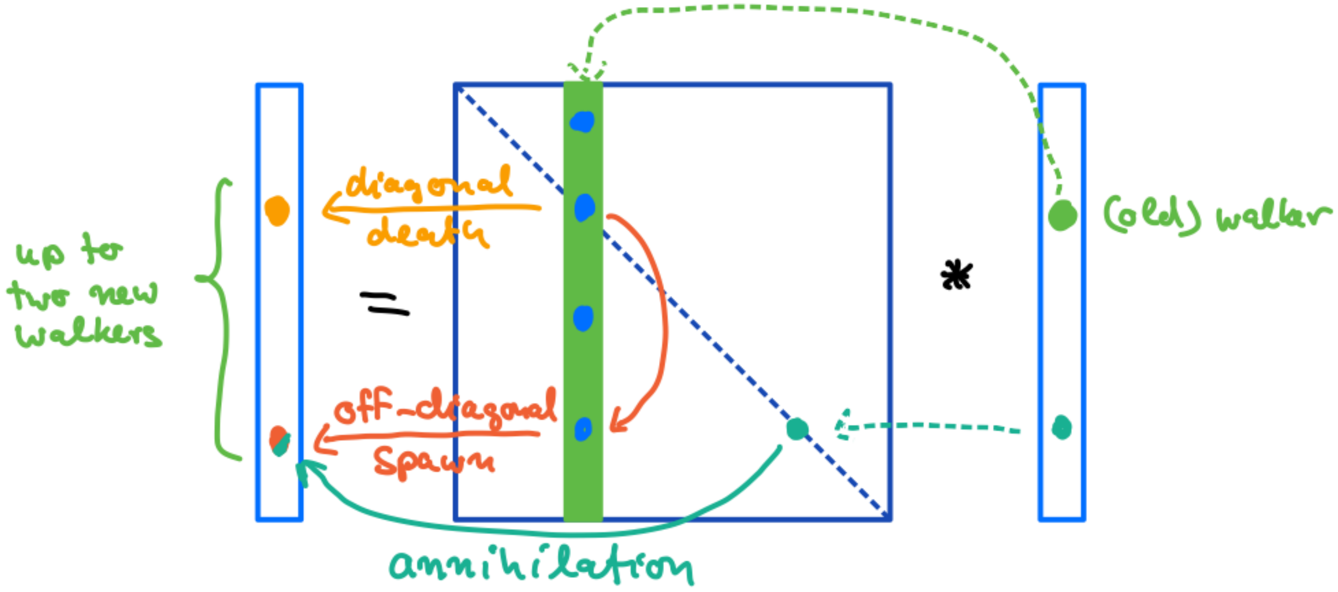
The Dodd-Walls Centre
for Photonics and Quantum Technology

Massey University
COLLEGE OF SCIENCES

Projector Monte Carlo and Exact Diagonalization with Rimu.jl



Joachim Brand

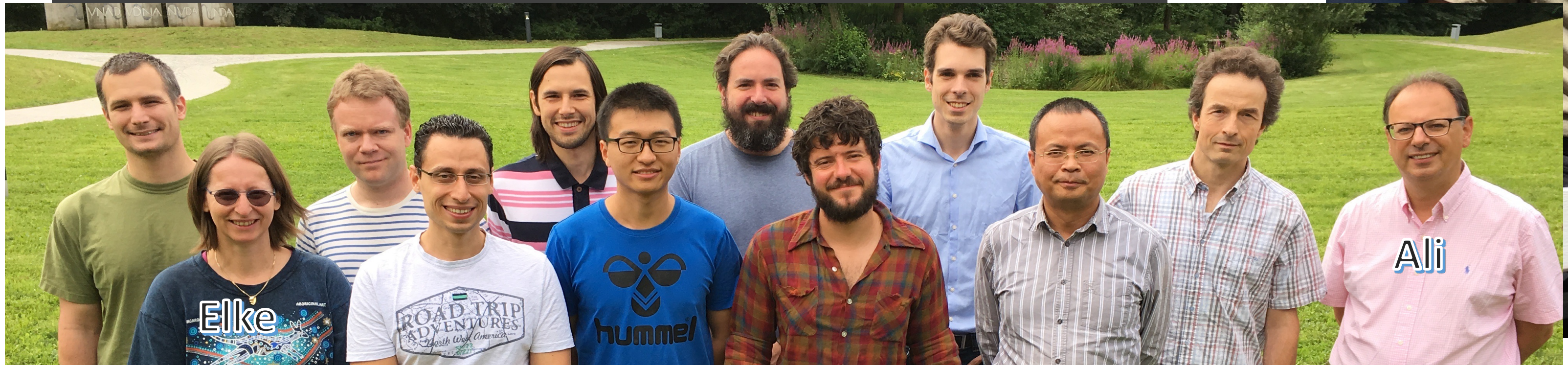
JuliaCon24 Eindhoven, 11 July 2024

Collaborators on Rimu.jl

Massey University:

- Matija Čufar
- Mingrui (Ray) Yang
- Chris Bradly
- Satyanand Kuwar

- Auckland University:
  - Elke Pahl
  - Jamie Taylor
- MPI Solid State Research Stuttgart:
  - Ali Alavi



Dodd-Walls Centre
for Photonic and Quantum Technologies
Te Whai Ao

- Government funded **Centre of Research Excellence** (re-funded through 2028)
- Main areas:
  - Ultra-cold atoms, quantum gases
  - Quantum sensing
  - Quantum optics
  - Nonlinear fibre optics
  - Photonic sensing
  - Biophotonics
- Funds:
  - Projects: fundamental to translational
  - Postdocs
  - PhD scholarships
  - Outreach

We want to solve / find…

Ground and excited states

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Time-independent Schrödinger equation

