

Consortium des Equipements de Calcul Intensif en Fédération Wallonie-Bruxelles

Introduction to Parallel Computing

damien.francois@uclouvain.be November 2023





Agenda

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

1.

General concepts

Why parallel? (simplified)

- 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

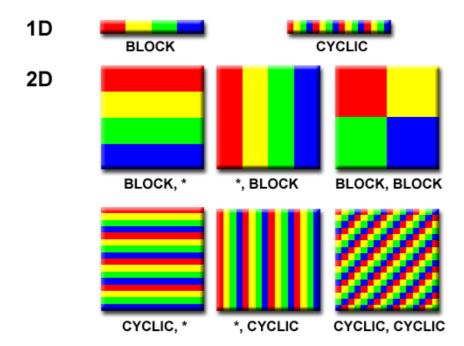
Parallelization involves:

Decomposition of the work

- Operation decomposition: task-level parallelism
 - Multiple programs (functional decomposition)
 - Multiple instances of the same program (SPMD)
- Data decomposition : data-level parallelism

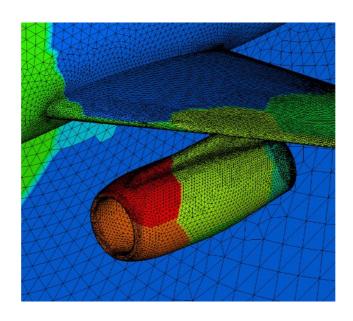
Decomposition of the work

- Operation decomposition: task-level parallelism
- Data decomposition : data-level parallelism
 - Block, cyclic



Decomposition of the work

- Operation 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 of the workers

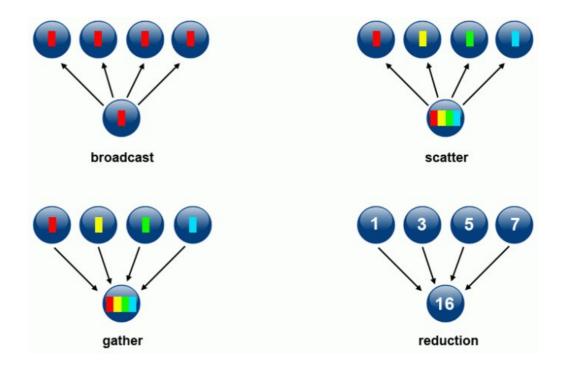
Synchronization of the workers

- high
 - Synchronous (SIMD) at the processor level; the same processor instruction for each worker at any time; (instruction level)
 - Fine-grained parallelism : subtasks communicate many times per second (typically at the loop level)
 - Coarse-grained parallelism: they do not communicate many times per second (typically function-call level)
 - Embarrassingly parallel: they rarely or never have to communicate (asynchronous)

