

HPC Cloud @ SURFsara

Design a Parallel Application

SURFsara HPC Cloud Workshop Jan 2015

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SURF SARA

Outline

- Parallel application:
 - What is the need? ... Laptop is not enough
 - How to make it parallel? ... Scalability
- Running a parallel application on the HPC cloud
- Hands-on: Extras!



SURFsara @SURFsara_NL · Jun 22

Why do I Need SURFsara Cloud Facility in My Research? #abl #cfd slideshare.net /aliabbasicivil ... via @SlideShare

Highly demanding applications for **compute** and **storage** resources to:

- Analyse larger computational domains
- Analyse larger volume of data
- Achieve higher accuracy
- Retrieve the results faster

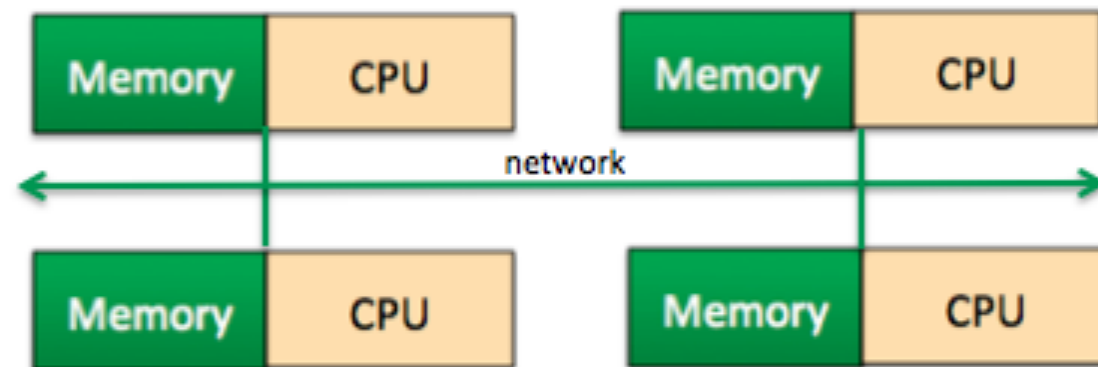


Scalability: system & software

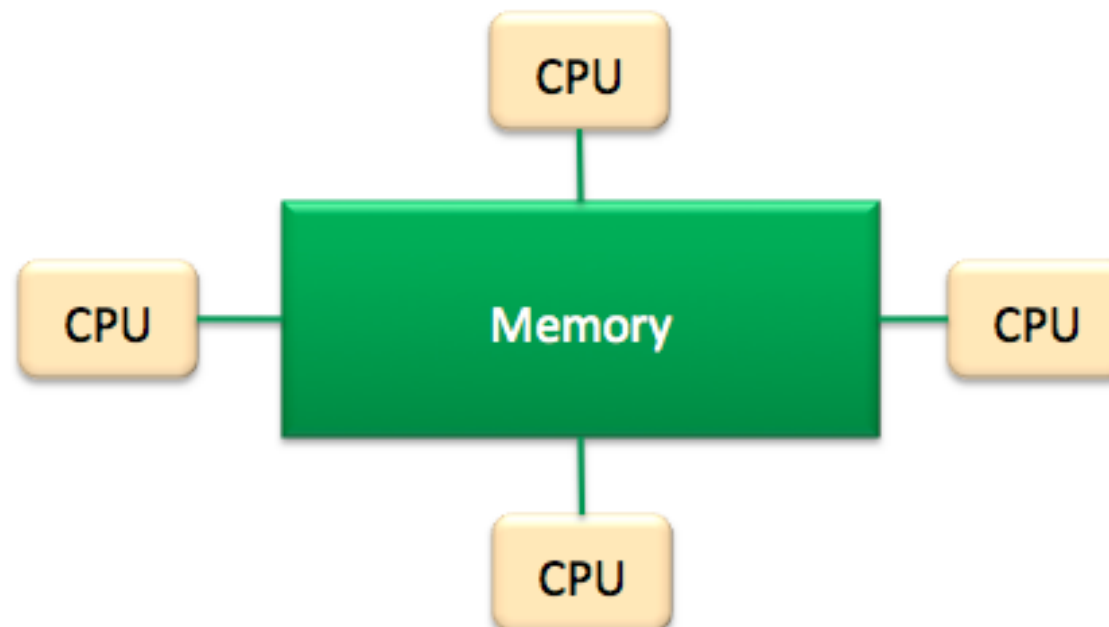
- System - add (virtual) hardware
 - Distributed memory systems
 - Shared memory systems
- Software - optimise the application
 - Develop code, e.g. MPI, OpenMP
 - Out of the box tools, e.g. Matlab, OpenFOAM, D-Flow FM

