TREX webinar (20/Tue./2024) @ Online ~ 10 min

TurboRVB package

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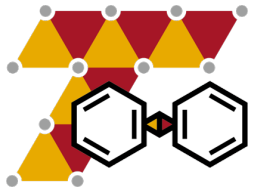
Our Quantum Monte Carlo packages



TurboRVB
Quantum Monte Carlo Package SISSA

QMC package (VMC, DMC, LRDMC, WF optimization).

K. Nakano*, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula*, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella* ***J. Chem. Phys.*** 152, 204121 (2020)

TurboGenius

Python wrappers and command-line interfaces.

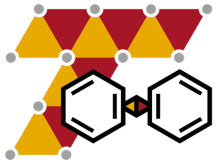
K. Nakano*, et al., ***J. Chem. Phys.*** 159, 224801 (2023)

Turbo Workflows

Workflow package realizing high-throughput calculations.

K. Nakano*, et al., ***J. Chem. Phys.*** 159, 224801 (2023)

TurboRVB features



TurboRVB
Quantum Monte Carlo Package SISSA

The main developer was Prof. Sandro Sorella.

The project is currently maintained by M. Casula and K. Nakano.

- Variational Monte Carlo (VMC) and Lattice regularized Diffusion Monte Carlo (LRDMC).

M. Casula et al., ***Phys. Rev. Lett*** 95, 100201 (2005)

- Flexible ansatz such as Antisymmetrized Geminal Power (AGP) and Pfaffian (Pf).

M. Casula et al., ***J. Chem. Phys. 119***, 6500 (2003)

C. Genovese et al., ***J. Chem. Theory Comput.*** 16, 6114 (2020)

- Atomic Forces by exploiting the algorithmic differentiation (AD).

S. Sorella et al., ***J. Chem. Phys.*** 133, 234111 (2010)

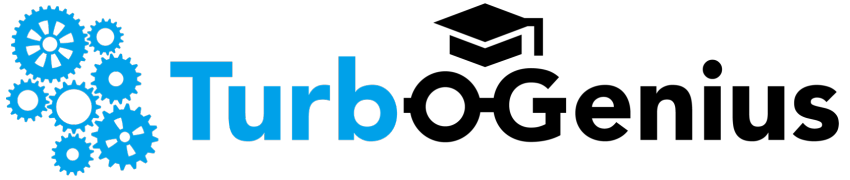
- Parallelized by MPI/OpenMP (hybrid) and GPU.

O. Kohulak et al., in prerаration (2023)

Python wrapper and workflows: TurboGenius

Listing 3. A python script to compute VMC energy of the hydrogen dimer

```python
# one needs "fort.10" (i.e., a WF file of the H2
    dimer) for this calculation.

# import modules
from turbogenius.vmc_genius import VMC_genius

# (1) create a vmc_genius instance
vmc_genius = VMC_genius(
    vmcsteps=600, # The number of MCMC steps
    num_walkers=40, # The number of walkers
)

# (2) generate an input file
vmc_genius.generate_input(input_name="datas_vmc.input")

# (3) launch a VMC run
vmc_genius.run(input_name="datas_vmc.input",
    output_name="out_vmc.o")

# (4) compute energy and forces with reblocking
vmc_genius.compute_energy_and_forces(bin_block=10,
    warmupblocks=10)

# print vmc energy
print(f"VMC energy = {vmc_genius.energy:.5f} +-
    {vmc_genius.energy_error:.5f} Ha")
```



https://github.com/kousuke-nakano/turbogenius

- QMC wrappers and command-line interfaces
- Implemented in object-oriented fashion by Python3
- Open-source under the BSD3 license (Jul. 2023-)

K. Nakano*, et al., ***J. Chem. Phys.*** 159, 224801 (2023)

TurboGenius paper recently published

The Journal of Chemical Physics ARTICLE pubs.aip.org/aip/jcp

TURBOGENIUS: Python suite for high-throughput calculations of *ab initio* quantum Monte Carlo methods

Cite as: J. Chem. Phys. 159, 224801 (2023); doi: 10.1063/5.0179003
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K. Nakano*, et al., ***J. Chem. Phys.*** 159, 224801 (2023)