Collaboration of the workers

Communication between workers

- Point to point
- Broadcast
- Scatter
- Gather
- Reduction

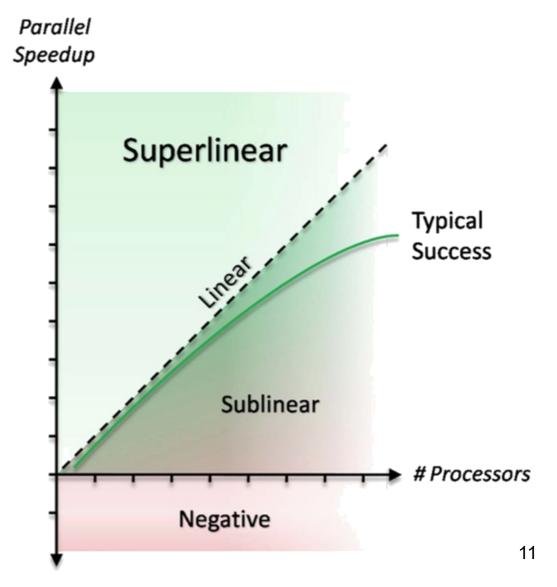


Does it work? Speedup, Efficiency, Scalability

Time for serial operations

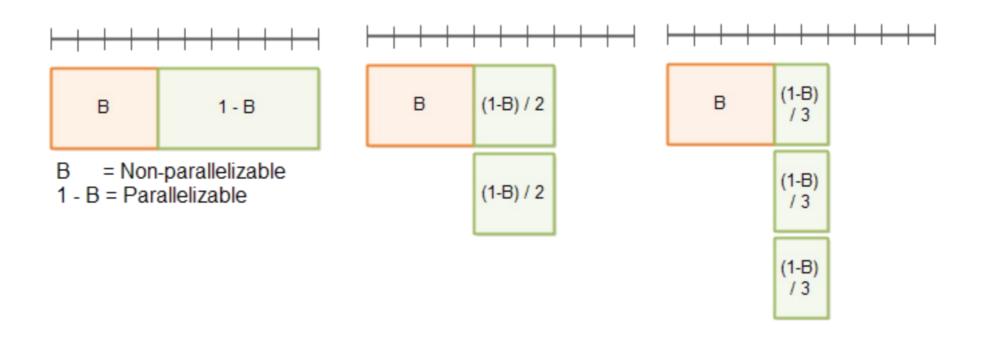
$$Speedup S = \frac{T_S}{T_P}$$
 Time for parallel operations

$$E = \frac{S}{p} = \frac{T_S}{pT_p}$$
 Number of processors



Challenge 1: Amdahl's Law

Not all the work can be decomposed



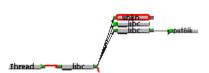
In parallel computing, Amdahl's law is mainly used to predict the theoretical maximum speedup for programs using multiple processors.

Challenge 2: Parallel overhead

Collaboration means communication and extra work

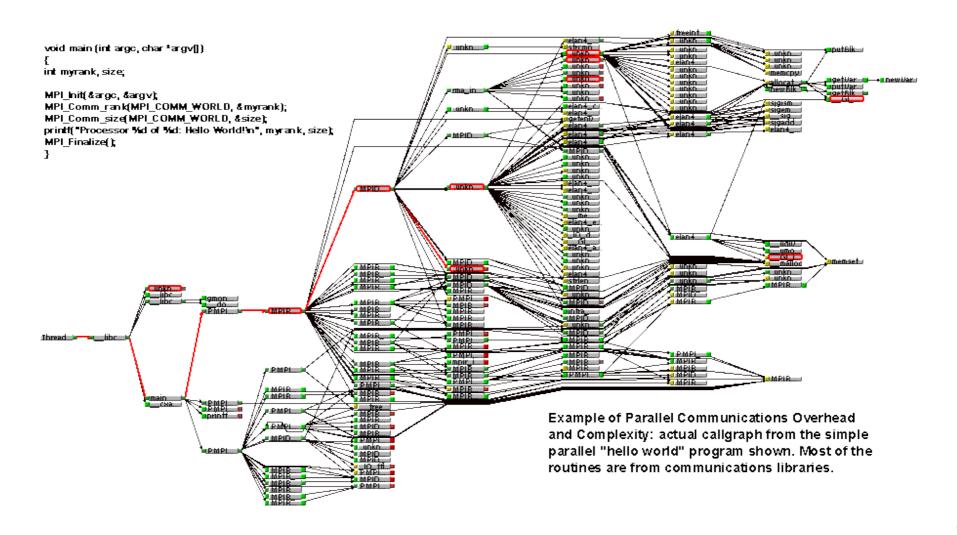
```
void main (int argo, char *argv[]) {

printf("Processor %d of %d: Hello World!\n",
}
```



Challenge 2: Parallel overhead

Collaboration means communication and extra work



Challenge 3: Load imbalance

Parallelization is efficient only if every worker has the same amount of work

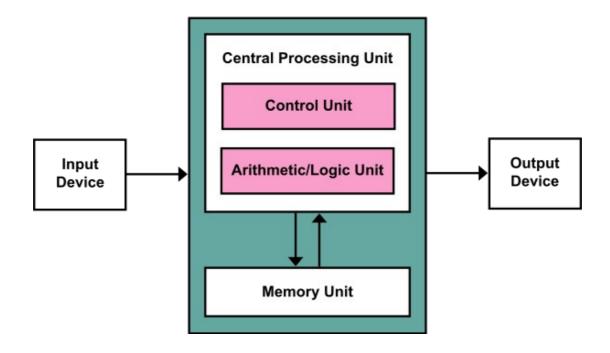


2.

