Tensor Optimization Algorithms and Libraries for Quantum Simulation

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Recent/ongoing research topics
(*-covered today)

- parallel matrix computations
  - matrix factorizations
  - eigenvalue problems
  - preconditioners
- tensor computations
  - tensor decomposition*
  - sparse tensor kernels*
  - tensor completion*
- simulation of quantum systems
  - tensor networks*
  - quantum chemistry
  - quantum circuits*
- fast bilinear algorithms
  - convolution algorithms
  - tensor symmetry*

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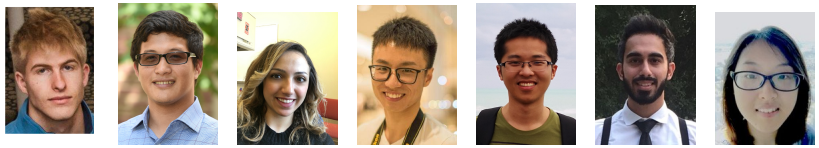

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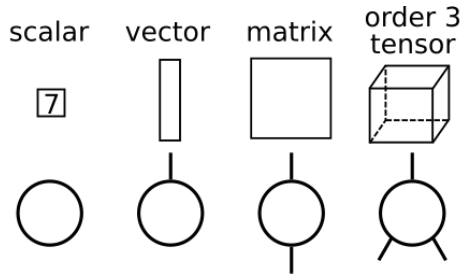
Outline

Tensors

A tensor is a collection of elements

- its dimensions define the size of the collection
- its order is the number of different dimensions
- specifying an index along each tensor mode defines an element of the tensor



A few examples of tensors are

- Order 0 tensors are scalars, e.g., $s \in \mathbb{R}$
- Order 1 tensors are vectors, e.g., $\boldsymbol{v} \in \mathbb{R}^n$
- Order 2 tensors are matrices, e.g., $\boldsymbol{A} \in \mathbb{R}^{m \times n}$
- An order 3 tensor with dimensions $s_1 \times s_2 \times s_3$ is denoted as $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{s_1 \times s_2 \times s_3}$ with elements t_{ijk} for $i \in \{1, \ldots, s_1\}, j \in \{1, \ldots, s_2\}, k \in \{1, \ldots, s_3\}$

Tensor Contractions

A tensor contraction multiplies elements of two tensors and computes partial sums to produce a third, in a fashion expressible by pairing up modes of different tensors, which may be expressed in Einstein summation notation (einsum)

tensor contraction	*einsum*
inner product	$w = \sum_i u_i v_i$
outer product	$w_{ij} = u_i v_{ij}$
pointwise product	$w_i = u_i v_i$
Hadamard product	$w_{ij} = u_{ij} v_{ij}$
matrix multiplication	$w_{ij} = \sum_k u_{ik} v_{kj}$
batched mat.-mul.	$w_{ijl} = \sum_k u_{ikl} v_{kjl}$
tensor times matrix	$w_{ilk} = \sum_j u_{ijk} v_{lj}$

General Tensor Contractions

Given tensor $\mathcal{U}$ of order $s+v$ and $\mathcal{V}$ of order $v+t$, a tensor contraction summing over v modes can be written as

$$w_{i_1 \ldots i_s j_1 \ldots j_t} = \sum_{k_1 \ldots k_v} u_{i_1 \ldots i_s k_1 \ldots k_v} v_{k_1 \ldots k_v j_1 \ldots j_t}$$

- Other contractions can be mapped to this form after transposition

Unfolding the tensors reduces the tensor contraction to matrix multiplication

- Combine consecutive indices in appropriate groups of size s ,t, or v
- If all tensor modes are of dimension n, obtain matrix–matrix product $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$ where $\boldsymbol{C} \in \mathbb{R}^{n^s \times n^t}$, $\boldsymbol{A} \in \mathbb{R}^{n^s \times n^v}$, and $\boldsymbol{B} \in \mathbb{R}^{n^v \times n^t}$
- Assuming classical matrix multiplication, contraction requires n^{s+t+v} elementwise products and $n^{s+t+v} - n^{s+t}$ additions

Emulation of Quantum Gates and Quantum Circuits

- Consider an n-qubit quantum state

$$|\psi\rangle = \sum_{\boldsymbol{i}\in\{0,1\}^n} t^{\psi}_{\boldsymbol{i}} \, |i_1 \cdots i_n\rangle \text{ with } t_{\boldsymbol{i}} \in \mathbb{C}$$

- Quantum circuits generally consist of 1-qubit and 2-qubit gates

$$|\phi\rangle = \boldsymbol{U}^{(s)} |\psi\rangle \Rightarrow t^{\phi}_{i_1\cdots i_n} = \sum_{j_s=0}^{1} u^{(s)}_{i_s j_s} t^{\psi}_{i_1\cdots i_{s-1} j_s i_{s+1}\cdots i_n}$$

$$|\phi\rangle = \boldsymbol{U}^{(s,t)} |\psi\rangle \Rightarrow t^{\phi}_{i_1\cdots i_n} = \sum_{j_s=0}^{1}\sum_{j_t=0}^{1} u^{(s)}_{i_s i_t j_s j_t} t^{\psi}_{i_1\cdots i_{s-1} j_s i_{s+1}\cdots i_{t-1} j_t i_{t+1}\cdots i_n}$$

- A quantum gate can be emulated as an $O(2^n)$-cost tensor contraction
- An n-qubit quantum circuit with depth D and $O(nD)$ gates can be simulated classically with $O(nD2^n)$ cost and $O(2^n)$ storage

