Compute Cluster Workshop

slurm

workload manager

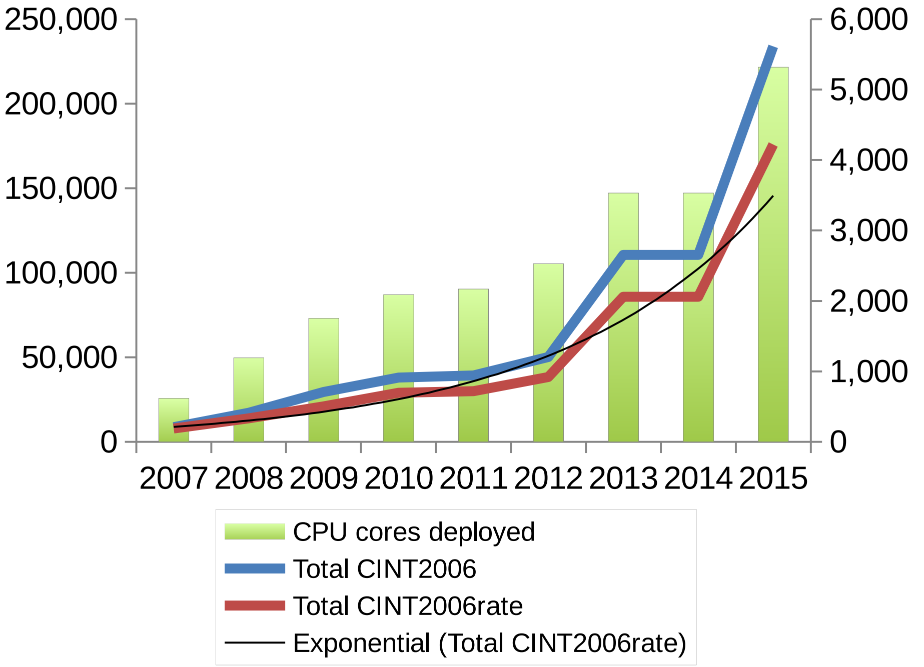
EMBL

Jurij Pečar

What is a compute cluster

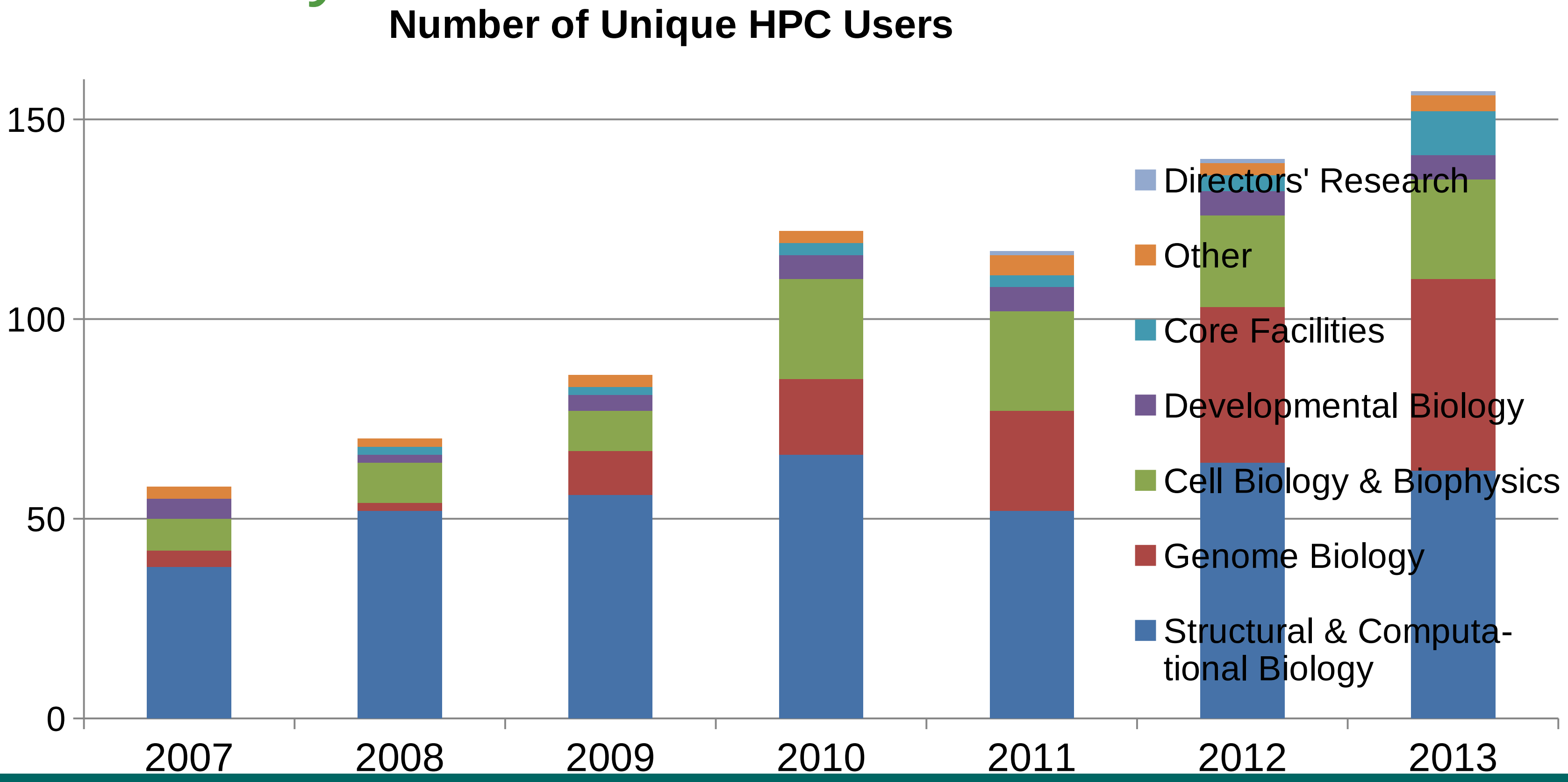
- Bunch of individual machines tied together in a special way
- Special software is used to represent those machines as a pool of shared resources
- This software gives you ability to ask for a chunk of this pool to run your software
- Tailored to batch processing (=jobs)
  - Interactive use possible
- You don’t care on which machine your job is running
  - If you do, you can ask for specific resources to be allocated to you