Hardware for parallel computing

Von Neumann (serial) architecture

An abstract view of early computers



Parallelism at the CPU (core) level

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

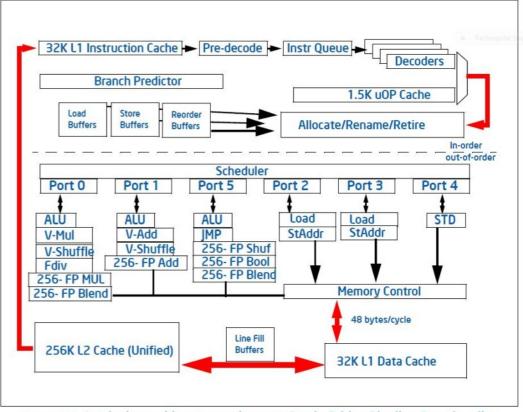
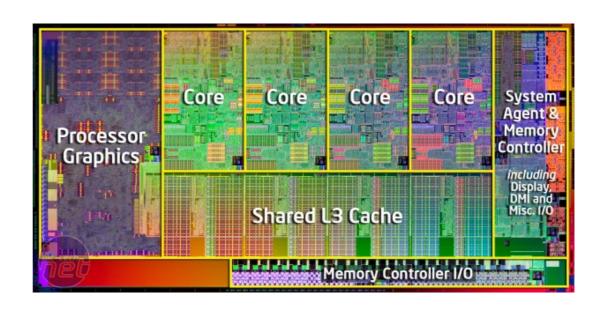


Figure 2-1. Intel microarchitecture code name Sandy Bridge Pipeline Functionality



Parallelism at the chip (socket) level

 Multicore parallelism



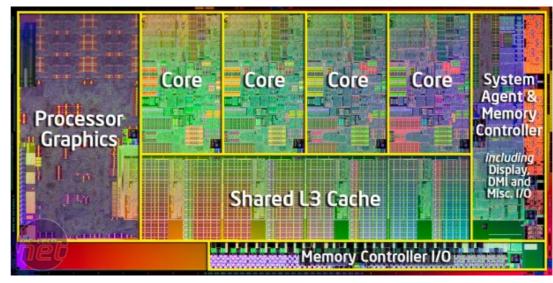
Parallelism at the computer level

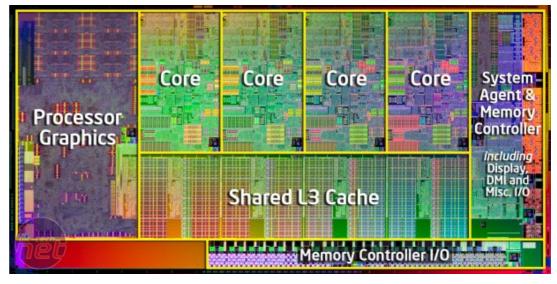


- Multi-socket parallelism
 - SMP
 - NUMA

Accelerators







Parallelism at the data center level



Multi-node parallelism





Parallelism 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.





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!

Parallelism at the data center level

Cloud computing "someone else's cluster"











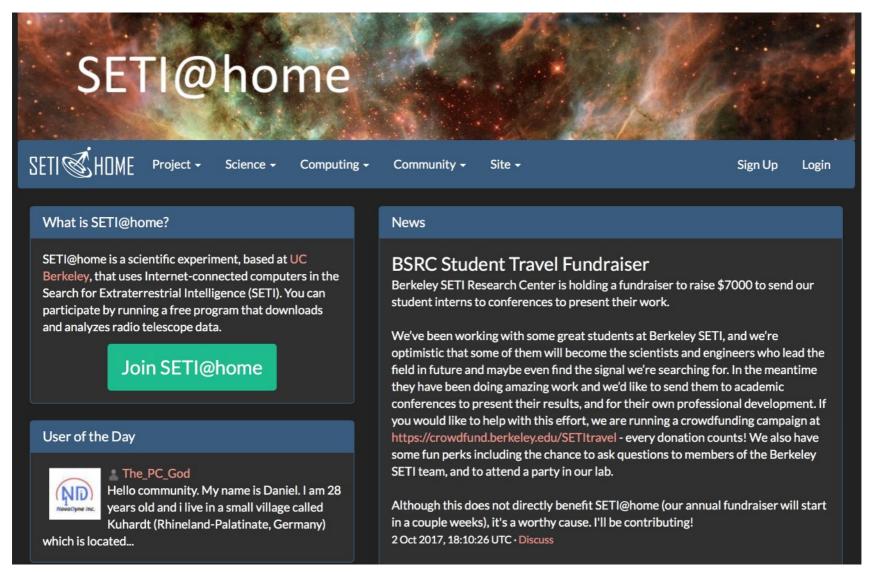
Parallelism at the world level

Grid computing – "cluster of clusters"



Parallelism at the world level

Distributed computing – "no unused cycle"



3.