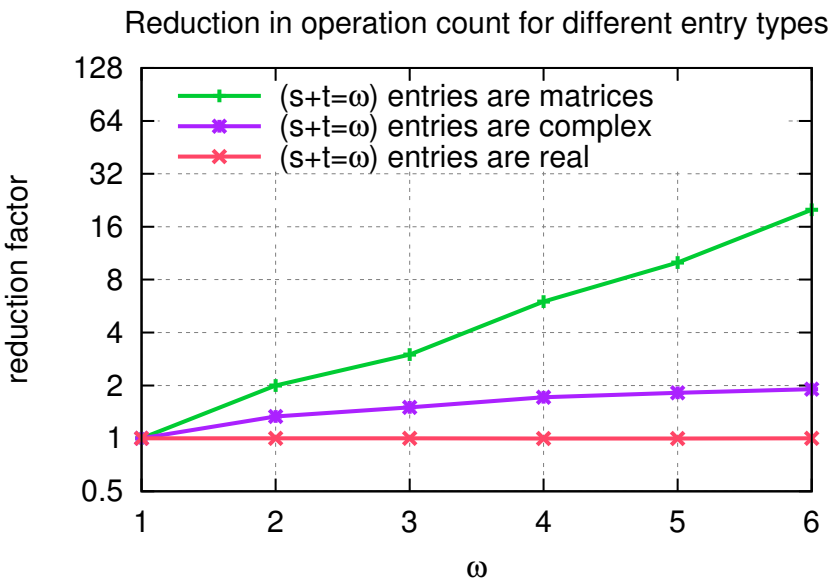
Symmetric Tensor Contractions

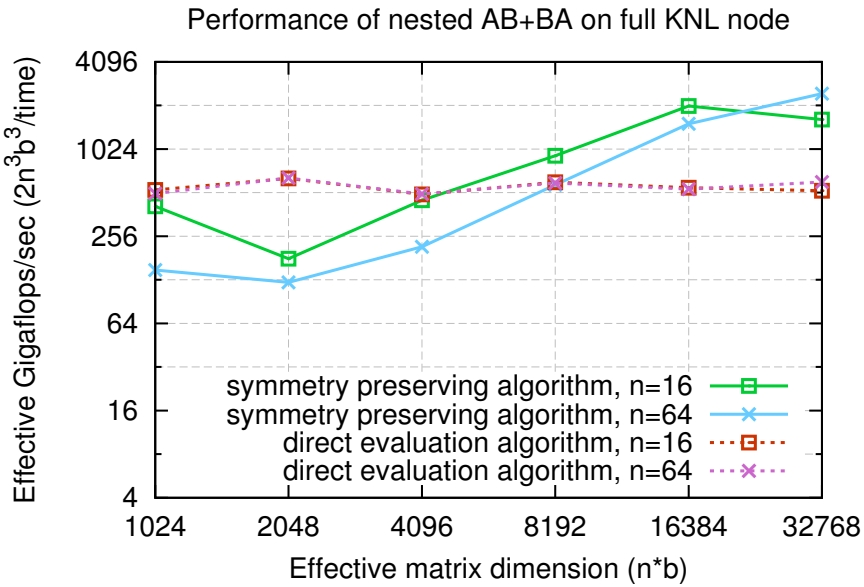
- Recall a symmetric tensor is defined by e.g.,
  $t_{ijk} = t_{ikj} = t_{kij} = t_{jki} = t_{jik} = t_{kji}$
- Tensors can also have skew-symmetry (also known as antisymmetry, permutations have $+/-$ signs), partial symmetry (only some modes are permutable), or group symmetry (blocks are zero if indices satisfy modular equation)
- The simplest example of a symmetric tensor contraction is

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} \quad \text{where } \boldsymbol{A} = \boldsymbol{A}^T$$

  it is not obvious how to leverage symmetry to reduce cost of this contraction

Permutational Symmetry in Tensor Contractions





New contraction algorithms reduce cost via permutational symmetry[1]

- Symmetry is hard to use in contraction e.g. $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ with $\boldsymbol{A}$ symmetric
- For contraction of order $s+v$ and $v+t$ tensors to produce an order $s+t$ tensor, previously known approaches reduce cost by $s!t!v!$
- New algorithm reduces number of *products* by $\omega!$ where $\omega = s+t+v$, leads to same reduction in *cost* for partially-symmetric contractions

$$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B} + \boldsymbol{B}\boldsymbol{A} \Rightarrow c_{ij} = \sum_k [(a_{ij} + a_{ik} + a_{jk}) \cdot (b_{ij} + b_{ik} + b_{jk})] - \ldots$$

[1] E.S, J. Demmel, CMAM 2020

Group Symmetry

- Tensors arising in physical simulations often have group structure that reflects conservation laws
  - Abelian group symmetries can be mapped to cyclic group, which can be used to define a block-sparse form of the tensors (here represented using extra modes), e.g.,

$$w_{aA,bB,iI,jJ} = \sum_{k,K,l,L} u_{aA,bB,kK,lL} v_{kK,lL,iI,jJ}.$$

    where for some group size G, we have symmetries, e.g.,

$$\begin{aligned} w_{aA,bB,iI,jJ} &\neq 0 \text{ if } A + B - I - J \equiv 0 \pmod{G}, \\ u_{aA,bB,kK,lL} &\neq 0 \text{ if } A + B + K + L \equiv 0 \pmod{G}, \\ v_{kK,lL,iI,jJ} &\neq 0 \text{ if } K + L - I - J \equiv 0 \pmod{G}. \end{aligned}$$

  - We can write each of these tensors using a reduced form and an irrep map,

$$w_{aA,bB,iI,jJ} = r^{(W)}_{aA,bB,iI,j} m_{ABIJ}$$

    where $m_{ABIJ} = 1$ if $A + B - I - J \equiv 0 \pmod{G}$ and $m_{ABIJ} = 0$ otherwise

