Python suites for implementing workflows with ab initio quantum Monte Carlo code

Kosuke Nakano, International School for Advanced Studies (SISSA), Japan Advanced Institute of Science and Technology (JAIST)

Ab initio quantum Monte Carlo study involves many complicated operations such as generating trial wave functions, optimizing variational parameters, and time-step (lattice-size) extrapolations. Automation of such tasks can decrease the required time for our work and reduce human errors as much as possible. We have recently developed python suites named "TurboGenius" and "TurboWorkflows" that allow us to implement workflows with ab initio quantum Monte Carlo code, "TurboRVB" [K. Nakano et al., J. Chem. Phys. 152, 204121 (2020)]. TurboGenius and TurboWorkflows are implemented by Python 3 in an object-oriented fashion. Users can utilize the provided modules as workflow templates or use the modules in their python scripts. TurboGenius also provides useful command-line interfaces by which users can quickly generate input files, run jobs, and analyze output results.

Ab-initio quantum Monte Carlo (QMC):

- Beyond DFT method. It explicitly considers the many-body electronic effect.
- Very high parallelization efficiency since the Monte Carlo Sampling is used.
- Computational order is much better than other high-accuracy methods.

TurboRVB Quantum Monte Carlo Package SISSA

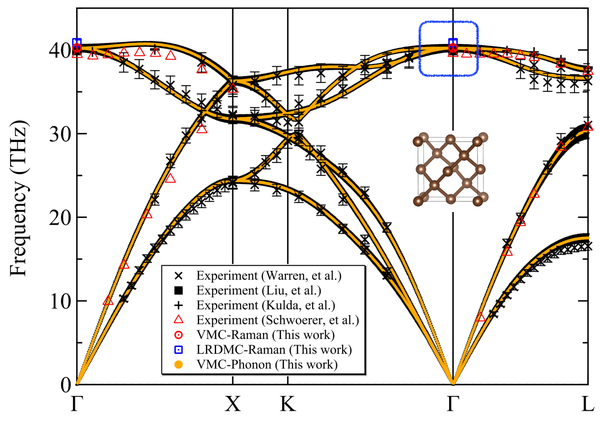
K. Nakano, et al., ***J. Chem. Phys.*** 152, 204121 (2020)

Being developed at SISSA in Trieste (Italy) under the supervision of Prof. Sandro Sorella.

- Implemented Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC)
- Computing Atomic Forces by exploiting the algorithmic differentiation (AD).
- Chosen as a Flagship code of Targeting Real Chemical accuracy at the EXascale (TREX) Project.

Application of TurboGenius (Phonon dispersion calculation)

combined with phonopy



Freq. of optical phonon at Γ

DFT-LDA	38.55 THz
VMC	40.65(38) THz
Experiment	40.35 THz

K. Nakano et al., ***Phys. Rev. B*** 103, L121110 (2021)

The result of phonon calculation of diamond on Fugaku.

Turbo-Genius (python wrappers):

TurboGenius

-Command line helpers

```
% turbogenius --help
Usage: turbogenius [OPTIONS] COMMAND [ARGS]...

Options:
--help Show this message and exit.

Commands:
convertfort10      convertfort10_genius
convertfort10mol   convertfort10mol_genius
convertpfaff       readforward_genius
convertwf          convert wavefunction
correlated-sampling correlated_sampling_genius
lrdmc              lrdmc_genius
lrdmcopt           lrdmcopt_genius
makefort10         makefort10_genius
prep               prep_genius
vmc                vmc_genius
vmcopt             vmcopt_genius
```

-Python classes

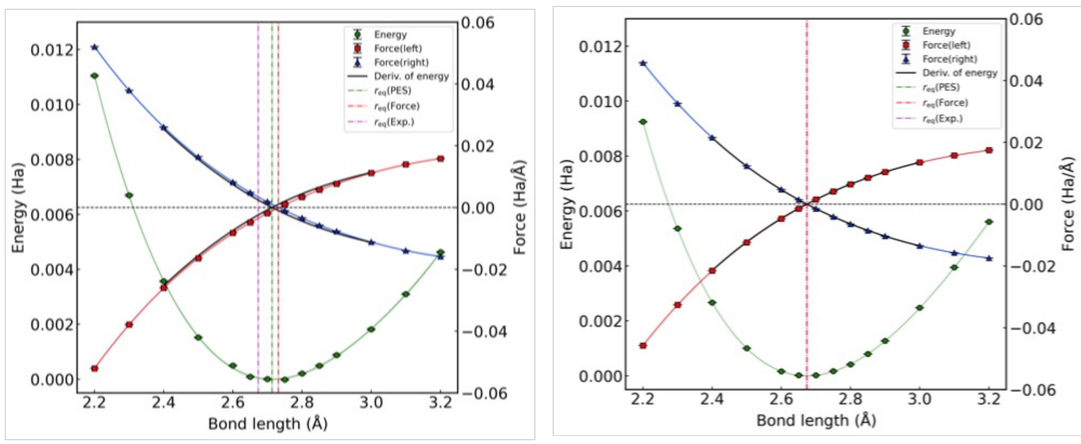
Parent Class	Class
-	Wavefuntion
Genius_IO	DFT_genius
	VMCopt_genius
	VMC_genius
	LRDMC_genius
	LRDMCopt_genius
	Correlated_sampling_genius

