Development of the Nanoconfinement Science Gateway

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***Abstract*—The nanoconfinement science gateway empowers users to simulate ions confined between material surfaces that are nanometers apart, and extract the associated ionic structure. The gateway facilitates investigations for a wide array of ionic and environmental parameters using standard molecular dynamics (MD) method for unpolarizable surfaces and an advanced MD technique for polarizable surfaces (dielectric interfaces). In this paper, we discuss the goals of the nanoconfinement science gateway and elucidate the plans for building it. We also discuss details of the current implementation, and provide a timeline for the future tasks.**

***Index Terms*—Science Gateways, Gateways 2017, Molecular Dynamics, Computational Nanotechnology, Ionic Structure, Nanoconfinement, Apache Airavata**

I. Introduction

Self-assembly of charged nanoparticles or biomacromolecules is governed to a large extent by the distribution of ions in confinement created by the assembling entities. It is therefore important to obtain an accurate knowledge of the structural information of ions trapped between dielectric interfaces representing the nanoparticle surfaces (Fig. 1). This ionic structure is determined by the competition between entropic and electrostatic interactions. In the case of nanoparticles exhibiting a different dielectric response compared to the surrounding environment, additional complications arise due to the presence of polarized charge at the interfaces. For a system with no dielectric mismatch across the interface, standard MD techniques suffice to give an accurate estimate for the ionic distribution. Advanced methods are needed to simulate ions near interfaces with dielectric mismatch. Taking cues from nature, we developed a methodology, the Car-Parrinello molecular dynamics (CPMD) for charged particles simulation, that enables the simulation of ions in conjunction with the update of the medium's dielectric response [1]. This on-the-fly CPMD method was employed successfully to simulate ions confined between two planar interfaces for a variety of ionic and environmental conditions [2].

Standard MD and CPMD simulations of ions in nanoconfinement are computationally intensive. A typical MD simulation of a system with 500 ions for 1 million steps (1 nanosecond of real-time dynamics) takes about 12 hours of simulation time on a single processor. CPMD on an average is approximately 5 times slower. Therefore, these methods employ parallel computing techniques to remain efficient and produce the necessary statistics on the output data. Currently, simulations are performed on multiple-core nodes (ranging from 8 to 32 processors) with OpenMP shared memory multiprocessing. This accelerates simulations by a factor of 10, thus enabling long simulations to generate research-level data within realistic timescales of hours to days. A typical mechanism for engaging community-at-large to disseminate such computational research is to make the code available and provide instructions to build and execute the code. But the learning curve in adopting and enhancing third party codes is generally steep and often leads to duplication of efforts [3]. Moreover, the intellectual thinking behind applying novel techniques like CPMD is hard to reproduce just from literature reading. Science Gateways alleviate such concerns by providing researchers and educators a user-friendly, web-based access to execute these simulation codes on computational resources in a seamless fashion. NanoHUB [4] is a popular example of the strengths of these computational platforms to reach a broad range of students, educators, and

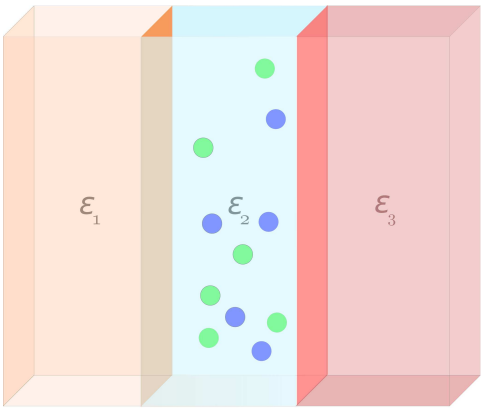


Fig. 1. Sketch of ions represented by blue and green circles confined by nanoparticle surfaces (reproduced from [1]). Surfaces are approximated as planar interfaces due to the size difference between ions and the assembling nanoparticles.