System architecture

- Distributed memory systems

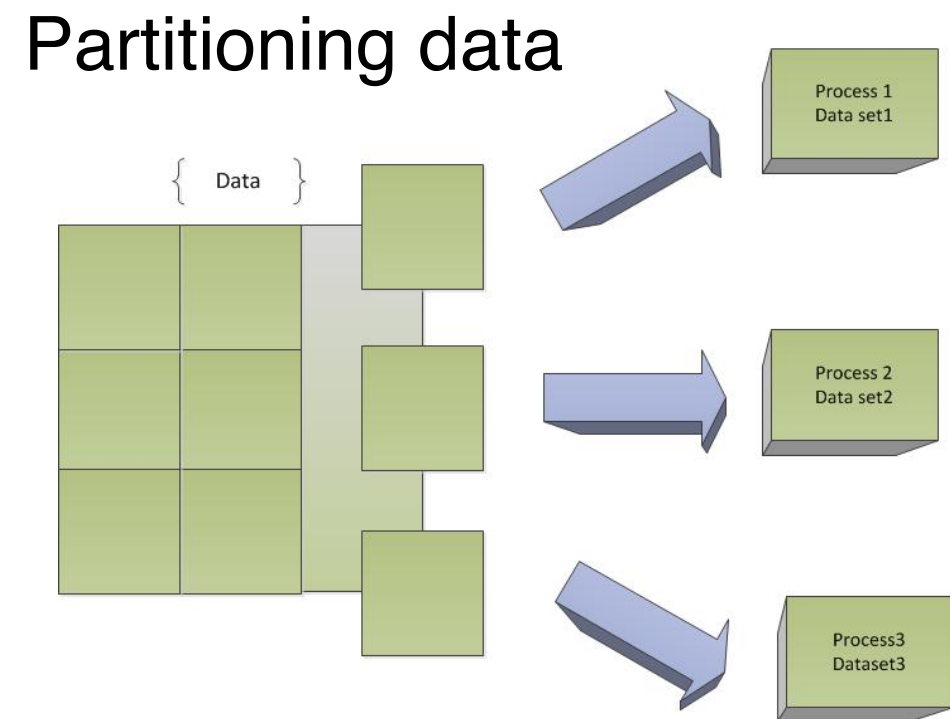
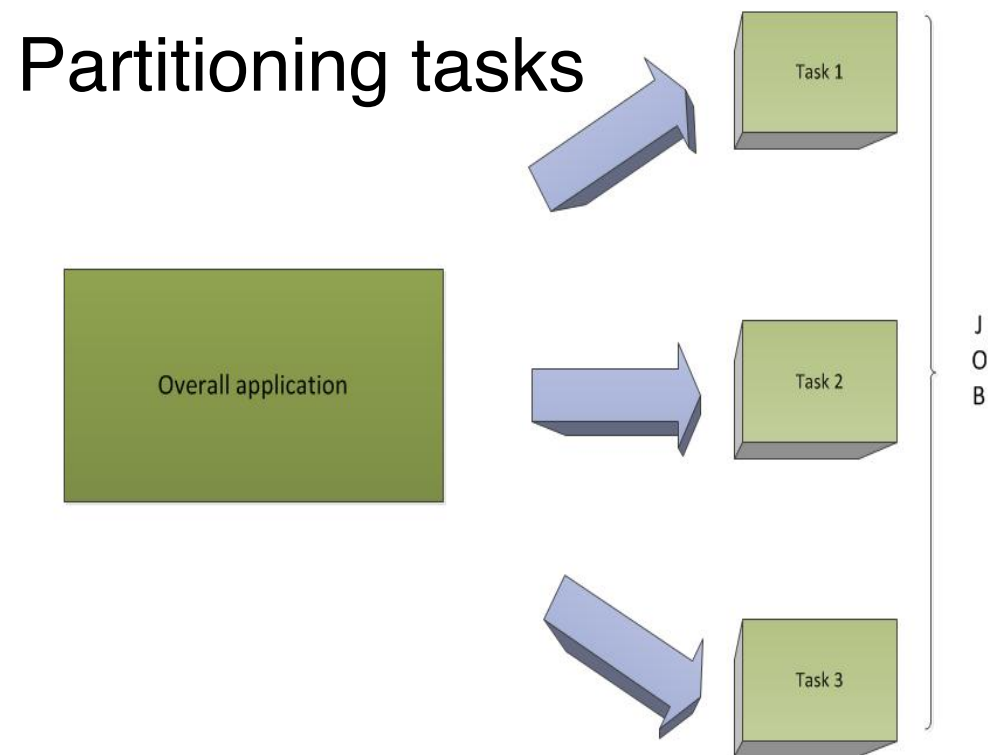


