



science + computing

| A Bull Group Company

Optimization of optimization runs, or, how do I get my results faster?

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| Jan Wender

| HPC Software and Services

Who I Am



Jan Wender

HPC Services and Software, science + computing ag:
Helping you to run your cluster most efficiently
Stuttgart Area, Germany | Information Technology and Services

Current HPC Services and Software, Team Leader at science + computing ag
Senior IT Consultant at science + computing ag

Past Assistant at EU-Project LINGUA
Research Assistant at Universität Trier
Student assistant at Universität Trier
[see all](#) ▾

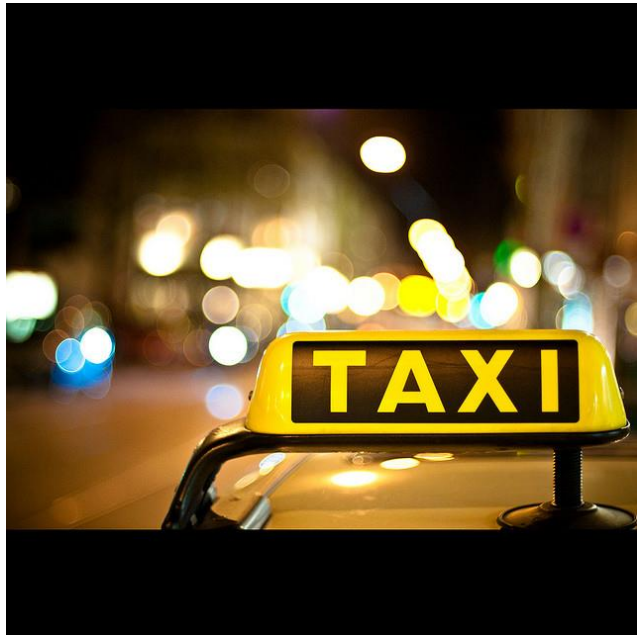
Education Universität Trier
Technische Universität Carolo-Wilhelmina zu Braunschweig

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How to Scale?



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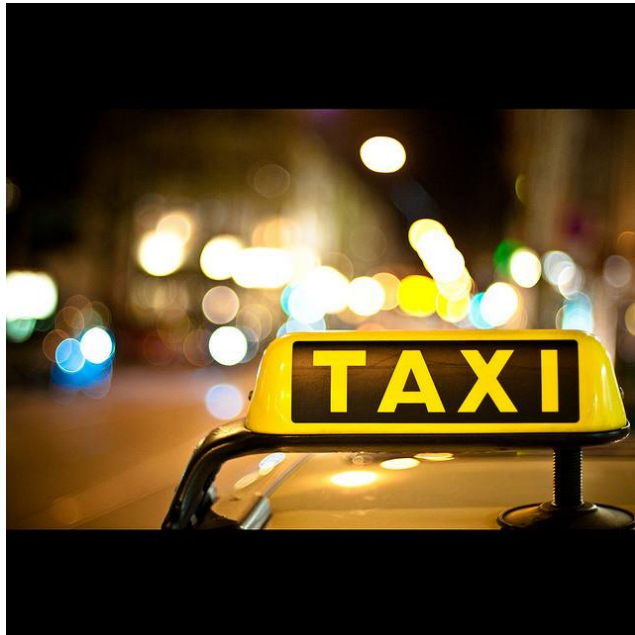
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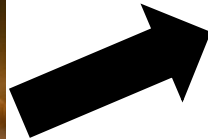
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Scale Up

Bigger is Better!



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Scale Out

If one is not enough, take two



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When Scale-Out goes wrong...