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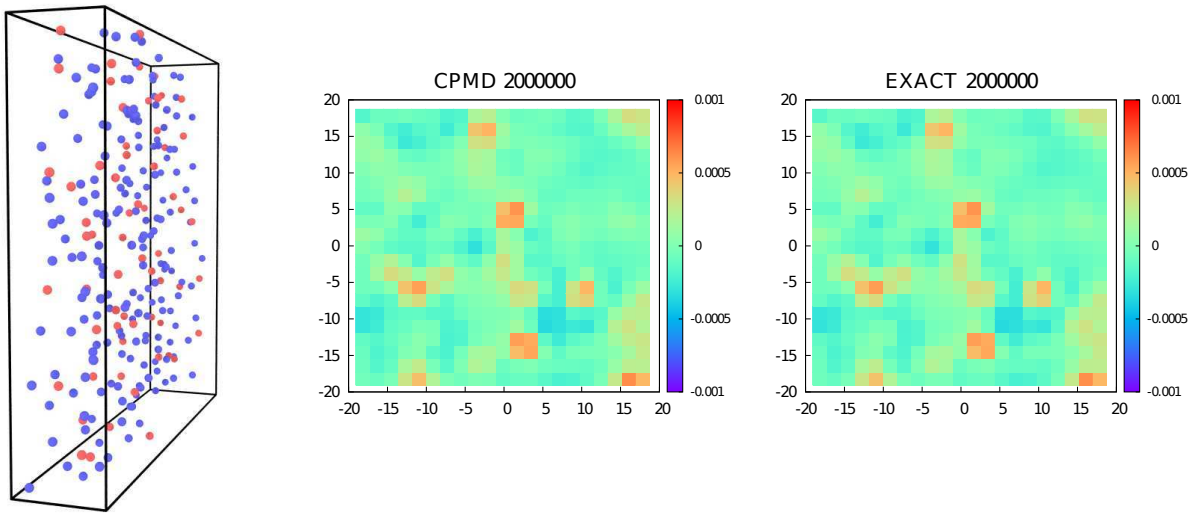


Fig. 2. A snapshot showing induced density map produced during a CPMD simulation (center) on one of the interfaces as a result of the instantaneous configuration of ions confined between the two interfaces (left). The induced charges in CPMD match with the exact values (right) signaling the success of the on-the-fly simulation.

researchers interested in nanoscale science and engineering [5]. Simulations may run on a range of resources including campus clusters and computational clouds. In addition to being excellent resource for learning the simulation methods and associated science, gateways accelerate the use of simulations using High Performance Computing (HPC) for testing new concepts, corroborating experiments and prototyping new designs.

II. Nanoconfinement Science Gateway

The goal of nanoconfinement science gateway [6] is to provide a web-based platform with sophisticated and user-friendly computing environment to engage with the nanoconfinement community by empowering them to launch and monitor simulations. The gateway integrates HPC resources at Indiana University and the NSF-Funded XSEDE resources [7]. Abstracting the complexities of using advanced cyberinfrastructure simplify the simulation experience of end users– the users do not need to learn the implementation details of HPC to understand and execute MD/CPMD methods.

The nanoconfinement gateway enables the users to explore the effects of nanoscale confinement on the distribution of ions. Simulations performed using this gateway provide the distributions of ions confined between macromolecular/nanoparticle interfaces that are nanometers apart. A variety of ionic and environmental attributes are available to investigate including electrolyte concentration, environmental dielectric profile, ion valency, and separation between the nanoparticle surfaces. Fig. 2 provides a snapshot of a CPMD simulation while it is producing data. Fig. 3 is an example simulation result provided for illustration purposes.

A general-purpose gateway enables the execution of the command line simulation tools from a web-based interface.