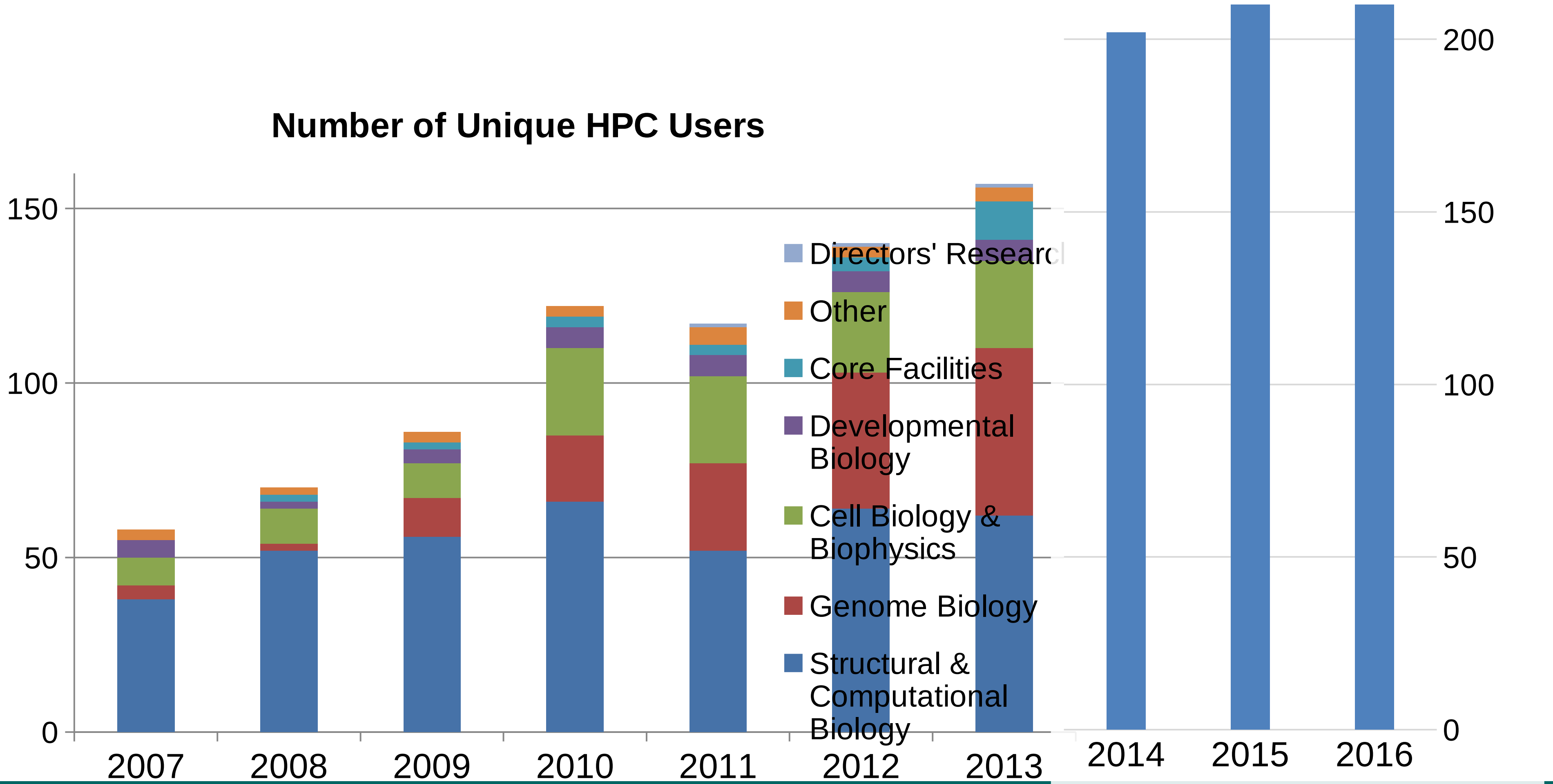
History



250,000
200,000
150,000
100,000
50,000
0
6,000
5,000
4,000
3,000
2,000
1,000
0
2007
2008
2009
2010
2011
2012
2013
2014
2015
CPU cores deployed
Total CINT2006
Total CINT2006rate
Exponential (Total CINT2006rate)

History


Number of Unique HPC Users
150
100
50
0
2007
2008
2009
2010
2011
2012
2013
Directors' Research
Other
Core Facilities
Developmental Biology
Cell Biology & Biophysics
Genome Biology
Structural & Computational Biology


Number of Unique HPC Users
150
100
50
0
2007
2008
2009
2010
2011
2012
2013
Directors' Researc
Other
Core Facilities
Developmental Biology
Cell Biology & Biophysics
Genome Biology
Structural & Computational Biology
200
150
100
50
0
2014
2015
2016

Existing cluster

- Hardware Managed by PlatformHPC
- Jobs managed by LSF
- /scratch managed by FhGFS

Why change

- PlatformHPC is
  - Inflexible
  - Outdated
  - Vendor lock-in
  - Expensive
- Better & open solutions exist, lets use them

Our choices

- Foreman for hardware deployment
- Puppet for configuration management
- Slurm for workload management
- We kept BeeGFS for /scratch

Slurm

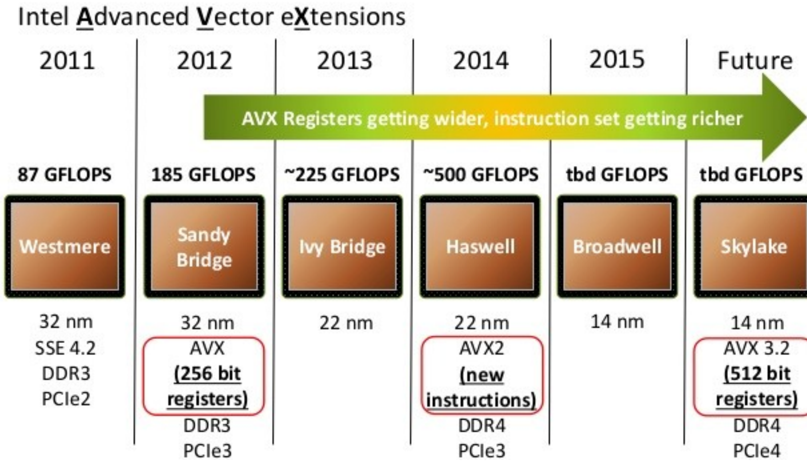
- “Simple Linux Utility for Resource Management”
- One of the most popular HPC schedulers
  - All new & experimental things are first developed for Slurm
- We deployed version 16.05
  - In the mean time new version already out ;)

