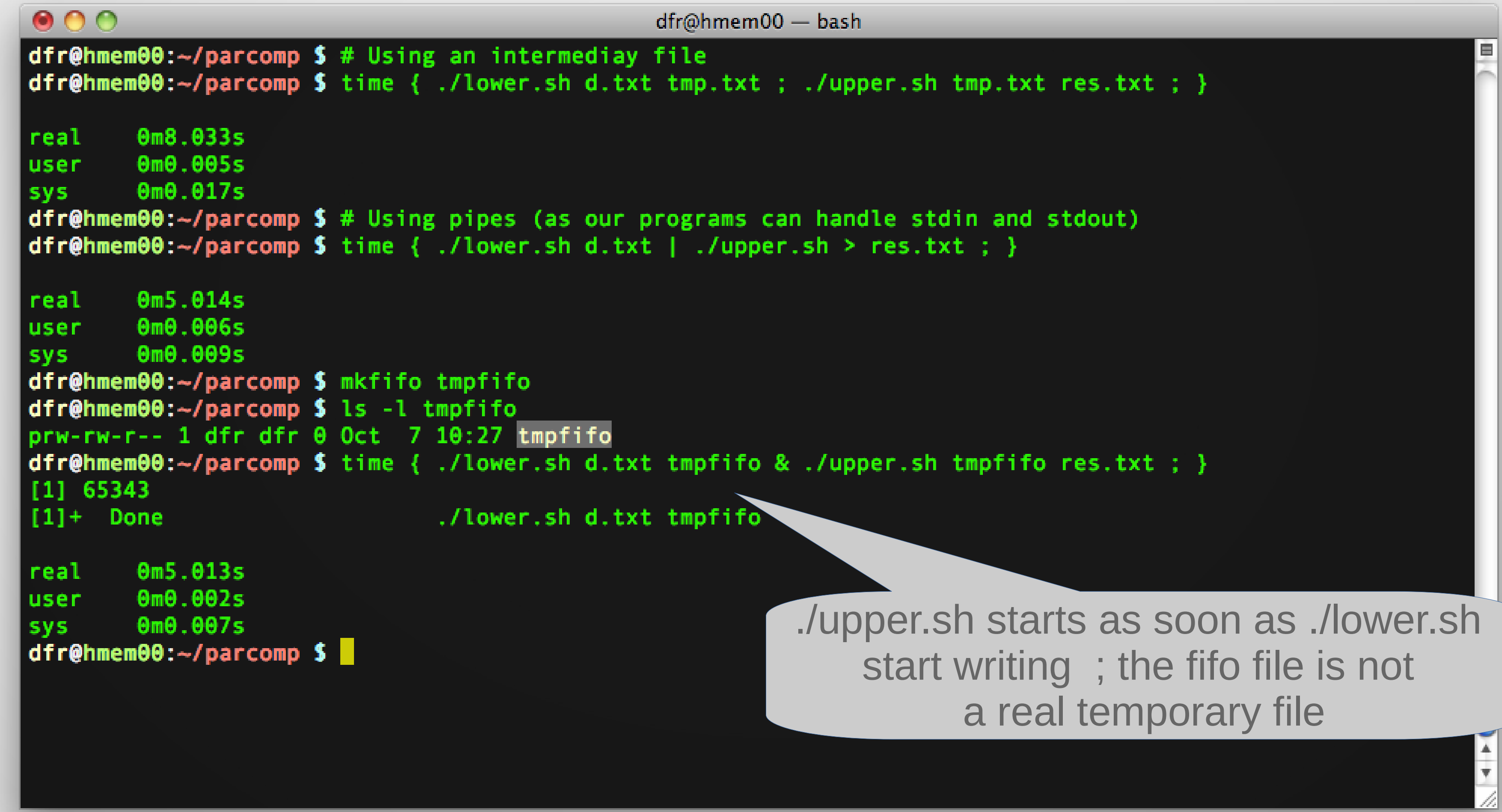


```
dfr@hmem00:~/parcomp $ # Using an intermediay file
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }

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 $
```

./upper.sh starts as soon as ./lower.sh
start writing ; no intermediate file

Several programs and one file

Using UNIX fifos for pipelining operations


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
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sys	0m0.017s
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dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt | ./upper.sh > res.txt ; }

