

# 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.

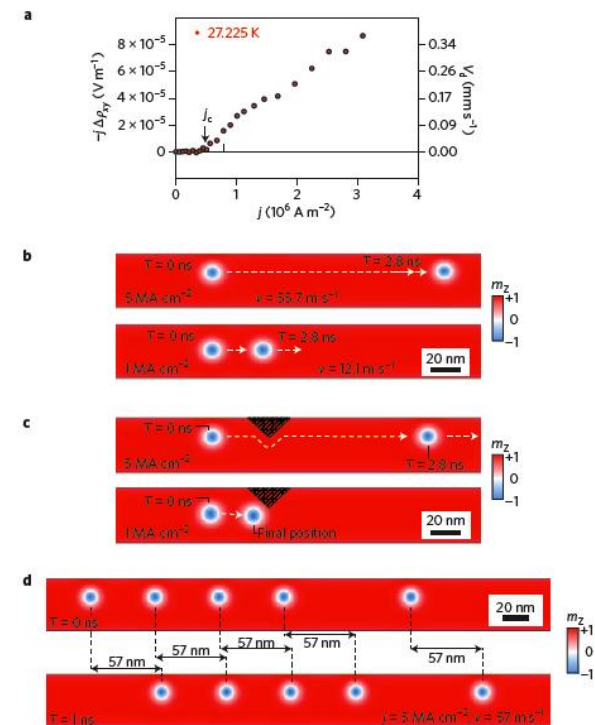
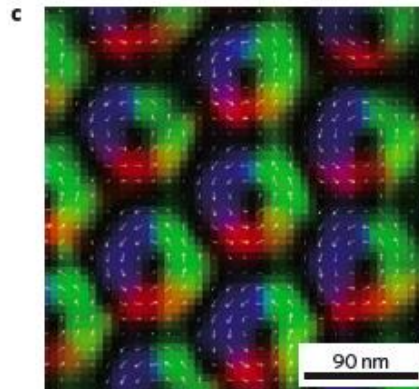
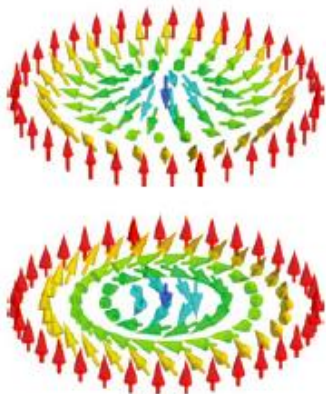
LETTERS

PUBLISHED ONLINE: 5 DECEMBER 2010 | DOI: 10.1038/NMAT2916

nature  
materials

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

X. Z. Yu<sup>1</sup>\*, N. Kanazawa<sup>2</sup>, Y. Onose<sup>1,2</sup>, K. Kimoto<sup>3</sup>, W. Z. Zhang<sup>3</sup>, S. Ishiwata<sup>2</sup>, Y. Matsui<sup>3</sup> and Y. Tokura<sup>1,2,4</sup>\*



