

### Why use an HPC?

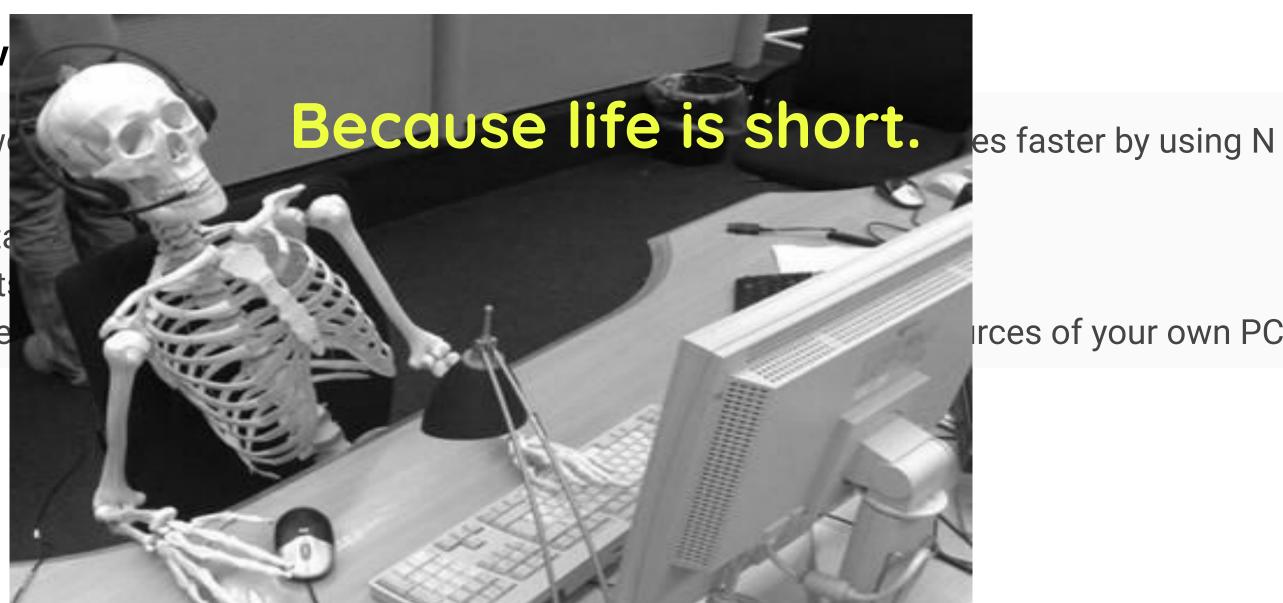
### The key goal is to solve the problems faster.

- Speed → Split the work between several processors: the program will run N-ish times faster by using N processors.
- Volume → large data analyses
- Cost → faster results, reduced wet lab analyses
- Efficiency and convenience → shared resources used 24/7, no need to use all resources of your own PC

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### Main Use Cases for HPC

### Clustered (Tightly coupled)

Modest IO requirements

- Fluid dynamics
- Weather forecasting
- Materials simulations
- Crash simulations

- Seismic processing
- Metagenomics
- Astrophysics
- Deep learning

# Heavy IO requirements

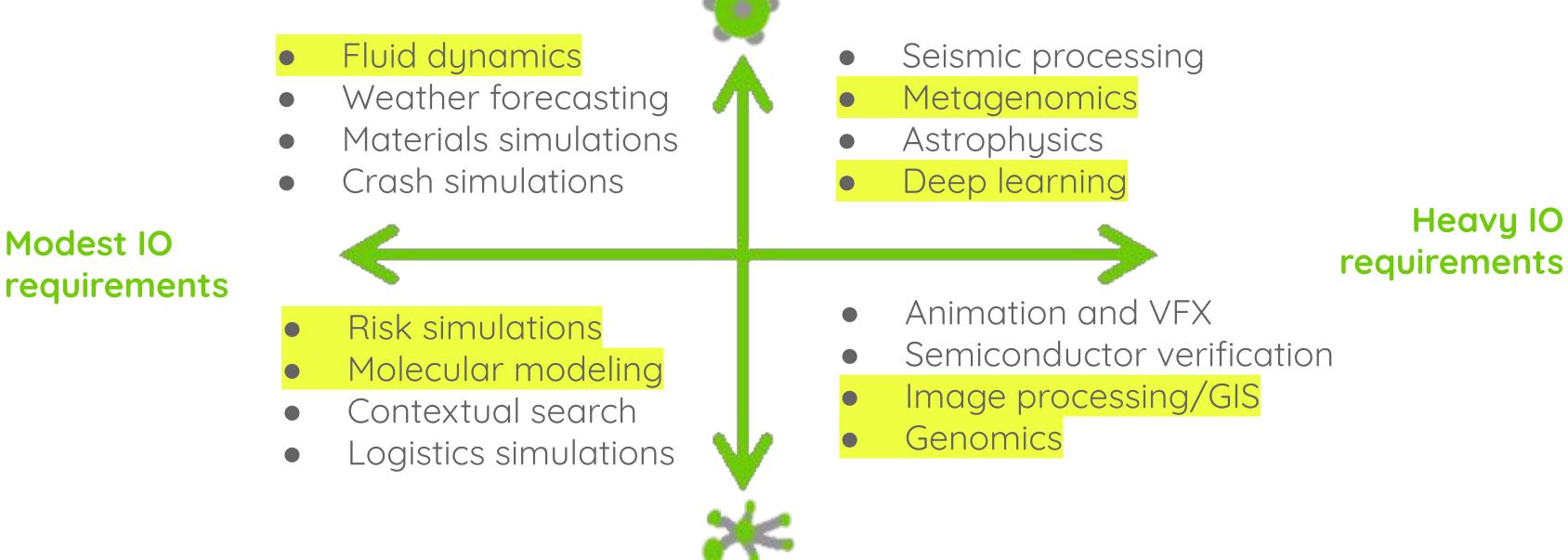
- Risk simulations
- Molecular modeling
- Contextual search
- Logistics simulations

