



## libmints



### Integrals 1/6, type-P

The "molecular" integrals module in Psi4 provides a uniform and convenient interface to 1e- and 2e- ints.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 7/36

## simint

Simint  
Simint  
Simint  
Simint

### Integrals 2/6, type-S

An alternate package for energy electron repulsion integrals. Specializes in vectorization for different microarchitectures.

Task: Find where libmints chooses between Libint2 and simint.

File/~Lines: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 8/36

## Libint2



### Integrals 3/6, type-I

The primary integrals dependency for Psi4, providing 2e- and many 1e- ints.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 9/36

## x2c



### Integrals 4/6, type-P

An implementation in libmints of ints for the exact-two-component exchange approach for scalar relativistic eff.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 10/36

## dkh



### Integrals 5/6, type-S

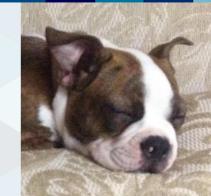
A dependency that provides ints to libmints for the Douglas-Kroll-Hess Hamiltonian for scalar relativistic effects.

Task: Find where enabling the dkh dep. makes CMake enable the Fortran lang.

File/~Lines: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 11/36

## ecpint



### Integrals 6/6, type-I

A dependency that provides E & deriv. 1e- ints for effective core potentials.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 12/36



## QCElemental



QC Deps 1/6, type-P

This Python module provides physical constants & periodic table but also parses your molecule string.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 13/36

## Libxc



QC Deps 2/6, type-S

The poster child for modular QC software, this C library provides exchange-correlation kernels and parameters for DFT functionals.

Task: Find where Psi4 grabs PBE0 from Libxc.

File/~Lines: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 14/36

## gau2grid



QC Deps 3/6, type-I

This C library vectorizes computing grid-2-gaussian collocation matrices.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 15/36

## OptKing



QC Deps 4/6, type-P

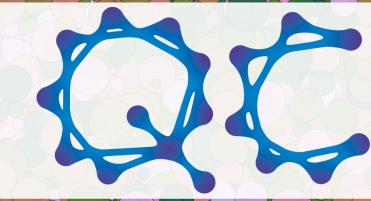
This Python module runs geometry optimizations and IRCs, driven by Psi4, QCEngine, or standalone.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 16/36

## QCEngine



QC Deps 5/6, type-S

This Python module runs QC software using QCSchema for I/O formats. Psi4 requires it for findif deriv, CBS mtds, MBE jobs, and DFT-D.

Task: Find one of two files where Psi4 sends AtomicInput schema to QCEngine.

File: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 17/36

## Libint2



QC Deps 6/6, type-I

This C++ library can be configured to provide integrals in 20 orderings.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 18/36



## ccenergy



### CC 1/6, type-P

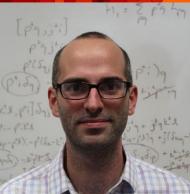
This suite of seven modules implements CC energies, derivatives, properties, and excited states.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 19/36

## fnocc



### CC 2/6, type-S

This module implements a wide variety of coupled-cluster energy methods very efficiently. It is named after the frozen natural orbitals approx.

Task: Which will fnocc \*not\* do? ccsd, qcisd(t), CONV, DF, CD, UHF, FNO, FC

NYI: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 20/36

## occ



### CC 3/6, type-I

The occ/dfocc pair runs CCD, CCSD(T), CCSD, & A-CCSD(T) but only for DF & CD.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

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## dlpno-cc



### CC 4/6, type-P

This in-development code builds upon DLPO-MP2 and is trialling the Einsums tensor library.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 22/36

## mrcc



### CC 5/6, type-S

This external project uses Psi4's SCF, then reads the orbitals to do any number of high-order expensive CC methods, with symmetry.

Task: `psi4.addons()` prints an availability list. What is the mrcc exe?

Exe: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 23/36

## psimrcc



### CC 6/6, type-I

This module runs Mukherjee (Mk) multi-ref CC atop 1- or 2-determinant ref.

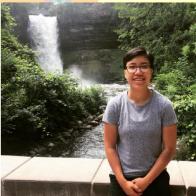
Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 24/36



## mp2f12



### MBPT 1/3, type-P

This in-development code for MP2 is the first since Psi3 to have F12 functionality.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 25/36

## dfmp2



### MBPT 2/3, type-S

Probably the first module written fresh for Psi4, dfmp2 runs RHF, UHF, & ROHF energies and RHF gradients, both all-electron and frozen-core.

Task: Find the user keyword that specifies the auxiliary basis for dfmp2.

Keyword: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 26/36

## detc1\_



### MBPT 3/3, type-I

If you've curious about MP12, detci is the module to call. V. small mols only.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 27/36

## CompositeJK



### SCF 1/3, type-P

This new class allows mix-and-match algorithms for Coulomb and Exchange. DFDIRJ, COSX, & LINK are the choices.

Task: Find & talk to the pictured GH user who is a primary developer for this module.

Dev's Initials: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 28/36

## LibXCFunctional



### SCF 2/3, type-S

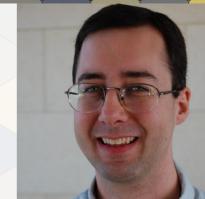
This class connects the Libxc data struct with the Psi4 Functional class. We can query Libxc's params for printing or alter its params for compute.

Task: Find a functional in Psi4 that needs its Libxc parameters "tweak"ed.

Functional: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 29/36

## detcas



### SCF 3/3, type-I

This offshoot of detci can run CASSCF and RASSCF both conventional and DF.

Task: (a) Sign up for a lightning talk -OR- (b) Find a trivial correction or clarification to docs or code comments, and make a PR thru GH website.

Talk Time/PR No.: \_\_\_\_\_

Trade these cards with other attendees to collect 'P', 'S', 'I' in the same category & fulfill their tasks. See lorlab for prize. 30/36



