Variational quantum Monte Carlo with neural network ansatz for open quantum systems

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GPU Day
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Open quantum systems

EPFL

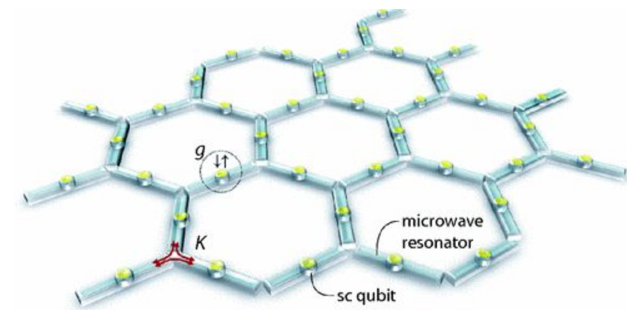
- Coupling to external environment
- Time evolution as Linbladian master equation

$$\dot{\hat{\rho}} = \underbrace{-\frac{i}{\hbar}\left[\hat{\mathcal{H}}, \hat{\rho}\right]}_{\text{unitary dynamics}} \underbrace{-\sum_j \frac{\gamma_j}{2}\left[\left\{\hat{K}_j^\dagger \hat{K}_j, \hat{\rho}\right\} - 2\hat{K}_j \hat{\rho} \hat{K}_j^\dagger\right]}_{\substack{\text{dissipative processes} \\ \hat{D} = \{\hat{K}_j\}}}$$

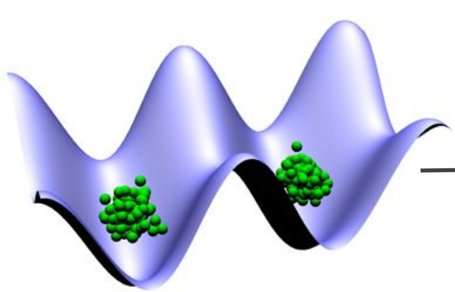
- Expressed as

$$\dot{\hat{\rho}} = \mathcal{L}(\hat{\rho})$$

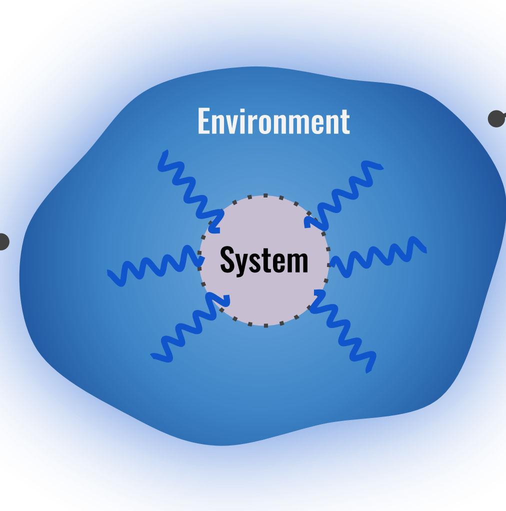
- Computational cost scales exponentially

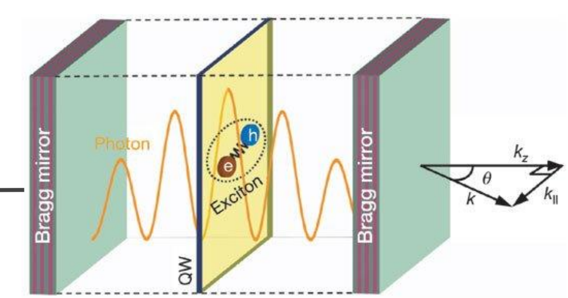


Koch et al., PRA (2010)



A. J. Daley, APS Viewpoint (2015)





Kasprzak et al., Nature (2006)

Lindbladian dynamics

- Formal solution

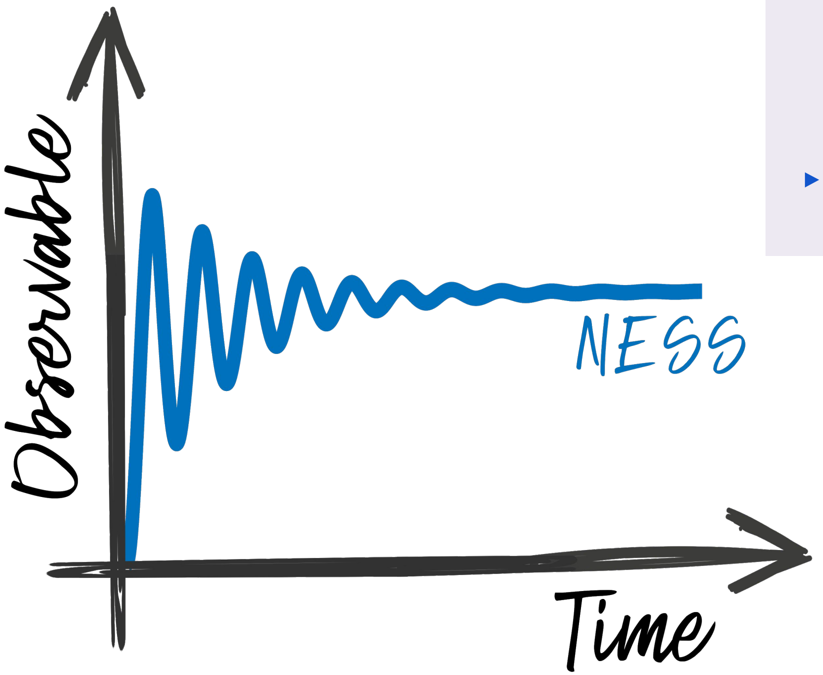
$$\hat{\rho}(t) = e^{\mathcal{L}t}\hat{\rho}(0)$$

- Long-time limit: **non-equilibrium steady state (NESS)**

$$\mathcal{L}(\hat{\rho}_{ss}) = \langle \rho_{ss}|\mathcal{L}|\rho_{ss}\rangle = 0$$

$$\mathcal{L}^\dagger\mathcal{L}(\hat{\rho}_{ss}) = \langle \rho_{ss}|\mathcal{L}^\dagger\mathcal{L}|\rho_{ss}\rangle = 0$$

- $\Longrightarrow$ Variational principle



What do we need?

- Variational ansatz for the density matrix
- Optimization method
- Stochastic sampling

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Variational ansatz for the density matrix

- $\mathcal{H} = \{|\boldsymbol{\sigma}\rangle\} = \{|\sigma_1, \sigma_2, \ldots, \sigma_N\rangle\}$
- **Ansatz**: map $\rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta})$
- Self-adjoint, positive semi-definite form

$$\rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \sum_{j=1}^{J} p_j(\chi) \cdot \psi_j(\boldsymbol{\sigma}, \chi)\psi_j^*(\boldsymbol{\eta}, \chi)$$