- Animation and VFX
- Semiconductor verification
- Image processing/GIS
- Genomics

Distributed/Grid (Loosely coupled)

### Main Use Cases for HPC

### Clustered (Tightly coupled)



Heavy IO

Distributed/Grid (Loosely coupled)

Table 1 High-performance computing architectures: advantages and drawbacks

Able to implement a digital circuit, which directly performs

tasks are executed on a dedicated hardware without any

purpose-specific tasks (unlike general-purpose software tools). Such

Integrated circuits containing an

array of programmable logic

blocks

FPGA - Field

Programmable

Gates Arrays

HPC type	Architecture	Advantages	Drawbacks	Computing paradigm
Computer cluster	Set of interconnected computers controlled by a centralized scheduler	Require minimal changes to the existing source code of CPU programs, with the exception of possible modifications necessary for message passing	Expensive, characterized by relevant energy consumption and requires maintenance	Multiple Instruction Multiple Data
Grid computing	Set of geographically distributed and logically organized (heterogeneous) computing resources	Require minimal changes to the existing source code of CPU programs, with the exception of possible modifications necessary for message passing	Generally based on 'volunteering': computer owners donate resources (e.g. computing power, storage) to a specific project; no guarantee about the availability of remote computers: some allocated tasks could never be processed and need to be reassigned; remote computers might not be completely trustworthy	Multiple Instruction Multiple Data
Cloud computing	Pool of computation resources (e.g. computers, storage) offered by private companies, attainable on demand and ubiquitously over the Internet	Mitigate some problems like the costs of the infrastructure and its maintenance	Data are stored on servers owned by private companies; issues of privacy, potential piracy, espionage, international legal conflicts, continuity of the service (e.g. owing to some malfunctioning, DDoS attacks, or Internet connection problems)	Multiple Instruction Multiple Data
GPU - Graphics Processing Units	formerly devoted to real-time	High number of programmable computing units allow the execution of thousands simultaneous threads. Availability of high-performance local memories	Based on a modified SIMD computing paradigm: conditional branches imply serialization of threads' execution. GPU's peculiar architecture generally requires code rewriting and algorithms redesign	Same Instruction Multiple Data (although temporary divergence is allowed)
MIC - Many Integrated Cores	Dedicated parallel co-processor installable in common desktop computers, workstations and servers	Similar to GPUs but based on the conventional ×86 instructions set: existing CPU code, in principle, might be ported without any modification. All cores are independent	Fewer cores with respect to latest GPUs. To achieve GPU-like performances, modification of existing CPU code to exploit vector instructions are required	Multiple Instruction Multiple Data

computational overhead (e.g. those related to the operating system) might be necessary to execute tasks using the highest clock frequency

Nobile, et al., Graphics processing units in bioinformatics, computational biology and systems biology, *Briefings in Bioinformatics*, Volume 18, Issue 5, September 2017, Pages 870–885, https://doi.org/10.1093/bib/bbw058.