Slurm terminology

- Step – single task run by scheduler (usually single command in job script)
- Job – resource allocation, steps run within it
- Job script – simple bash script that combines resource allocation requests and job steps
- Partition – collection of resources with some common attributes (also known as queue)
- Features – set of labels applied to different compute nodes
- Constraint – set of labels job is asking for
- Account – ID used for slurm accounting purposes (equals to primary group)

Current hardware (H1 2017)

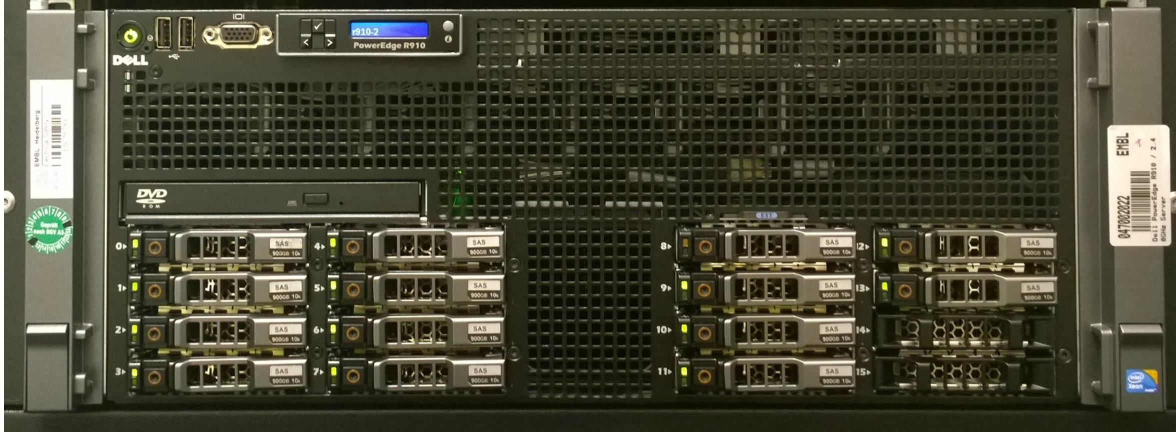
- 8 “bigmem” Westmere nodes (240 cores)
- 84 SandyBridge nodes (1344 cores)
- 162 Haswell nodes (3888 cores)
- 2 GPU nodes:
  - gpu1 with SandyBridge and 3x K20
  - gpu2 with Broadwell and 8x P100
- BeeGFS scratch storage



State of transition (as of Q1 2017)

- 54 Haswell nodes under slurm
- 28 SandyBridge nodes under slurm
- 4 bigmem nodes under slurm
- Both gpu nodes under slurm
- Scratch still directly connected to LSF nodes
- Software environment mostly usable
  - About 20 softwares still on to-do list

Bigmem nodes



- Hardware: Dell R910
- CPU: 4x E7-4870 (10 cores, 2.4GHz, SSE4.2)
- Memory: 1TB @ 1066Mhz
- Local /tmp as tmpfs, 9TB @ 2GB/s
- Network: 10Gb/s
- Features: HT, cpu2.4GHz, net10G, westmere
- Dell end-of-support 2015/3/29, 3rd party support still available

SandyBridge nodes

- Hardware: IBM HS23
- CPU: 2x E5-2670 (8 cores, 2.6GHz, AVX)
- Memory: 256 GB @ 1600Mhz
- Local /tmp as tmpfs, 258 GB @ 3GB/s
- Network: 1Gb/s per blade, 10Gb/s per chassis
- Features: HT, cpu2.6GHz, avx, sandybridge

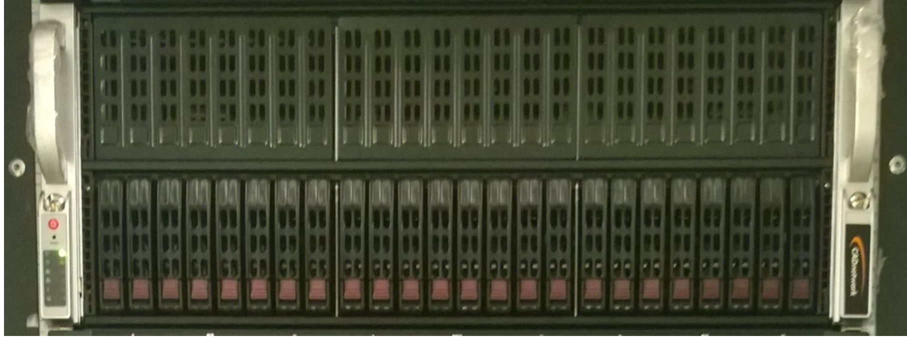
Haswell nodes

- Hardware: Fujitsu BX2560M1
- CPU: 2x E5-2680v3 (12 cores, 2.5GHz, AVX2)
- Memory: 256 GB @ 2133Mhz
- Local /tmp as tmpfs, 258GB @ 3GB/s
- Network: 10Gb/s per blade, 20Gb/s per chassis
- Features: noHT, HT, cpu2.5GHz, avx2, net10G, haswell

GPU nodes: gpu1

- Hardware: Supermicro
- CPU: 2x E5-2630 (6 cores, 2.3GHz, AVX)
- Memory: 64 GB @ 1333Mhz
- GPU: 3x Nvidia K20m (Kepler, 5GB memory @ 208GB/s)
- Local /tmp as tmpfs, 1.6TB @ 2GB/s
- Network: 1Gb/s
- Features: noHT, cpu2.3GHz, avx, gpu=K20, sandybridgbe