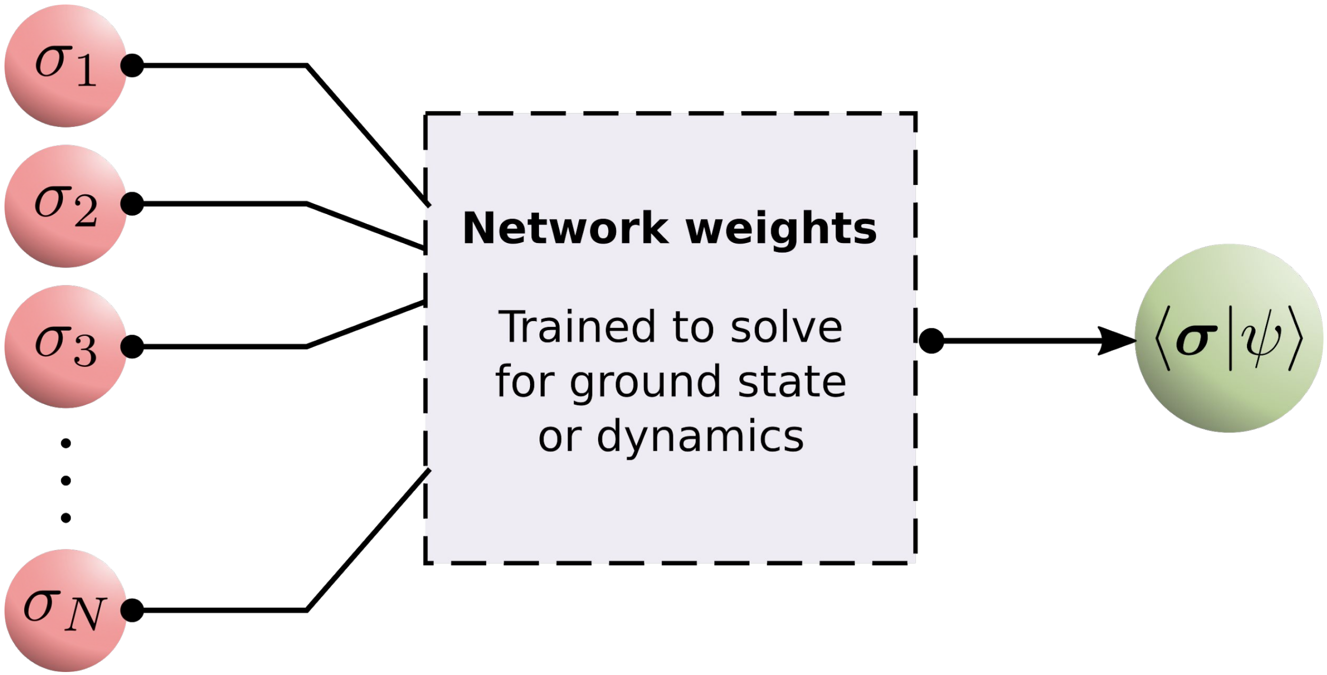
- What do we use for $\psi_j(\boldsymbol{\sigma}, \chi)$?
- Tensor networks? Jastrow wave-function?
- Neural network representation by Carleo and Troyer [Science 355, 602]

$$\begin{pmatrix} \rho_{1,1} & \rho_{1,2} & \cdots & \rho_{1,n} \\ \rho_{2,1} & \rho_{2,2} & \cdots & \rho_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{n,1} & \rho_{n,2} & \cdots & \rho_{n,n} \end{pmatrix}$$

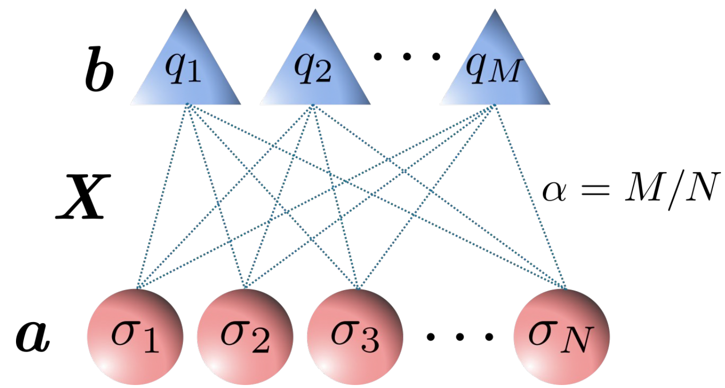
$$\downarrow$$

$$\rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta})$$

Neural Network Quantum States



Restricted Boltzmann-machine



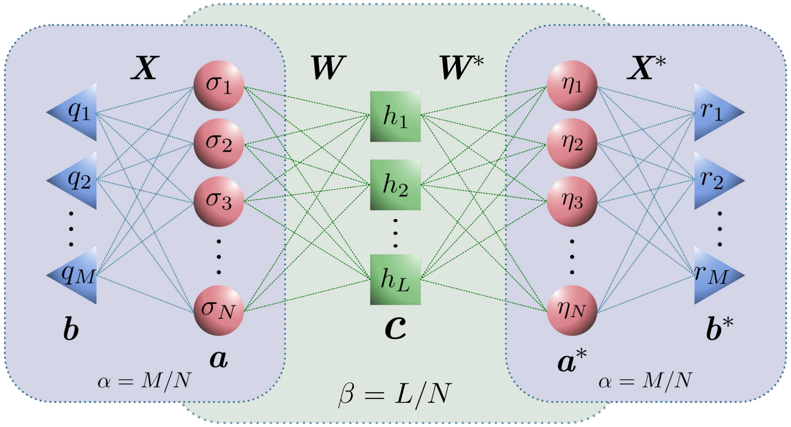
$$\psi(\boldsymbol{\sigma}, \chi) = \sum_{\{q\}} e^{\mathcal{H}(\boldsymbol{\sigma}, \{q\})} = \sum_{\{q\}} e^{\left(\sum_i a_i \sigma_i + \sum_m b_m q_m + \sum_{m,i} q_m \sigma_i X_{mi}\right)} = P(\boldsymbol{\sigma})$$

- The network is connected by Ising interactions
- The probability of a spin configuration is the Boltzmann-weight of the Ising Hamiltonian
- Connection to tensor networks
  [Cirac et al., PRX 8, 011006]

- Intrinsically non-local correlations
- No dimensionality constraints
- High accuracy (representability theorems)

Neural Network Density Matrix

$$\rho_\chi(\boldsymbol{\sigma},\boldsymbol{\eta}) = \sum_{j=1}^{J} p_j(\chi)\cdot\psi_j(\boldsymbol{\sigma},\chi)\psi_j^*(\boldsymbol{\eta},\chi)$$



$$\rho_\chi(\boldsymbol{\sigma},\boldsymbol{\eta}) = e^{\left(\sum_i a_i\sigma_i\right)} e^{\left(\sum_i a_i^*\eta_i\right)} \times \prod_{l=1}^{L}\cosh\left(c_l+\sum_i W_{li}\sigma_i+\sum_i W_{li}^*\eta_i\right)$$
$$\times\prod_{m=1}^{M}\cosh\left(b_m+\sum_i X_{mi}\sigma_i\right)\times\prod_{n=1}^{M}\cosh\left(b_n^*+\sum_i X_{ni}^*\eta_i\right)$$

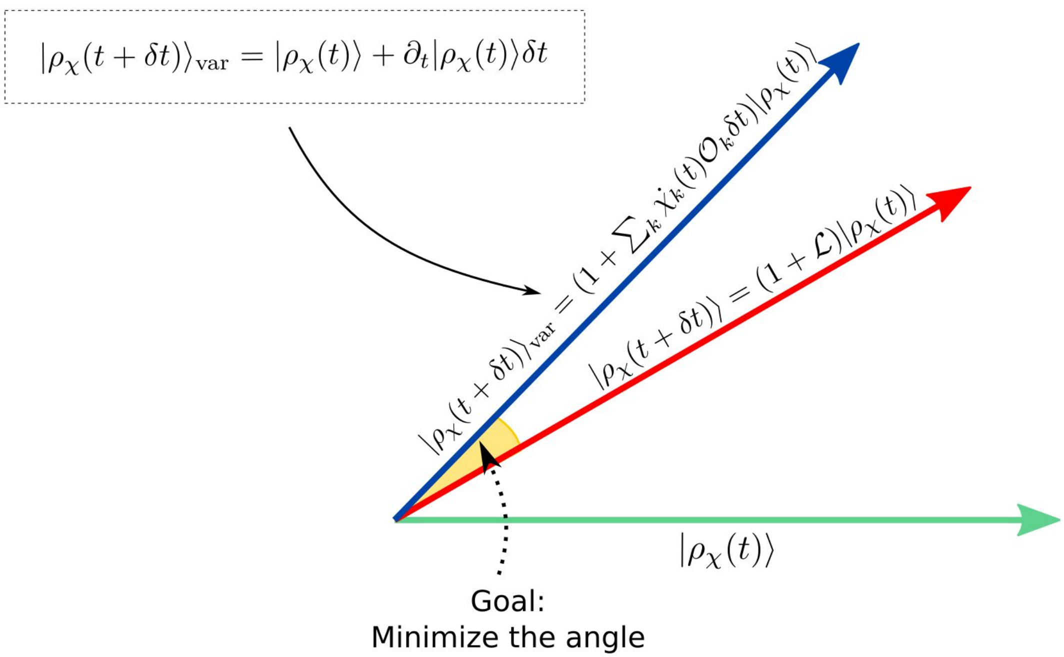
- The representative power depends on the number of hidden nodes and ancillary bits
- Numerically efficient, analytical derivatives