Booth, Thom, Alavi, JCP (2009)
Cleland, Booth, Alavi, JCP (2010)

Finite temperature physics
(canonical density matrix / partition function)

$$\hbar\frac{d\hat{\rho}}{d\beta} = -\frac{1}{2}\left\{\hat{H},\hat{\rho}\right\}$$

Bloch equation

Blunt *et al.* PRB (2014)

Quantum dynamics

$$i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$$

Schrödinger equation

McClean, Parkhill, Aspuru-Guzik, PNAS (2013), PRA (2015)
Guther et al. PRL (2018)

Driven dissipative dynamics
(open quantum system)

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \sum_i\left(\hat{L}_i\hat{\rho}\hat{L}_i^\dagger - \frac{1}{2}\left\{\hat{L}_i^\dagger\hat{L}_i,\hat{\rho}\right\}\right)$$

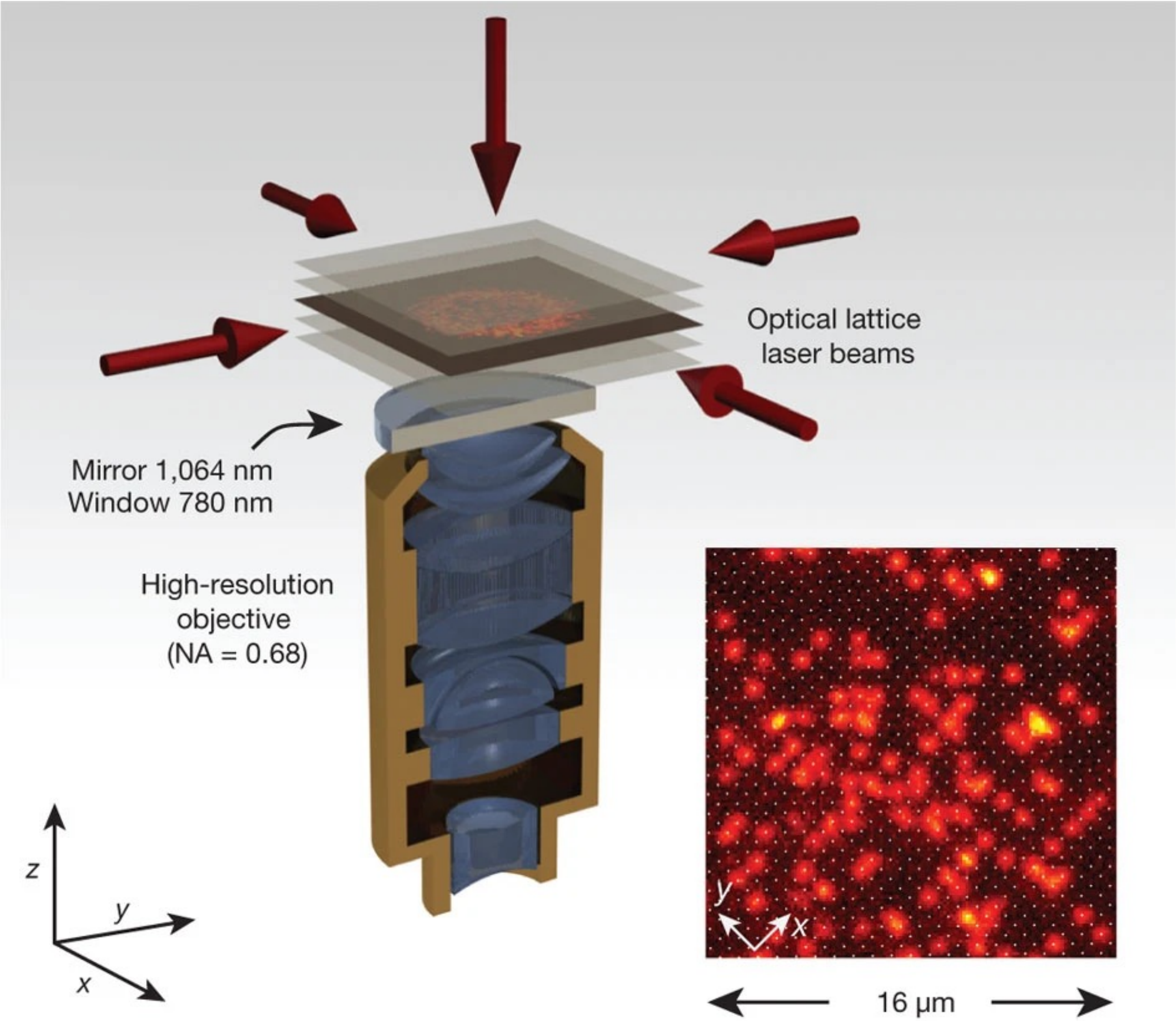
(Lindblad) quantum master equation

Nagy, Savona PRA (2018)

…with quantum Monte Carlo

Available algorithms and implementations based on Full Configuration Interaction Quantum Monte Carlo (FCIQMC)

Motivation: The physics of ultracold atoms and molecules



Laser-cooled ultracold gases of atoms or molecules can engineer synthetic quantum many-body systems, e.g. the Bose-Hubbard model.

Quantum gas microscopes can probe the quantum state with single-atom and single site resolution.

