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Boosted Imaginary Time Evolution of Matrix Product States

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Imaginary Time Evolution

- Given a Hamiltonian $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$, Imaginary Time Evolution (ITE) finds its ground state $|\phi_0\rangle$ by applying the non-unitary operator $\hat{T} = e^{-\hat{H}\tau}$ on some state $|s\rangle = \sum_j a_j|\phi_j\rangle$,

$$|\psi(\tau)\rangle = N(\tau)e^{-H\tau}|s\rangle = N(\tau)\sum_j e^{-E_j\tau}a_j|\phi_j\rangle\,,$$

where $N(\tau)$ is a normalisation constant.

- If $\langle s|\phi_0\rangle \neq 0$, $\frac{e^{-E_j\tau}a_{j\neq 0}}{e^{-E_0\tau}a_0}$ decays exponentially with time, and therefore $\tau \to \infty, |\psi(\tau)\rangle \to |\phi_0\rangle$

Boosted Imaginary Time Evolution (BITE) in 2D

Performing ITE for $\Delta\tau$ on $|s\rangle$ gives

$$|t\rangle = N(\Delta\tau)\left(e^{-E_0\Delta\tau}|\phi_0\rangle + e^{-E_1\Delta\tau}|\phi_1\rangle\right).$$

BITE Reflection Operator

Defining the BITE reflection operator

$$\hat{R}(|v\rangle) = 2|v\rangle\langle v| - \hat{I},$$

the n^{th} reflected state, $n \in \mathbb{N}$, is given by

$$|r_n\rangle = \hat{R}(|r_{n-1}\rangle)|r_{n-2}\rangle\,,$$

where $|r_0\rangle = |t\rangle$.

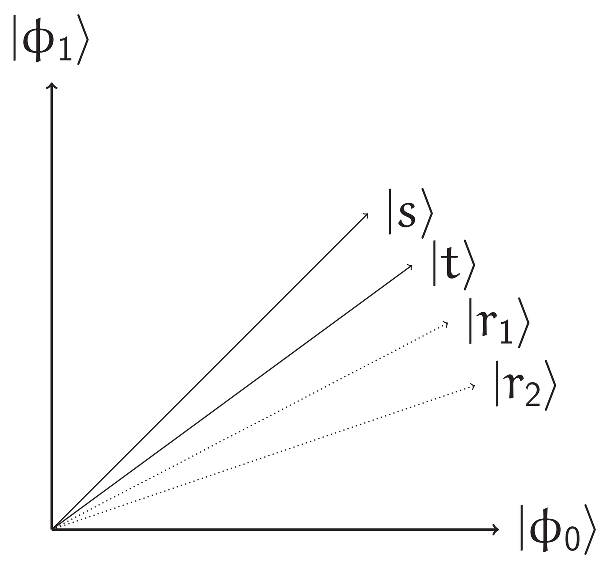

Figure 1: The state $|r_1\rangle$ is produced by reflecting $|s\rangle$ about $|t\rangle$. The state $|r_2\rangle$ is produced by reflecting $|t\rangle$ about $|r_1\rangle$.

Efficient boosting

$|r_n\rangle$ is given by the recurrence relation

$$|r_n\rangle = 2\langle r_{n-1}|r_{n-2}\rangle|r_{n-1}\rangle - |r_{n-2}\rangle = 2\langle t|s\rangle|r_{n-1}\rangle - |r_{n-2}\rangle\,.$$

As $|r_n\rangle$ is in the plane spanned by $|s\rangle$ and $|t\rangle$, one can write

$$|r_n\rangle = \alpha_n|t\rangle + \beta_n|s\rangle\,,$$

with the recurrence relations

$$\alpha_n = 2\langle t|s\rangle\alpha_{n-1} - \alpha_{n-2},\ \text{and}\ \beta_n = -\alpha_{n-1},$$

with the initial conditions $\alpha_{-1} = 0$ and $\alpha_0 = 1$. It follows that the homogeneous recurrence relation for $|r_n\rangle$ has the close form expression

$$|r_n\rangle = \frac{1}{\sin(\theta)}\left(\sin((n+1)\theta)|t\rangle - \sin(n\theta)|s\rangle\right),$$

where $\cos(\theta) = \langle t|s\rangle$.