real	0m5.014s
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sys	0m0.009s
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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 $ 
```
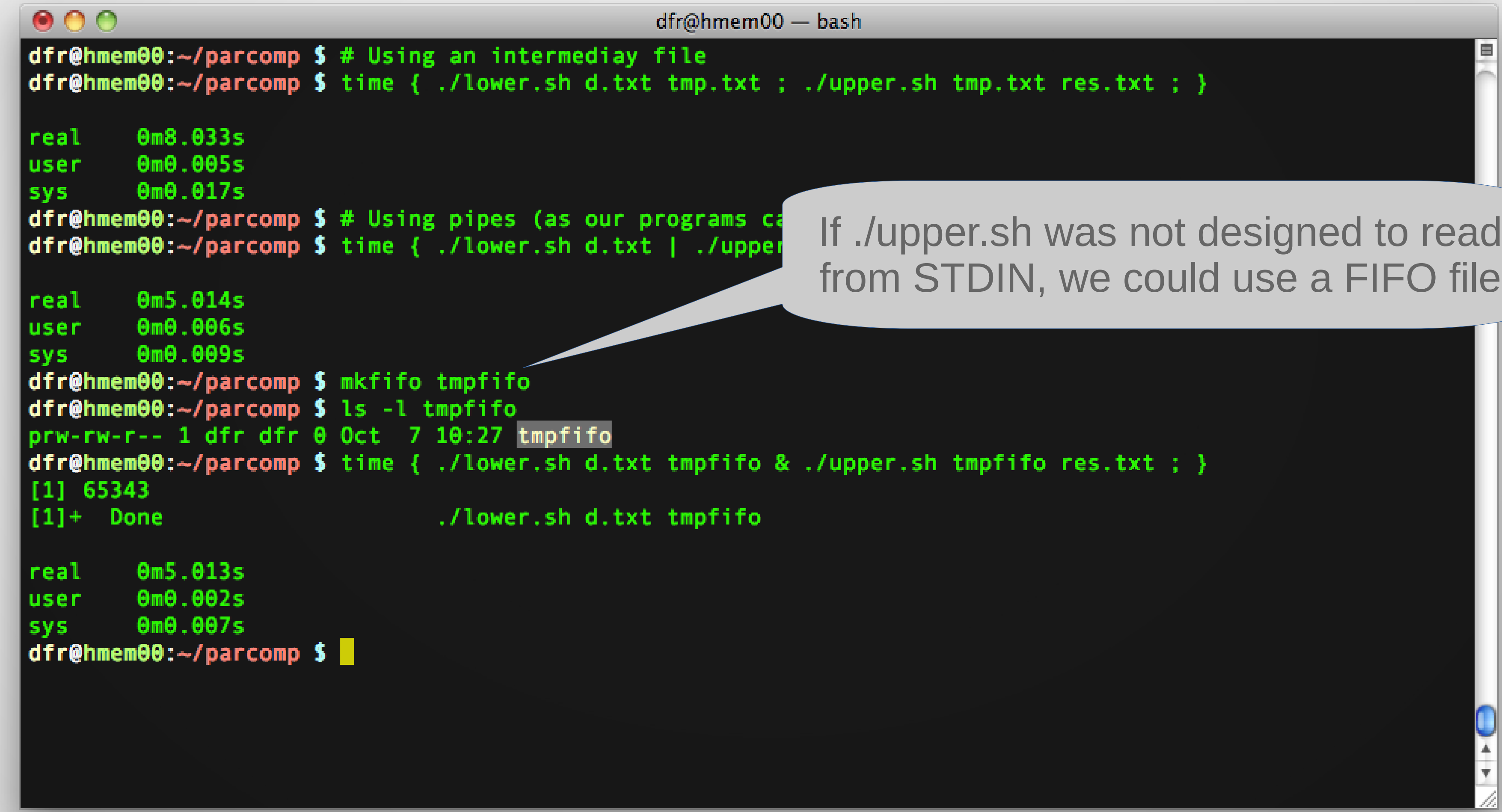

./upper.sh starts as soon as ./lower.sh start writing ; the fifo file is not a real temporary file

Several programs and one file



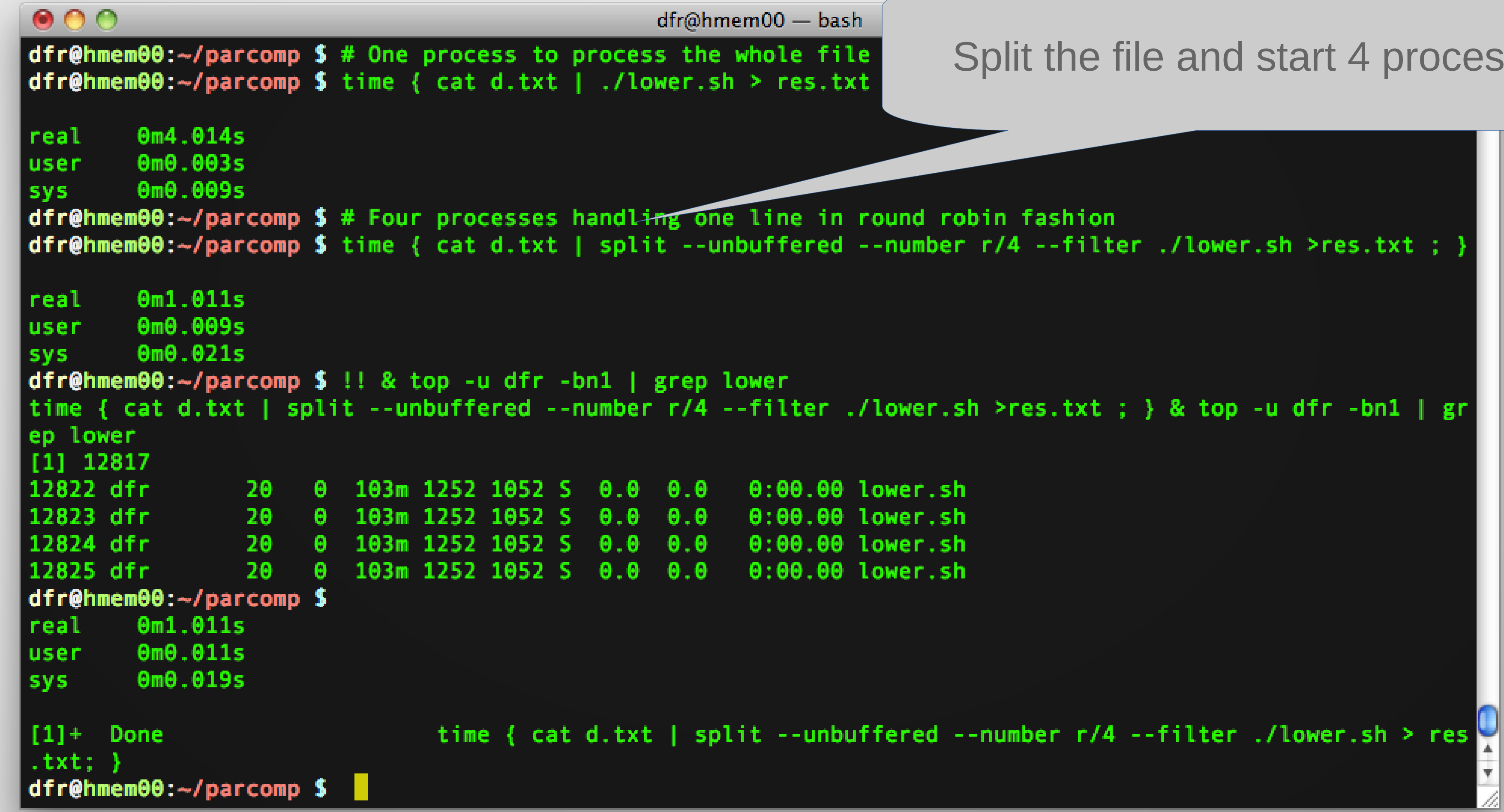
dfr@hmem00 — bash

