Unified nanoscale gateway to HPC and Grid environments

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The wide use of nanotechnology

Skyrmions on the track

Albert Fert, Vincent Cros and João Sampaio

Magnetic skyrmions are nanoscale spin configurations that hold promise as information carriers in ultradense memory and logic devices owing to the extremely low spin-polarized currents needed to move them.

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nature materials

Near room-temperature formation of a skyrmion crystal in thin-films of the helimagnet FeGe

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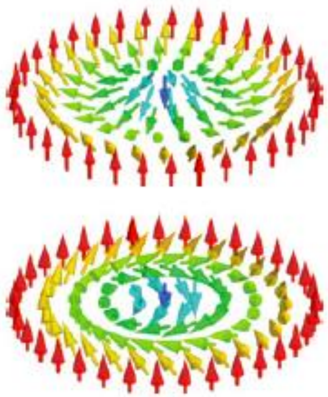

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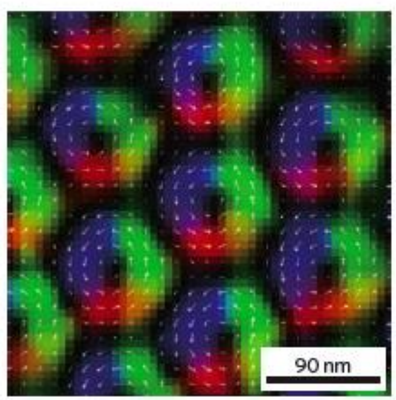
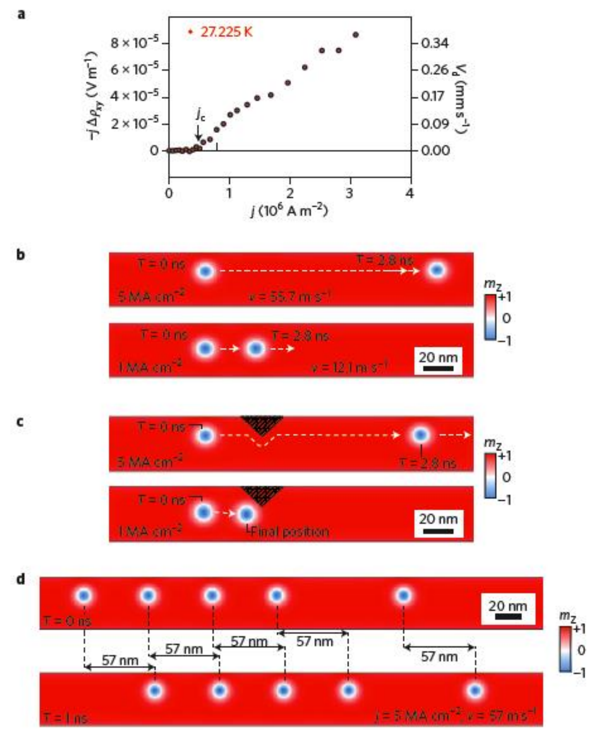
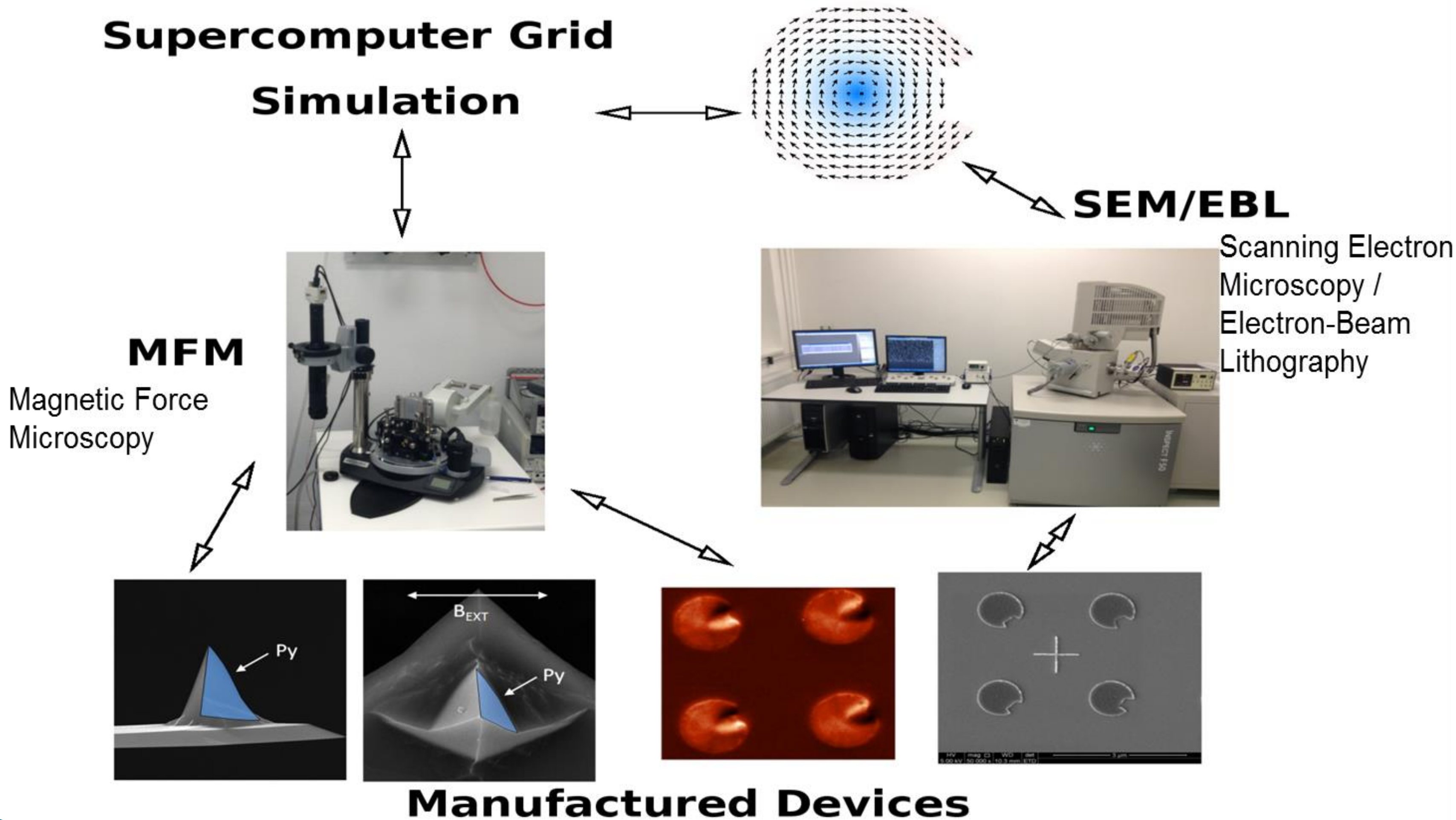