What do we need?

- Variational ansatz for the density matrix
- Optimization method
- Stochastic sampling

Stochastic Reconfiguration (SR) for open quantum systems

- Well adapted for Hamiltonian problems [Sorella et al., J. Chem. Phys. 127, 014105]
- Efficient and robust
- Accounts for the correlation between the variables



Stochastic Reconfiguration (SR) for open quantum systems

$$\partial_t \chi_k = \sum_{k'} S^{-1}_{kk'} F_{k'}$$

Linear system to be solved at each iteration step

Sparse solvers for large number of parameters [Choi et al., SIAM, **33**, 1810]

- Real time evolution

$$F_k = -\frac{\partial \langle\langle \mathcal{L} \rangle\rangle}{\partial \chi_k} = -\frac{\partial}{\partial \chi_k} \frac{\langle \rho_\chi | \mathcal{L} | \rho_\chi \rangle}{\langle \rho_\chi | \rho_\chi \rangle}$$

- Steady state

$$F_k = -\frac{\partial \langle\langle \mathcal{L}^\dagger \mathcal{L} \rangle\rangle}{\partial \chi_k} = -\frac{\partial}{\partial \chi_k} \frac{\langle \rho_\chi | \mathcal{L}^\dagger \mathcal{L} | \rho_\chi \rangle}{\langle \rho_\chi | \rho_\chi \rangle}$$

- SR = Steepest descent if S is the identity
- Euler approximation: $\chi(t+\delta t) = \chi(t) + \nu \cdot S^{-1}(t) F(t)$

$$O_k(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \frac{1}{\rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta})} \cdot \frac{\partial \rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta})}{\partial \chi_k}$$

$$F_k = \langle\langle O_k^* \mathcal{L} \rangle\rangle - \langle\langle \mathcal{L} \rangle\rangle \langle\langle O_k^* \rangle\rangle$$

$$S_{kk'} = \langle\langle O_k^* O_{k'} \rangle\rangle - \langle\langle O_k^* \rangle\rangle \langle\langle O_{k'} \rangle\rangle$$

What do we need?

- Variational ansatz for the density matrix
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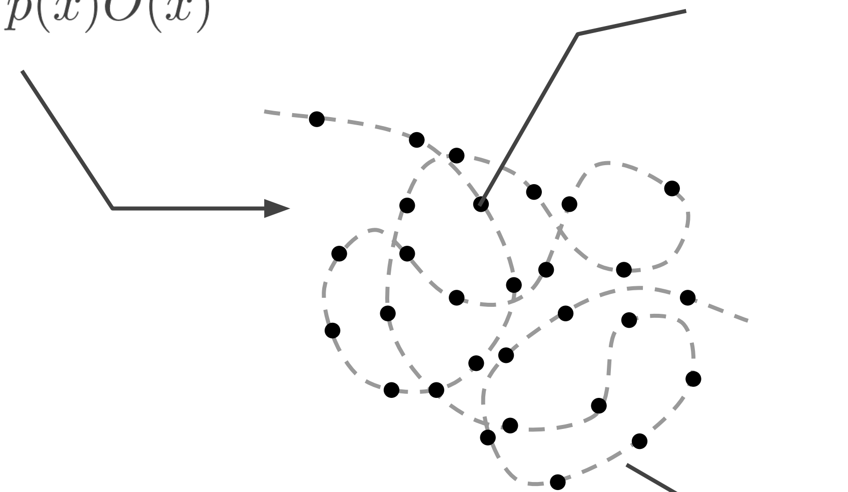
Stochastic sampling

$$\langle O \rangle = \sum_x p(x) O(x)$$

$$\mathcal{A}(X_i \to X_j) = \min\left(1, \frac{p(X_j) \cdot \mathcal{Q}(j|i)}{p(X_i) \cdot \mathcal{Q}(i|j)}\right)$$



$$\langle O_{MC} \rangle = \frac{1}{N} \sum_i^N O(X_i)$$

Stochastic sampling

$$\langle O \rangle = \sum_x p(x) O(x)$$

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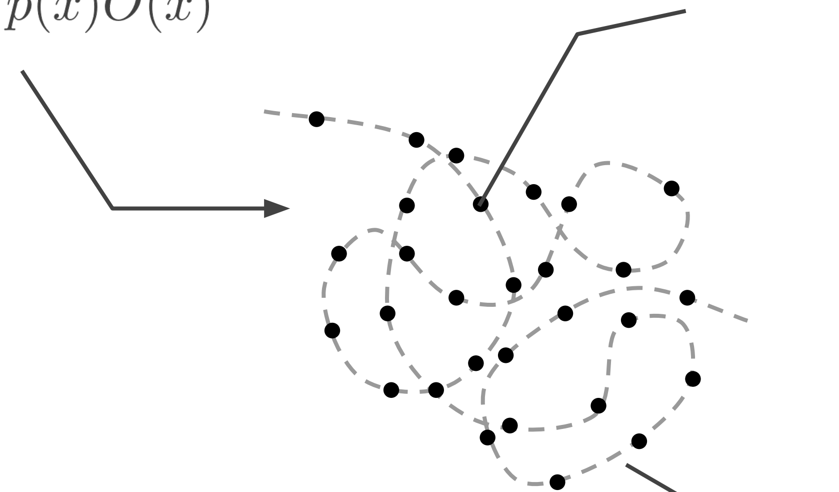

$$\langle O_{MC} \rangle = \frac{1}{N}\sum_i^N O(X_i)$$

- Let's rewrite the linear system for MCMC sampling

$$F_k = \sum_{\boldsymbol{\sigma},\boldsymbol{\eta}} |\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\rho_\chi\rangle|^2 \cdot \left(\frac{\partial \ln\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\rho_\chi\rangle}{\partial \chi_k}\right)^* \frac{\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\mathcal{L}|\rho_\chi\rangle}{\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\rho_\chi\rangle}$$
$$- \sum_{\boldsymbol{\sigma},\boldsymbol{\eta}} |\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\rho_\chi\rangle|^2 \cdot \frac{\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\mathcal{L}|\rho_\chi\rangle}{\langle \boldsymbol{\sigma},\boldsymbol{\eta}|\rho_\chi\rangle} \sum_{\boldsymbol{\sigma}',\boldsymbol{\eta}'} |\langle \boldsymbol{\sigma}',\boldsymbol{\eta}'|\rho_\chi\rangle|^2 \cdot \left(\frac{\partial \ln\langle \boldsymbol{\sigma}',\boldsymbol{\eta}'|\rho_\chi\rangle}{\partial \chi_k}\right)^*$$