# 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).

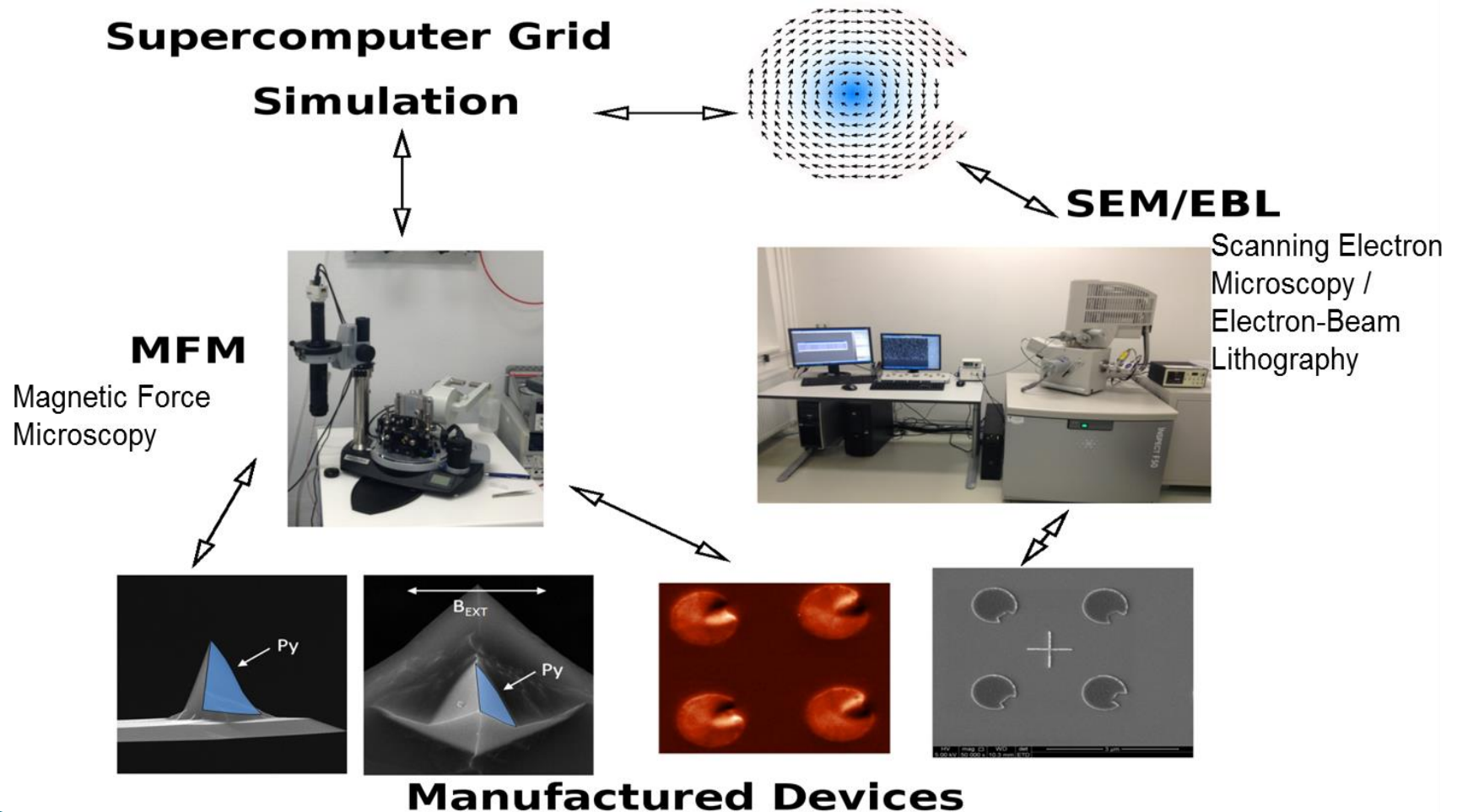
## ▶ Nanoscale simulations

- 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

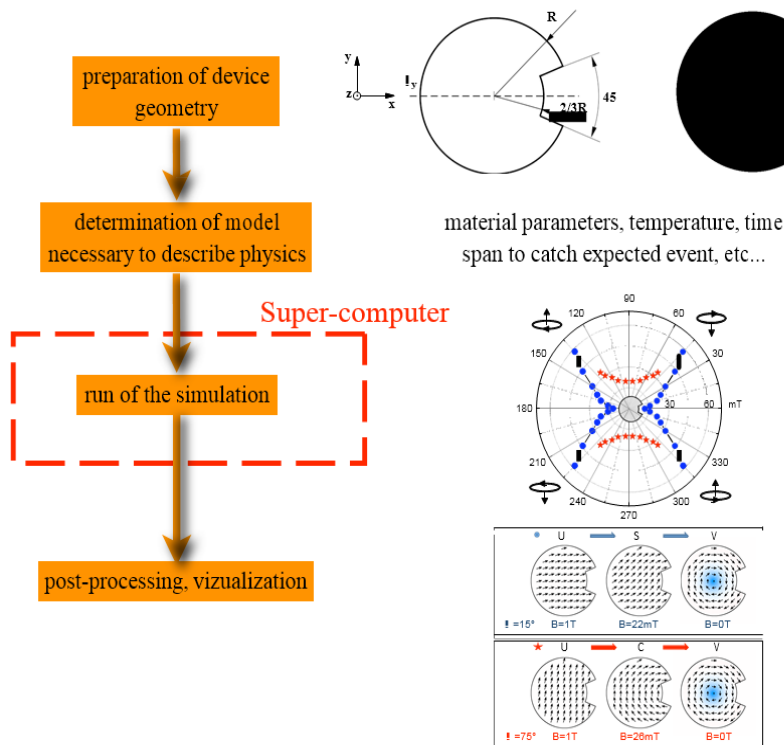
- are CPU time consuming,
- require algorithms' involvements and HPC supports to increase simulation speeds and efficiency
- used software packages for simulations:
  - OOMMF: Object Oriented Micro Magnetic Framework
  - Magpar: implementation of finite elements method solver for micro-magnetics