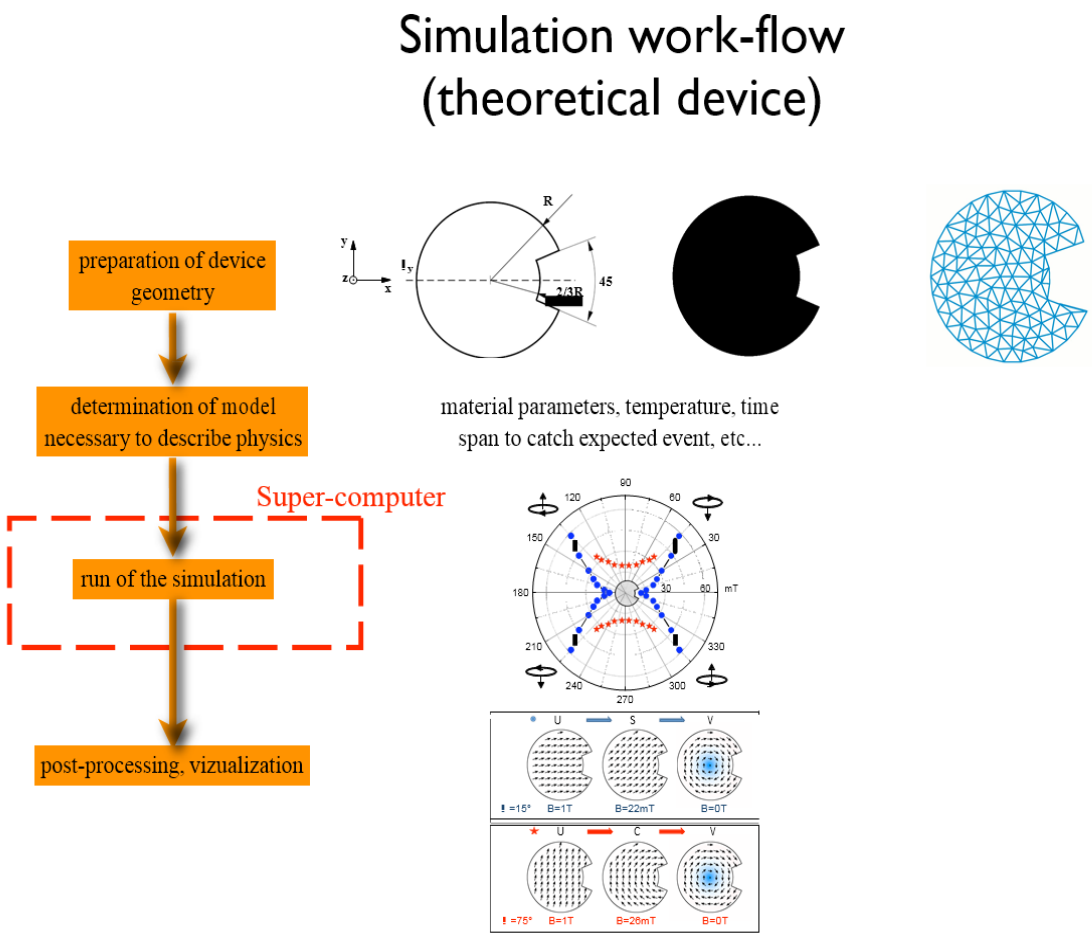
Micro-magnetism nanotechnology and HPC simulations

