LINCOLN

Learning Complex Networks

INFN Sezione di Perugia, Italy

17 July 2023

The IS

LINCOLN (Learning Complex Networks)
Responsabile Nazionale (E. Orlandini)

Sezioni coinvolte (PD, BO, FI, **PG**, CS, CT)

Goal: *The aim of the IS is to study a variety of complex networks (e.g. neural networks; quantum networks; polymer networks; networks in proteins and chromatin; ecological and social networks) by using advanced theoretical tools. In particular, the objective is to develop techniques to exploit and control the properties of complex networks and the processes living on them.*

Involved scientists from PG-UNICAM

2023: 9 associated researchers, 7.7FTE

- Brodoloni Luca (PhD student, Unicam, 100%)
- Cantori Simone (PhD student, Unicam, 100%)
- Costa Emanuele (PhD student, Unicam, 100%)
- Di Patti Francesca (RTDB, UniPG, 100%)
- Mancini Stefano (PO, Unicam, 20%, R. L. till 20-07-2022)
- Marini Bettolo Marconi Umberto (Senior associate, 50%)
- Midei Giovanni (PhD student, Unicam, 100%)
- Pilati Sebastiano (PA, Unicam, 100%, R. L. since 21-07-2022)
- Scriva Giuseppe (PhD student, Unicam, 100%)

2022:

- Costa Emanuele (PhD Student UniCam, 100%)
- Di Patti Francesca (RTDB UniPG, 100%)
- Pilati Sebastiano (RTDB UniCam, 100%)
- Scriva Giuseppe (PhD Student UniCam, 100%)

RECENT RESEARCH ACTIVITIES

Deep learning for quantum many-body physics

E. Costa, G. Scriva, R. Fazio, S. Pilati, *Deep-learning density functionals for gradient descent optimization*, Phys. Rev. E **106**, 045309 (2022)
H. J. Kulik et al., *Roadmap on Machine learning in electronic structure*, Electronic Structure **4**, 023004 (2022)
F. Pellicani, D. Dal Ben, A. Perali, S. Pilati, *Machine Learning Scoring Functions for Drug Discovery from Experimental and Computer-Generated Protein–Ligand Structures: Towards Per-Target Scoring Functions*, Molecules **28**, 1661 (2023)

Quantum Monte Carlo simulations of ultracold atoms

G. Spada, S. Pilati, S. Giorgini, *Thermodynamics of a dilute Bose gas: A path-integral Monte Carlo study*, Phys. Rev. A **105**, 013325 (2022)
G. Spada, S. Giorgini, S. Pilati, *Path-Integral Monte Carlo Worm Algorithm for Bose Systems with Periodic Boundary Conditions*, Cond. Matt. **7**, 30 (2022)
G. Bertaina, M. G. Tarallo, S. Pilati, *Quantum Monte Carlo study of the role of p-wave interactions in ultracold repulsive Fermi gases*, Phys. Rev. A **107**, 053305 (2023)

Combining adiabatic and gate-based quantum computer with deep learning

S. Cantori, D. Vitali, S. Pilati, *Supervised learning of random quantum circuits via scalable neural networks*, Quantum Sci. & Technol. **8**, 025022 (2023)
G. Scriva, E. Costa, B. McNaughton, S. Pilati, *Accelerating equilibrium spin-glass simulations using quantum annealers via generative deep learning*, SciPost Phys. **15**, 018 (2023)

BEC-BCS crossover in multiband superconductors

G. Midei, A. Perali, *Tunable BCS-BEC crossover, reentrant, and hidden quantum phase transitions in two-band superconductors with tunable valence and conduction bands*, Phys. Rev. B **107**, 184501 (2023)

Geometro-thermodynamics

C. Cafaro, O. Luongo, S. Mancini and H. Quevedo, *Thermodynamic length, geometric efficiency and Legendre invariance*, Physica A **590**, 126740 (2022) [20%]
B. Alessio, L. Orlando, M. Stefano, *Inflationary entanglement*, Phys. Rev. D **107**, 103512 (2023) [20%]

Recent theses:

- PhD in Science and Technology, curriculum in Physics, F. Pellicani, Ligand-Protein Binding Affinity Prediction Using Machine Learning Scoring Functions, 20-1-2023, UniCam
- L.M. Fisica, S. Cantori, *Benchmarking quantum computers via deep learning*, 8-2-2022 UniCam
- L.M. Fisica, L. Brodoloni, *Supervised learning of atomization energies via 3D convolutional neural networks*, 5-7-2022 UniCam
- L.M. Fisica, E. Pasquali, *Generative deep learning for medical imaging*, 5-7-2022 UniCam

Recent talks:

- S. Pilati, *Accelerating spin-glass simulations using quantum annealers through deep learning*, University of Bologna, 22-2-2022
- F. Di Patti, Synchronization in simplicial complexes, Assemblea del GNFM – gruppo nazionale di fisica matematica, Montecatii Terme, 5-7/5/2022
- F. Di Patti, Dinamiche collettive e formazione di pattern in sistemi di reazione-diffusione su reti complesse, 25/3/2022, UniPG

ON-GOING/FUTURE RESEARCH ACTIVITIES

QMC simulations of Bose-Bose mixtures

- G. Spada, S. Pilati, S. Giorgini, *Attractive solution of binary Bose mixtures: Liquid-vapor coexistence and critical point*, arXiv:2304.12334 (2023)
- G. Pascual, G. Spada, S. Pilati, S. Giorgini, J. Boronat, Thermal-induced Local Imbalance in Repulsive Binary Bose Mixtures, arXiv:2302.13659 (2023)
- G. Spada, L. Parisi, G. Pascual, N. G. Parker, T. P. Billam, S. Pilati, J. Boronat, S. Giorgini, Phase separation in binary Bose mixtures at finite temperature, arXiv:2211.09574 (2023)
- Droplet formation in 2D Bose-Bose mixtures

Deep-learning for density functional theory

- E. Costa, R. Fazio, S. Pilati, Deep learning non-local and scalable energy functionals for quantum Ising models, arXiv:2305.15370 (2023)
- Time-dependent DFT for quantum spin models

Benchmarking gate-based quantum computers

- G. Scriva, N. Astrakhantsev, S. Pilati, and G. Mazzola, *Challenges of variational quantum optimization algorithms in presence of measurement shot noise* (in preparation)

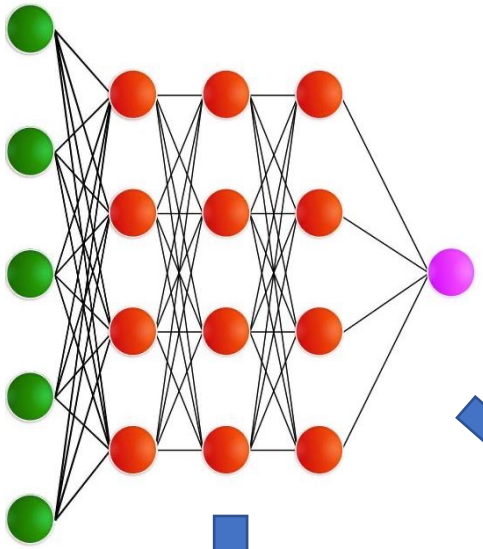
Pattern formation and collective dynamics in reaction and diffusion systems on networks and continuous spaces

- M. Fondi, F. Di Patti and E. Perrin, *The acquisition of additional feedback loops may optimize and speed up the response of quorum sensing*, BioRxiv (2022)
- F. Di Patti, M. Camarena Sainz, Y. Ugartechea Chirino, R. Arbel–Goren, E. Alvarez–Buylla, D. Fanelli and J. Stavans, *Stochastic Turing Patterns of Trichomes in Arabidopsis Leaves* (in preparation)

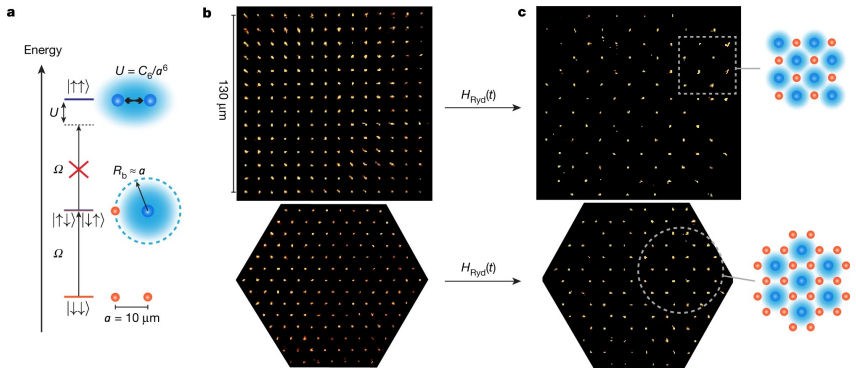
Neural QMC simulations of quantum spin glasses and Rydberg-atom in optical tweezers

- Spin-glass transition in mean-field, short-range quantum spin models, Rydberg-atom quantum simulators