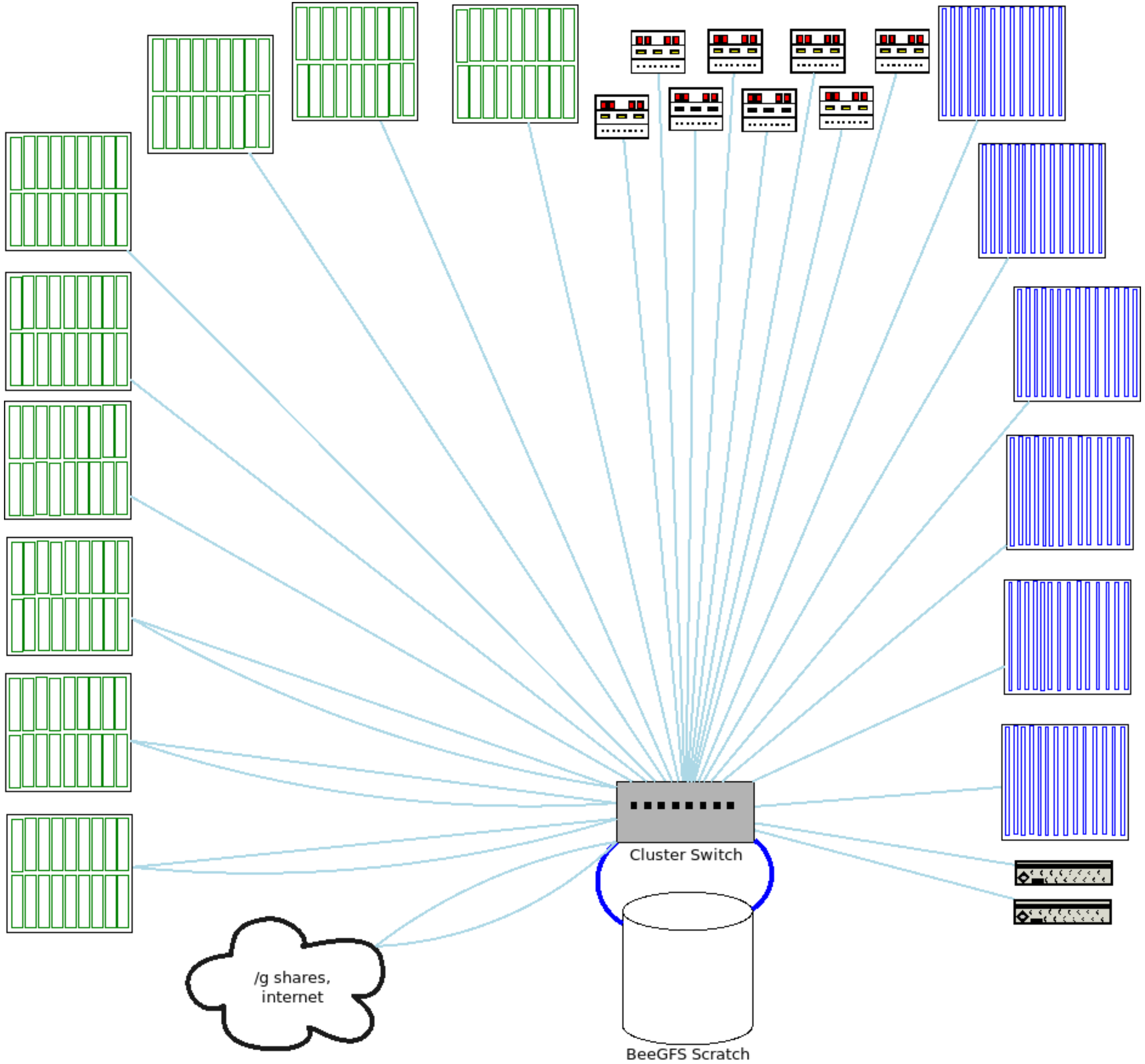
GPU nodes: gpu2



- Hardware: Supermicro
- CPU: 2x E5-2680 (28 cores, 2.4GHz, AVX2)
- Memory: 512 GB @ 2400Mhz
- GPU: 8x Nvidia P100 (Pascal, 16GB memory @ 732 GB/s)
- Local /tmp as tmpfs, 197GB @ 3GB/s
- Network: 10Gb/s
- Features: HT, cpu2.4GHz, avx2, gpu=P100, broadwell

/scratch

- Hardware: Dell + NetApp
- Memory: 256 GB per server
- Network: 40Gb/s per server
- 120 disks, 350TB usable space
- 4 NVMe cards, 16TB flash cache



EMBL

Hardware lifecycle

- Gather requests throughout the year
- Shopping begins in second half of the year
- New hw deployed by end of year
- Goes into production in beginning of next year

Software environments

- Base OS: CentOS 7.3
- SEPP: /g/software/bin
  - Might still work, but no guarantees
  - Planned to be phased out
- SBgrid:
  - Commercial offering
  - source /programs/sbgrid.shrc
- Environment modules
  - module avail

Each one is designed to be the only one in use

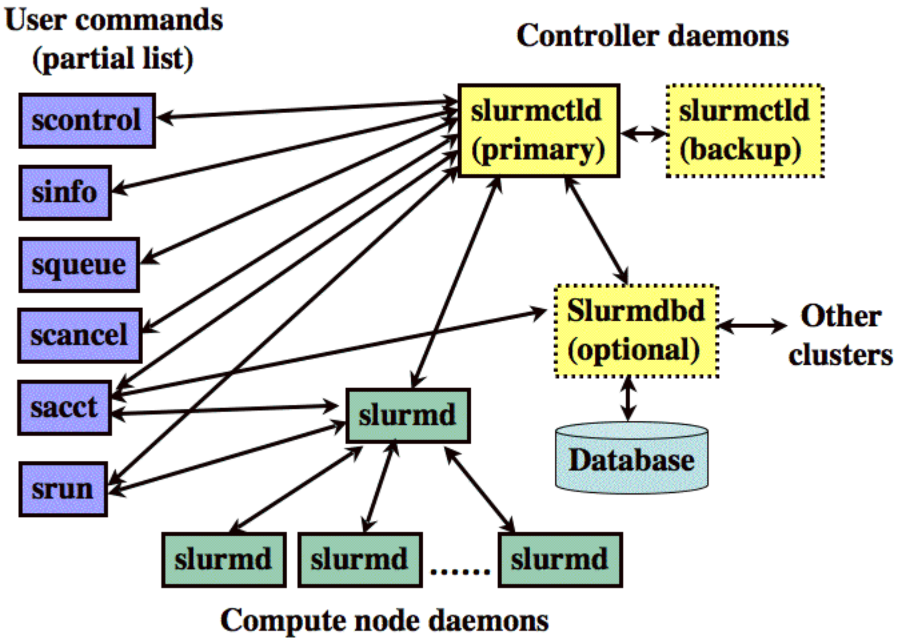
Do not mix them or undefined things will happen

Environment Modules

- Used with Lmod
- Provided by EasyBuild
  - Repeatable software builds
  - Hardware optimized builds
    - Currently building for Nehalem, SandyBridge and Haswell
  - Large community
  - Road map towards containers

LIKELIHOOD YOU WILL GET CODE WORKING BASED ON HOW YOU'RE SUPPOSED TO INSTALL IT:
VERY LIKELY
APP STORE OR PACKAGE MANAGER
GITHUB LINK
SOURCEFORGE LINK
GEOCITIES/TRIPOD LINK
COPY-AND-PASTE EXAMPLE CODE FROM PAPER'S APPENDIX
ANYTHING THAT "REQUIRES ONLY MINIMAL CONFIGURATION AND TWEAKING"
UNLIKELY

