



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

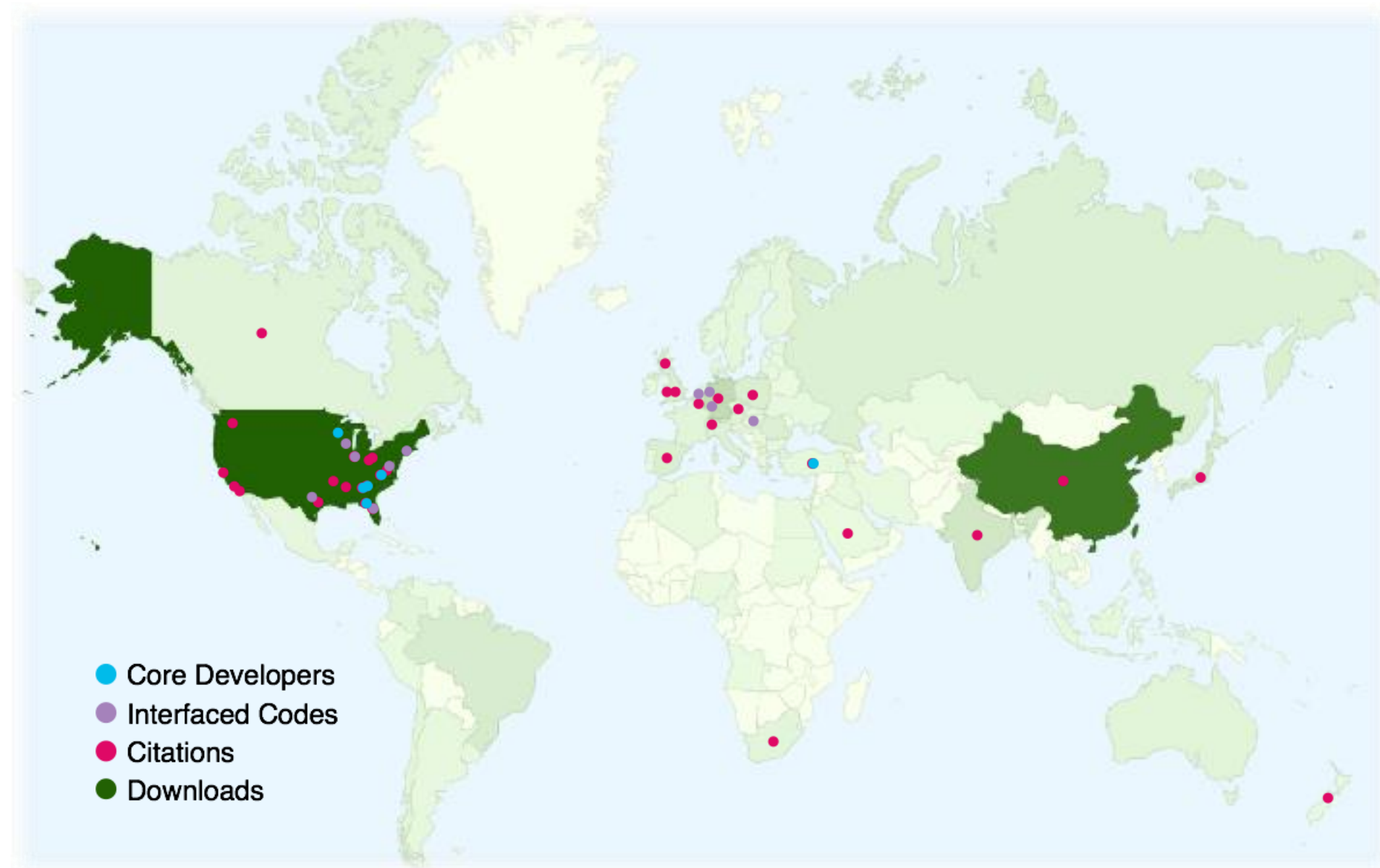
C. David Sherrill

*School of Chemistry and Biochemistry*

