Dynamical Features of Complex Systems: A Molecular Simulation Study

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Overview

- Introduction
- Benchmarking and Analyzes
- Scientific Results
- Publications & Collaborations

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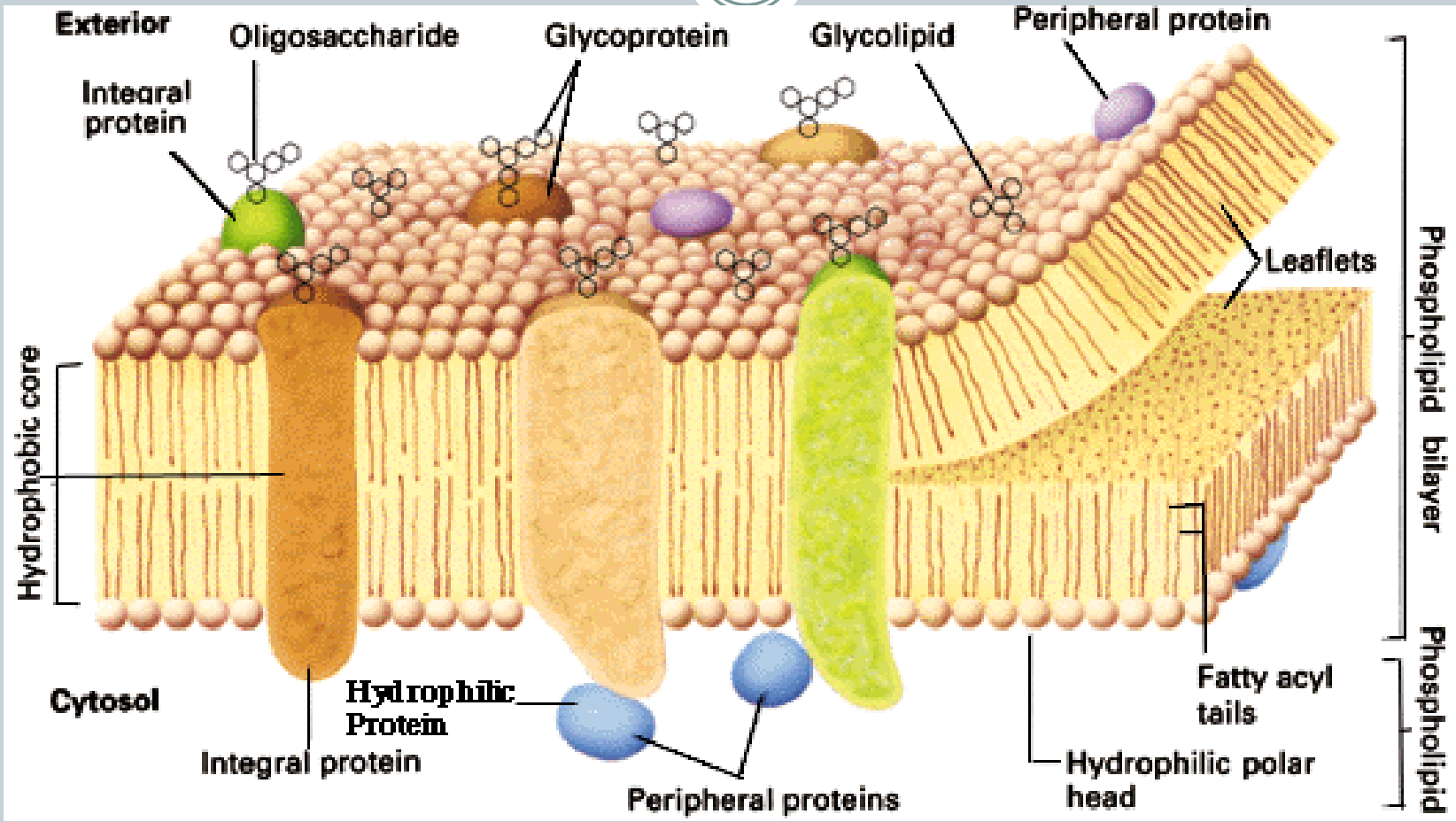
Introduction

