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.

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

a

b

c

d

90 nm

20 nm

20 nm

20 nm

20 nm

20 nm

20 nm
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

Supercomputer Grid
Simulation

SEM/EBL
Scanning Electron Microscopy / Electron-Beam Lithography

MFM
Magnetic Force Microscopy

Manufactured Devices

[Images of various equipment and simulations related to micro-magnetism nanotechnology and HPC simulations]
Simulation workflows: theoretical and real devices

Simulation work-flow (theoretical device)

- preparation of device geometry
- determination of model necessary to describe physics
- run of the simulation
- post-processing, visualization

Cloud

Scientist manufacture a number of REAL DEVICES

automated determination of device geometry

trying various models for simulated devices

run run run ... of the simulation

post-processing, check if the results coincide with the experiments

YES

NO

Interpret results
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
Typical simulation of the angular dependence of the vortex nucleation field

Typical simulation of the temperature dependence of the vortex nucleation field

Advantages of HPC approach:
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<table>
<thead>
<tr>
<th>Nano-magnetic device (diameter)</th>
<th>Number of simulations</th>
<th>Simulation time</th>
<th>Output data</th>
<th>Machine</th>
</tr>
</thead>
<tbody>
<tr>
<td>70 nm Desired aim</td>
<td>1</td>
<td>20 min</td>
<td>-</td>
<td>PC</td>
</tr>
<tr>
<td>500 nm fabricated in nanotechnology laboratory at the end of 2013</td>
<td>51 smaller sim. (4)</td>
<td>4.5 days</td>
<td>232 MB</td>
<td>PC</td>
</tr>
<tr>
<td></td>
<td>100 bigger sim. (4)</td>
<td>8 hours</td>
<td>3.5 GB</td>
<td>cluster HPC / Grid</td>
</tr>
</tbody>
</table>
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
Nano simulations

Check request input parameters

Check input nano-image

Unique request’s indicator

Simulation statuses

Simulation results and logs

Cancel request at any time

Show simulation results from:

Result history
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.
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.
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 end-users.
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)
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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