PSI4

OPEN-SOURCE QUANTUM CHEMISTRY

psicode.org

International Developers Conference, Georgia Tech, Nov 14-15
http://www.psicode.org

Participating Institutions:

- Georgia Tech
- Virginia Tech
- Emory University
- University of Georgia
- NIH
- ETH Zurich
- Ataturk University
- Florida State University
- Bethel University
- Chemical Semantics, Inc.
- University of Memphis
- University of Tromso

Topics:

- Development Updates
- Common Driver for Quantum Chemistry
- Parallelization
- The Psi4 Development Ecosystem
- Psi4 Object-Oriented Design

5300+ downloads
71 citations (ISI “Hot Paper”)
Totally Free and Open Source

Reception of Psi4 by the Community

C. David Sherrill

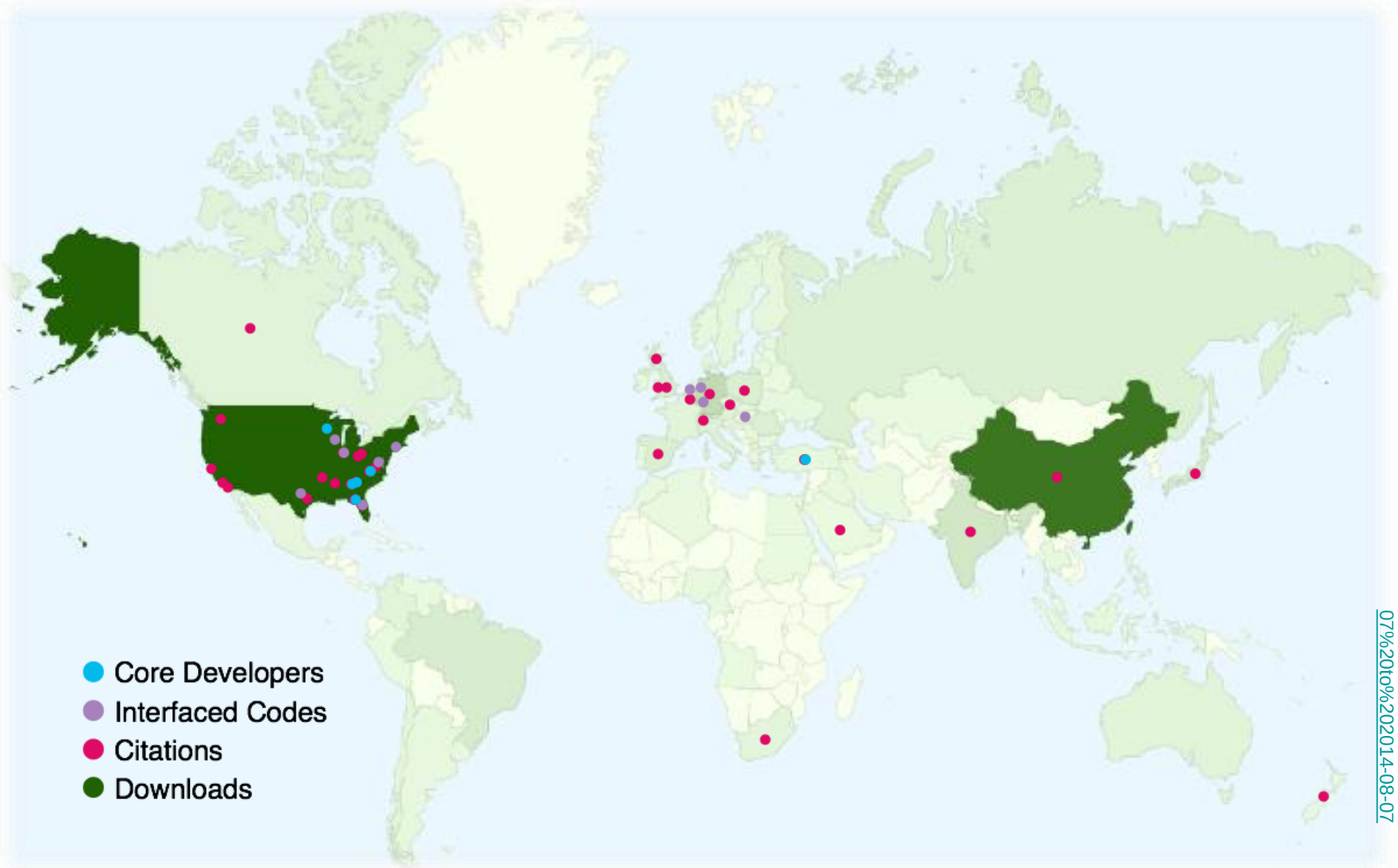
School of Chemistry and Biochemistry

School of Computational Science and Engineering

Georgia Institute of Technology

Georgia Institute of Technology
Center for Computational Molecular Science and Technology

PSI4 **Across the Map**



http://sourceforge.net/projects/psicode/files/stats/map?dates=2013-04-07%20to%202014-08-07