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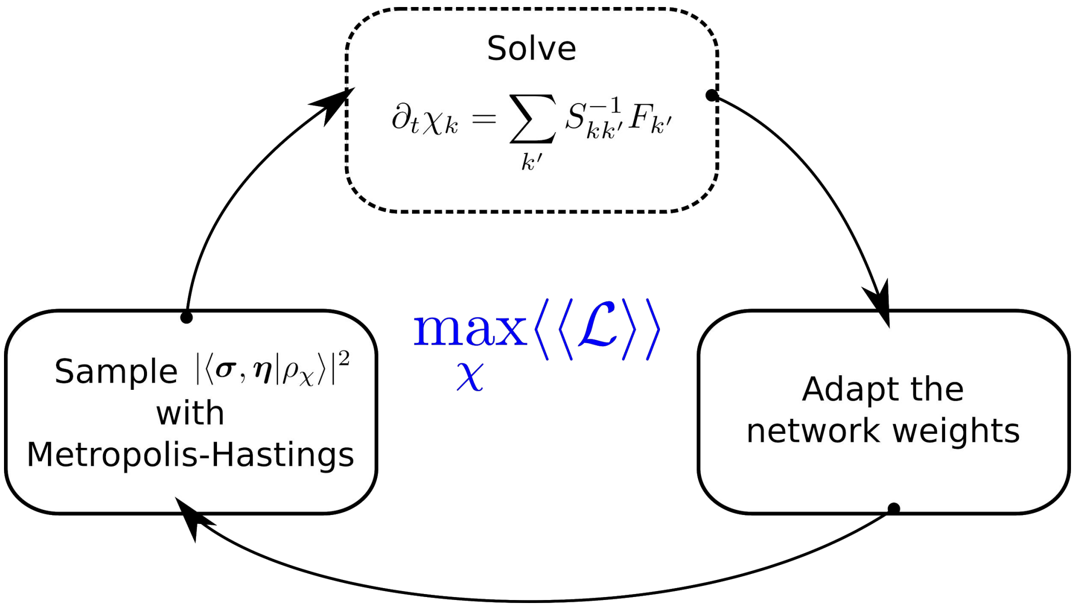
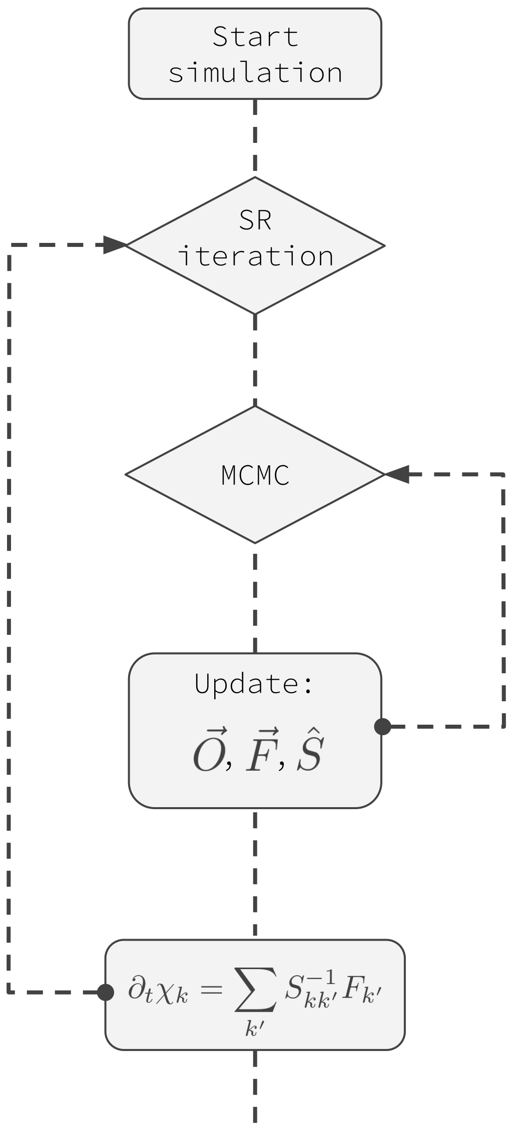
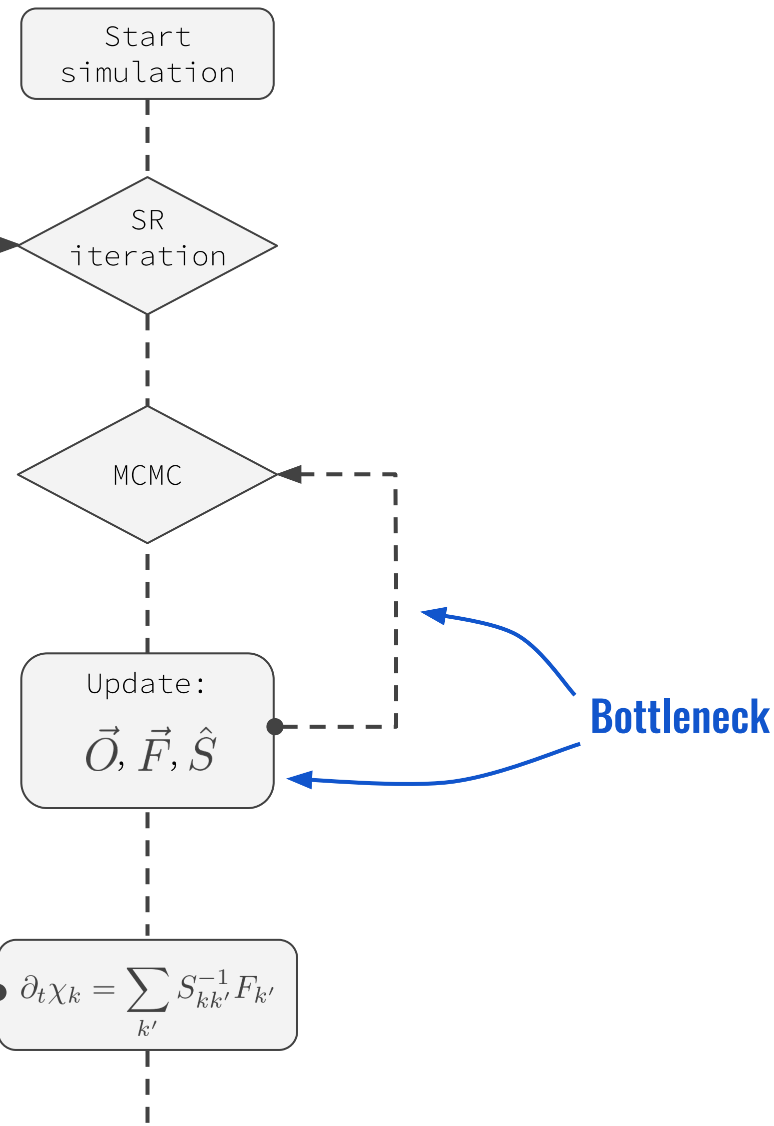


