Preparation

Generate a JAGP ansatz from a chosen basis set and a structure

makefort10.x

JAGP

Conversion

JAGP → JSD ansatz for a DFT calc.

convertfort10mol.x

JSD

DFT

Optimize coefficients of molecular orbitals by SCF calculation

prep.x

JSD

JSD → JAGP ansatz

convertfort10.x

JAGP

Correlated sampling

Check if the conversion is successful

readforward.x

JAGP

VMC optimization

Find an optimal variational parameter set

turborvb.x

VMC evaluation

Compute observables (energy, forces, etc…)

turborvb.x

LRDMC

Extrapolation with several different lattice spaces

turborvb.x

Preparation

Generate a JAGP ansatz from a chosen basis set and a structure

makefort10.x

JAGP

Conversion

JAGP → JSD ansatz for a DFT calc.

convertfort10mol.x

JSD

DFT

Optimize coefficients of molecular orbitals by SCF calculation

prep.x

JSD

convertfort10(mol).x

JSD → JAGP(n) ansatz

convertfortpfaff.x

JAGP → JPf ansatz

JAGP

JAGPn

JPf

turborvb.x

VMC optimization

Find an optimal variational parameter set

turborvb.x

Ionic dynamics

Langevin MD
Path Integral MD

turborvb.x

VMC evaluation

Compute observables (energy, forces, etc…)

turborvb.x

LRDMC

Extrapolation with several different lattice spaces

readforward.x

Post-processing

Correlated sampling, Electron and Ionic correlation functions, etc…