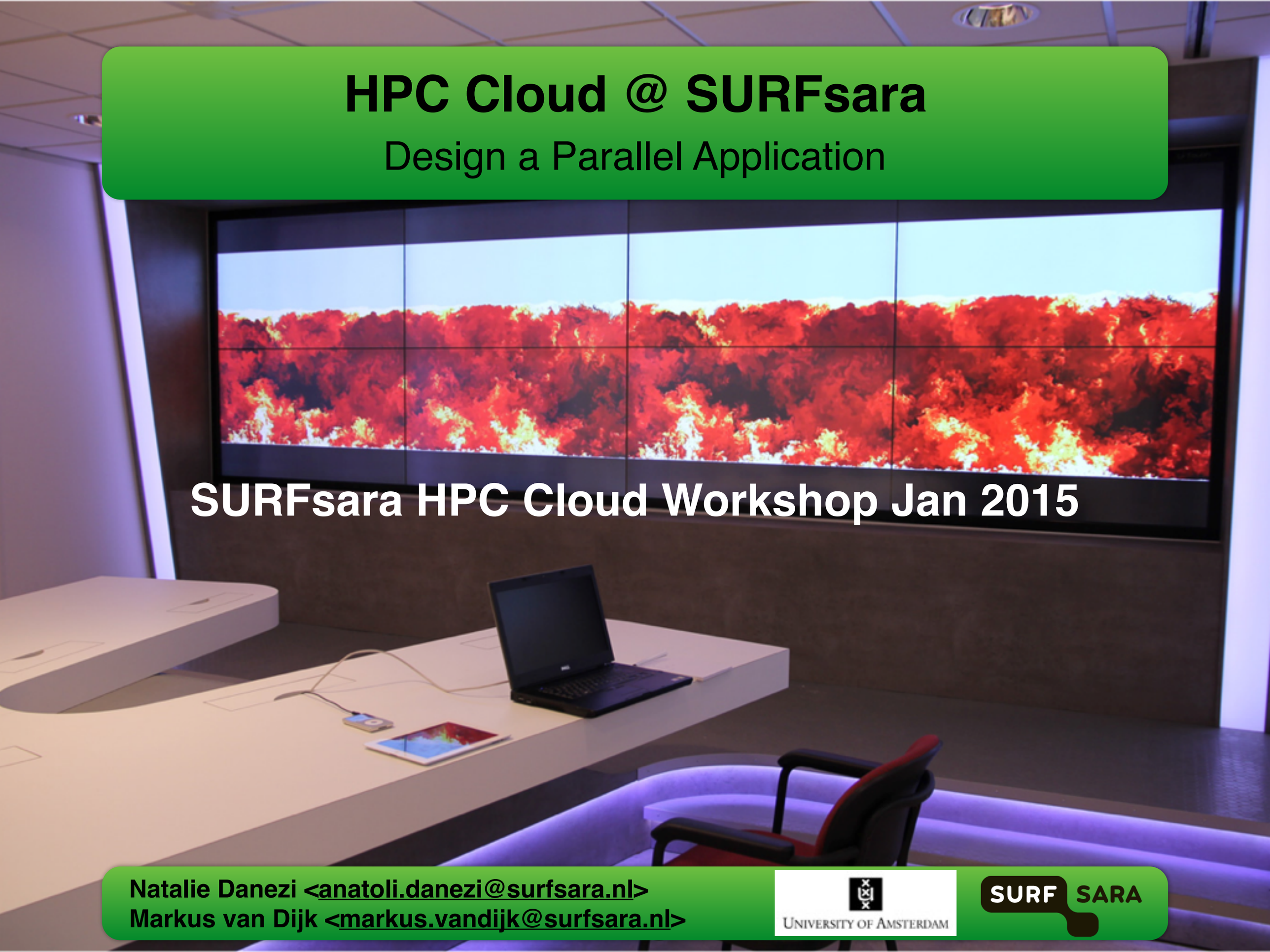
HPC Cloud @ SURFsara

Design a Parallel Application



SURFsara HPC Cloud Workshop Jan 2015

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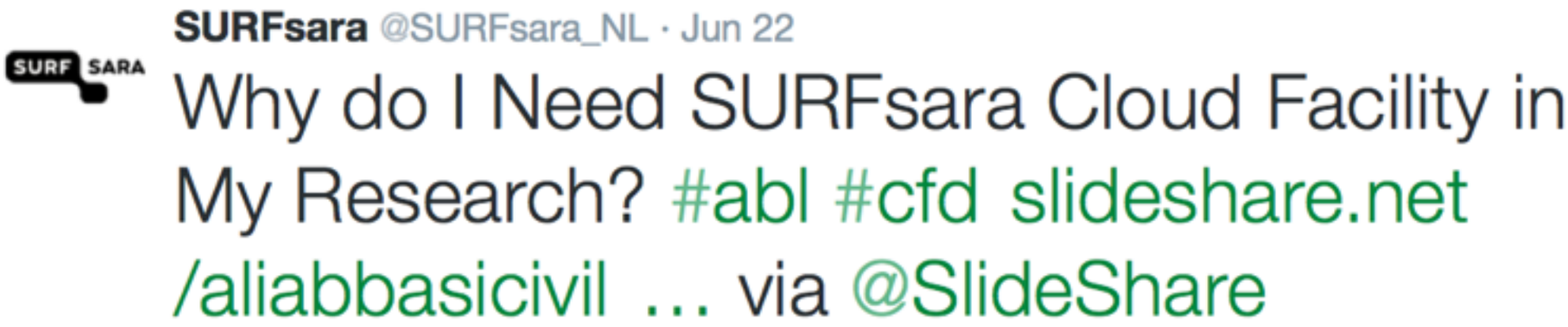
SURF SARA

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!



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