- Shared memory systems



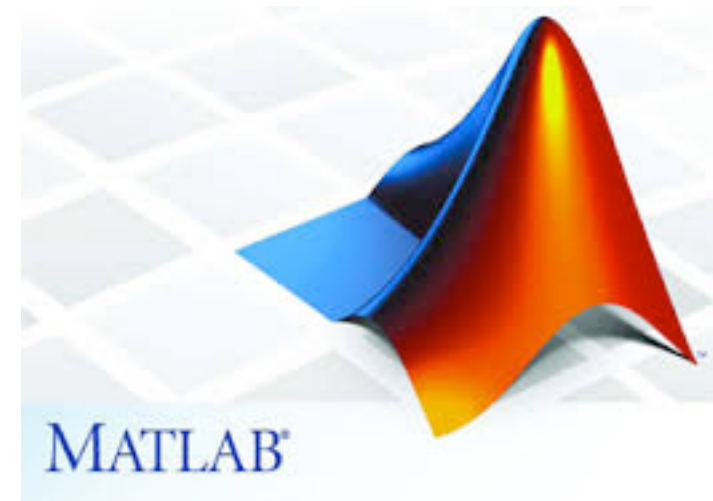
Software optimisation (1)

- Develop your code - find opportunities for parallelisation
 - OpenMP, MPI - advanced programming skills
 - Optimisation techniques - partitioning tasks / data



Software optimisation (2)