Block Contraction Approach to Group Symmetry

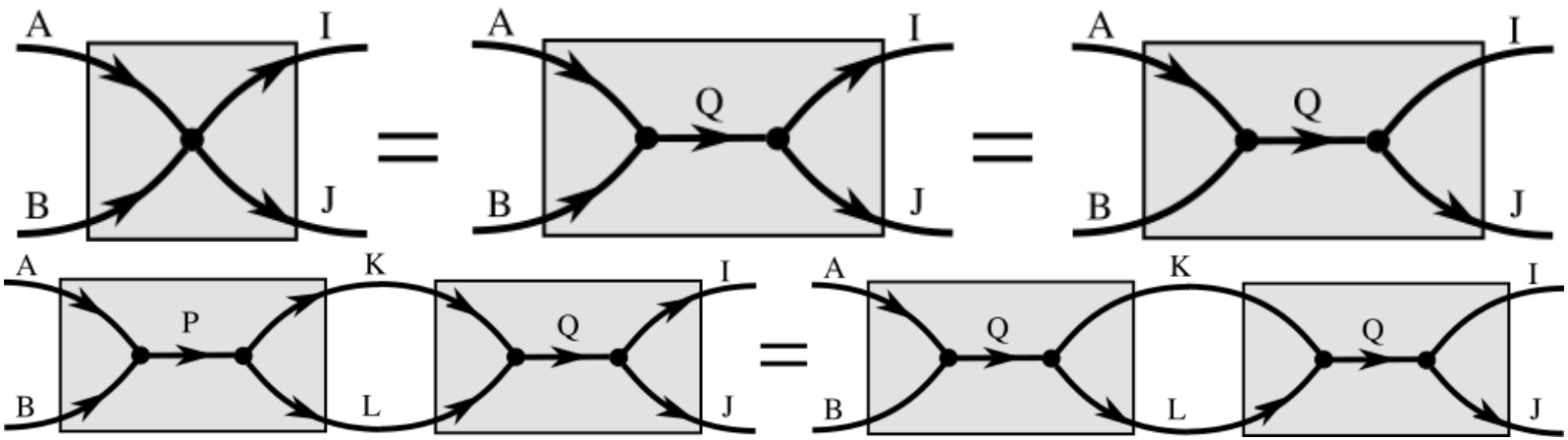
Algorithm 3.1 Loop nest to perform group symmetric contraction $w_{aA,bB,iI,jJ} = \sum_{k,K,l,L} u_{aA,bB,kK,lL} v_{kK,lL,iI,jJ}$.

for $A = 1, \ldots, G$ **do**
  for $B = 1, \ldots, G$ **do**
    for $I = 1, \ldots, G$ **do**
      $J = A + B - I \bmod G$
      for $K = 1, \ldots, G$ **do**
        $L = -A - B - K \bmod G$
        $\forall a, b, i, j, \quad w_{aA,bB,iI,jJ} = \sum_{k,l} w_{aA,bB,iI,jJ} + u_{aA,bB,kK,lL}, v_{kK,lL,iI,jJ}$
      end for
    end for
  end for
end for

Group Symmetry in Tensor Contractions

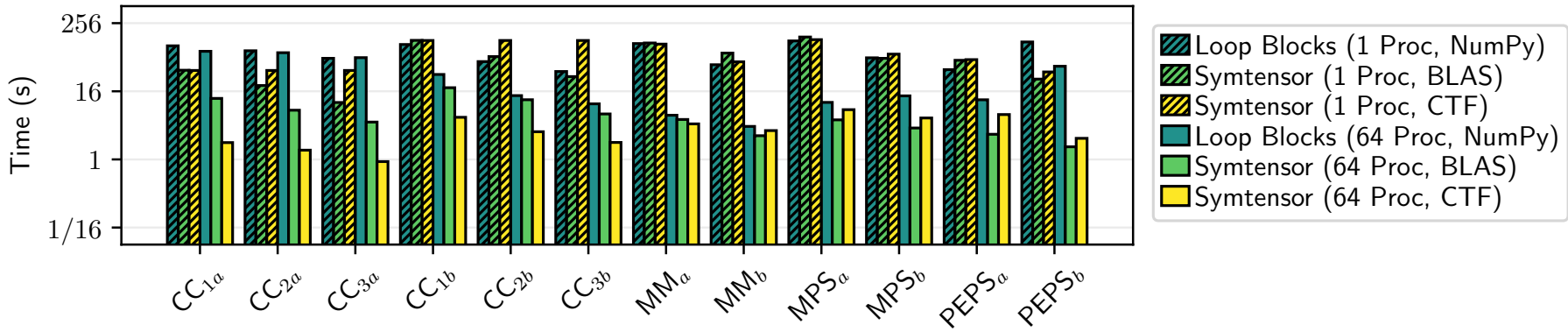
New contraction algorithm, *irreducible representation alignment* uses new reduced form to handle group symmetry (momentum conservation, spin, quantum numbers, etc.) without looping over blocks or sparsity[1]

$$\begin{aligned}\hat{w}_{aA,b,i,jJ,Q} &= w_{aA,b,Q-A \bmod G,i,-J-Q \bmod G,jJ}, \\ &= \sum_{L,k,l} \hat{u}_{aA,b,k,lL,Q} \hat{v}_{k,lL,i,jJ,Q}.\end{aligned}$$



[1] collaboration with Yang Gao, Phillip Helms, and Garnet Chan at Caltech, to appear on arxiv, July 2020

Automation of Group Symmetric Contractions



- Group symmetric tensors represented programmatically by
  - a dense reduced tensor (containing unique data)
  - an implicit sparse tensor (irrep map) describing the group symmetry
- At contraction time reduced form is transformed so as to align irrep maps (introduce Q index)
- Users can write symmetry-oblivious code

Library for Massively-Parallel Tensor Computations

Cyclops Tensor Framework[1] sparse/dense generalized tensor algebra

- Cyclops is a C++ library that distributes each tensor over MPI
- Used in chemistry (PySCF, QChem)[2], quantum circuit simulation (IBM/LLNL)[3], and graph analysis (betweenness centrality)[4]
- Summations and contractions specified via Einstein notation

```
E["aixbjy"] += X["aixbjy"] - U["abu"]*V["iju"]*W["xyu"]
```

- Best distributed contraction algorithm selected at runtime via models
- Support for Python (`numpy.ndarray` backend), OpenMP, and GPU
- Simple interface to core ScaLAPACK matrix factorization routines

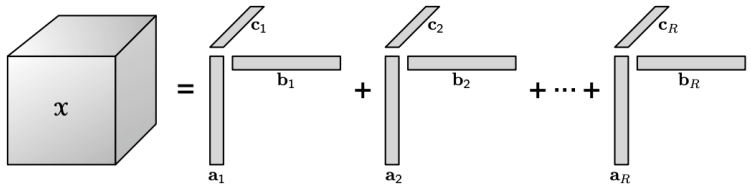
[1] https://github.com/cyclops-community/ctf