Wrappers for each binary!

K. Nakano et al., *in preparation* (2022)

Application of TurboWorkflows (Potential energy surface)

- Li_2 dimer (LRDMC with JDFT)
- Li_2 dimer (LRDMC with JAGPs)



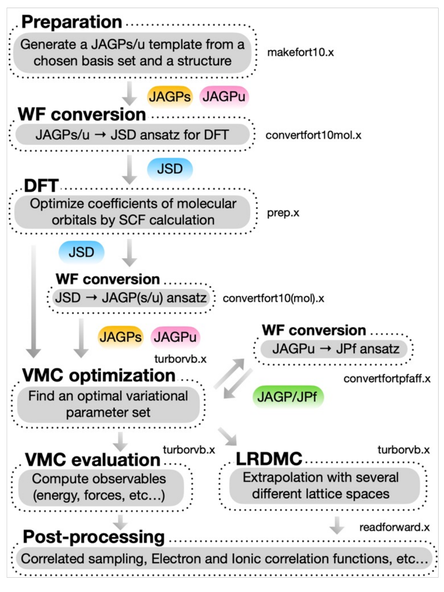
- Unbiased DMC forces can be realized in general??

K. Nakano et al., ***J. Chem. Phys.*** 156, 034101 (2022)

Turbo-Workflows (High-throughput pkg.):

Turbo Workflows

-Complicated workflows



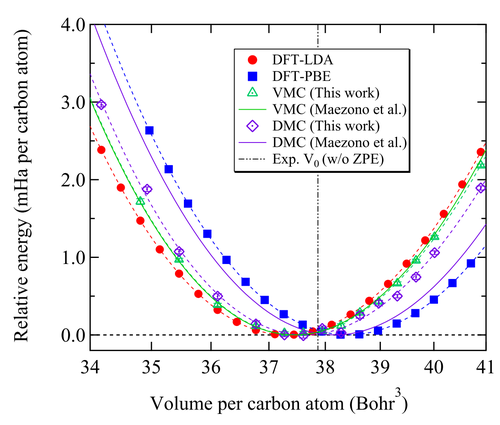
-Implemented by python !!

```
#******************
#! VMC
#******************
vmc_dir=os.path.join(root_dir, "03vmc")
os.makedirs(vmc_dir, exist_ok=True)

copy_files=["fort.10", "pseudo.dat"]
for file in copy_files:
    shutil.copy(os.path.join(vmcopt_dir,file), os.path.join(vmc_dir, file))
os.chdir(vmc_dir)

vmc_genius=VMC_genius(
                vmcsteps=vmc_steps,
                num_walkers=vmc_num_walkers,
                )

vmc_genius.generate_input()
vmc_genius.run()
vmc_genius.compute_energy_and_forces(bin_block=vmc_bin_block, warmupblocks=vmc_war

energy, error= vmc_genius.energy, vmc_genius.energy_error
print(f"VMC-JDFT energy = {energy:.5f} +- {error:3f} Ha")

os.chdir(root_dir)
```

Enabling us do high-throughput calculation!

K. Nakano et al., *in preparation* (2022)

Application of TurboWorkflows (Equation of States)



Anstaz: JDFT (WF=LDA)

Equilibrium lattice Parameters

VMC	6.693(1) Bohr
DMC	6.702(1) Bohr
Experiment	6.7193(5) Bohr

Underestimated…

- Nodal Surface optimization is needed?
- Finite-size extrapolation is needed?

Future works!

K. Nakano et al., ***Phys. Rev. B*** 103, L121110 (2021)

Future works

Supported by TREX Targeting Real chemical accuracy at the EXascale

Public release of TurboRVB (under discussion), TurboGenius (BSD-3 License), and TurboWorkflows (BSD-3 License).

TurboRVB Quantum Monte Carlo Package SISSA TurboGenius Turbo Workflows

Applications of TurboWorkflows. Any suggestions and collaborations are welcome!!! High-T_c superconductors. etc..