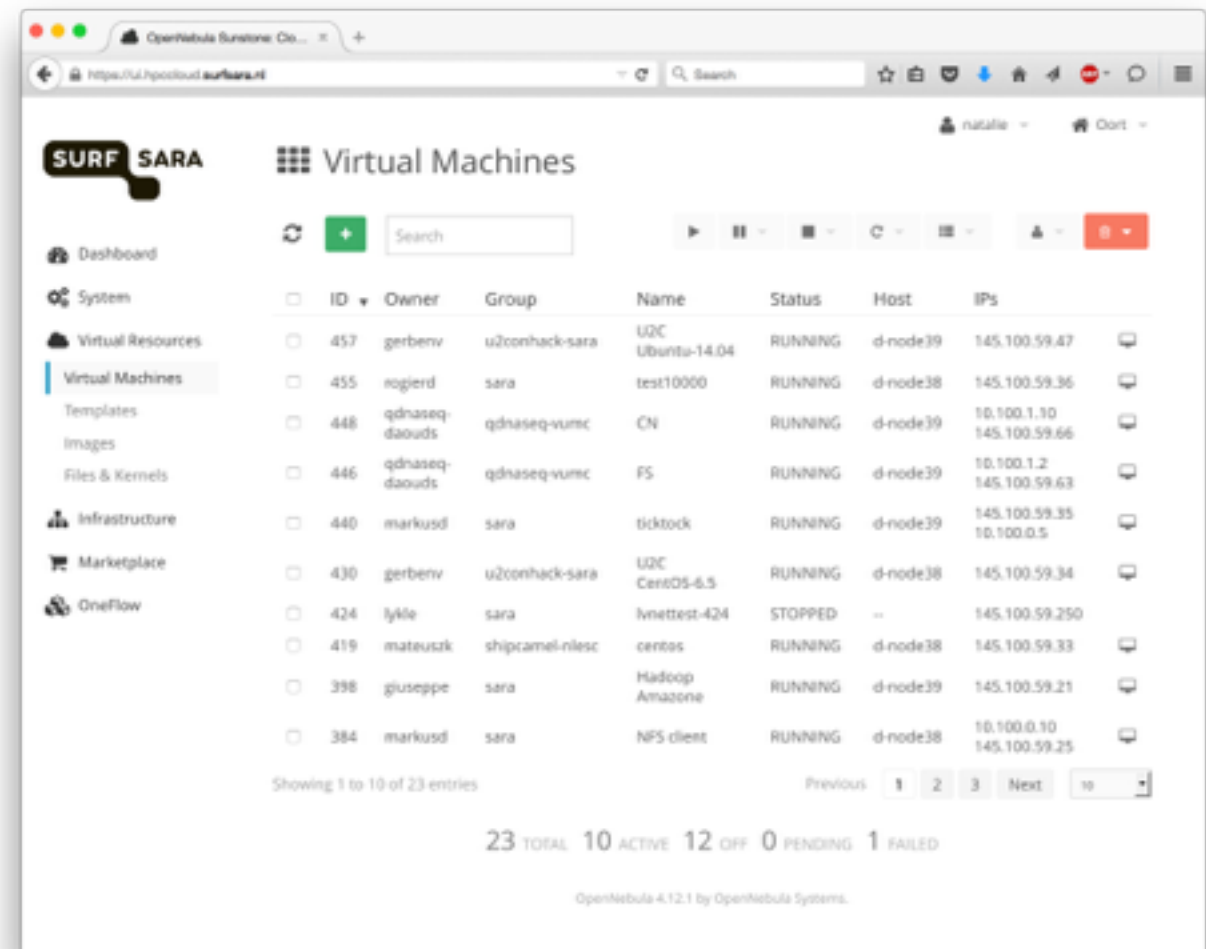
- Out of the box tools



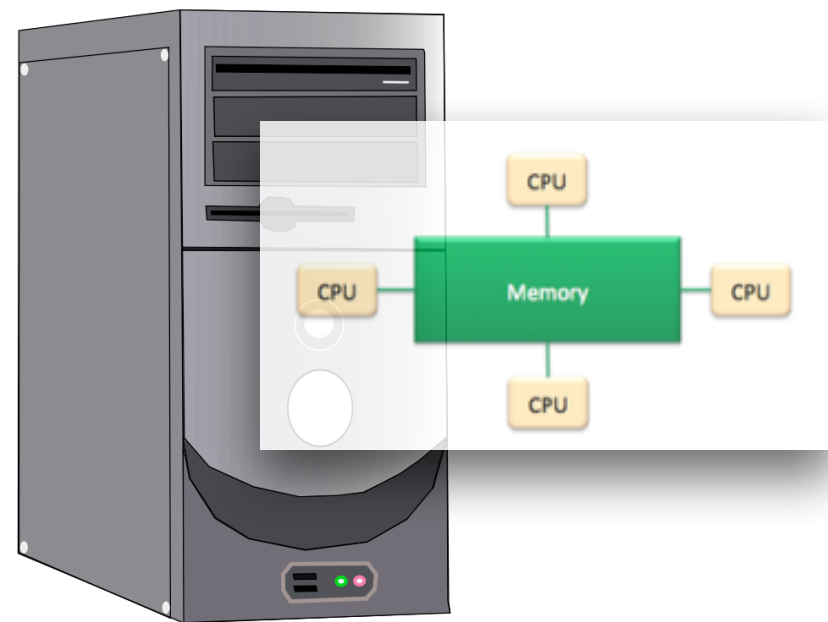
Open  FOAM

Running a parallel application on the HPC cloud

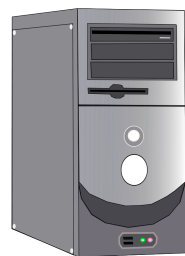
- Access the UI
- Prepare OS Image
- Create the Template
- Instantiate VM(s)
 - single-VM, single-core
 - single-VM, multi-core
 - multi-VM, multi-core
(master/workers cluster)



