QTensorNet: A High-Performance Tensor-Network-Based Toolkit for Many-Body Quantum Simulations

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Outline

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- A short introduction to TNs
- Existing Toolkits
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- Decorated Square-Kagome Heisenberg Antiferromagnet
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Motivation

- **Simulation Bottleneck:**
  The dimension of the Hilbert space of an N-particle quantum system grows exponentially with N, making exact diagonalization and unitary dynamics simulation infeasible for realistic system sizes.

- **Quantum Computation:**
  Classical simulation of many-body quantum systems becomes crucial for the development, validation, and benchmarking of quantum algorithms and quantum hardware architectures.

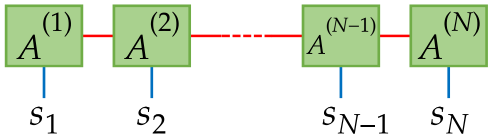
- **Role of Tensor Networks (TNs):**
  Tensor network approaches exploit the area law for entanglement entropy to efficiently approximate low-energy states of Hamiltonians of gapped systems with local interactions, enabling the simulation of such systems that are otherwise inaccessible to conventional methods.

TNs & Thin SVD

Matrix Product State (MPS):

$|\Psi\rangle_N = \sum_{\{s_i=1,\dots,d\}} \psi_{s_1,\dots,s_N} |s_1 \dots s_N\rangle$, where $\psi_{s_1,\dots,s_N}$ is a d^N-dimensional tensor.

$\psi_{s_1, s_2,\dots,s_N} = A^{(1)}_{1, s_1, \alpha_1} A^{(2)}_{\alpha_1, s_2, \alpha_2} \dots A^{(N-1)}_{\alpha_{N-2}, s_{N-1}, \alpha_{N-1}} A^{(N)}_{\alpha_{N-1}, s_N, 1}$ ⇒

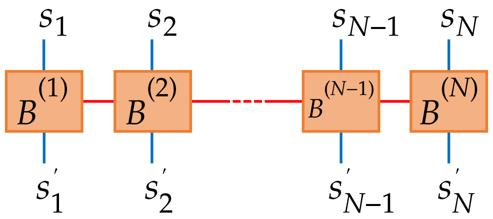


Number of parameters: $d^N \to dN\chi^2_{max}$

Matrix Product Operator (MPO):

$\widehat{O} = \sum_{\{s_i=1,\dots,d\}} \sum_{\{s'_j=1,\dots,d\}} o_{s_1,\dots,s_N, s'_1,\dots,s'_N} |s_1 \dots s_N\rangle \langle s'_1 \dots s'_N|$, where $o_{s_1,\dots,s_N, s'_1,\dots,s'_N}$ is a $d^N \times d^N$-dimensional tensor.

$o_{s_1,\dots,s_N, s'_1,\dots,s'_N} = B^{(1)}_{1, (s_1, s'_1), \beta_1} B^{(2)}_{\beta_1, (s_2, s'_2), \beta_2} \dots B^{(N-1)}_{\beta_{N-2}, (s_{N-1}, s'_{N-1}), \beta_{N-1}} B^{(N)}_{\beta_{N-1}, (s_N, s'_N), 1}$ ⇒



Number of parameters: $d^N \times d^N \to d^2N\chi^2_{max}$

Thin Singular Value Decomposition (SVD):

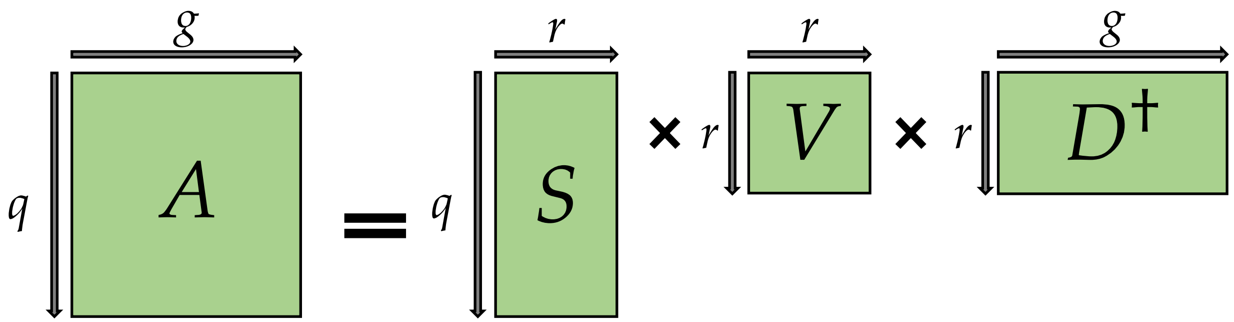
$A_{n,m} = S_{n,k} V_{k,k} (D^\dagger)_{k,m}$, $A \in \mathbb{C}^{q\times g}$, $S^\dagger S = I$, $D^\dagger D = I$.