Fig. from Sherson et al. Nature 467, 68 (2010)

What is Rimu? - Dacrydium Cupressinum

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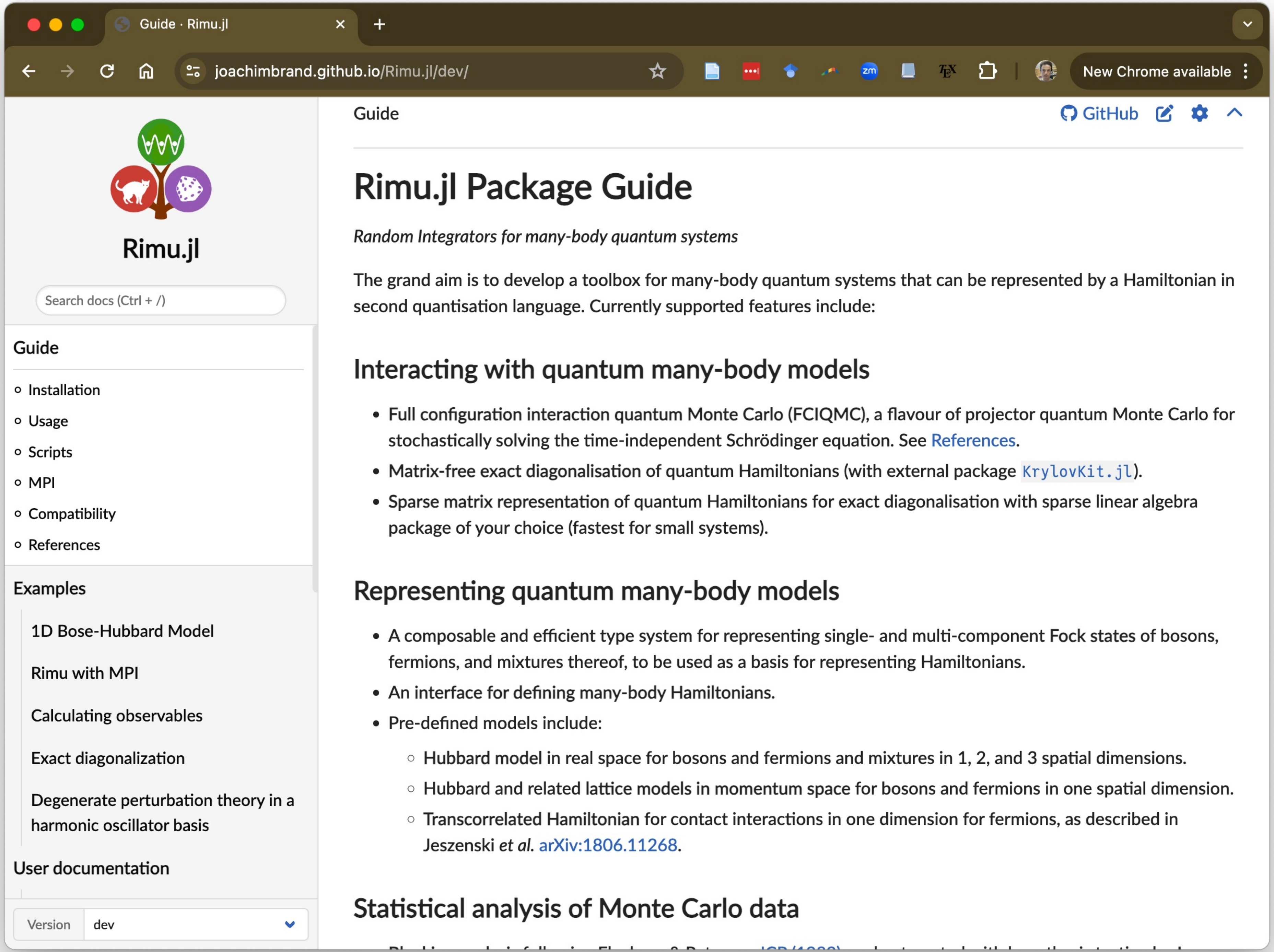

Guide · Rimu.jl

joachimbrand.github.io/Rimu.jl/dev/

New Chrome available

Rimu.jl

Search docs (Ctrl + /)

Guide

- Installation
- Usage
- Scripts
- MPI
- Compatibility
- References

Examples

1D Bose-Hubbard Model

Rimu with MPI

Calculating observables

Exact diagonalization

Degenerate perturbation theory in a harmonic oscillator basis

User documentation

Version dev

Guide

GitHub

Rimu.jl Package Guide

Random Integrators for many-body quantum systems

The grand aim is to develop a toolbox for many-body quantum systems that can be represented by a Hamiltonian in second quantisation language. Currently supported features include:

Interacting with quantum many-body models

- Full configuration interaction quantum Monte Carlo (FCIQMC), a flavour of projector quantum Monte Carlo for stochastically solving the time-independent Schrödinger equation. See References.
- Matrix-free exact diagonalisation of quantum Hamiltonians (with external package `KrylovKit.jl`).
- Sparse matrix representation of quantum Hamiltonians for exact diagonalisation with sparse linear algebra package of your choice (fastest for small systems).

Representing quantum many-body models

- A composable and efficient type system for representing single- and multi-component Fock states of bosons, fermions, and mixtures thereof, to be used as a basis for representing Hamiltonians.
- An interface for defining many-body Hamiltonians.
- Pre-defined models include:
  - Hubbard model in real space for bosons and fermions and mixtures in 1, 2, and 3 spatial dimensions.
  - Hubbard and related lattice models in momentum space for bosons and fermions in one spatial dimension.
  - Transcorrelated Hamiltonian for contact interactions in one dimension for fermions, as described in Jeszenski *et al.* arXiv:1806.11268.

Statistical analysis of Monte Carlo data

Open-source package
Developed since 2016

So far:

- Bosons, fermions, mixtures
- Hubbard, Transcorrelated
- Exact diagonalization
- FCIQMC

Future:

- Time evolution
- Spinor gases, spin-orbit coupling
- Open quantum systems

Why full configuration interaction quantum Monte Carlo?