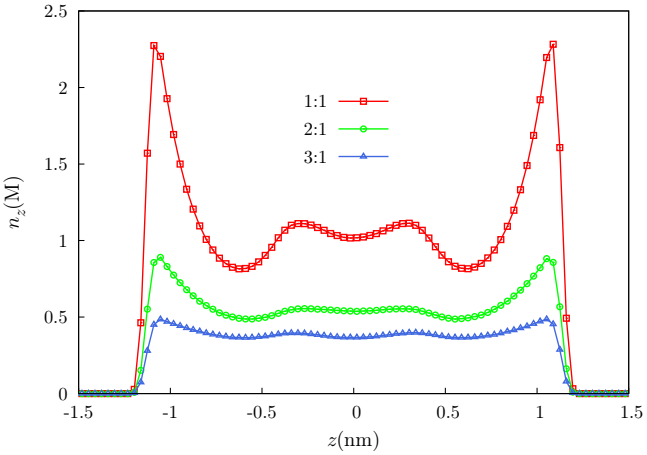


Fig. 3. Researcher's view of a sample result on the gateway using the MD simulation: distributions of ions described by n_z (in units of Molars) as a function of z (nm). Ions are confined by two surfaces at -1.5 nm and 1.5 nm. Different symbols denote ions of valencies 1, 2, and 3. Figure reproduced from [1].

The gateway also allows the users to track multiple simulations with easily accessible mechanisms that enable the comparison of different simulation results. Beyond these advantages, the goal of our gateway is to build application-specific input generation, output visualization, and data production that enables us to address the needs of the targeted nanoscience community interested in the behavior of ions near nanoparticle surfaces and related material phenomena. We also expect the gateway to enhance the performance of our simulation tools through feedback from users on computing-related and nanoscale-application-specific issues and results. This will

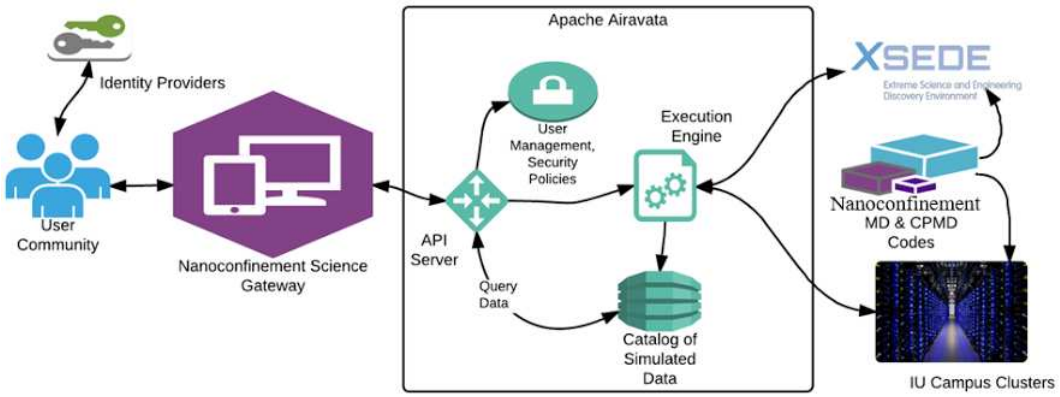


Fig. 4. Conceptual architecture diagram of the nanoconfinement science gateway.

contribute towards developing user-tested, user-informed, and user-friendly tools for online portals such as nanoHUB.

III. Implementation Details

The nanoconfinement gateway is built over Apache Airavata [8] Science Gateway framework. Building over an existing framework allows for rapid prototyping and keeps the focus on the science without getting distracted into cyberinfrastructure (HPC) details. Airavata is an open source software framework that enables gateway providers to compose, manage, execute, and monitor large scale applications and workflows on distributed computing resources such as local clusters, supercomputers, computational grids, and computing clouds. The nanoconfinement gateway user interfaces are built over the Apache Airavata's reference PHP based gateway which consumes Airavata's programming language-independent API.

