

Consortium des Equipements de Calcul Intensif en Fédération Wallonie-Bruxelles

Introduction to Parallel Computing

damien.francois@uclouvain.be December 2022



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 \rightarrow more storage capacity

Parallelization involves:

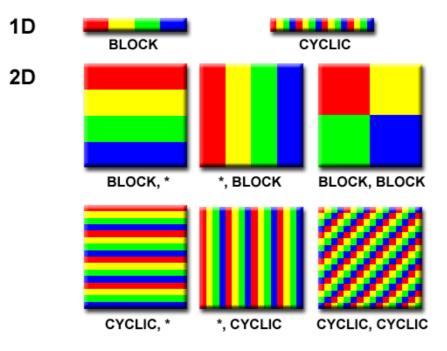
- decomposition of the work
 - distributing instructions to processors
 - distributing data to memories
- *collaboration* of the workers
 - **synchronization** of the distributed work
 - communication of data

Decomposition of the work

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

Decomposition of the work

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

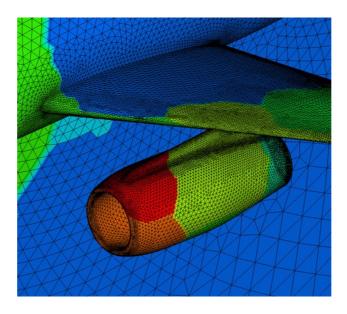


https://nyu-cds.github.io/python-mpi/04-decomposition/

7

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



Parallelization involves:

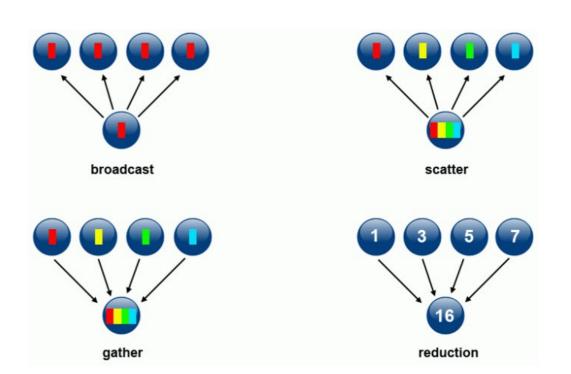
Collaboration of the workers

- 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)
- Iow Embarrassingly parallel : they rarely or never have to communicate (asynchronous)

Parallelization involves:

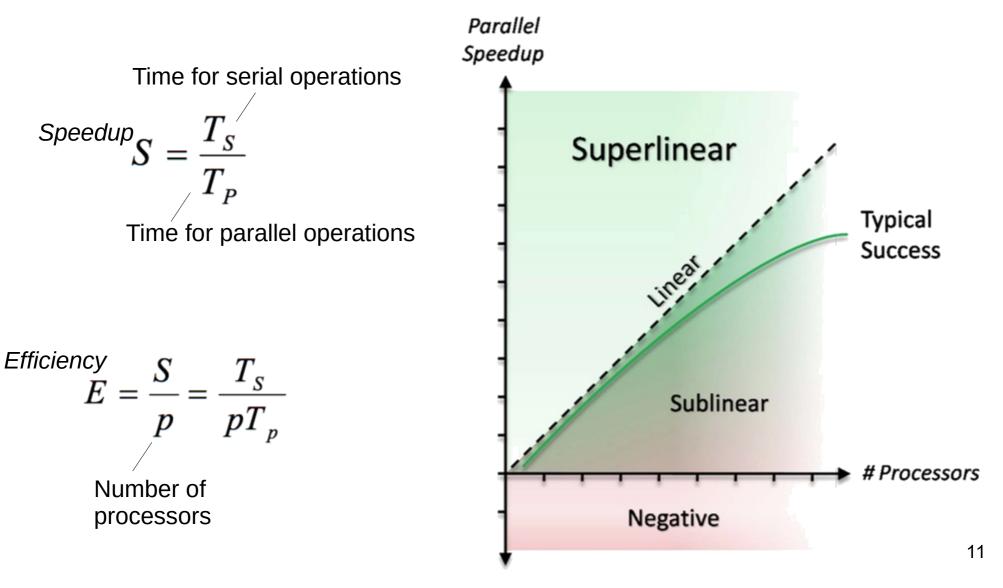
Collaboration of the workers

- Communication between workers
 - Point to point
 - Broadcast
 - Scatter
 - Gather
 - Reduction



https://hpc.llnl.gov/documentation/tutorials/introduction-parallel-computing-tutorial

