Andrey Asadchev

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Education objective

- Ph.D. in Chemistry with emphasis on Computational Chemistry

Education

- **Valdosta State University (VSU)** — Valdosta, GA
  B.S., Computer Science Major — May 2005
  B.S., Mathematics Minor — May 2005

- **Iowa State University (ISU)** — Ames, IA
  Ph.D., Physical Chemistry — expected Dec 2011

Research interests

- CPU and memory efficient algorithms.
- Chemistry and Linear Algebra algorithms on GPU accelerators.
- Distributed memory algorithms and communication.
- Two electron integral methods, many-body methods, e.g. MP2, CC.
- Domain specific embedded languages, e.g tensor expressions.
- Higher-order programming and template meta-programming.
- Symbolic computations and automatic code generation.

Teaching interests

- Applied Mathematics and Computer Science for Science students
- Advanced C++ and template meta-programming

Research experience

- **Dr. Thomas Manning, Valdosta State Univeristy, 2004-2005**
  Linux Beowulf Cluster
  Modeling of C8, C10, C12, and C14 cyclic systems

- **Dr. Mark Gordon, Iowa State University/Ames Lab, 2005-present**
  Parallel CI methods
  GAMESS on IBM Blue Gene and Cray XT4
  Massively parallel MP2 program, Supercomputing 08
  Uncontracted Rysq quadrature on GPU, NCSA 09
  Uncontracted Rys Quadrature Implementation of up to G Functions on Graphical Processing Units, JCTC 10

Related Work Experience

- **Research Assistant, Valdosta State University, Chemistry Dept, 2003-2004**
  Chemistry projects with Dr. Thomas Manning.

- **Teaching Assistant, Valdosta State University, Chemistry Dept, 2004**
  General Chemistry.

- **Teaching Assistant, Iowa State University, 2005-2006**
  General Chemistry recitations and labs.

- **Research Assistant, Iowa State University/Ames Lab, 2006-present**
  Quantum Chemistry codes and applications.

Current projects

- C++ implementation of HF, MP2, DFT, CC methods in CPU/GPU environment
- CC algorithms with N^3 memory overhead
- Tensor/matrix expressions
- CUDA/Boost interfacing, e.g ublas/CUBLAS bindings.

Relevant computer experience

- C++, C, Python, Fortran, Java
- Standard Template Library and Boost
- MPI, ARMCI, OpenMP, CUDA
- POSIX system programming
- Mathematica, Matlab/Octave
- UNIX administration

Presentations and Publications

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

- **Performance of Electronic Structure Calculations on BG/L and XT4 Computers**
  A.Asadchev, B.M.Bode, M.S.Gordon, *Journal of Computational and Theoretical Nanoscience, 2009 6(6)*

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

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

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