Useful links

- Our website

https://turborvb.sissa.it

- TurboRVB GitHub

https://github.com/sissaschool/turborvb

- TurboGenius GitHub

https://github.com/kousuke-nakano/turbogenius

- TurboWorkflows GitHub

https://github.com/kousuke-nakano/turboworkflows

- Tutorials Collections

https://github.com/kousuke-nakano/turbotutorials

Established unbiased VMC forces by TurboRVB

Unbiased and affordable atomic forces in *ab initio* Variational Monte Carlo

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(Dated: January 1, 2024)

Ab initio quantum Monte Carlo (QMC) is a state-of-the-art numerical approach for evaluating accurate expectation values of many-body wavefunctions. However, one of the major drawbacks that still hinders widespread QMC applications is the lack of an affordable scheme to compute unbiased atomic forces. In this study, we propose a very efficient method to obtain unbiased atomic forces and pressures in the Variational Monte Carlo (VMC) framework with the Jastrow-correlated Slater determinant ansatz, exploiting the gauge-invariant and locality properties of its geminal representation. We demonstrate the effectiveness of our method for H_2 and Cl_2 molecules and for the cubic boron nitride crystal. Our framework has a better algorithmic scaling with the system size than the traditional finite-difference method, and, in practical applications, is as efficient as single-point VMC calculations. Thus, it paves the way to study dynamical properties of materials, such as phonons, and is beneficial for pursuing more reliable machine-learning interatomic potentials based on unbiased VMC forces.

K. Nakano*, et al., arXiv:2312.17608, under review (2024).

VMC force calculations with HF/DFT orbitals

We should keep in mind that variational parameters (p_i) are ***implicitly*** dependent on atomic positions.

$$\mathbf{F}_\alpha = -\frac{dE(\mathbf{R}_\alpha, p_i)}{d\mathbf{R}_\alpha} = -\left\langle \frac{\partial}{\partial \mathbf{R}_\alpha} E_{\mathrm{L}} \right\rangle$$

Hellmann–Feynman (PW, LO)

$$- 2\left\langle (E_{\mathrm{L}} - E) \frac{\partial \log \Psi_{\mathrm{T}}}{\partial \mathbf{R}_\alpha} \right\rangle$$

Pulay (only for LO)

$$- \left\langle \sum_{i=1}^{N_p} \frac{\partial E}{\partial p_i} \frac{dp_i}{d\mathbf{R}_\alpha} \right\rangle$$

Variational term (PW, LO)

(This doesn't exist in KS-DFT)