```
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 ca
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt | ./upper

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 $
```

If ./upper.sh was not designed to read from STDIN, we could use a FIFO file

One program and one large file

The split command distributes data from stdin to program



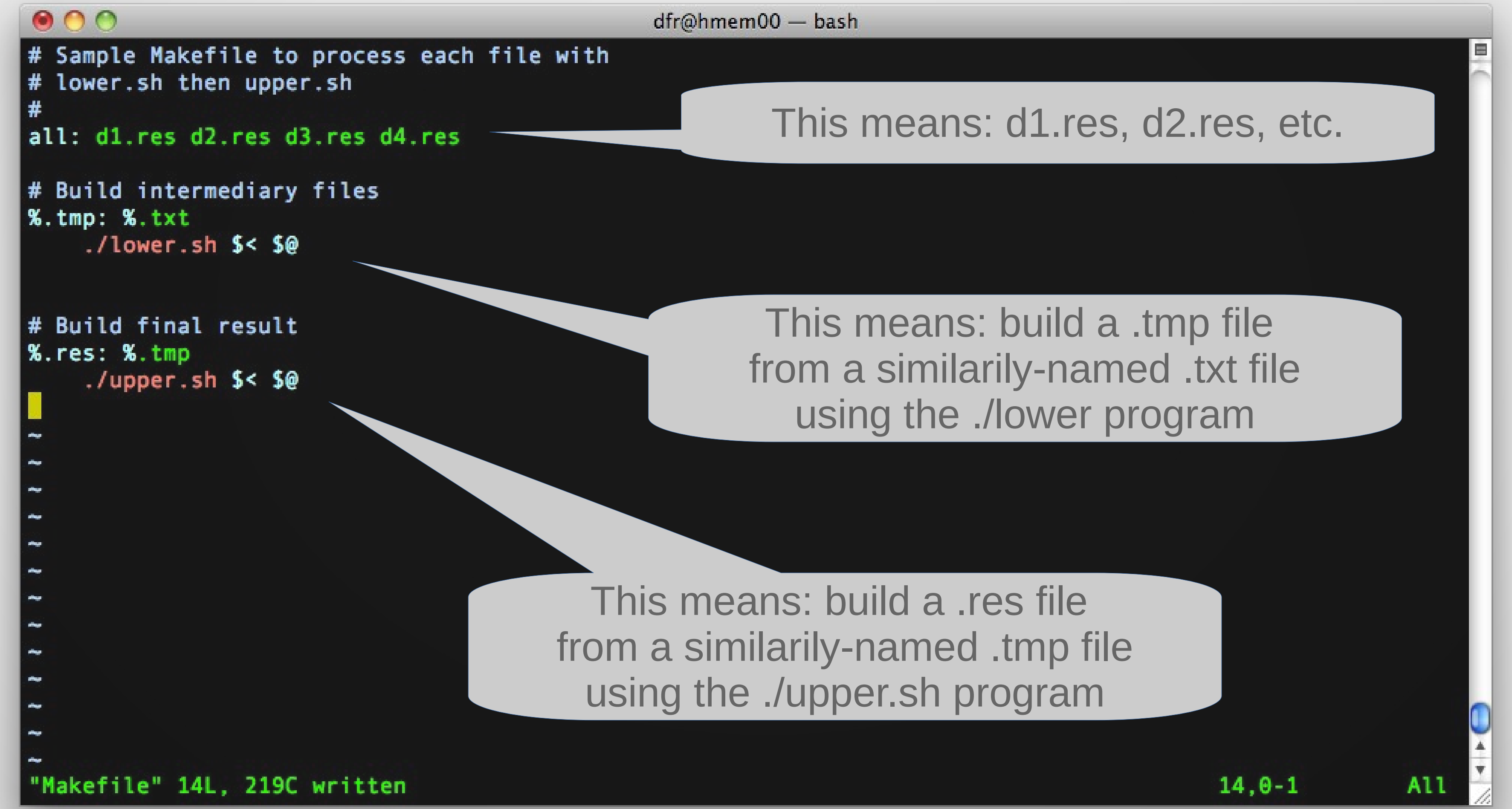
Split the file and start 4 processes

