High Performance Computing: A brief introduction and demonstration

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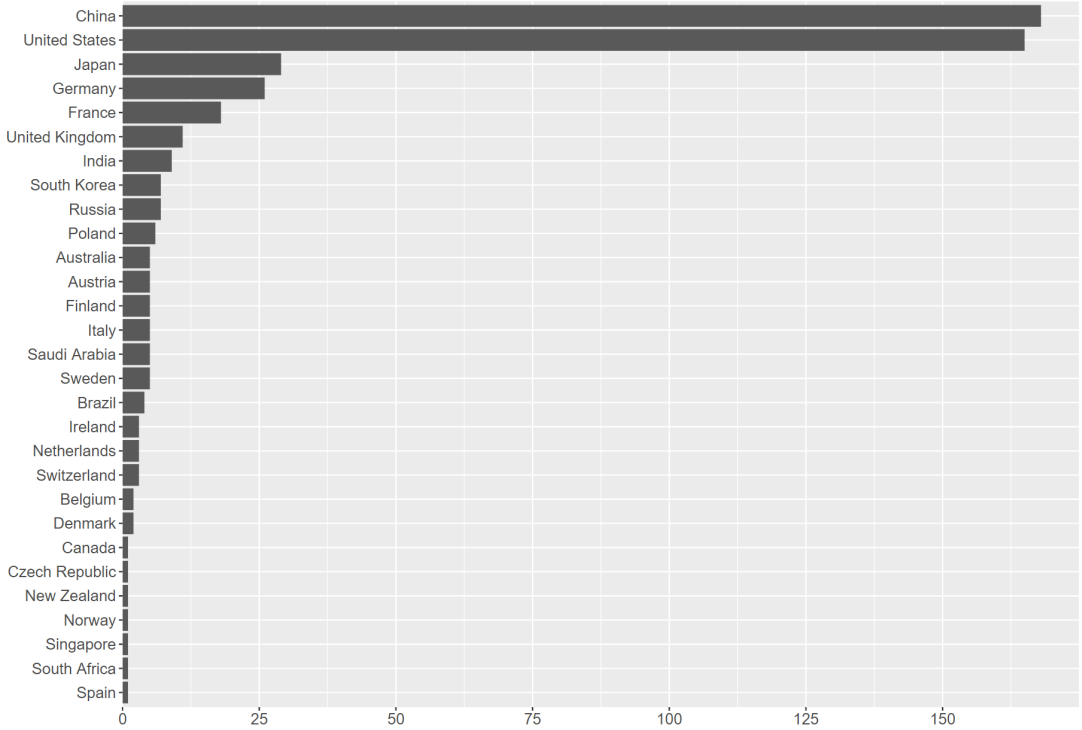
Need for CPU

- Demand for CPU is usually very high in practical study, and increase significantly as the number of molecules involved.

Hexacene adsorption project	Structural relaxation	Single-point self-consistent calculation
Number of CPU cores	64	256
Requested memory (GB)	128	512
Typical running time for a convergent calculation (hour)	20	8
Estimated total committed CPU hours (hour)	30000	300000
Estimated total disk occupied (GB)	40	3000

TOP 500

- The TOP500 project ranks and details the 500 most high performance computer systems in the world. (HPC ~ “supercomuters”)



TOP 500

- The TOP500 project ranks and details the 500 most high performance computer systems in the world. (HPC ~ “supercomuters”)

Rank	Rmax Rpeak (PFLOPS)	Name	Model	Processor	Interconnect	Vendor	Site country, year	Operating system
1	93.015 125.436	*Sunway TaihuLight*	Sunway MPP	SW26010	Sunway[13]	NRCPC	National Supercomputing Center in Wuxi China, 2016[13]	Linux (Raise)
2	33.863 54.902	*Tianhe-2*	TH-IVB-FEP	Xeon E5–2692, Xeon Phi 31S1P	TH Express-2	NUDT	National Supercomputing Center in Guangzhou China, 2013	Linux (Kylin)
3	17.590 27.113	*Titan*	Cray XK7	Opteron 6274, Tesla K20X	Gemini	Cray	Oak Ridge National Laboratory United States, 2012	Linux (CLE, SLES based)
4	17.173 20.133	*Sequoia*	Blue Gene/Q	A2	Custom	IBM	Lawrence Livermore National Laboratory United States, 2013	Linux (RHEL and CNK)
5	14.015 27.881	*Cori*	Cray XC40	Xeon Phi 7250	Aries	Cray	National Energy Research Scientific Computing Center United States, 2016	Linux (CLE)
6	13.555 24.914	*Oakforest-PACS*	Fujitsu	Xeon Phi 7250	Intel Omni-Path	Fujitsu	Joint Center for Advanced High Performance Computing, Kashiwa Japan, 2016	Linux
7	10.510 11.280	*K computer*	Fujitsu	SPARC64 VIIIfx	Tofu	Fujitsu	Riken Advanced Institute for Computational Science (AICS) Japan, 2011	Linux
8	9.779 15.988	*Piz Daint*	Cray XC50	Xeon E5-2690v3, Tesla P100	Aries	Cray	Swiss National Supercomputing Centre Switzerland, 2016	Linux (CLE)
9	8.587 10.066	*Mira*	Blue Gene/Q	A2	Custom	IBM	Argonne National Laboratory United States, 2012	Linux (CNK)
10	8.101 11.079	*Trinity*	Cray XC40	Xeon E5–2698v3	Aries	Cray	Los Alamos National Laboratory United States, 2015	Linux (CLE)

