Environment expansion for MPS time evolution

Jesse Osborne [1] Ian McCulloch [2]

[1]Max Planck Institute for Quantum Optics

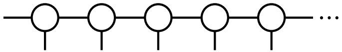
[2]National Tsing Hua University

SQAI–NCTS Workshop on Quantum Technologies and Machine Learning

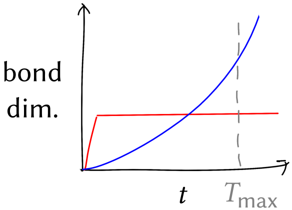
28 August 2025

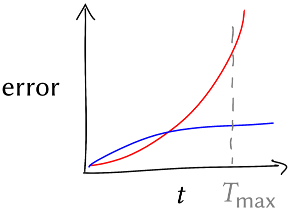
Time evolution of matrix product states

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle = \cdots$$



- In general, entanglement entropy grows linearly
- For fixed error, need to increase bond dimension
- Conversely, for fixed bond dimension, error will grow

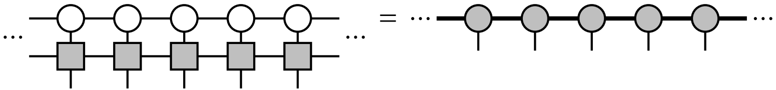




Reach $T_{\max}$ once cost or error becomes too large

MPS time evolution methods

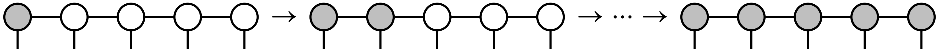
Approximation of time-evolution operator $U(\Delta t) = e^{i\hat{H}\Delta t}$



- TEBD Vidal PRL **91**, 147902 (2003); **93**, 040502 (2004)
- MPO evolution Zaletel et al. PRB **91**, 165112 (2015); Van Damme et al. SciPost Phys. **17**, 135 (2024)
- Inherently increases bond dimension (need to truncate)

Time-dependent variational principle (TDVP)

Haegeman et al. PRL **107**, 070601 (2011); PRB **94**, 165116 (2016)



- Local updates: fixed bond dimension

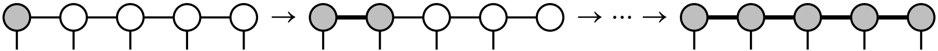
TDVP optimality?

PRL **107,** 070601 (2011) PHYSICAL RE

the TDVP equations are also invariant under time reversal (see [12] for a Trotter-based approach that recovers time-reversal invariance). This approach does not require any truncation and is thus globally optimal within the manifold $\mathcal{M}_{\text{uMPS}}$.

- TDVP is ‘optimal’ for a fixed bond dimension
- But increasing entanglement requires increasing the bond dimension
- Two-site TDVP? More expensive

Better: single-site TDVP with environment expansion

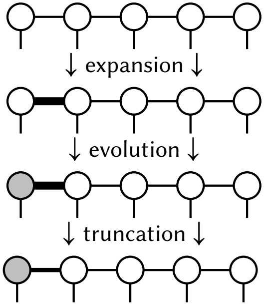


Many approaches (also for DMRG):

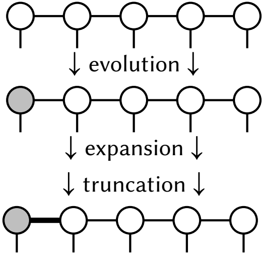
- White PRB **72**, 180403 (2005)
- Dolgov & Savostyanov SIAM J. Sci. Comput. **36**, A2248 (2014)
- Hubig et al. PRB **91**, 155115 (2015)
- Yang & White PRB **102**, 094315 (2020)
- Dunnet & Chin PRB **104**, 214302 (2021)
- Xu et al. JACS Au **2**, 335 (2022)
- Gleis et al. PRL **130**, 246402 (2023); arXiv:2501.12291; Li et al. PRL **133**, 026401 (2024)
- McCulloch & JJO arXiv:2403.00562; in preparation

Pre- and post-expansion

Pre-expansion



Post-expansion

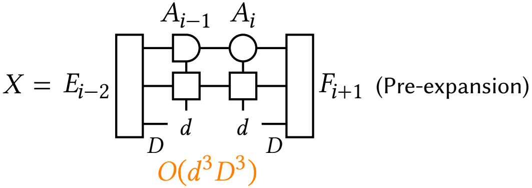


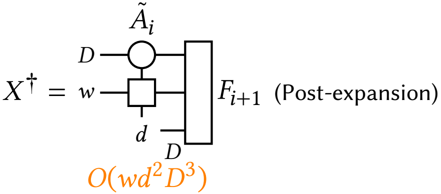
- Add new DoFs *before* evolution, then discard in truncation afterwards
- Two-site TDVP, ...

- Add new DoFs *after* evolution during the truncation step
- Subspace expansion/3S, ...