- **Interest in modeling of complex systems using molecular dynamics (MD) simulation has increased dramatically, and the parallel implementation makes it possible the fully understanding interesting phenomena and events, which occurs on long timescale and impossible to get from real experiments.**
  - *M. E. Tuckerman, D. A. Yarne, S. O. Samuelson, A. L. Hughes and G. J. Martyna, "Exploiting Multiple Levels of Parallelism in Molecular Dynamics Based Calculations via Modern Techniques and Software Paradigms on Dis-tributed Memory Computers," Computer Physics Com-munications, Vol. 128, No. 1-2, 2000, pp. 333-376. doi:10.1016/S0010-4655(00)00077-1*
  - *M. E. Tuckerman and G. J. Martyna, "Understanding Modern Molecular Dynamics Methods: Techniques and Applications," The Journal of Physical Chemistry, Vol. 104, No. 2, 2000, pp. 159-178. doi:10.1021/jp992433y*
- **During last decade the usage of parallel computational resources and supercomputers leads to the significant progress in bio-systems modeling. Increasing in system dimensions and simulation time became possible with the linear in-crease of computational resources of distributed computing infrastructures.**
  - *W. Dubitzky, A. Schuster, P. Sloot, M. Schroeder and M. Romberg, "Distributed, High-Performance and Grid Computing in Computational Biology," Lecture Notes in Bioinformatics, Vol. 4360, 2007, p. 192.*

Introduction: Cell Model Membranes



Lipid bilayers have long been investigated for many years as a structural model for biological membranes.

