Usage of IMP Science Gateway for Molecular Dynamics Simulations of Various Metal-Organic Nanostructures

Yuri Gordienko,
Elena Zasimchuk,
Valentin Tatarenko,

G.V.Kurdyumov Institute for Metal Physics (IMP), National Academy of Sciences of Ukraine, Kyiv, Ukraine
e-mail: gord@imp.kiev.ua

Lyudmila Steblenko,
Olexiy Krit,
Dmytro Kalinichenko

Taras Shevchenko Kyiv National University, Kyiv, Ukraine

Lina Sartinska

Frantsevich Institute for Problems in Materials Science, National Academy of Sciences of Ukraine, Kyiv, Ukraine

ABSTRACT

The general description is given for the "IMP Science Gateway" portal created on the basis WS-PGRADE and gUSE technologies for parallel and distributed computing in various heterogeneous distributed computing infrastructures (DCI) including clusters, service grids, desktop grids, clouds. Several typical use cases are considered for molecular dynamics simulations of complex behavior of various nanostructures (nanoindentation of graphene layers, defect system relaxation in metal nanocrystals, thermal stability of boron nitride nanotubes, etc.). The advantages and drawbacks of the approach are outlined in the context of its practical applications in materials science, physics and chemistry.

Keywords

Distributed computing infrastructure, cluster, service grid, desktop grid, cloud, science gateway, WS-PGRADE, gUSE, molecular dynamics, graphene, boron nitride nanotubes, metal nanocrystals.

1. INTRODUCTION

Currently new materials are of great interest that have nanoscale structure (nanomaterials) and unique properties, for example, metal nanocrystals, nanoscale non-metallic (organic) tubes like carbon nanotubes (CNT), boron nitride nanotubes (BNNT), other organic nanoscale materials (graphene, etc.) and their complicated ensembles. Molecular dynamics (MD) simulations of nanoscale processes are very promising. They are especially perspective in the wide range of physical parameters, because of the possibility for "parameter sweeping" parallelism. Actually, MD simulations can be performed in a brute force manner in the available heterogeneous distributed computing infrastructure (DCI) based, for example, on Desktop Grids (DGs), Service Grids (SGs), clusters, cloud resources. The recent advances in computing algorithms and infrastructures, especially in development of DCIs, allow us to solve these tasks efficiently without expensive scaling-up. DCIs on the basis of the BOINC SZDG, XtremWeb-HEP, OurGrid, and EDGeS [1-5] platforms for high-performance distributed computing are very promising ways to use the heterogeneous computing resources, especially by means of the science gateway technology on the basis of WS-PGRADE platform [6]. The main objective of the work is to demonstrate the capabilities of the proposed specific science gateway (SG) on the basis of WS-PGRADE platform for MD simulations and further data post-processing on the basis of LAMMPS [7] and other packages like R for statistical analysis, MolTemplate for atomic configuration, Debyer for X-ray analysis (https://code.google.com/p/debyer/), etc. Several typical workflows were created for simulation of several physical processes with various demands for the computing resources: tension of metal nanocrystals under different physical conditions, tension of ensemble of metal nanocrystals under the same conditions, manipulations with complex nanostructures like indentation of graphene membranes, thermal stability of BNNT, etc.

2. OVERVIEW OF SCIENCE GATEWAY TECHNOLOGY

The science gateway portal "IMP Science Gateway" (Fig. 1) at the premises of G.V.Kurdyumov Institute for Metal Physics (IMP) National Academy of Sciences of Ukraine, is based on the WS-PGRADE portal and gUSE technologies. The WS-PGRADE portal technology is a web based front end of the gUSE infrastructure. gUSE (grid User Support Environment) is a framework of high-level services to achieve an interoperation between the distributed computing infrastructures (DCIs) and the user communities. WS-PGRADE supports the development and submission of distributed applications executed on the computational resources of the Grid. The resources of the "Grid" (including clusters, service grids, desktop grids, clouds) are connected to the gUSE by a single point back end, the DCI-Bridge [6]. The main idea of WS-PGRADE+gUSE approach is: "The Portal is within the reach of anyone from anywhere" [8]. The development and execution functionalities are separated and fitted to the different expectations of the following two main user groups:

- The common users with limited power and permissions, like ordinary scientists from materials science, physics, chemistry, etc. (referenced as "end users") need only a restricted manipulation possibility. They get the simulation applications in the ready state, to trim it and submit it with a minimal effort.
- The full power users, like designers of thientific processes and related simulation workflows (referenced as "developers"), need to build and to fit the application to be as comfortable as possible for common users.