```
dfr@hmem00:~/parcomp $ # One process to process the whole file
dfr@hmem00:~/parcomp $ time { cat d.txt | ./lower.sh > res.txt

real    0m4.014s
user    0m0.003s
sys     0m0.009s
dfr@hmem00:~/parcomp $ # Four processes handling one line in round robin fashion
dfr@hmem00:~/parcomp $ time { cat d.txt | split --unbuffered --number r/4 --filter ./lower.sh >res.txt ; }

real    0m1.011s
user    0m0.009s
sys     0m0.021s
dfr@hmem00:~/parcomp $ !! & top -u dfr -bn1 | grep lower
time { cat d.txt | split --unbuffered --number r/4 --filter ./lower.sh >res.txt ; } & top -u dfr -bn1 | gr
ep lower
[1] 12817
12822 dfr       20   0  103m 1252 1052 S  0.0  0.0   0:00.00 lower.sh
12823 dfr       20   0  103m 1252 1052 S  0.0  0.0   0:00.00 lower.sh
12824 dfr       20   0  103m 1252 1052 S  0.0  0.0   0:00.00 lower.sh
12825 dfr       20   0  103m 1252 1052 S  0.0  0.0   0:00.00 lower.sh
dfr@hmem00:~/parcomp $
real    0m1.011s
user    0m0.011s
sys     0m0.019s

[1]+  Done                    time { cat d.txt | split --unbuffered --number r/4 --filter ./lower.sh > res
.txt; }
dfr@hmem00:~/parcomp $
```

Need recent version of Coreutils/8.22-goolf-1.4.10

Several programs and many files

A Makefile describes dependencies and is executed with ‘make’



```
# Sample Makefile to process each file with
# lower.sh then upper.sh
#
all: d1.res d2.res d3.res d4.res