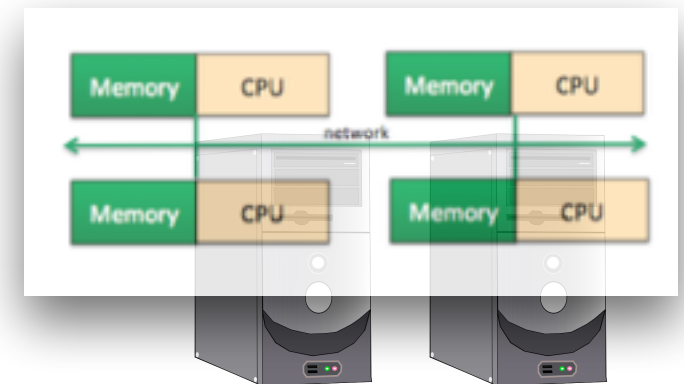
Scaling up vs. Scaling out



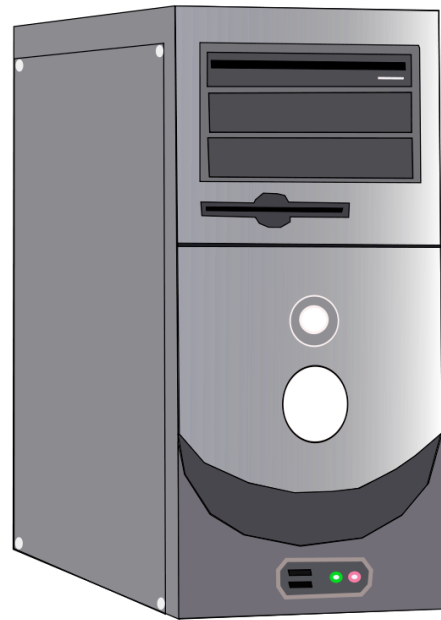
Scale up



Scale out



Scaling up



Scale up



- HPC Cloud Applications
 - High memory node (up to 1TB memory per VM)
 - Multicore VMs (up to 64 cores per VM)
 - Big data (hundreds of GB storage drives)
- See example in ‘Extras’: calculate pi with OpenMP

Scaling out (1)

- HPC Cloud Applications
 - Multiple independent VMs
 - E.g. performing the same application
 - Up to your quota limit & capacity



Scale out

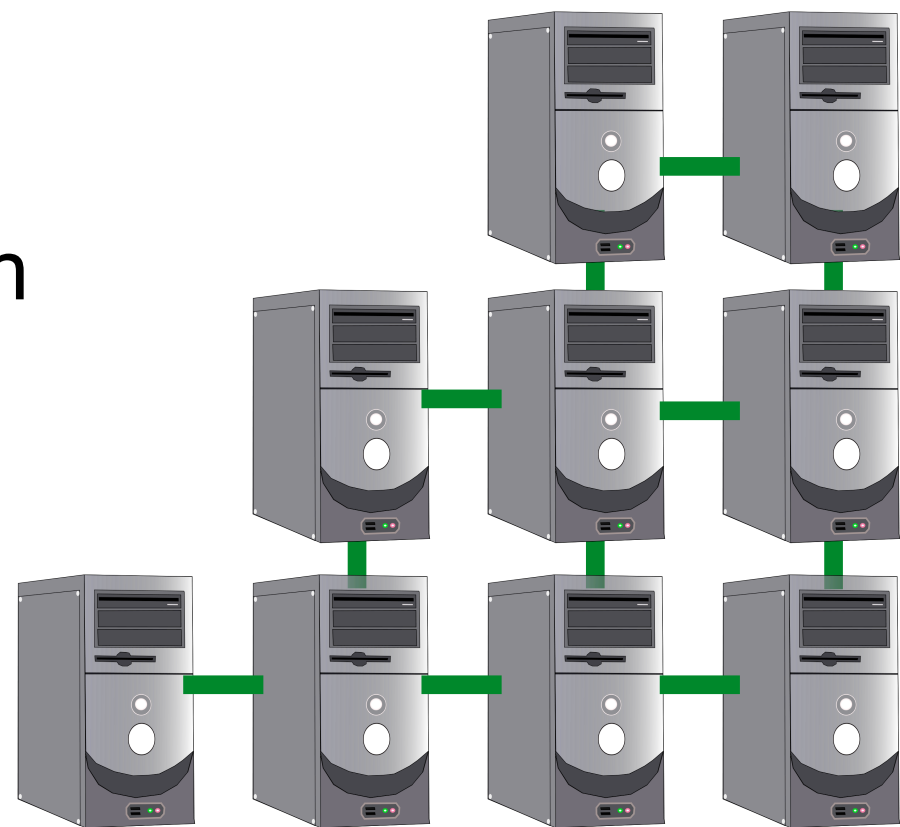


Scaling out (2)

- HPC Cloud Applications
 - Multiple interconnected VMs
 - E.g. clusters, master/workers architecture
 - Up to your quota limit & capacity
- See example in 'Extras': xBeach with MPI