"IMP Science Gate" portal (Fig. 1) provides a scientific workflow management for both application developers and

end users, and supports various DCIs including clusters, service grids, desktop grids and clouds.

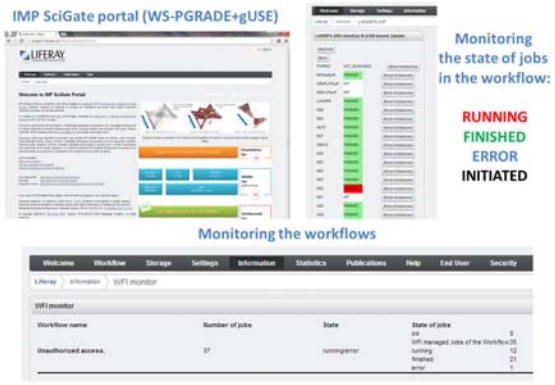


Fig. 1. The graphical user interface, monitoring abilities and flags for state of jobs at "IMP Science Gate" portal.

"IMP Science Gate" portal provides a simple way of creating, submitting, observing and retrieving of one or a multi job workflow (Fig. 2).

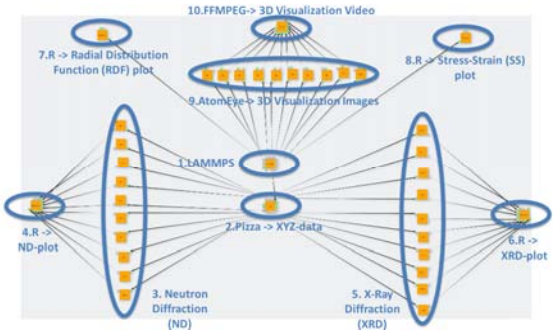


Fig. 2. The scheme of the workflow created by means of WS-PGRADE workflow management technology for MD simulations.

The typical process of the complex workflow creation and management can be demonstrated by the following example of tension of metal nanocrystals under different physical conditions with the following steps:

- signing in "IMP Science Gate" portal (top left part in Fig. 1);
- create a graph scheme for the basic blocks of the workflow (yellow bricks with small squares in Fig. 2);
- determine (create and name) a workflow from the graph;
- configure the workflow (links between yellow bricks in Fig. 2);
- start execution of the workflow;
- monitor the current status of execution (top right and bottom parts of Fig. 1);
- check the MD simulation results obtained by LAMMPS package (tables in the red rectangles in the center of Fig. 3);
- check the MD simulations results converted by Pizza script package for post-processing (table in the red rectangle in the bottom of Fig. 3);
- check the intermediate post-processed visualizations of atomic positions obtained by AtomEye package (images in the top part of Fig. 3);
- check the intermediate post-processed results of X-ray analysis (of the MD simulations results) obtained by Debyer package (tables in the blue rectangles in the bottom part of Fig. 3);
- get the final post-processed results (of the MD simulations results) after X-ray analysis, radial distribution function (RDF) analysis, and stress-strain (SS) analysis obtained by R package (plots in the green rectangles at the left and right sides of Fig. 3);
- get the final post-processed video of visualizations of atomic positions obtained by FFMPEG package (video in the violet rectangle in the top part of Fig. 3).

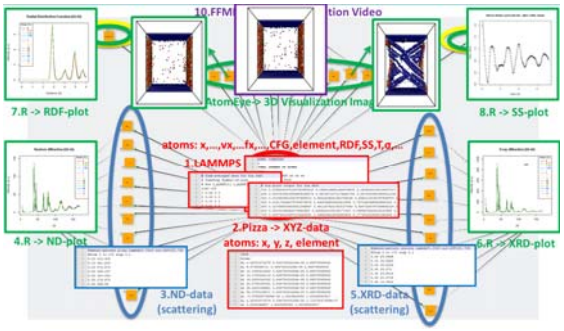


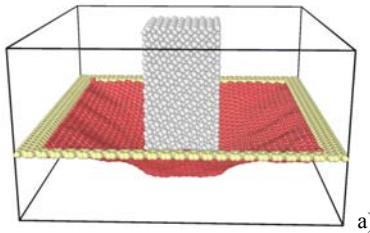
Fig. 3. The typical workflow with the actual MD simulation results, intermediate post-processed data, and final results (plots, visualization images and video).