Generally programmed using a descriptive language (e.g. VHDL, Verilog [18]),

which can be cumbersome. Debugging using digital circuits simulators might

be complicated and not realistic. Experience with circuit design optimization

Dedicated hardware

### Table 1 High-performance computing architectures: advantages and drawbacks

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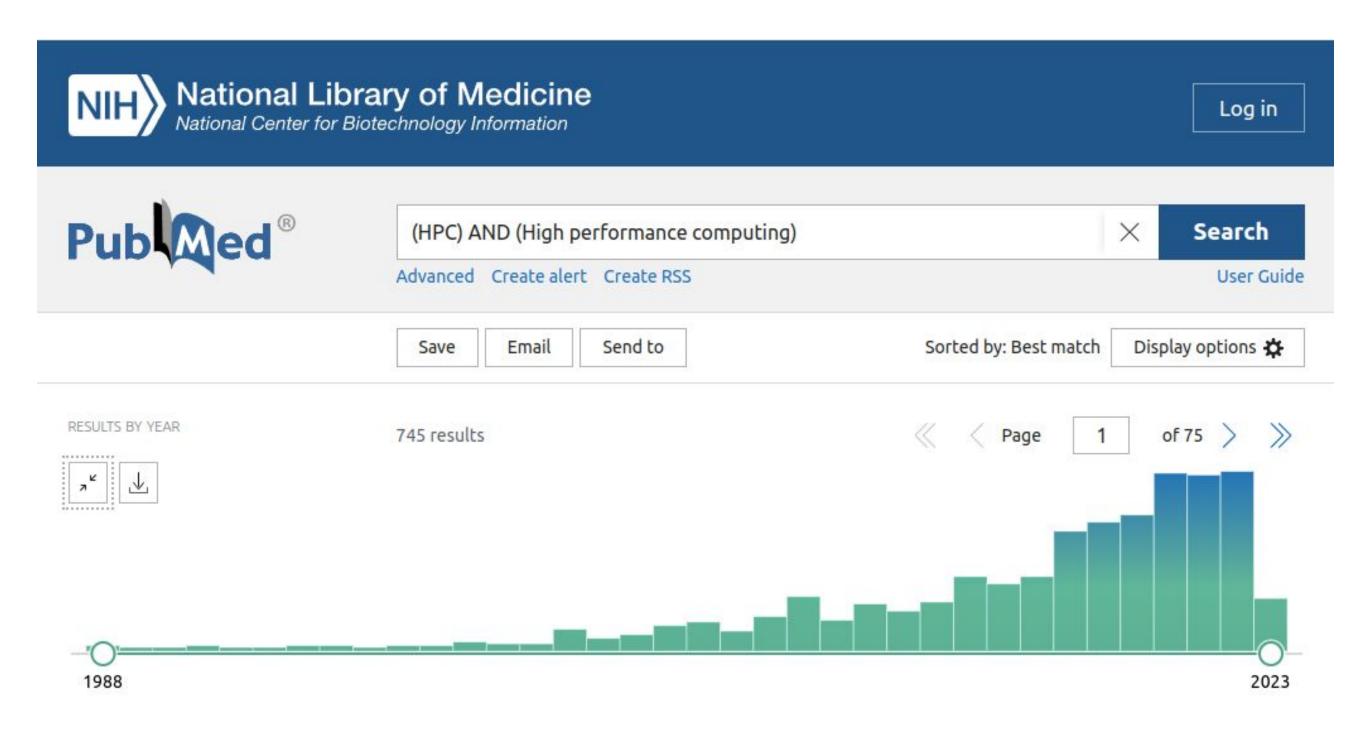
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which can be cumbersome. Debugging using digital circuits simulators might

Dedicated hardware

### HPC in Life Sciences recent papers:

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Jean-Paul Courneya

Alexa Mayo, AHIP

**High-Performance Computing** 

### HPC in Life Sciences recent papers

Editorial Published: 18 July 2018 Special Issue on High Performance Computing in Biomedical Informatics Luping Zhou, Islem Rekik, Chenggang Yan & Guorong Wu Research Open Access Published: 16 December 2022

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Profiling the BLAST bioinformatics application for load

balancing on high-performance computing clusters

Trinity Cheng, Pei-Ju Chin, Kenny Cha, Nicholas Petrick & Mike Mikailov ⊠

BMC Bioinformatics 23, Article number: 544 (2022) | Cite this article

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Biol Methods Protoc. 2022; 7(1): bpac032.

PMCID: PMC9767868 PMID: 36561335

Published online 2022 Nov 15. doi: 10.1093/biomethods/bpac032

Teaching computational genomics and bioinformatics on a high performance computing cluster—a primer

Arun Sethuraman™

Neuroinformatics 16, 283 (2018) | Cite this article Briefings in Bioinformatics Brief Bioinform. 2017 Sep; 18(5): 870-885 Published online 2016 Jul 7. doi: 10.1093/bib/bbw058 PMID: 2 High Performance Computing PP-Distance Algorithms to Generate X-ray Spectra from 3D Graphics processing units in bioinformatics, computational biology and systems biology by 🤗 César González 🔭 🖂 🧿 🧶 Simone Balocco 2 🦁 👰 Jaume Bosch ³, 🥷 Juan Miguel de Haro ³ 🧓 🥷 Maurizio Paolini 4, Antonio Filgueras <sup>3</sup> , a Carlos Álvarez <sup>3</sup> and Ramon Pons <sup>1,\*</sup> Institut de Química Avançada de Catalunya (IQAC-CSIC), 08034 Barcelona, Spain Is high performance computing a <sup>2</sup> Department of Mathematics and Informatics, Universitat de Barcelona, 08007 Barcelona, Spain requirement for novel drug discovery and 3 Barcelona Supercomputing Center (BSC), 08034 Barcelona, Spain 4 INTEL, 20090 Assago, Italy how will this impact academic efforts? Savíns Puertas-Martín [0], Antonio J. Banegas-Lun Juana L. Redondo [0], Pilar M. Ortigosa [0], Ol'ha ( Pages 981-985 | Received 16 Oct 2019, Accepted 17 Apr 2021 Computing Using VDJServer V1: A Method by the 20 September 2022 / Accepted: 22 September 2022 / Published: 27 September 2022 6 Download citation 
☐ https://doi.org/10.1080/174 **AIRR Community** Scott Christley, Ulrik Stervbo & Lindsay G. Cowell ≥ on beha to Tackle Pandemic Crisis

Exscalate4CoV: Innovative High Performing Computing (HPC) Strategies

by Andrea R. Beccari 1 0 and A Giulio Vistoli 2,\* 🖂 0 Protocol Open Access | First Online: 28 May 2022