Here, S is a left singular vectors,

V is a diagonal matrix of singular values,

$D^\dagger$ is a right singular vectors.

⇒



Time-Dependent Variational Principle

Variational formulation of the Schrödinger equation:

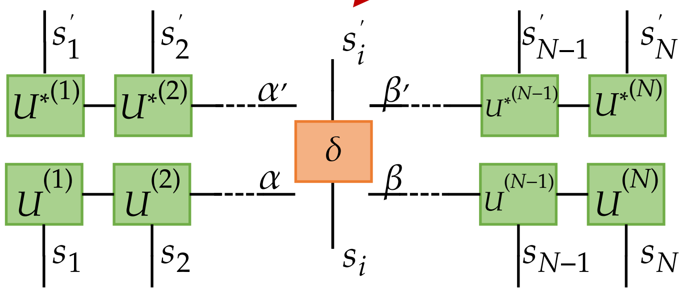
$$\min_{\left|\Psi^{TN}(t)\right\rangle} \left| \frac{d}{dt}\left|\Psi^{TN}(t)\right\rangle + \frac{i}{\hbar}\hat{H}(t)\left|\Psi^{TN}(t)\right\rangle \right|^2 \quad \forall\, t \in [t_{min}, t_{max}]$$

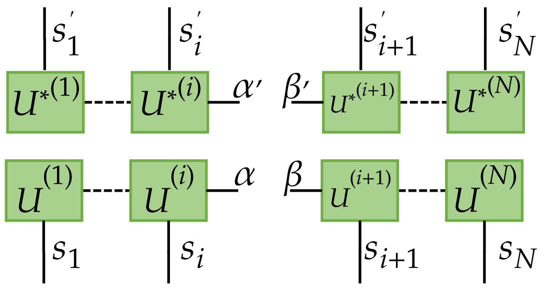
The tangent space projection operator (only loop-free TNs):

$$\frac{d}{dt}\left|\Psi^{TN}(t)\right\rangle = -\frac{i}{\hbar}\hat{P}_{\left|\Psi^{TN}(t)\right\rangle}\hat{H}(t)\left|\Psi^{TN}(t)\right\rangle$$

$$\hat{P}_{\left|\Psi^{TN}\right\rangle} = \sum_{i=1}^{N} \underbrace{\mathbb{I}^{(i)} \otimes \sum_{Q_i} \left|q_1^{[i]},\dots,q_{r_i}^{[i]}\right\rangle\left\langle q_1^{[i]},\dots,q_{r_i}^{[i]}\right|} - \sum_{(i,j)_k} \underbrace{\sum_{q_k, q_k^{'}} \left|q_k^{'[j]}\right\rangle\left\langle q_k^{'[j]}\right| \otimes \left|q_k^{[i]}\right\rangle\left\langle q_k^{[i]}\right|}$$

Here, $\left|q_k^{[i]}\right\rangle$ is the orthonormal basis state of the TTN segment attached to site i through link q_k when the network is orthogonalized around i.





