

Python
INTERPRETER
Python-2.0

dot matrix multiplication

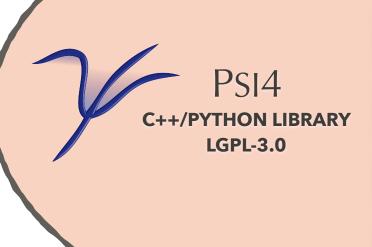
einsum generalized tensor contractions

linalg.solve linear matrix equation solution

linalg.eigh Hermitian matrix eigenv. decomp.

linalg.norm matrix & vector norm flavors

linalg.pinv generalized SVD matrix inv.



core.BasisSet gbs parsing, aux selection, manip.
core.MintsHelper 1 & 2e<sup>-</sup> ints, transformations

core.Matrix.asarray data container & exchange

core.Wavefunction orbital info & subsets

core.JK Coulomb & exchange mat. algorithms

energy('HF') reference for post-HF

core.Molecule geometry parsing, manip.

BLAS·LAPACK FORTRAN LIBRARY

**BSD-3-Clause** 

## Get these contents with

- > git clone https://github.com/psi4/psi4numpy.git
- > conda install psi4 -c psi4