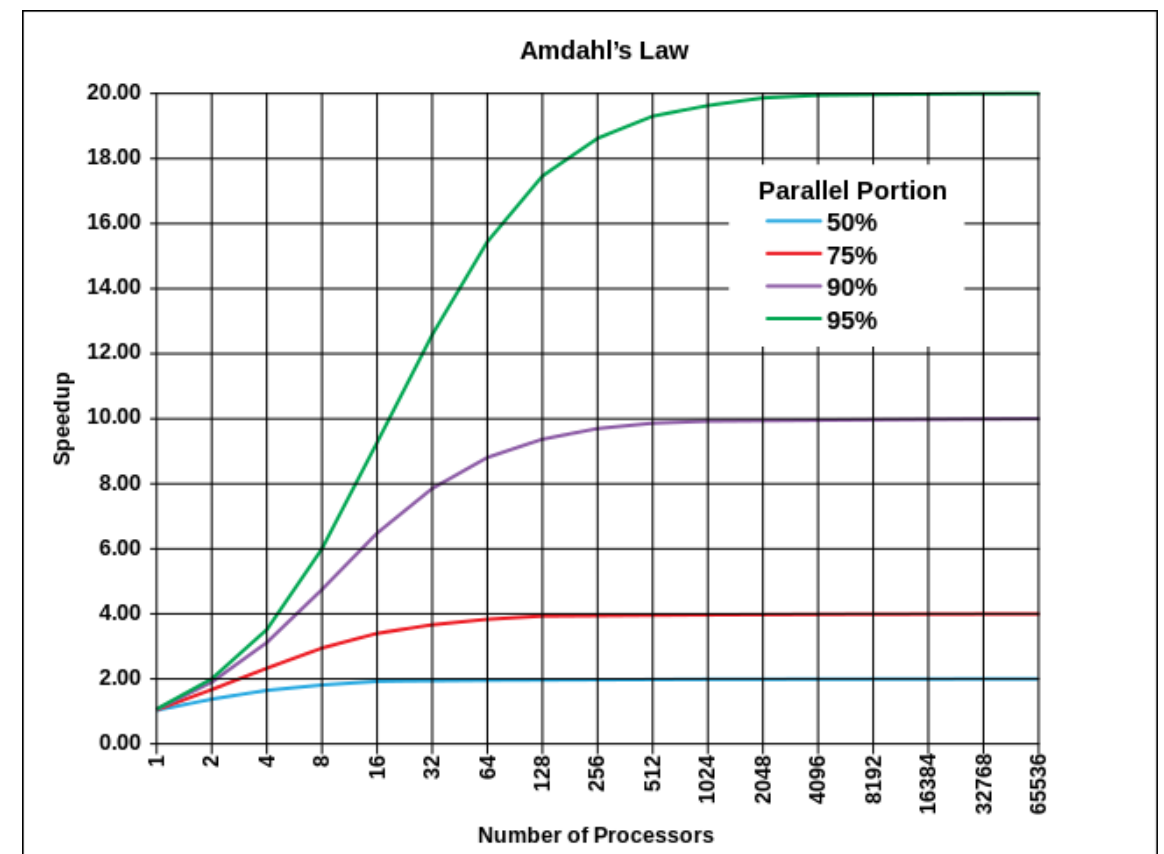


Scale out



What makes HPC difficult?

- Scaling up
 - ◉ Amdahl's law
 - ◉ Easy, but expensive
- Scaling out
 - ◉ More machines - more problems
 - ◉ Machines fail
 - ◉ Networks fail
 - ◉ Heterogeneous hardware
 - ◉ Latencies
 - ◉ Data locality
- Key questions...



Key questions

Define your specific requirements:

- Number of cores, Memory, Wall-clock time, data volumes
- Pipelines: what is shared in tasks, what needs to be communicated
- Data locality (private or shared)
- Wall-clock vs. CPU time
- Operating system, software (licensing programs) and databases
- Network interfaces (private or public) - virtual cluster
- Balance effort: system / software scalability



Hands-on: Extras

- Continue from:

[https://doc.hpcccloud.surfsara.nl/UvAworkshop-2016-01-25/
UvAworkshop-2016-01-25](https://doc.hpcccloud.surfsara.nl/UvAworkshop-2016-01-25/UvAworkshop-2016-01-25)

- Finish Part A & B
- Move to Extras!