

# Quantum Many-Body Simulations of Double Dot System

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# Introduction

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# Quantum-Dot

- Small semiconductor nanostructures
- 2-10 nanometers with 10—50 particles

# Quantum-Dot Model

- Schrödinger equation
  - $\mathcal{H}|\psi\rangle = E|\psi\rangle$

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- $$\mathcal{H} = -\frac{1}{2} \sum_i \nabla_i^2 + \sum_{i < j} f(\mathbf{r}_i, \mathbf{r}_j) - \frac{1}{2} \sum_k \frac{\nabla_k^2}{M_k} + \sum_{k < l} g(\mathbf{R}_k, \mathbf{R}_l) + V(\mathbf{R}, \mathbf{r})$$

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- Born-Oppenheimer Approximation
  - Ignore Nuclei
  - $\sum_k \frac{\nabla_k^2}{M_k}$  gone
  - $\sum_{k<l} g(\mathbf{R}_k, \mathbf{R}_l)$  constant

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# Quantum-Dot Model

- Interaction

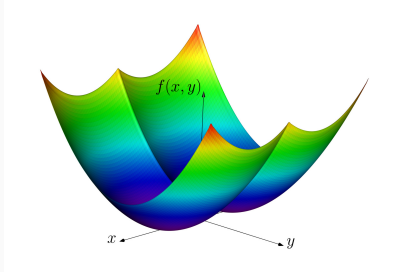
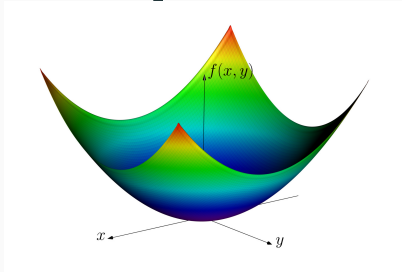
- $f(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$

# Quantum-Dot Model

- Interaction: Coulomb repulsion
  - $f(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$
- Confinement: Harmonic Oscillator<sup>1</sup>, Double-Well<sup>2</sup>

$$V(\mathbf{r}) = \frac{1}{2} \omega m r^2$$

$$V(\mathbf{R}, \mathbf{r}) = \frac{1}{2} m \omega^2 (r^2 - \delta R|x| + R^2)$$



<sup>1</sup>S. Kvaal. “Harmonic Oscillator Eigenfunction Expansions, Quantum dots, and Effective Interactions”. In: *Phys. Rev. B* 80 (4 2009), p. 045321.

<sup>2</sup>M. J. A. Schuetz et al. “Nuclear Spin Dynamics in Double Quantum Dots: Multistability, Dynamical Polarization, Criticality, and Entanglement”. In: *Phys. Rev. B* 89 (19 2014), p. 195310.

# Methods

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# Hartree-Fock Variational Monte-Carlo

$$E_0 \leq \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

# Methods: Slater Determinant and Energy Functional

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- Pauli Principle

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- Pauli Principle
- Slater Determinant
  - $\Psi_T^{\text{AS}} = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \mathcal{P}_P \prod_i \psi_i$
  - $\Psi_T^{\text{S}} = \sqrt{\frac{\prod_{i=1}^N n_i!}{N!}} \sum_P \mathcal{P}_P \prod_i \psi_i$

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- Slater Determinant
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  - $\Psi_T^{\text{S}} = \sqrt{\frac{\prod_{i=1}^N n_i!}{N!}} \sum_P \mathcal{P}_P \prod_i \psi_i$
- $E[\Psi] = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \sum_p \langle p | \mathcal{H}_0 | p \rangle + \frac{1}{2} \sum_{p,q} [\langle pq | f_{12} | pq \rangle \pm \langle pq | f_{12} | qp \rangle]$
- $\mathcal{H}_0 = -\frac{1}{2} \sum_i \nabla_i^2 + V(r)$