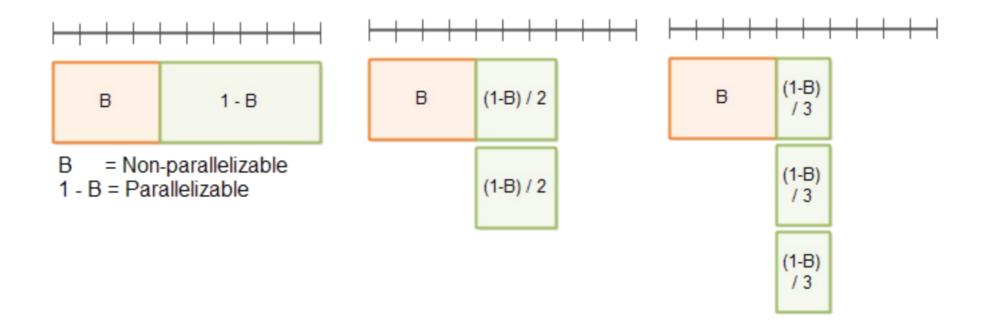
Does it work? Speedup, Efficiency, Scalability



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

Challenge 1: Amdahl's Law

Not all the work can be decomposed

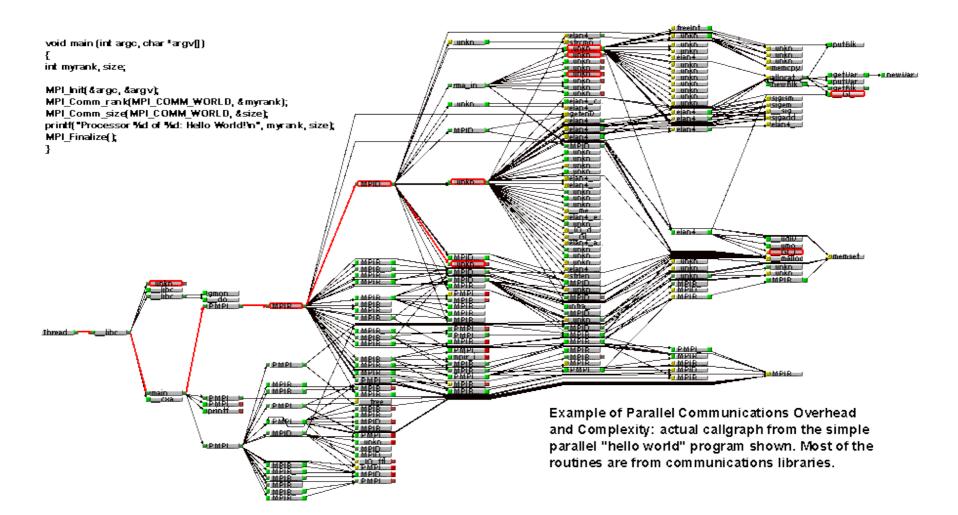


In parallel computing, Amdahl's law is mainly used to predict the theoretical maximum speedup for programs using multiple processors.