Implementation



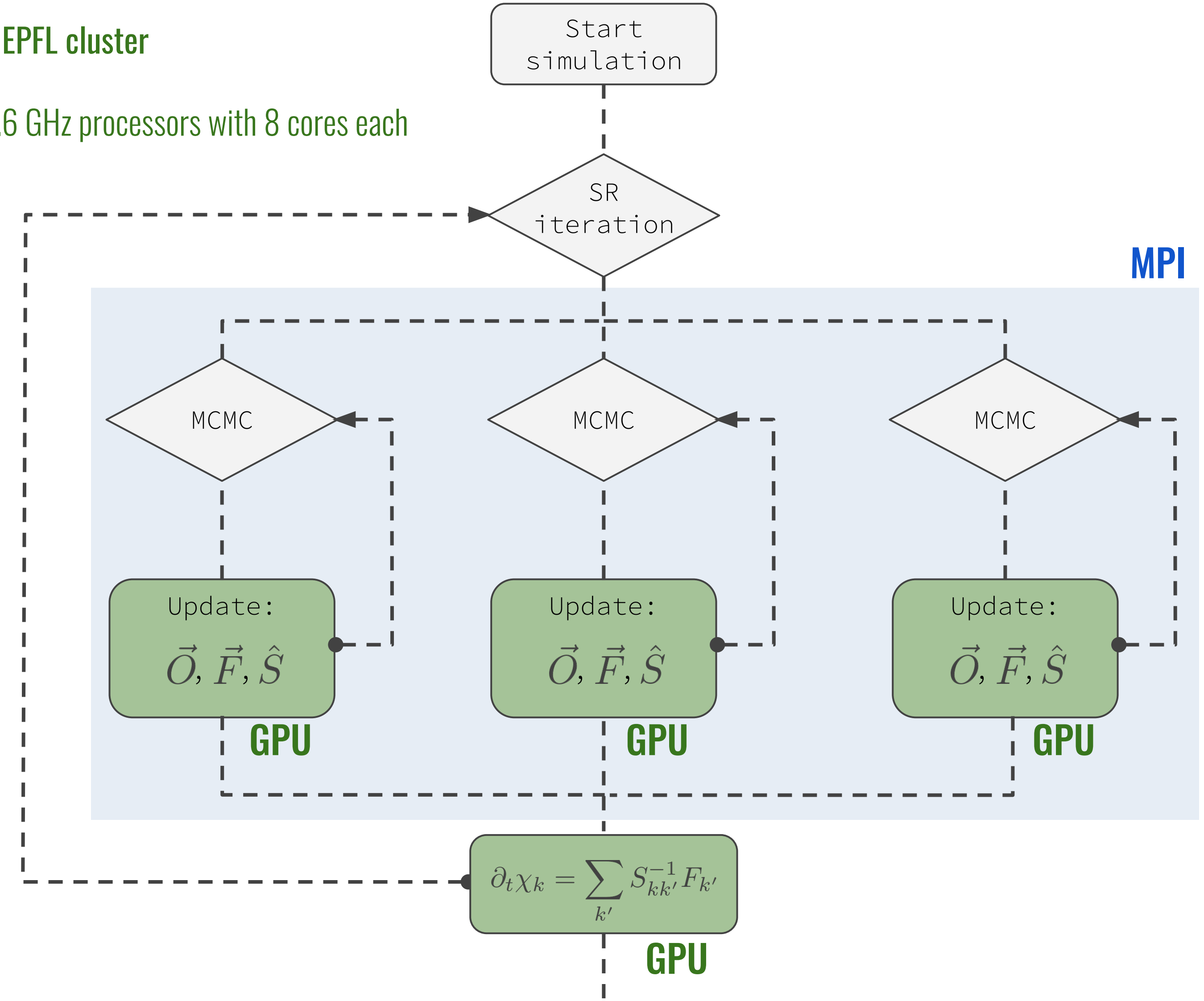
Implementation



Implementation

GPU SPEED UP: 20X

Python3.6 on EPFL cluster
Nodes:
2 Ivy Bridge 2.6 GHz processors with 8 cores each
4 K40 NVIDIA



Results: Spin lattices

XYZ Heisenberg model - 2D

$$\hat{\mathcal{H}} = \sum_{\langle i,j \rangle} \left(J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z \right)$$

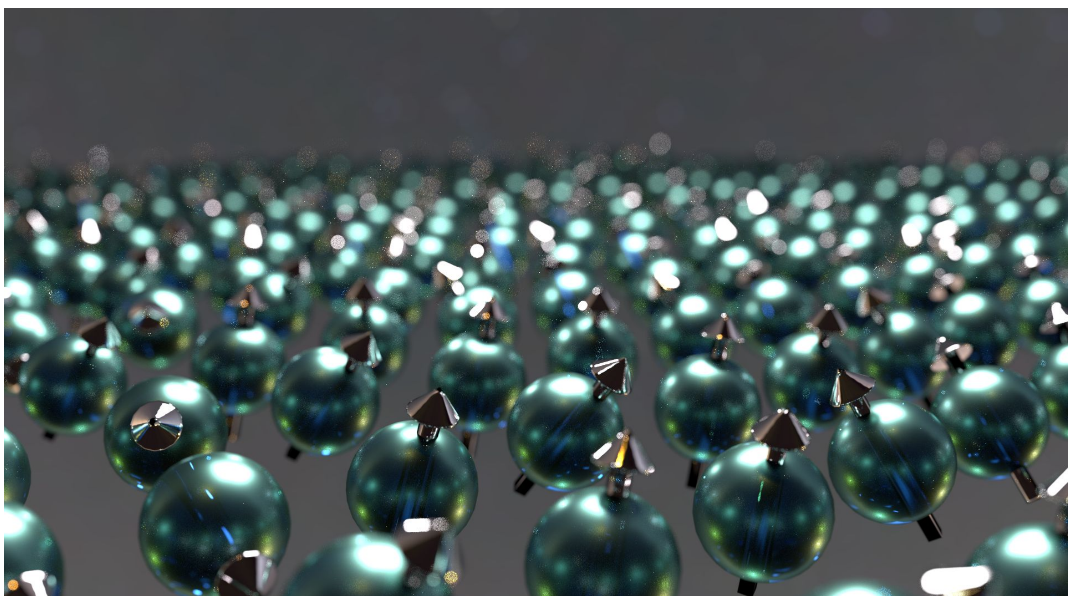
$$\hat{D} = \{\hat{\sigma}_i^-\}$$

Rydberg Ising model - 1D

$$\hat{\mathcal{H}} = \frac{U}{2} \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j + \Omega \sum_i \hat{\sigma}_i^x$$

$$\hat{n}_i = \frac{1}{2}(1 + \hat{\sigma}_i^z)$$

$$\hat{D} = \{\hat{n}_i\}$$



Transverse field Ising model - 1D

$$\hat{\mathcal{H}} = J_z \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + h \sum_i \hat{\sigma}_i^x$$

$$\hat{D} = \{\hat{\sigma}_i^-\}$$

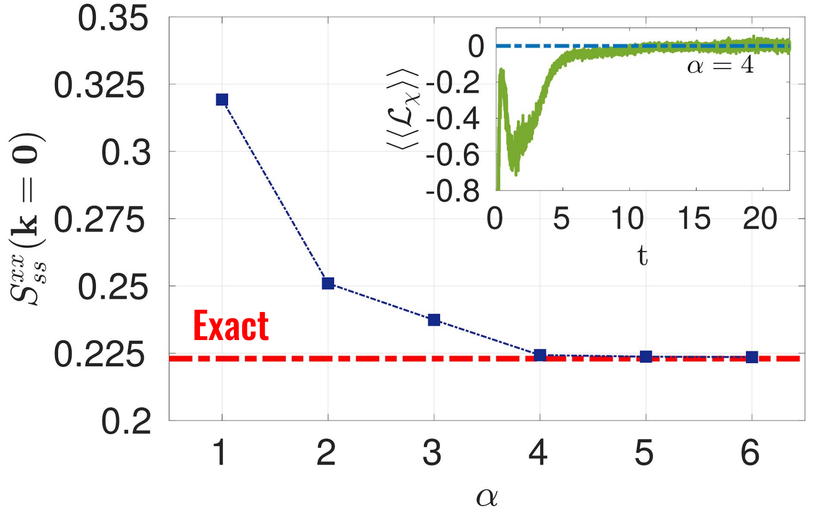
XYZ Heisenberg model - 2D - steady state