# Micro-magnetism nanotechnology and HPC simulations

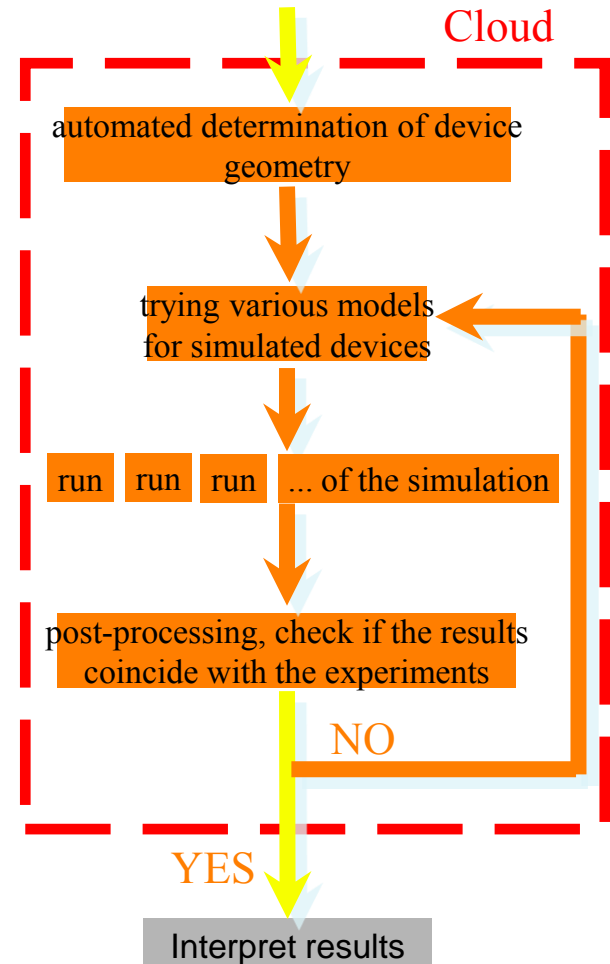


# Simulation workflows: theoretical and real devices

## Simulation work-flow (theoretical device)



Scientist manufacture  
a number of 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

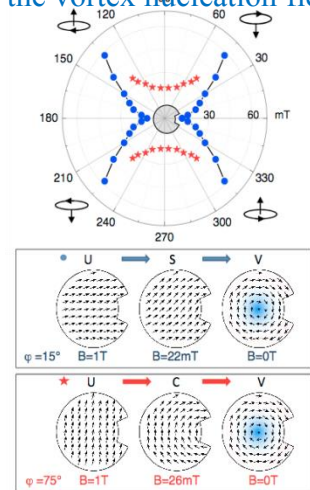
# OOMMF experiments on PC and IISAS HPC cluster

Table 1: Performance results of micromagnetic simulations

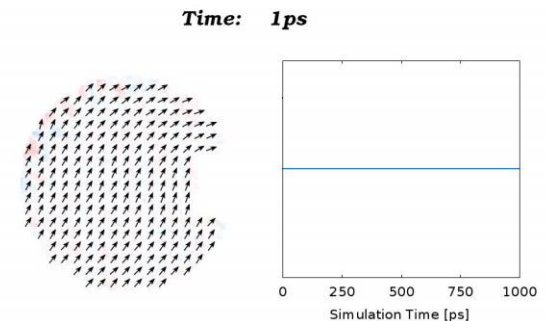
Nano-magnetic device (diameter)	Number of simulations	Simulation time	Output data	Machine
70 nm Desired aim	1	20 min	-	PC
500 nm fabricated in nanotechnology laboratory at the end of 2013	51 smaller sim. <sup>(4)</sup>	4,5 days	232 MB	PC
	100 bigger sim. <sup>(4)</sup>	8 hours	3,5 GB	cluster HPC / Grid

- 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



The diagram illustrates the architecture of a Cloud-based Web Application. It shows a user (person icon) interacting with a laptop, which connects through a firewall (brick wall icon) to a Web Server (server rack icon). The Web Server is connected to an Application Server (server rack icon) via a network (cloud icon). The Application Server is connected to a GRID of High Performance Capacity (represented by three server racks icon). The Application Server also has a monitor displaying a graph.