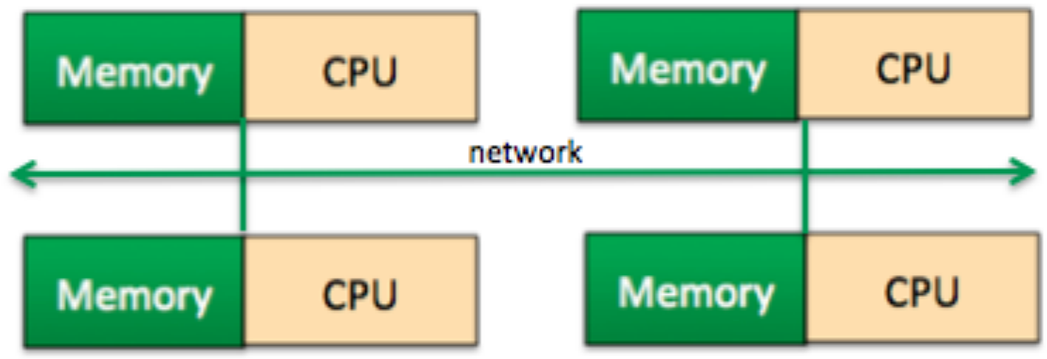
Examples?

Scalability: system & software

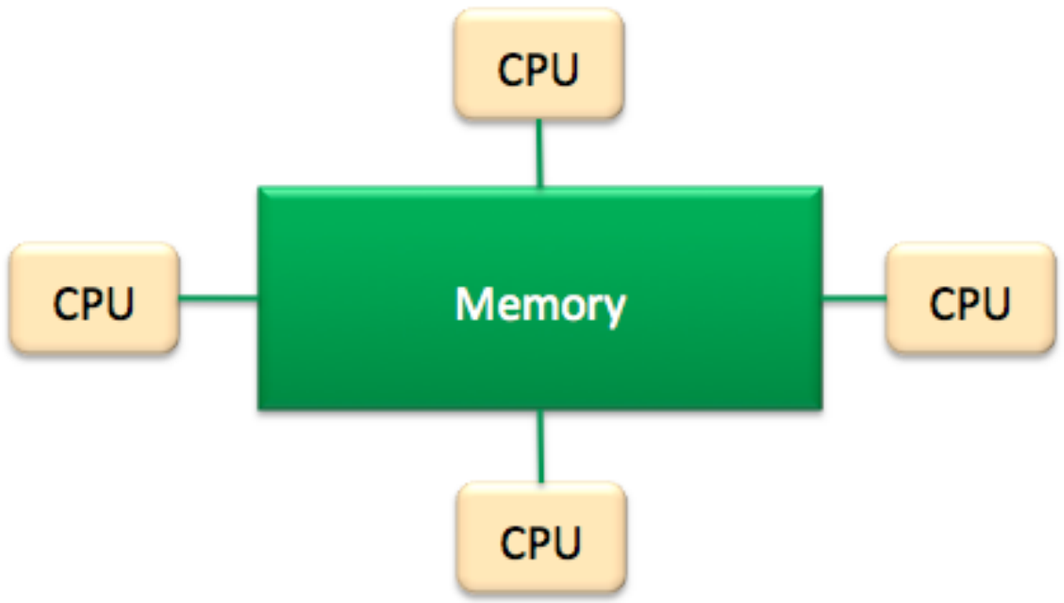
- System - add (virtual) hardware
  - Distributed memory systems
  - Shared memory systems
- Software - optimise the application
  - Develop code, e.g. MPI, OpenMP
  - Out of the box tools, e.g. Matlab, OpenFOAM, D-Flow FM