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

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



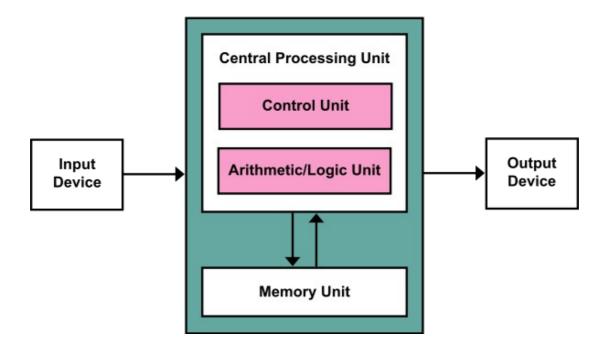
https://hpc-wiki.info/hpc/Load_Balancing



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)

. . .

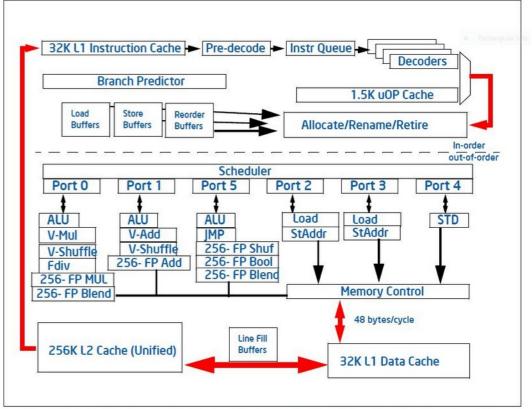
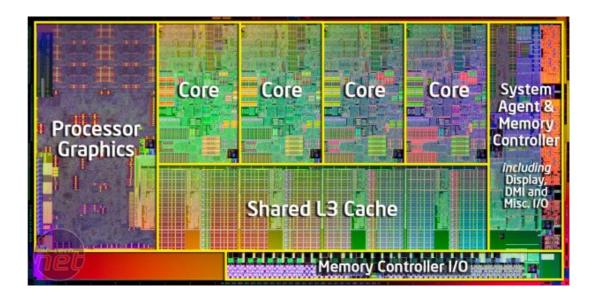


Figure 2-1. Intel microarchitecture code name Sandy Bridge Pipeline Functionality



Parallelism at the chip (socket) level

• Multicore parallelism

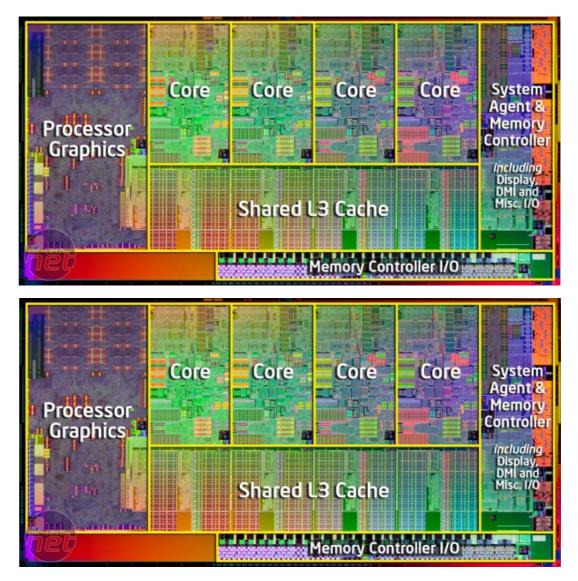


Parallelism at the computer level



- Multi-socket parallelism
 - SMP
 - NUMA
- Accelerators





Parallelism at the data center level



Multi-node parallelism





Parallelism at the data center level

Cluster computing

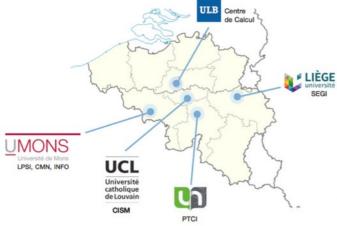


Consortium des Équipements de Calcul Intensif

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"