Programming paradigms and programming models

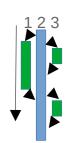
Is parallization automagic?

- **ILP**: yes, by the CPU and/or the compiler
- SIMD: mostly, by the compiler, but it can be fooled by your code (→ pragmas)
- Intra-node: can be if the library/software you use is designed for it (→ *_NUM_THREADS env vars, be aware of NUMA placement issues)
- **GPUs**: can be if the library/software you use is designed for it (→ CUDA_VISIBLE_DEVICES env vars, be aware of GPU/CPU memory transfers)
- Inter-node: never automagic. You will at least need to explicitly start processes (→ be aware of the network capabilities)

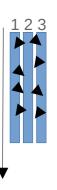
Main parallel programming paradigms

Task-farming:

 Master program distributes work to worker programs (leader/follower); or

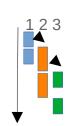


- Worker programs pick up tasks from pool (work stealing).
- **SPMD** (Single program multiple data)
 - A single program that contains both the logic for distributing work and computing
 - Multiple instances are started and "linked" together
 - Instances are identified with a distinct index



Other parallel programming paradigms

- MPMD (Multiple program multiple data)
- Pipelining: workers take care of a subtask in the processing chain and pass the intermediate result to the next worker



- Divide and Conquer :
 - workers are spawned at need and report their result to the parent



Speculative parallelism : workers are spawned and result possibly discarded

```
CPU1: If (very_long_computation())
CPU1: then
CPU1: do A
CPU1: else
CPU1: do B
```

```
CPU1: res=very_long_computation()
CPU2: do A
CPU3: do B
CPU1: if (res) discard B else discard A
```



Programming models

- Single computer:
 - CPUs: PThreads, OpenMP, TBB, OpenCL, ...
 - Accelerators: CUDA, OpenCL, OpenAcc/OpenMP, SYCL, Hipp, ROCm, ...
- Multi-computer:
 - Clusters:
 - Message passing: MPI, PVM
 - PGAS: CoArray Fortran, UPC, Global Arrays
 - Clouds: MapReduce, Spark RDD
 - Distributed computing: BOINC

4.

User tools

that GNU/Linux offers

- 4.1 Parallelized tools
- 4.2 Job control and parallel processes
- 4.3 Basic tools
- 4.4 GNU Parallel

4.1. Parallelized utilities

Some tools have a parallelized counterpart, or parallel options. Examples:

serial		parallel
gzip grep ssh sort scp bc	 ← → → ← → → ← → → ← → → 	pigz ripgrep, singrep clustershell sortparallel bbcp bcx

Consider the following example program

```
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
dfr@hmem00:~/parcomp $ ./lower.sh d.txt
dfr@hmem00:~/parcomp $
```

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

Run the program twice

```
● ● ●
                                               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
```

Run the program twice and measure the time it takes

```
● ● ●
                                               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 ; };
```

Run the program twice and measure the time it takes

```
● ● ●
                                               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
user
        0m0.019s
```

4.2. Job control & Parallel processes in Bash

Run the program twice "in the background" and measure the time

```
● ● ●
                                               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
        0m0.004s
user
        0m0.019s
SVS
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
                              ./lower.sh d2.txt r2.txt
[2]+ Done
real
        0m4.011s
        0m0.004s
user
        0m0.005s
dfr@hmem00:~/parcomp $
```

4.2. Job control & Parallel processes in Bash

Parallel for loop in Bash:

(...) & : creates a sub-shell with all commands in the bloc and start it in the background wait : barrier to synchronize all sub-shells