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Workstation vs. Cluster

High-End-Workstation

- 1 Node, 2 CPUs
- per CPU
 - 4 – 8 (18) Cores
 - Freq. up to 3.5 GHz (2.3 GHz)
- 8 – 16 (36) Cores
- bis 512 GB RAM

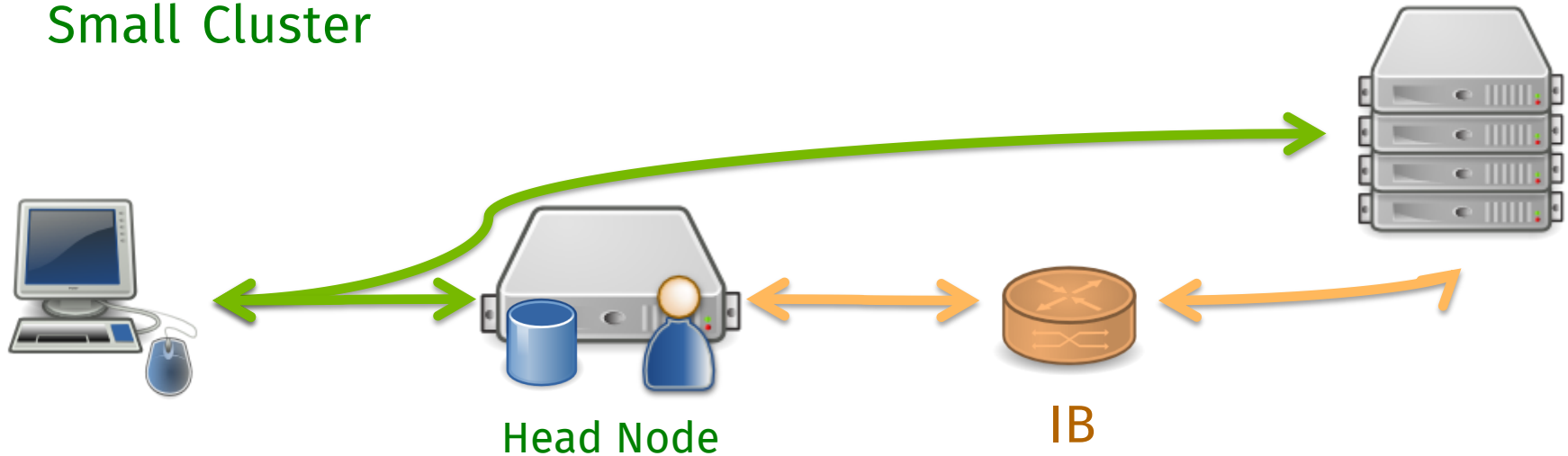
Cluster

- Several Nodes (z.B. 5)
- per CPU
 - 10 or 12 Cores
 - Freq. up to 2.6 GHz
- 100 – 120 Cores
- bis 1280/2560 GB RAM