*School of Computational Science and Engineering*

*Georgia Institute of Technology*

# 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

- ADF

Visscher; FDE solvation

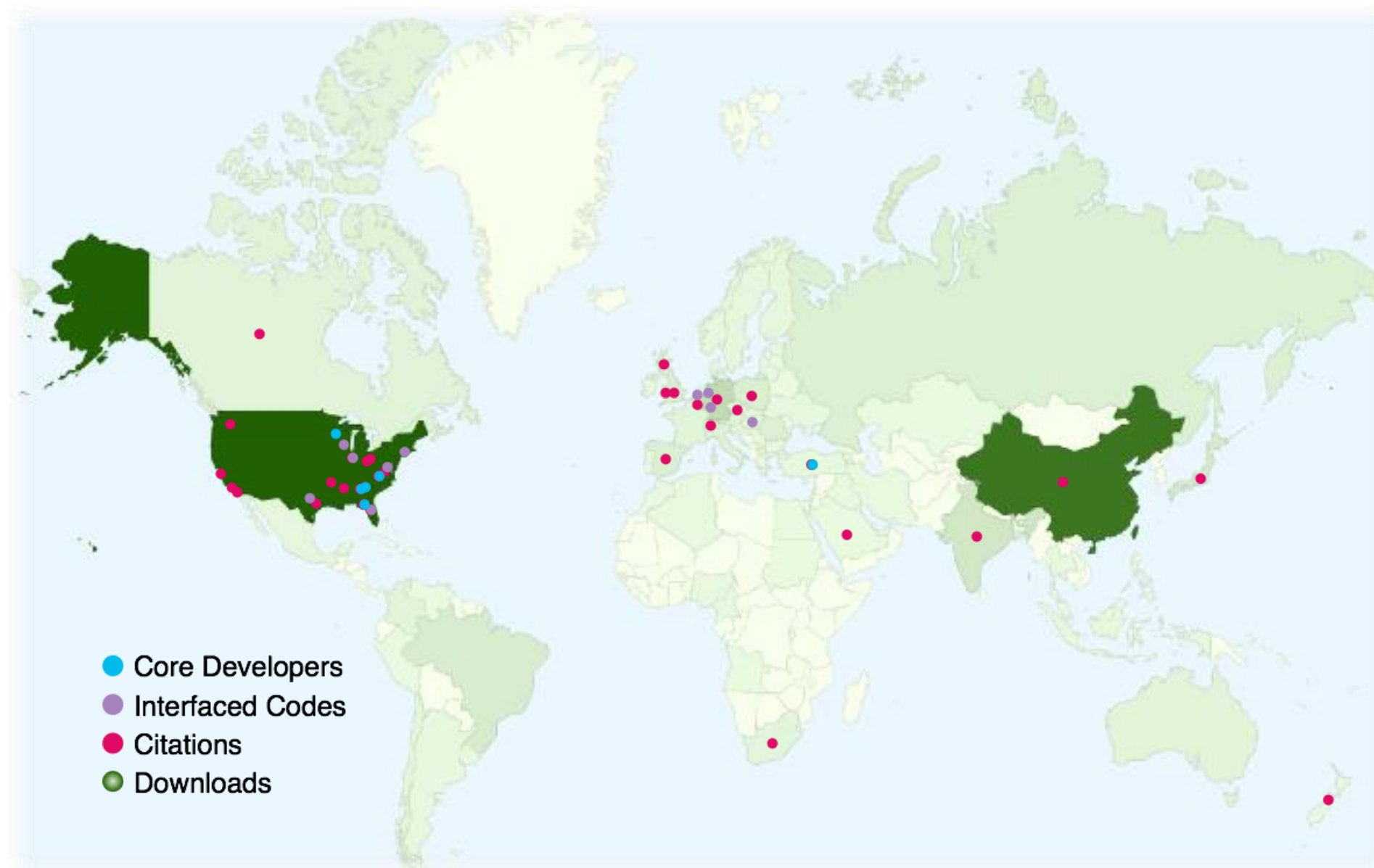