Stop criterion

Energy of the n^{th} reflected state $|r_n\rangle$ is

$$E_n = \alpha_n^2E_t + \alpha_{n-1}^2E_i - 2\alpha_n\alpha_{n-1}E_{it},$$

where $E_t = \langle t|\hat{H}|t\rangle$, $E_s = \langle s|\hat{H}|s\rangle$ and $E_{st} = \langle s|\hat{H}|t\rangle$.

E_n is calculated until $E_{n+1} > E_n$, and $|r_n\rangle$ is found using the closed form expression.

BITE algorithm

- Imaginary time evolve an initial state $|s\rangle$ by a single step $\Delta\tau$ to produce a state $|t\rangle$.
- Calculate the overlap $\langle t|s\rangle$ and the terms E_t, E_s and E_{st} and the series of energies $E_n < E_{n+1}$. Compute the corresponding state $|r_n\rangle$.
- Imaginary time evolve $|r_n\rangle$ by a single step to produce a new initial state $|s'\rangle$, and by two steps to produce a new evolved state $|t'\rangle$.
- Repeat steps 1-3 using the new states $|s'\rangle$ and $|t'\rangle$ as the initial states until the energy converges.

BITE in 3D

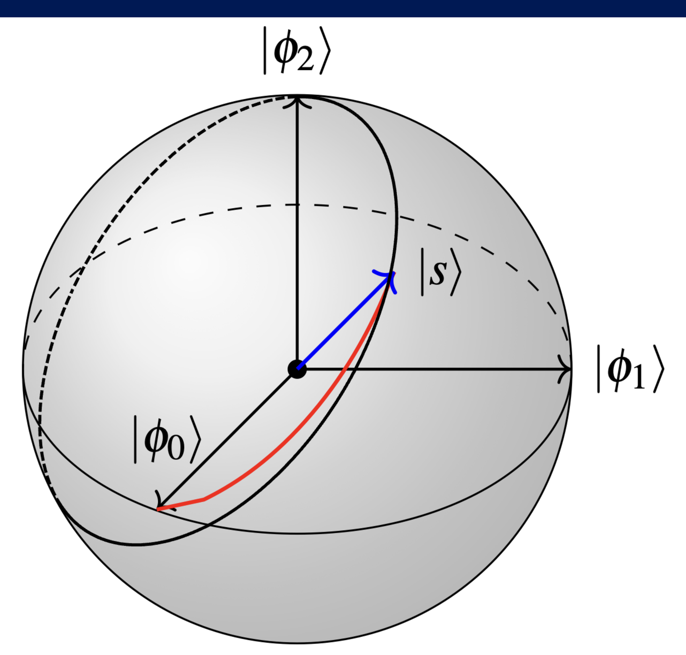

Figure 2: A visualisation of BITE in a norm conserving 3D Hilbert space. The blue vector represents the initial state $|s\rangle$ and the red curve is a trajectory resulting from imaginary time evolution. BITE can access any state on the the black great circle spanned by $|s\rangle$ and $|t\rangle$ (not shown).

Results

As a test case, we use the transverse field Ising model on a 1D spin chain given by

$$\hat{H} = -J\sum_{i,j}X_iX_j - g\sum_i Z_i,$$

with $n = 100$ sites, open boundary conditions, $J = 0.5$ and $g = 1.5$, $\Delta\tau = 0.001$.