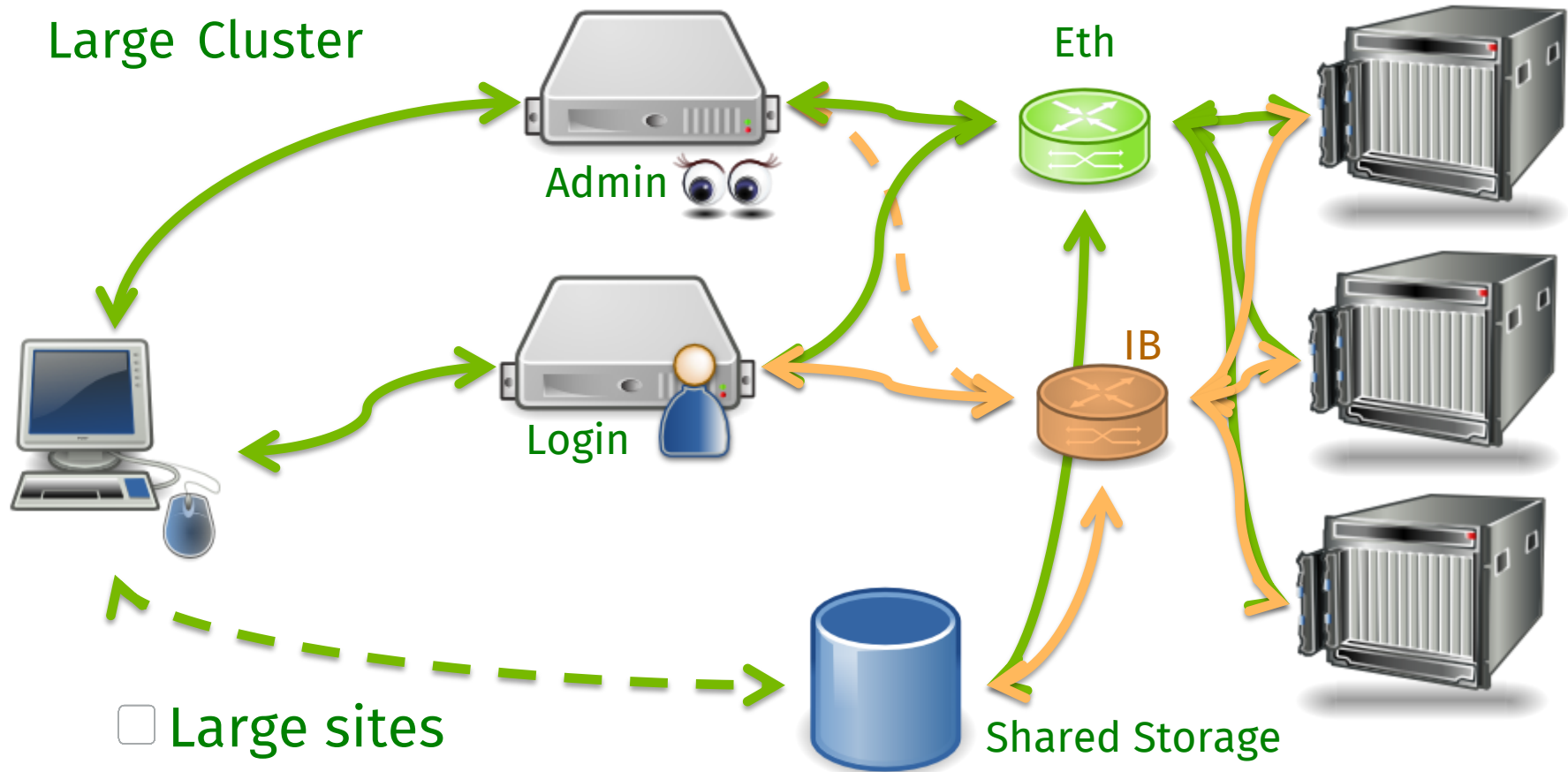
Structure of a HPC Cluster

Small Cluster