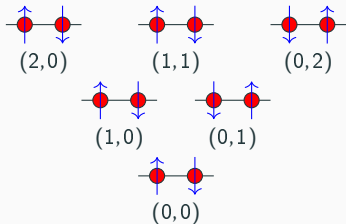


# Methods: Hartree-Fock

- Assumptions
  - The Born-Oppenheimer approximation holds.
  - All relativistic effects are negligible.
  - The wavefunction can be described by a single *Slater determinant*.
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  - Fock-operator:  $\mathcal{F} \equiv \mathcal{H}_0 + \mathcal{J} \pm \mathcal{K}$ 
    - $\mathcal{J} \equiv \langle \psi_k^* | f_{12} | \psi_k \rangle = \int \psi_k^*(\mathbf{r}) f_{12} \psi_k(\mathbf{r}) d\mathbf{r}$
    - $\mathcal{K} \equiv \langle \psi_k^* | f_{12} | \psi \rangle = \int \psi_k^*(\mathbf{r}) f_{12} \psi(\mathbf{r}) d\mathbf{r}$
    - $\mathcal{F} | \psi \rangle = \boldsymbol{\varepsilon} | \psi \rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \dots, \varepsilon_N)$

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    - $\mathcal{F} | \psi \rangle = \boldsymbol{\varepsilon} | \psi \rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \dots, \varepsilon_N)$
  - $N+1$  equations to be solved.

## Methods: Hartree-Fock

- Integrate out spin
- Pair spins as:  $\{\psi_{2I-1}, \psi_{2I}\} = \{\phi_I(\mathbf{r})\alpha(s), \phi_I(\mathbf{r})\beta(s)\}$



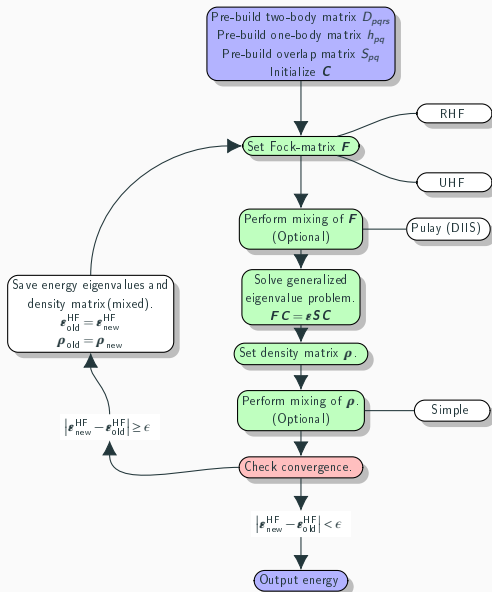
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- Expand:  $\phi_i(\mathbf{r}) = \sum_{p=1}^L C_{pi} \chi_p(\mathbf{r})$
- Roothan-Hall:  $\mathbf{F}\mathbf{C}_i = \epsilon \mathbf{S}\mathbf{C}_i$ 
  - $F_{pq} = h_{pq} + \sum_{pq} \rho_{pq} (2D_{prqs} \pm D_{prsq})$
  - $h_{pq} \equiv \langle p | h | q \rangle$
  - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi} C_{qi}^*$
  - $D_{pqrs} \equiv \langle pq | f_{12} | rs \rangle$
  - $S_{pq} \equiv \langle p | q \rangle$
- Poople-Nesbet:  $\mathbf{F}^+ \mathbf{C}^+ = \epsilon \mathbf{S} \mathbf{C}^+, \mathbf{F}^- \mathbf{C}^- = \epsilon^- \mathbf{S} \mathbf{C}^-$ 
  - $F_{pq}^{\pm} = h_{pq} + \sum_{k_{\pm}} \sum_{rs} C_{rk_{\pm}}^{\pm\dagger} C_{sk_{\pm}}^{\pm\dagger} [D_{prqs} - D_{prsq}] + \sum_{k_{\mp}} \sum_{rs} C_{rk_{\mp}}^{\mp\dagger} C_{sk_{\mp}}^{\mp\dagger} D_{prqs}$