3. TYPICAL USE CASES

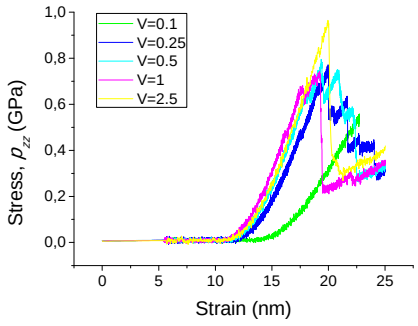
The several use cases are presented below where different workflows were designed by WS-PGRADE workflow manager and used for computations in the DCI by means of gUSE technology.

3.1. Nanoindentation of Graphene Layers

Molecular dynamics computer simulation of nanoindentation was performed for monolayer graphene membrane in an atomic force microscope (Fig. 4a).



a)



b)

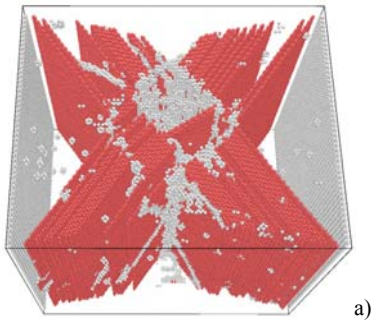
Fig. 4. Nanoindentation of the graphene membrane (red color — mobile graphene atoms, yellow color — fixed graphene atoms, gray color – nanoindentor atoms) (a) for different speeds (A/pm) of the nanoindentor (b).

The elastic properties and tensile strength were investigated for different physical conditions (speed nanoindentor, radius head nanoindentor, material nanoindentor, the free surface area of the grapheme membrane), and methodological parameters (type of building is idealized and real solid nanoindentor). The distributed

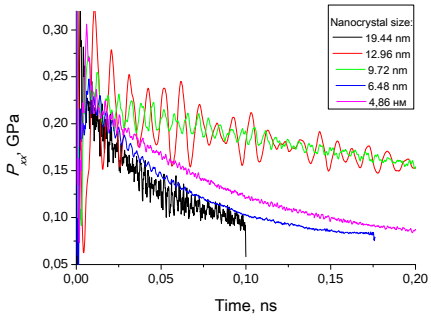
computing grid-infrastructure was used on the basis of the 'IMP Science Gateway' portal in IMP NASU (http://scigate.imp.kiev.ua) using WS-PGRADE and gUSE technologies [5, 6]. It is shown that the graphene membrane deforms and collapses within a wide range of strain values and applied forces (within the range 1.5-3 mN); internal tensile stresses along the axis – 0.6-0.8 GPa (Fig. 4b). For a defect-free graphene under uniaxial tension, this corresponds to the tensile strength of 80-150 GPa and Young's modulus of 0.8-1.2 TPa. These results confirm and significantly extend the known experimental data of nanoindentation in a narrow range of parameters [9] and the previous results of computer simulation of uniaxial tension of defect-free graphene [10]. They exhibit a nonlinear dependence of the elastic and strength properties of an ideal defect-free graphene on the physical conditions and guidelines of the experimental parameters. It is shown that atomically perfect (defect-free) nanomaterials (for example, graphene), depending on the experimental conditions may have a complex mechanical behavior beyond the linear regime of deformation.

3.2. Defect System Relaxation in Metal Nanocrystals

This use case is related to the molecular dynamics simulation of relaxation behavior of nanocrystals after the uniaxial tension (Fig. 5a).



a)



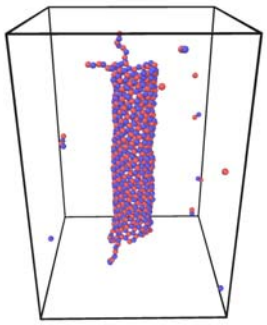
b)

Fig. 5. The evolution of the defect substructure in Al nanocrystal (after 15 ps, defects only are shown: gray color — point defects, red color — stacking faults) (a), and oscillation of the internal stress P_{xx} for different nanocrystal sizes (b).

