Update on the Psi4 Project

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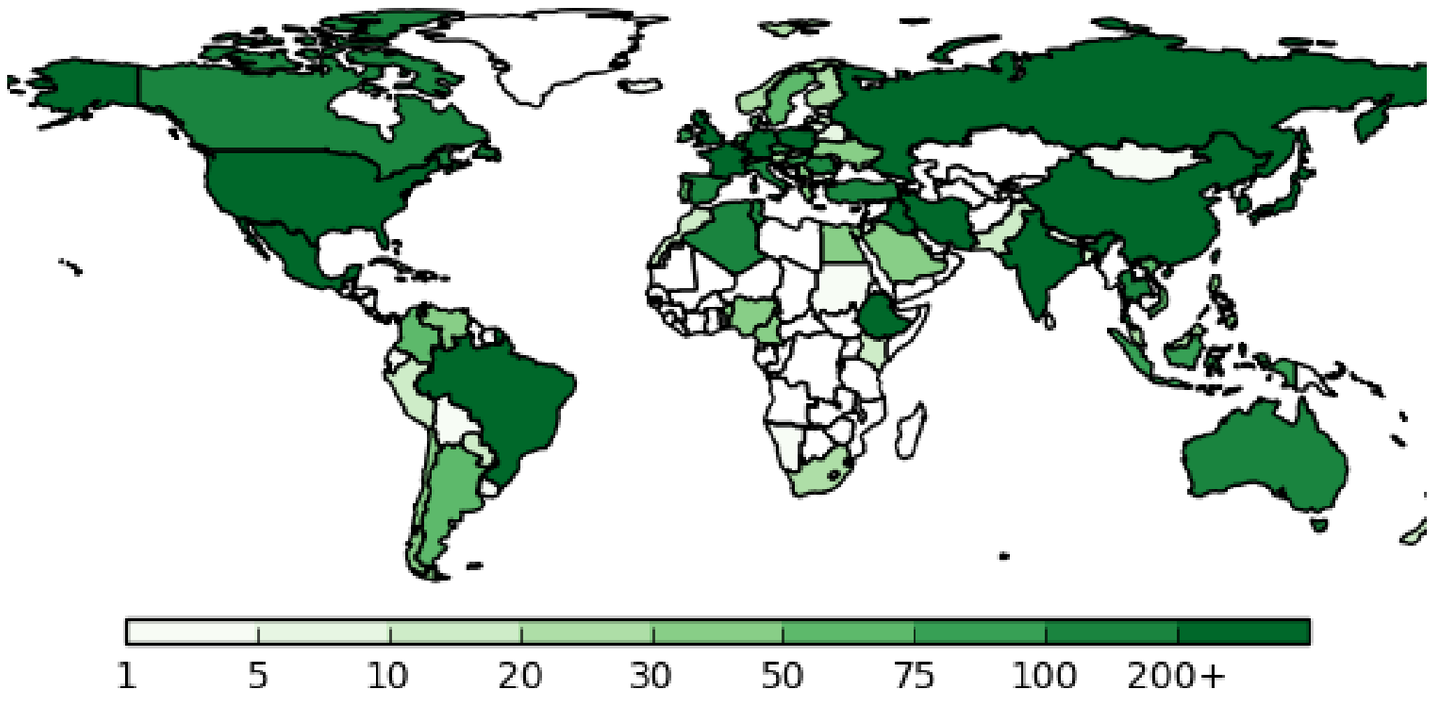
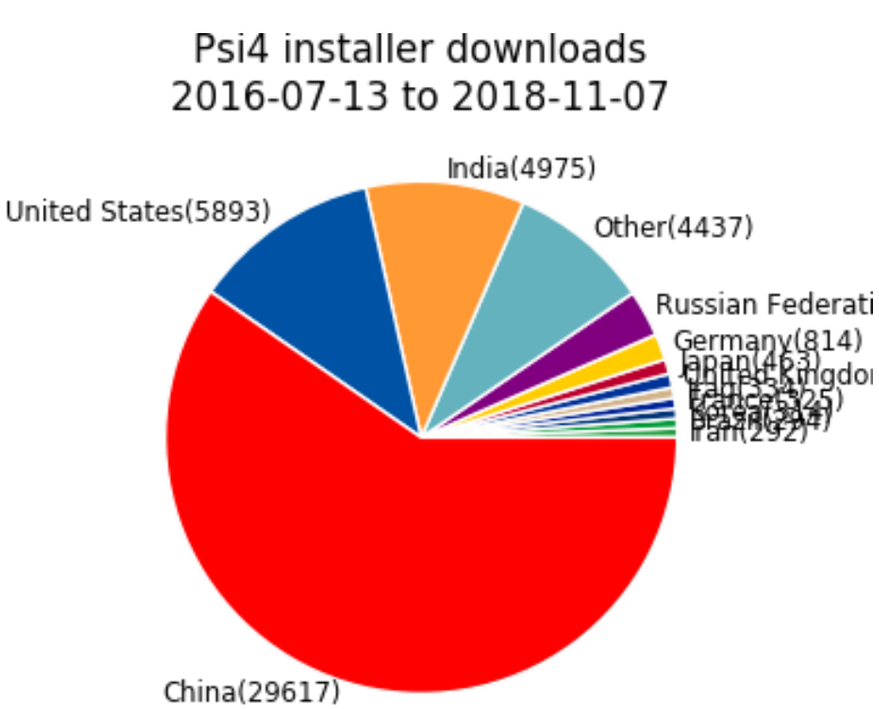
STATUS