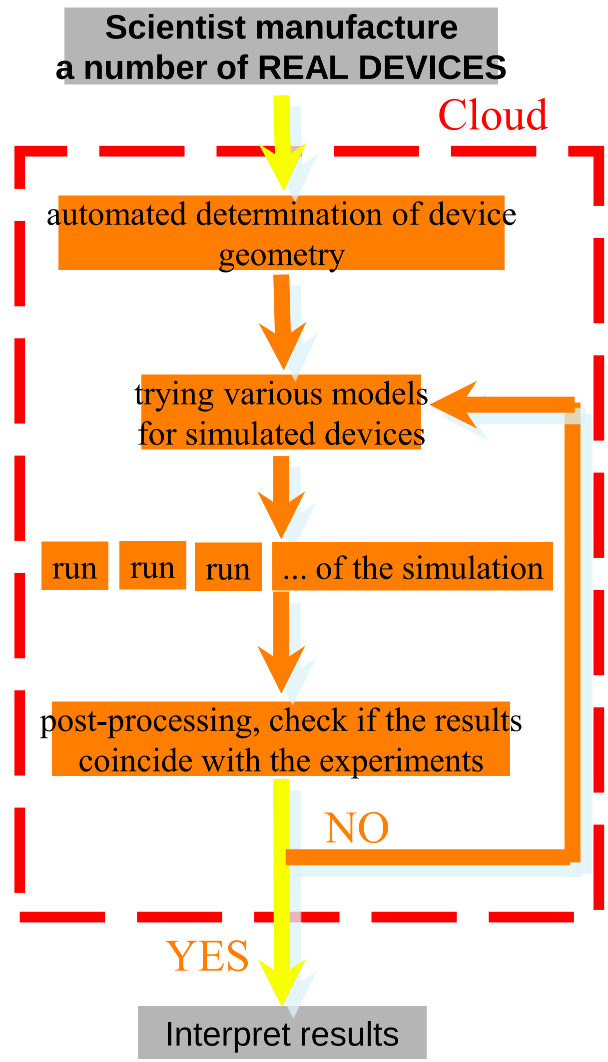
- Micromagnetism
  - new phenomena & exotic magnetic arrangements like vortices or skyrmions are investigated for practical applications e.g. information storage (memory medium).
- Nanoscale simulations
  - Help to understand underlying processes in physics of magnetic devices on sub-micrometer scale:
  - Solving magnetic dynamics described by non-linear Landau-Lifshitz-Gilbert partial differential equation,
  - Searching for (meta)stable magnetic configurations minimizing total energy functional for given systems (steepest descent, conjugated gradients, simulated annealing, meta-dynamics algorithm)
- These simulations of dynamical processes in magnetic devices
  - are CPU time consuming,
  - require algorithms' involvements and HPC supports to increase simulation speeds and efficiency
  - used software packages for simulations:
    - OOMMF: Object Oriented Micro Magnetic Framework
    - Magpar: implementation of finite elements method solver for micro-magnetics