# Methods: Hartree-Fock



- Variational Principle

# Methods: Variational Monte-Carlo

- Variational Principle
- Rewrite expectation value:  $\frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \int \frac{\Psi^* \mathcal{H} \Psi}{\int \Psi^* \Psi dr} dr = \int \frac{|\Psi|^2 E_L}{\int \Psi^* \Psi dr} dr$ 
  - $E_L(R; \alpha) \equiv \frac{1}{\Psi} \mathcal{H} \Psi$
  - $P(R) \equiv \frac{|\psi_T|^2}{\langle \Psi_T | \Psi_T \rangle}$

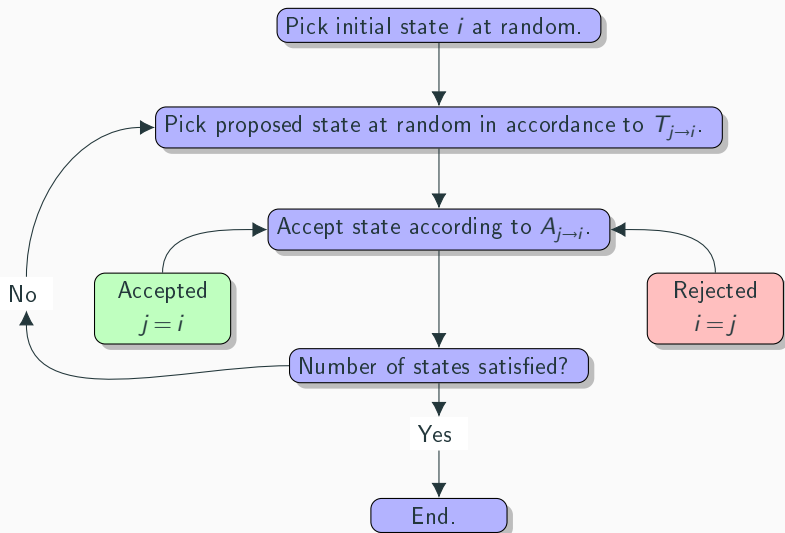
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  - $P(R) \equiv \frac{|\psi_T|^2}{\langle \Psi_T | \Psi_T \rangle}$
- Metropolis-Hastings Algorithm
  - $r^{\text{new}} = r^{\text{old}} + \Delta t \xi$
  - $A_{i \rightarrow j} = \min\left(\frac{P_{i \rightarrow j}}{P_{j \rightarrow i}} \frac{T_{i \rightarrow j}}{T_{j \rightarrow i}}, 1\right)$

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  - Importance Sampling
    - $r^{\text{new}} = r^{\text{old}} + D \Delta t F^{\text{old}} + \sqrt{\Delta t} \xi$
    - $F = \frac{2}{\Psi} \nabla \Psi$
    - $\frac{T(b, a, \Delta t)}{T(a, b, \Delta t)} = \sum_i \exp\left(-\frac{(r_i^{(b)} - r_i^{(a)} - D \Delta t F_i^{(a)})^2}{4 D \Delta t} + \frac{(r_i^{(a)} - r_i^{(b)} - D \Delta t F_i^{(b)})^2}{4 D \Delta t}\right)$

## Methods: Variational Monte-Carlo





# Wavefunction

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$$\phi_i(\mathbf{r}) = \sum_{p=1}^L C_{pi} \chi_p(\mathbf{r})$$

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$$\langle \phi_i(\mathbf{r}) | \phi_j(\mathbf{r}) \rangle$$

$$\langle \phi_i(\mathbf{r}) | x_d^k | \phi_j(\mathbf{r}) \rangle$$

$$\langle \phi_i(\mathbf{r}) | \nabla^2 | \phi_j(\mathbf{r}) \rangle$$

$$\langle \phi_i(\mathbf{r}_1) \phi_j(\mathbf{r}_2) | f_{12} | \phi_k(\mathbf{r}_1) \phi_l(\mathbf{r}_2) \rangle$$