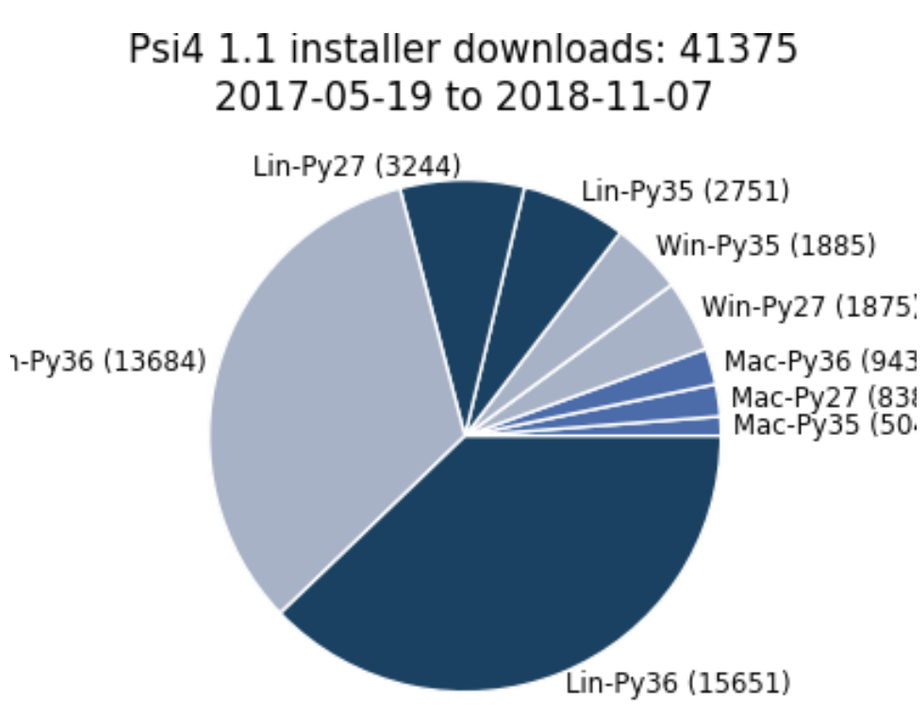
Psi4: The Papers

- J. M. Turney et al., *WIREs: Comput. Mol. Sci*. **2**, 556 (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
  - 379 citations as of November 2018
- R. M. Parrish et al., *JCTC* **13**, 3185 (2017)
  - 98 citations as of November 2018
- Psi4NumPy: D. G. A. Smith et al., *JCTC* **14**, 3504 (2018)
  - 1 citation as of November 2018