PSI4 **Across the Map**

- MRCC

  Kállay; arbitrary order CC/CI

- DFTD3

  Grimme; dispersion correction

- Molden

  Schaftenaar

  orb., density visualization

- WebMO

  Polik & Schmidt

  GUI/web server

- ERD

  Flocke; $2e^-$ integrals

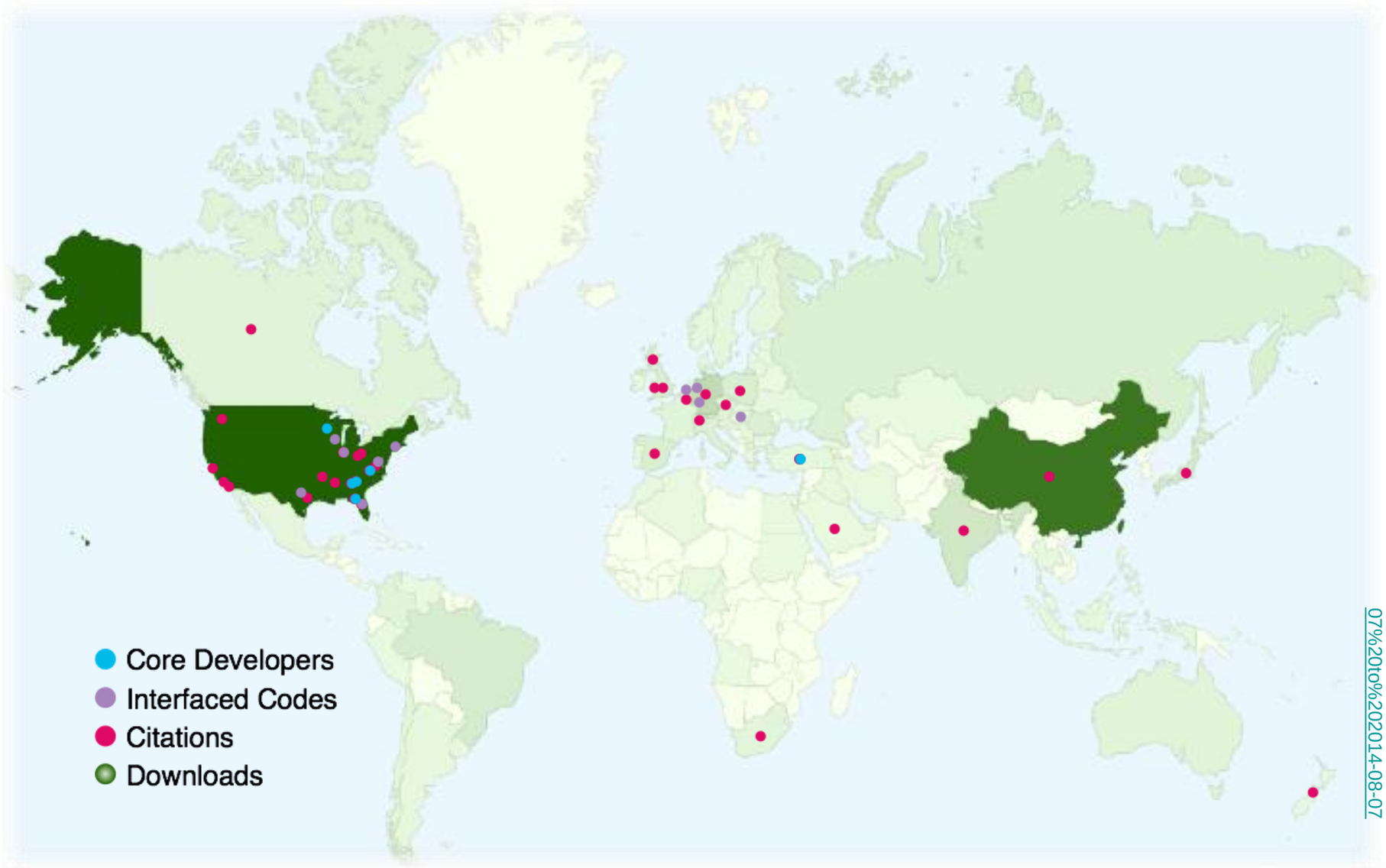
- libefp

  Kaliman & Slipchenko