Projector quantum Monte Carlo

- Solve the time-independent Schrödinger equation

$$\hat{H}|\Psi\rangle = E_0|\Psi\rangle$$

- Find stochastic averages for the ground state energy and properties

Existing projector Monte Carlo methods

- Green's function Monte Carlo (GFC: Kalos, PR 1962)
- Diffusion Monte Carlo (DMC: JB Anderson, JCP 1975)
- Auxiliary-field quantum Monte Carlo (AFQMC)
- Path integral ground-state Monte Carlo (PIGS)

Why "Full configuration interaction quantum Monte Carlo" (FCIQMC: Booth, Thom, Alavi, JCP 2009)?
It a natural extension of exact diagonalization / FCI.

Full configuration interaction quantum Monte Carlo (FCIQMC)

Major developments

- Integer formulation (Booth, Thom, Alavi, JCP 2009)
  First formulation of algorithm
- Initiator rule (Cleland, Booth, Alavi, JCP 2010)
  Approximation that softens the sign problem
- Population dynamics with sign problem (Spencer, Blunt, Foulkes, JCP2012)
  Improved understanding of the nature of the sign problem in FCIQMC
- Semistochastic FCIQMC and floating-point coefficients (Petruziello *et al.* PRL 2012)
  Reduces noise and improves efficiency
- Vector compression theory; fast randomized iterations (Lim, Weare, SIAM Review 2017)

Our work

- Improved population control (Yang, Pahl, Brand, JCP 2020)
- Analysis of population control bias (Brand, Yang, Pahl, PRB 2022)

Starting point: Fock basis states

Represent Hamiltonian in a basis of Fock states / number states /Slater determinants (if fermions)

$$|\Psi_0\rangle = \sum_{\bar{n}} c_{\bar{n}} |\bar{n}\rangle$$

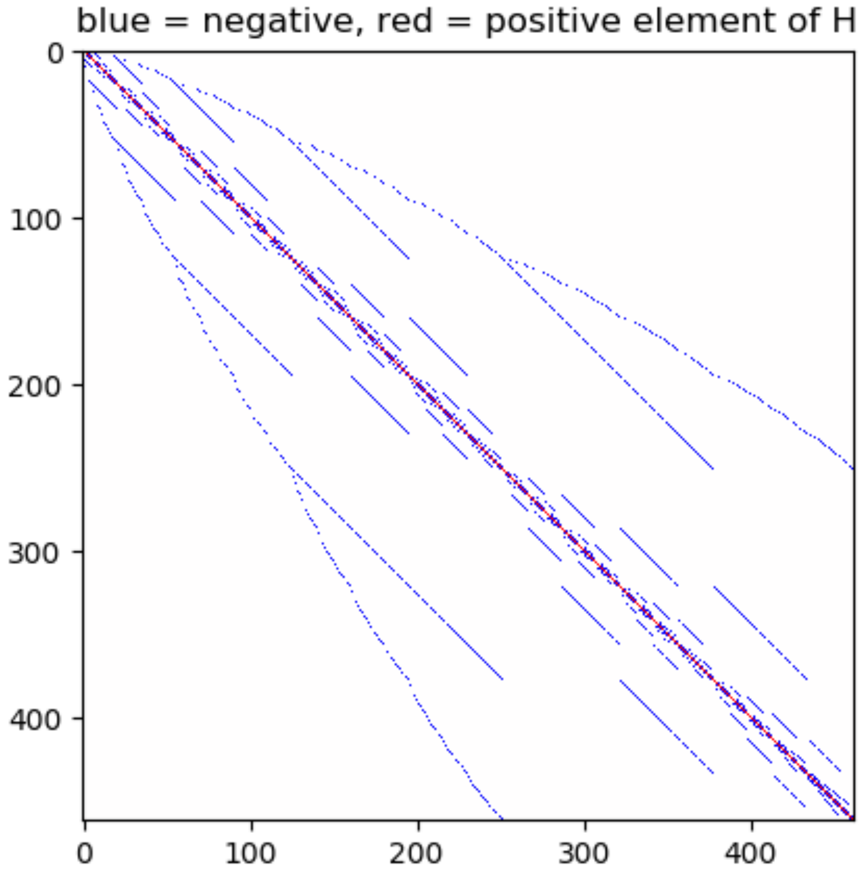
$$|n_1, n_2, \ldots, n_M\rangle = \prod_{i=1}^{M} \frac{1}{\sqrt{n_i!}} \left(\hat{a}_i^\dagger\right)^{n_i} |\mathrm{vac}\rangle$$

E.g. Bose Hubbard model with *N*=6 particle in *M*=6 sites

$$\hat{H} = -J \sum_{\langle i,j\rangle} \hat{a}_i^\dagger \hat{a}_j + U \sum_i \hat{n}_i(\hat{n}_i - 1)$$

… becomes a matrix with elements

$$(\mathbf{H})_{\bar{n},\bar{m}} = \langle n_1, n_2, \ldots, n_M | \hat{H} | m_1, m_2, \ldots, m_M \rangle$$



N = 6, M = 6, dim H = 462

Projector Monte Carlo principles

Representing the Hamiltonian as a matrix, turns the Schrödinger equation into a **generic linear algebra problem**:

$$\mathbf{H}\mathbf{c}_0 = E_0\mathbf{c}_0$$

Iteration equation:

$$\mathbf{c}^{(n+1)} = \mathbf{T}\mathbf{c}^{(n)} \quad \text{with} \quad \mathbf{T} = \mathbf{1} + \delta\tau\left(S^{(n)}\mathbf{1} - \mathbf{H}\right) \quad \text{(for FCIQMC)}$$

Discretised imaginary time evolution, or power method.