[2] E.S., D. Matthews, J. Hammond, J.F. Stanton, J. Demmel, JPDC 2014

[3] E. Pednault, J.A. Gunnels, G. Nannicini, L. Horesh, T. Magerlein, E. S., E. Draeger, E. Holland, and R. Wisnieff, 2017

[4] E.S., M. Besta, F. Vella, T. Hoefler, SC 2017

CP Decomposition



- For a tensor $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{n \times n \times n}$, the CP decomposition[1] is defined by matrices $\boldsymbol{U}$, $\boldsymbol{V}$, and $\boldsymbol{W}$ such that

$$t_{ijk} = \sum_{r=1}^{R} u_{ir} v_{jr} w_{kr}$$

- For an order N tensor, the decomposition generalizes as follows,

$$t_{i_1 \ldots i_d} = \sum_{r=1}^{R} \prod_{j=1}^{d} u_{i_j r}^{(j)}$$

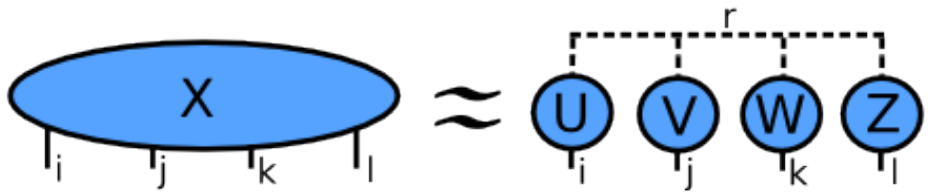
- Its rank is generally bounded by $R \leq n^{d-1}$

[1] Kolda and Bader, SIAM Review 2009

Alternating Least Squares for CP Decomposition

Consider rank R CP decomposition of an $s \times s \times s \times s$ tensor

$$x_{ijkl} \approx \sum_{r=1}^{R} u_{ir} v_{jr} w_{kr} z_{lr}$$



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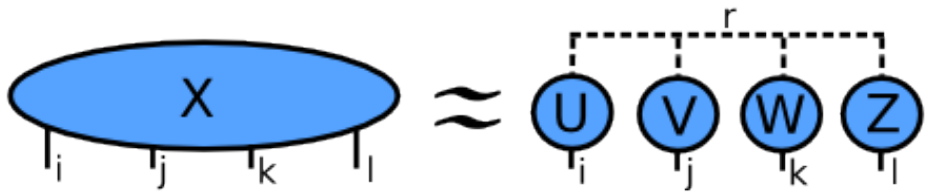
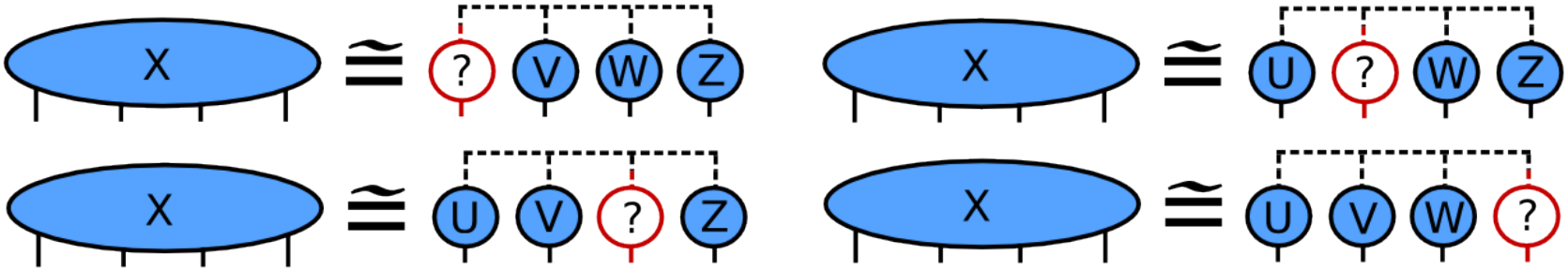


ALS updates factor matrices in an alternating manner

$$\min_{\boldsymbol{A}^{(n)}} f(\boldsymbol{A}^{(1)}, \ldots, \boldsymbol{A}^{(N)}) = \frac{1}{2} ||\boldsymbol{\mathcal{X}} - [\![\boldsymbol{A}^{(1)}, \cdots, \boldsymbol{A}^{(n)}, \cdots, \boldsymbol{A}^{(N)}]\!]||_F^2,$$



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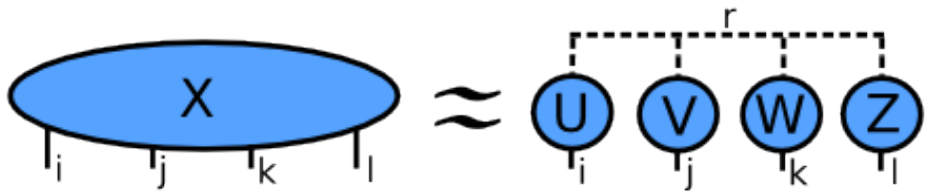