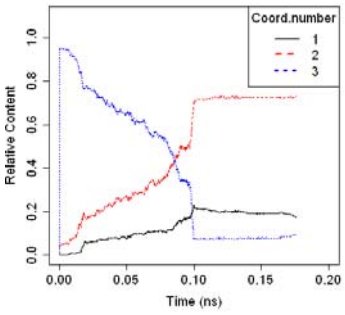
The periodic time dependence of internal stress (Fig. 5b) and the distribution of defects in the crystal structure was observed for different relaxing objects (single crystals of Al, Cu, and Si), physical conditions (tensile rate, size and orientation of the nanocrystals) and methodological parameters (potential type, boundary conditions, and others). The oscillatory nature of the relaxation of internal stresses is associated with the periodic rearrangement of the metastable defect substructure (point defects, dislocations, stacking faults and their intersections) (Fig. 5a). The evolution of the defect substructure is accompanied by a transition from the exponential decay for small nanocrystals (Fig. 5b) to periodic oscillations with the sharp increase of the oscillation period with increase of the nanocrystal sizes (Fig. 5c), due to the involvement of defect substructures in a wider range scales in the process of relaxation, interaction and self-organization [11]. These results confirm and significantly extend the known experimental data on the oscillatory nature of the relaxation processes and mechanisms of evolution of the initial defect substructure of crystals after ultrasound and magnetic effects [12, 13].

3.3. Thermal Stability of Boron Nitride Nanotubes

Boron nitride nanotubes (NTNB) possess exceptional physical properties, which are a prerequisite for their wide practical applications in the future.



a)



b)

Fig. 6. The collapse of NTNB (after 0.1 ns, nitrogen atoms are shown by red and boron atoms — by blue color) (a), the dynamics of the collapse for (6,6) NTNB (length of 5 nm) characterized by changes in portions of atoms with different coordination numbers (b).

It is known that NTNB, unlike the carbon nanotubes (CNTs) has a higher thermal stability [14]. In this use case, MD simulation is applied for investigation of thermal stability of NTNB with different chirality, size and perfection of structure (Fig. 1a). The dynamics (Fig. 1b) and temperature dependence of the NTNB collapse was observed for NTNBs with various chiralities, sizes and perfection of structure, as well as the simulation parameters (type of potential, boundary conditions, thermal conditions, etc.). It is shown that the NTNB collapse proceeds by separation of atoms from NTNB open caps. Wherein the NTNB collapse temperature (T_c) for the ideal infinitely long (under the periodic boundary conditions) NTNBs without open caps is considerably higher than T_c for the real (finite size) NTNBs with open caps. It is shown that the presence of defects leads to decrease of T_c and reduces thermal stability of NTNBs. Dynamics of the NTNB collapse depends on their chirality (zigzag, armchair, etc.), but the mechanism of their collapse

(by separation of atoms from the open caps) remains unchanged. These results confirm and significantly extend the known experimental data on the thermal stability of NTNBs [14, 15].

4. CONCLUSIONS

The general purpose and application specific workflows for computer simulations of complex natural processes in materials science, physics, and chemistry can be easily designed and used in practice on the basis of the available "workflow management" technologies. One of the ways to prepare and use scientific workflows was applied and demonstrated at "IMP Science Gateway" portal created on the basis of: WS-PGRADE technology for workflow management and gUSE technology for parallel and distributed computing in various heterogeneous distributed computing infrastructures (DCI) including clusters, service grids, desktop grids, clouds. Several typical scientific applications were considered as use cases of its usage. It is shown that the physical characteristics evaluated on the basis of MD simulations in the proposed SSG on the basis of LAMMPS are in satisfactory agreement with the experimental data and allowed to discover the new aspects of operation and manipulation of nanomaterials. Porting MD-applications to heterogeneous DCI by means of "scientific gateway" ideology is easy and efficient, if WS-PGRADE platform is used, and parameter decomposition and sweeping parallelism are possible. As a result, molecular dynamics simulations of complex behavior of various nanostructures (nanoindentation of graphene layers, defect system relaxation in metal nanocrystals, thermal stability of boron nitride nanotubes, etc.) can be effectively carried out in the heterogeneous DCI with a quite short learning curve.

The obvious advantages are as follows: smooth access to heterogeneous DCI and software, division of user roles (admin: portal activities, power user: principal scientist, common user: scientists, students), possibility to make more complex workflows (with additional modules, ad hoc changes, etc.), low level of added complexities (no changes in binaries, no changes in input/output formats, all changes by scripts & command line arguments**),** short learning curve for usual scientists.

Some non-critical drawbacks of the approach include: non-standard file naming convention (alphanumeric only), which can cause problems with legacy code with special symbols, tacit "stdout" and "stderr" information style for some errors in WS-PGRADE.