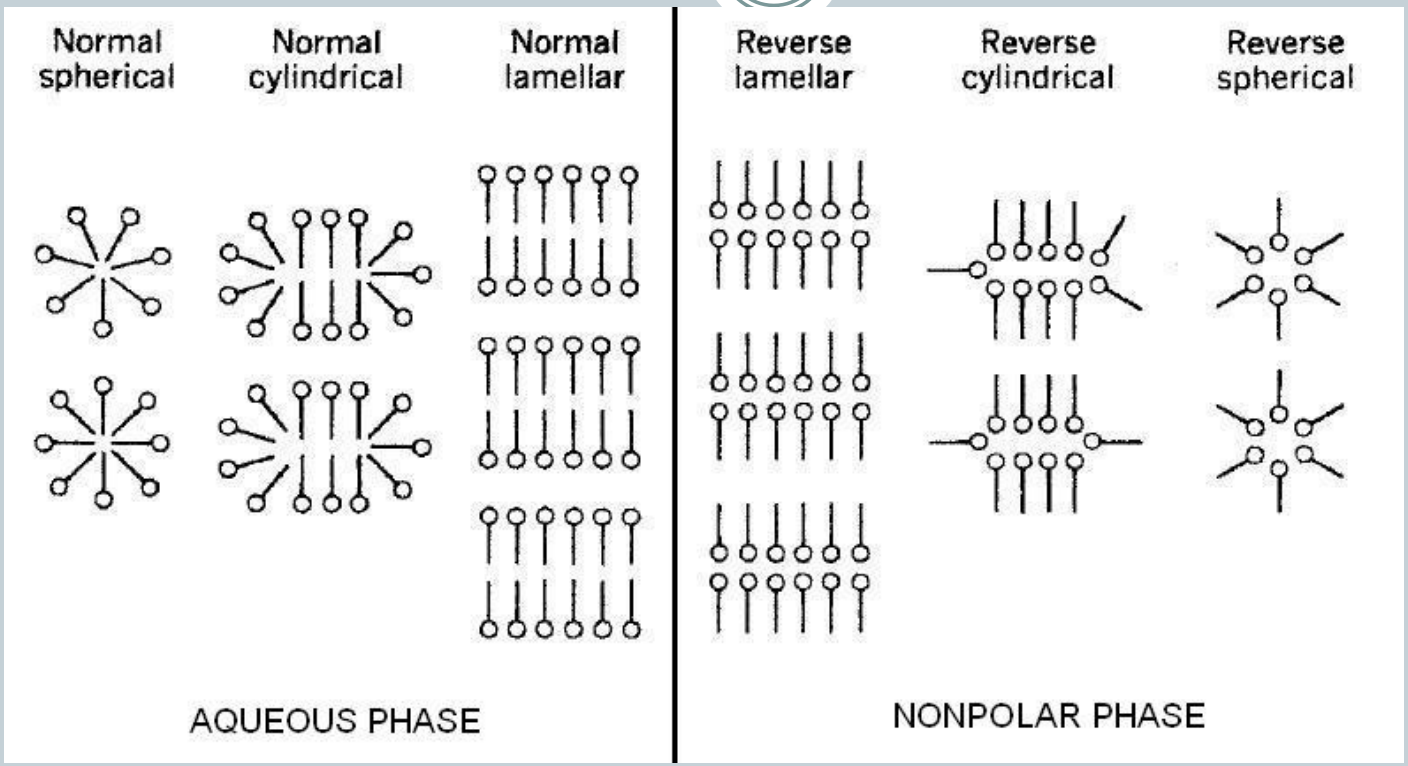
Introduction: Surfactants

- **Surfactants can be considered as a simple model for biological membranes.**

- **Surfactants are usually organic compounds that are amphiphilic, meaning they contain both hydrophobic groups "tails" and hydrophilic groups "heads“ and are classified into four groups; anionic, cationic, non-ionic, and zwitterionic (dual charge).**

- ***in everyday life, soaps, shampoos, etc…surfactants – is blend of “surface acting agents”***

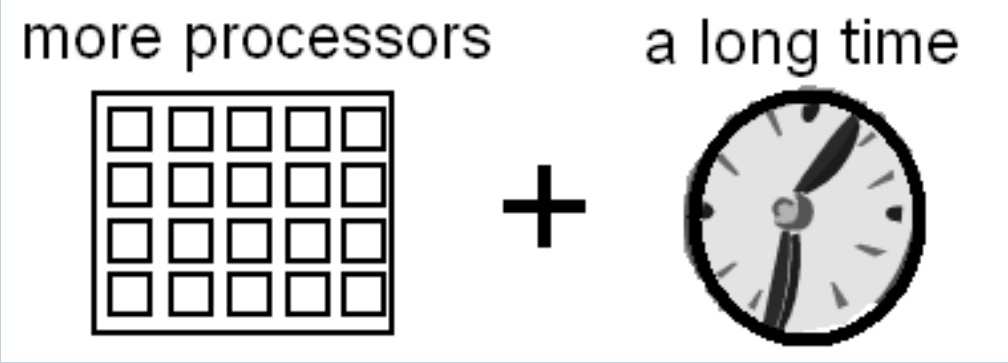
Introduction: Surfactants self-organization



- Surfactants self-organize various structures ranging from micelles to lamella depending on their molecular structure, temperature and concentration. The critical micelle concentration (CMC) is defined as the concentration of surfactants above which micelles and other structures form.

Introduction: HPC Needs

- In order to mimic the real membrane (erythrocyte, *E.coli*, etc) or the complex system, we should add the number of atoms (adding some components, e.g. cholesterol, lipids, proteins) – i.e. increase the number of processors means an increase of the system size in order to get more realistic model.
- More Time ! - will make it possible to describe of many interesting phenomena (like phase transitions, *trans-gauche* isomerizations, folding effects, rotations, flip-flop, etc), which occur on the tens of nanosecond time scale.