- Truncation fixes computational cost/error (fixed bond dim./singular value cutoff)
- Can use both pre- and post-expansion

Incorporate extra DoFs from SVD of





Randomized SVD: If we want k expansion vectors

- Multiply by $dD \times (k + p)$ Gaussian random matrix Ω (p: oversampling ~ 10)
- QR decomposition $QR = X\Omega$
- SVD $USV^\dagger = Q^\dagger X$, keeping k singular values
- Append extra states QU onto MPS tensor

Much cheaper: $O(dwkD^2)$ (linear in d); typically, we use $k = 0.1D$

Benchmark setup

XX model (= free fermions)

$$\hat{H} = \frac{1}{2} \sum_j \left(\hat{S}_j^- \hat{S}_{j+1}^+ + \hat{S}_j^+ \hat{S}_{j+1}^- \right)$$

Initial state

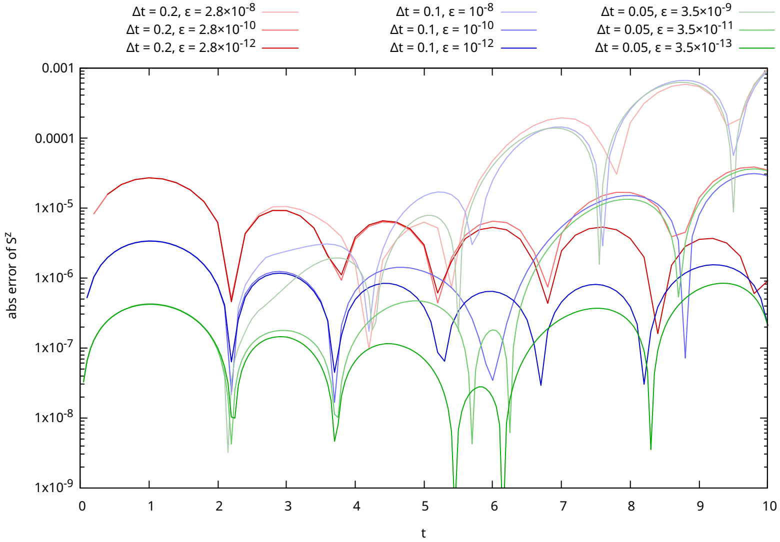
$$|\Psi(0)\rangle = |\cdots \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \cdots\rangle$$

Exactly solvable: dynamics described in terms of Bessel functions

$$S_j^z(t) = -\frac{(-1)^j}{2} J_0(2t)$$

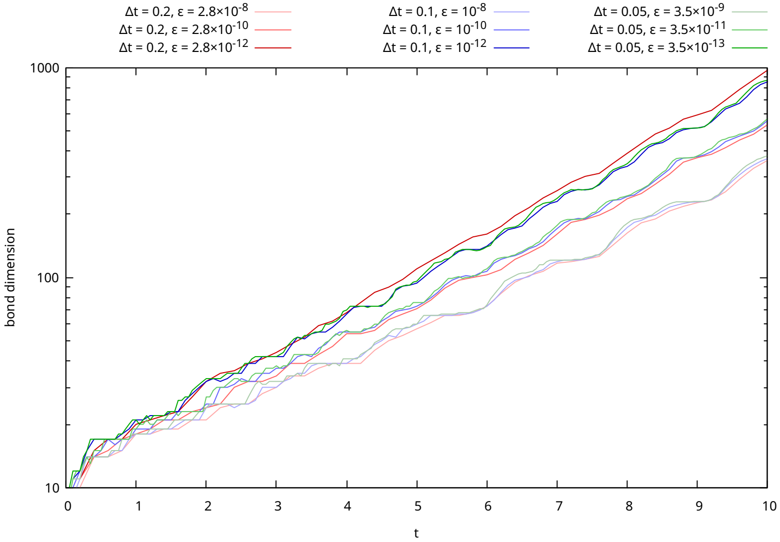
We use infinite TDVP (repeat TDVP on unit cell of iMPS a couple of times)

Results



- Δt: timestep
- ε: DM cutoff
- Early t error: Δt
- Late t error: ε
- Need to adjust ε if we decrease Δt ($\varepsilon \sim \Delta t^{1.5}$?)

Results



Δt = 0.2, ε = 2.8×10^-8
Δt = 0.2, ε = 2.8×10^-10
Δt = 0.2, ε = 2.8×10^-12
Δt = 0.1, ε = 10^-8
Δt = 0.1, ε = 10^-10
Δt = 0.1, ε = 10^-12
Δt = 0.05, ε = 3.5×10^-9
Δt = 0.05, ε = 3.5×10^-11
Δt = 0.05, ε = 3.5×10^-13
1000
100
10
bond dimension
0
1
2
3
4
5
6
7
8
9
10
t

Conclusion

- Single-site TDVP: two kinds of environment expansion (pre- & post-)
- Acceleration via randomized SVD (linear in d)
- Fixed bond dimension vs fixed truncation error
- Early time error dominated by timestep, late by truncation

Code: `https://github.com/mptoolkit`