Fig. 4 provides a high level conceptual summary of nanoconfinement science gateway powered by Apache Airavata. Users (left) authenticate to a gateway, which in turn interacts with Apache Airavata's API server. The API server routes requests from users to the appropriate internal components, which provide access to data and metadata, execute nanoconfinement simulations on remote resources, and move data between resources.

The gateway's front end is currently based on the Airavata PHP Gateway built over Laravel framework. Building over a widely used framework such as Airavata has alleviated basic issues like cross-browser compatibility. This enables us to focus on core gateway functionality while outsourcing browser-specific challenges to a large Airavata community dedicated to resolution of these issues. The input parameters are classified into physical parameters specific to the material system and algorithm/computing parameters specific to MD/CPMD method and computational resources. We have simplified the number and description of the physical input parameters, e.g. confinement width, ion valency, salt concentration (Figure 5). The user also specifies the simulation job parameters (simulation timestep, wall time limit, etc.). The output of this simulation are the datafiles that contain the ionic distributions and movies of ion dynamics in confinement. These data files

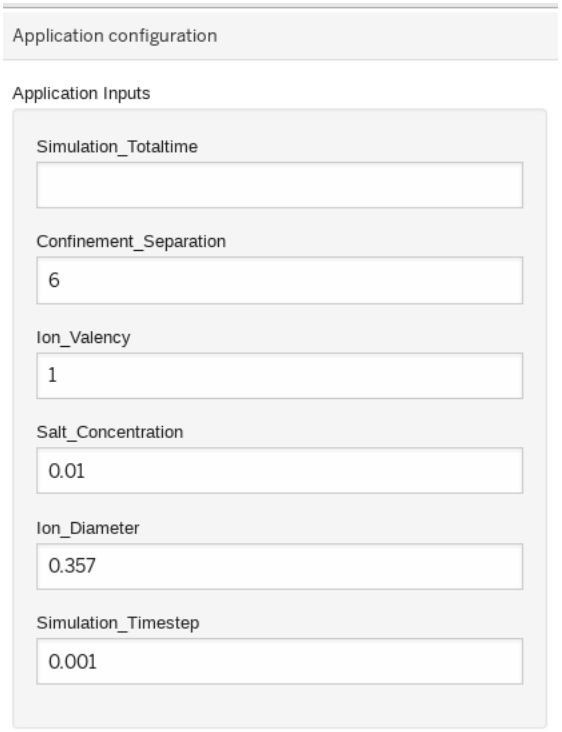


Fig. 5. End-user view of the input parameters for the nanoconfinement science gateway.

are text files that can be plotted using visualization software such as Gnuplot for simple 2D plots and Ovito for simulation movies. Our future plans include enabling seamless output visualization through this gateway.

The Apache Airavata community is moving from the laravel framework into python based Django framework to align with application specific customizations and for seamless integration with Jupyter Ipython Notebooks. These improvements align well with the nanoconfinement gateway road map. We will migrate over the current gateway into Django framework and will further extend it to incorporate the input specification and post processing tools.