Introduction: HPC Needs

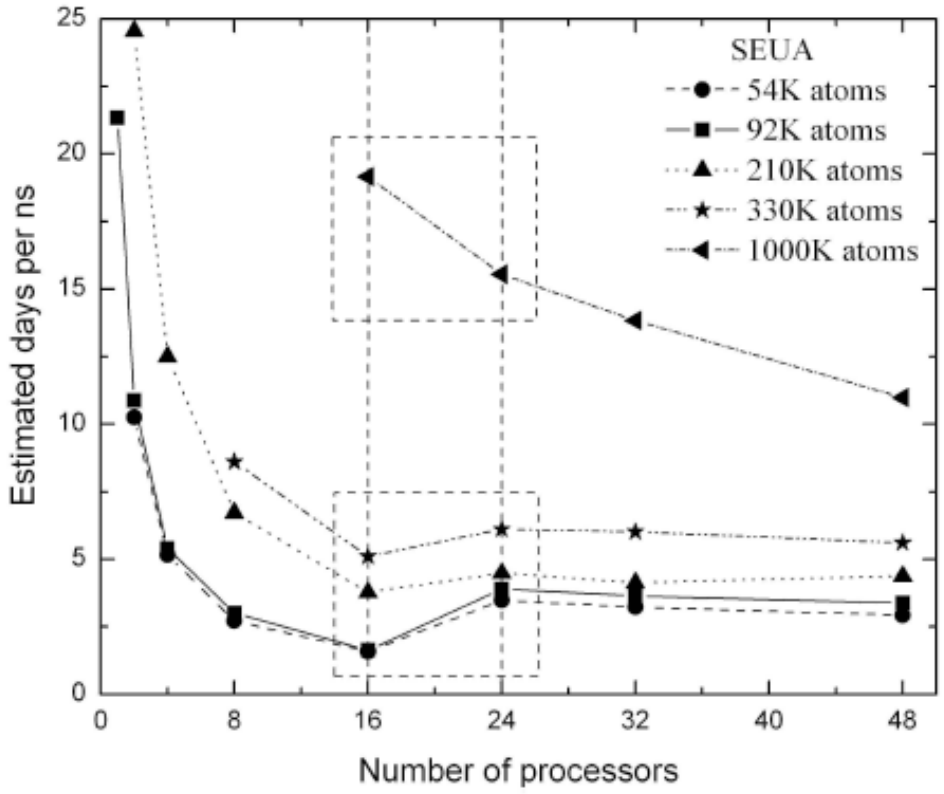


Figure 3. The NAMD performance and the estimation of days/ accordingly for 1000K, 330K, 210K 92K and 54K atoms.

Introduction: Molecular Dynamics Study of Complex Systems

Parallel molecular dynamics simulation of Sodium dodecylsulfate (SDS) – polymer systems (inverse micellar and lamellar) depending on the temperature and the polymer concentration. First, parallel MD simulation (about 100-200ns) of SDS/decanol/water bilayer (about 300.000 atoms) system with PDADMAC has been done, varying the polymer concentration from 2.6% to 10%, as well as the temperature of the system. SDS/water/oil inverse micellar system (up to 500.000 atoms) in presence of polyampholytes by varying the system pH and the hydrophobicity of the embedded polyampholyte has been created and simulated.

- **Problems Solved**

  The investigations will help us understand the mechanism of interaction of anionic SDS and cationic/anionic/noncharged polymer and to receive important information on the dynamical and structural features of mentioned systems.

- **Impact**

  The results of the proposed investigations will make an important contribution to basic research in Colloid Physics.

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Benchmarking and Analyzing: HPC Implementation

- **Computational Recourses:** Bulgarian BlueGene/P supercomputer (2048).
  Armenian National Grid Infrastructure - Armcluster (128 procs, Myrinet), and AM-05-YSU Grid site (128 cores, Infiniband)