# Build intermediary files
%.tmp: %.txt
    ./lower.sh $< $@


# Build final result
%.res: %.tmp
    ./upper.sh $< $@

~
~
~
~
~
~
~
~
~
~
~
~
~
"Makefile" 14L, 219C written                                   14,0-1        All
```

This means: d1.res, d2.res, etc.

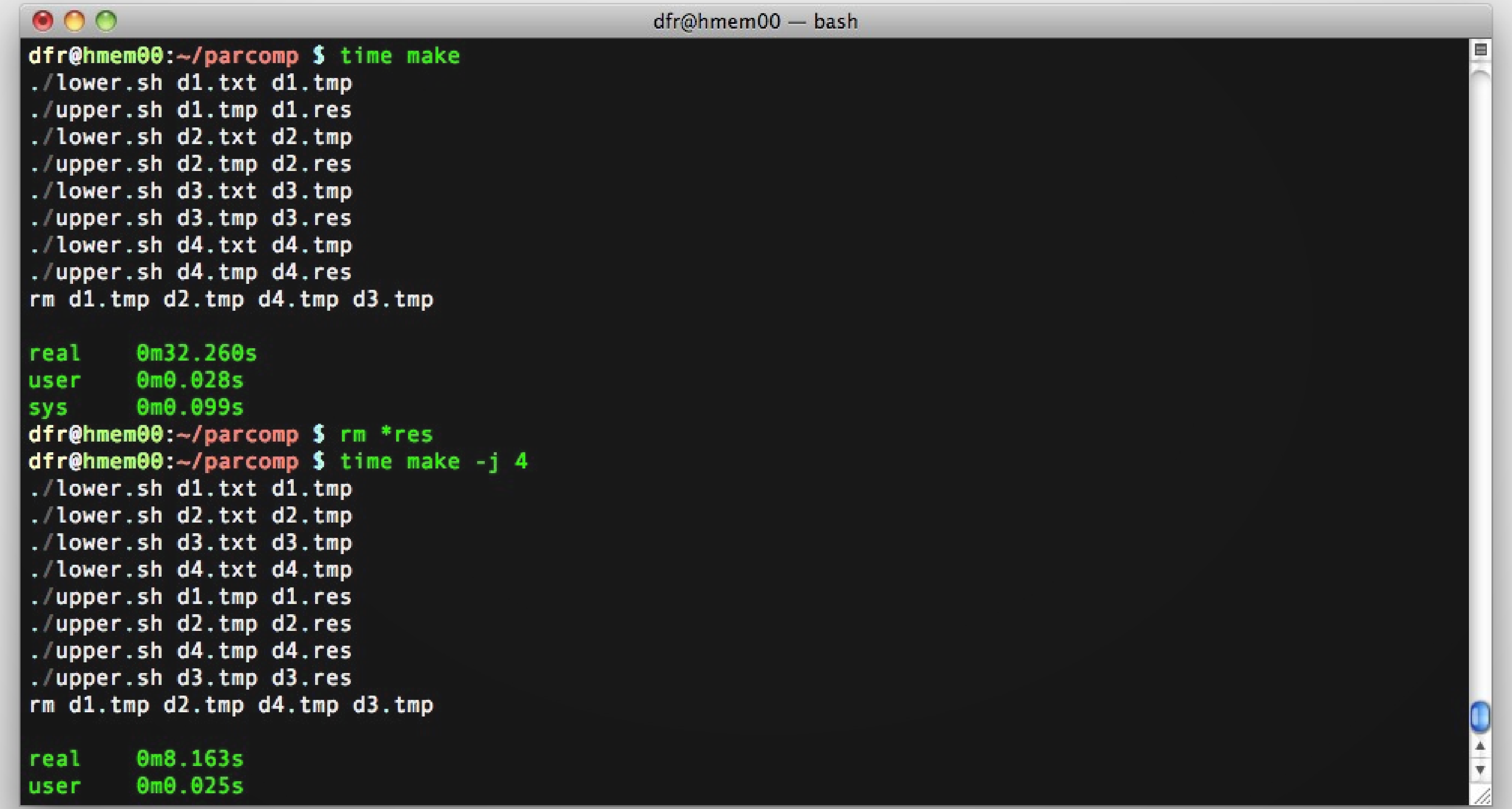
This means: build a .tmp file
from a similarily-named .txt file
using the ./lower program

This means: build a .res file
from a similarily-named .tmp file
using the ./upper.sh program

https://www.gnu.org/software/make/manual/html_node/index.html

Several programs and many files

The ‘make’ command can operate in parallel



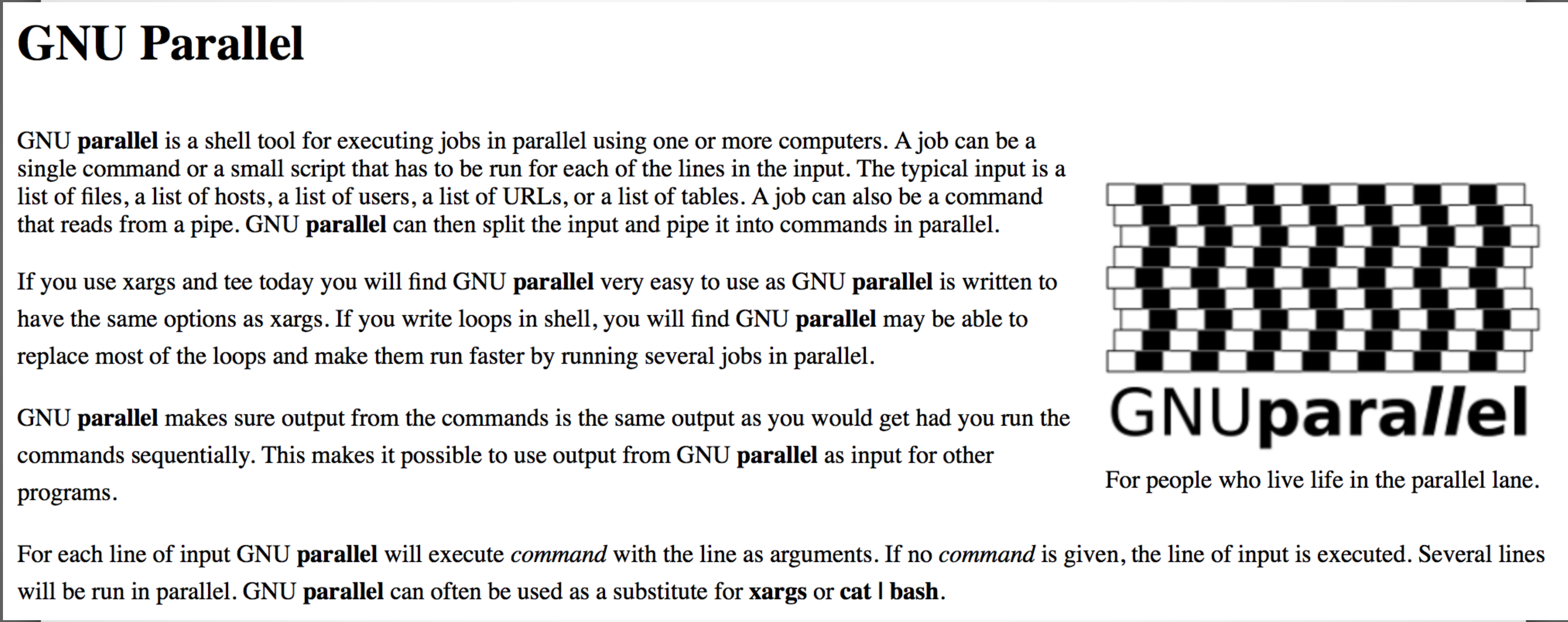
dfr@hmem00 — bash

```
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.