4.3.1. One program and many files

The xargs command distributes data from stdin to program Equivalent to ./lower.sh d1.txt; 0 0 0 dfr@hmem00 - bash ./lower.sh d2.txt; dfr@hmem00:~/parcomp \$ 1s d?.txt d1.txt d2.txt d3.txt d4.txt ./lower.sh d3.txt : dfr@hmem00:~/parcomp \$ ls d?.txt | xargs -n 1 echo "File: " ./lower.sh d3.txt; 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 0m0.010s user 0m0.006s dfr@hmem00:~/parcomp \$ time { ls d?.txt | xargs -n 1 -P 4 ./lower.sh > /dev/null ; } 0m4.014s real 0m0.008s user 0m0.016s dfr@hmem00:~/parcomp \$ Equivalent to ./lower.sh d1.txt & ./lower.sh d2.txt & ./lower.sh d3.txt & ./lower.sh d3.txt & wait

4.3.2. 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 - bash
dfr@hmem00:~/parcomp $ # Using an intermediay file
dfr@hmem00:~/parcomp $ time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }
        0m8.033s
real
        0m0.005s
user
        0m0.017s
SVS
```

4.3.2. 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 - 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
        0m0.005s
user
SVS
        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
        0m0.006s
user
        0m0.009s
```

4.3.2. 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
user
                            A FIFO file is a "fake" file to which
SVS
       0m0.017s
dfr@hmem00:~/parcomp $
                           a process can write at the end and
dfr@hmem00:~/parcomp $
                            another can read at the beginning
dfr@hmem90:~/parcomp $ mkfifo tmpfifo
dfr@hmem00:~/parcomp $ ls -1 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
                            ./lower.sh d.txt tmpfifo
[1]+ Done
real
       0m5.013s
       0m0.002s
user
       0m0.007s
SVS
                                                        ./upper.sh starts reading as soon
dfr@hmem00:~/parcomp $
                                                             as ./lower.sh starts writing
```

4.3.3. One program and one large file

The split command distributes data from stdin to program

```
● ● ●
                                              dfr@hmem00 - bash
dfr@hmem00:~/parcomp $ # One process to process the whole file
                                                                    Split the file and start 4 processes
dfr@hmem00:~/parcomp $ time { cat d.txt | ./lower.sh > res.txt
real
        0m4.014s
        0m0.003s
user
SVS
        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
        0m0.009s
user
        0m0.021s
```

Need recent version of Coreutils/8.22-goolf-1.4.10

4.3.3. One program and one large file

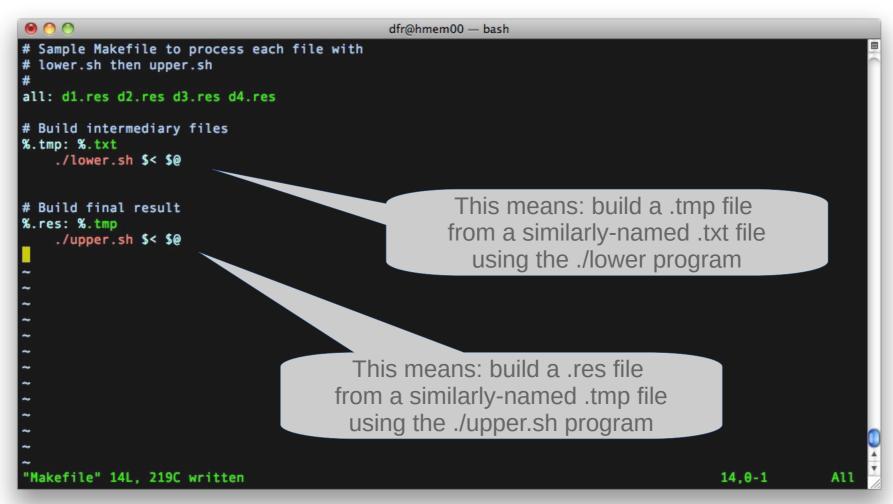
The split command distributes data from stdin to program

```
● ● ●
                                             dfr@hmem00 - bash
                                                                  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
        0m0.003s
user
SVS
        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
       0m0.009s
user
       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 5 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
       0m0.011s
user
SVS
       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

4.3.4. Several programs and many files

A Makefile describes dependencies and is executed with 'make'



4.3.4. Several programs and many files

The 'make' command can operate in parallel

```
0 0 0
                                               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
        0m0.099s
SVS
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
        0m0.025s
user
```

4.3. Basic tools

Summary

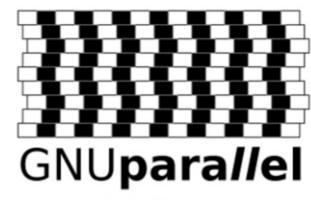
- You have either
 - one very large file to process
 - with one program: split
 - with several programs: fifo (or pipes)
 - many files to process
 - with one program xargs
 - with many programs make