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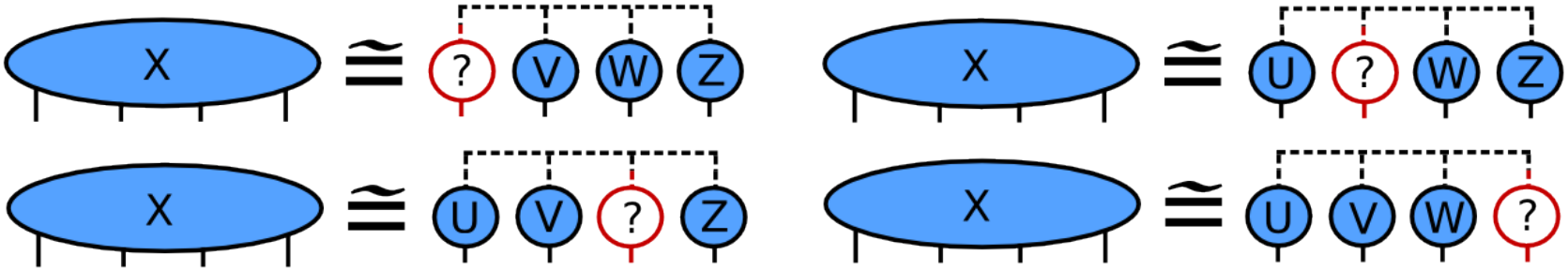
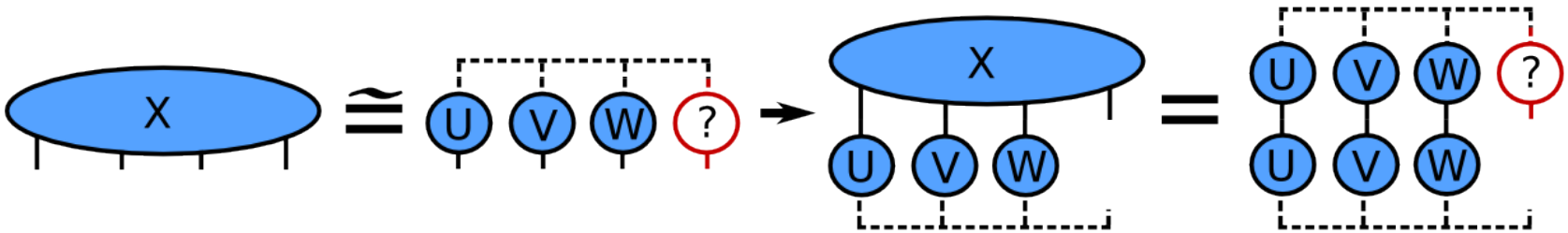
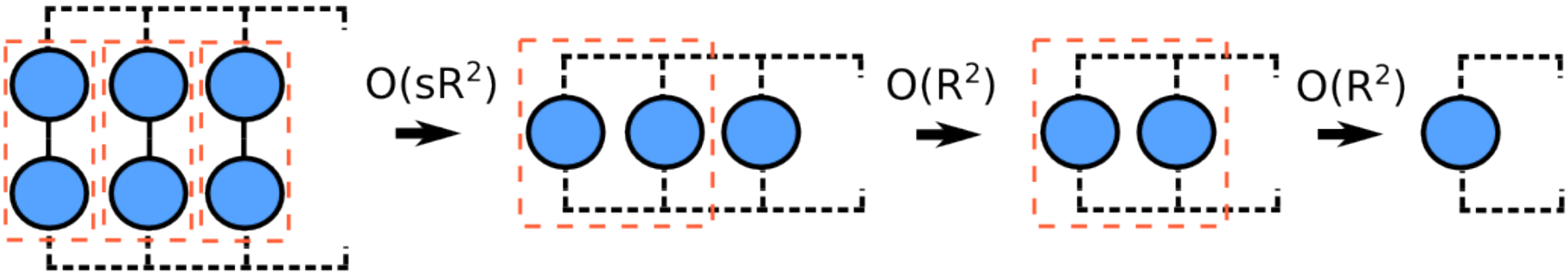


Each quadratic subproblem is typically solved via normal equations



Tensor Contractions in CP ALS

The normal equations are cheap to compute



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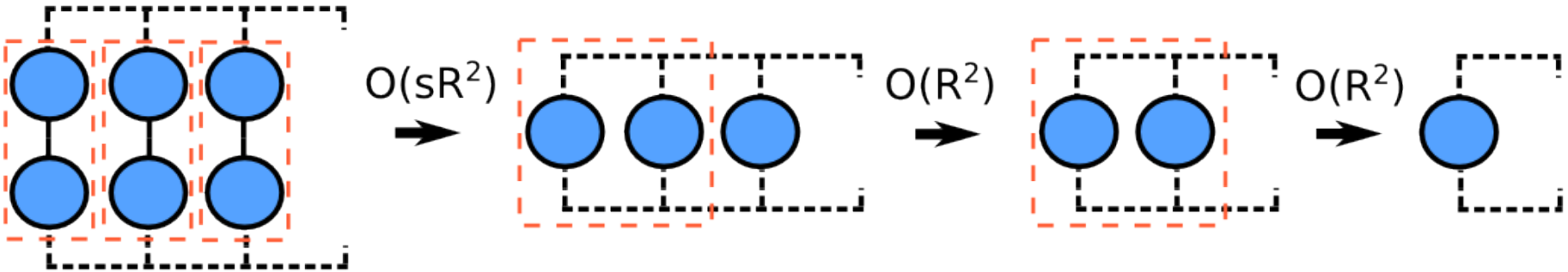
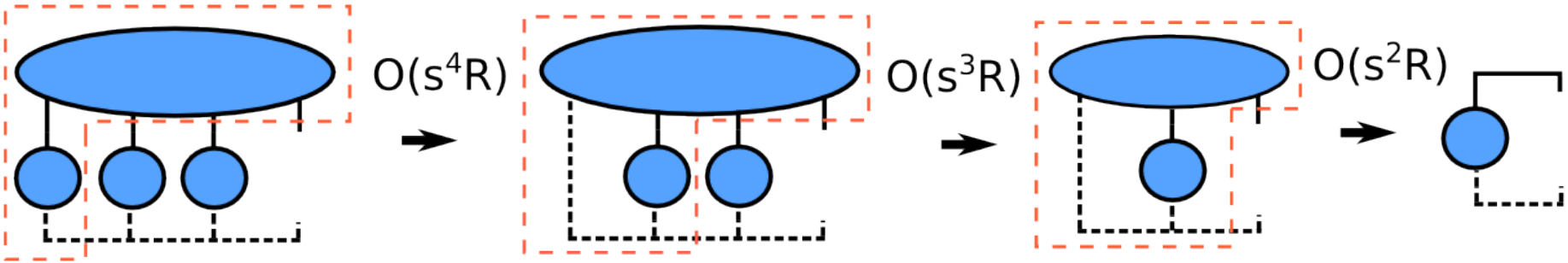
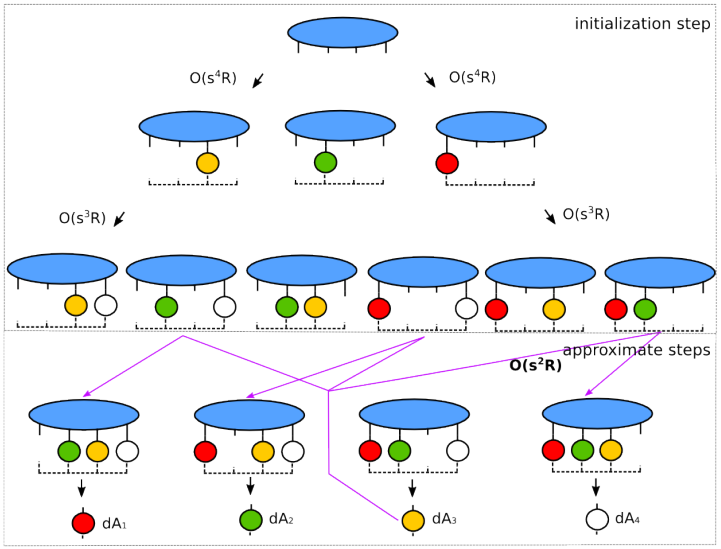
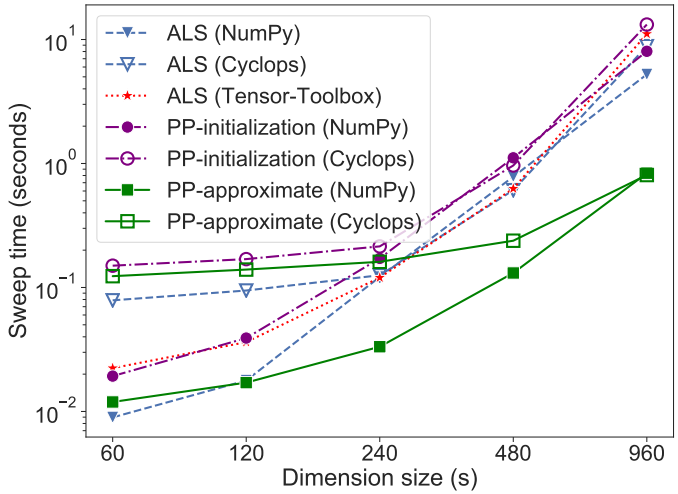