Density Matrix Renormalization Group

Variational formulation for the ground-state problem:

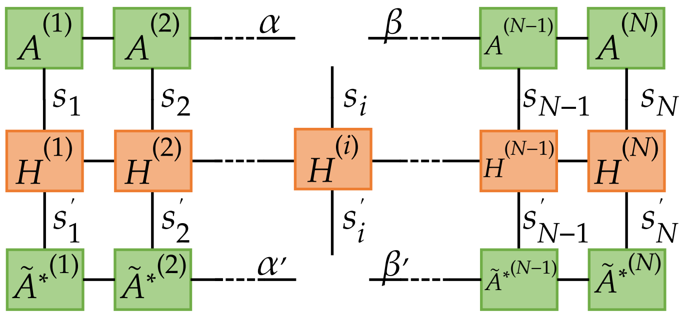
$$min_{|\Psi^{TN}\rangle} \langle \Psi^{TN} | \hat{H} | \Psi^{TN} \rangle$$

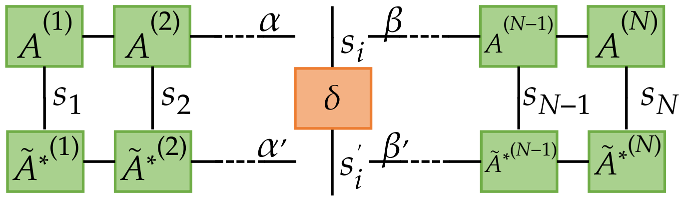
$$\text{at } \langle \Psi^{TN} | \Psi^{TN} \rangle = 1$$

Lagrange multiplier method:

$$L = \langle \Psi^{TN} | \hat{H} | \Psi^{TN} \rangle - \lambda \left(\langle \Psi^{TN} | \Psi^{TN} \rangle - 1 \right)$$

$$\frac{\delta L}{\delta \widetilde{A^{(i)}}^{*}} = 0 \;\rightarrow\; \hat{H}^{(i)}_{eff} \widetilde{A^{(i)}} = \lambda^{(i)}_{min} \hat{N}^{(i)} \widetilde{A^{(i)}}$$





Existing Toolkits

The most widely used and functional TN toolkits are iTensor and TeNPy.

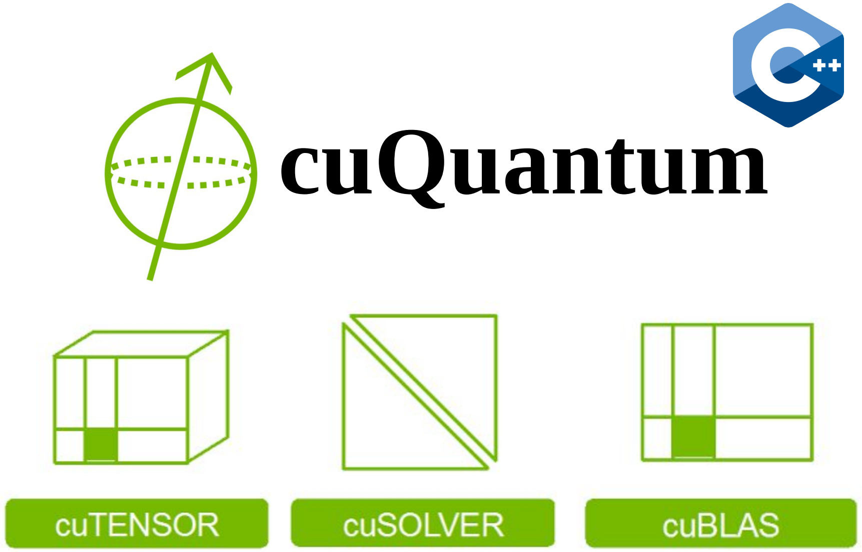
- iTensor features:
  - Utilizes a single CPU or GPU
  - Provides intuitive "smart index" algebra
  - Focuses mainly on MPS/MPO
  - Makes custom geometries hard to build
- TeNPy features:
  - Utilizes only a CPU
  - Focuses mainly on MPS/MPO
  - Makes custom geometries hard to build

An alternative is Nvidia-developed cuQuantum package.

- cuQuantum benefits:
  - utilizes one or more GPUs via MPI
  - provides high-performance implementations of SVD/QR decomposition, tensor construction, and gradient calculation
  - Allows any tensor architecture to be built
  - Offers strong optimization of contraction paths
- cuQuantum issues:
  - Lacks ready-to-use implementations of most physical TN algorithms
  - Remains hardware-locked exclusively to NVIDIA ecosystems