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Towards Portable Large-Sci Part of the Methods in Molecular Biology book series (MIMB

EXSCALATE, Dompé Farmaceutici S.p.A., Via Tommaso De Amicis 95, I-80131 Napoli, Italy

Dipartimento di Scienze Farmaceutiche, Università degli Studi di Milano, Via Mangiagalli 25, I-20133 Milano, Italy

Author to whom correspondence should be addressed.

igh-Performance Computing in Cardiovascular Medicine of Multi-Dimensional Data Analysisre. Shinichi Goto

ar dinamics, Artificial intelligence, Neural network, Machine learning

Phylogenetics and Phylodynamics Using BEAGLE

Guy Baele ☑, Daniel L. Ayres, Andrew Rambaut, Marc A. Suchard & Philippe Lemey

Hyperparameter Tuning with I Int. J. Mol. Sci. 2022, 23(19), 11576; https://doi.org/10.3390/ijms231911576 Learning for Imbalanced Alzheimer's Disease Data

Yuankai Huo ⊠, Justin Blaber, Stephen M. Damon, Brian D. Boyd, Shun by 🙎 Fan Zhang 1,2,\* 🖂 💿 🙎 Melissa Petersen 1,2 🖂 🧸 Leigh Johnson 1,3 🖂 🧟 James Hall 1,2 🖾 and Parvathaneni, Camilo Bermudez Noguera, Shikha Chaganti, Vishwesh N Sid E. O'Bryant <sup>1,2</sup> □

Appl. Sci. 2022, 12(13), 6670; https://doi.org/10.3390/app12136670

Biocomputing 2023, pp. 541-545 (2022)

#### HIGH-PERFORMANCE COMPUTING MEETS HIGH-PERFORMANCE MEDICINE

Anurag Verma, Jennifer Huffman, Ali Torkamani, and Ravi Madduri

Bioinformationist, Health Sciences and Human Services Library, Uni

High-performance computing service for bioinformatics

Published online 2018 Oct 1, doi: 10.5195/imla.2018.512

Associate Director for Services, Health Sciences and Human Service 21201

https://doi.org/10.1142/9789811270611\_0050 | Cited by: 0

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e Methods in Molecular Biology book series (MIMB, volume 1910)

High-Performance Computing in Bayesian

\* Author to whom correspondence should be addressed

# Some topics covered and tools used

- protein folding
- drugs design
- genomics
  - WGS
  - RNAseq
  - proteome
  - metabolome
- ecology
- large datasets
- precision medicine
- ML/AI
- simulations

- AlphaFold
- Nextflow workflow managers
- CI/CD
- containers

- Quantum computing is coming
- cloud vs on-prem
- GPU
- Future directions in HPC

Heroes



And what happens when you accidentally delete ¼ of your temporary results

ttps://doi.org/10.1093/molbev/msaa15



# Run 4\*100k simulations in few days

- when to make the job start (waiting in the queue)
- "auto"launching launcher and set a waiting time
- Keep working on the cluster while simulating and fairplay
- Control in real time how much memory your job is using

```
🔞 🗐 🗊 wflow_fsc_cluster.sh (ebianco on marvin.s.upf.edu /gpfs42/robbyfs/homes/users/ebianco/SCRIPTS) - gedit
Save
 1 #!/bin/bash
 2 #mar 17 abr 2018 10:43:18 CEST
 3 #script to:
 4 # (1) run fastsimcoal simulation
 5 # (2) send the script to convert apr file to vcf individually
          (or in blocks defined by variable $rep, default is rep=10 )
 7 #to launch it
 8 # sbatch -t 30-00 -x mr-01-[01-02] -J fsc.$model ~/SCRIPTS/wflow fsc cluster.sh $model
 9 # squeue -o "%.18i %.9P %.8j %.8T %.10M " -u ebianco
10
11 #SBATCH -o fsc.%j.out
12 #SBATCH -e fsc.%j.err
13 #SBATCH -- job-name=fsc
14 #SBATCH --cpus-per-task=12
15 #SBATCH --partition=normal
16 #SBATCH --mem-per-cpu=4g
17 #SBATCH --mail-type=all
18 # SBATCH --mail-type=fail
19
20 module load fastsimcoal2/2.6.0.3
21
22 model=$1
24 SCRIPTF="/homes/users/ebianco/SCRIPTS"
26 #check if variables are set correctly
27 if [[ ! $model ]]
28 then
29 echo -e "ERROR: model is not specified. \nScript must be run as \nsbatch wflow_fsc.sh \$model \$numsim \$numsamp \$rep[optional]"
30 exit 1
31 fi
32
33 #run fastsimcoal after checking if model files are present in running folder
34 # if [[ -a $model.tpl && -a $model.est ]]
35 # then
36 time fsc26 -t $model.tpl -n 15 -e $model.est -E 25000 -q -c 12
38 rm -f $model/sust.*.out
39 # else
40 # echo "ERROR: no $model.tpl or $model.est file in running folder."
41 # exit 1
42 # fi
43
44 exit 0
```

# When to make a job start (waiting in the queue)

sbatch --dependency=after:\$j launcher\_sust.sh \$model \$m

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sbatch --dependency=after:\$j launcher\_sust.sh \$model \$m

#### -d, --dependency=<dependency list>

Defer the start of this job until the specified dependencies have been satisfied completed. <dependency\_list> is of the form <type:job\_id[:job\_id][,type:job\_id[:job\_id]]> or <type:job\_id[:job\_id][?type:job\_id[:job\_id]]>. All dependencies must be satisfied if the "," separator is used. Any dependency may be satisfied if the "?" separator is used. Many jobs can share the same dependency and these jobs may even belong to different users. The value may be changed after job submission using the scontrol command. Once a job dependency fails due to the termination state of a preceding job, the dependent job will never be run, even if the preceding job is requeued and has a different termination state in a subsequent execution.