But forming the right-hand sides ($\boldsymbol{M}^{(n)}$) requires expensive MTTKRP (matricized tensor-times Khatri-Rao product)



Pairwise Perturbation Algorithm





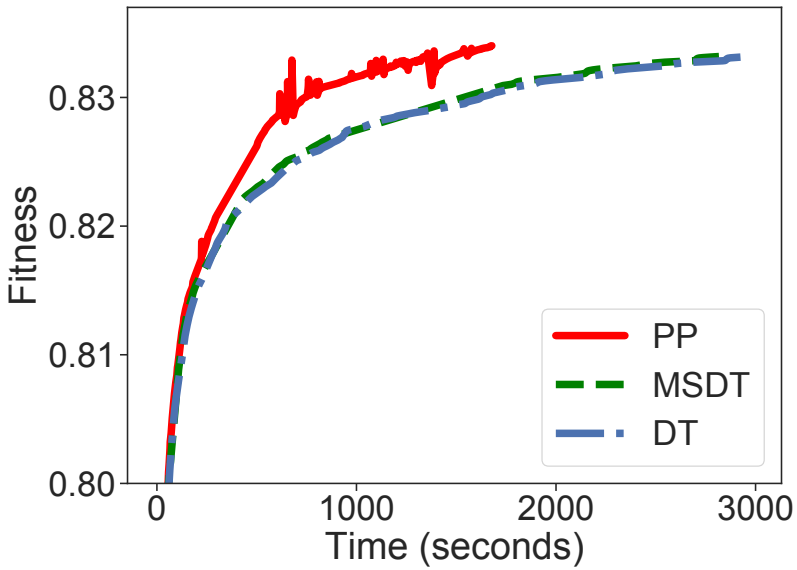
New algorithm: pairwise perturbation (PP)[1] approximates ALS

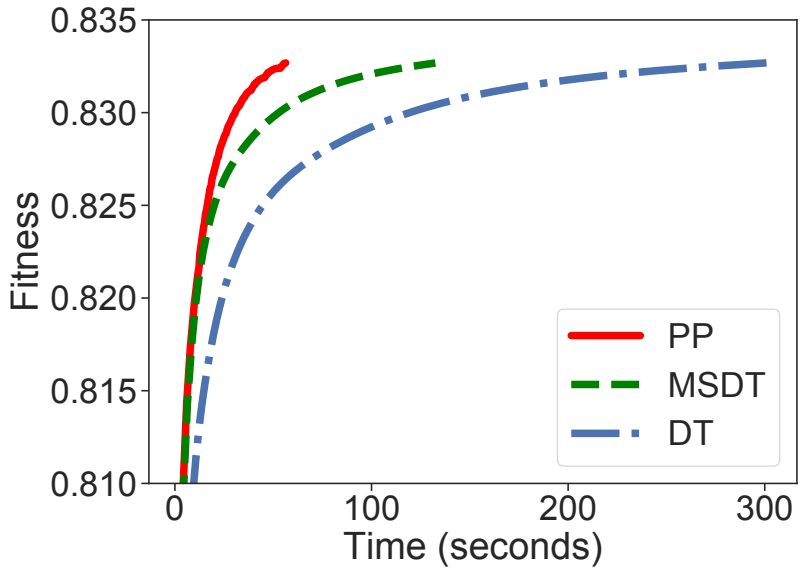
- based on perturbative expansion of ALS update to approximate MTTKRP
- approximation is accurate when ALS updates stagnate
- rank $R < s^{N-1}$ CP decomposition:
  - ALS sweep cost $O(s^N R) \Rightarrow O(s^2 R)$, up to 33x speed-up