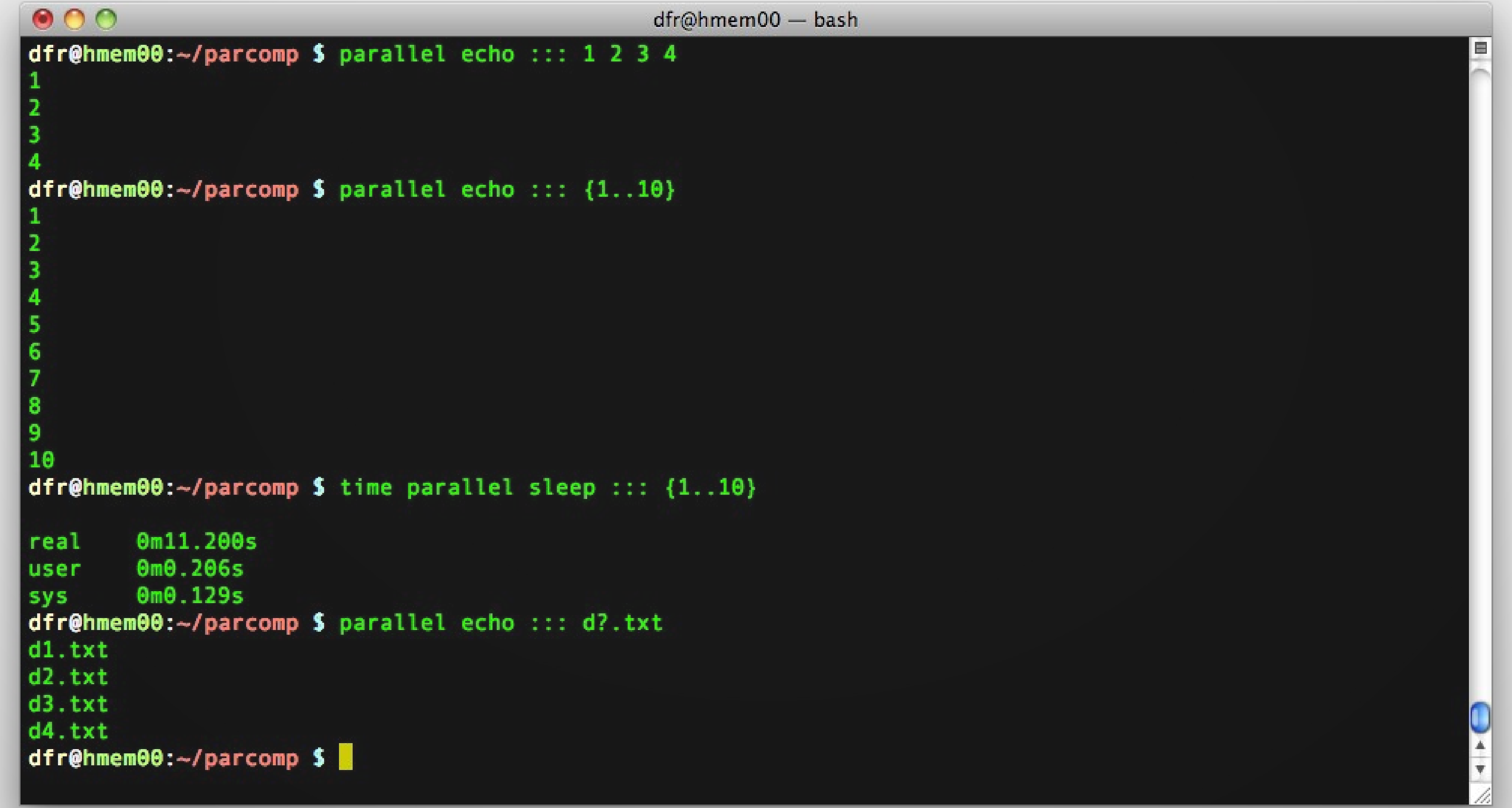
For people who live life in the parallel lane.

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
Might not be available everywhere