#### after:job\_id[:jobid...]

This job can begin execution after the specified jobs have begun execution.

#### afterany:job\_id[:jobid...]

This job can begin execution after the specified jobs have terminated.

#### afterburstbuffer:job\_id[:jobid...]

This job can begin execution after the specified jobs have terminated and any associated burst buffer stage out operations have completed.

#### aftercorr:job\_id[:jobid...]

A task of this job array can begin execution after the corresponding task ID in the specified job has completed successfully (ran to completion with an exit code of zero).

#### afternotok:job\_id[:jobid...]

This job can begin execution after the specified jobs have terminated in some failed state (non-zero exit code, node failure, timed out, etc).

#### afterok:job\_id[:jobid...]

This job can begin execution after the specified jobs have successfully executed (ran to completion with an exit code of zero).

#### expand:job\_id

Resources allocated to this job should be used to expand the specified job. The job to expand must share the same QOS (Quality of Service) and partition. Gang scheduling of resources in the partition is also not supported.

#### singleton

This job can begin execution after any previously launched jobs sharing the same job name and user have terminated.

# "Auto"launching launcher and set a waiting time

sbatch --begin=now+5minutes launcher\_sust.sh \$model \$m

## "Auto"launching launcher and set a waiting time

sbatch --begin=now+5minutes launcher\_sust.sh \$model \$m

#### --begin=<time>

Submit the batch script to the Slurm controller immediately, like normal, but tell the controller to defer the allocation of the job until the specified time.

Time may be of the form *HH:MM:SS* to run a job at a specific time of day (seconds are optional). (If that time is already past, the next day is assumed.) You may also specify *midnight*, *noon*, *fika* (3 PM) or *teatime* (4 PM) and you can have a time-of-day suffixed with *AM* or *PM* for running in the morning or the evening. You can also say what day the job will be run, by specifying a date of the form *MMDDYY* or *MM/DD/YY YYYY-MM-DD*. Combine date and time using the following format *YYYY-MM-DD[THH:MM[:SS]]*. You can also give times like *now* + *count time-units*, where the time-units can be *seconds* (default), *minutes*, *hours*, *days*, or *weeks* and you can tell Slurm to run the job today with the keyword *today* and to run the job tomorrow with the keyword *tomorrow*. The value may be changed after job submission using the **scontrol** command. For example:

```
--begin=16:00
--begin=now+1hour
--begin=now+60 (seconds by default)
--begin=2010-01-20T12:34:00
```

#### Notes on date/time specifications:

- Although the 'seconds' field of the HH:MM:SS time specification is allowed by the code, note that the poll time of the Slurm scheduler is not precise enough to guarantee dispatch of the job on the exact second. The job will be eligible to start on the next poll following the specified time. The exact poll interval depends on the Slurm scheduler (e.g., 60 seconds with the default sched/builtin).
- If no time (HH:MM:SS) is specified, the default is (00:00:00).
- If a date is specified without a year (e.g., MM/DD) then the current year is assumed, unless the combination of MM/DD and HH:MM:SS has already passed for that year, in which case the next year is used.

# Keep working on the cluster while simulating and fairplay

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

~/SCRIPTS/wflow\_sust\_cluster.sh \$model \$mult

## Keep working on the cluster while simulating and fairplay

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

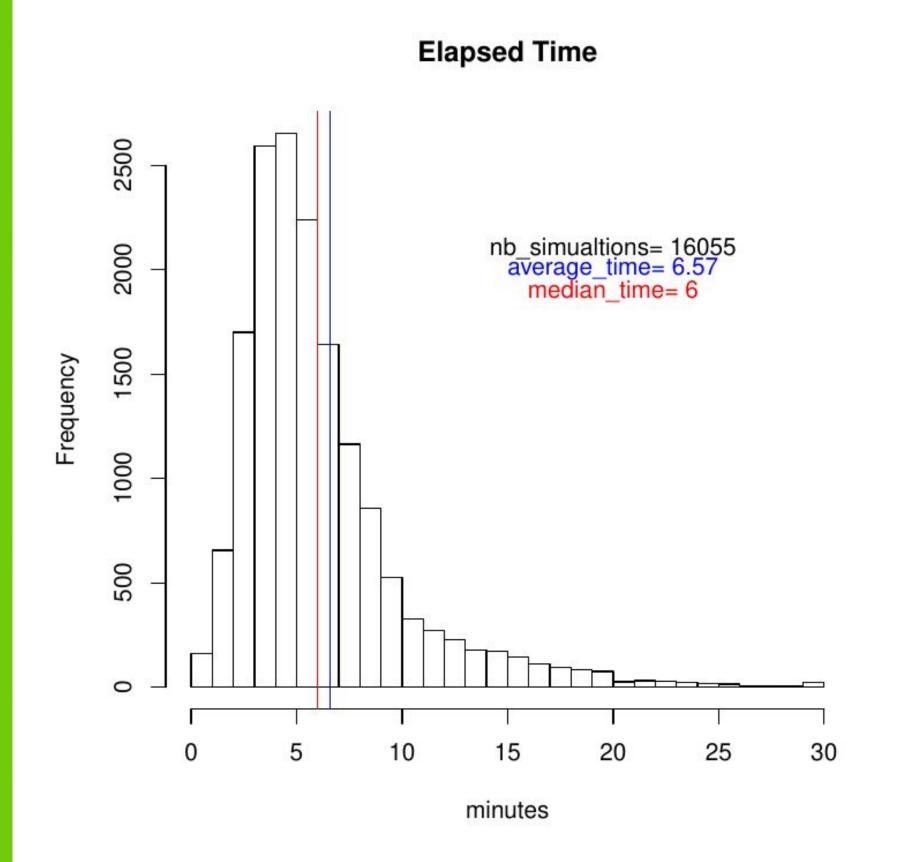
~/SCRIPTS/wflow\_sust\_cluster.sh \$model \$mult