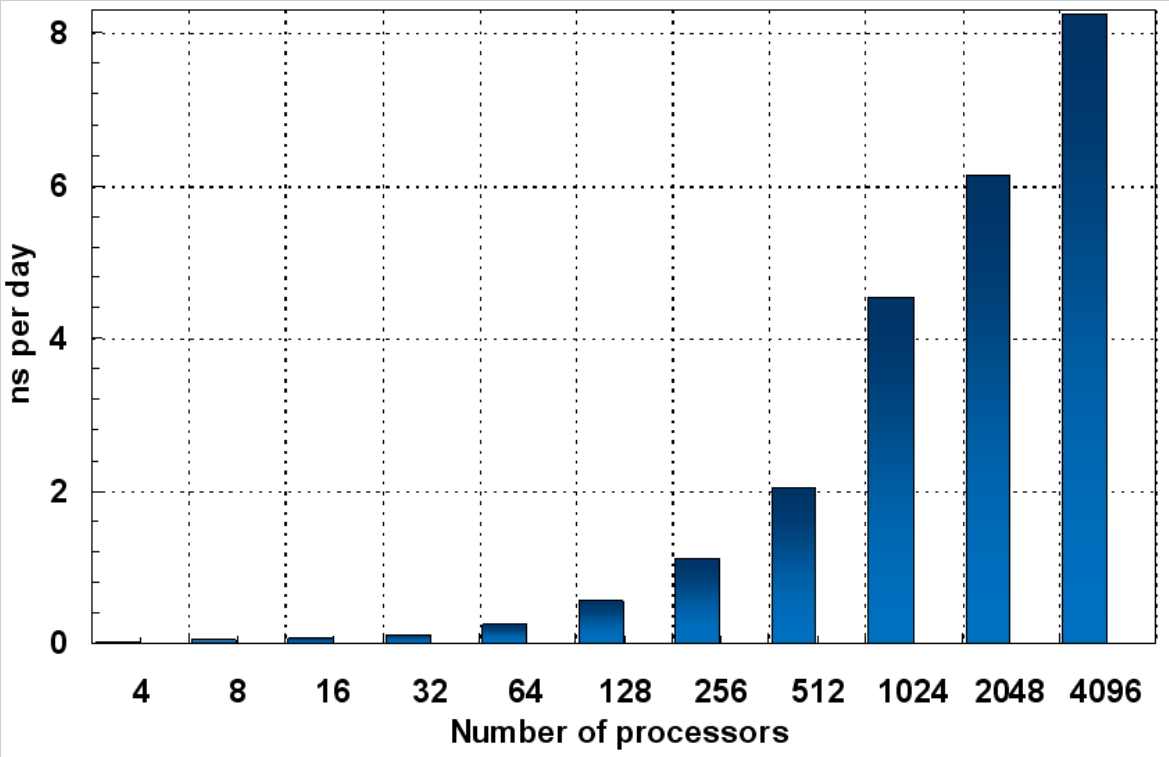
- **Using Software Packages:** The latest versions of GROMACS and NAMD software packages have been successfully installed on the Armcluster and the Grid sites (AM-03-YSU, AM-05-YSU) located in the Yerevan State University. The packages are available on the Bulgarian BlueGene supercomputer.

- **Scalability:** The application is based on NAMD and GROMACS packages, which are parallel molecular dynamics scalable codes designed for high-performance simulation of large biomolecular systems.

- **Benchmarking:** The environments of the Armenian national grid infrastructure and the Bulgarian BlueGene/P have been used as platforms for a series of benchmarks. The parallel scaling (parallel performance up to 48 cores) of NAMD code has been investigated by estimation of the sensitivity of interconnection on speedup and benchmark results – testing the parallel performance of Myrinet, Infiniband and Gigabit Ethernet networks. The bencharmiking up to 4096 cores have been done on Bulgarian BlueGene/P

Benchmarking

NAMD benchmarking on BlueGene/P ~210K system



- The benchmarking of GROMACS package shows that with standard implementation (without any optimized testing by means of "g_tune_pme" code) the spatial decomposing is more efficient than the particle decomposition and that the clusters with high-performance network interconnections (such as Myrinet and Infiniband) show better results compared to Gigabit connectivity. The results as a scientific output will be presented soon.