Micro-magnetism nanotechnology and HPC simulations



Simulation workflows: theoretical and real devices





Computational capacity requirements of nanoscale simulations

- Modelling system of nano-magnetic device (desired theoretical case):
  - 70nm wide in diameter, which is usual for practical applications
  - Simulation requires cca. 20 min on PC with 2GHz processor with discretization mesh of 1nm
- Real ability is to fabricate devices of the size 500nm in diameter
  - Behaviors of the 500nm large device is qualitatively different
  - Simulations for real 500nm wide device were above nanotechnology scientists time limit on their computational capacity ☹
- Current research: to get reliable results nanoscientists need to:
  - Repeat simulations with various different realizations of stochastic noise to acquire some reliable statistics
  - Run simultaneously multiple instances of simulations with various random noise to accelerate process
- Advantages of HPC/Grid approach:
  - More and bigger simulations, bigger amount of produced data
  - Much more faster simulations, which can not be realized without HPC

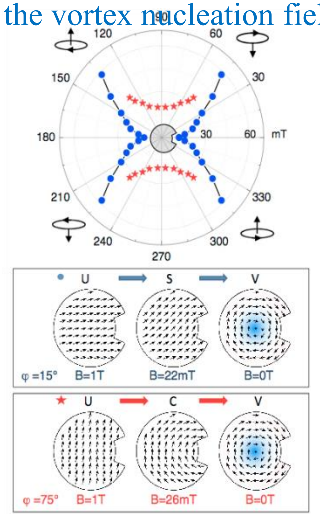
OOMMF experiments
on PC and IISAS HPC cluster

Table 1: Performance results of micromagnetic simulations

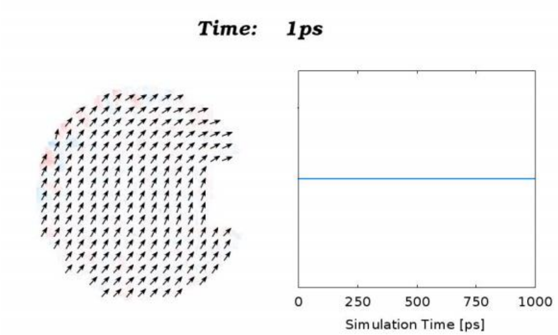
Nano-magnetic device (diameter)	Number of simulations	Simulation time	Output data	Machine
70 nm Desired aim	1	20 min	-	PC
500 nm fabricated in nanotechnology laboratory at the end of 2013	51 smaller sim. (4)	4,5 days	232 MB	PC
	100 bigger sim. (4)	8 hours	3,5 GB	cluster HPC / Grid

- Advantages of HPC approach:
  - More and bigger simulations, bigger amount of produced data
  - Much more faster simulations, which can not be realized without HPC