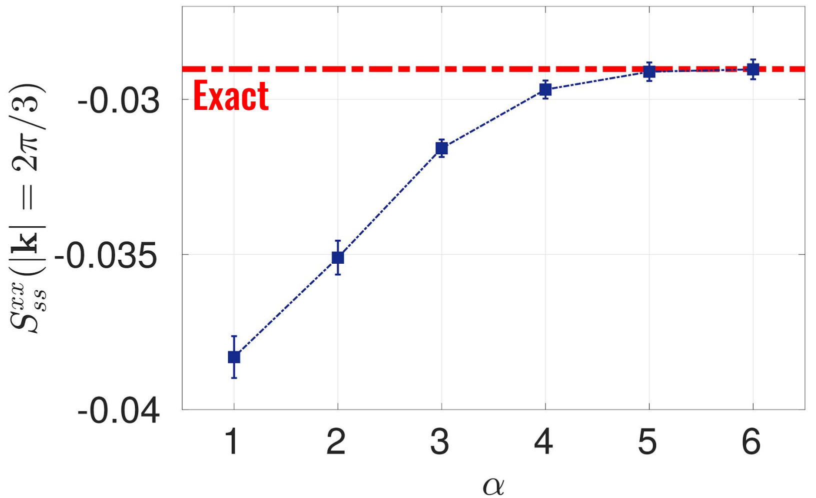
$$\hat{\mathcal{H}} = \sum_{\langle i,j \rangle} \left(J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z \right)$$

$$\hat{D} = \{ \hat{\sigma}_i^- \}$$

- Steady state spin structure factor

$$S_{ss}^{xx}(\mathbf{k}) = \frac{1}{N(N-1)} \sum_{\mathbf{j} \neq \mathbf{l}} e^{-i\mathbf{k}(\mathbf{j}-\mathbf{l})} \langle \hat{\sigma}_{\mathbf{j}}^x \hat{\sigma}_{\mathbf{l}}^x \rangle$$





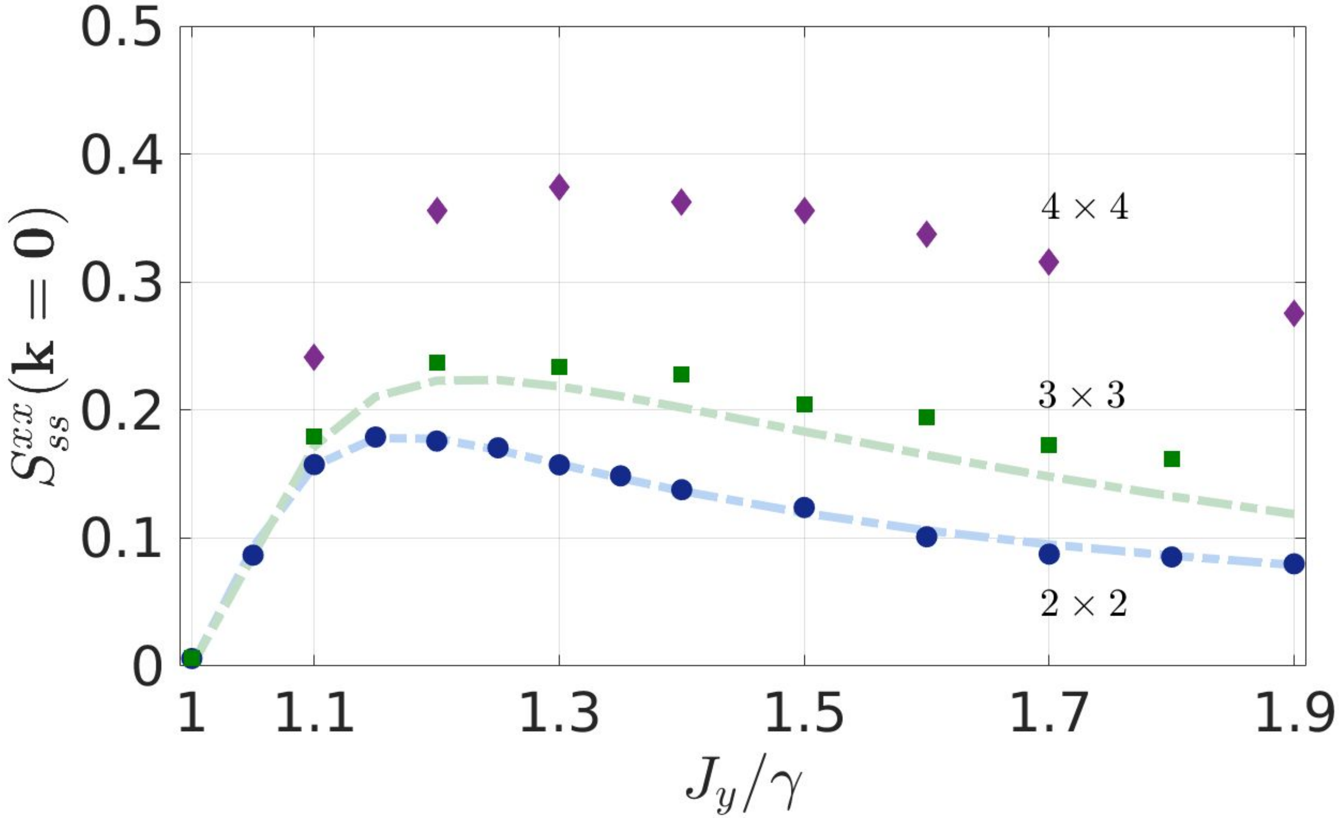
3×3 lattice

$J_x/\gamma = 0.9,\ J_y/\gamma = 1.2,\ J_z/\gamma = 1.0$

XYZ Heisenberg model - phase transition

$$\hat{\mathcal{H}} = \sum_{\langle i,j \rangle} \left(J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z \right)$$