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

• Syntax: parallel command ::: argument list

```
dfr@hmem00 - bash
dfr@hmem00:~/parcomp $ parallel echo ::: 1 2 3 4
dfr@hmem00:~/parcomp $ parallel echo ::: {1..10}
dfr@hmem00:~/parcomp $ time parallel sleep ::: {1..10}
real
        0m11.200s
user
        0m0.206s
        0m0.129s
dfr@hmem00:~/parcomp $ parallel echo ::: d?.txt
d1.txt
d2.txt
d3.txt
dfr@hmem00:~/parcomp $
```

• Syntax: {} as argument placeholder.

```
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 $
```

Multiple parameters and --xapply

```
0 0 0
                                               dfr@hmem00 - bash
dfr@hmem00:~/parcomp $ parallel echo ::: 1 2 3 4 ::: A B
1 B
dfr@hmem00:~/parcomp $ parallel --xapply echo ::: 1 2 3 4 ::: A B C D
2 B
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
  and A
2 and B
  and C
  and D
  and A
3 and B
  and C
3 and D
  and A
```

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

```
0 0 0
                                              dfr@hmem00 - bash
dfr@hmem00:~/parcomp $ cat experiments.csv
Number, Letter
2,B
dfr@hmem00:~/parcomp $ parallel --colsep ',' --header '\n' echo {Number} {Letter} ::: experiments.csv
2 B
dfr@hmem00:~/parcomp $
```

A terminal for every job

Using --tmux GNU parallel can start a terminal for every job run:

```
seq 10 20 | parallel --tmux 'echo start {}; sleep {}; echo done {}'
```

This will tell you to run something similar to:

```
tmux -S /tmp/tmsrPr00 attach
```

Using normal **tmux** keystrokes (CTRL-b n or CTRL-b p) you can cycle between windows of the running jobs. When a job is finished it will pause for 10 seconds before closing the window.

Interactivity

GNU parallel can ask the user if a command should be run using --interactive:

```
parallel --interactive echo ::: 1 2 3
```

```
echo 1 ?...y
echo 2 ?...n
1
echo 3 ?...y
3
```

Timing

Some jobs do heavy I/O when they start. To avoid a thundering herd GNU **parallel** can delay starting new jobs. **--delay** *X* will make sure there is at least *X* seconds between each start:

```
parallel --delay 2.5 echo Starting {}\;date ::: 1 2 3
```

```
Starting 1
Thu Aug 15 16:24:33 CEST 2013
Starting 2
Thu Aug 15 16:24:35 CEST 2013
Starting 3
Thu Aug 15 16:24:38 CEST 2013
```

Progress information

Based on the runtime of completed jobs GNU parallel can estimate the total runtime:

```
parallel --eta sleep ::: 1 3 2 2 1 3 3 2 1
```

```
Computers / CPU cores / Max jobs to run
1:local / 2 / 2

Computer:jobs running/jobs completed/%of started jobs/
Average seconds to complete
ETA: 2s 0left 1.11avg local:0/9/100%/1.1s
```

With a joblog GNU parallel can be stopped and later pickup where it left off. It it important that the input of the completed jobs is unchanged.

```
parallel --joblog /tmp/log exit ::: 1 2 3 0
cat /tmp/log
parallel --resume --joblog /tmp/log exit ::: 1 2 3 0 0 0
cat /tmp/log
```

```
Seg Host Starttime
                      Runtime Send Receive Exitval Signal Command
        1376580069.544 0.008
                                                        exit 1
       1376580069.552 0.009 0 0
                                                        exit 2
  : 1376580069.560 0.012
                                                        exit 3
        1376580069.571 0.005
                                                        exit 0
                      Runtime Send Receive Exitval Signal Command
Seq Host Starttime
        1376580069.544 0.008
                                                        exit 1
        1376580069.552 0.009
                                                        exit 2
       1376580069.560 0.012
                                                        exit 3
       1376580069.571 0.005
                                                        exit 0
  : 1376580070.028 0.009
                                                        exit 0
        1376580070.038 0.007
                                                        exit 0
```

Other interesting options

--pipe Split a file

Use remote servers through SSH

-j n Run n jobs in parallel

-kKeep 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.

Homework

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 ; }
```

Summary

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