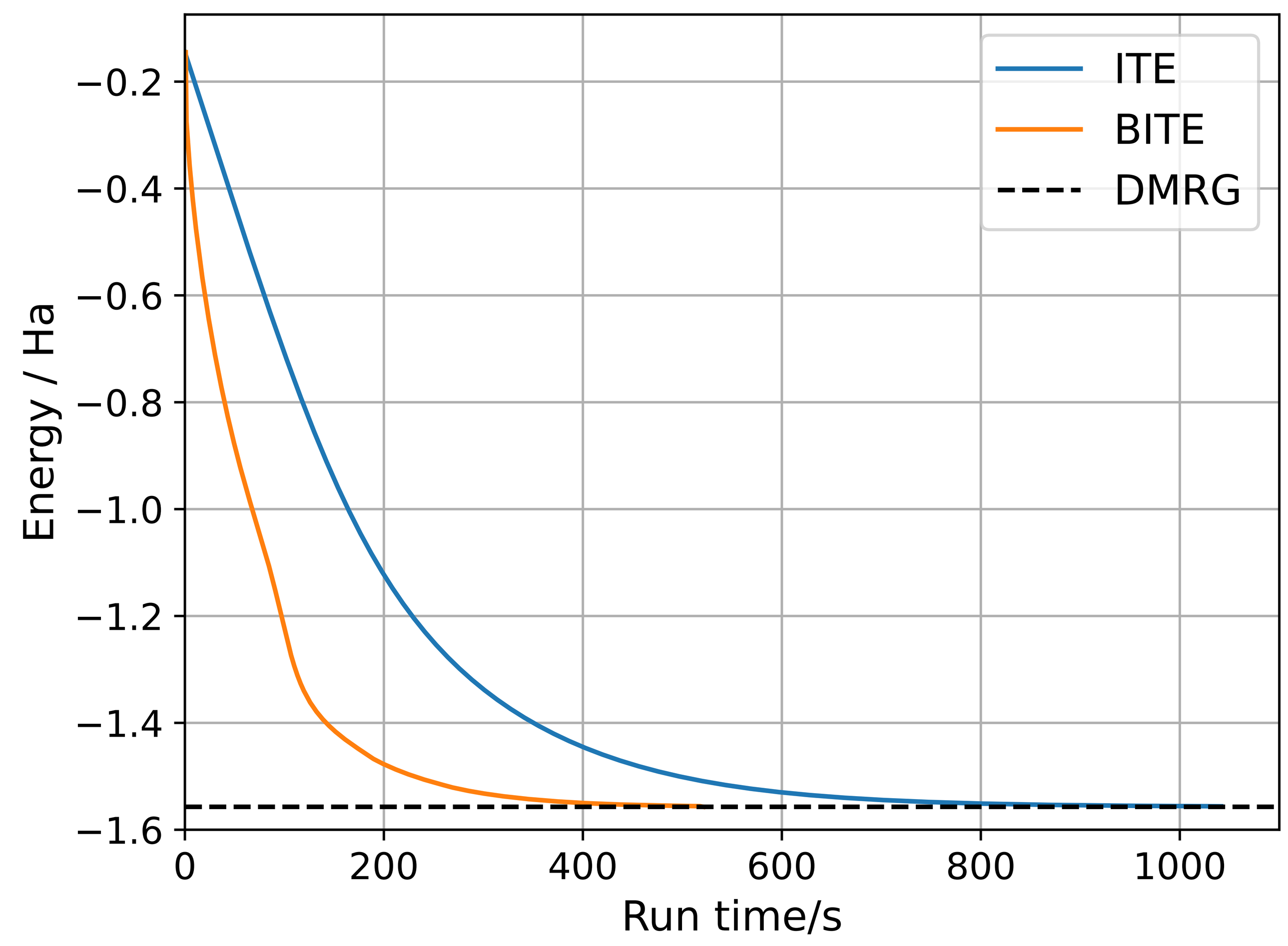

Figure 3: The energy per site of the MPS vs run time for ITE and the BITE algorithms. Dashed black line is the DMRG energy.