## Wavefunction: Single-Well

- Hermite Function:  $\psi_n(\mathbf{r}) \equiv \prod_d N_d H_{n_d}(\sqrt{\omega} x_d) \exp(-\frac{\omega}{2} x_d^2)$

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- Solution in polar<sup>3</sup>

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- $\psi_n(\mathbf{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \mathbf{r}, \mathbf{0}\right)$

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- Solution in Cartesian<sup>6</sup>

$$\langle g_i(\mathbf{r}) | g_j(\mathbf{r}) \rangle$$

$$\langle g_i(\mathbf{r}) | x_d^k | g_j(\mathbf{r}) \rangle$$

$$\langle g_i(\mathbf{r}) | \nabla^2 | g_j(\mathbf{r}) \rangle$$

$$\langle g_i(\mathbf{r}_1) g_j(\mathbf{r}_2) | f_{12} | g_k(\mathbf{r}_1) g_l(\mathbf{r}_2) \rangle$$

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<sup>6</sup>J. Olsen T. Helgaker P. Jørgensen. *Molecular Electronic-Structure Theory*. Wiley, 2014. isbn: 978-0-47-196755-2. doi: 10.1002/9781119019572.



# Wavefunction: Single-Well Integral Elements

$$\langle \psi_i^{\text{HO}} | \psi_j^{\text{HO}} \rangle = N_i \delta_{ij}$$

$$\langle \psi_i^{\text{HO}} | h^{\text{HO}} | \psi_j^{\text{HO}} \rangle = N_i \epsilon_i^{\text{HO}} \delta_{ij}$$

$$\langle \psi_i^{\text{HO}} \psi_j^{\text{HO}} | \frac{1}{r_{12}} | \psi_k^{\text{HO}} \psi_l^{\text{HO}} \rangle = \frac{aN_{ijkl}}{\sqrt{2\omega}} \sum_{tuvw} H_{tuvw}^{ijkl} \sum_{pq}^{t+v,u+w} E_p^{tv} E_q^{uw} (-1)^q \zeta_{p+q} \left( \frac{\omega}{2}, \mathbf{0} \right)$$

$$E_t^{i+1,j} = \frac{1}{2(\alpha + \beta)} E_{t-1}^{ij} - \frac{\beta}{\alpha + \beta} (A_x - B_x) E_t^{ij} + (t+1) E_{t+1}^{ij}$$

$$E_t^{i,j+1} = \frac{1}{2(\alpha + \beta)} E_{t-1}^{ij} - \frac{\alpha}{\alpha + \beta} (A_y - B_y) E_t^{ij} + (t+1) E_{t+1}^{ij}$$

$$E_0^{00} = K_{AB}$$

$$\zeta_{t+1,u}^n = t \zeta_{t-1,u}^{n+1} + X_{AB} \zeta_{t,u}^{n+1}$$

$$\zeta_{t,u+1}^n = u \zeta_{t,u-1}^{n+1} + Y_{AB} \zeta_{t,u}^{n+1}$$

$$\zeta_{00}^n = \left( \frac{-2\alpha\beta}{\alpha + \beta} \right)^n \zeta_n \left( \frac{\alpha\beta}{\alpha + \beta} R_{AB}^2 \right)$$

$$\zeta_n(x) = \int_{-1}^1 \frac{u^{2n}}{\sqrt{1-u^2}} e^{-u^2 x} du$$

$$\zeta_{t+1,u,v}^n = t \zeta_{t-1,u,v}^{n+1} + X_{AB} \zeta_{t,u,v}^{n+1}$$

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## Wavefunction: Double-Well

- Perturbation of harmonic oscillator:  $U^{\text{DW}}(r) = V^{\text{HO}}(r) + V_n^{\text{DW}}(r)$