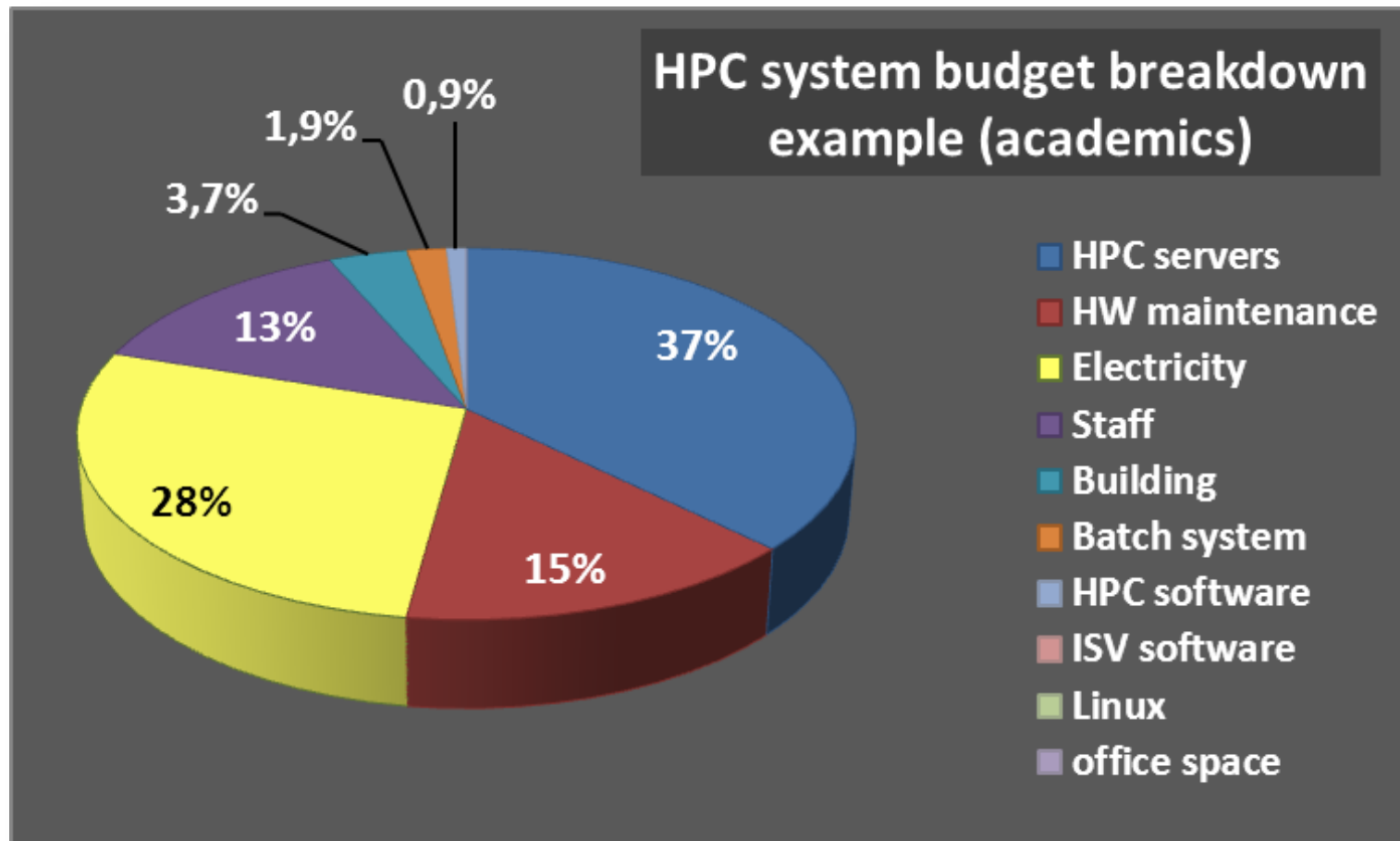
- Small sites
- ~5 Compute Nodes
- Headnode including Storage, also Login Node