  fragment potentials

- Gaussian

  Many-body expansion



http://sourceforge.net/projects/psicode/files/stats/map?dates=2013-04-07%20to%202014-08-07

- ADF

  Visscher; FDE solvation

- PubChem

  NIH; structure look-up

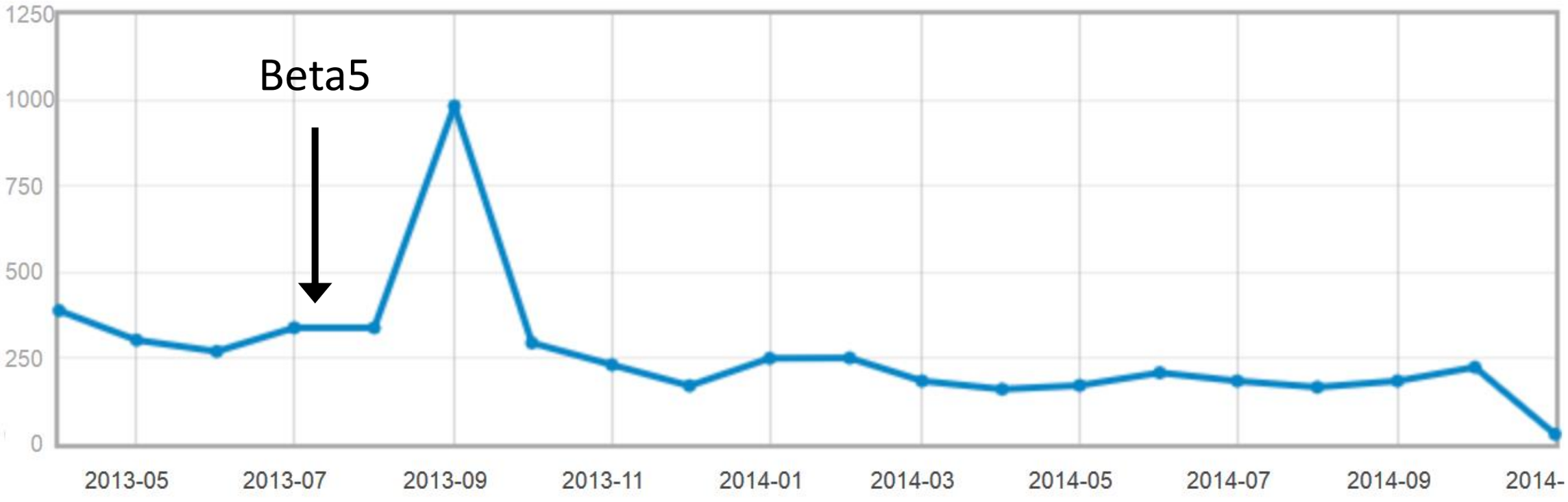
- CFOUR

  Gauss & Stanton

  CC/MBPT/properties/etc.