$\because \delta E / \delta \Psi = 0$

J. Tiihonen, et al., ***J. Chem. Phys.*** 154, 204111 (2021)

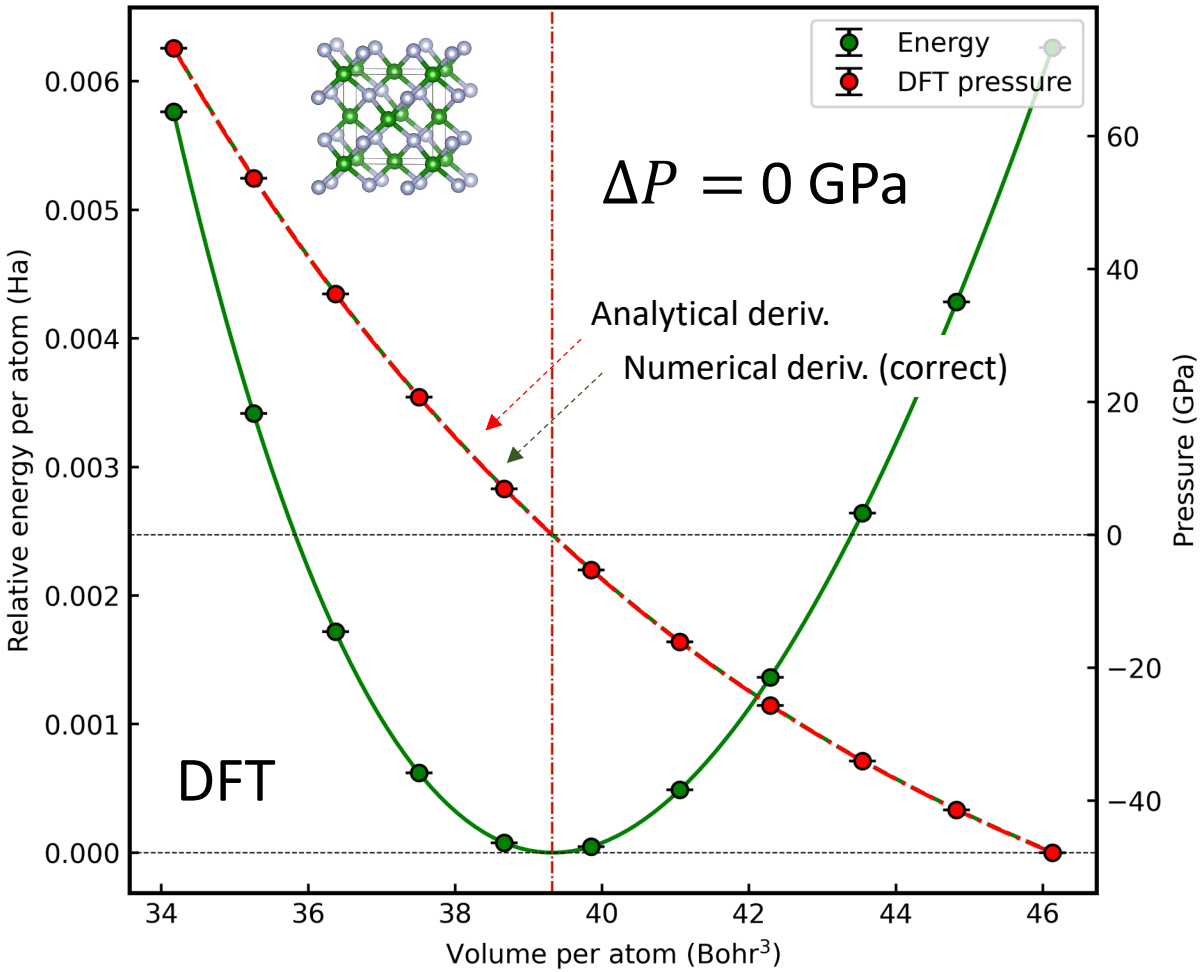
K. Nakano, et al., ***J. Chem. Phys***. 156, 034101 (2022)

The variational term has a finite value when a variational parameter in a given WF is **NOT** optimized.