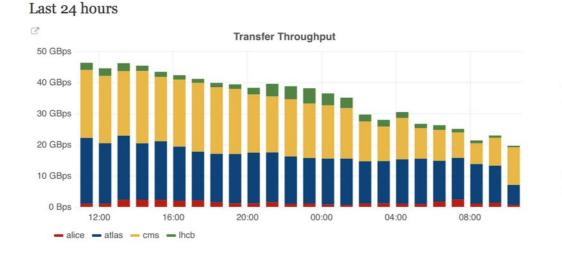


Parallelism at the world level

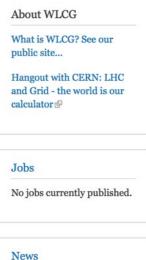
Grid computing – "cluster of clusters"

Ŵ	•		mputing Grid						Q
Home	Collaboration	Meetings	Grid Operations	Security	Tools	Docs & Ref	Getting Started	Public site	
Home									

Welcome to the Worldwide LHC Computing Grid



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.



News

TEG Reports

2

- Computing Model Update available
- Technology Market Cost Trends

Parallelism at the world level

Distributed computing - "no unused cycle"



SETI

Project - Science - Computing -

- Community - Site -

Sign Up Login

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 paradigms and programming models

Is parallization automagic?

- ILP: yes
- SIMD: mostly, but the compiler 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*)

If you are in charge of parallization, see next slides...

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

If (very_long_computation) then do A else 28 do B

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



User tools that GNU/Linux offers

4.1 Parallelized tools4.2 Job control and parallel processes4.3 Basic tools4.4 GNU Parallel

4.1. Parallelized utilities

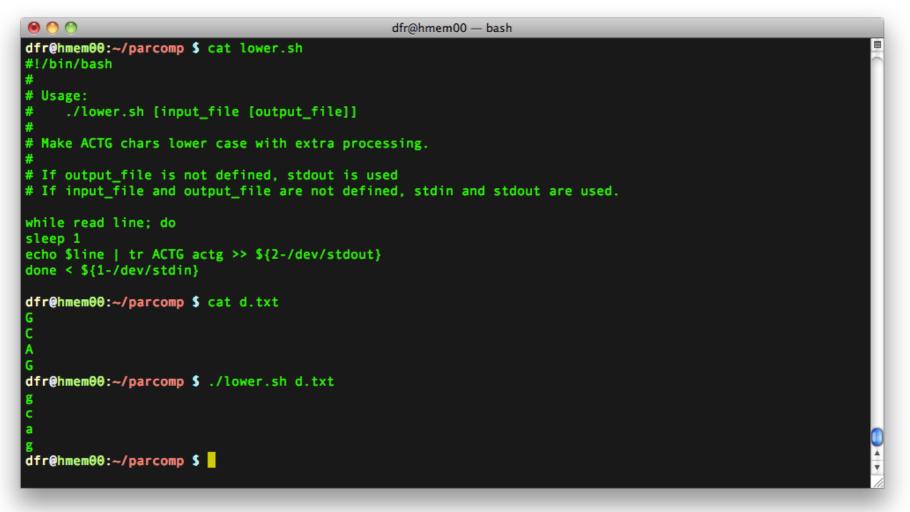
Some tools have a parallelized counterpart. Examples:

serial

gzip pigz grep ripgrep ssh clustershell sort sort –parallel scp bbcp bc bcx

parallel

Consider the following example program



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

Run the program twice

00	dfr@hmem00 — bash	
r@hmemθθ:~/parcomp \$ # Fore	ground: commands end with ';'	
<pre>r@hmem00:~/parcomp \$ time {</pre>	<pre>./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt ;</pre>	
r@hmem00:~/parcomp \$		

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

Run the program twice and measure the time it takes

```
0 0
                                              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 ; };
```

34

Run the program twice and measure the time it takes

00	dfr@hmem00 — bash	
	# Foreground: commands end with ';'	E .
r@hmem00:~/parcomp \$	<pre>time { ./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt ; };</pre>	
al 0m8.033s		
er 0m0.004s		
s 0m0.019s		
r@hmem00:~/parcomp \$		

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

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

```
0 0
                                               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
SVS
dfr@hmem00:~/parcomp $
```