Deep learning

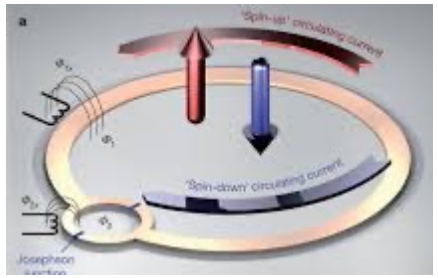


Quantum simulators (e.g., Rydberg atoms)



P. Scholl et al., Nature 595, 233–238 (2021).

Quantum annealers (D-Wave Systems)



Gate-based quantum computers (e.g., IBM, Google, …)

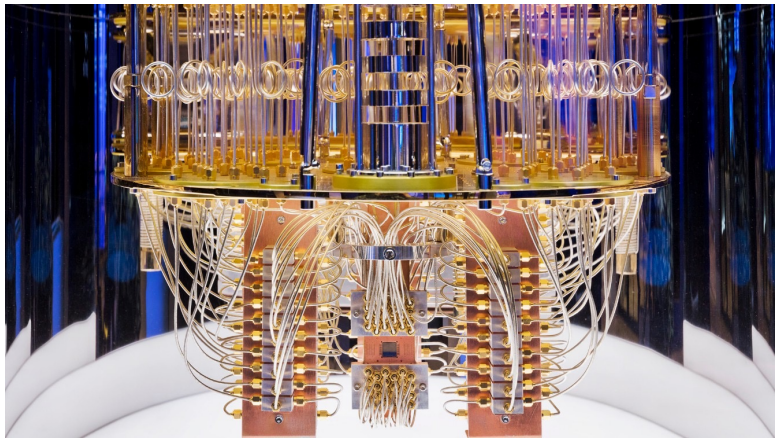
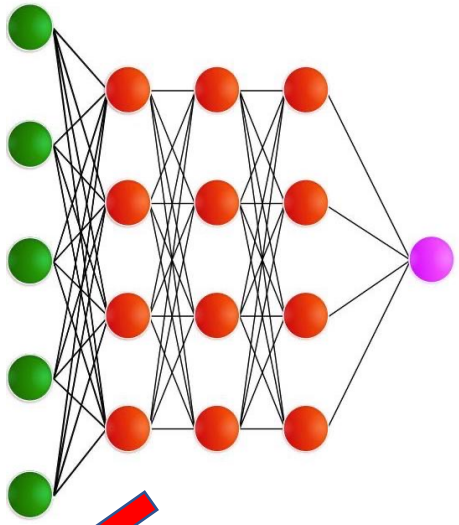


Image from: https://www.esa.int/ESA_Multimedia/Images/2020/11/Interior_of_IBM_s_quantum_computer

Quantum annealers

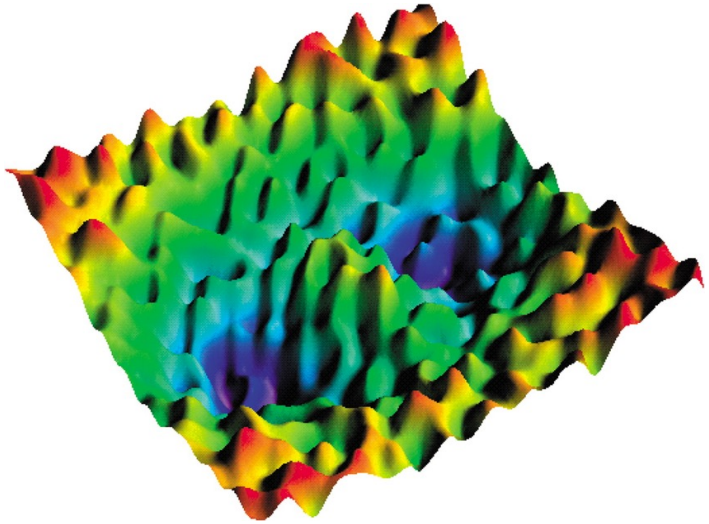
Classical deep learning



Low-T equilibrium properties of spin glasses

$$H = \sum_{ij} J_{ij} x_i x_j$$

Energy landscape



NEURAL MONTE CARLO SIMULATIONS

McNaughton, Milošević, Perali, SP, PRE (2020)

Proposal matrix in Metropolis-Hastings algorithm: $w_{\mathbf{x}\prime\mathbf{x}} = p_{\mathrm{NETWORK}}(\mathbf{x}')$ (use ancestral sampling)

Acceptance probability: $A_{\mathbf{x}'\mathbf{x}} = \min\left(1, \frac{p_{\mathrm{BOLTZ}}(\mathbf{x}')w_{\mathbf{x}\mathbf{x}\prime}}{p_{\mathrm{BOLTZ}}(\mathbf{x})w_{\mathbf{x}\prime\mathbf{x}}}\right)$

We need: $p_{\mathrm{BOLTZ}}(\mathbf{x}) > 0 \implies p_{\mathrm{NETWORK}}(\mathbf{x}) > 0$

if: $p_{\mathrm{NETWORK}}(\mathbf{x}) \cong p_{\mathrm{BOLTZ}}(\mathbf{x}) \longrightarrow A_{\mathbf{x}'\mathbf{x}} \cong 1$ → efficient simulation!

if: $p_{\mathrm{NETWORK}}(\mathbf{x}) \cong 0$ where $p_{\mathrm{BOLTZ}}(\mathbf{x}) \approx 1$ → ergodicity problem!

