Max A. Maximov

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Citizenship Status

U.S. Permanent Resident

Outline

An enthusiastic, adaptive, and fast-learning person with a broad and acute interest in molecular simulations. I particularly enjoy collaborating with scientists from different disciplines, to solve new challenges, develop new skills and get sharpen already existing ones. I have a solid professional experience working as a senior software engineer at Dell, combined with B.S. and M.S. education in computational physics, Ph.D. in Chemical Engineering, and Co-Op with Colgate on molecular dynamics simulation of amino acids at mineral surfaces.

I am currently finishing my Ph.D. studies, recently defended my thesis, making final edits, and completing my co-op. I am open to work since August 2021.

Current Position

Ph.D. in Chemical Engineering at New Jersey Institute of Technology
Computational Lab for Porous Materials
Scientific advisor: Prof. Gennady Gor
http://porousmaterials.net
Thesis: Advances in Modeling Gas Adsorption in Porous Materials for the Characterization Applications
The manuscript is available at https://mmaximov.net/dissertation
09/2017 – 08/2021

Education

Ph.D. in Chemical Engineering, New Jersey Institute of Technology *08/2021*
M.S. in Applied Math and Physics, Computational Physics dept, St Petersburg State University *2013*
B.S. in Physics, Computational Physics dept, St Petersburg State University *2011*

Professional Experience

Colgate-Palmolive, *Co-Op* (Remote, US) *06/2020 – Ongoing*

Molecular dynamics modeling of Colgate®Sensitive Pro-Relief™ toothpaste components using Gromacs and LAMMPS. The project aims to explain the role of certain amino acids in the adhesion between calcium carbonate particles themselves and the dentin surface. Forces, density profiles, and free energies were calculated. Publication and patent are in preparation.

Dell Software, *Senior Dev Staff Software Engineer* (St Petersburg, Russia) *10/2013 – 08/2017*

Developed software for system administrators, namely worked on various distributed cloud and on-premise email server (including Gmail and Office 365) migration and Active Directory recovery products helping to build a common platform for company products.

Key accomplishments:

- Integrated and consulted external teams to integrate five different products with minimal breaking changes.
- Developed a large-scale parallel log analysis tool capable of processing and searching in dozens of gigabytes of logs using Elasticsearch and own utility written in Go.
- Solved many customer cases where I had to investigate complex problems with network and security. Each case helped me to improve the product and tools to facilitate the resolution of the cases and deployment of hotfixes.
- Designed from scratch a fast and stable acceptance test suite in AWS cloud for a legacy product with minimal change of source code. I also wrote a plugin for a test utility that was reused by other teams.
- During the development of a new command-line API, found and fixed bugs in PowerShell by contributing to the official repository, which fix is now being used in pretty much all up-to-date Windows machines.
- Shared knowledge in the common portal, participated in test games, sync-ups, delivered own talks.

Programming skills

Python (numpy, scipy, sympy, pandas, scikit-learn, tensorflow, pytorch, rdkit, numba, jupyter), C++ (Boost, MPI, CUDA, Akka), Matlab/Octave, Maple, R, .NET, Haskell, Scheme, Scala, Go, Java, OpenCV, ANTLR, [N,J,g]Unit, LaTeX, cloud (AWS, Windows Azure), databases (Elastic, Solr, Lucene, MS SQL, PostgreSQL, SQLite, MySQL)

Simulation Software

LAMMPS, Gromacs, RASPA, Ovito, Avogradro, VMD, Packmol, Moltemplate, little experience with Gaussian

Additional Education

Computer Science Center, school affiliated with JetBrains, Yandex, St Petersburg Academic University, 2014 – 2015

Awards

- NJIT Service and Research Award, 2021
- NJIT Graduate Student Early Publication Award, 2019
- Travel Grant for International Workshop on Characterization of Porous Materials from the National Science Foundation, 2018

PhD Projects (in relevant order)

Pore-size distribution of opals

- Implemented Derjaguin-Broekhoff-de Boer and Frenkel-Halsey-Hill theories for capillary condensation.
- Collaborated with an experimentalist.
- Implemented non-negative least squares regression with Tikhonov (ridge) regularization for the adsorption integral equation to find the pore-size distribution from the experimental adsorption isotherm.

Links to: video, slides, paper, source code

Cell tracking using computer vision

- Implemented a segmentation algorithm for shortest, long and dead-end parts in a maze where the cells were placed to. Specifically, I first detected horizontal, vertical, and junction parts, then represented them as a graph and found the distances and dead-ends nodes.
- Calculated the likelihood for a cell (fibroblast) to divide (mitosis) for each type of path over the whole dataset as well as the preference of the path.
- Improved an already existing CV code to recognize the cells and made the algorithm to automatically detect the labeling errors.

Links to: slides, paper

Machine learning prediction of vapor pressure using Graph Convolutional Neural Networks. (unpublished)

- Scrapped a large dataset with SMILES strings and vapor pressure data from three different sources (PubChem, NIST, ChemIDplus).
- Reported dozens of species with errors in the NIST database by automatically detecting the errors (mostly because the temperature had wrong units).
- Unfortunately, the precision was not good enough. The further plan is to implement develop new features and compare the results with group contribution methods.