QTensorNet

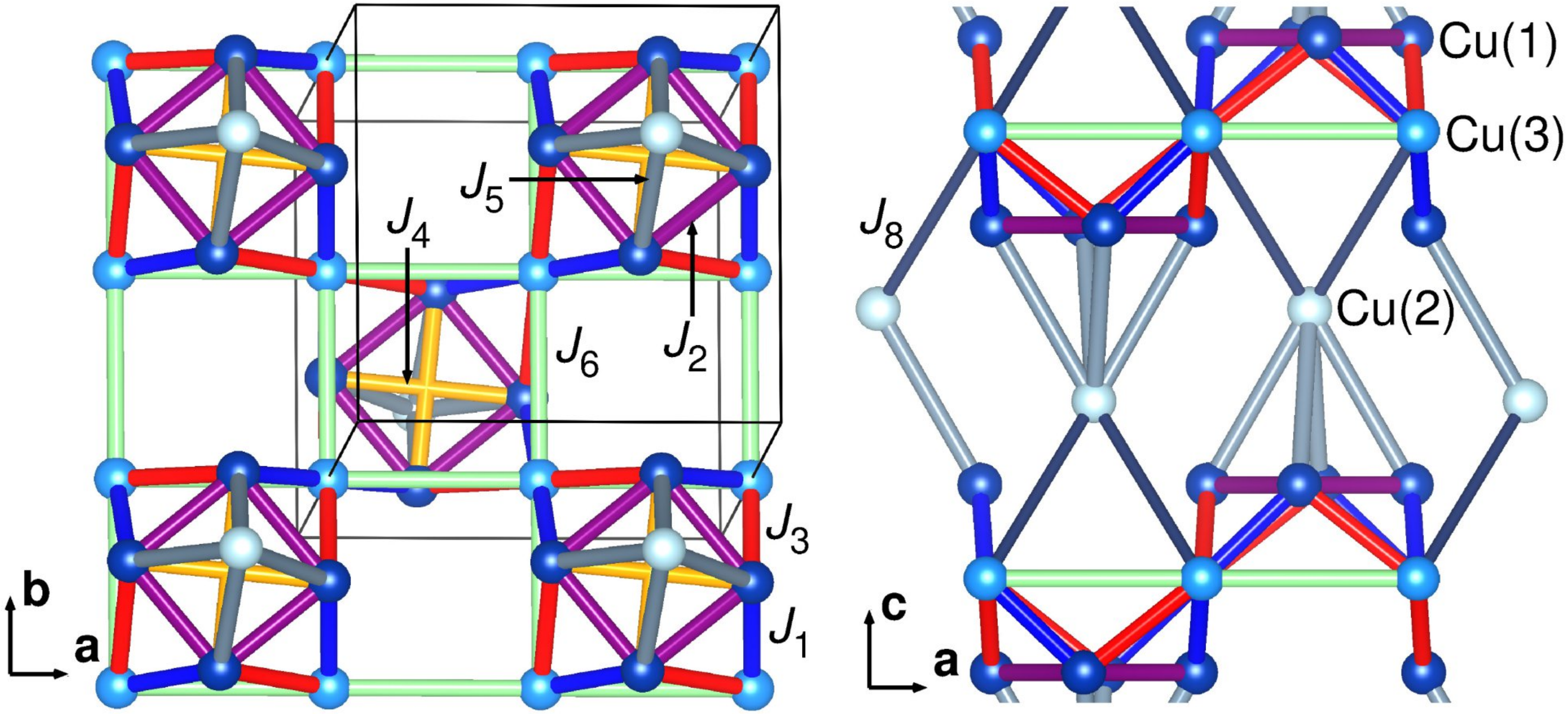
- Currently, the toolkit supports any single-level, loop-free tensor network.
- The toolkit utilizes a single Nvidia GPU (or multiple GPUs via MPI) for contraction of a tensor network.
- The toolkit uses cuSOLVER, cuTENSOR, and cuBLAS to solve linear algebra problems.
- The TEBD, DMRG & TDVP methods are implemented.
- Basic operations for operator algebra and Hilbert space vectors represented as TNs are implemented.



Github: https://github.com/YauheniTalochkaN/QTensorNet

Decorated Square-Kagome Heisenberg Antiferromagnet

Nabokoite $KCu_7TeO_4(SO_4)_5Cl$



M.G. Gonzalez, Y. Iqbal, J. Reuther, H.O. Jeschke, Field-induced spin liquid in the decorated square-kagome antiferromagnet nabokoite $KCu_7TeO_4(SO_4)_5Cl$, (2024). https://doi.org/10.48550/arXiv.2410.10385.