Linjian Ma

[1] Linjian Ma, E.S. arXiv:1811.10573

Parallel Pairwise Perturbation Algorithm





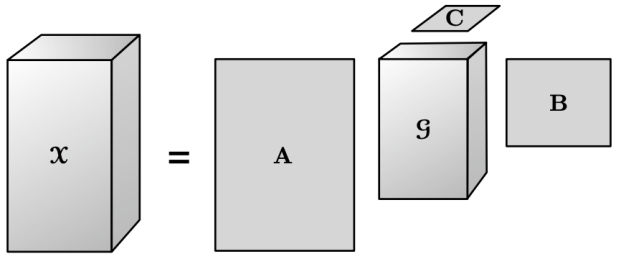
Effective parallelization by decomposing MTTKRP into local MTTKRPs [1]

$$\boldsymbol{U} = \text{MTTKRP}(\boldsymbol{\mathcal{T}}, \boldsymbol{V}, \boldsymbol{W}) \Rightarrow \boldsymbol{U}_i = \sum_{j,k} \text{MTTKRP}(\boldsymbol{\mathcal{T}}_{ijk}, \boldsymbol{V}_j, \boldsymbol{W}_k)$$

- processor (i, j, k) owns $\boldsymbol{\mathcal{T}}_{ijk}$, $\boldsymbol{V}_j$, and $\boldsymbol{W}_k$
- pairwise perturbation can be used to approximate local MTTKRPs
- multi-sweep dimension-tree (MSDT) amortizes terms across sweeps

[1] Linjian Ma, E.S. IPDPS 2021

Tucker Decomposition



- The Tucker decomposition[1] expresses an order d tensor via a smaller order d core tensor and d factor matrices
  - For a tensor $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{n \times n \times n}$, the Tucker decomposition is defined by core tensor $\boldsymbol{\mathcal{Z}} \in \mathbb{R}^{R_1 \times R_2 \times R_3}$ and factor matrices $\boldsymbol{U}$, $\boldsymbol{V}$, and $\boldsymbol{W}$ with orthonormal columns, such that

$$t_{ijk} = \sum_{p=1}^{R_1} \sum_{q=1}^{R_2} \sum_{r=1}^{R_3} z_{pqr} u_{ip} v_{jq} w_{kr}$$

  - If an exact Tucker decomposition exists, it can be computed via SVD (HoSVD)
  - HOOI method optimizes in an alternating manner among $(\boldsymbol{U}, \boldsymbol{\mathcal{Z}})$, $(\boldsymbol{V}, \boldsymbol{\mathcal{Z}})$, $(\boldsymbol{W}, \boldsymbol{\mathcal{Z}})$

[1] Kolda and Bader, SIAM Review 2009

Randomized Methods for Sparse Tensor Decomposition

- When seeking a low-rank $R = O(1)$ decomposition for a sparse tensor, sketching schemes have been shown to be efficient
- In this regime, Tucker can be used to construct a CP decomposition
- Leverage score sampling on the rank-constrained least squares problem $\min_{\boldsymbol{X},\mathrm{rank}(\boldsymbol{X})\leq R} \|\boldsymbol{AX}-\boldsymbol{B}\|_F$ leads to a state-of-the-art cost-accuracy trade-off[1] to effectively approximate HOOI (ALS)

Algorithm for Tucker	LS solve cost	Sample size (m)
ALS	$O(\mathrm{nnz}(\boldsymbol{\mathcal{T}})R^{N-1})$	/
ALS + TensorSketch[2]	$\tilde{O}(mR^N + msR)$	$O(R^{2(N-1)} \cdot 3^{N-1}/(\epsilon^2\delta))$
ALS + TTMTS[2]	$\tilde{O}(msR^{N-1})$	$O(R^{2(N-1)} \cdot 3^{N-1}/(\epsilon^2\delta))$
ALS + TensorSketch[1]	$\tilde{O}(mR^{2N-2} + sR^{N-1})$	$O\big((R^{(N-1)} + 1/\epsilon^2) \cdot (3R)^{(N-1)}/\delta\big)$
ALS + leverage scores[1]	$\tilde{O}(mR^{2N-2} + sR^{N-1})$	$O(R^{(N-1)}/(\epsilon^2\delta))$

[1] Linjian Ma and E.S., arXiv:2104.01101

[2] O. Malik and S. Becker, 2018 (assuming unconstrained LSQ)

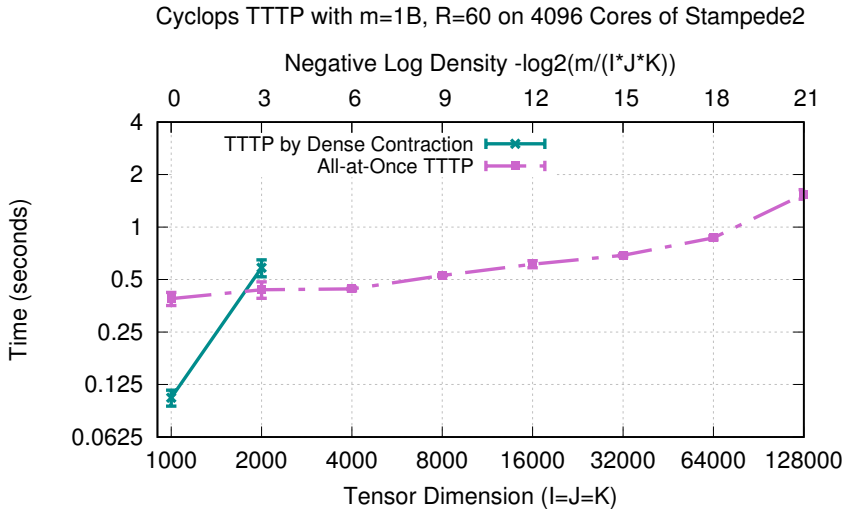
Tensor Completion

- The tensor completion problem seeks to build a model (e.g., CP decomposition) for a partially-observed tensor
- For an order three tensor $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{n \times n \times n}$, given a set of observed entries t_{ijk} for $(i,j,k) \in \Omega$, we seek to minimize

$$\sum_{(i,j,k)\in\Omega} \underbrace{(t_{ijk} - \sum_{r} u_{ir} v_{jr} w_{kr})^2}_{\text{loss function}} + \lambda^2(\|\boldsymbol{U}\|_2^2 + \|\boldsymbol{V}\|_2^2 + \|\boldsymbol{W}\|_2^2)$$

- Completion objective differs from decomposition of a sparse tensor, as it excludes unobserved entries
- Other loss functions than quadratic loss are often interest for different tensor data