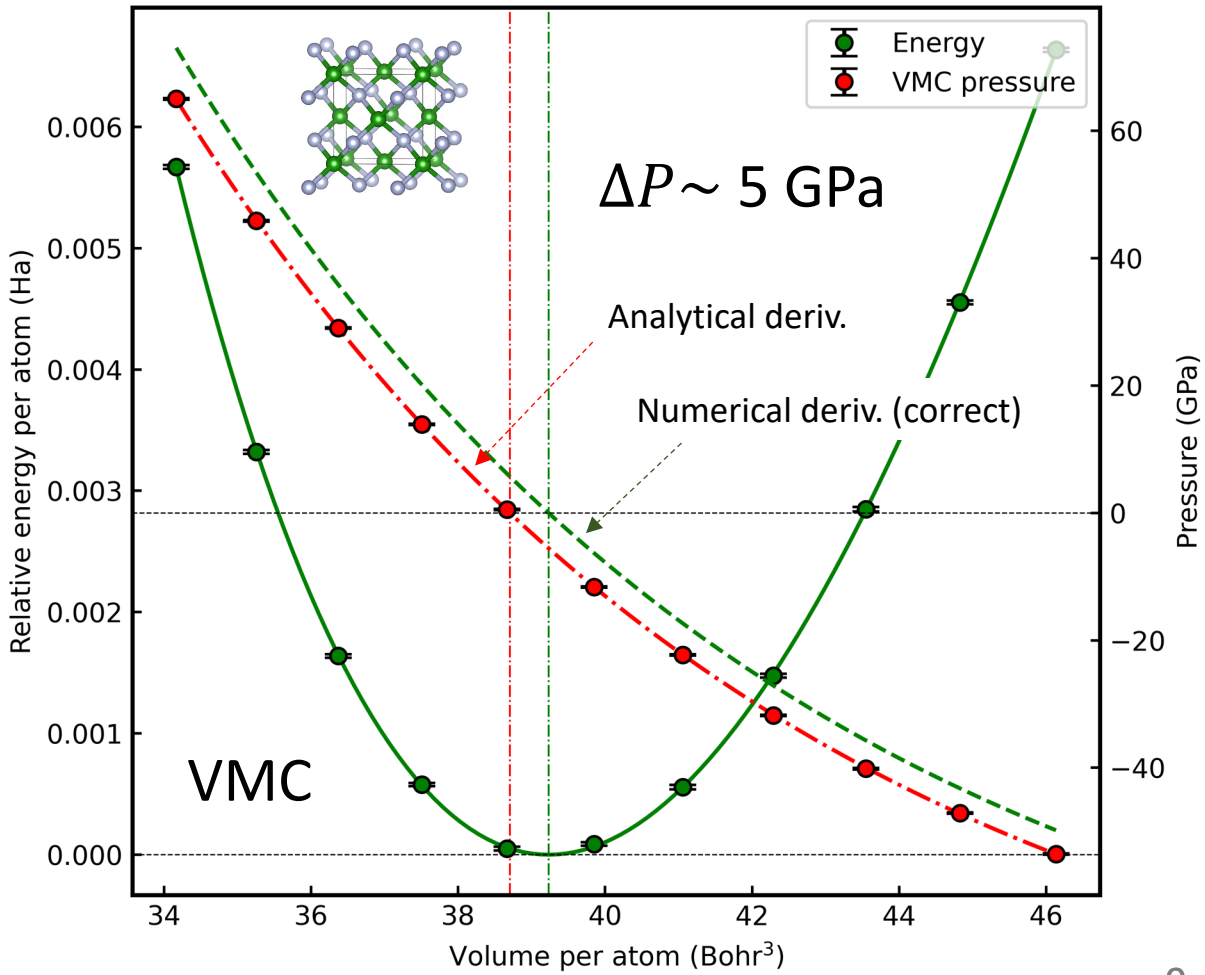
For large systems, one CANNOT afford to optimize all. **Jastrow Slater-Determinant (JSD)**.

Pressure bias in DFT and VMC calculations for BN

Cubic BN, Quantum Espresso: **DFT with LDA-PZ**



Cubic BN, TurboRVB: **VMC with JSD ansatz**



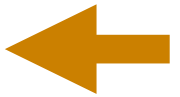
Compensation of the missing term

A solution is very simple: explicitly computing the missing term!

$$\mathbf{F}_\alpha = -\frac{dE(\mathbf{R}_\alpha, p_i)}{d\mathbf{R}_\alpha} = -\left\langle \frac{\partial}{\partial \mathbf{R}_\alpha} E_{\mathrm{L}} \right\rangle$$

