Yuriy Khalak

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QUALIFICATIONS

Expertise	Artificial intelligence, software automation and infrastructure, parallel programming, efficient and security conscious code, problem solving, collaborative R&D, pharma, game development, technical writing.
Programming	Python, C/C++, Perl, Bash, JavaScript; MPI, OpenMP.
Key Technologies:	
Machine Learning	PyTorch, Diffusers, scikit-learn, Neptune, TensorBoard.
Python	NumPy, SciPy, Matplotlib, pandas, Django (with REST and SQLite).
CI/CD & Agile	Git, GitHub/GitLab, Jira, pytest, unittest.
Development Tools	Jypyter notebook, Spyder, Visual Studio 2022, VS Code, gcc/g++, icc, make, CMake, gdb, valgrind.
Game Development	Ogre3D, Godot, pygame, JavaScript Canvas, Blender.
Linux	Ubuntu, openSUSE, console tools, Emacs, OpenSSH, Apache.
Theoretical Chemistry	Gromacs, LAMMPS, NWChem, CPMD, RDKit, ASE, MDAnalysis.
Languages	Fluent: English, Ukrainian; Intermediate: French.

RECENT PROJECTS

- TerrainDiffusion (09.2024): a generative diffusion model for realistic terrain without the need for post-processing with erosion simulations.
- BraneSpace (07.2024-10.2024): an Asteroids-inspired 2D space game with a custom physics engine. Written in Python 3 with pygame graphics and NumPy math. Compiled for interpreter-free release with Nuitka.
- LogistiX (03.2023-current): an in-development browser game about managing military logistics. Driven by Django REST framework and SQLite on the server and JavaScript Canvas on the client side.

WORK HISTORY

Software Developer **06.2024 – 07.2024**
Freelancing through UpWork **Moncton, NB, Canada**

- Created an automated system (Python 3, NumPy, SciPy) for fitting models of light scattering in non-homogeneous media to experimental data. Worked directly with the client to understand their operational requirements and choose an appropriate model. Provided ongoing support by adapting the code to evolving input formats and overcoming numerical instability at extreme parameter values.

Postdoctoral Researcher **05.2019 – 05.2022**
Max Planck Institute for Multidisciplinary Sciences **Göttingen, Germany**

Built software for automated drug design.

- Built and published an active learning approach (Python 3, PyTorch) for computational ligand optimization by training ML models on an expanding set of theoretical binding free energies. Built a system for dynamically computing, caching, and distributing molecular features to remote training nodes while minimizing network load and tuning model hyper-parameters.
- Created scalable software (Python 3, C++, Perl) for predicting binding of drug candidates with molecular dynamics simulations distributed across a compute cluster. Produced an automated workflow to manage and analyze multi-step distributed calculations and graphically report the predictions. Delivered it to an industrial partner for in-house use and adapted it for AWS infrastructure.

EDUCATION

Doctorate (PhD equivalent) **03.2015 – 02.2019**
Eindhoven University of Technology **Eindhoven, Netherlands**

- Wrote tools (C/C++, Python 2) for automatic parameterization and refinement of molecular dynamics models from quantum mechanical calculations.
- Implemented explicit simulation (C++, SSE2) of polarization effects into a branch of Gromacs, a high-performance engine for chemical simulations.
- Added support for periodic quantum systems to the VOTCA-XTP library (C++).

MSc -> PhD (unfinished) in Chemistry: Nanotechnology **09.2013 – 12.2014**
University of Waterloo **Waterloo, ON, Canada**

BSc with Combined Honours in Biology and Physics **09.2009 – 04.2013**
Dalhousie University **Halifax, NS, Canada**

AWARDS

- Natural Sciences and Engineering Council of Canada Alexander Graham Bell Canada Graduate Scholarship 2013, MSc level
- NSERC University Undergraduate Student Research Awards (USRA) 2010, 2011, and 2012
- First Place in Dalhousie University Computer Science Day Software Competition 2009
- Third Place in UNBSJ High School Programming Competition 2008, 2009

KEY PUBLICATIONS AND TALKS

Y. Khalak. Learning to Bind: Active Learning for *In Silico* Ligand Optimization. (November 2022). Université de Moncton, Moncton, Canada.

Y. Khalak, G. Tresadern, D. F. Hahn, B. L. de Groot, & V. Gapsys (2022). Chemical space exploration with active learning and alchemical free energies. *Journal of Chemical Theory and Computation*, *18*(10), 6259-6270.

Y. Khalak, G. Tresadern, M. Aldeghi, H. M. Baumann, D. L. Mobley, & B. L. de Groot, V. Gapsys (2021). Alchemical absolute protein–ligand binding free energies for drug design. *Chemical Science*, *12*(41), 13958-13971.

Y. Khalak, B. Baumeier, and M. Karttunen (2018). Improved general-purpose five-point model for water: TIP5P/2018. *The Journal of chemical physics*, *149*(22), 224507.