Structure of a HPC Cluster

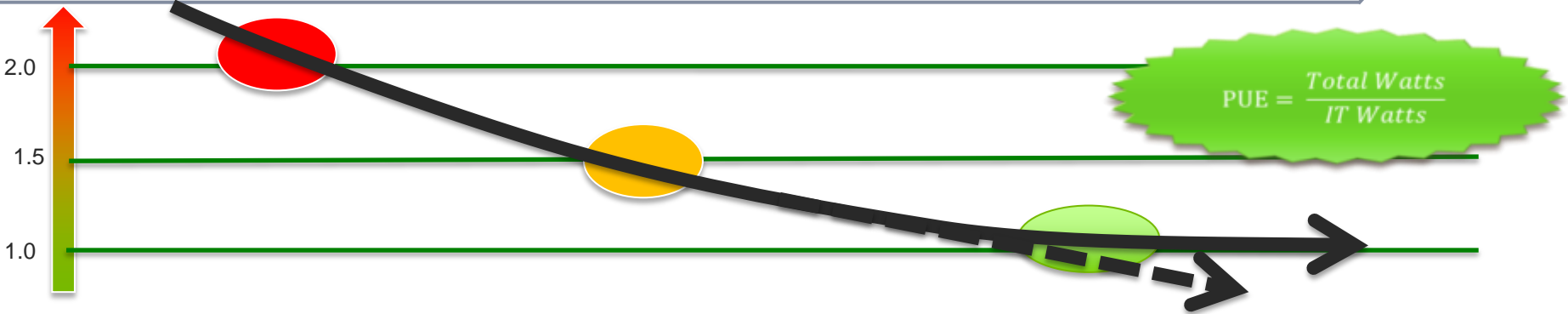


- Large sites
 - Thousands of Nodes
- Dedicated Nodes
- Dedicated Storage

Energy Consumption



Cooling & Power Usage Effectiveness



Air-cooled
 10(-20) kW/rack
 Room 20° C
 A/C water 7-12° C

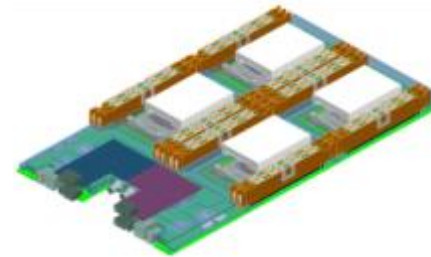
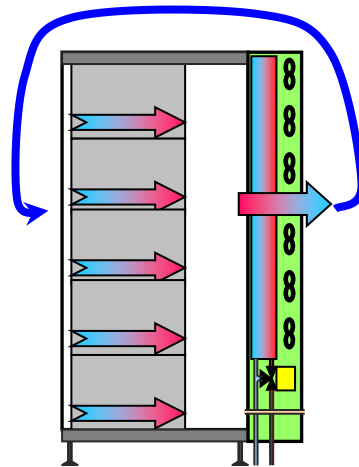
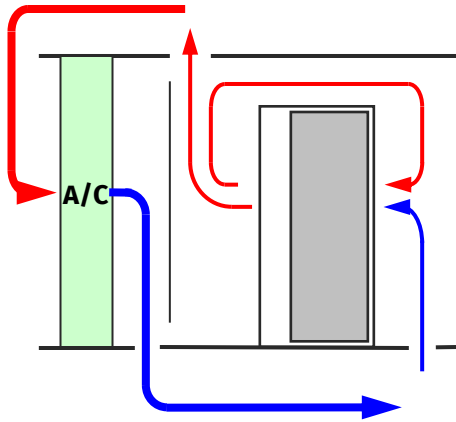
PUE ≥ 1.7