Related work:

- K. A. Nicoli et al., PRE 101, 023304 (2020): MCMC+autoregressive n. for ferromagnetic models.
- F. Noè et al., Science 365, 1147 (2019): normalizing flows for complex-molecule simulations.
- X. Ding et al., J. Phys. Chem. B, 124, 10166 (2020): normalizing flows for free-energy computations.
- M. Gabrié et al., arXiv:2105.12603 (2021): adaptive MCMC via normalizing flows.
- G. S. Hartnett, M. Mohseni,arXiv:2001.00585v2 (2020): spin-glass simulations via normalizing flows.

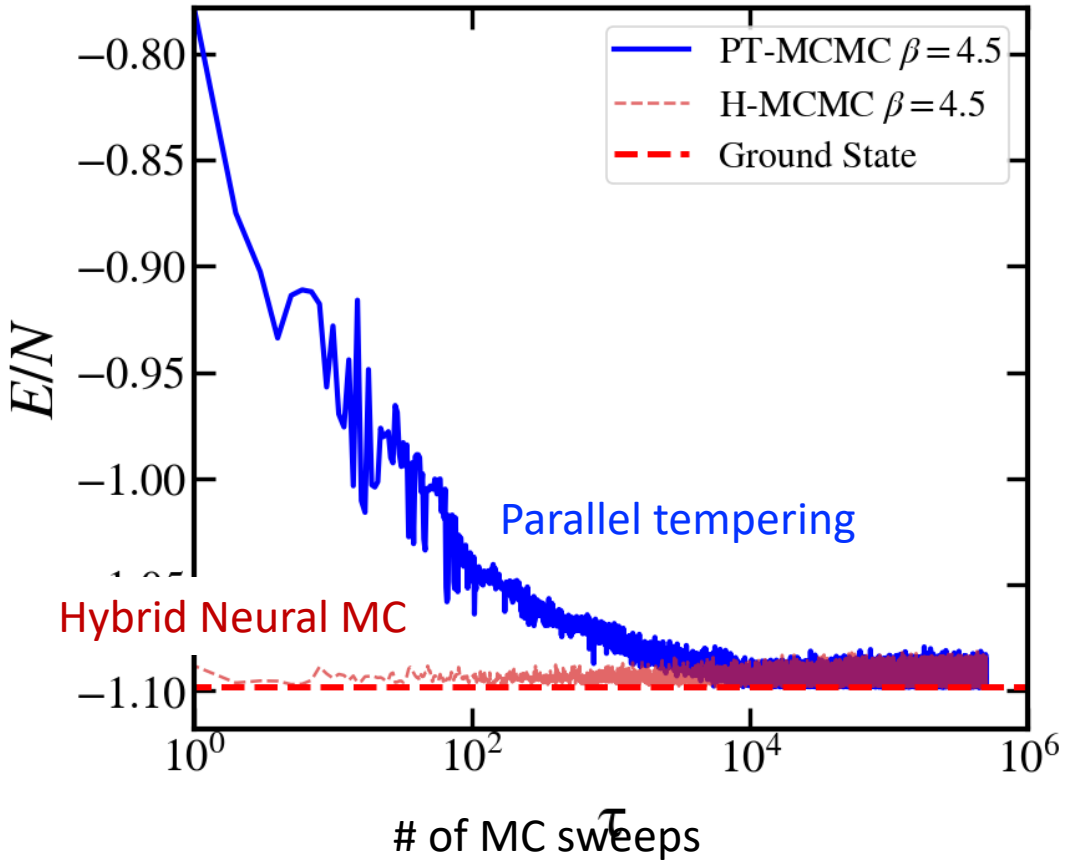
Hybrid neural simulation of a spin glass at low T