Slurm architecture



Slurm commands

- `salloc` – allocate resources and spawn a shell
- `srun` – run a single job step
- `sbatch` – submit a job script
- `scancel` – kill a running job
- `squeue` – reports the state of jobs in the queue
- `sinfo` – reports the state of queues and nodes

Rosetta stone

User command	PBS	LSF	Slurm
Job submission	`qsub [script file]`	`bsub [script file]`	`sbatch [script file]`
Job deletion	`qdel [job id]`	`bkill [job id]`	`scancel [job id]`
Job status (by job)	`qstat [job id]`	`bjobs [job id]`	`squeue [job id]`
Job status (by user)	`qstat -u [username]`	`bjobs -u [username]`	`squeue -u [username]`
Queue list	`qstat -Q`	`bqueues`	`squeue`
Node list	`pbsnodes -l`	`bhosts`	`sinfo -N`

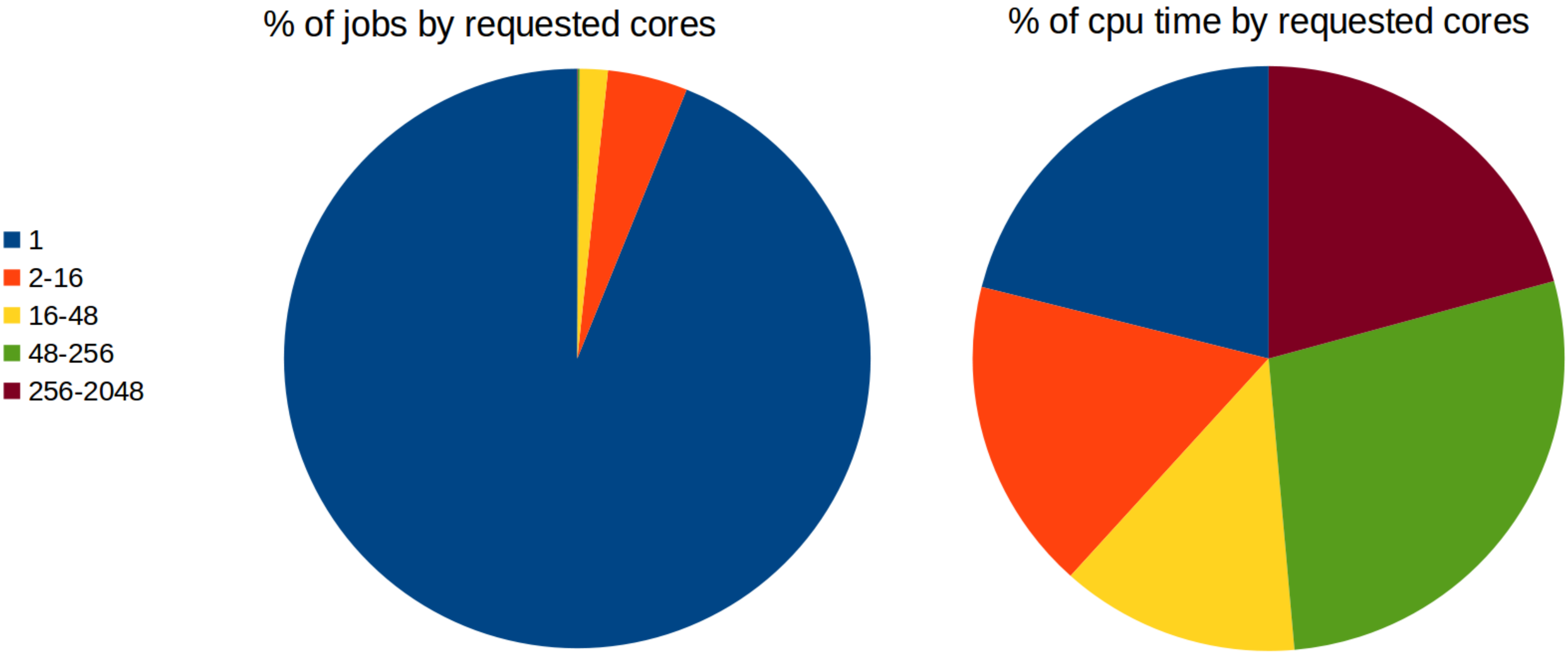
Slurm wrappers for LSF commands

- `bsub`
- `bkill`
- `bjobs`
- `lsid`

Slurm wrappers for PBS commands

- `qsub`
- `qdel`
- `qstat`
- `qalter`
- `qhold`
- `pbsnodes`

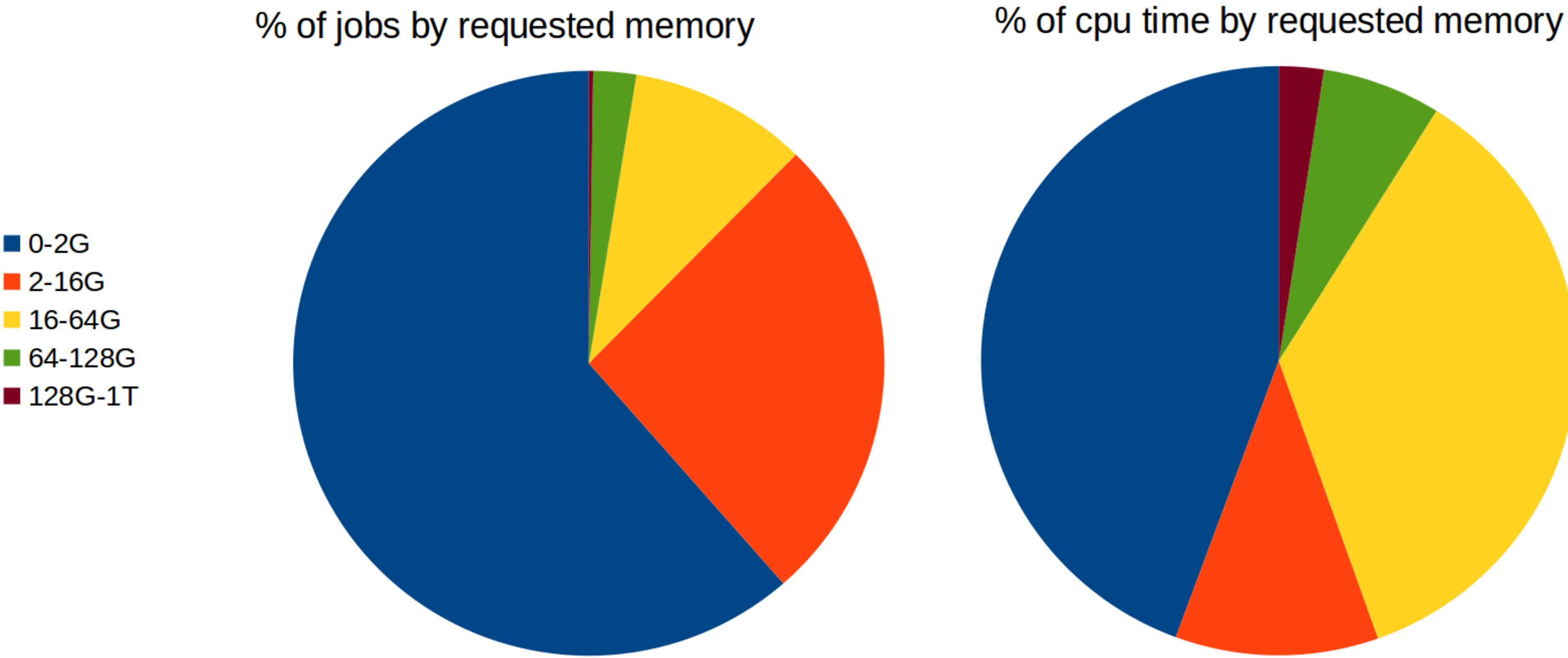
From LSF logs ...