Water-cooled doors
 40 kW/rack
 Room 20° C
 Water 7-12° C

PUE ~ 1.4

Direct-Liquid-cooling
 80 kW/rack
 Room up to 30° C
 Water Up to 40 °C

PUE < 1.1



Co-generation

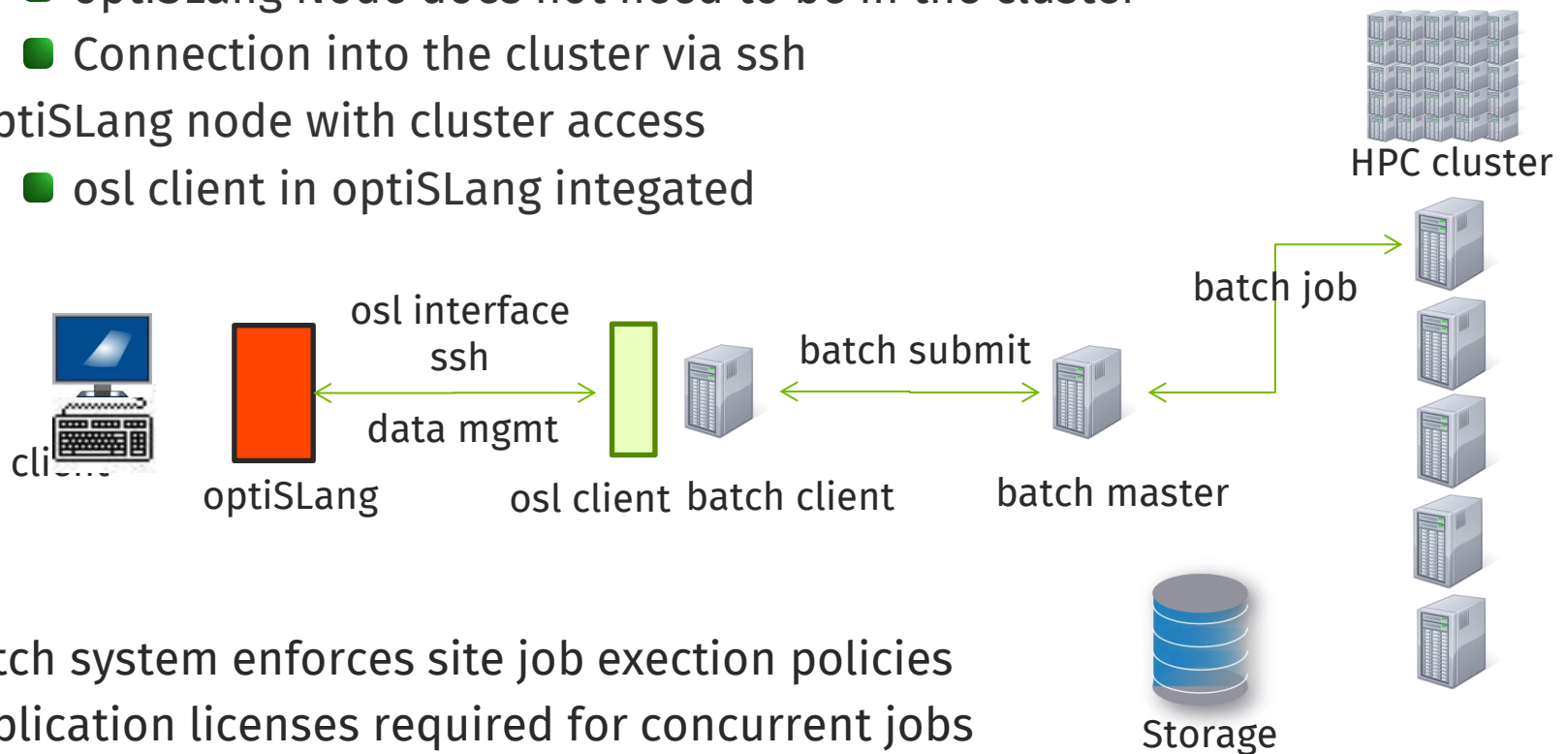
optiSLang Batch-Jobs

Access to the Cluster

- Generic Interfaces
- optiSLang Node does not need to be in the cluster
- Connection into the cluster via ssh

optiSLang node with cluster access

- osl client in optiSLang integrated



Batch system enforces site job execution policies
Application licenses required for concurrent jobs

Batch Policies

Possible configurations for prioritization of optiSLang jobs

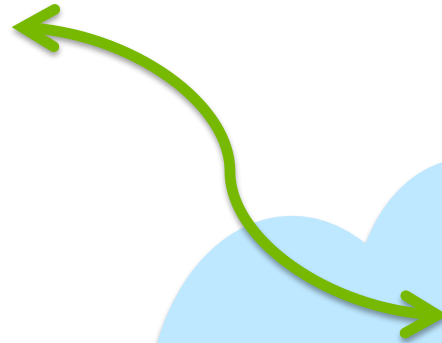
■ Examples LSF:

- SLAs: allow a number of optiSLang jobs to run concurrently when there are jobs available
- Guarantee a number of slots for optiSLang jobs
- Preempt lower priority jobs for high priority optiSLang jobs
- Give equal or higher priority to jobs of different users

