Andrey Asadchev

Contact Information

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Summary

Computational scientist passionate about C++, high-performance computing, and low-level code optimization. Interests include C++ template expressions and meta-programming, parallel linear algebra, computational chemistry, machine learning, hobby electronics, and gardening.
US permanent resident (green card), Canada permanent resident
Fluent in English, native Russian speaker, conversational level of French.

Education

PhD, Physical Chemistry, Dec 2012
Iowa State University, Ames, IA

- Emphasis on computational quantum chemistry.
- Dissertation: *Modernizing the core quantum chemistry algorithms*, http://lib.dr.iastate.edu/etd/12915/

BSc, Computer Science, May, 2005
Valdosta State University, Valdosta, GA

- Magna Cum Laude

Technical Skills

Programming Languages:	C++/11/14/17, Python, C, FORTRAN 77/90
C++ Concepts:	Object oriented design, metaprogramming, expression templates
C++ Libraries:	Standard Template Library (STL), Boost, pybind11
Machine Learning:	Tensorflow, Scikit
Scientific Computing:	BLAS, LAPACK, Eigen, Trillions, Mathematica, Matlab/Octave
Parallel Programming:	CUDA, MPI, TBB, OpenMP, ARMCI
Parallel I/O:	HDF5, NetCDF, Lustre, PVFS
Code optimization:	SSE and AVX vectorization with intrinsics/assembly
Performance analysis:	Linux perf, Intel VTune/Parallel Studio, PAPI
Debugging:	gdb, Valgrind, DDT, TotalView
Build tools:	CMake, autotools
Collaboration:	git, Atlassian stack (JIRA, Stash), Agile
HPC Environments:	IBM BlueGene, Cray XT, OpenMPI, MPICH, PBS/Torque/SLURM
UNIX/Linux:	POSIX API programming, bash shell scripting, Linux administration

Work and Research Experience

Virginia Tech, Blacksburg, VA
Research Scientist **2020 - Present**

Development of electron integral methods for current and emerging processor architectures, Python/C++ integration.

- Development of experimental high-performance electron integral library (Libintx)
- Obara-Saika 3-center 2-electron code suitable for GPU and SIMD CPU architectures
- High-efficiency J-Engine and Fock-exchange GPU code
- Python/C++ integration in TiledArray and MPQC
- Various codebase enhancements to reduce compilation time and memory

Infosys Limited, Palo Alto, CA
Senior Product Technical Architect **2017 - 2020**

Development and integration of machine learning features in Infosys products

- Integrated Tensorflow into Infosys ML offerings.
- Introduced C++/Python interoperability via PyBind11 to allow for rapid development and prototyping.
- ML RESTful WebService implementation via Flask.
- Continuous enhancement of core code base and build system.

Skytree, Inc., San Jose, CA
HPC C++ Developer **2013 - 2017**

Participated in the development of the Skytree C++ Machine Learning (ML) product.

- Refactored the C++ codebase according to modern C++ patterns;
  reduced the number of lines of code, improved maintainability and compilation speed.
- Identified and resolved key computational and memory bottlenecks;
  significantly improved overall execution time and reduced memory footprint.
- Implemented core dense and sparse linear algebra objects and kernels.
- Designed and implemented several distributed ML algorithms using OpenMP and MPI.
- Worked with data scientists to address feature requests and resolve bugs.

Virginia Tech, Blacksburg, VA
PostDoctoral Researcher **2012 - 2013**

Participated in the development of Massively Parallel Quantum Chemistry (MPQC) package.

- Modernized the MPQC C++ code base by using Boost and Eigen linear algebra library.
- Ported MPQC to CMake; simplified build and deployment across various HPC platforms.
- Developed fully distributed OpenMP/MPI sparse Davidson eigensolver with out-of-core capabilities, scalable to 1000s of cores.
- Conducted pilot research to optimize key computational kernels on SSE/AVX processors.

Iowa State University, Ames, IA
Research Assistant **2008 - 2012**

Developed computational chemistry C++ library (libcchem) with GPU capabilities and FORTRAN bindings.

- Implemented automatically generated vectorized C++ Rys Quadrature algorithm;
  30-40% faster than the original FORTRAN code.
- Implemented scalable multi-threaded Hartree-Fock algorithm with constant memory overhead.
- Implemented Rys Quadrature and Hartree-Fock algorithms on GPU using CUDA C++;
  showed speedups on the order of 10-17 times.
  In the process resolved several issues in Boost C++ libraries due to CUDA compiler.
- Designed and implemented distributed in-core and out-of-core data storage suitable for matrix and tensor computations with C++ object oriented interface and integration with BLAS.
- Implemented scalable distributed perturbation theory and Coupled Cluster algorithms with low memory footprint and ability to utilize GPU devices via CuBLAS.
  The implementation showed orders of magnitude reduction in memory use, as well as improvement in speed and overall scalability (1000s of cores), over the original FORTRAN code.

Ames Laboratory, Ames, IA
Research Assistant **2006 - 2008**

Participated in the development of The General Atomic and Molecular Electronic Structure System (GAMESS).

- Ported GAMESS to Blue Gene and Cray XT using ARMCI library
- Implemented tools to run GAMESS in various MPI and batch system environments
- Replaced FORTRAN code with BLAS/LAPACK calls, parallelized linear algebra routines;
  improved overall program performance, allowed GAMESS to scale to 1000s of cores.

Open Source Projects

- https://github.com/asadchev/pyxcc - Experimental Python computational chemistry package
- https://github.com/asadchev/libintx - High-performance electron integral library

Teaching Experience

Virginia Tech, Blacksburg, VA
(SICM)2 Summer School **2013**

- Taught GPU/CUDA programming workshop to computational sciences graduate students.

Iowa State University, Ames, IA
Chemistry Instructor **2005 - 2006**

- Taught general chemistry lab and recitation sections.

Publications and Presentations

A Fast and Flexible Coupled Cluster Approach
A. Asadchev, M. S. Gordon
Journal of Chemical Theory and Computation 2013 9(8)

New Multithreaded Hybrid CPU/GPU Approach to Hartree–Fock
A. Asadchev, M. S. Gordon
Journal of Chemical Theory and Computation 2012 8 (11)

Uncontracted Rys Quadrature Implementation of up to G Functions on graphical processing units (GPUs)
A. Asadchev, V. Allada, J. Felder, B. M. Bode, M. S. Gordon, T. L. Windus
Journal of Chemical Theory and Computation 2010 6(3)

Accelerating Quantum Chemistry Research using GPUs
A. Asadchev, J. Felder
GPU Technology Conference, NVIDIA, San Jose, 2009

Uncontracted Rys Quadrature on GPU
A. Asadchev
Path to Petascale, NCSA, 2009

Performance of Electronic Structure Calculations on Blue Gene/L and Cray XT4
A. Asadchev
IEEE/ACM Supercomputing 2008 Poster