System architecture

- Distributed memory systems



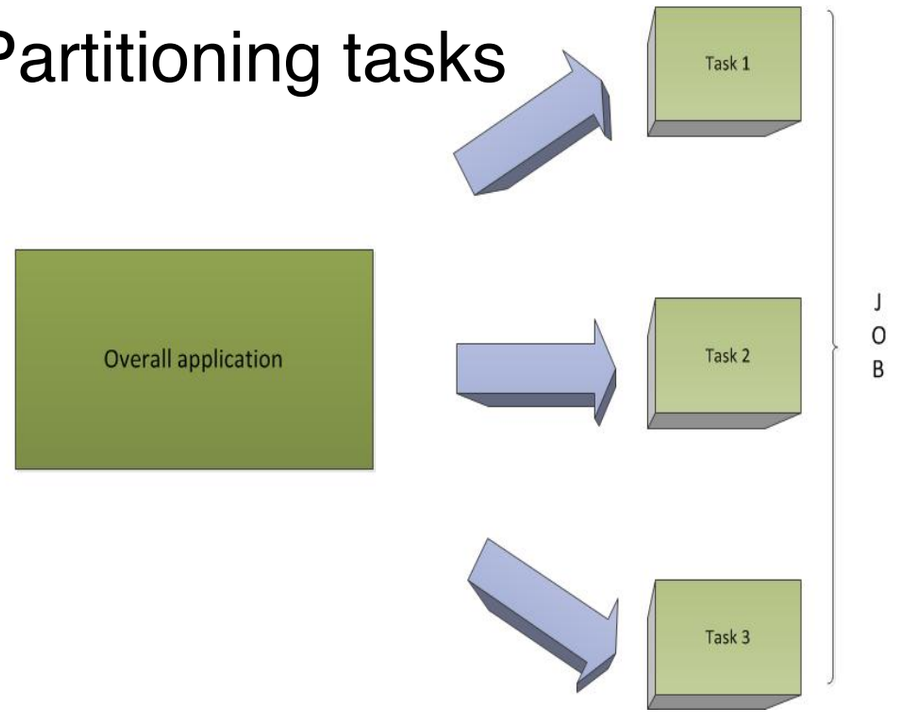
- Shared memory systems



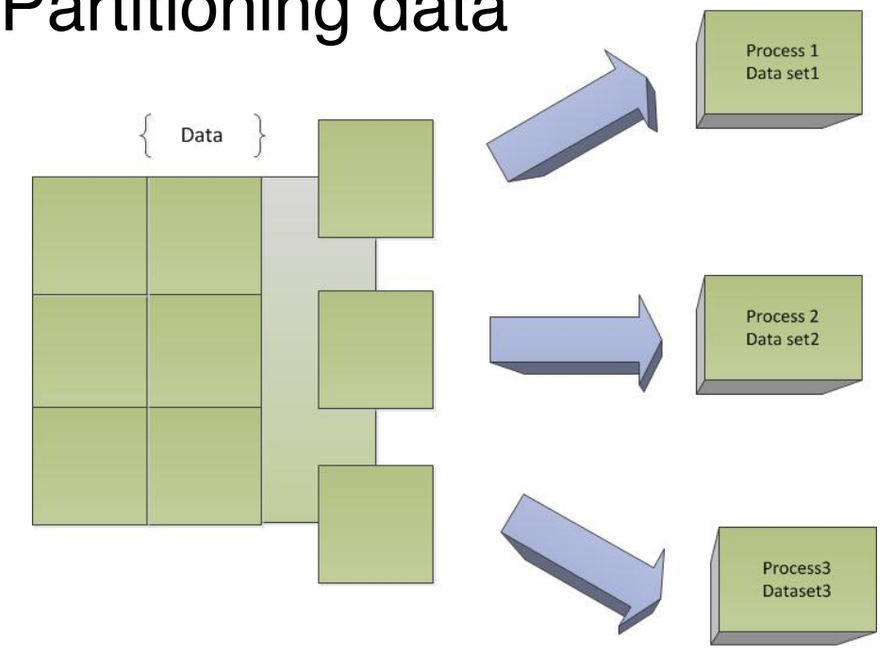
Software optimisation (1)