The nanoconfinement simulation codes are ported and de-

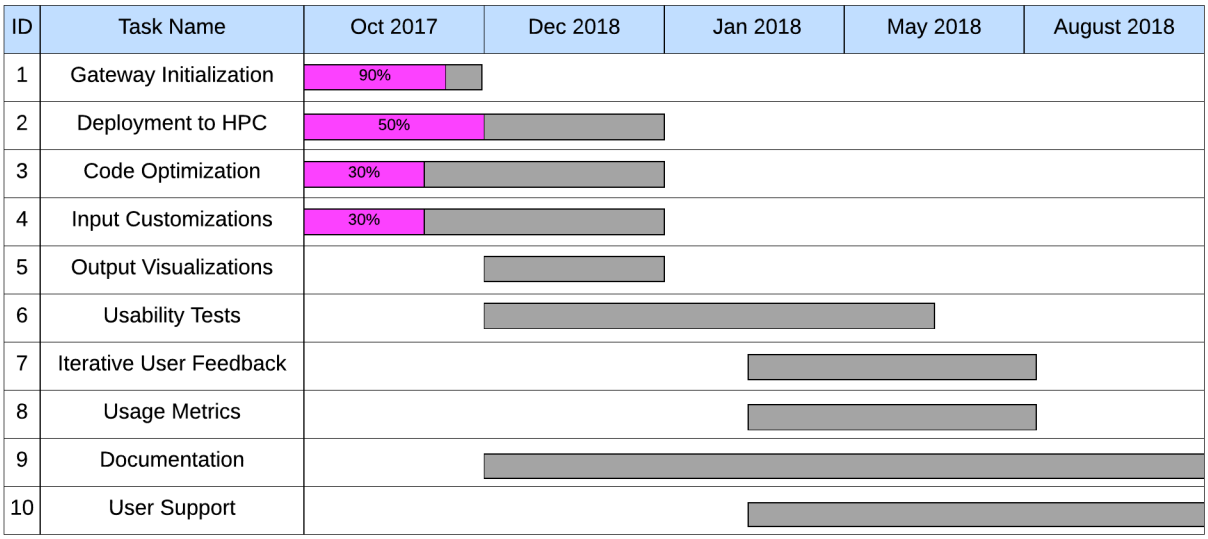


Fig. 6. Development tasks and timeline of nanoconfinement science gateway.

ployed on XSEDE computational resources. We have registered the descriptions of various input and output parameters with the Apache Airavata system. These descriptions are used by the Airavata components to generate the artifacts required to expose the application as a service. Any gateway administrator can then access these wrapped application services and facilitate user executions on target compute resources. The resulting abstractions reduce human inefficiencies by providing a uniform interface for the scientist and hiding unnecessary complexities.

The current versions of the code are optimized for CPUs with OpenMP multithreading. The CPU cycles for the gateway users are provided through XSEDE [7] startup allocation and Indiana University's BigRed II cluster. The simulations have successfully executed on both the BigRed II cluster and Comet resources available through XSEDE. As we onboard users, we would like to reduce the execution wall time. We will first profile the code with Allinea MAP profiler [9]. Based on profiling and benchmarking, we will subsequently optimize the simulation code with multi-node MPI-based parallelization and explore performance gains by GPU accelerations or XSEDE Stampede 2's Many Integrated Core Architecture (Knights Landing).

Current codes with openMP parallelization for 16 threads lead to a run time of 1 hour for a mid-size candidate system of 500 ions simulated for 1 million time steps. We plan to make the method more efficient by using MPI. Our initial testing has shown that using MPI can lead to a speed up of 3-5 depending on the system size. Improving the efficiency of the simulation method using MPI will be a key computing challenge moving forward. The source codes for the MD version of the ions in nanoconfinement simulation are hosted on GitHub; we plan to release CPMD code in immediate future. Through this, we expect to nucleate a community of researchers including students and faculty to use our gateway. We will provide user support related to the simulation codes and the underlying scientific questions. We will seek help from infrastructure providers (e.g. XSEDE, Indiana University research computing team) for issues related to cyberinfrastructure (e.g. file systems, job failures, network issues).

IV. Outlook

In this short paper, we introduce the nanoconfinement science gateway and discuss its goals and implementation details. At this early stage, we do not have the usage metrics for the gateway. However, as noted in the previous section, we have a detailed implementation plan. We provide the current development status of the gateway and a timeline for key tasks involved in its future development (Fig. 6). The key tasks center around input/output customizations, code optimization, HPC benchmarking, and user-testing metrics.

We will employ different mechanisms to evaluate this project including the number of users of the gateway as well as the number of contributors and issues on GitHub. The gateway will be used in teaching of modeling and simulation courses at Indiana University. Student feedback will be employed to enhance the user-friendliness and performance of the gateway. The gateway will enable the development of user-tested and user-friendly computational tools for deployment in online portals such as nanoHUB [5].

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