Psi4 Downloads



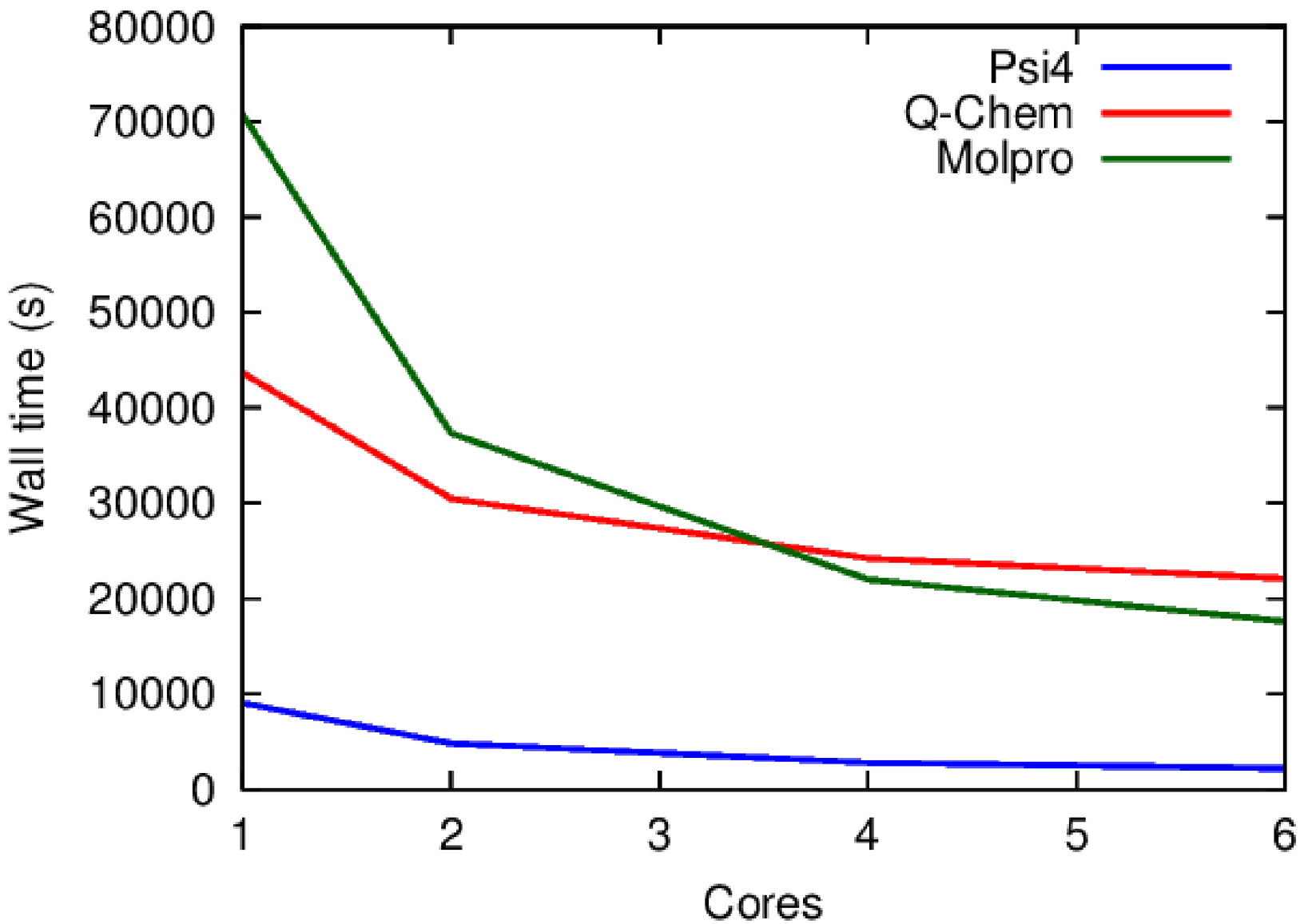




Performance

- For many types of computations, we are competitive with or better than commercial codes

Benzene dimer, DF-FNO-CCSD(T)/aug-cc-pVDZ with 99.5% occupancy (conventional for Molpro)



Anecdotal Feedback

- Lots of favorable comments from users and developers
- Psi4 seems to getting a lot of attention
- Positive comments about ease of installation

STRATEGY

Goals of the Psi4 Project

- Provide free, open-source software for quantum chemistry
- Make the code fast
- Make the code easy to use
- Provide good documentation for users
- Provide a robust infrastructure for rapid development of new theoretical methods
- Make the code friendly to reusable libraries, add-ons, plugins, etc. Promote development of reusable software components
- *Make Psi4 the premier free quantum chemistry program*

Who is in our Target Audience?

In priority order…

1. End users who want to do chemistry with a QC program
2. Educators who want to train students in QC
3. Developers who want to create / implement a method

Help these groups before helping others

Strengths

- Open-source license earns us points with users, developers, collaborators, and funding agencies; we were one of the first serious QC codes in this space
- Generally fast code
- Easy to use
- Compared to most other QC codes, cleaner code and better software development practices
- Good documentation for users

Weaknesses

- Not yet fully featured --- some QC projects can’t be done (or done as easily) with Psi4
  - Analytic DFT Hessians
  - IR intensities
  - ECP’s (in progress)
  - TDDFT
  - GPU capabilities
  - Gradients for solvent models

Opportunities

- Interoperability (with plugins, libraries, other QC codes, MM codes, …)
- Massive-scale automation
- Educational outreach (free, WebMO integration, Jupyter integration, …)

Strategic Aims

- Make Psi full featured (e.g., analytic SCF Hessians, IR intensities, ECP's, TDDFT)
- Make Psi the best code for multi-core architectures
- Add at least reasonable GPU support
- Make Psi truly user-friendly by adding GUI capabilities (e.g., interface to Avogadro 2)
- Leverage existing libraries wherever possible; let others solve some of our problems
- … and what then??