$$\hat{D} = \{\hat{\sigma}_i^-\}$$



$J_x/\gamma = 0.9,\ J_z/\gamma = 1.0$

$\alpha = \beta = 3$

Rydberg Ising dynamics - 1D

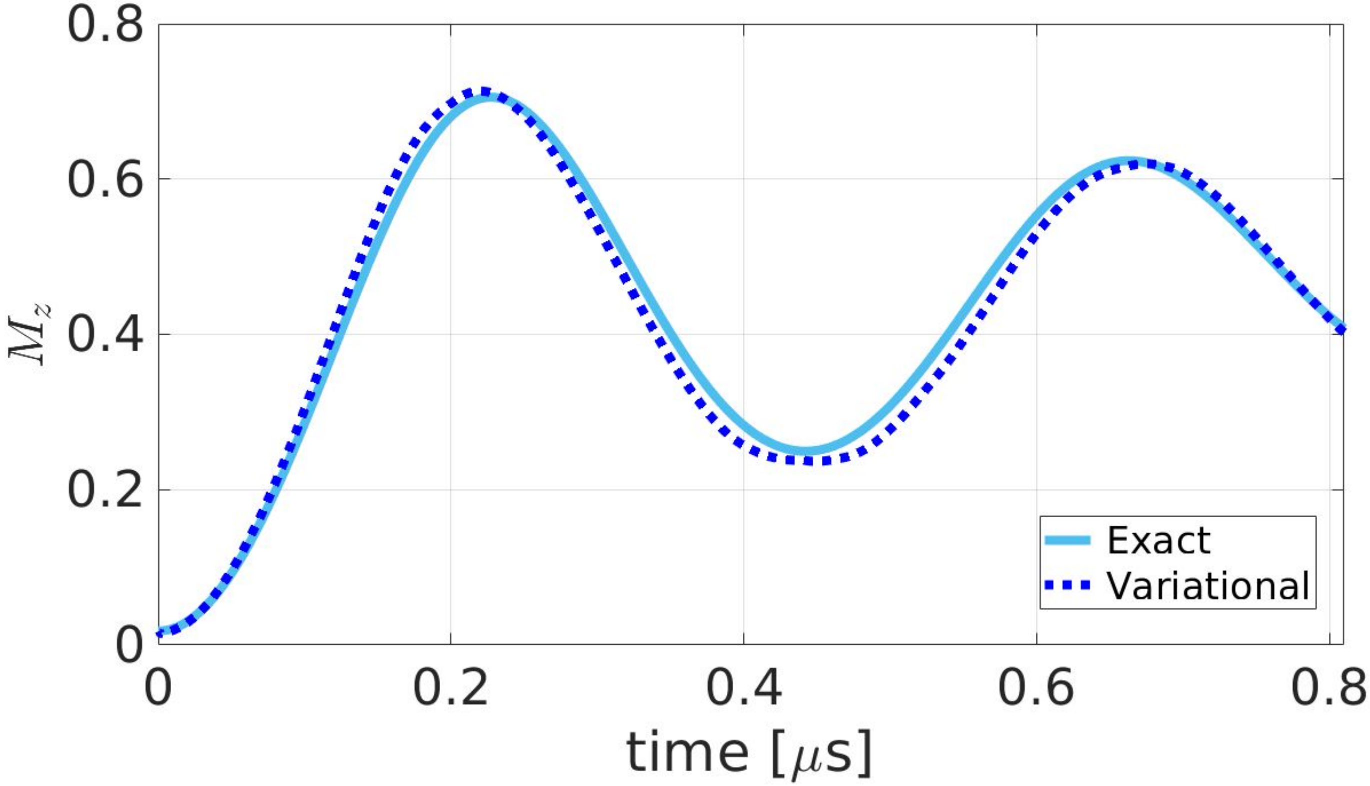
$$\hat{\mathcal{H}} = \frac{U}{2}\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j + \Omega\sum_i\hat{\sigma}_i^x$$

$$\hat{n}_i = \frac{1}{2}(1+\hat{\sigma_i^z})$$

$$\hat{D} = \{\hat{n}_i\}$$

- Magnetization

$$M_z = \frac{1}{N}\sum_{i=1}^{N}\mathrm{Tr}(\hat{\rho}\hat{\sigma}_i^z)$$

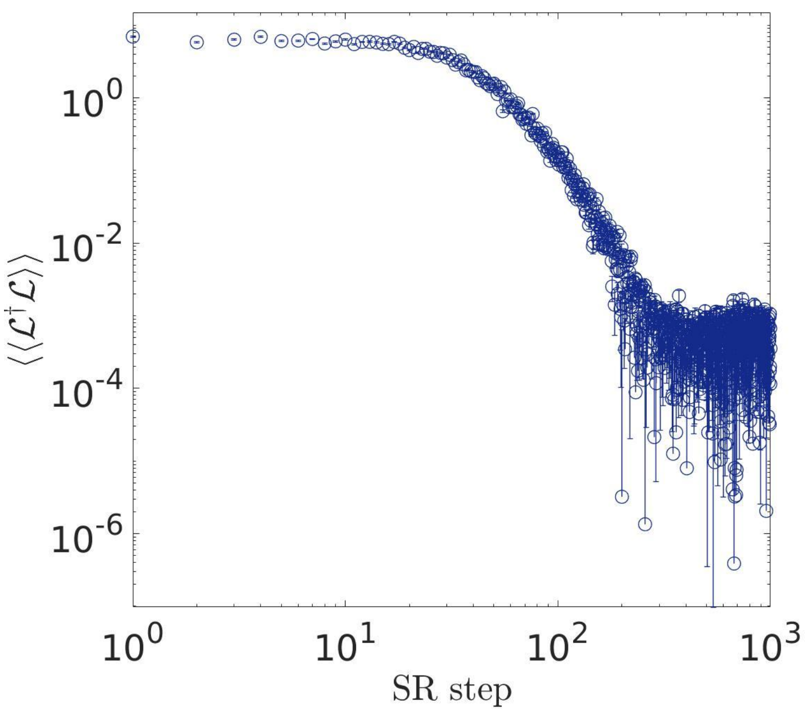


$$\alpha = \beta = 1, 6\text{ spins}, \frac{\Omega}{2\pi} = 0.9\text{ MHz}, \frac{U}{h} = 2.7\text{ MHz}$$

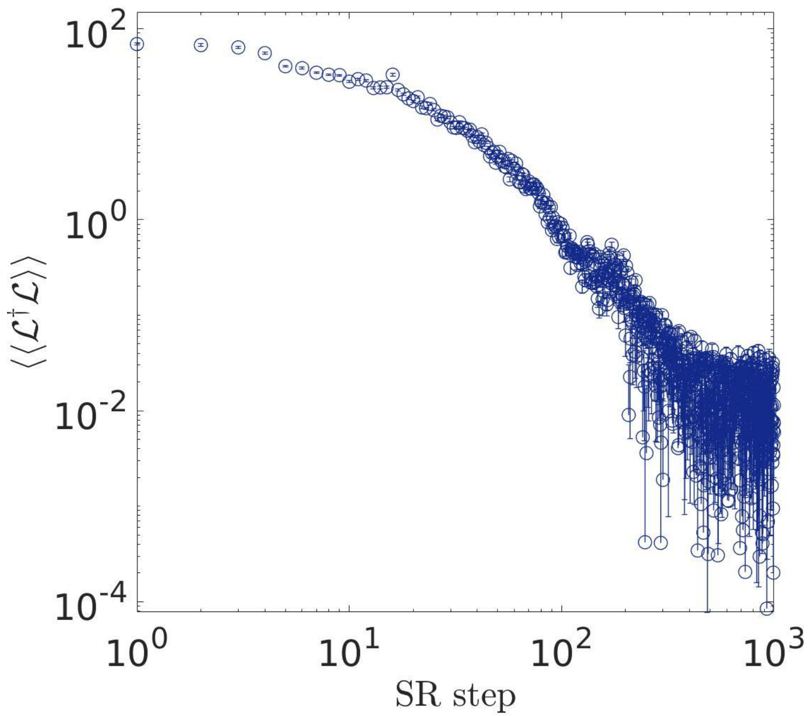
Transverse field Ising model - 1D

$$\hat{\mathcal{H}} = J_z \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + h \sum_i \hat{\sigma}_i^x$$

$$\hat{D} = \{\hat{\sigma}_i^-\}$$



5 spins



25 spins

$$\alpha = \beta = 1,\ J_z/\gamma = 0.5,\ h = 0.5$$

Conclusion

- Neural network ansatz for open quantum systems
- Efficient and robust optimization
- Adapted for many-core computing
- Results for different spin models
- Including phase transition and real time evolution
- Working version for bosons

Thank you for your attention!

https://doi.org/10.1103/PhysRevLett.122.250501

Featured

- PRL Viewpoint: https://physics.aps.org/articles/v12/74
- EPFL article: https://news.epfl.ch/news/simulating-quantum-systems-with-neural-networks/
- Engadget: https://www.engadget.com/2019/07/05/ai-simulates-quantum-systems/