HPC is also in Universities

- Monash University: Monarch, 2000-core CPU

```
localmachine$ ssh jsmith@msgln6.its.monash.edu
jsmith@msgln6.its.monash.edu.au's password:

Last login: Mon Oct  7 12:01:22 2013 from localmachine.monash.edu.au

*******************************************************
*                                                     *
* Please limit local CPU-intensive processes to       *
* one at a time and no more than 30 mins. in          *
* duration. It is recommended to use qsub to          *
* execute longer jobs.                                *
*                                                     *
* It is recommended that jobs indicate:               *
*                                                     *
*   #$ -l h_rt=hh:mm:ss    (for walltime)             *
*   #$ -l h_vmem=nG        (for mem req'ts)           *
*                                                     *
* For example:                                        *
*   #$ -l h_rt=16:00:00    (for 16 hours)             *
*   #$ -l h_vmem=2G        (for 2GB mem)              *
*                                                     *
*******************************************************

jsmith@msgln6~> _
```

HPC is also in Universities

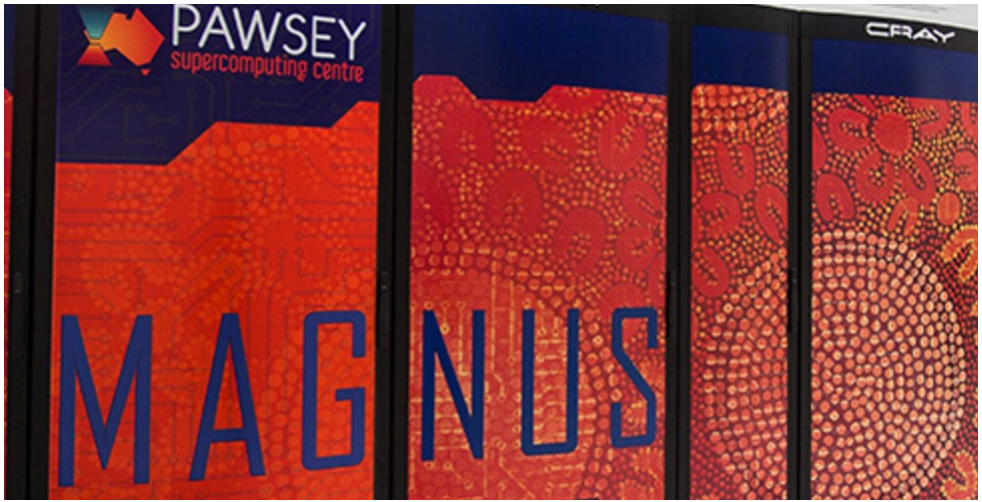
- Central South University: http://hpc.csu.edu.cn
- 1420-core CPU