- ▶ 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

Nano simulations

Result history

Please fill parameters, select the image and click the Submit button

Oxs\_ImageAtlas

IMAGE

Choose File

20140501\_080808\_nano\_image.ppm

OK

XRANGE

1e-7

OK

YRANGE

1e-7

OK

ZRANGE

4e-8

OK

Oxs\_UZeeman

B\_START (x y z)

0 1 0.001 0

OK

B\_END (x y z)

0 0 0

OK

B\_STEPS

50

OK

Oxs\_TimeDriver

M\_START (x y z)

1 0 0

OK

Send notification after simulation

EMAIL

jaroslav.tobik@gmail.com

Submit

Clear the form

2.97MB/s

100%

1.5 MB

00:00:00

'# MIF 2.1

#

set PI [expr {4\*atan(1.)}]

set MUO [expr {4\*\$PI\*1e-7}]

Specify Oxs\_ImageAtlas:atlas {

xrange {0 1e-7}

yrange {0 1e-7}

zrange {0 4e-8}

image nano\_image.ppm



Other parameters

Send request

Successful image transfer

Successful simulation specification

# Nanoscale gateway

## Simulation results and history

The screenshot shows a web interface titled "Nano simulations" and "Result history". It features a filter bar for "Show simulation results from:" with options: "Last month", "Last week", "Last day", and "Last 10". Below this is a table of simulation requests. Each row includes a timestamp, input parameters (MIF2, PPM), action buttons (Result data, Error log, Output log, Remove), and a status message. Callouts point to specific elements: "Unique request's indicator" points to the timestamp; "Check request input parameters" points to the MIF2 button; "Check input nano-image" points to the PPM button; "Simulation statuses" points to the status messages; "Simulation results and logs" points to the Result data, Error log, and Output log buttons; and "Cancel request at any time" points to the Remove button.

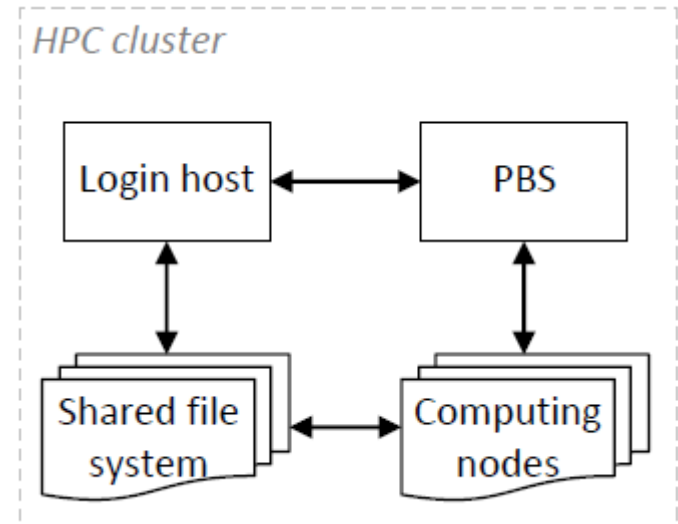
Request at	MIF2	PPM	Result data	Error log	Output log	Remove	Status
2014.03.07 12:26:20							Finished at 2014.03.07 12:42:10 after 0h15m50s
2014.05.01 08:08:08							Finished at 2014.05.03 15:33:00 after 7h24m52s
2014.05.13 08:53:28							Finished at 2014.05.13 09:00:27 after 0h6m59s
2014.05.13 11:31:17							Submitted at 2014.05.13 11:33:05
2014.05.13 11:33:08							Waiting after 0h2m5s

Callouts:

- Unique request's indicator
- Check request input parameters
- Check input nano-image
- Simulation statuses
- Simulation results and logs
- Cancel request at any time