#### -t, --time=<time>

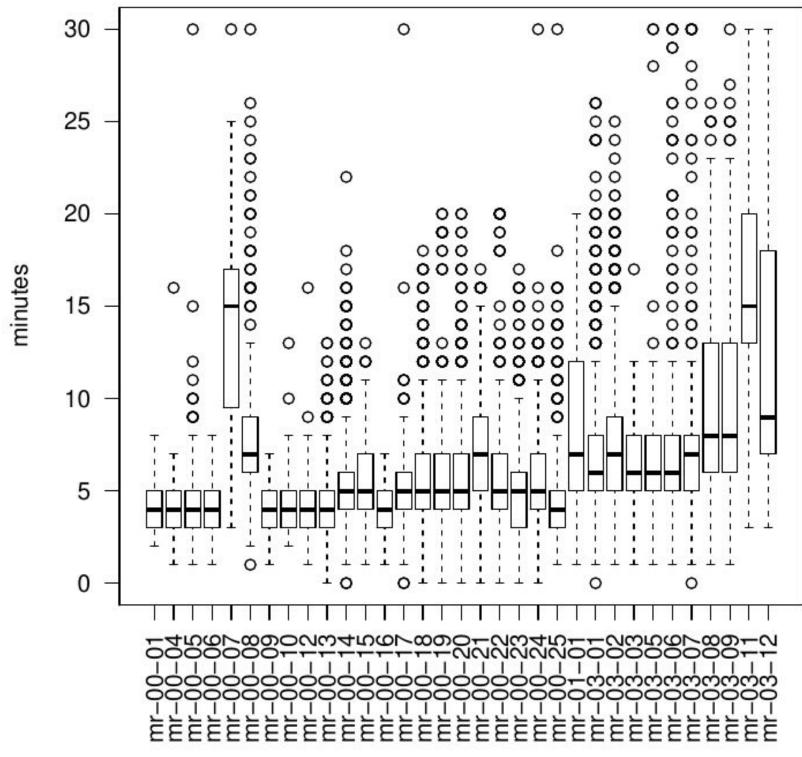
Set a limit on the total run time of the job allocation. If the requested time limit exceeds the partition's time limit, the job will be left in a PENDING state (possibly indefinitely). The default time limit is the partition's default time limit. When the time limit is reached, each task in each job step is sent SIGTERM followed by SIGKILL. The interval between signals is specified by the Slurm configuration parameter **KillWait**. The **OverTimeLimit** configuration parameter may permit the job to run longer than scheduled. Time resolution is one minute and second values are rounded up to the next minute.

A time limit of zero requests that no time limit be imposed. Acceptable time formats include "minutes", "minutes:seconds", "hours:minutes:seconds", "days-hours", "days-hours:minutes" and "days-hours:minutes:seconds".

### Homemade benchmark



### Elapsed time per node



## Keep working on the cluster while simulating and fairplay

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

~/SCRIPTS/wflow\_sust\_cluster.sh \$model \$mult

-x, --exclude=<node name list>

Explicitly exclude certain nodes from the resources granted to the job.

#### -w, --nodelist=<node name list>

Request a specific list of hosts. The job will contain *all* of these hosts and possibly additional hosts as needed to satisfy resource requirements. The list may be specified as a comma-separated list of hosts, a range of hosts (host[1-5,7,...] for example), or a filename. The host list will be assumed to be a filename if it contains a "/" character. If you specify a minimum node or processor count larger than can be satisfied by the supplied host list, additional resources will be allocated on other nodes as needed. Duplicate node names in the list will be ignored. The order of the node names in the list is not important; the node names will be sorted by Slurm.