GNU Parallel

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

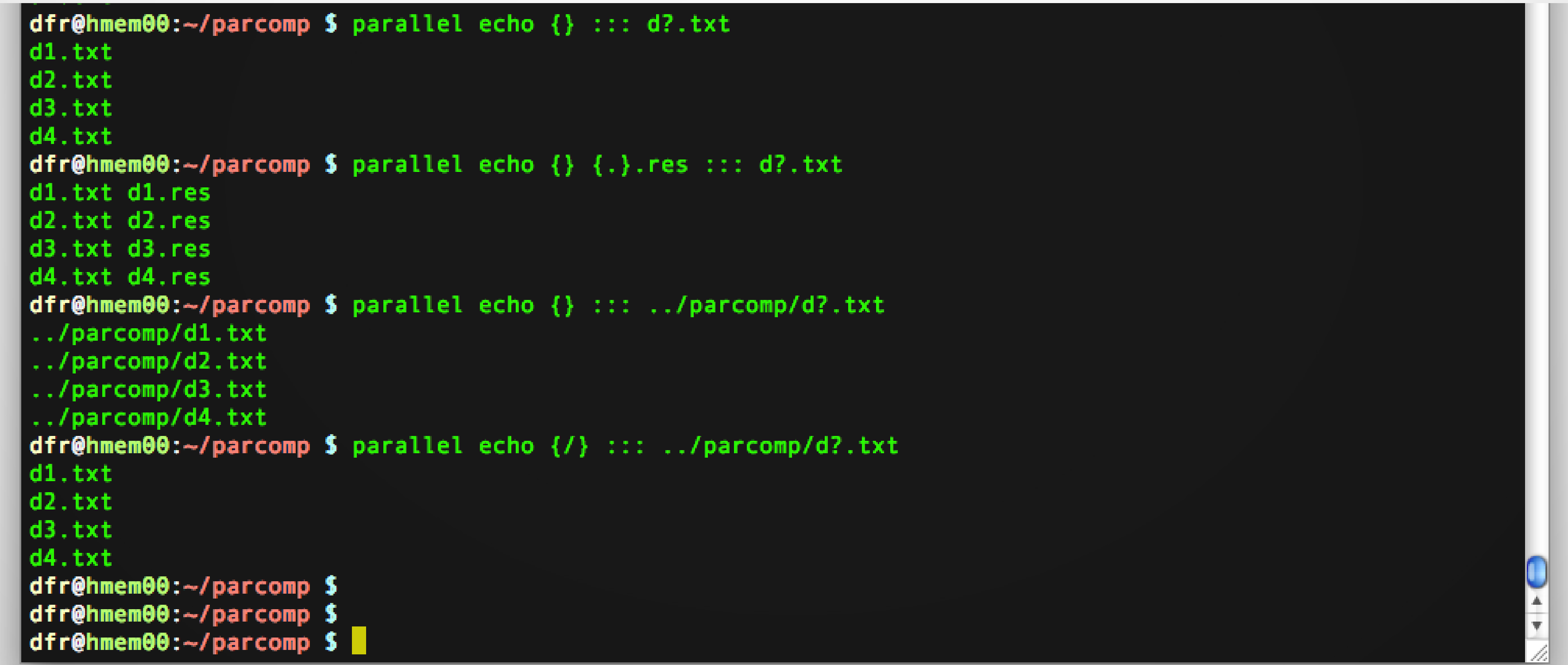


dfr@hmem00 — bash

```
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

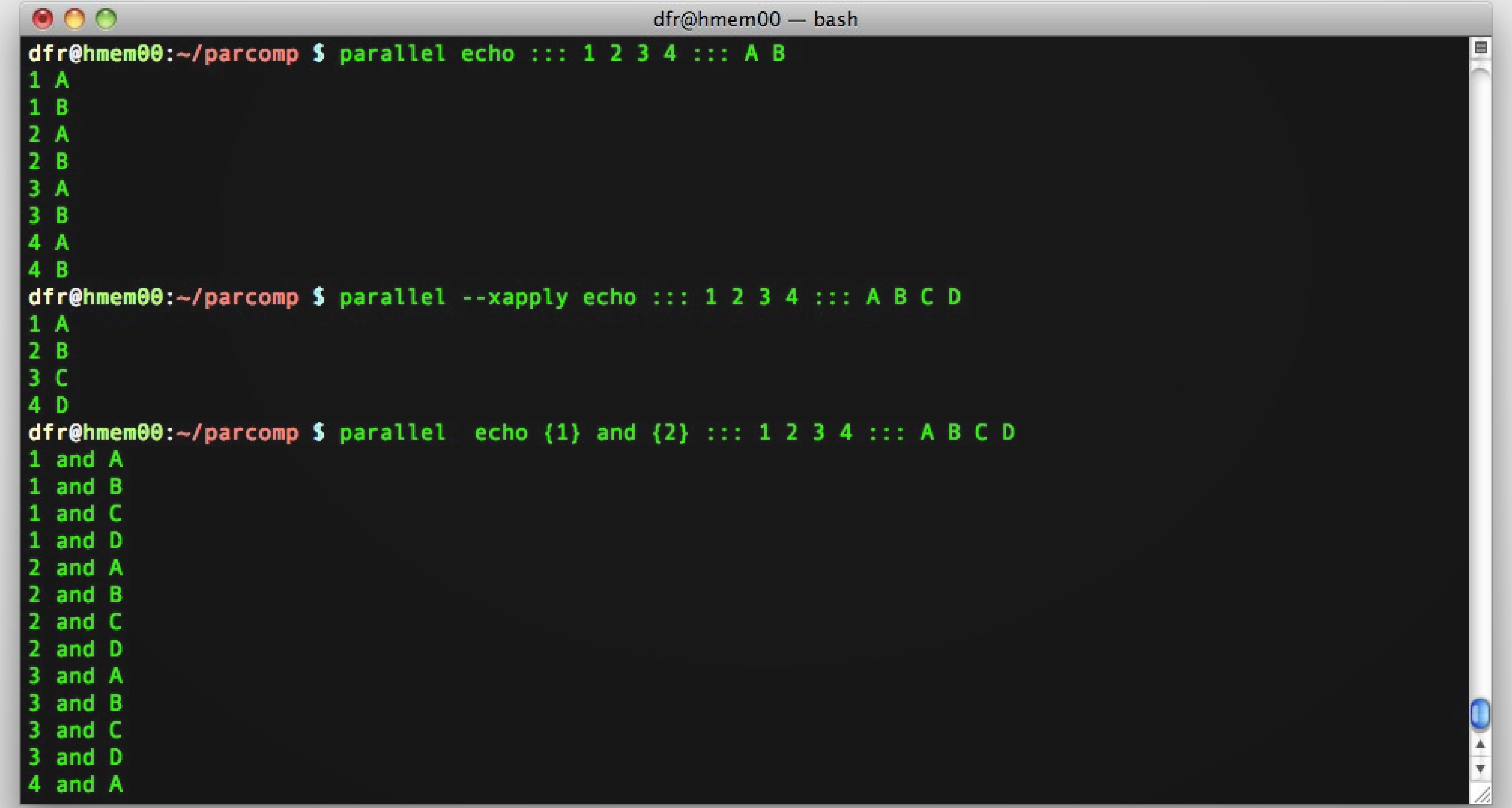
- Syntax: {} as argument placeholder.



