

Consortium des Equipements de Calcul Intensif en Fédération Wallonie-Bruxelles

Introduction to Parallel Computing

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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

Also: energy consumption is a cubic function of clock frequency so using 2 ⁴ compute units is 8 times cheaper than using one unit with double the frequency

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

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

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

printf(Processor %d of %d: Hello World!'n",

}



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

Why wouldn't it work?

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





Hardware for parallel computing

Von Neumann (serial) architecture

An abstract view of early computers



https://en.wikipedia.org/wiki/Von_Neumann_architecture

Parallelism at the CPU (core) level

An abstract view of modern CPUs

- Instruction-level parallelism (ILP)
 - Instruction pipelining
 - Out-of-order execution
 - Speculative execution

. . .

- Simultaneous multithreading (SMT)
- 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"

X	Vorldw	/L_C	mputing Grid							•
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

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- Computing Model Update available
- Technology Market Cost Trends

Parallelism at the world level

Distributed computing - "no unused cycle"





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

Programming paradigms (logic of work sharing and organizing) Programming models (software libraries and APIs)

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 1 CPU1: do A CPU1: else 2 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



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, or parallel options. Examples:

serial		parallel
gzip grep ssh sort scp bc	$ \begin{array}{c} & \longrightarrow \\ & \longleftarrow \\ & & & \end{pmatrix} $	pigz ripgrep, singrep clustershell sortparallel bbcp bcx

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	
dfr@hmem00:~/parcomp \$ # Foreg	ground: commands end with ';'	
<pre>dfr@hmem00:~/parcomp \$ time {</pre>	./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt	
real 0m8.033s		
user 0m0.004s		
dfr@hmem00:~/parcomp \$ # Backs		
<pre>dfr@hmem00:~/parcomp \$ time {</pre>		
[1] 49722		
[1] - Done		
[2]+ Done		
real 0m4.011s		
user 0m0.004s		
sys 0m0.005s		
arrennemou		
		Ă
		*

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 ; };
```

Run the program twice and measure the time it takes

0 0	dfr@hmem00 — bash	
dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$	<pre># Foreground: commands end with ';' time { ./lower.sh d1.txt r1.txt ; ./lower.sh d1.txt r2.txt ; };</pre>	
real 0m8.033s user 0m0.004s sys 0m0.019s		
dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$ [1] 49722	<pre># Background, in parallel: commands end with '&' and 'wait' necessary time { ./lower.sh d2.txt r1.txt & ./lower.sh d2.txt r2.txt & wait ; }; </pre>	
[2] 49723 [1]- Done [2]+ Done		
real 0m4.011s user 0m0.004s sys 0m0.005s dfr@hmem00:~/parcomp \$		
		115

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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 $
```

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

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	
dfr@hmem00:~/parcomp dfr@hmem00:~/parcomp	<pre>\$ # Using an intermediay file \$ time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }</pre>	
real 0m8.033s user 0m0.005s sys 0m0.017s dfr@hmem00:~/parcomp dfr@hmem00:~/parcomp	\$ # Using pipes (as our programs can handle stdin and stdout) \$ time { ./lower.sh d.txt ./upper.sh > res.txt ; }	
<pre>real 0m5.014s user 0m0.000s sys 0m0.009s dfr@hmem00:~/parcomp dfr@hmem00:~/parcomp prw-rw-r 1 dfr dfr dfr@hmem00:~/parcomp [1] 65343 [1]+ Done</pre>		
real 0m5.013s user 0m0.002s sys 0m0.007s dfr@hmem00:~/parcomp	\$	

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

00	dfr@hmem00 — bash	
dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$	<pre># Using an intermediay file time { ./lower.sh d.txt tmp.txt ; ./upper.sh tmp.txt res.txt ; }</pre>	
real 0m8.033s user 0m0.005s sys 0m0.017s dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$	<pre># Using pipes (as our programs can handle stdin and stdout) time { ./lower.sh d.txt ./upper.sh > res.txt ; }</pre>	
real 0m5.014s user 0m0.006s sys 0m0.009s		
<pre>dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$ prw-rw-r 1 dfr dfr 0 dfr@hmem00:~/parcomp \$ [1] 65343 [1]+ Done</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