# Job array: Keep working on the cluster while simulating and fairplay

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

~/SCRIPTS/wflow\_sust\_cluster.sh \$model \$mult

#### -a, --array=<indexes>

Submit a job array, multiple jobs to be executed with identical parameters. The *indexes* specification identifies what array index values should be used. Multiple values may be specified using a comma separated list and/or a range of values with a "-" separator. For example, "--array=0-15" or "--array=0,6,16-32". A step function can also be specified with a suffix containing a colon and number. For example, "--array=0-15:4" is equivalent to "--array=0,4,8,12". A maximum number of simultaneously running tasks from the job array may be specified using a "%" separator. For example "--array=0-15%4" will limit the number of simultaneously running tasks from this job array to 4. The minimum index value is 0. the maximum value is one less than the configuration parameter MaxArraySize. NOTE: currently, federated job arrays only run on the local cluster.

# Job array: Keep working on the cluster while simulating and fairplay

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

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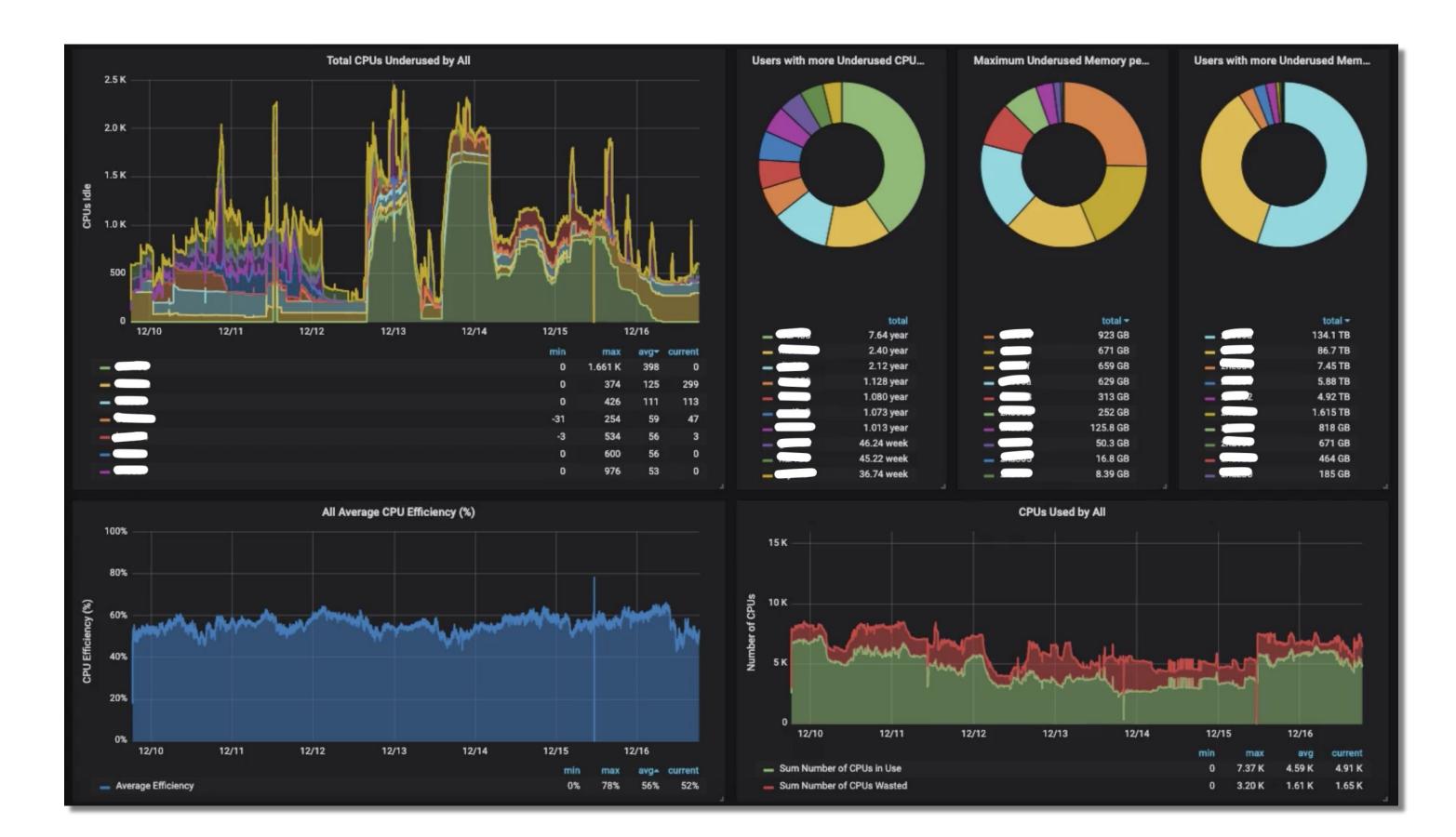
Keep working on the cluster while simulating of wflow\_sust\_cluster.sh (ebianco on marvin.s.upf.edu/gpfs42/robbyfs/ho

