PSI4

AB INITIO QUANTUM CHEMISTRY

Wiley Interdisciplinary Reviews

PSI4 Paper

A preview of the PSI4 code and its capabilities has been published online in *Wiley Interdisciplinary Reviews: Computational Molecular Science. (DOI: 10.1002/wcms.93)*

Updated Public Beta Now Available *July 3, 2013*

Note to previous users: Update any mention of PsiMod to psi4 in .psi4rc or input files

Recent PSI4 Results

Density fitting / Cholesky decomposition (DF/CD) CCSD(T) is now available. DF/CD

PSI4 Capabilities

Coupled Cluster Methods
Large-Scale SAPTn

PSI4 GitHub Feed

7 weeks ago by Justin Turney:
Removes MADNESS

WSSSPE Communities Panel:
Education and Training

Pivotal question:

How can we educate developers to produce complex, agile, and sustainable domain-specific software?

"Advanced Techniques for Scientific Programming and Collaborative Development of Open Source Software Packages at the International Centre for Theoretical Physics (ICTP)"

Ivan Girotto (ICTP, Trieste), Axel Kohlmeyer (Temple U.),
David Grellscheid (IPPP, UK), Shawn T. Brown (PSC & CMU)

- Motivation, structure, and outcomes of a three-week workshop held at the International Centre for Theoretical Physics in March 2013
- Focused on Quantum ESPRESSO, a plane-wave density-functional theory (DFT) package for condensed-matter physics (mostly FORTRAN-90, multiple executables)
- Participants included developers and would-be developers of the package with a wide range of experience with development tools and techniques.
- Future workshops planned, including one in 2014 for the LAMMPS molecular dynamics code

“On the Development of Sustainable Software for Computational Chemistry”

T. Daniel Crawford (Virginia Tech)

- Current challenges facing computational chemistry software-development efforts and a community-wide effort to overcome them
- Educational infrastructure in chemistry is a major obstacle to training of theorists capable of developing sustainable software.
- A two-week software summer school was held at Virginia Tech in late July 2013 training ~25 graduate students from 17 different theoretical chemistry groups.
- A second summer school is planned for 2014 at Stony Brook University.

“Experiments in Sustainable Software Practices for Future Architectures”

Charles R. Ferenbaugh (LANL)

- "Exascale Tutorial" series: year-long, part-time "boot camp" to educate experienced developers in new architectures and languages (C++, CUDA, OpenCL) (2010)
- Four-year-long Software Infrastructure for Future Technologies (SWIFT) project to produce a prototype multi-physics code suitable to run on future architectures (2011)
- First experiences at LANL with the disciplined development practices that are common in the software industry
- Recognized a conflict between intense software development and the “interrupt drive” culture at LANL

Overarching Issues

- Complexity/opacity of scientific problems
- Lack of cross-education
- Cultural inertia

Code Complexity

- Computational chemistry and physics programs contain hundreds of thousands to millions of lines of hand-written code.
- Often written in an amalgam of languages: F77, F90, F95, HPF, C, C++, Python, etc.
- Evolved in an *ad hoc* manner over decades because "problems being addressed are not always fully understood." (Girotto)

Lack of Cross-Education

- Chemistry and physics students receive little to no training in software development.
- Most computer science students lack the underlying knowledge of the scientific domains to develop creative software solutions.
- Neither group receives appreciable credit within their own communities for collaboration.
- Workshops were able to find at least some common ground between the two groups.

Cultural Inertia

- Graduate programs in chemistry and physics require a modicum of coursework between the bachelor and Ph.D., giving students little opportunity to overcome deficiencies.
- The "just get the physics working" (Ferenbaugh) approach to code development pervades the vast majority of groups.
- Credit for software development is a major obstacle – especially within the scientific cultures that judge productivity of their members.

Ending on a Positive Note!

- Many of these problems are now widely recognized, both by the active researchers and funding agencies.
- The workshops described in the Girotto, Crawford, and Ferenbaugh papers, in particular, were very successful in closing the education gap among the domain scientists that participated.
- Education/indoctrination efforts that aggressively span entire communities can lead to a sea-change in domain-specific software development.