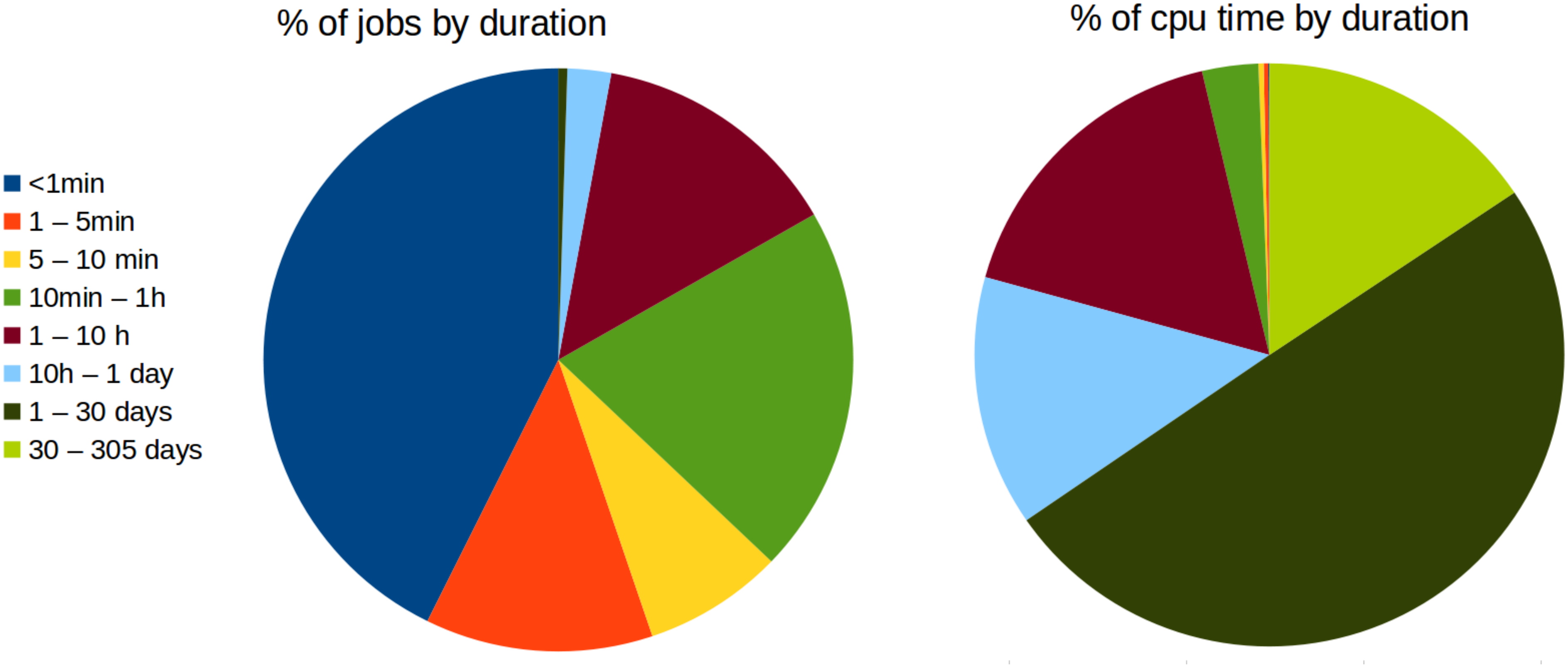
% of jobs by requested cores

% of cpu time by requested cores

From LSF logs ...



From LSF logs ...