- PubChem

NIH; structure look-up

- CFOUR

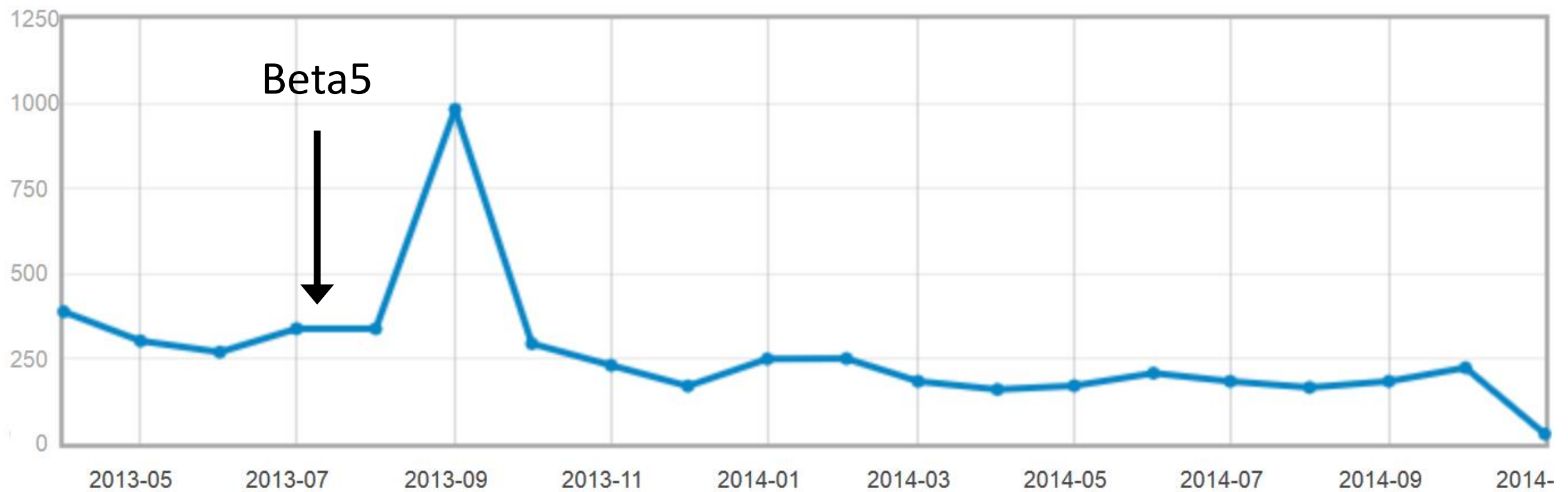
Gauss & Stanton

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) $\delta$ MP2]