Fixed point (long time limit):

Coefficient vector $\mathbf{c}^{(n)} \to \mathbf{c}_0$

Scalar shift $S^{(n)} \to E_0$

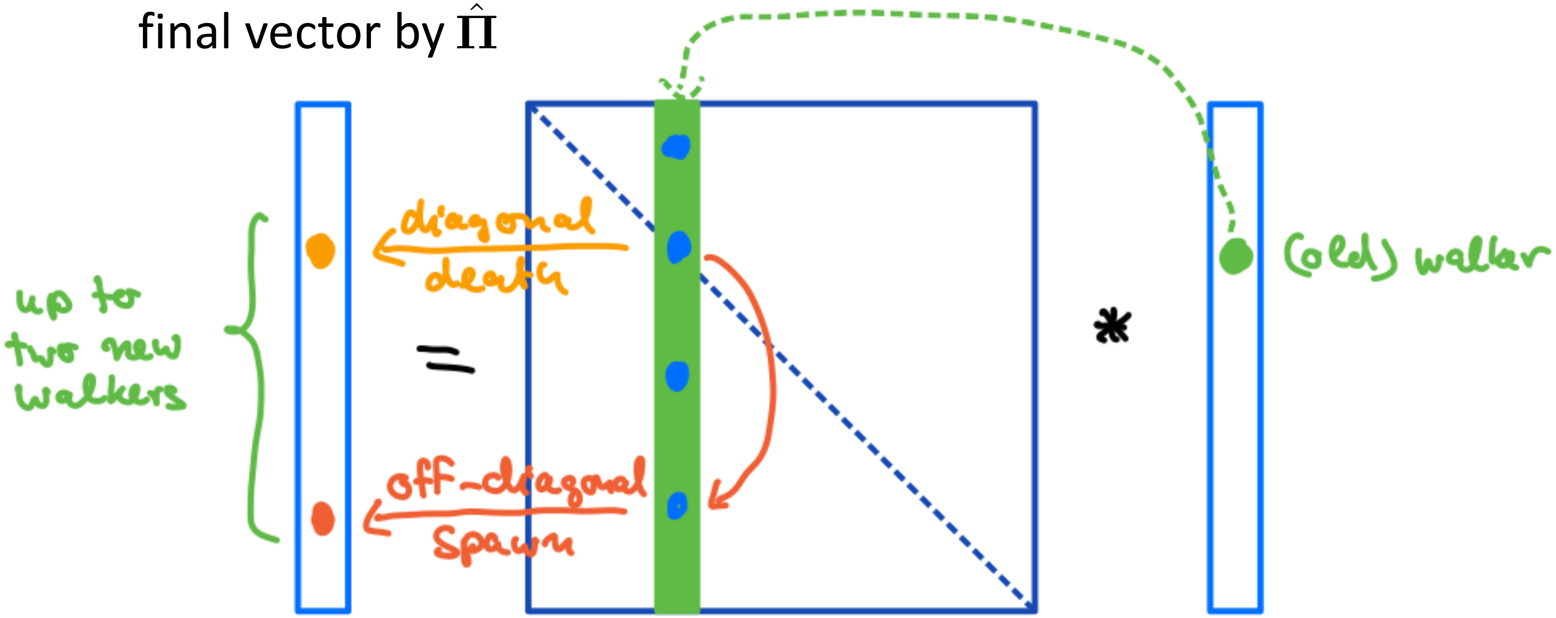
Code example

Stochastic sampling procedure

$$\mathbf{c}^{(n+1)} = \hat{\mathbf{\Pi}}\,\hat{\mathbf{T}}\mathbf{c}^{(n)}$$

Compression of
final vector by $\hat{\mathbf{\Pi}}$

Compression of
column vector in $\hat{\mathbf{T}}$ = stochastic spawning



DynamicSemistochastic style:
No vector compression in $\hat{\mathbf{T}}$ if the number of nonzero offdiagonals is less than the number of walkers in the coefficient c_i.

Parallelisation using native Julia threading

Data structure **PDVec**:
A vector of segmented Julia **Dict**s (hash tables) with one segment per thread.
Only configurations with non-zero coefficient (after stochastic projection) are stored.