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- Integral-Elements

$$\langle \psi_p^{\text{DW}} | \psi_q^{\text{DW}} \rangle = \delta_{pq}$$

$$\langle \psi_p^{\text{DW}} | h^{\text{DW}} | \psi_q^{\text{DW}} \rangle = \epsilon_p^{\text{DW}} \delta_{pq}$$

$$\langle \psi_p^{\text{DW}} \psi_q^{\text{DW}} | \frac{1}{r_{12}} | \psi_r^{\text{DW}} \psi_s^{\text{DW}} \rangle = \sum_{ijkl} C_{tp}^{\text{DW}} C_{uq}^{\text{DW}} C_{vr}^{\text{DW}} C_{ws}^{\text{DW}} \langle \psi_t^{\text{HO}} \psi_u^{\text{HO}} | \frac{1}{r_{12}} | \psi_v^{\text{HO}} \psi_w^{\text{HO}} \rangle$$

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- NQS:  $J_{\text{NQS}} = e^{-\sum_{i=1}^N \frac{(r_i - a_i)^2}{2\sigma^2}} \prod_j \left( 1 + e^{b_j + \sum_{i=1}^N \sum_{d=1}^D \frac{x_i^{(d)} w_{i+d,j}}{\sigma^2}} \right)$

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- Hartree-Fock:  $\Phi_{ij} = \sum_l C_{jl} \psi_{n_l}^{\text{HO}}(\sqrt{\omega} r_i)$
- Modified Hartree-Fock:  $\Phi_{ij} = \sum_l C_{jl} \psi_{n_l}^{\text{HO}}(\sqrt{\alpha\omega} r_i)$
- Padé-Jastrow:  $J_{\text{Padé}} = \prod_{i < j} e^{\frac{a_{ij} r_{ij}}{1 + \beta r_{ij}}}$
- NQS:  $J_{\text{NQS}} = e^{-\sum_{i=1}^N \frac{(r_i - a_i)^2}{2\sigma^2}} \prod_j \left( 1 + e^{b_j + \sum_{i=1}^N \sum_{d=1}^D \frac{x_i^{(d)} w_{i+d,j}}{\sigma^2}} \right)$
- Padé-NQS:  $J = J_{\text{Padé}} J_{\text{NQS}}$

# Wavefunction: Slater-Jastrow

- Slater determinant:  $\psi = \det(\Phi(\mathbf{R}; \boldsymbol{\alpha})) \xi(s)$
- Modified Hermite:  $\Phi_{ij} = \psi_{n_j}^{\text{HO}}(\sqrt{\alpha\omega} r_i) = \prod_d N_d H_{n_d}(\sqrt{\alpha\omega} x_d) e^{-\frac{\alpha\omega}{2} x_d^2}$
- Hartree-Fock:  $\Phi_{ij} = \sum_l C_{jl} \psi_{n_l}^{\text{HO}}(\sqrt{\omega} r_i)$
- Modified Hartree-Fock:  $\Phi_{ij} = \sum_l C_{jl} \psi_{n_l}^{\text{HO}}(\sqrt{\alpha\omega} r_i)$
- Padé-Jastrow:  $J_{\text{Padé}} = \prod_{i < j} e^{\frac{a_{ij} r_{ij}}{1 + \beta r_{ij}}}$
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- Padé-NQS:  $J = J_{\text{Padé}} J_{\text{NQS}}$

# Implementation

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- C++ and Eigen



# Implementation

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- C++ and Eigen
  - Performance

# Implementation

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- C++ and Eigen
  - Performance
  - Generalization

# Implementation

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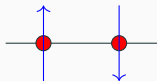
- C++ and Eigen
  - Performance
  - Generalization
- Python

# Implementation

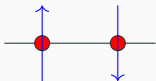
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- C++ and Eigen
  - Performance
  - Generalization
- Python
  - Generate C++ code