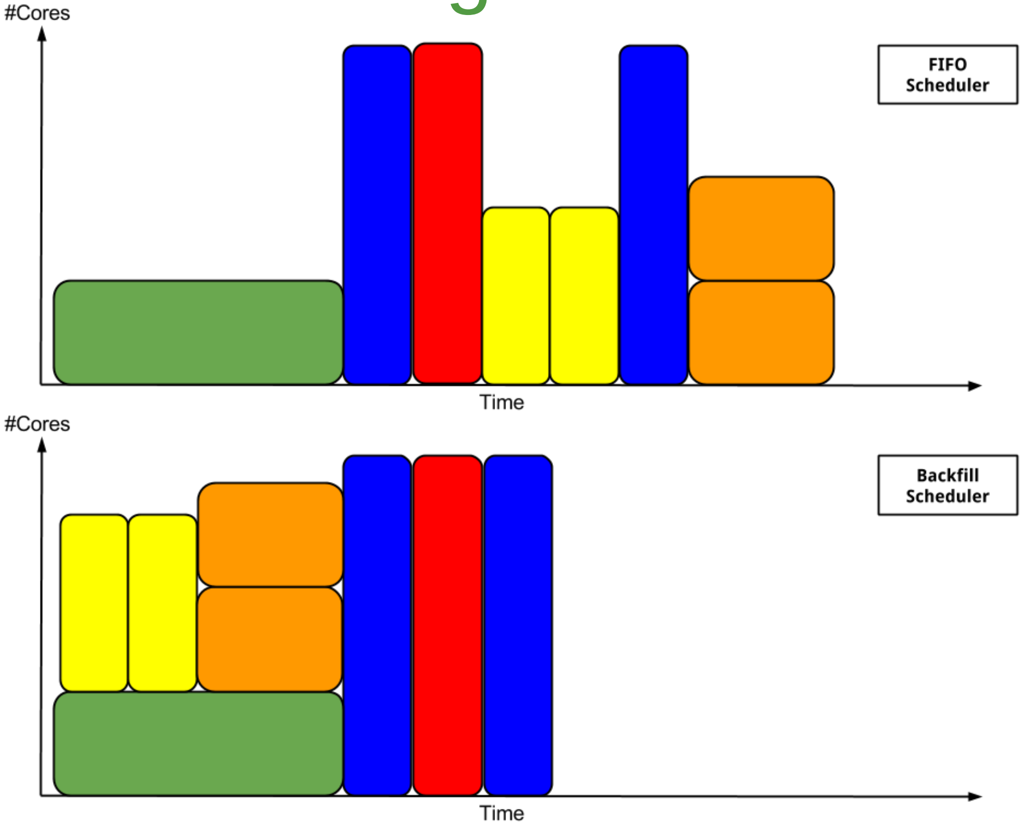


Queues

- Organized by duration
  - If you know or can estimate, tell Slum how long your job will run
- Default queue: htc
  - Max runtime 1h, max memory per core 16GB
- 1day, 1week, 1month

- Hw specific:
  - bigmem
  - gpu

Backfill scheduling



Where to find help

- Wiki: https://wiki.embl.de/cluster/
- chat.embl.org #cluster
- itsupport@embl.de
- clusterNG mailing list
- Meetings as needed
  - When there are new things to announce and explain
- Bio-IT meetings, Coding Club

For more information

- www.vi-hps.org
- www.prace-ri.eu

Exercise: login

- Use ssh to login to `login.cluster.embl.de`

Exercise: slurm resources

- View partitions: `sinfo -l`
- View node info: `sinfo -Nl`
- View node features: `sinfo -No “%N %f”`

Slurm node states

- Idle
- Mixed
- Allocated
- Draining
- Drained
- Down
- Unknown

Exercise: modules

- List available modules: `module avail`
- Search available modules: `module spider <modulename>`
- Detailed description of a module: `module whatis <modulename>`
- Help for a specific module: `module help <modulename>`

Exercise: toolchains

- Run `gcc -v` and observe the version
- `module load foss`
- Run `gcc -v` again and observe the version
- `module list`
- `module purge`
- `module list`

Exercise: dependencies

- `module load snakemake`
- `module list`
- `module load matplotlib`
- `module list`
- `snakemake -h`
- What happens?

How to handle that

Merit by Markus Fritz

Exercise: job environment

- `module purge`
- `module load foss`
- `srun gcc -v`

Exercise: interactive job

- `module purge`
- `salloc`
- `hostname`
- `env | grep SLURM`
- srun hostname
- exit

Exercise: default resources

- salloc
- srun grep Cpus_allowed_list /proc/self/status
- srun cat /sys/fs/cgroup/memory/slurm/uid_$(id -u)/job_$SLURM_JOBID/memory.limit_in_bytes
- exit

Exercise: asking for resources

-
  ```
  salloc -N 1 -n 4 --mem=500
  ```

-
  ```
  srun grep Cpus_allowed_list /proc/self/status
  ```

-
  ```
  srun cat /sys/fs/cgroup/memory/slurm/uid_$(id -u)/job_$SLURM_JOBID/memory.limit_in_bytes
  ```

-
  ```
  exit
  ```

Exercise: asking for resources

- `salloc -N 1 -n 1 --mem=300G`

Exercise: asking for resources

- `salloc -N 1 -n 1 --mem=300G -p bigmem`

- srun grep Cpus_allowed_list /proc/self/status

- srun cat /sys/fs/cgroup/memory/slurm/uid_$(id -u)/job_$SLURM_JOBID/memory.limit_in_bytes

- exit

Exercise: asking for features

- `salloc -N 1 -n 4 -C HT`
- srun grep Cpus_allowed_list /proc/self/status
- exit
- `salloc -N 1 -n 4 -C noHT`
- srun grep Cpus_allowed_list /proc/self/status
- exit

Features table

	avx	avx2	broadwell	cpu 2.3 GHz	cpu 2.4 GHz	cpu 2.5 GHz	cpu 2.6 GHz	gpu=K20	gpu=P100	haswell	HT	net10G	noHT	sandybridge	westmere
htc	x	x				x	x			x	x	x	x	x	
1day	x	x				x	x			x	x	x	x	x	
1week	x	x				x	x			x	x	x		x	
1month	x	x				x	x			x	x	x		x	
bigmem					x							x			x
gpu	x	x	x	x	x			x	x		x	x	x		

Data movement

- Your work is highly data intensive
- Data and compute should be as close as possible to achieve best performance
- Slurm provides per-job $TMPDIR and $SCRATCHDIR
- Nodes have at least 250GB @ 2GB/s of TMPDIR, **use it!**
- If you can’t, use $SCRATCHDIR

- Use /g shares only as a source of input data and a place to store results

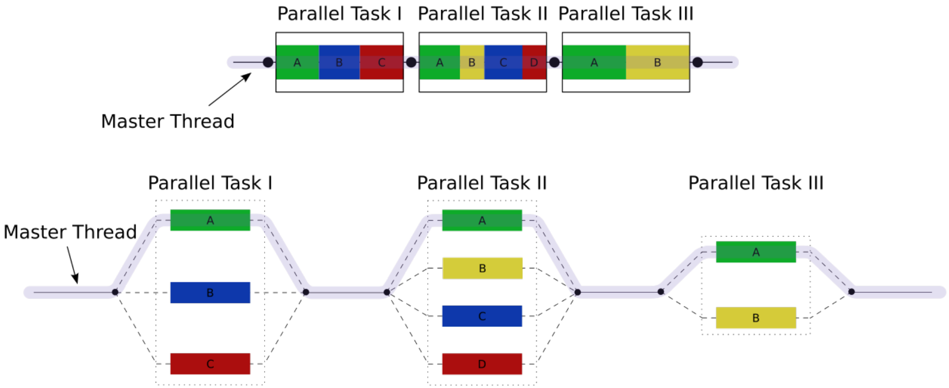
Example: Data movement

- This job script illustrates a method of copying input to many nodes

```
#!/bin/bash
#SBATCH -t 03:00
#SBATCH -p 1day
#SBATCH -N 4
#SBATCH -n 96
#SBATCH --tmp=50G

#copy to node local tmp
srun -N $SLURM_NNODES cp
/g/somewhere/project/input_data $TMPDIR/

module load …
#do stuff …

#wrap up
srun -N $SLURM_NNODES cp $TMPDIR/results
/g/somewhere/project/output
```