Benchmarking: Comparison

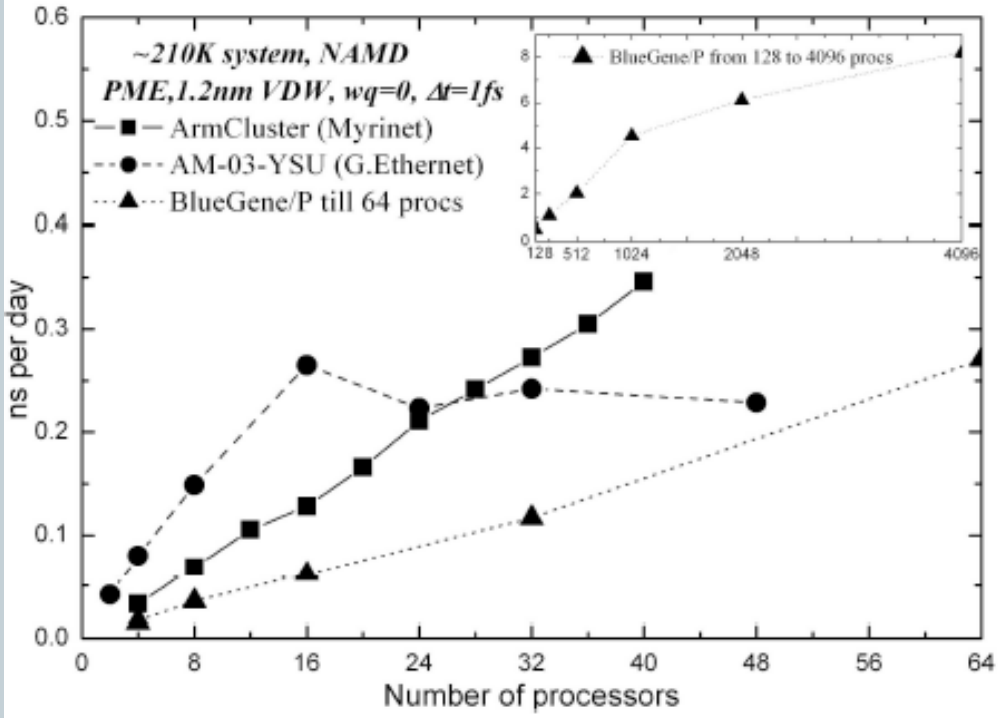


Figure 2. The NAMD performance and the estimation of ns per day against the number of processors for BlueGene/P, ArmCluster and AM-03-YSU sites.

Benchmarking: Conclusion

Thus, the benchmarking results show that for complex systems consisting more than 200K atoms the usage of supercomputers is rather efficient than the computational facilities of the ArmGrid infrastructure.

For relatively small systems up to 200-300K atoms, with the increase of processors we track that the computation spend more time on communications between processors, as in case of Grid sites of the ArmGrid infrastructure, whereas the benchmarking on BlueGene/P shows almost gradually increase of speed of calculation with the increase of processors.

Note that for relatively small amount of processors (up to 64 processors) the speed of calculation is surely better on ArmGrid sites due to the type of processors (BlueGene/P with PowerPC 450 - 850MHz vs worker nodes with Intel 2.0GHz to 3.06GHz frequency).

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Scientific Results

- IBM BlueGene (1024 cores): SDS/wat/oil with embedded polyampholytes at pH=4. Currently, ~ 70ns simulation run was carried out at pH=9. Up to 100ns of experiment have been done by changing the pH.

- Micellar system (sodium pentadecylsulfonate (SPDS) /water system near the critical micellar concentration) with about 2.500.000 (using Gromacs).The latter was reached the 93ns checkpoint.

- Series of simulations of mentioned micellar system (SPDS/water) changing the concentration ratio. It was stated that depending on concentration of amphiphilic material, the relaxation time of self-organization of small oligomers is changed.

- The increasing of water concentration correspondingly leads to the decrease the formation time, as clearly seen in snapshots provided below.

Scientific Results

- Using atomic scale simulation we have investigated inverse micellar system with presence of polyampholyte at pH=9. Currently ~70ns parallel molecular dynamics (MD) simulation was carried out for a sodium dodecyl sulfate (SDS) /polyampholyte/toluene/pentanol/water system. Analysis of the pre-results shows almost stable microdroplet during the whole simulation time, however additional run needs to reach equilibrium and compare to experimental findings. It is also run the mentioned system at pH=4, which will make it possible to reveal the mechanism of droplet-droplet interactions in dependence on pH, as well give us information about the localization of polyampholyte. The system runs on the Armenian Grid Infrastructure and on the Bulgarian Supercomputer BlueGene/P using 512 cores.

- The simulation of micellar system (sodium pentadecylsulfonate (SPDS) /water system near the critical micellar concentration) with about 2.500.000 atoms is in progress and currently 93ns of simulation run was finished. Due to the huge size of trajectories, only the output pdb files are written. The testing analysis is planning to do at 100ns of simulation time.