The "scientific gateway" ideology — using workflow manager (like WS-PGRADE) and resource manager (like gUSE) at the premises of the science portal (like "IMP Science Gateway" portal) — is very efficient in the context of its practical applications in materials science, physics and chemistry.

5. ACKNOWLEDGEMENT

The work presented here was partially funded by EU FP7 SCI-BUS (SCIentific gateway Based User Support) project, No. RI-283481, and partially supported in the framework of the research theme "Introduction and Use of Grid Technology in Scientific Research of IMP NASU" under the State Targeted Scientific and Technical Program to Implement Grid Technology in 2009-2013.

REFERENCES

[1] F. Cappello, S. Djilali, G. Fedak, T. Herault, F. Magniette, V. Neri, O. Lodygensky, "Computing on large-scale distributed systems: Xtremweb architecture, programming models, security, tests and convergence with grid", *Future Generation Computer Systems*, **21**(3), pp.417-437, 2005.

[2] W. Cirne, F. Brasileiro, N. Andrade, L. Costa, A. Andrade, R. Novaes, M. Mowbray, "Labs of the world, unite!!!", *Journal of Grid Computing*, **4**(3), pp.225-246, 2006.

[3] P. Kacsuk, J. Kovacs, Z. Farkas, A. Marosi, G. Gombas, Z. Balaton, "SZTAKI desktop grid (szdg): a flexible and scalable desktop grid system", *Journal of Grid Computing*, **7**(4), pp.439-461, 2009.

[4] Yu.G. Gordienko, O. Baskova, O. Gatsenko, "Enabling High-Performance Distributed Computing to e-Science by Integration of 4th Generation Language Environments with Desktop Grid Architecture and Convergence with Global Computing Grid", *Proceedings of Cracow Grid Workshop'10*, Cracow, Poland, pp. 234-243, 2011.

[5] O. Gatsenko, L. Bekenev, E. Pavlov, Yu.G. Gordienko, "From Quantity to Quality: Massive Molecular Dynamics Simulation of Nanostructures Under Plastic Deformation in Desktop and Service Grid Distributed Computing Infrastructure", *Computer Science*, **14**, pp.27-44, 2013.

[6] P. Kacsuk, "P-grade portal family for grid infrastructures", *Concurrency and Computation: Practice and Experience Journal*, **23**:3, pp.235-245, 2011.

[7] S. Plimpton, "Fast parallel algorithms for short-range molecular dynamics", *Journal of Computational Physics*, **117**(1), pp.1–19, 1995

[8] WS-PGRADE Portal User Manual, version 3.4.3, 2012 (http://sourceforge.net/projects/guse/).

[9] C. Lee, X. Wei, J.W. Kysar, J. Hone, "Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene", *Science*, **321**, pp.385-388, 2008.

[10] A. Gatsenko, A. Baskova, B. Bandalak, V. Tatarenko, Yu. Gordienko, "Application of Desktop Grid Technology in Material Science", *5th Int. Conf. "Distributed Computing and Grid-technologies in Science and Education" GRID'2012* (Dubna, Russia) pp.123-129, 2012.

[11] Yu. Gordienko, "Molecular Dynamics Simulation of Defect Substructure Evolution and Mechanisms of Plastic Deformation in Aluminium Nanocrystals", *Metallofizika i Noveishie Tekhnologii*, **33**, No.9, pp.1217-1247, 2011 (in Ukrainian).

[12] L.P. Steblenko, O.M. Krit, A.N. Kuryliuk, J.L. Kobzar, S.N. Naumenko, "Features of the magnetomechanical effect in silicon crystals due to the influence of the gradient of the magnetic field", *Metallofizika i Noveishie Tekhnologii*, **32**, No.5, pp.697-703, 2010 (in Russian).

[13] V.A. Makara, O.O. Korotchenkov, D.V. Kalinichenko, A.B. Nadtochiy, L.P. Steblenko, "Change of the elastic-stress state of the subsurface layer of silicon under the influence of cavitation and magnetic fields", *Metallofizika i Noveishie Tekhnologii*, **33**, No.12, pp.1627-1635, 2011 (in Ukrainian).

[14] C. Zhi, Y. Bando, C.Tang, D. Golberg, "Boron Nitride Nanotubes", *Materials Science and Engineering R*, **70**, pp.92-111 (2010).

[15] L.L. Sartinska, Catalyst-Free Synthesis of Nanotubes and Whiskers in an Optical Furnace and a Gaseous Model for Their Formation and Growth, *Acta Materialia*, **59**, No.11, pp.4395-4403 (2011).