This work was carried out in collaboration with Dr. Pavel Maksimov, Bogoliubov Laboratory of Theoretical Physics, JINR.

Decorated Square-Kagome Heisenberg Antiferromagnet

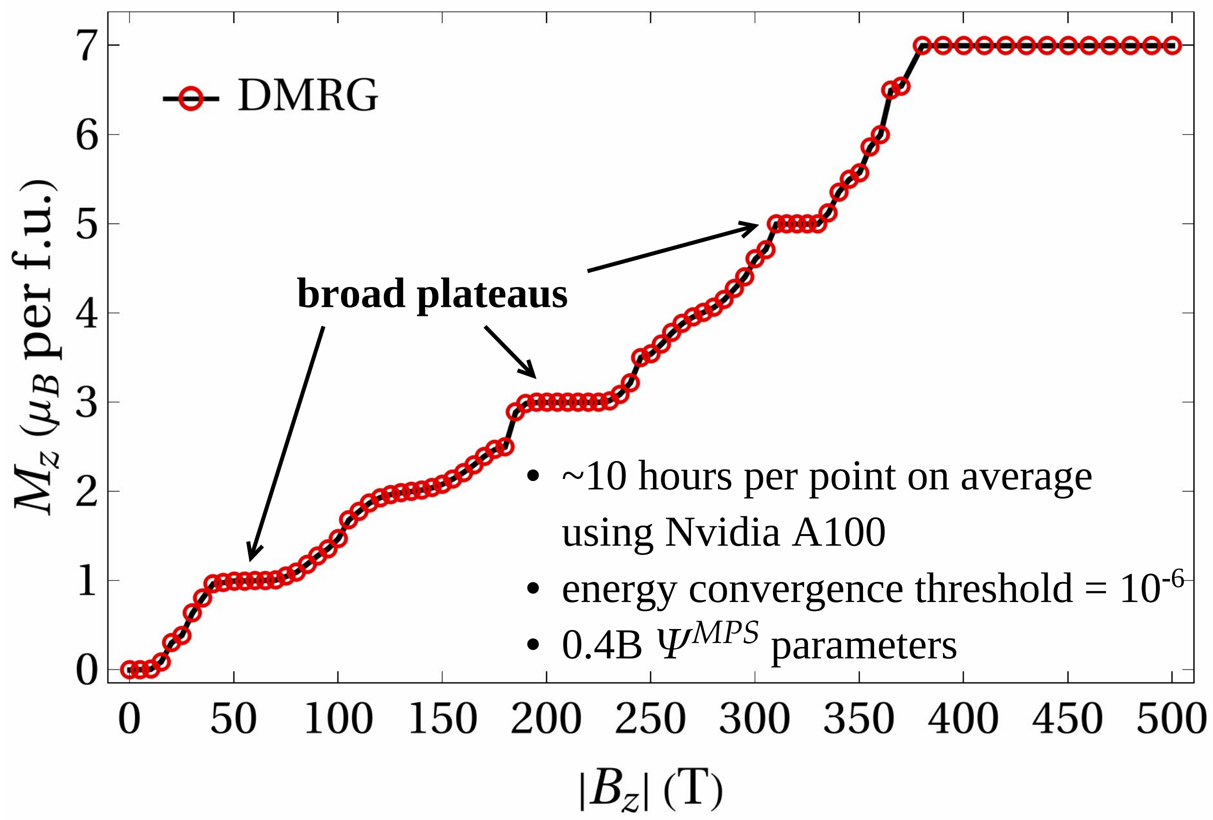
$$\hat{H} = -g\mu_B \frac{\hbar}{2}\sum_{i=1}^{N} B_z \hat{\sigma}_{z,\,i} + \frac{\hbar^2}{4}\sum_{i<j} J_{i,j}\hat{\vec{\sigma}}_i \cdot \hat{\vec{\sigma}}_j$$