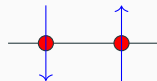
## Implementation: Cartesian



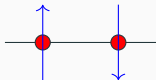
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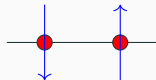
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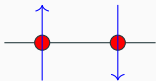
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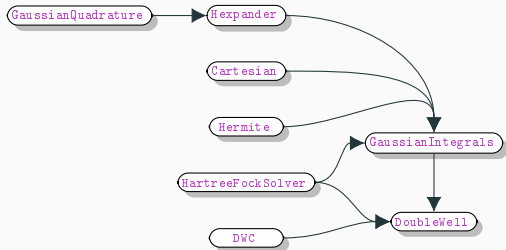


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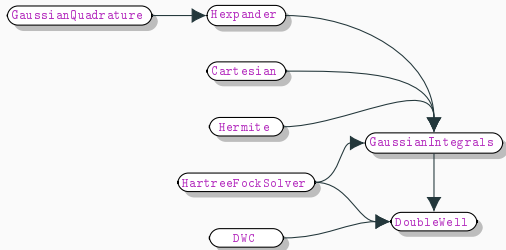


(0,0)

# Implementation: Hartree-Fock

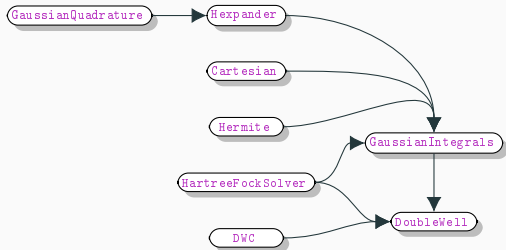


# Implementation: Hartree-Fock



- Parallelization
  - Two-body element is computationally expensive
  - $$S_i = \sum_{j=0}^{P_i} \prod_d (n_{j_d} + 1)$$

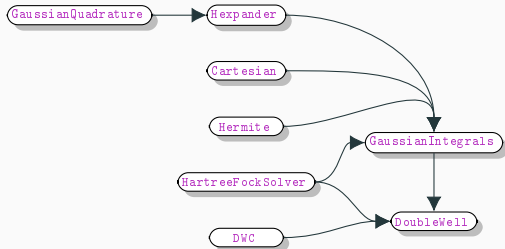
# Implementation: Hartree-Fock



- Parallelization
  - Two-body element is computationally expensive
  - $$S_i = \sum_{j=0}^{P_i} \prod_d (n_{j_d} + 1)$$
- Hartree-Fock algorithm only run on one process

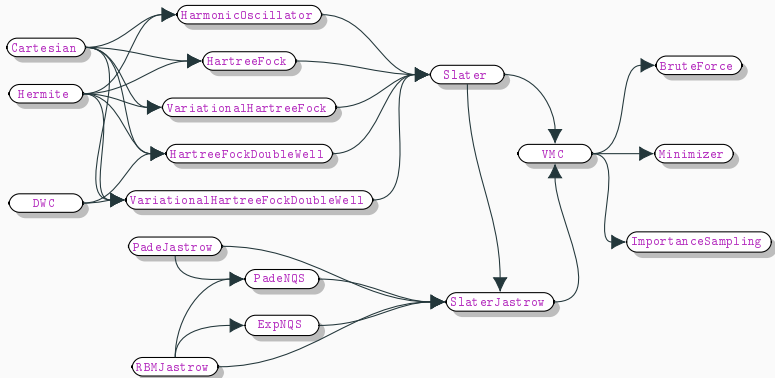


# Implementation: Hartree-Fock



- Parallelization
  - Two-body element is computationally expensive
  - $$S_i = \sum_{j=0}^{P_i} \prod_d (n_{jd} + 1)$$
- Hartree-Fock algorithm only run on one process
- Tabulation of Two-Body matrix

# Implementation: Variational Monte-Carlo



## Summary and Conclusion

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Questions?

# Questions

Questions?