OpenMP

- Shared memory parallelism
- A method to parallelize within the same node
- Obeys 10+ environment variables
- Slurm sets OMP_NUM_THREADS based on cpus requested by job



Exercise: OpenMP

- Prepare this job script
- Use `sbatch` to submit it
- Vary number of tasks per node
- Observe “Number of threads” and “Best rate Triad” differences

```
#!/bin/bash
#SBATCH -t 00:01:00
#SBATCH -N 1
#SBATCH --ntasks-per-node 1 #vary this 1..24

module load STREAM
stream_1Kx10M
```

Exercise: OpenMP and placement

- Try --hint=compute_bound or memory_bound
- Vary number of tasks per node
- Observe “Number of threads” and “Best rate Triad” differences

```
#!/bin/bash
#SBATCH -t 00:01:00
#SBATCH -N 1
#SBATCH --ntasks-per-node #1..24
#SBATCH --hint=

module load STREAM
stream_1Kx10M
```

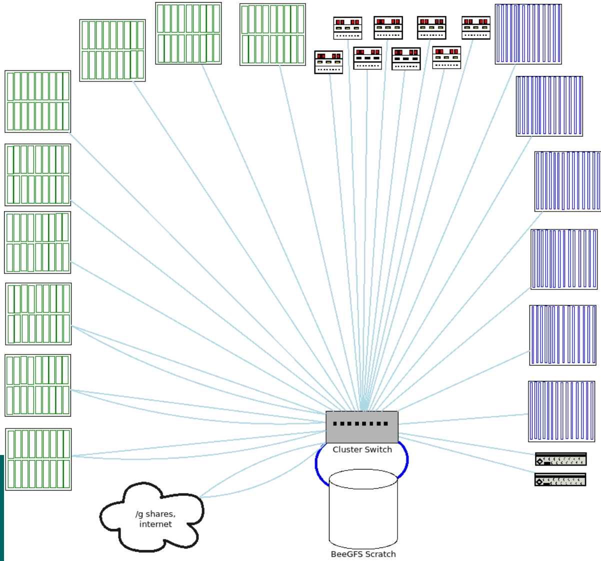
MPI

- Distributed memory parallelism
- A method to parallelize across many nodes
  - Also suitable for some problems within the same node
- Our OpenMPI build integrated with slurm

Exercise: MPI

- Submit this job script
- Observe numbers
- Add `#SBATCH -C net10G`
- Observe numbers
- Add `#SBATCH --switches=1`
- Observe numbers

```
#!/bin/bash
#SBATCH -t 00:05:00
#SBATCH -n 2
#SBATCH -N 2

module load OSU-Micro-Benchmarks
echo $SLURM_NODELIST

mpirun osu_bw
mpirun osu_latency
```



Exercise: notifications

- Slurm can send you emails
- They include some job efficiency statistics
- Useful to tune your exact resource request

```
#!/bin/bash
#SBATCH -t 00:01:10
#SBATCH -N 1 -n 1
#SBATCH -J stress
#SBATCH --mail-type BEGIN,END,FAIL
#SBATCH --mail-user=your.mail@embl.de

#do something
module load stress

cd $TMPDIR
stress -t 60 -c 1 -i 1 -m 1 -d 1
```

Exercise: GPU

- Slurm implements gpu as "generic resource" (gres)
- You can ask for some number of them
- Use constraint to select specific gpu model
- Check wiki for exact gpu/cpu hardware offers

```
#!/bin/bash
#SBATCH -p gpu
#SBATCH -n 6
#SBATCH --mem=50G
#SBATCH -C gpu=P100
#SBATCH --gres=gpu:2

#run relion on 6 cpu cores and 2 gpus
module load RELION

#do relion stuff ...
```

Why is my job queued?

- Your job sits in the queue in state PENDING
- Use `scontrol show job [job id]` to understand why

```
JobId=828772 JobName=CL3d_round2K2.sh
   UserId=dauden(21588) GroupId=cmueller(574) MCS_label=N/A
   Priority=4294155964 Nice=0 Account=cmueller QOS=normal
   JobState=PENDING Reason=Resources Dependency=(null)
   ...
```

Exercise: why did my job fail?

- Submit such job script
- Use sacct -j [jobid] to determine exit code and failing step
- Anything non-zero is a problem
- Standard ones defined in /usr/include/sysexits.h
- Bash has a couple of its own
- Every software can implement its own ...

```
#!/bin/bash
#SBATCH -t 00:01:00
#SBATCH -N 1
#SBATCH -n 1

#do something that fails …
exit 1
```

Best practices: Slurm

- Use salloc to experiment and test
- Use srun to run single commands from your scripts or external workflow managers (such as snakemake)
- Use sbatch and job scripts for everything where you want to preserve information about environment used (module load statements)
- Use notifications to fine tune your memory and runtime requests

Best practices: R

- While capable of using multiple threads via OpenMP, no performance benefit has been seen
- Recommend to use it with -n 1
- If possible, try parallelizing it with MPI (at least three ways to do that)
- Explore alternatives (like Julia)

Best practices: GPU

- Gpu1 offers 12 cores and 3 GPUs
- Gpu2 offers 28 cores and 8 GPUs
- Slurm knows which GPU is closest to which core
- If software knows about OpenMP or MPI, try to use 2-3 cores per GPU, otherwise use 1
- Use --hint=nomultithread to tell slurm to give you cores and not threads

How to approach parallelization

- Single operation over large dataset
  - Think of splitting it into smaller chunks and do them at the same time
- If you’re doing things in loops, look for independent data
  - Typically “for [all elements of an array] do ...”
- Figure out a way to execute these loop steps in parallel
  - Use some form of shared memory model
    - Parallel loop constructs
    - Independent workers
  - Use some tool that helps you with that

One of the options: Jug

- Demo by Renato Alves

Conclusion

- To achieve best performance:
  - Put data and compute as close together as possible
  - Use memory instead of disk
  - Identify independent data and implement some parallelism on it

Q & A

Thanks