sbatch -x mr-01-[01-02] --time=30 --array=0-9 -J sust.\${m}.\${model} \

~/SCRIPTS/wflow\_sust\_cluster.sh \$model \$mult

```
Open ▼
 1 #!/bin/bash
 2 #SBATCH -o sust.%j.out
 3 # SBATCH -- job-name=sust
 4 #SBATCH --cpus-per-task=1
 5 #SBATCH --partition=normal
 6 #SBATCH --mem-per-cpu=10G
 7 # SBATCH --mail-type=end
 8 #SBATCH --mail-type=fail
11 ss="${SLURM ARRAY TASK ID}"
12 ss=$((ss+1))
13 mult=$2
14 s=$((ss+mult))
15 model=${1}
16
17 cd /gpfs42/robbyfs/scratch/lab_dcomas/ebianco/DEMO/$model
19 outname=${model}_${s}
21 if I ! Soutname I
22 then
23 echo "WARNING: no outname specified, exit."
24 exit 1
25 fi
27 echo "Converting Soutname"
29 rm -fr Soutname/
31 mkdir Soutname
32 cd Soutname
34 python ~/SCRIPTS/arp2selink_cluster.py $outname 15
36 bash wflow_${outname}.sh
37
38 exit 0
39
                       sh ▼ Tab Width: 8 ▼
                                              Ln 21, Col 18
```

### Control in real time how much memory your job is using - job monitoring tool



### Control in real time how much memory your job is using - without job monitoring tool

- scontrol show jobid \$JOBID
- squeue -t R -u \$USER  $\rightarrow$  to see in which node your job is running
- interactive -m 1 -w <node>
- top

```
ebianco@marvin:/homes/users/ebianco/DEMO/POSTPR/p-values
top - 10:06:33 up 13 days, 19:57, 0 users, load average: 11.06, 10.83, 10.27
Tasks: 425 total, 8 running, 417 sleeping,
                                                o stopped,
%Cpu(s): 34.5 us, 0.1 sy, 0.0 ni, 65.4 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
KiB Mem : 26385593+total, 21930035+free, 42007624 used, 2547968 buff/cache
KiB Swap: 8388604 total, 8384696 free,
                                              3908 used. 22034067+avail Mem
   PID USER
                     NI
                           VIRT
                                                  %CPU %MEM
                                                                TIME+ COMMAND
                 PR
                                   RES
                                           SHR S
115251 ebianco
                      0 5768200
                                  5.49
                                          4528 R 100.0
                                                       2.1
                                                             25:23.98 R
                 20
170308 mbogaer+
                      0 3546604
                                          1920 R 100.0
                                                            12879:46 i_baypass
                                  3.49
                 20
                                                       1.3
                                         1968 R 100.0
 60456 asantini
                         938912 921208
                                                       0.3 542:59.64 hgs
                 20
                 20
                          14.6g
                                         13940 S 100.0 1.2 47:46.60 java
105448 adedios
                                   3.0g
                                  5.3g
112066 ebianco
                 20
                      0 5743200
                                          4704 R 100.0
                                                       2.1
                                                             31:53.20 R
123451 ebianco
                                  4.99
                                          4664 R 100.0
                      0 5287080
                                                      2.0
                                                              7:50.24 R
                 20
133028 xfarre
                 20
                         180312
                                33656
                                                        0.0
                                                              1185:34 codeml
                                           884 R 100.0
                      0 3356648 471444 117792 S 100.0 0.2
147993 sdeb
                 20
                                                              2334:13 MATLAB
148257 sdeb
                      0 3291112 474312 117724 S 100.0
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148376 sdeb
                 20
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                      0 2050016
                                  1.0g
                                       10588 R 100.0
                                                              1124:13 python
165293 xfarre
                 20
                                                        0.4
 13469 root
                 0 -20
                                 12.7g 611168 S
                                                       5.1 108:34.38 mmfsd
                          28.9g
                                                   0.7
127293 ebianco
                         172572
                                  2716
                                          1668 R
                                                   0.7 0.0
                                                              0:00.12 top
                 20
                          13216
                                   752
                                                   0.3 0.0
                                                              3:43.33 rngd
 1297 root
                 20
                                          604 S
                         384544
                                                   0.3 0.0
                                                              1:31.44 dsm_ism_srvmgrd
 2149 root
                 20
                                  1912
                                          1356 S
                                                   0.0 0.0
                                                              8:28.13 systemd
                                          2612 S
     1 root
                 20
                         193432
                                  6388
                                                   0.0 0.0
                                                              0:00.54 kthreadd
                                             0 S
                 20
                      0
                                     0
     2 root
                 20
                                                   0.0 0.0
                                                              0:04.75 ksoftirgd/0
                      0
     3 root
                                             0 S
                                             0 S
                                                              0:00.04 kworker/0:0H
                  0 -20
                                     0
                                                   0.0 0.0
     5 root
                                                              0:00.71 migration/0
                                             0 S
                                                   0.0 0.0
                                     0
     8 root
                 rt
                                             0 S
                                                   0.0 0.0
                                                              0:00.00 rcu bh
                              0
                                     0
     9 root
                 20
                                                              9:48.37 rcu sched
                                             0 S
                                                   0.0 0.0
    10 root
                 20
                                     0
                                                   0.0 0.0
                                                              0:00.00 lru-add-drain
                  0 -20
                              0
                                     0
                                             0 S
    11 root
```

### In conclusion:

- All disciplines in Life Science can benefit from HPC
- Work smarter: user your resources at their best performance
  - reduce analysis time,
  - reduce costs,
  - reduce wetlab tests
- Be fair, and FAIR (Findability, Accessibility, Interoperability, and Reuse)
  - document and comment all your codes! (It's for your own benefit)



# Questions?

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