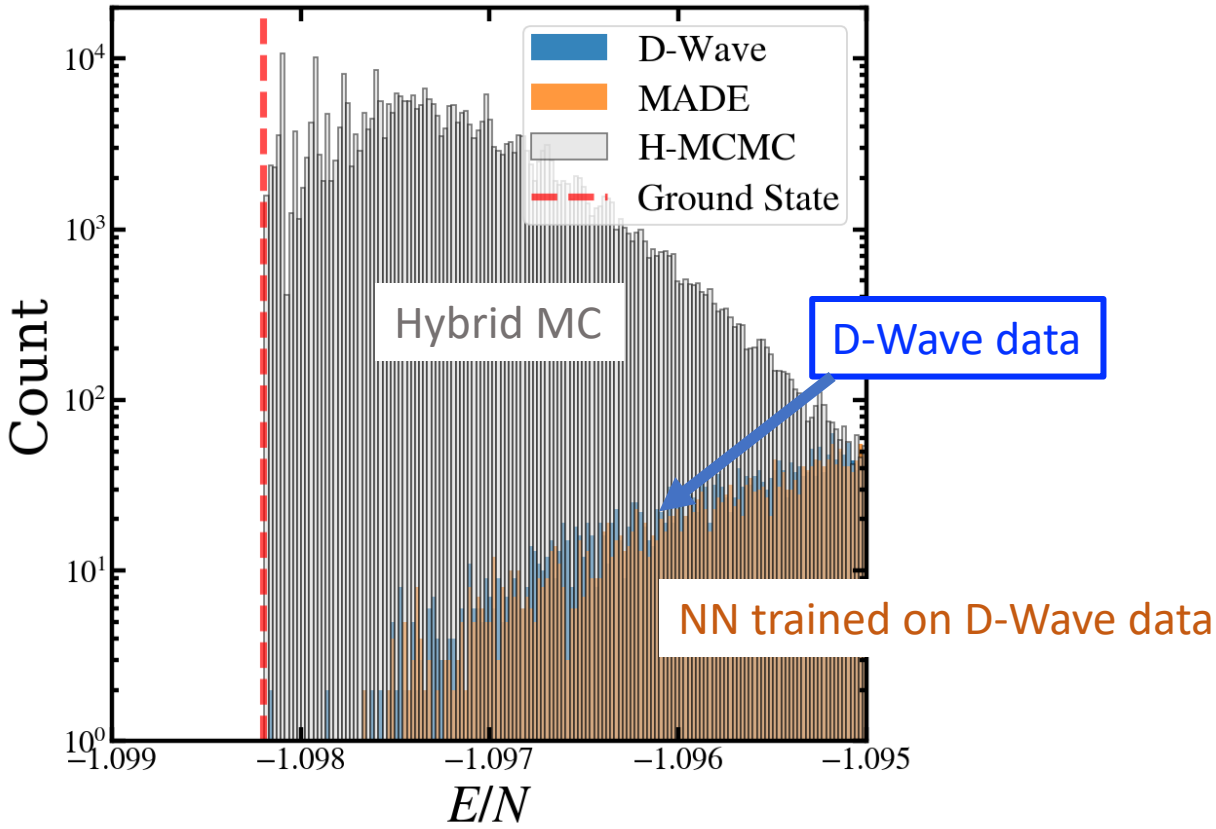
G. Scriva, E. Costa, B. McNaughton, S. Pilati, *Accelerating equilibrium spin-glass simulations using quantum annealers via generative deep learning*, SciPost Phys. **15**, 018 (2023)

NN trained on D-WAVE data

Annealing time: $100\mu s$

β/J = 4.5
2D square lattice N=484
Nearest and next-nearest neighbor interaction
Uniform random couplings