$$\mathbf{c}^{(n+1)} = \hat{\mathbf{\Pi}}\,\hat{\mathbf{T}}\mathbf{c}^{(n)}$$

$\mathbf{c}^{(n)}$

Initial vector

Parallelisation using native Julia threading

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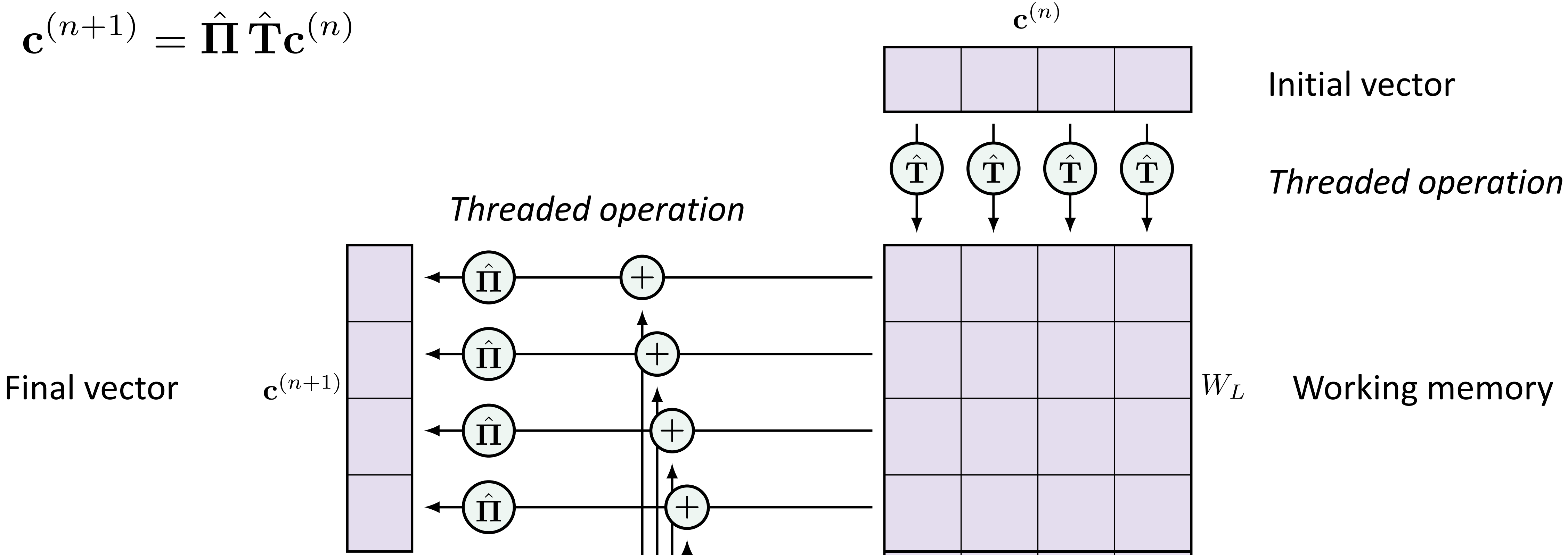
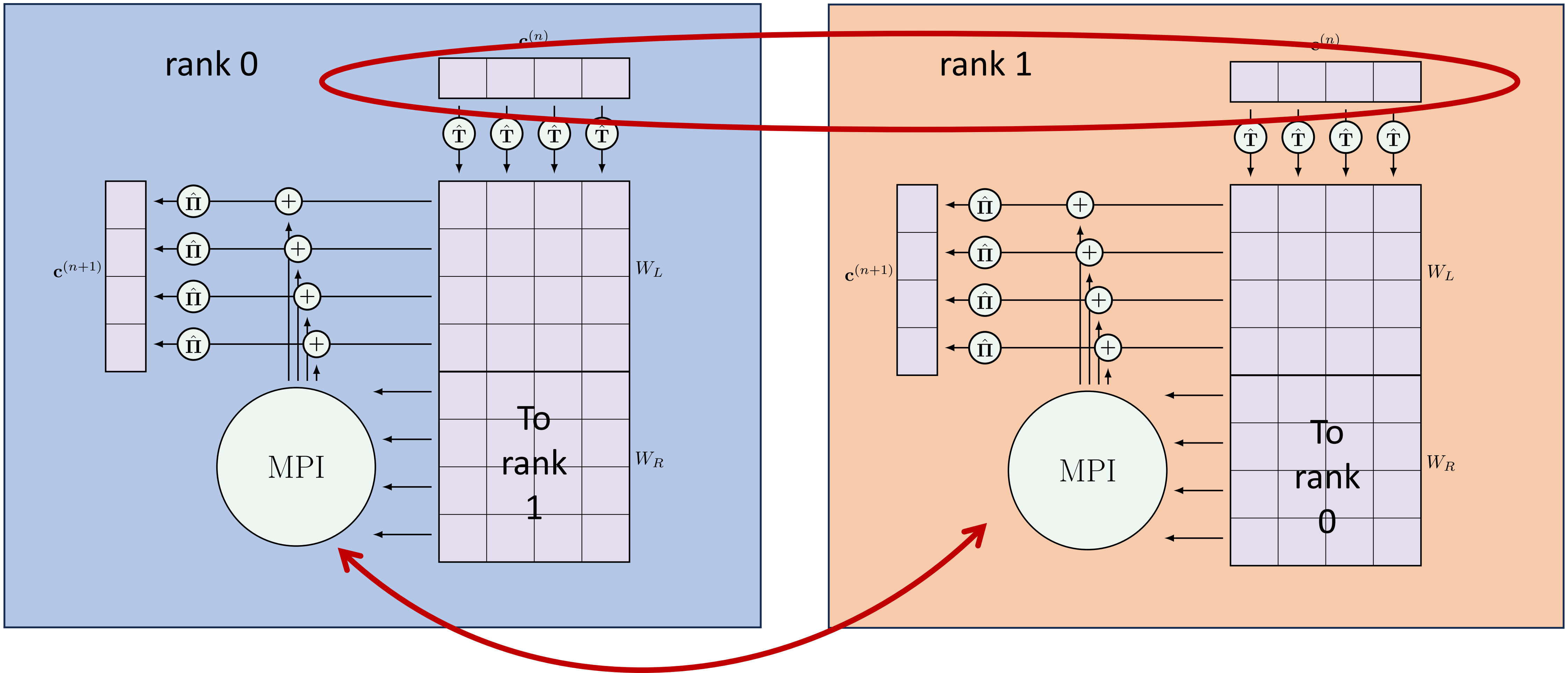
$$\mathbf{c}^{(n+1)} = \hat{\mathbf{\Pi}}\,\hat{\mathbf{T}}\mathbf{c}^{(n)}$$