	dfr@hmem00 - bash # One process to process the whole file time { cat d.txt ./lower.sh > res.txt
real 0m4.014s user 0m0.003s sys 0m0.009s dfr@hmem00:~/parcomp \$ dfr@hmem00:~/parcomp \$	# Four processes handl ing one line in round robin fashion time { cat d.txt splitunbufferednumber r/4filter ./lower.sh >res.txt ; }
real 0m1.011s user 0m0.009s sys 0m0.021s	
<pre>dfr@hmem00:~/parcomp \$ time { cat d.txt spli</pre>	! & top -u dfr -bn1 grep lower unbufferednumber r/4filter ./lower.sh >res.txt : } & top -u dfr -bn1 gr
ep lower	
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 dfr@hmem00:~/parcomp \$ real 0m1.011s user 0m0.011s sys 0m0.019s	103m 1252 1052 5 0.0 0.0 0:00.00 Lower.sh
<pre>[1]+ Done .txt; } dfr@hmem00:~/parcomp \$</pre>	time { cat d.txt splitunbufferednumber 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	
./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 al.tmp a2.tmp a4.tmp a3.tmp	
real Am32 26As	
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 dl.tmp dl.res	
./upper.sh d2.tmp d2.res	
./upper.sn d4.tmp d4.res	
rm d1 tmp d2 tmp d4 tmp d3 tmp	
<u></u>	
real 0m8.163s	
user 0m0.025s	

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 but you can install it

• Syntax: parallel command ::: argument list



• 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

00	dfr@hmem00 — bash	1
dfr@hmem00:~/parcomp \$ parallel echo ::: 1 2 1 A 1 B 2 A 2 B 3 A 3 B 4 A	3 4 ::: A B	
4 B		
dfr@hmem00:~/parcomp \$ parallelxapply echo 1 A 2 B 3 C 4 D dfr@hmem00:~/parcomp \$ parallel echo {1} and 1 and A 1 and B 1 and C 1 and D	b ::: 1 2 3 4 ::: A B C D d {2} ::: 1 2 3 4 ::: A B C 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		

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

● ○ ○	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>	
dfr@hmem00:~/parcomp \$ parallelcolsep ',' 1 A 2 B 3 B 3 A 4 C 5 C 5 A dfr@hmem00:~/parcomp \$	header '\n' echo {Number} {Letter} :::: experiments.csv

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.

https://www.gnu.org/software/parallel/parallel_tutorial.html

Interactivity

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

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

Output:

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

https://www.gnu.org/software/parallel/parallel_tutorial.html

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

Output:

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

https://www.gnu.org/software/parallel/parallel_tutorial.html

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

Output:

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
```

Output:

Seq 1 2 3 4	Host : : :	Starttime 1376580069.544 1376580069.552 1376580069.560 1376580069.571	Runtime 0.008 0.009 0.012 0.005	Send 0 0 0 0	Receive 0 0 0 0	Exitval 1 2 3 0	Signal 0 0 0 0	Command exit 1 exit 2 exit 3 exit 0
Seq 1	Host :	Starttime 1376580069.544	Runtime 0.008	Send 0	Receive 0	Exitval 1	Signal 0	Command exit 1
2	:	1376580069.552	0.009	0	0	2	0	exit 2
3	:	1376580069.560	0.012	0	0	3	0	exit 3
4	:	1376580069.571	0.005	0	0	0	0	exit 0
5	:	1376580070.028	0.009	0	0	0	0	exit 0

• Split a file with --pipe

\varTheta 🕙 🔿 dfr@hmem00	— bash
dfr@hmemθθ:~/parcomp \$ cat *.csv	
Number,Letter	
1, A second second	
2,B	
3,B	
3,R A C	
5.0	
5,A	
dfr@hmem00:~/parcomp \$ tail -n +2 *.csv parallel -kN	<pre>1recend '\n'pipe echo -n "JOB{#} : ;cat;"</pre>
JOB1 :1,A	일이 이 것 것 같아요. 이 같은 이 것 같아요. 것 것 같아요. 이 것 같아요. 것 것 같아요. 이 것
JOB2 :2,B	
JUB3 :3,B	
10B5 :4 C	
JOB6 :5.C	
J0B7 :5,A	
dfr@hmem00:~/parcomp \$	
	T

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

- Multiple programs and one file (not suitable for that)
- 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