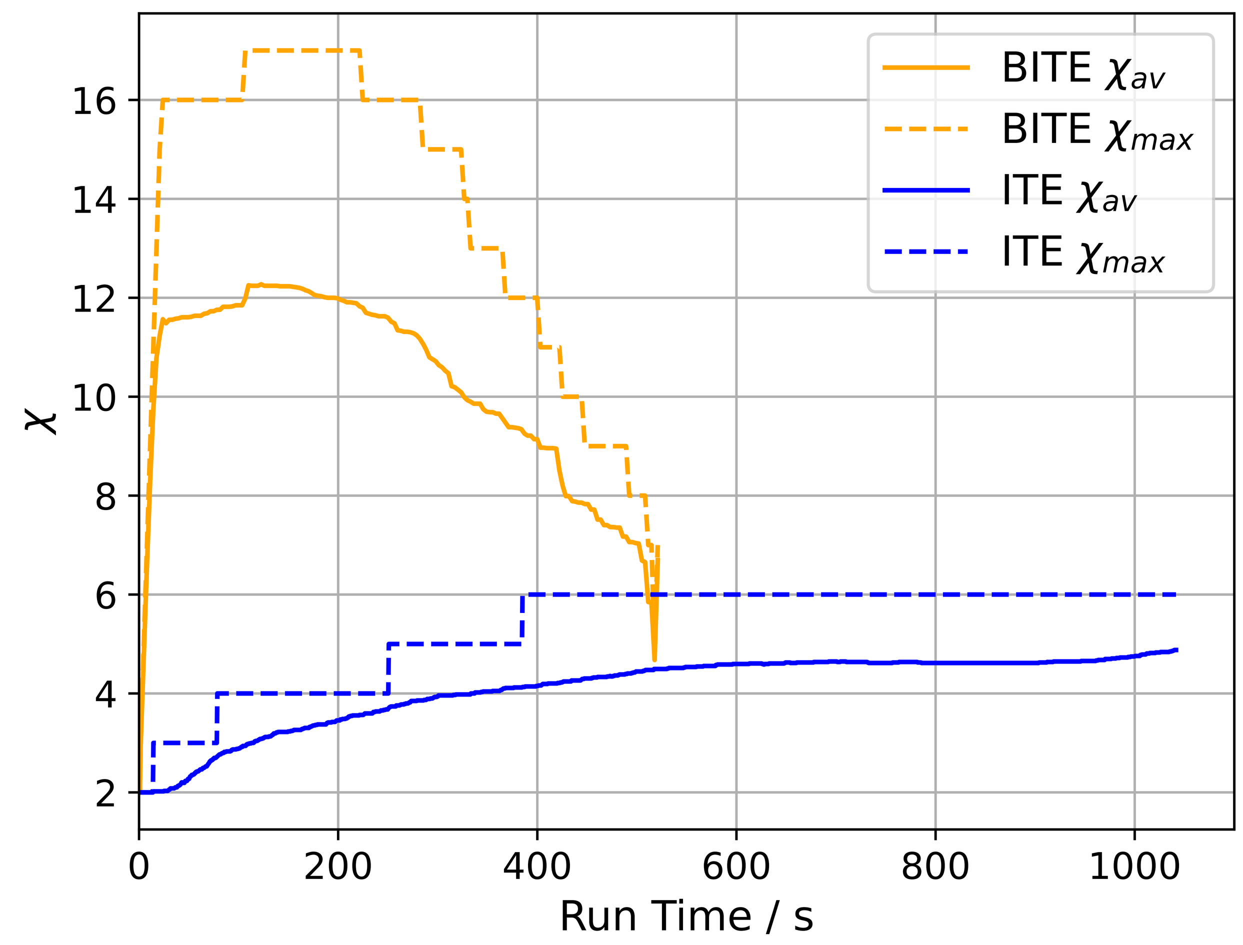

Figure 4: Average and maximum bond dimension at each point in the BITE and ITE calculations. χ_{av} is averaged over all matrices in the MPS.

Results

Table 1: Run time, maximum and average (over the entire calculation) bond dimension and fidelity of the final state with the ground state for various time step sizes.

Method	$\Delta\tau$	t_r	χ_{max}	χ_{av}	$\lvert\langle\phi_0\vert\psi\rangle\rvert^2$
ITE	0.001	1042	6	4.1	0.953
BITE	0.001	521	17	10.2	0.998
ITE	0.005	204	7	4.5	0.956
BITE	0.005	156	16	6.3	0.959
ITE	0.01	105	7	4.8	0.960
BITE	0.01	79	16	5.8	0.957

Conclusions

- Here we present a novel quantum-inspired classical algorithm that has the potential to speed-up the convergence of imaginary time evolution of matrix product states to a ground state.
- We have presented a proof-of-concept demonstration of the method applied to the 1D transverse field Ising model with open boundary conditions.
- In this work we have focused on the 1D case where DMRG is typically a better method than ITE. However, it may be possible to extend the BITE method to 2D where the use of imaginary time evolution is more prevalent.

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