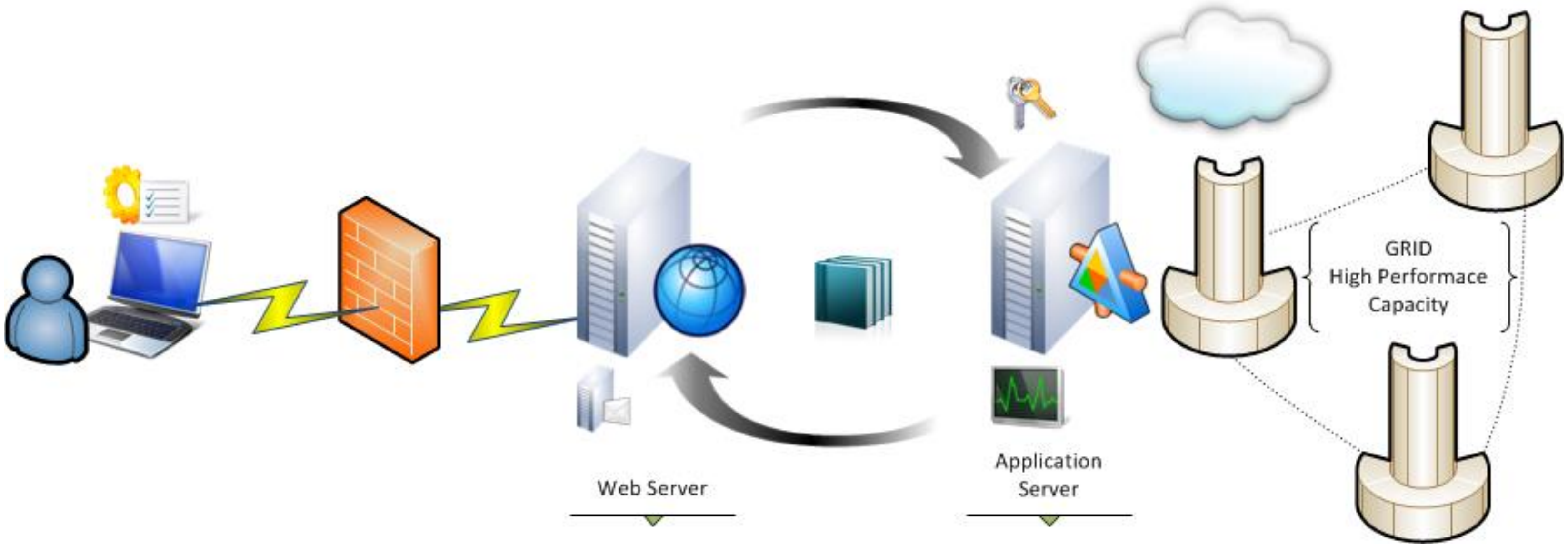
Typical simulation of the angular dependence
of the vortex nucleation field