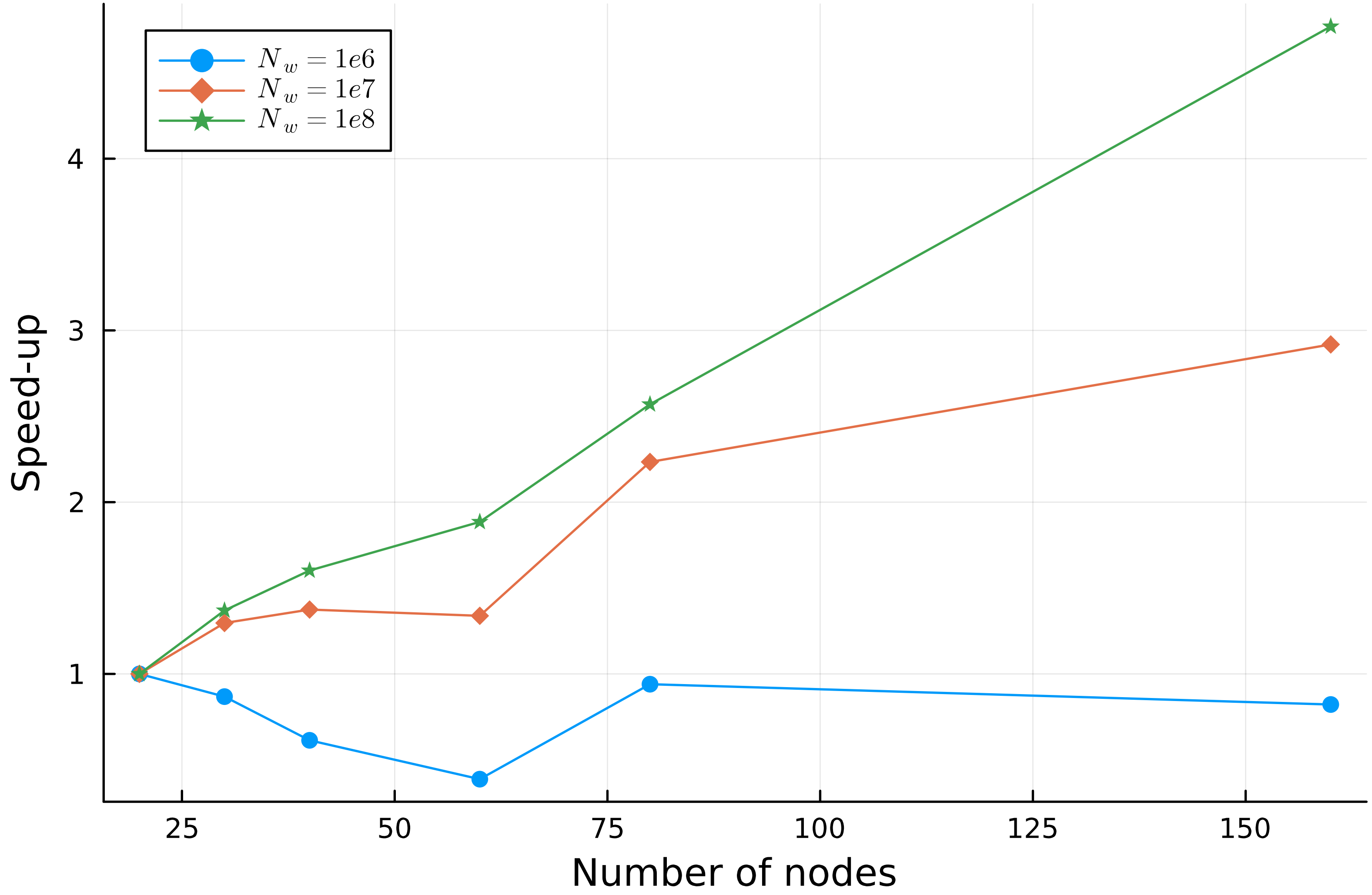


Adding distributed parallelism with MPI

Data structure **PDVec** is distributed across nodes.



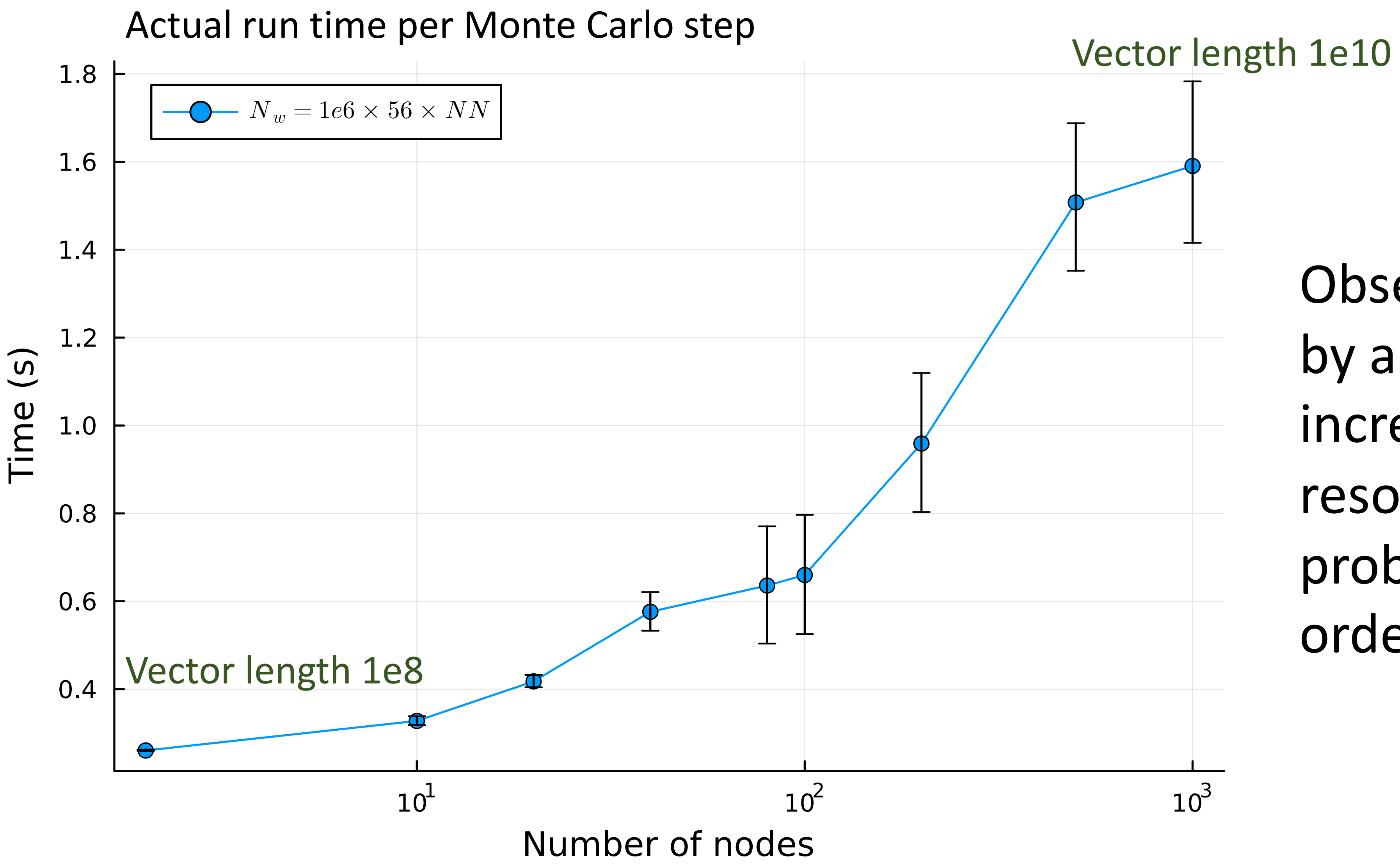
Strong scaling (first results) on Frontier (Oak Ridge National Lab)