```
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

- Multiple parameters and --xapply

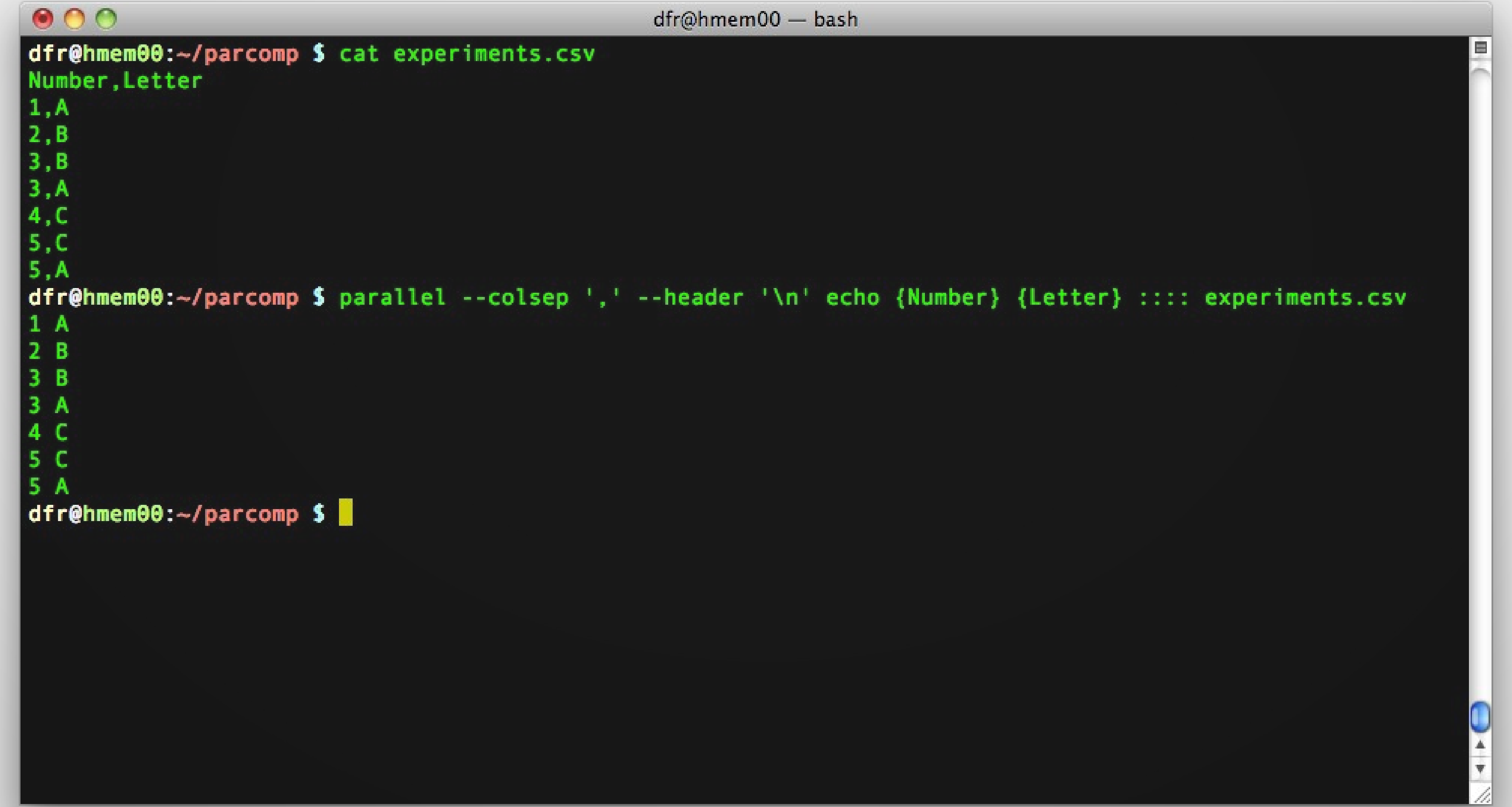


dfr@hmem00 — bash

```
dfr@hmem00:~/parcomp $ parallel echo ::: 1 2 3 4 ::: A B
1 A
1 B
2 A
2 B
3 A
3 B
4 A
4 B
dfr@hmem00:~/parcomp $ parallel --xapply echo ::: 1 2 3 4 ::: A B C D
1 A
2 B
3 C
4 D
dfr@hmem00:~/parcomp $ parallel  echo {1} and {2} ::: 1 2 3 4 ::: A B C D
1 and A
1 and B
1 and C
1 and D
2 and A
2 and B
2 and C
2 and D
3 and A
3 and B
3 and C
3 and D
4 and A
```

GNU Parallel

- When arguments are in a file : use :::: (4x ':')


dfr@hmem00 — bash

```
dfr@hmem00:~/parcomp $ cat experiments.csv
Number,Letter
1,A
2,B
3,B
3,A
4,C
5,C
5,A
dfr@hmem00:~/parcomp $ parallel --colsep ',' --header '\n' echo {Number} {Letter} :::: experiments.csv
1 A
2 B
3 B
3 A
4 C
5 C
5 A
dfr@hmem00:~/parcomp $
```

Other interesting options

`--pipe`	Split a file
`-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.

Home work

Reproduce the examples from the previous slides 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 ; }
```