Typical simulation of the temperature dependence of the vortex nucleation field

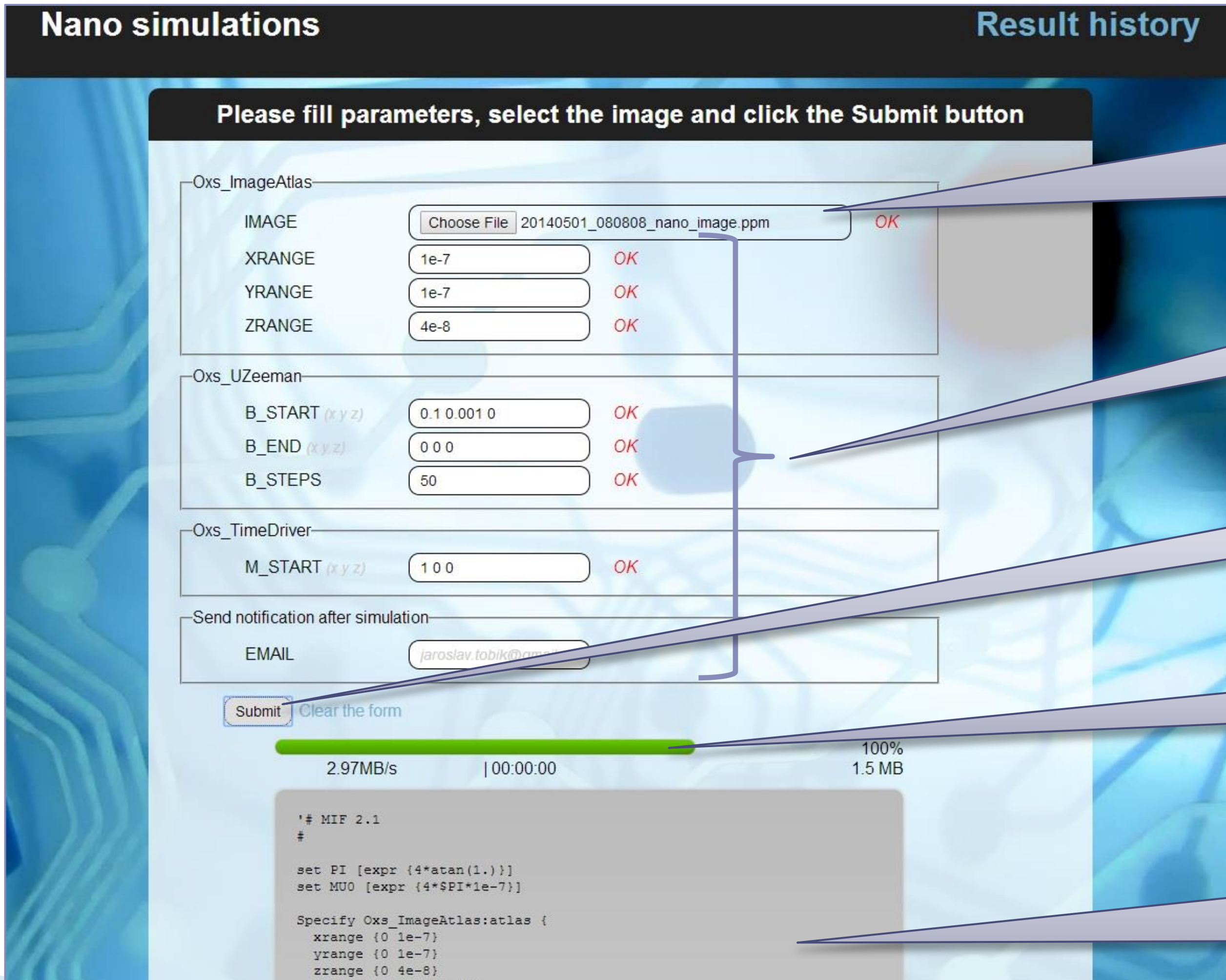


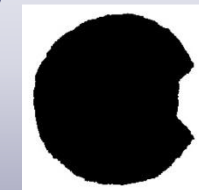
IISAS nanoscale gateway: system architecture



- User-friendly gateway to HPC/Grid/Cloud computational power
- Suitable for repeated simulations: sending simulations request and receiving simulations results
- Do not requires from end-users deep IT knowledge on HPC computing nor Grid/Cloud computing
- Customizable for generic HPC/Grid/Cloud jobs