Download Statistics

- First publicly released on April 7, 2013
- Since then, 5,312 downloads
- Checkouts from Git are not tracked



Sourceforge Downloads

PSI4: The Paper

- J. M. Turney et al., *WIREs: Comput. Mol. Sci*. **2**, 556 (2012)
- Published July/August 2012
- ISI “Highly Cited Paper”: In the top 1% of the field of Chemistry based on a highly cited threshold for the field and publication year
- 71 citations as of November 2014

Outside Groups Citing the PSI4 Paper (2014)

- Holger Bettinger [SAPT]
- Ken Jordan
- Steven Wheeler [SAPT]
- Ekaterina Izgorodina, Monash, Australia [DF-CCSD(T), CBS]
- E. Fabiano, National Nanotechnology Laboratory, Italy [MP2, MP4, QCISD(T), CCSD(T), SAPT, CBS]
- Sebastian Wouters, Ghent, Belgium [RHF orbitals to input into DMRG]
- Thomas Beck, U. Cincinnati [DF-MP2]
- Yuji Mochizuki, Rikkyo Univ., Japan [ADC]
- Peter Pulay [cited as a program package with high-level correlated energies and gradients]
- Jean-Luc Bredas [SAPT, fractional occupation RSH DFT]

Outside Groups Citing the PSI4 Paper (2014)

- Clemence Corminboeuf [SAPT]
- Michael Gilson [SAPT]
- Y. B. Wang, Guizhou U., China [SAPT]
- Greg Tschumper [SAPT]
- Jiri Sponer [SAPT]
- Georg Jansen [mentions SAPT available in PSI4]
- (Hollman/Schaefer/Valeev used PSI4 Python interface and NumPy to develop toy code of concentric atomic density fitting)
- John Herbert [SAPT]
- Grant Hill, U. Sheffield [SAPT2+(3)δMP2]

Observations on Citations

- Majority are for SAPT capabilities --- something they basically can’t get elsewhere
- Even when Psi4 is used for SAPT, the users don’t go ahead and use it for other features (e.g., DFT); they frequently use 3 packages in a single study, each for its “signature feature”
- Probably just reflects how slow people are to change their habits

Comments about Psi4 From the Community

- George Schatz (October 2013): “We haven’t downloaded it yet because it sounded like the code was still in beta”
- Anonymous force field developer (used our CC code in a recent study): “You guys are younger and more energetic, and you seem to be more willing to collaborate than people associated with some other packages”
- Anonymous commercial developer: “We’re getting a lot of pushback because we’re not open source. Maybe I should look at what you guys are doing.”

Feedback from ETH (via Rollin King)

"As I talked with several professors today at ETH, they all noted that it was important to them that PSI4 was open source." Sentiments were expressed that closed-source codes:

- Reduce the impact of a theoretical work by reducing the number of users
- Impair the development of the field, requiring others to redo past work
- Contradict the spirit of publication, in which work/results are presented publicly
- Abuse the privilege of taxpayer-provided resources for personal gain
- Restrict some types of opportunities for collaboration