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

Partitioning tasks

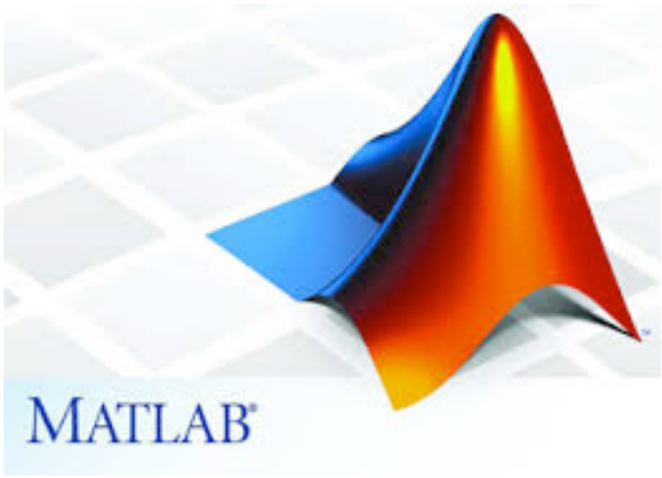


Partitioning data



Software optimisation (2)

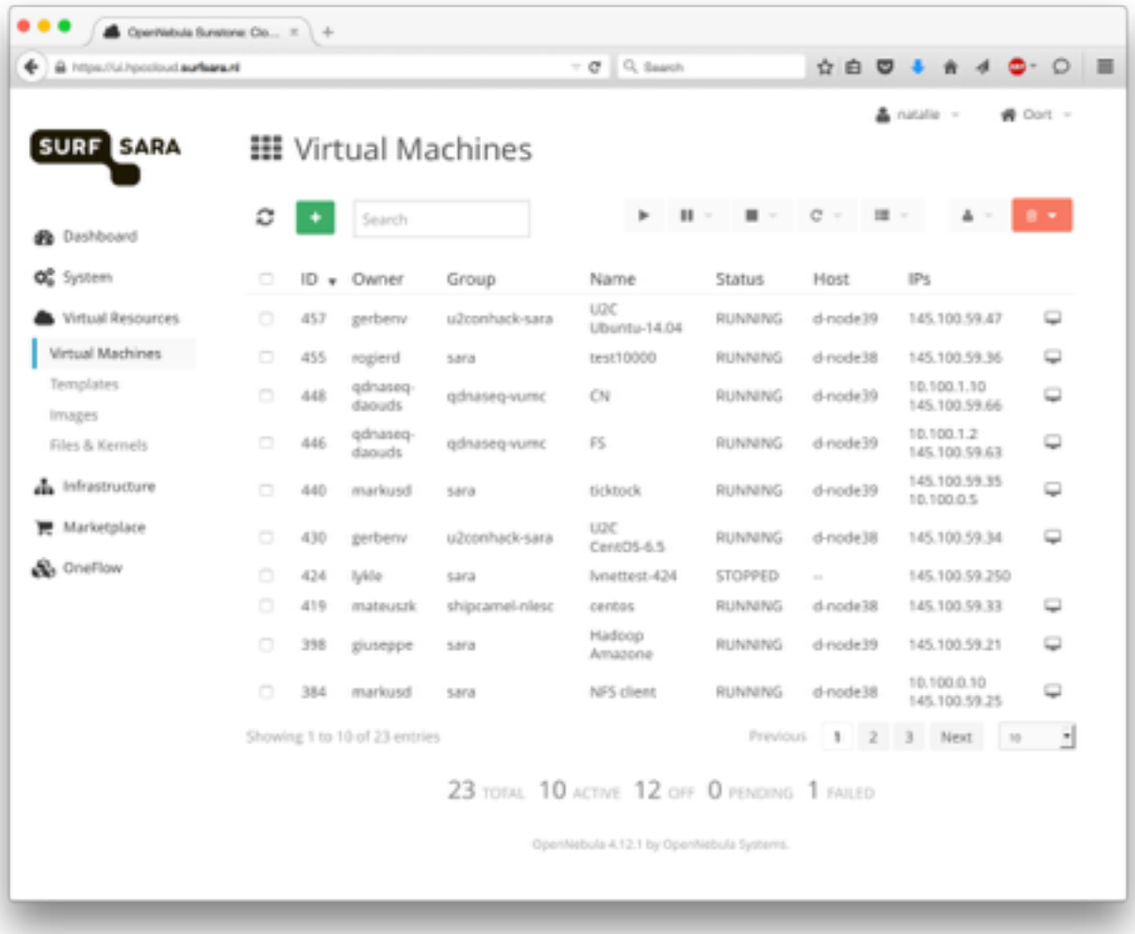
- Out of the box tools



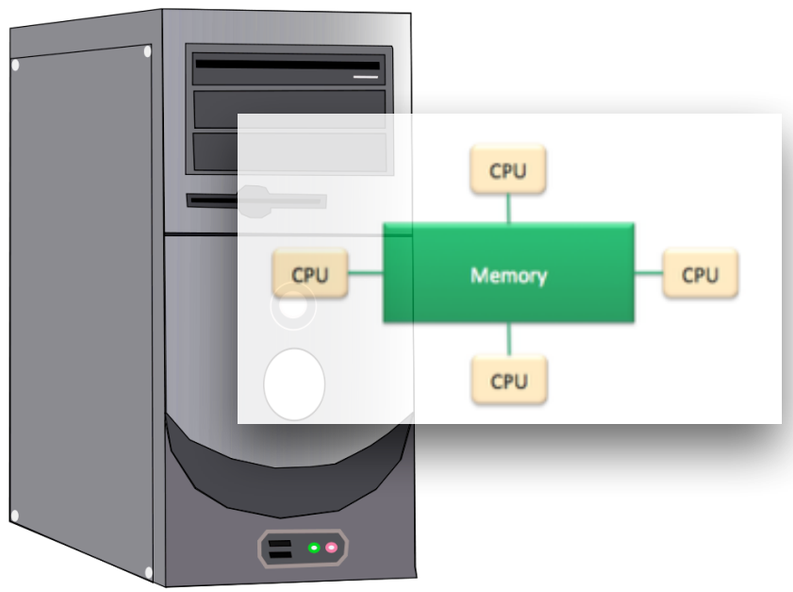
Running a parallel application on the HPC cloud

- 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

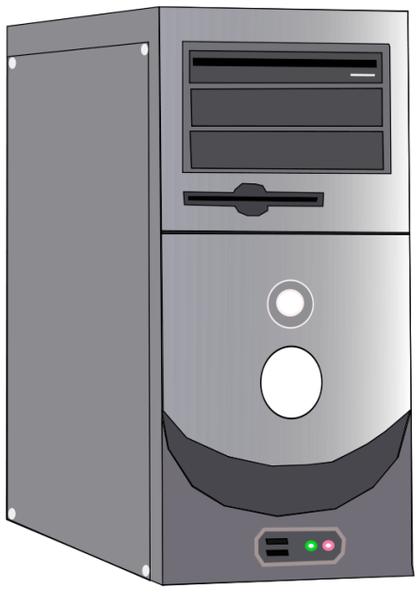


Scale up

Scale out

How?

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

How?

Scaling out (1)