Model:
6x6 Bose Hubbard model with 36 bosons and 1 impurity; dimension 8×10^{21}

Each node has 56 cores (threads).

Weak scaling

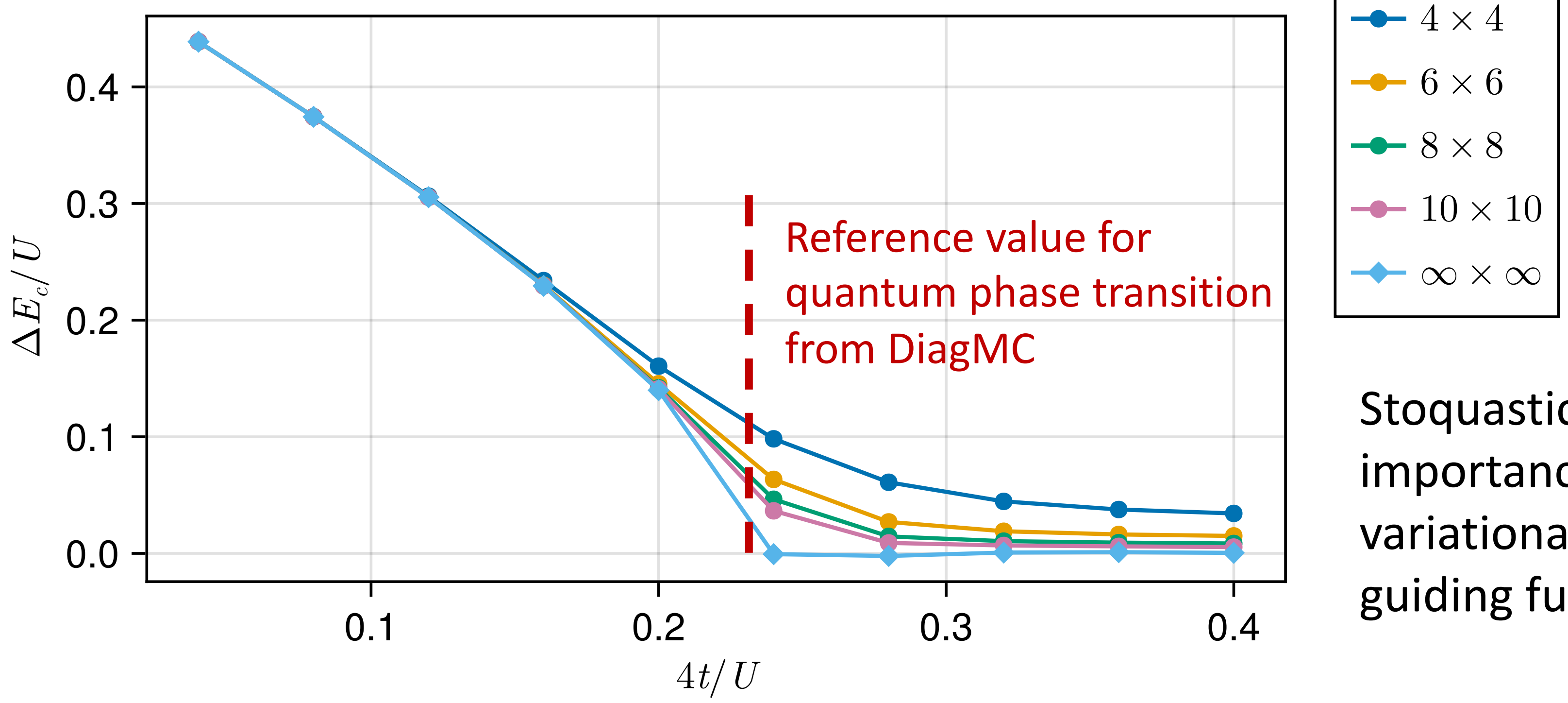


Observe a slow down by a factor of six when increasing the resources and problem size by 3 orders of magnitude.

Physics results: Mott-insulator superfluid transition in the 2D Bose-Hubbard model

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

Charge gap $\Delta E_C = E_{L+1} + E_{L-1} - 2E_L$



Dimension:
3×10^{8}
2×10^{20}
1×10^{37}
5×10^{58}

Stoquastic FCIQMC problem using importance sampling with variationally optimized (1-parameter) guiding function

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...with **Rimu.jl**

Collaborators welcome!

Funding (much appreciated)

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