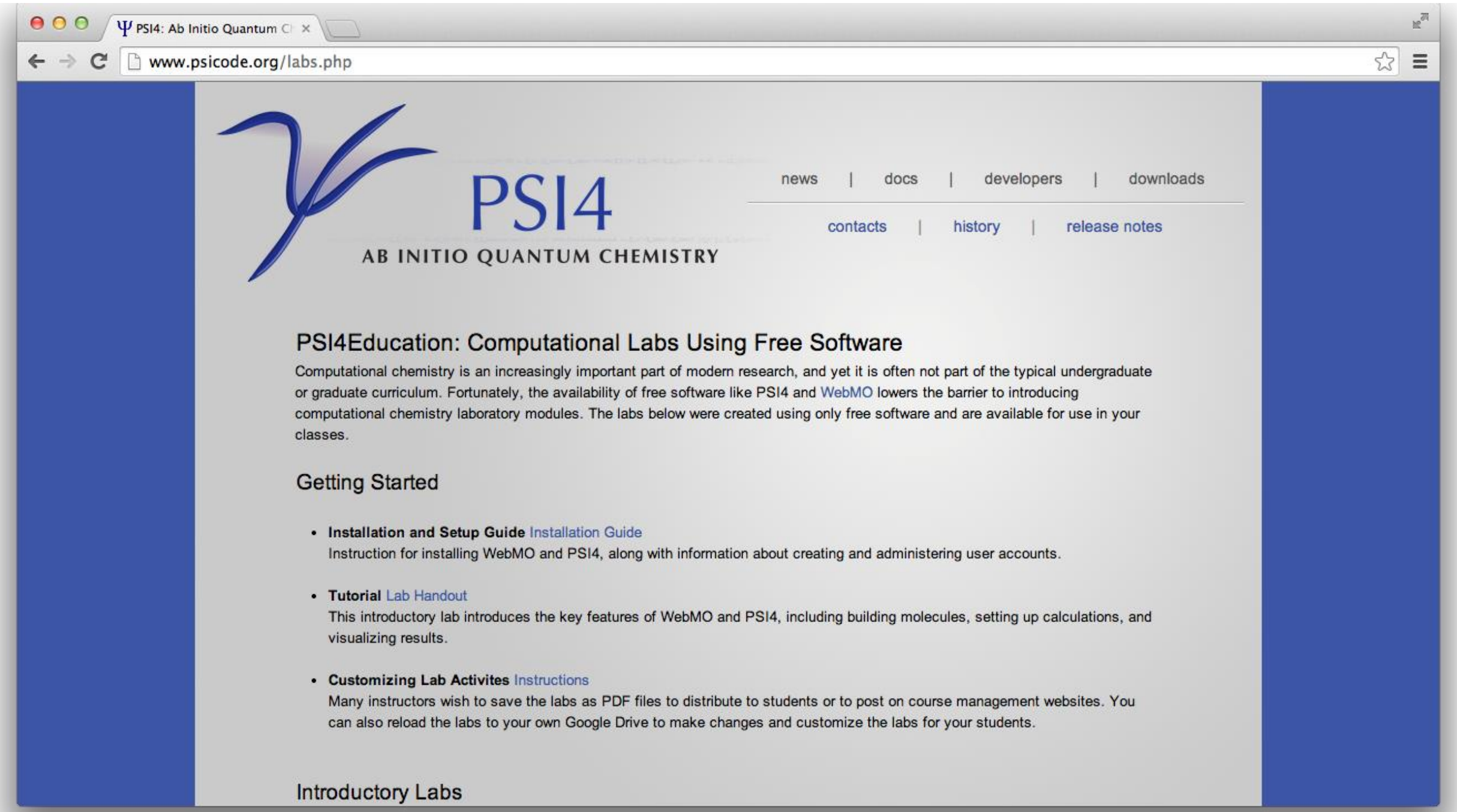
Feedback from Nate DeYonker (U Memphis)

- Wants DK integrals
- Wants to be able to use MCSCF to get symmetry averaged HF orbitals for high symmetry cases
- Wants to be able to use seudocanonical/natural/DFT orbitals in ccenergy (raises general question of orbital handling)