Nanoscale gateway: simulation request with parameters





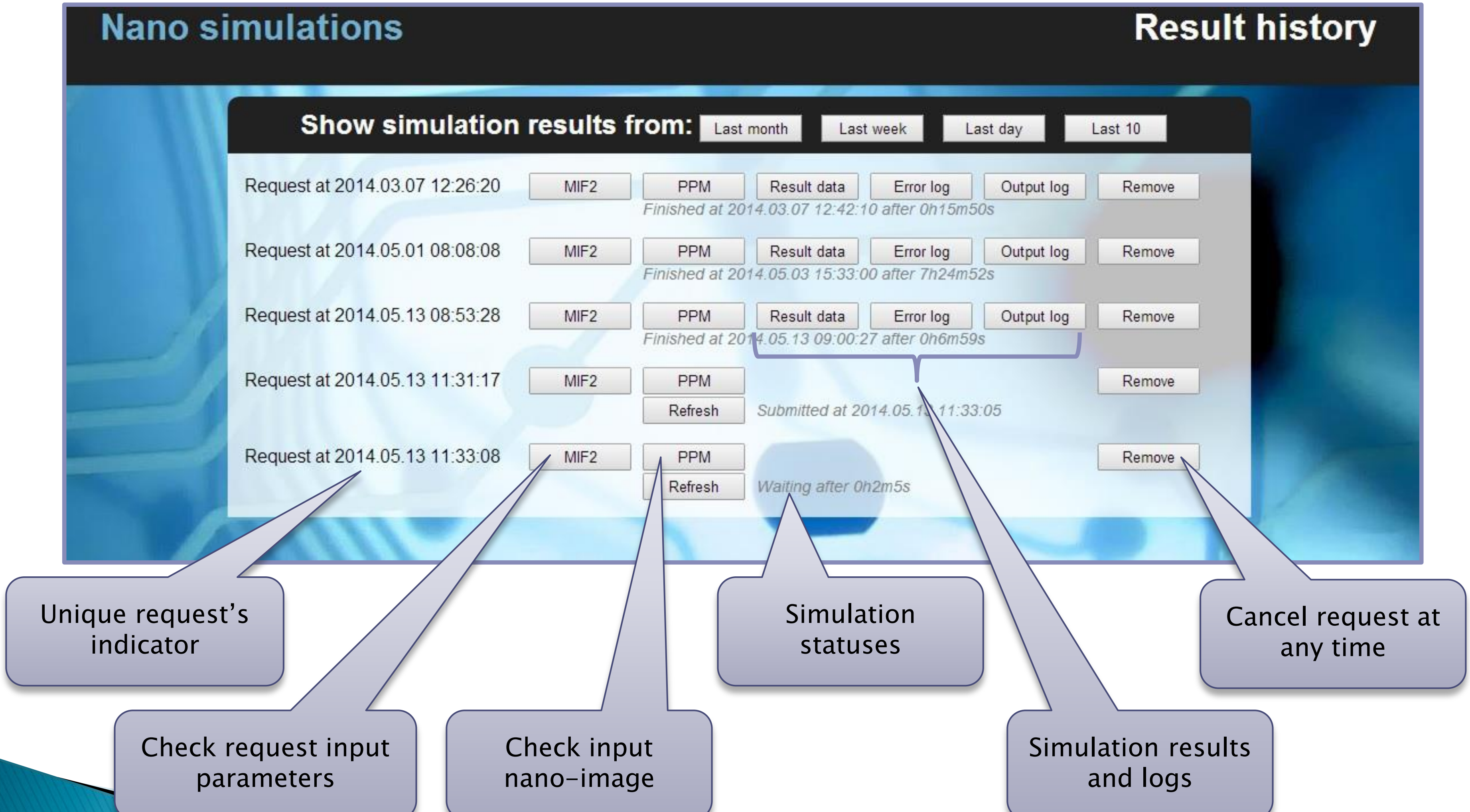
Other parameters

Send request

Successful image transfer

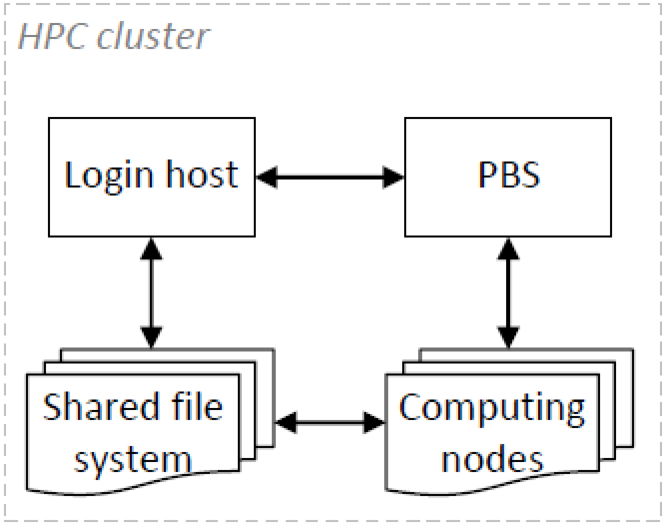
Successful simulation specification

Nanoscale gateway
Simulation results and history



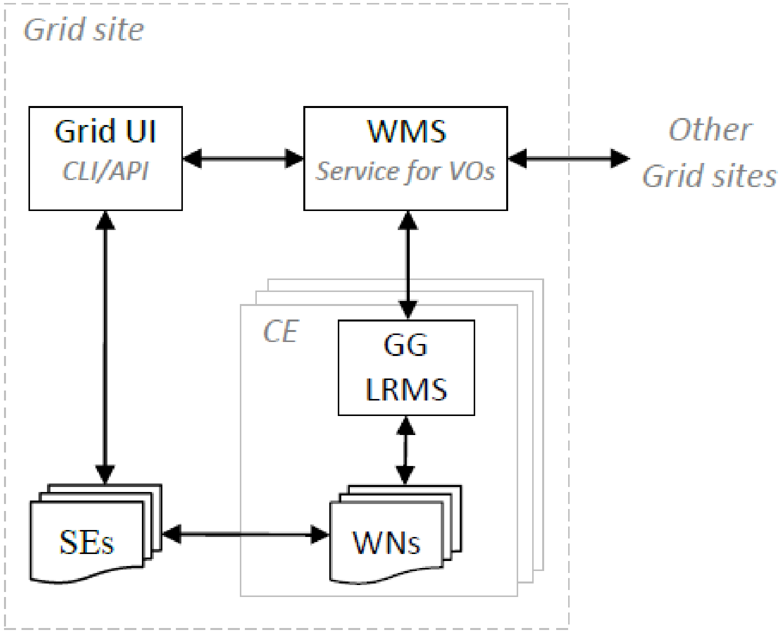
Running simulations in HPC cluster

- PBS workload management system is usually used to submit and start a job on HPC cluster. PBS has three primary roles:
  - Queuing
  - Scheduling
  - Monitoring
- PBS provides a set of commands that the user can apply for the job management operations. For the job submission the command ***qsub*** is used to which a batch-job script describing the application you want to run, is passed as an input argument.
- The command returns a job identifier which is referred to in any actions involving the job, such as checking the job state, modifying, tracking, or deleting the job.



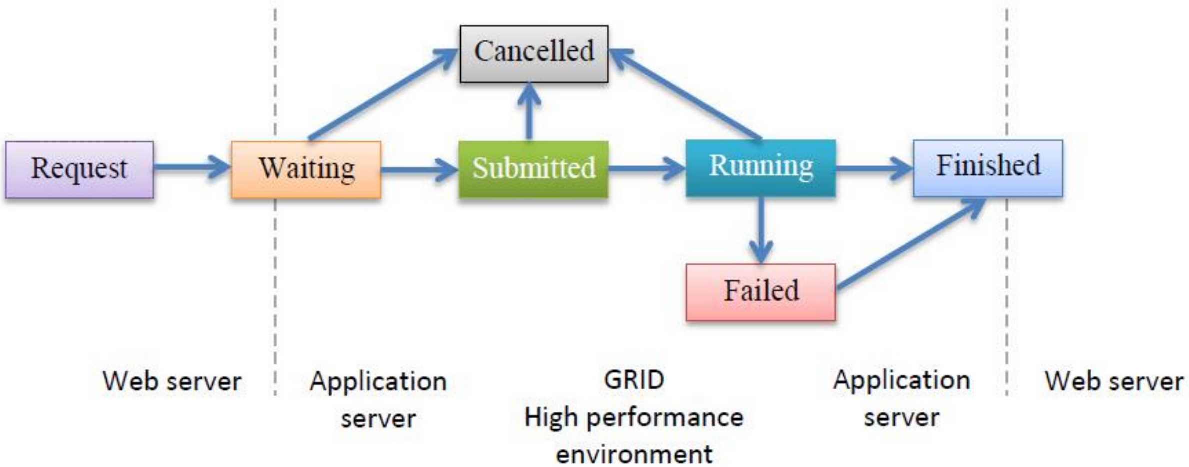
Running simulations in Grid

- Users access to Grid infrastructure through Grid User Interface (UI).
  - Grid UI is different from the gateway UI
  - Grid UI is marked as the Application server in our gateway architecture
- From the Grid UI, the user authenticates to use Grid (EGI) resources and can take advantage of all functionalities offered by the Information, Workload and Data management systems, which are parts of the Grid middleware EMI.
- Grid UI provides
  - CLI (Command Line Interface) and
  - API (Application Programming Interface) tools to perform basic Grid operations.



IISAS nanoscale gateway: simulation states

- Monitoring simulations' statuses
- Monitoring IISAS HPC cluster workload
- Unified statuses for HPC and Grid/Cloud jobs: simplified and unified job states for end-users



- The gateway job states are unified and simplified for endusers.
- They are also little different from
  - HPC job states (*Held, Queued, Waiting, Running, Completed, Exiting, Suspend, Moved*)
  - Grid job states (*Submitted, Waiting, Ready, Scheduled, Running, Aborted, Done, Cleared*)

Conclusion

- Advantages of HPC/Grid approach:
  - More and bigger simulations, bigger amount of produced data
  - Much more faster simulations, which can not be realized without HPC
- Advantages of gateway approach
  - Hides the complexity of the Grid middleware and makes the access to HPC/Grid resources transparent and comfortable
  - Helps scientists in other research areas to concentrate better on their work
  - Customizable for generic HPC/Grid/Cloud jobs

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