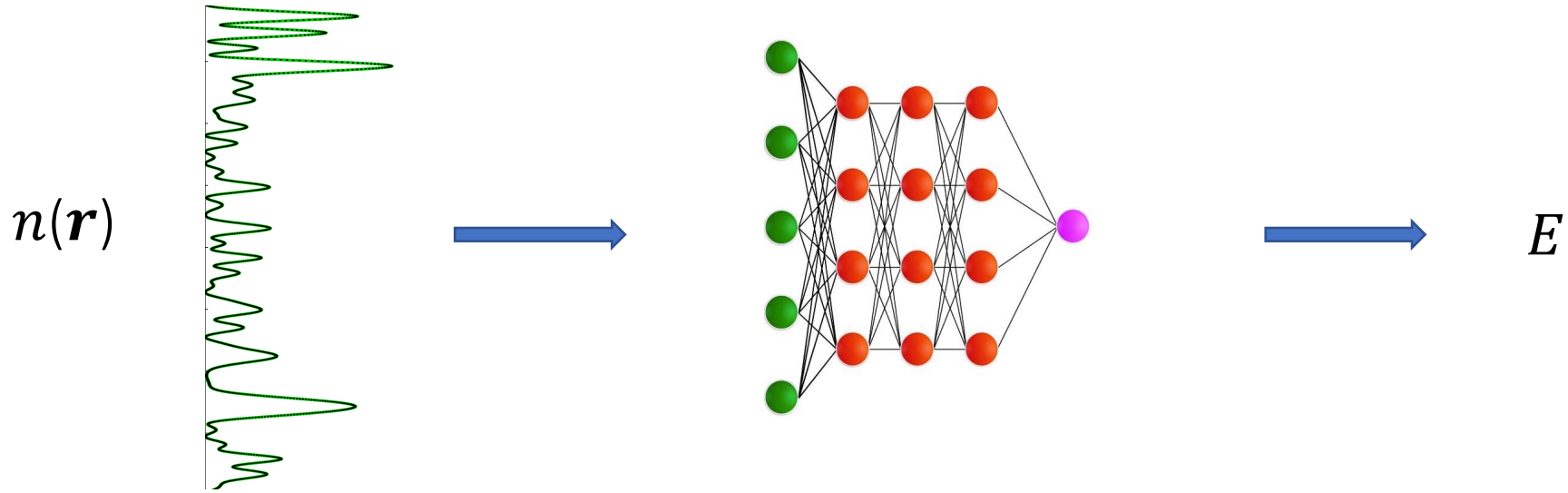
Deep learning density functional theory

QM $\quad |\psi_0\rangle \quad \Rightarrow \quad E_0 = \langle\psi_0|\hat{H}|\psi_0\rangle$

DFT $\quad n_0(\boldsymbol{r}) \quad \Rightarrow \quad E_0 = E[n_0(\boldsymbol{r})]$ (1° Hohenberg-Kohn theorem)

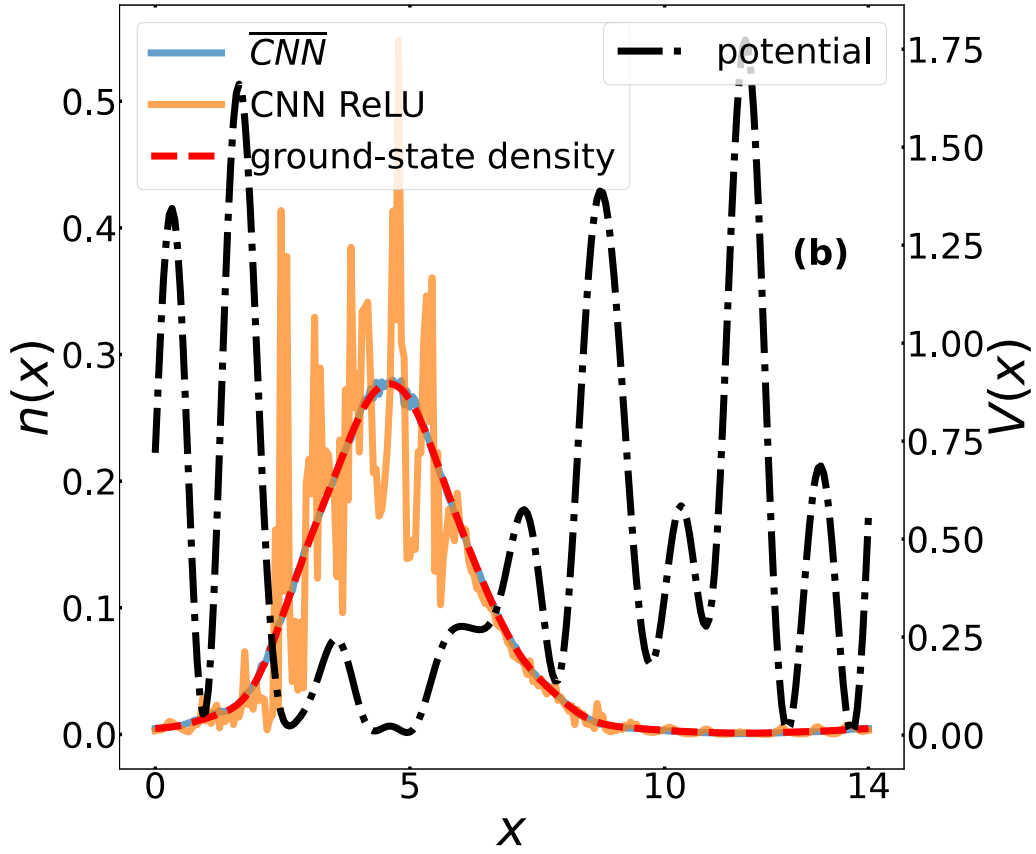
$E_0 \leq E[n(\boldsymbol{r})]$ (2° Hohenberg-Kohn theorem)

The functional $E[n(\boldsymbol{r})]$ is unknown! $\Rightarrow$ deep learning



DFT of atoms in optical speckle disorder

- Instability in gradient-descent minimization with common deep NNs.
- Inter-channel averaging to avoid instability.