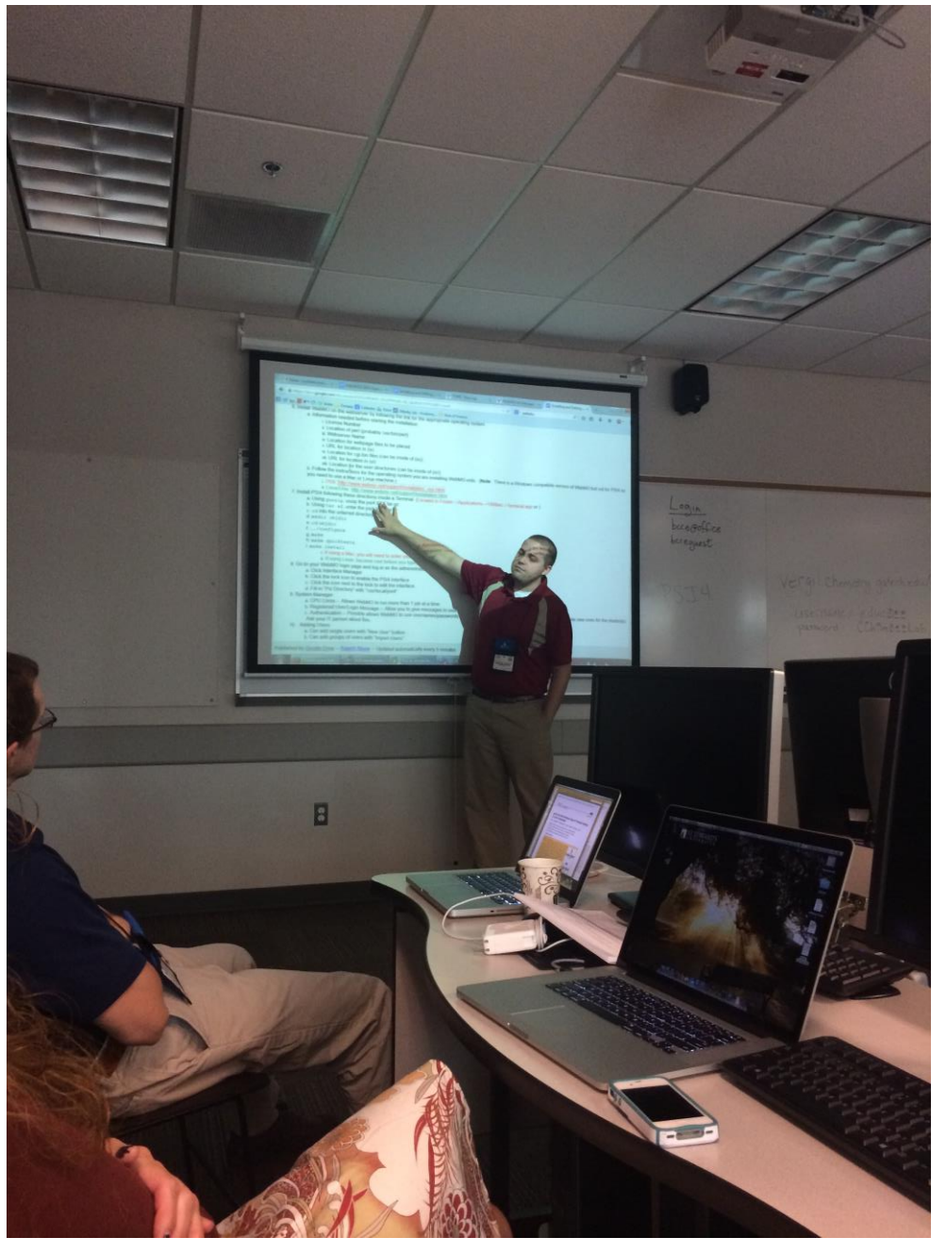
NPA Capabilities

- Tymofii Nikolaienko has a Java version of NBO and would like to discuss integration with PSI4
- I think we don’t want to be calling Java libraries from PSI4; maybe we could be calling it as a binary
- I encouraged him to think about translating to a reusable C++ library

PSI4Education: An open lab manual



PSI4Education Workshop
Held at BCCE August 5, 2014



- Premiere of our free, open-source lab manual based on free software
- 25 chemical educators (community college through universities)
- Hands-on experience using Psi4/WebMO

PSI4Education Team

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Cal Poly

Ryan Fortenberry
Georgia Southern

Matthew Kennedy
Georgia Tech

Tricia Shepherd
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Collaboration with WebMO:

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