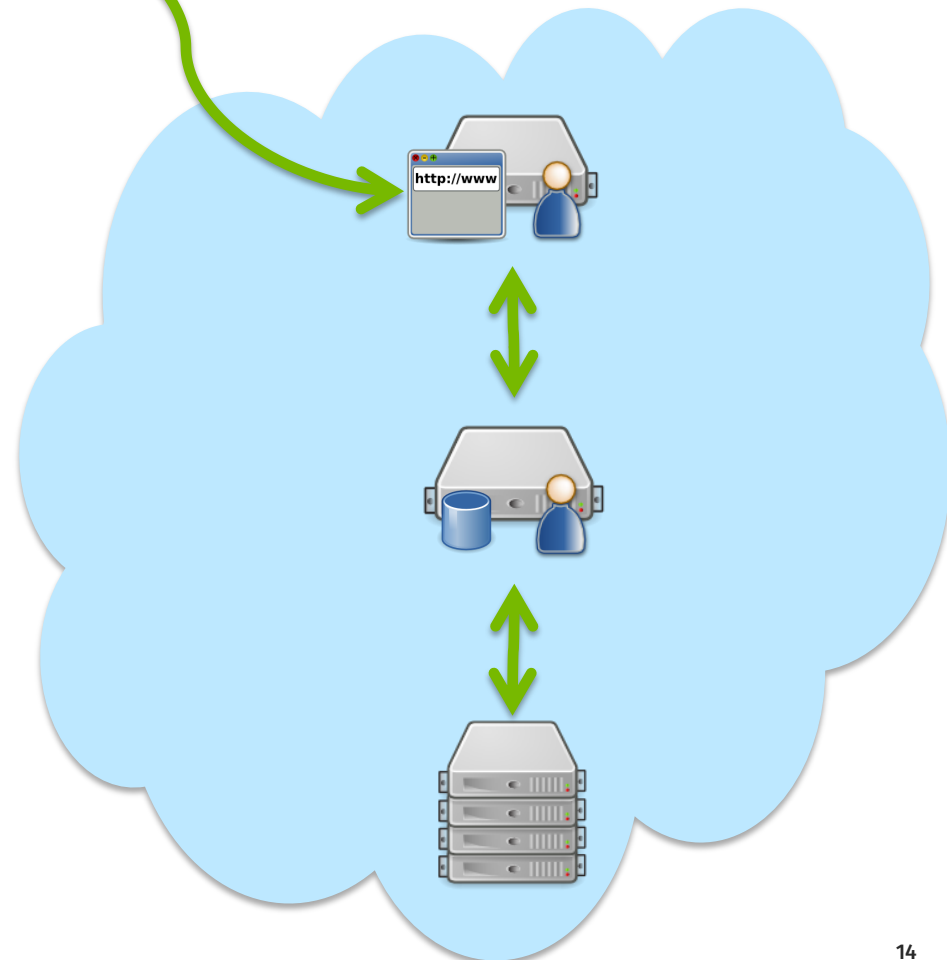
```
Begin ServiceClass
NAME          = optiSLangJob
PRIORITY      = 10
GOALS         = [velocity 11 timeWindow (1:9:00-5:17:00)]
End ServiceClass

Begin ServiceClass
NAME          = slaOptimizeLong
GOALS         = [ guarantee ]
ACCESS_CONTROL = QUEUES[ long ]
AUTO_ATTACH   = y
DESCRIPTION   = Guaranteed slots
End ServiceClass
```

HPC in the Cloud



- Access via Portal
- Remote Visualisierung
- Benefits
 - Provider operated
 - High Availability
 - Flexible Usage
 - Pay per use
- Challenges
 - Data Transfer
 - Application Licensing
 - Security
- Utilization?