Scientific Results: Snapshot

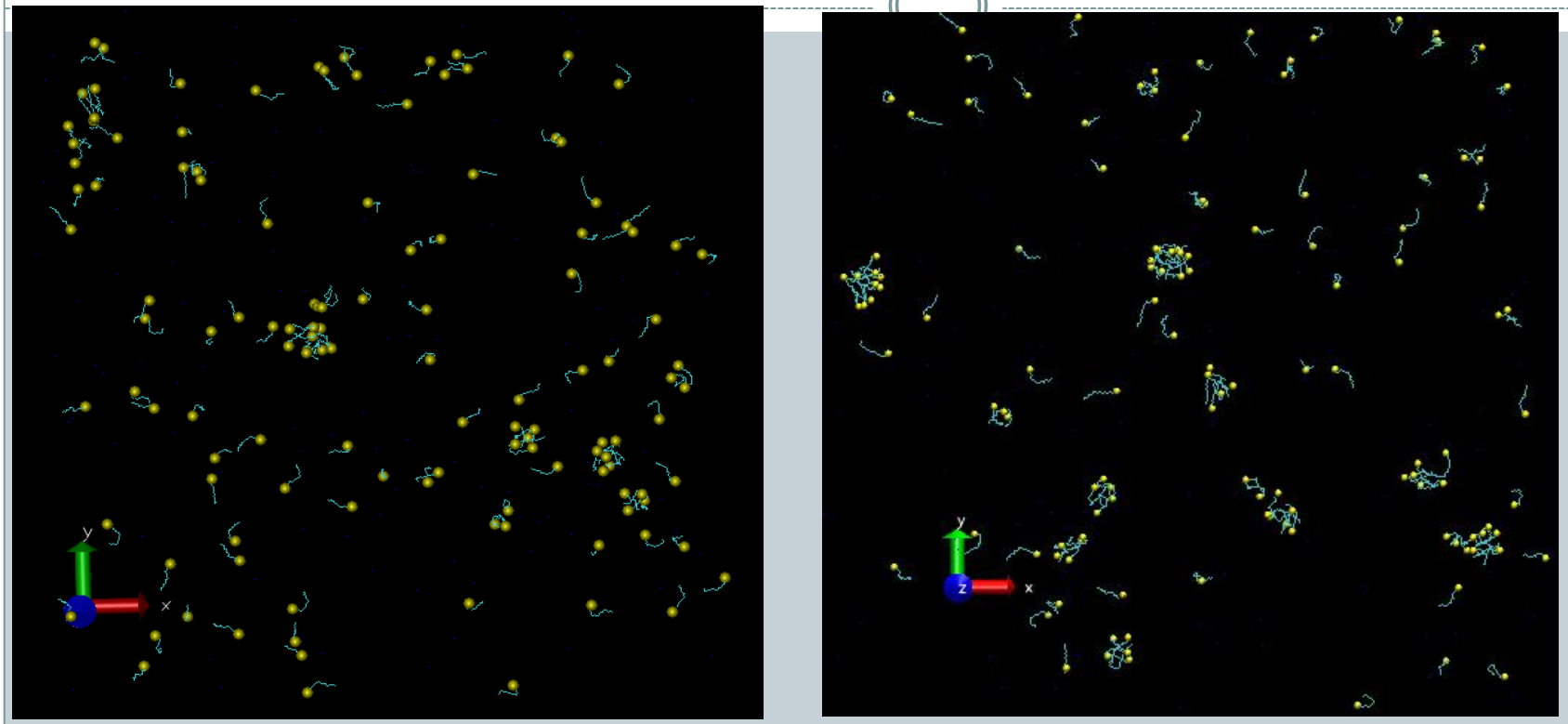

Figure 1.SPDS/water system (8mM) at 45ns(left) and 93ns(right) checkpoints

- The snapshot shows that at 45ns checkpoint we track the organization of small oligomers consisting of 5-7 SDS molecules. In case of 93ns the oligomer size increases and reached more than 11 SDS molecules.