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

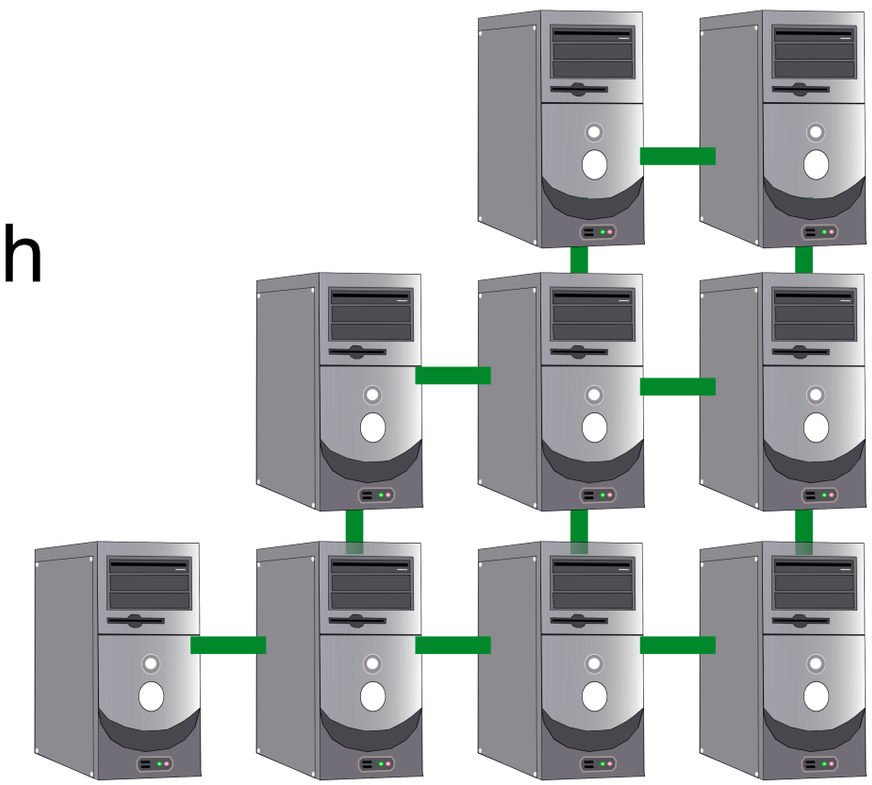
Scale out

How?

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

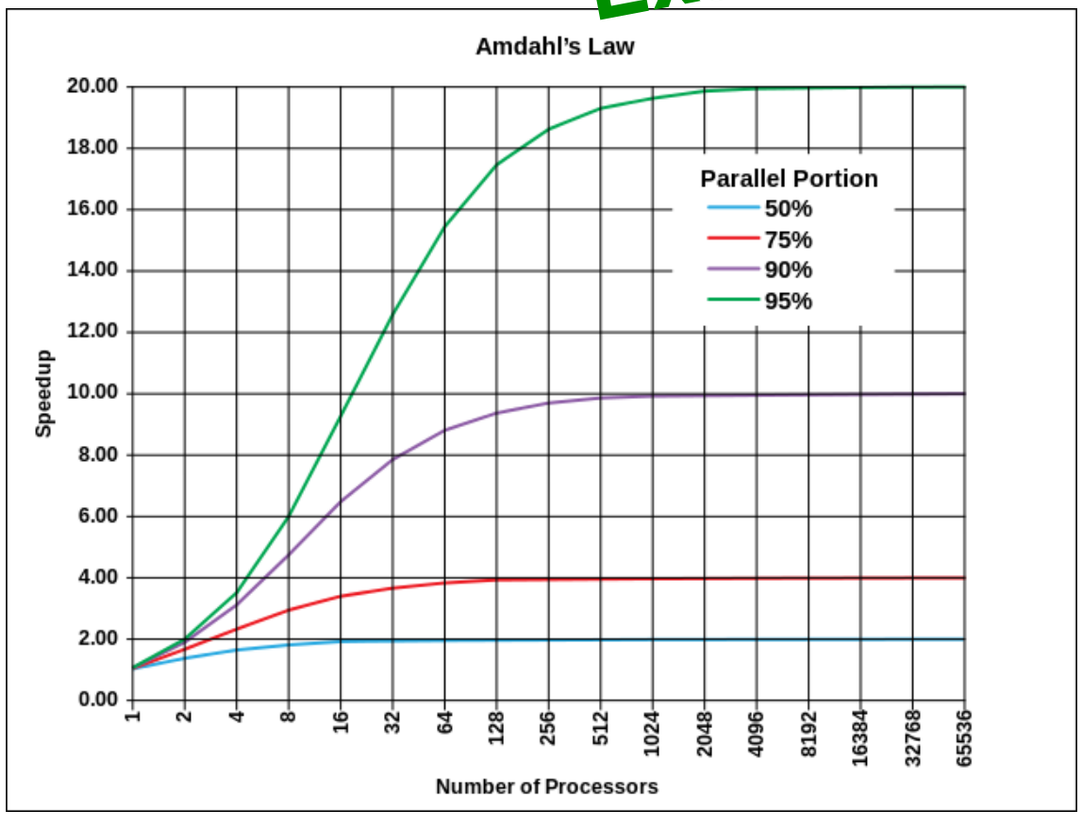
Scale out



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…

Examples?



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.hpccloud.surfsara.nl/UvAworkshop-2016-01-25/UvAworkshop-2016-01-25

- Finish Part A & B
- Move to Extras!