4.2. Job control & Parallel processes in Bash

Parallel for loop in Bash:

```
for i in {1..10}; do | for i in {1..10}; do
  command1
  command2
done
```

```
command1
 command2
done; wait
```

 (\ldots) & : 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



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

0 0	dfr@hmem00 — bash	
	<pre>\$ # Using an intermediay file \$ time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }</pre>	
	<pre>\$ # Using pipes (as our programs can handle stdin and stdout) \$ time { ./lower.sh d.txt ./upper.sh > res.txt ; }</pre>	
real 0m5.013s user 0m0.002s sys 0m0.007s dfr@hmem00:~/parcomp	\$	

4.3.2. Several programs and one file

Using UNIX fifos for pipelining operations



4.3.3. One program and one large file

The split command distributes data from stdin to program

● ● ● ● fr@hmem00:~ fr@hmem00:~				ocess	the	file	Split tl	he fi	le an	d s	tart	4 p	oroc	esse	es
ıser 0m0.									r ./low	ver.s	¦h ≻r	es.tx	<t;}< th=""><th></th><th></th></t;}<>		
ıser 0m0	.011s .009s .021s													L	
Ifr@hmem00:- ime { cat (p lower [1] 12817															
2825 dfr fr@hmem00:- eal 0m1 ser 0m0 ys 0m0															
1]+ Done txt;															

Need recent version of Coreutils/8.22-goolf-1.4.10

4.3.3. One program and one large file

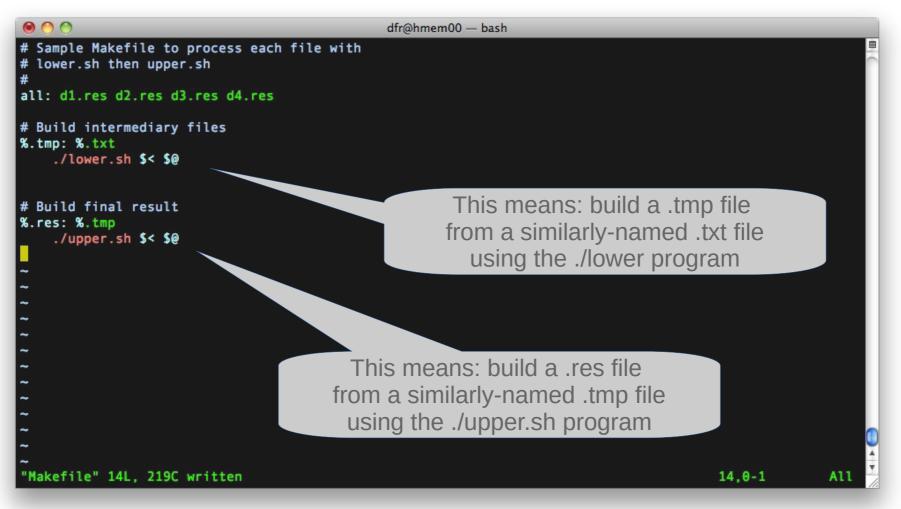
The split command distributes data from stdin to program

<pre></pre>						s the		le	Split the file and start 4 processes
real 0m4.014s user 0m0.003s sys 0m0.009s dfr@hmem00:~/parco dfr@hmem00:~/parco									robin fashion mber r/4filter ./lower.sh >res.txt ; }
ep lower								./lower	er.sh >res.txt ; } & top -u dfr -bn1 gr
[1] 12817 12822 dfr 20	•	102-	1353	1052	5 0.0		0:00.00	1.000	
12822 dfr 20				1052			0:00.00		
						0.0			
				1052		0.0	0:00.00		
12825 dfr 20 dfr@hmem00:~/parco real 0m1.011s user 0m0.011s sys 0m0.019s	ө тр \$	103m	1252	1027	5 0.0	0.0	0:00.00	Lower.	sn
<pre>[1]+ Done .txt; } dfr@hmem00:~/parco</pre>	mp \$	•	time	e { ca	t d.txt	sp]	litunb	uffered	dnumber r/4filter ./lower.sh > res