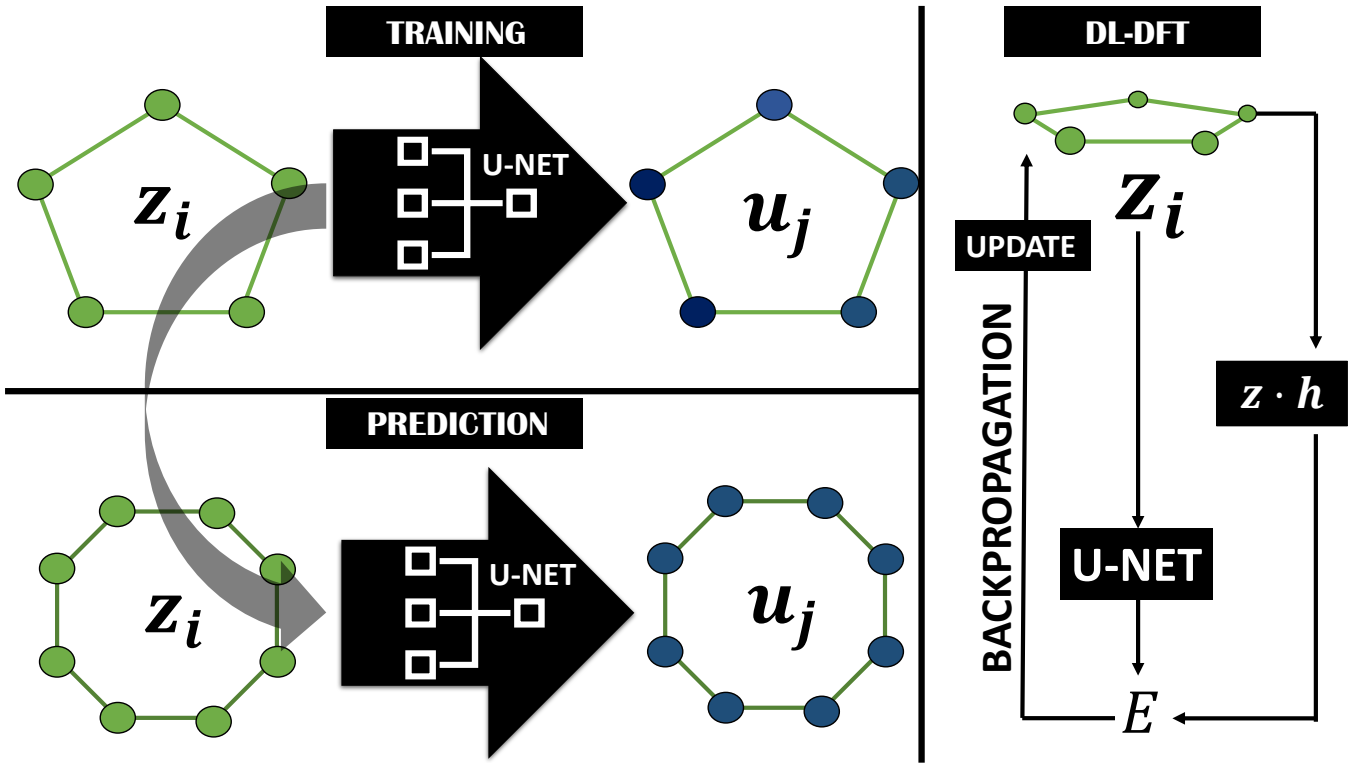
E. Costa, G. Scriva, R. Fazio, S. Pilati, *Deep-learning density functionals for gradient descent optimization*, Phys. Rev. E **106**, 045309 (2022)