Bull's HPC on Demand offer

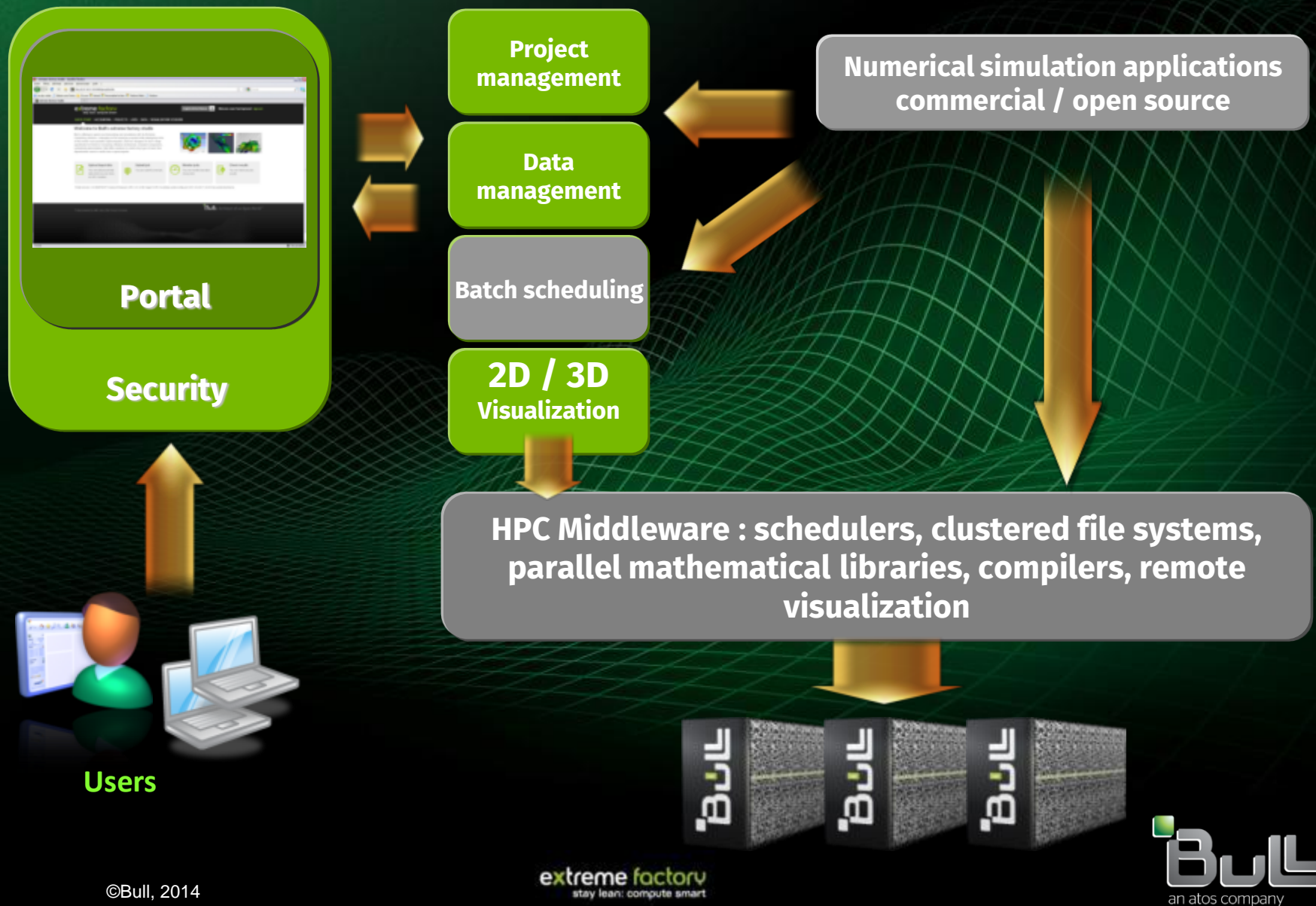
extreme factory

- ✓ performing compute infrastructure based on Bullx solutions
- ✓ Setup and operated by Bull HPC experts
- ✓ High level of service with total security
- ✓ Web portal access
- ✓ A quick and easy response to your innovation needs
- ✓ No requirement for heavy investment



To compute smart !

An operational scientific 'cloud'



Remote pre-/post-processing

The screenshot displays the 'extreme factory studio' web application in a Mozilla Firefox browser. The page title is 'Voir session de visualisation - TestML-VMD001'. The interface includes a navigation menu with options like 'français (France)', 'Welcome Marc Levrier!', and 'Terminer la session'. Below the navigation, there are several menu items: 'DÉMARRAGE RAPIDE', 'COMPTABLES', 'ADMINISTRATION', 'LES APPLICATIONS', 'CLIENTS', 'JOBS', 'DONNÉES', and 'SESSIONS DE VISUALISATION'. The main content area shows a 'Graphical Representations' panel with a 'Selected Molecule' dropdown set to 'D: alanin.pdb'. Below this, there are 'Create Rep' and 'Delete Rep' buttons, and a table with columns 'Style', 'Color', and 'Selection'. The 'VMD Main' panel is also visible, showing a menu with 'File', 'Molecule', 'Graphics', 'Display', 'Mouse', 'Extensions', and 'Help'. A table in the 'VMD Main' panel lists molecule information:

ID	T	A	D	F	Molecule	Atoms	Frames	Val
0	T	A	D	F	alanin.pdb	66	1	0

At the bottom of the 'VMD Main' panel, there are controls for 'Sphere Scale' (set to 1.0) and 'Sphere Resolution' (set to 8). The main visualization area shows a 3D ball-and-stick model of a protein structure. The status bar at the bottom left indicates 'Terminé' and the bottom right shows 'Non paramétré'.

Questions?

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