Link to slides

Ultrasound adsorption isotherms simulation

- Processed ultrasound adsorption data and calculated the bulk and shear moduli change.
- Modeled these data using Grand Canonical Monte Carlo method with near-quantitative agreement.
- Showed a relation between the bulk modulus and the pore size, which can be a promising method for characterization.

Link to paper

Simulation of Three-Dimensional Ordered Mesoporous (3DOm) carbons

- Derived and implemented the integrated potential for a complex geometry. The potentials can also be useful for other Monte Carlo and DFT modeling.
- Modified Monte Carlo code to support the potential and simulated gas adsorption in these pores to figure out the role of interconnections, which many studies neglect.

Link to paper

Kinetic Monte Carlo algrotithm (KMC) for vapor-liquid equilibrium (unpublished)

- Performed benchmarks with Grand Canonical Monte Carlo simulations.
- Plan to implement a GPU-optimized version of it. Going to be published.

Teaching Experience

- Teaching Numerical Methods in Chemical Engineering with Python seminar, which was also mandatory for CHE491 Independent Study course (10 participants, 7 classes; link to evaluation), NJIT, 2019
- Mentoring Marcos Molina and Taylor Kvist during the 3DOm carbons project, NJIT, 2019 – 2021
- Supervision of high school and B.S. students during summer 2018 – 2020 in the scope of the vapor-liquid equilibrium in organic compounds relevant to the atmospheric chemistry project and the isothermal modulus of square-well fluids project, NJIT

Publications

6. ***Maximov M. A.***, Molina M. and Gor G. Y., The Effect of Interconnections on Gas Adsorption in Materials with Spherical Mesopores: a Monte Carlo Simulation Study, ***J. Chem. Phys.***, 154(11):114706, 2021 **10.1063/5.0040763**
5. Emelianova A., ***Maximov M. A.***, and Gor G. Y., Solvation pressure in spherical mesopores: Macroscopic theory and molecular simulations, ***AIChE J***, 67(3):e16542, 2020 **10.1002/aic.16542**
4. ***Maximov M. A.***, Galukhin A. V., and Gor G. Y., Pore-Size Distribution of Silica Colloidal Crystals from Nitrogen Adsorption Isotherms, ***Langmuir***, 35(47):14975-14982, 2019 **10.1021/acs.langmuir.9b02252**
3. ***Maximov M. A.*** and Gor G. Y., Molecular Simulations Shed Light on Potential Uses of Ultrasound in Nitrogen Adsorption Experiments, ***Langmuir***, 34(51):15650–15657, 2018 **10.1021/acs.langmuir.8b02909**
2. Dobrzanski C. D., ***Maximov M. A.***, and Gor G. Y., Effect of Pore Geometry on the Compressibility of a Confined Simple Fluid, ***J. Chem. Phys.***, 148(5):054503, 2018 **10.1063/1.5008490**
1. Pham Q. L., Rodrigues L. N., ***Maximov M. A.***, Chandran V. D., Bi C., Chege D., Dijamco T., Stein E., Tong N. A. N., Basuray S., Voronov R. S., Cell Sequence and Mitosis Affect Fibroblast Directional Decision-Making During Chemotaxis in Microfluidic Mazes, ***Cell Mol Bioeng***, 11(6):483–494, 2018 **10.1007/s12195-018-0551-x**

Conference Presentations

Maximov M. A., Galukhin A. V., and Gor G. Y., Pore-Size Distribution of Silica Colloidal Crystals from Nitrogen Adsorption Isotherms, ***AIChE Annual Meeting***, online, 2020 (poster and oral)

Maximov M. A. and Gor G. Y., Pore Size Estimation from Ultrasonic Measurements during Nitrogen Adsorption Experiment, ***AIChE Annual Meeting***, Orlando, FL, 2019 (oral)

Maximov M. A. and Gor G. Y., Ultrasound propagation in fluid-saturated nanoporous media, ***Transport In Disordered Environments***, Princeton, NJ, 2019 (poster)

Maximov M. A. and Gor G. Y., Molecular Simulations Shed Light on Potential Uses of Ultrasound in Nitrogen Adsorption Experiments, ***The 22nd Meeting of the North-East Corridor Zeolite Association***, Philadelphia, PA, 2018 (poster)

Maximov M. A. and Gor G. Y., Analysis of Ultrasonic Measurements during Nitrogen Adsorption Experiments, ***1st North American Symposium on Dynamic Vapor Sorption Science***, Philadelphia, PA, 2018 (poster)

Maximov M. A. and Gor G. Y., Kinetic Monte Carlo methods for calculation of fluid phase equilibria, ***Molecular Simulations Mini-Workshop***, Newark, NJ, 2018 (oral)

Maximov M. A. and Gor G. Y., Compressibility of Nitrogen Adsorbed in Vycor Glass, ***8th International Workshop "Characterization of Porous Materials: From Ångströms to Millimeters***", Delray Beach, FL, 2018 (poster)

Maximov M. A. and Gor G. Y., Argon Adsorption in Three-Dimensional Ordered Mesoporous (3DOm) Carbons: Monte Carlo Molecular Simulation Study, ***Annual Meeting of the APS Mid-Atlantic Section***, Newark, NJ, 2017 (poster)