# 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)

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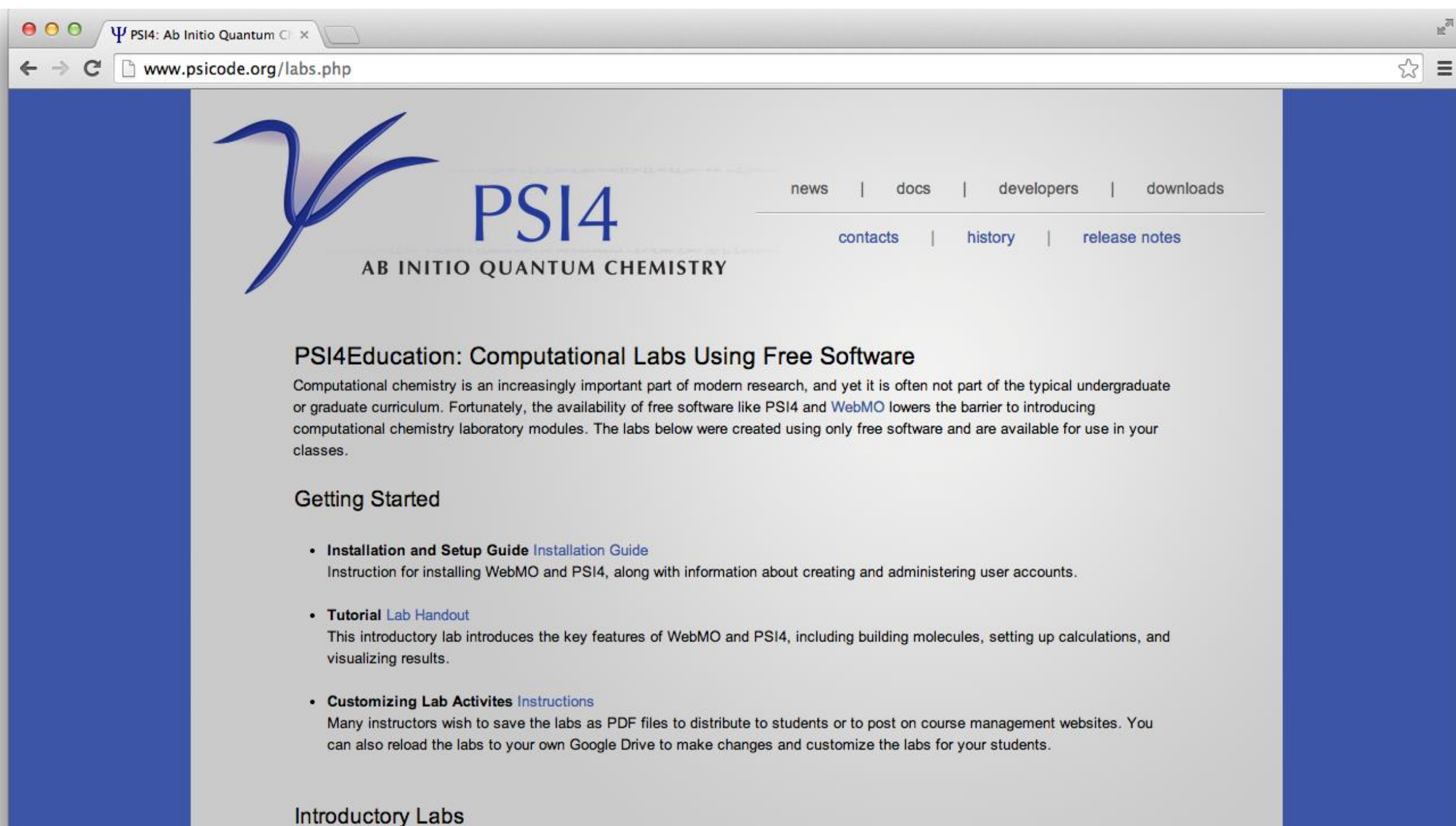
- Wants DK integrals
- Wants to be able to use MCSCF to get symmetry averaged HF orbitals for high symmetry cases
- Wants to be able to use pseudocanonical/natural/DFT orbitals in ccenergy (raises general question of orbital handling)

# NPA Capabilities

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- 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



The screenshot shows a web browser window with the address bar displaying `www.psicode.org/labs.php`. The page features a blue header with the PSI4 logo (a stylized blue psi symbol) and the text "PSI4 AB INITIO QUANTUM CHEMISTRY". To the right of the logo is a navigation menu with links: "news", "docs", "developers", "downloads", "contacts", "history", and "release notes". The main content area has a blue sidebar on the left and a white background for the text. The text includes the title "PSI4Education: Computational Labs Using Free Software", a paragraph about computational chemistry, a "Getting Started" section with three bullet points, and a section titled "Introductory Labs".

PSI4  
AB INITIO QUANTUM CHEMISTRY

news | docs | developers | downloads  
contacts | history | release notes

## PSI4Education: Computational Labs Using Free Software

Computational chemistry is an increasingly important part of modern research, and yet it is often not part of the typical undergraduate or graduate curriculum. Fortunately, the availability of free software like PSI4 and [WebMO](#) lowers the barrier to introducing computational chemistry laboratory modules. The labs below were created using only free software and are available for use in your classes.

### Getting Started

- **Installation and Setup Guide** [Installation Guide](#)  
Instruction for installing WebMO and PSI4, along with information about creating and administering user accounts.
- **Tutorial** [Lab Handout](#)  
This introductory lab introduces the key features of WebMO and PSI4, including building molecules, setting up calculations, and visualizing results.
- **Customizing Lab Activities** [Instructions](#)  
Many instructors wish to save the labs as PDF files to distribute to students or to post on course management websites. You can also reload the labs to your own Google Drive to make changes and customize the labs for your students.