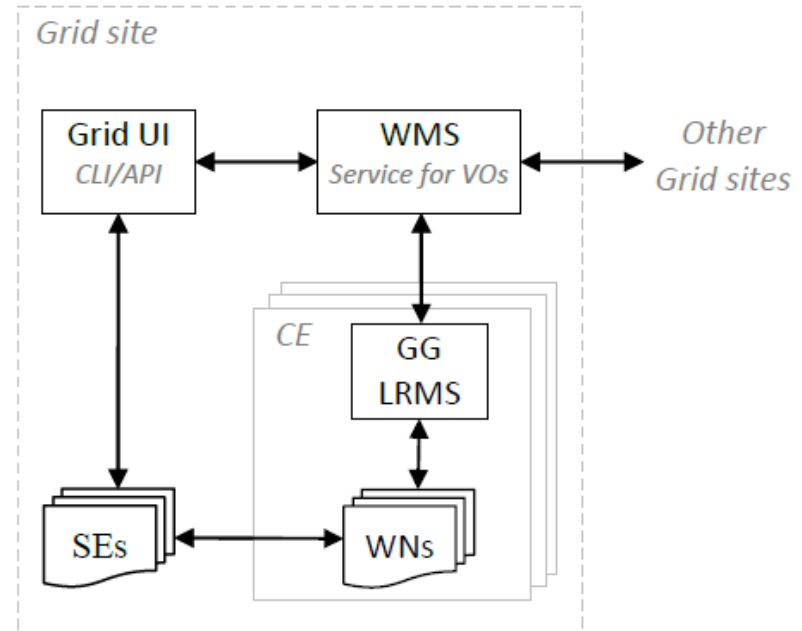
# Running simulations in HPC cluster

- ▶ 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.



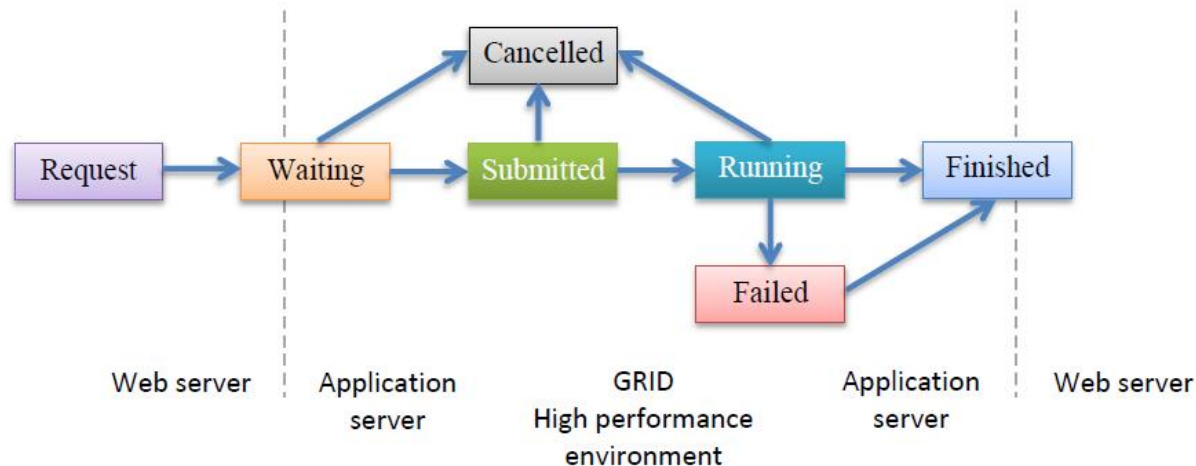
# Running simulations in Grid

- ▶ 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

# Acknowledgements

- ▶ This work is supported by projects:
    - KC INTELINSYS ERDF ITMS 26240220072
    - EGI-InSPIRE EU FP7-261323 RI,
    - CLAN APVV-0809-11 and
    - VEGA No. 2/0054/12
  
  - ▶ Micro-magnetism simulations and the gateway realization were achieved on the hardware equipment obtained within project
    - SIVVP ERDF ITMS 26230120002
- 

# Thank you for attention

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G. Nguyen, L. Hluchý, J. Tóbik, V. Šipková, M. Dobrucký, J. Astaloš, V. Tran, R. Andok:  
"Unified nanoscale gateway to HPC and Grid environments",  
5th Symposium on Information and Communication Technology 2014,  
pp. 85–91, ACM 978–1–4503–2930–9/14/12, ISBN: 978–1–4503–2930–9,  
DOI 10.1145/2676585.2676591