DFT for quantum spin models via scalable neural networks

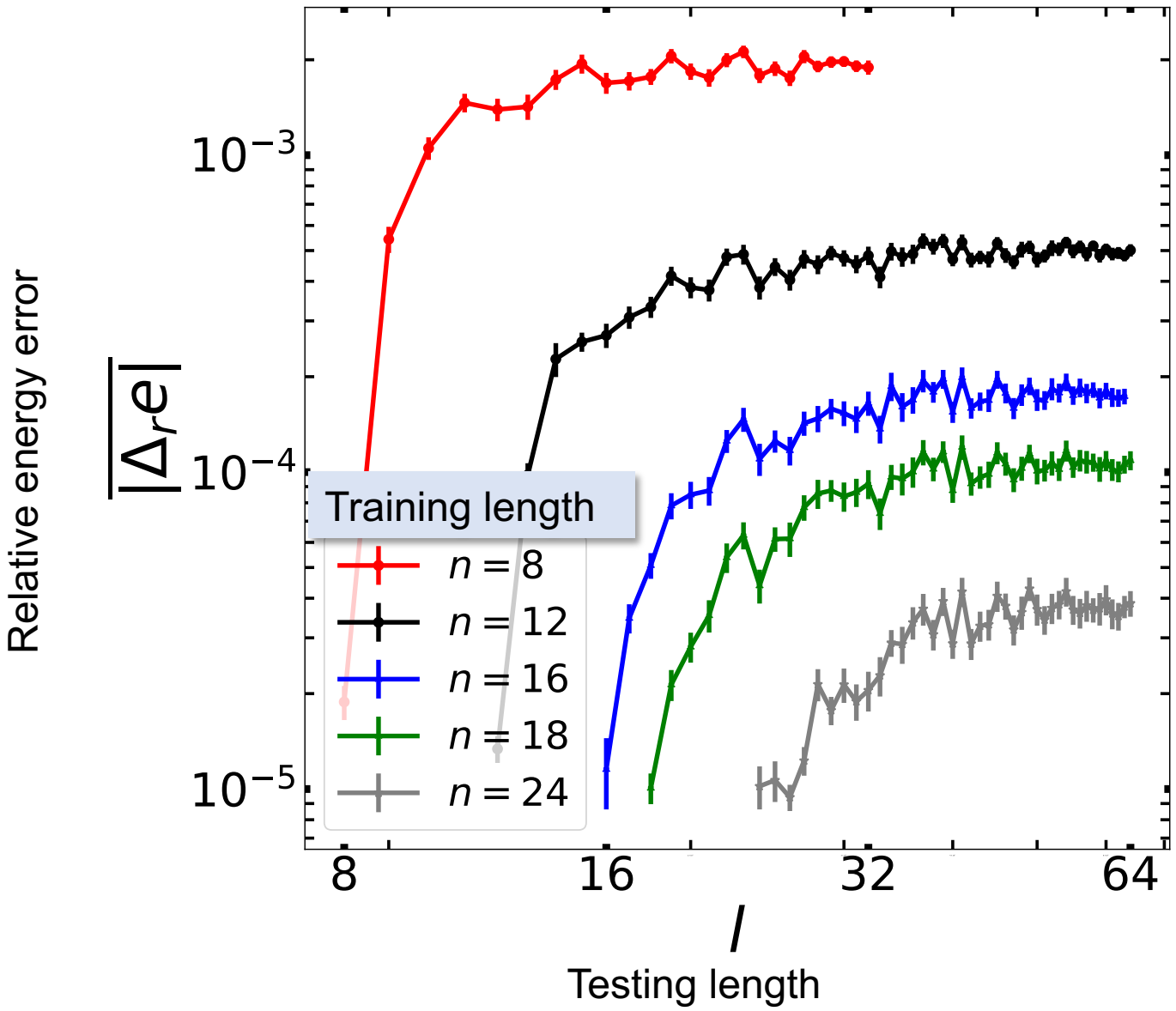
Hamiltonian: $H = -J \sum_i \sigma_i^z \sum_i \sigma_{i+1}^z - \Gamma \sum_i \sigma_i^x$

Functional: $E[\boldsymbol{z}]$

$z_i = -\langle \sigma_j^x \rangle$ $\quad\quad$ $u_j = -J \langle \sigma_j^z \sigma_{j+1}^z \rangle$



Predicting energies for larger systems than those used for training



E. Costa, R. Fazio, S. Pilati, Deep learning non-local and scalable energy functionals for quantum Ising models, arXiv:2305.15370 (2023) Under review in PRB

Future goal:
dynamics via time-dependent DFT

Expected results for 2023-2024:

QMC simulations of Bose-Bose mixtures

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G. Pascual, G. Spada, S. Pilati, S. Giorgini, J. Boronat, *Thermal-induced Local Imbalance in Repulsive Binary Bose Mixtures*, arXiv:2302.13659 (2023) (under review in PRA)

G. Spada, L. Parisi, G. Pascual, N. G. Parker, T. P. Billam, S. Pilati, J. Boronat, S. Giorgini, *Phase separation in binary Bose mixtures at finite temperature*, arXiv:2211.09574 (2023) (under review in SciPost Physics)

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Main collaborations:

S. Giorgini, G. Spada (UniTN); J. Boronat (UPC, Barcelona); G. Mazzola (U. Zurich); R. Fazio (ICTP, UniNA); D. Fanelli, M. Fondi (UniFI); J. Stavans (Weizmann)

Financial request: 12 K€ for travel (conferences & scientific collaborations)