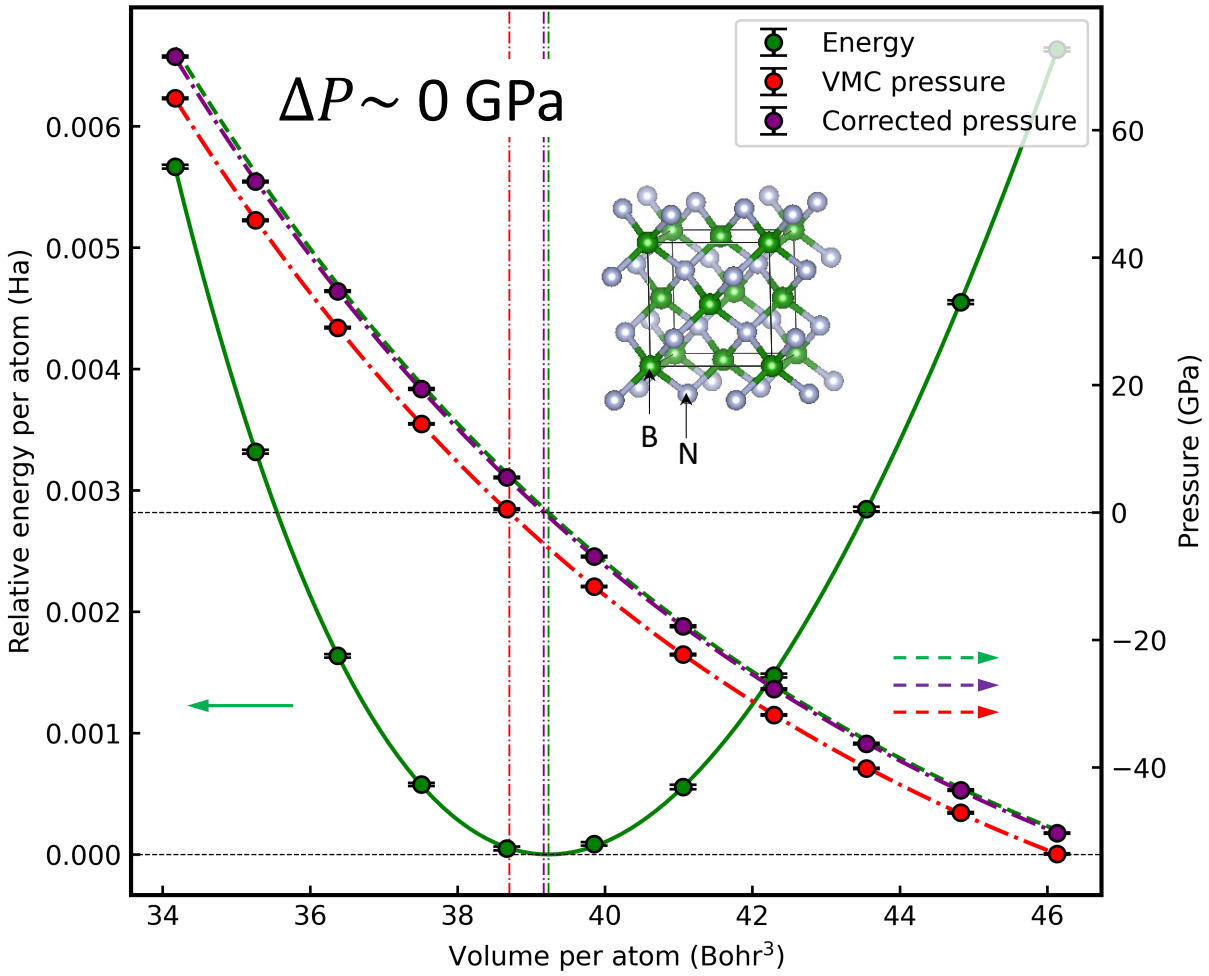
$$- 2\left\langle (E_{\mathrm{L}} - E) \frac{\partial \log \Psi_{\mathrm{T}}}{\partial \mathbf{R}_\alpha} \right\rangle$$

$$- \left\langle \sum_{i=1}^{N_p} \frac{\partial E}{\partial p_i} \frac{dp_i}{d\mathbf{R}_\alpha} \right\rangle$$



Compute this!

Application to Crystal (c-BN, 2x2x2, 256 el.)



K. Nakano*, et al., arXiv:2312.17608, under review (2024).

$$\mathbf{P}^{\mathrm{c}}_{\alpha} = -\langle \sum_{i,j}^{L,L} \frac{\partial E}{\partial \lambda_{i,j}} \frac{d\lambda_{i,j}}{dV} \rangle$$

TABLE II. Equilibrium lattice parameters and volumes per atom obtained by fitting the EOS, and from the regular VMC pressure and the corrected one. Zero point energy and temperature effects are not included.

Source	Lattice (Å)	Volume (Bohr^3)
EOS	3.5962(3)	39.232(9)
VMC pressure	3.5800(1)	38.704(5)
Corrected pressure	3.5943(2)	39.169(5)
Experiment	3.594 [a]	39.160 [a]

[a] These values are taken from Ref. 49.

Perspectives

- Refactoring is in progress.
- Better documentations and tutorials.

Any suggestion is appreciated!

Thank you very much for your attention