Scientific Results: Snapshots

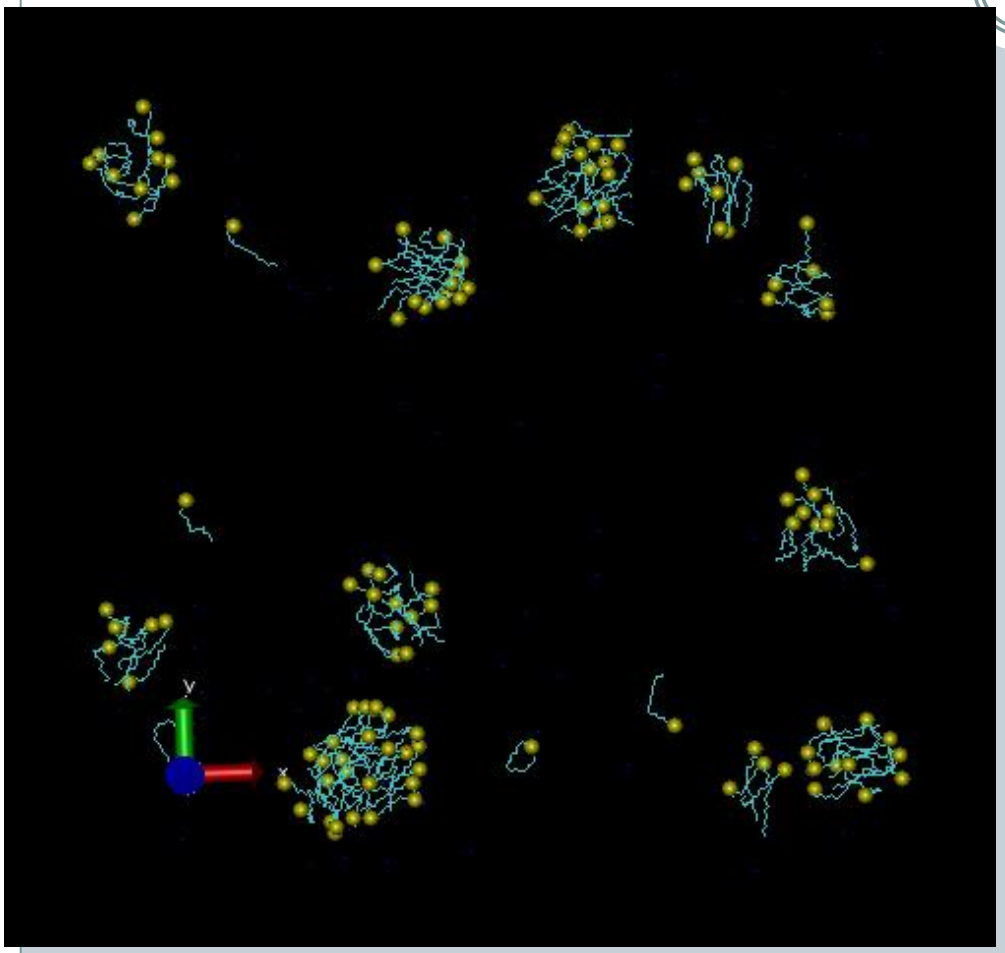

Figure 2.SPDS/water system (33mM) at 38ns checkpoint

- The mentioned system at 33mM concentration shows the decrease of the formation time of small oligomers and at same time interval we track the organization of small oligomers consisting of ~30 SDS molecules. Note that, at higher concentrations(263mM system), the aggregation of whole micelle (128 SPDS molecules) was completed at ~40ns of simulation run.

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Publications & Collaborations: Recent Publications (Published)

- A. Poghosyan, L. Arsenyan, H. Astsatryan, M. Gyurjyan, H. Keropyan, A. Shahinyan, NAMD Package Benchmarking on the Base of Armenian Grid Infrastructure, Journal of Communications and Network, Scientific Research Publishing, vol. 04, 2012, PP. 34-40, DOI: 10.4236/cn.2012.41005

- A. Shahinyan, P. Hakobyan, L. Arsenyan, A. Poghosyan, The study of lyotropic liquid crystal structure using the molecular dynamics method, Journal of Molecular Crystals and Liquid Crystals, 2012, DOI:10.1080/15421406.2012.687174.

- A.A.Shahinyan, L.H.Arsenyan, A.H.Poghosyan, The Study of Phase Diagram of the Surfactant/Water System by Molecular Dynamics Simulation, Book of Abstracts of 5th Japan – Russia International Workshop "Molecular Simulation Studies in Material and Biological Sciences", Joint Institute for Nuclear Research, Dubna, Russia, September 9 – 12, 2012.

- A. Poghosyan, L. Arsenyan, H. Astsatryan, Comparative NAMD Benchmarking of Complex System on Bulgarian BlueGene/P, IEEE Proceedings of the Distributed Computing and Visualization Systems Conference, Opatija, Croatia, pp. 319-321.

Publications & Collaborations: Publications (under review)

- A. Poghosyan, L. Arsenyan, A. Shahinyan, Molecular dynamics study of long chain alkyl sulfonate/water system, Elsevier Journal Colloid and Interface Science

Publications & Collaborations: Collaboration

- Institut für Chemie of Universität Potsdam, Potsdam, Germany
- International Center for Theoretical Physics, Trieste, Italy