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'



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

4.3.4. Several programs and many files

The 'make' command can operate in parallel

000	dfr@hmem00 — bash	
dfr@hmem00:~/parcomp \$ time make		
./lower.sh d1.txt d1.tmp		\sim
./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		<u> </u>

Summary

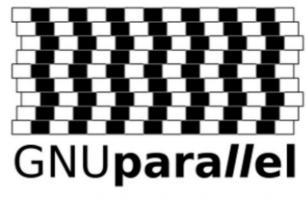
- You have either
 - one very large file to process
 - with one program: split
 - with several programs: fifo (or pipes)
 - many files to process
 - with one program xargs
 - with many programs make

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.

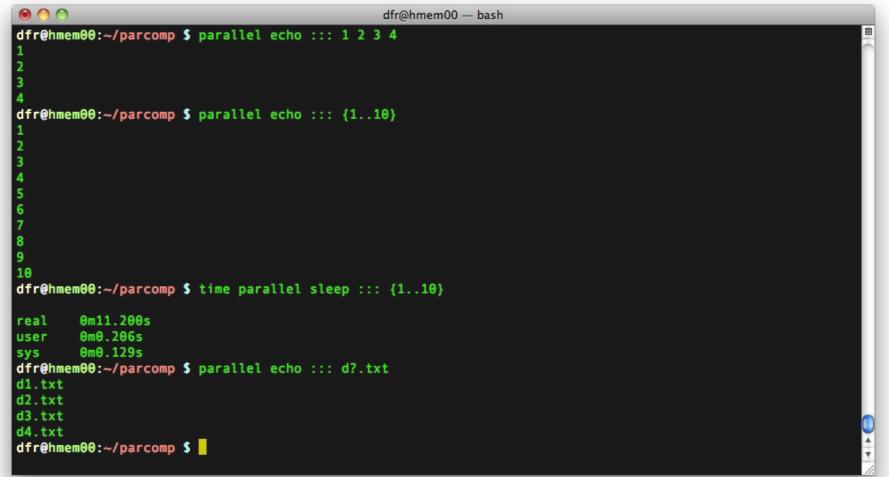


For people who live life in the parallel lane.

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



• Syntax: {} as argument placeholder.

d1.txt	
d2.txt	
d3.txt	
d4.txt	
<pre>dfr@hmem00:~/parcomp \$ parallel echo {} {.}.res ::: d?.txt</pre>	
d1.txt d1.res	
d2.txt d2.res	
d3.txt d3.res	
d4.txt d4.res	
<pre>dfr@hmem00:~/parcomp \$ parallel echo {} :::/parcomp/d?.txt</pre>	
/parcomp/d1.txt	
/parcomp/d2.txt	
/parcomp/d3.txt	
/parcomp/d4.txt	
<pre>dfr@hmem00:~/parcomp \$ parallel echo {/} :::/parcomp/d?.txt</pre>	
d1.txt	
d2.txt	
d3.txt	
d4.txt	
dfr@hmem00:~/parcomp \$	
dfr@hmem00:~/parcomp \$	T
dfr@hmem00:~/parcomp \$	

• Multiple parameters and --xapply

O O dfr@hmem00 — bash	
<pre>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</pre>	
4 B dfr@hmemθθ:~/parcomp \$ parallelxapply echo ::: 1 2 3 4 ::: A B C D 1 A 2 B 3 C 4 D	
<pre>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</pre>	
3 and A 3 and B 3 and C 3 and D 4 and A	

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

000	dfr@hmem00 — bash
<pre>dfr@hmem00:~/parcomp \$ cat experiments.csv Number,Letter 1,A 2,B 3,B 3,A 4,C 5,C</pre>	
5,A	header '\n' echo {Number} {Letter} :::: experiments.csv

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.

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