### Introductory Labs

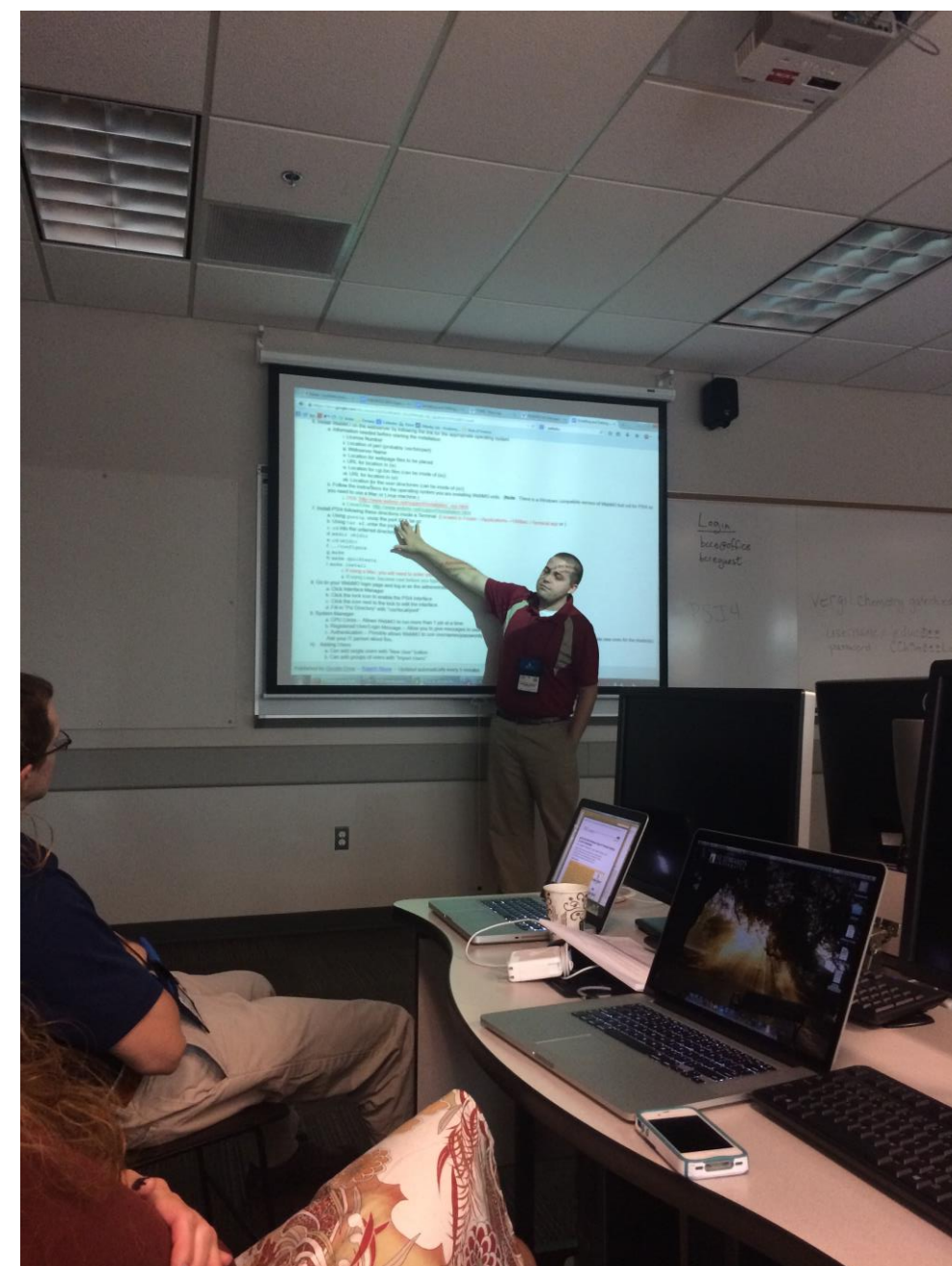


# PSI4Education Workshop

## 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



Ashley Ringer McDonald  
Cal Poly



Ryan Fortenberry  
Georgia Southern



Matthew Kennedy  
Georgia Tech



Tricia Shepherd  
St. Edwards

## Collaboration with WebMO:



J.R. Schmidt  
Wisconsin



Will Polik  
Hope College