$4 \times 4 \times 7$ cluster = 112 spins

$|\Psi\rangle \rightarrow \Psi^{MPS}$ $\quad \chi_{max}^{MPS} = 1500$

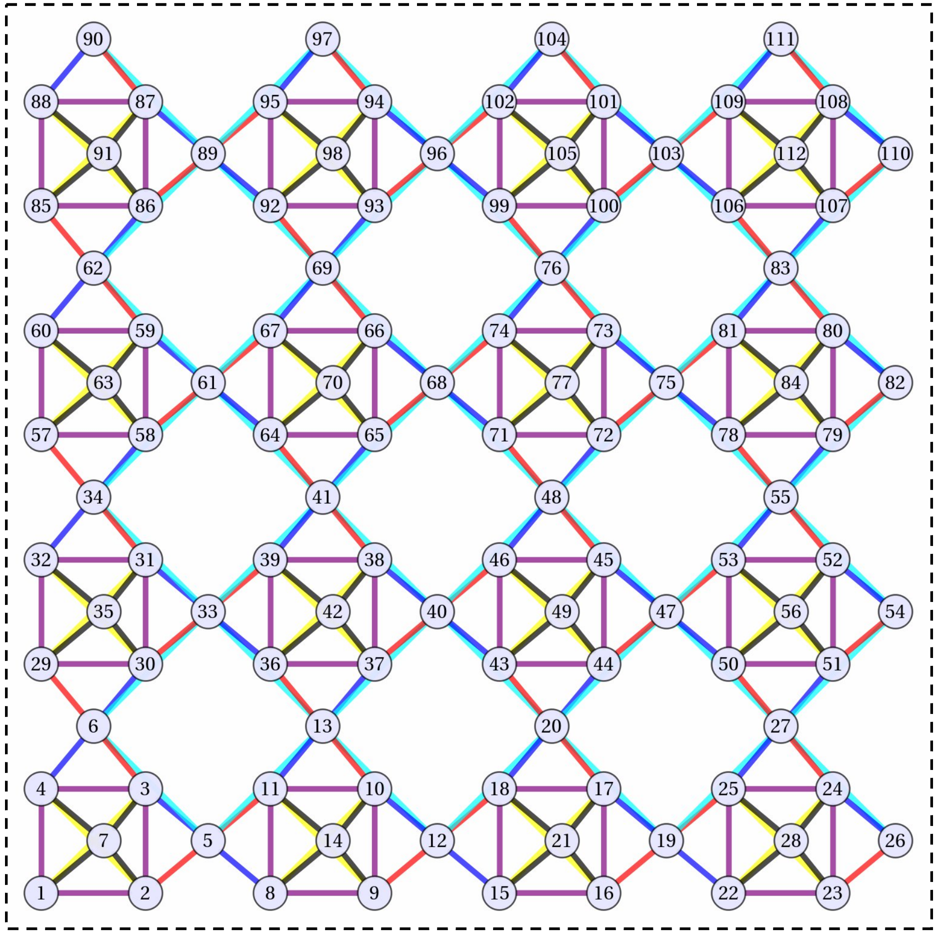
$\hat{H} \rightarrow H^{MPO}$ $\quad \chi_{max}^{MPO} = 300$

$$M_z = \frac{1}{16}\left\langle \Psi_{gs}^{MPS} \left| \sum_{i=1}^{N} \hat{\sigma}_{z,\,i} \right| \Psi_{gs}^{MPS} \right\rangle$$



- $J_1 =$ 0.1723 meV
- $J_2 =$ 10.1685 meV
- $J_3 =$ 14.2186 meV
- $J_4 =$ 14.6495 meV
- $J_5 =$ 13.0983 meV
- $J_6 =$ 2.6714 meV

Periodic Boundary Conditions



Conclusions & Outlook

- QTensorNet was developed as a high-performance, GPU-accelerated toolkit for the efficient simulation of many-body quantum systems using tensor network methods.
- The ground-state magnetization dependence on the external magnetic field for a 112-spin cluster of nabokoite was calculated using QTensorNet, predicting broad plateaus at M_z = 1, 3, and 5 μ_B per f.u.
- Neural-network-inspired optimization techniques and numerical orthogonalization methods will be integrated into QTensorNet to enable support for loopy tensor networks, such as PEPS and MERA.

Acknowledgments

I sincerely thank the support team of the GOVORUN supercomputer and personally Maxim Zuev for the assistance with software installation and configuration.

Thank you for attention!