National Computing Facilities in Australia

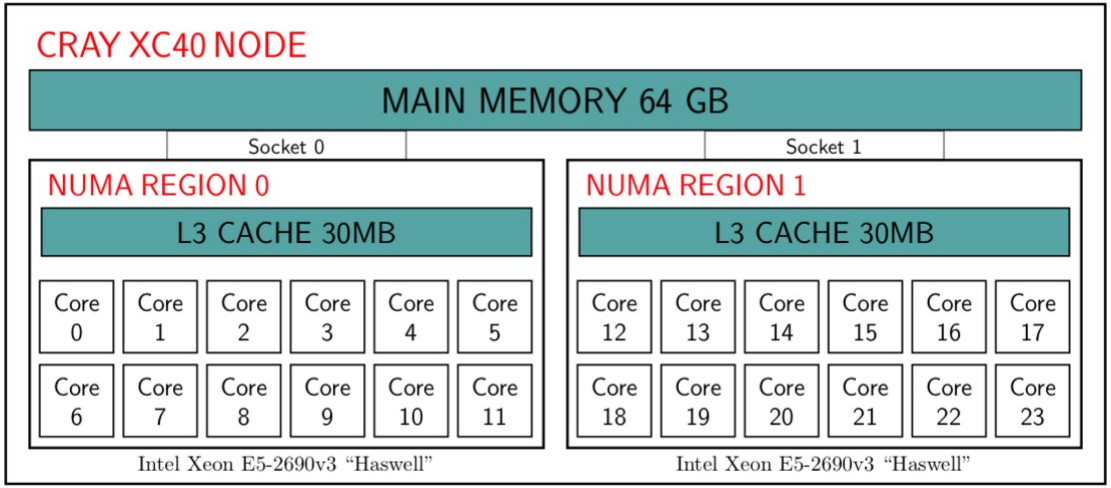
- **Raijin**
- 57,472 cores (Intel Xeon Sandy Bridge)
- 160 TB memory
- 1.5 MW power, 100 tonnes of water in cooling.

National Computing Facilities in Australia

- Pawsey Supercomputing Center
- Most powerful public research supercomputer in Southern Hemisphere
- 35,712 cores

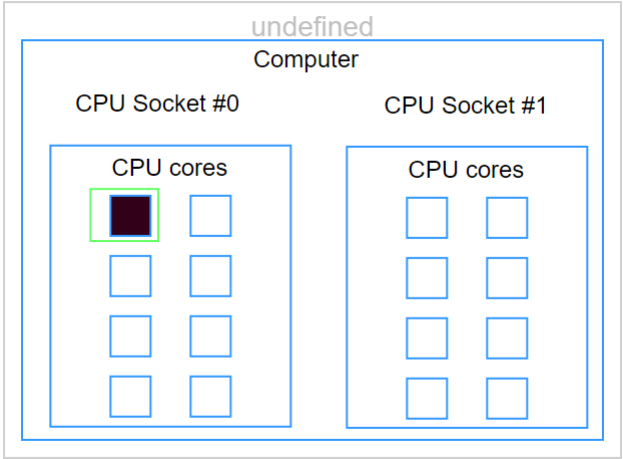


HPC Structure



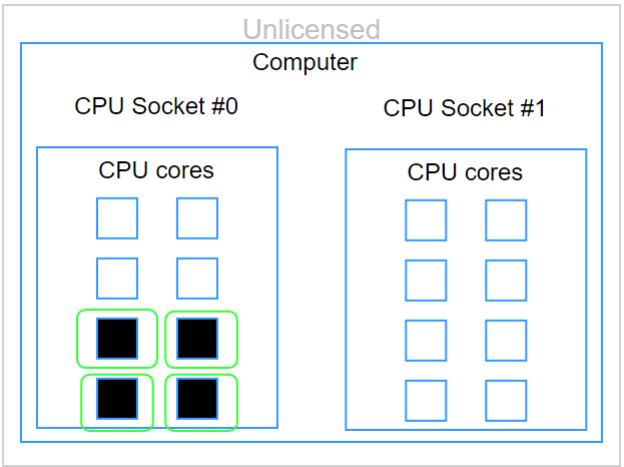
Requesting CPUs

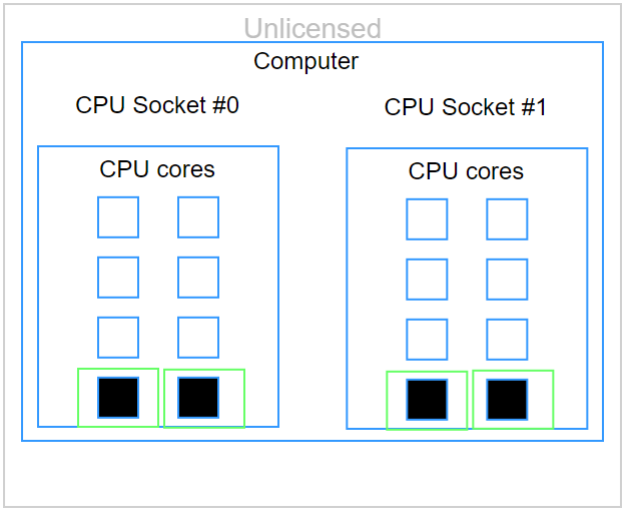
- Serial job - use only one core on one processor



Requesting CPUs

- Parallel jobs – requesting multiple CPUs on one node or across nodes





Accessing HPC, Move/Transfer Files

- **DEMO**