Three flavours of machine learning

Supervised

- Labelled data

$$[(\mathbf{x_1}, \mathbf{y_1}), \ldots, (\mathbf{x_N}, \mathbf{y_N})]$$

- E.g. handwriting-recognition

Unsupervised

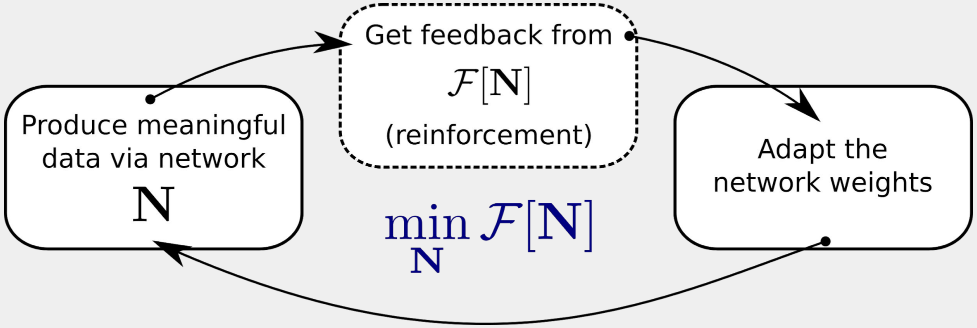
- Unlabelled data

$$[\mathbf{x_1}, \ldots, \mathbf{x_N}]$$

- E.g. cluster analysis

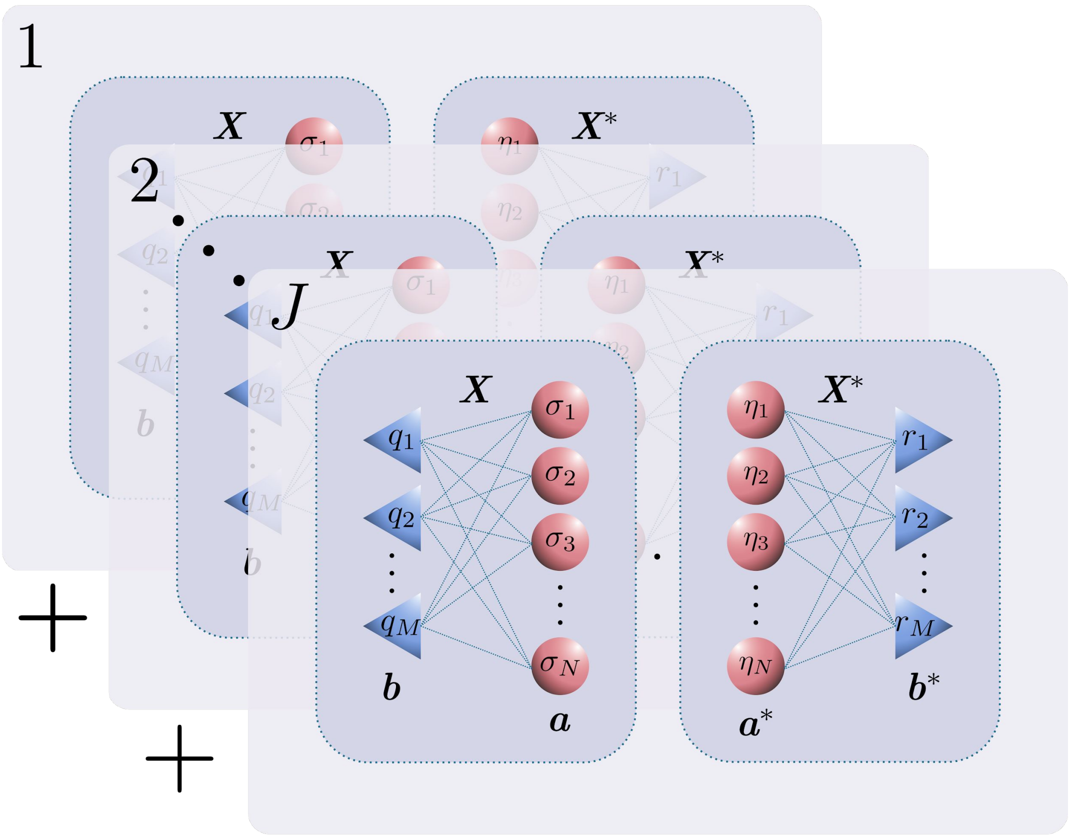
Reinforcement learning

- Generates data, gets feedback, solves the task



- E.g. playing go or Variational Monte Carlo

Neural Network Density Matrix



$$\rho_\chi(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \sum_{j=1}^{J} p_j(\chi) \cdot \psi_j(\boldsymbol{\sigma}, \chi)\psi_j^*(\boldsymbol{\eta}, \chi)$$

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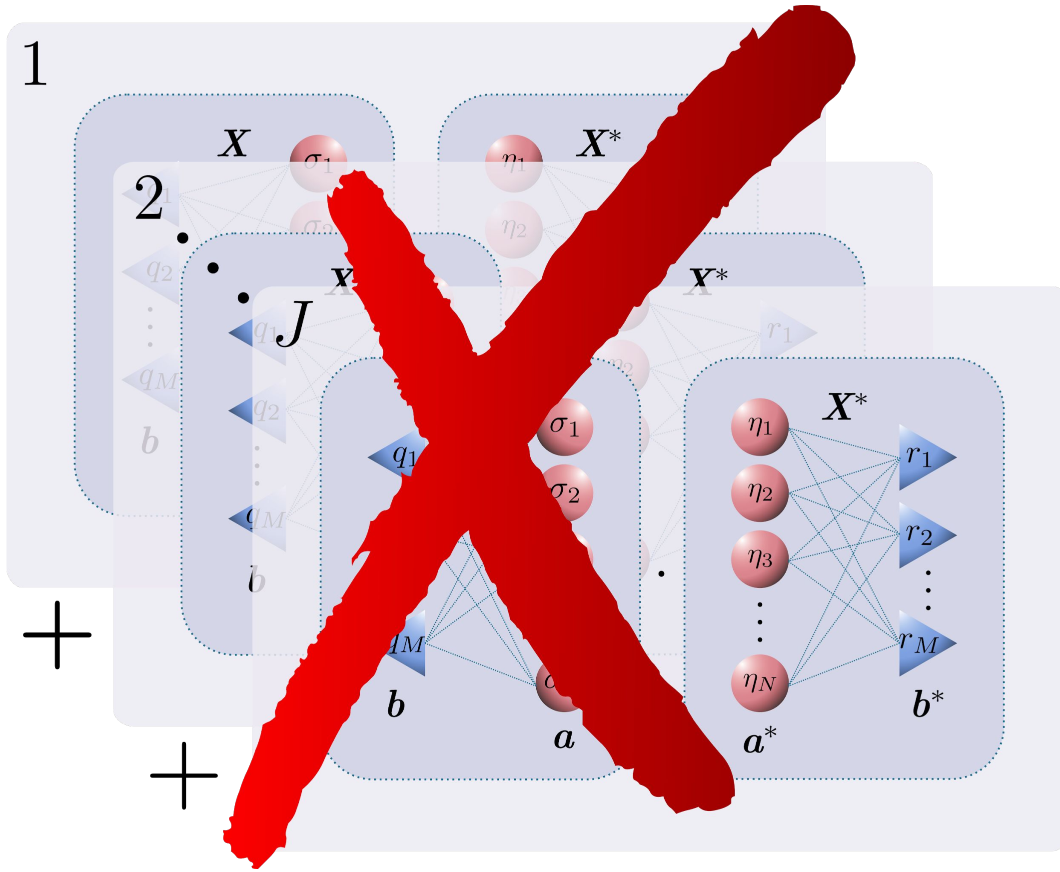

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