Tensor Completion



- Via the Cyclops Python interface, we have implemented parallel (over MPI) completion with SGD, CCD, ALS (with iterative and direct solves), and Gauss-Newton, with support for generalized loss[1]
- Tensor times tensor product (TTTP) routine enables CP tensor completion

$$r_{ijk} = \sum_r t_{ijk} u_{ir} v_{jr} w_{kr}$$

- For ALS, explicit parallel direct solves[2] are fastest

[1] Navjot Singh, Zecheng Zhang, Xiaoxiao Wu, Naijing Zhang, Siyuan Zhang, and Edgar Solomonik arXiv:1910.02371

[2] Shaden Smith, Jongsoo Park, and George Karypis, 2016

Hamiltonians as Tensor Network Operators

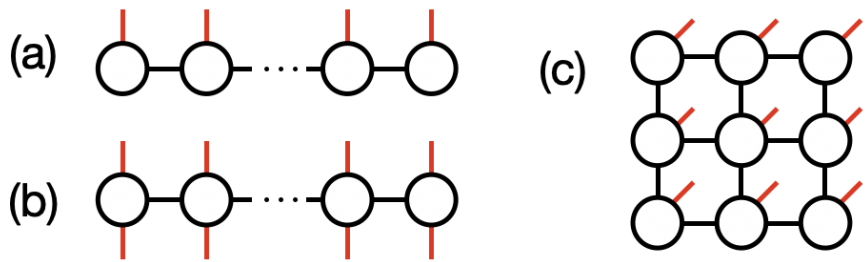
- Tensor network methods use tensor decompositions to represent quantum systems
- These methods are most natural for lattice spin systems such as the Heisenberg model and the simpler transverse field Ising model

$$H = \sum_{\langle i\, j\rangle} J^z Z_i Z_j + \sum_i h_x X_i$$

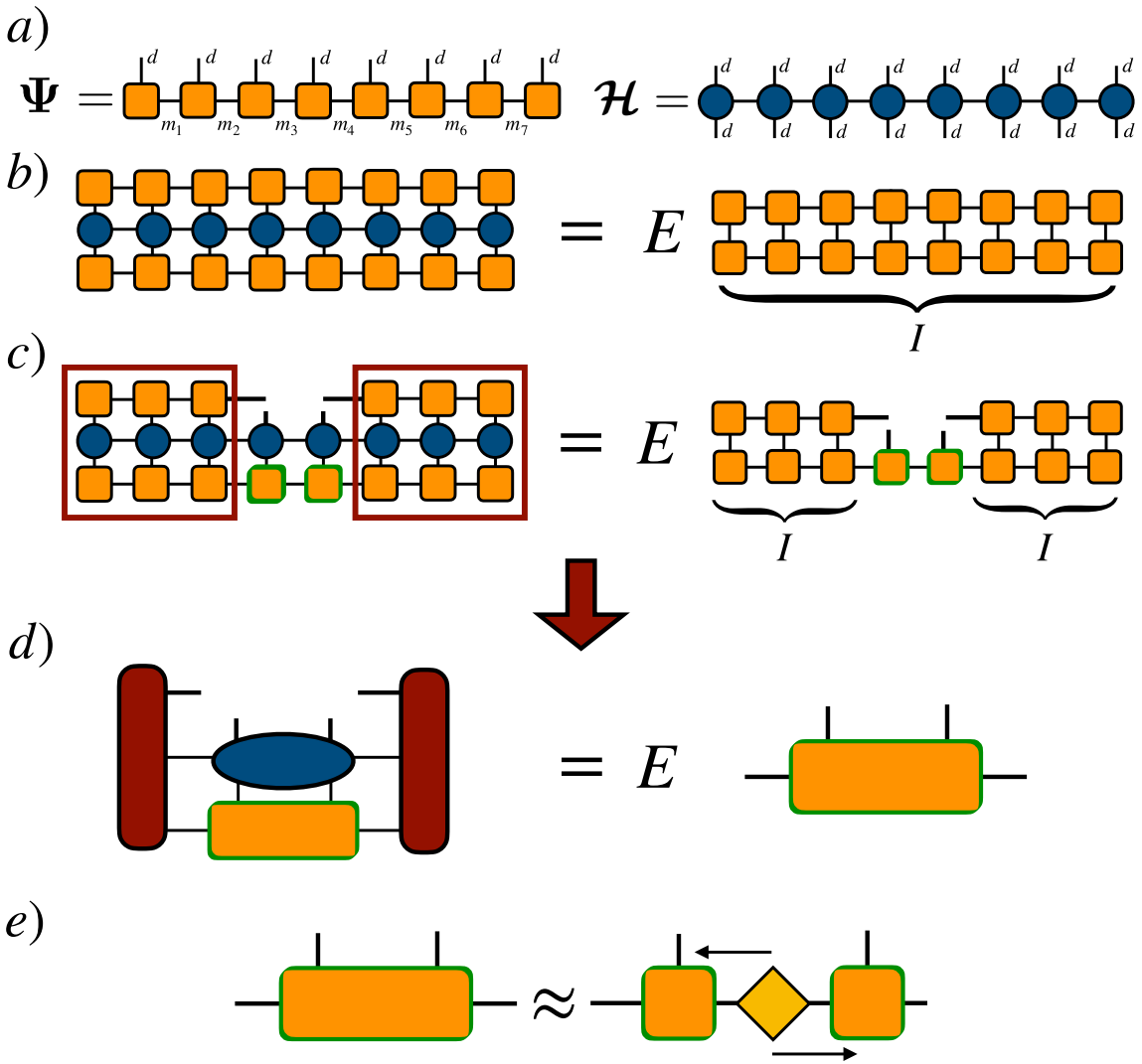
  where $\langle i\, j\rangle$ denote neighboring sites on a 2D lattice
- In the 1D case, 2-qubit operators such as $Z_i Z_{i+1}$ can be written as

$$\boldsymbol{H} = \boldsymbol{Z} \otimes \boldsymbol{Z} \otimes \boldsymbol{I} \otimes \cdots \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{Z} \otimes \boldsymbol{Z} \otimes \boldsymbol{I} \otimes \cdots \otimes \boldsymbol{I} + \cdots$$

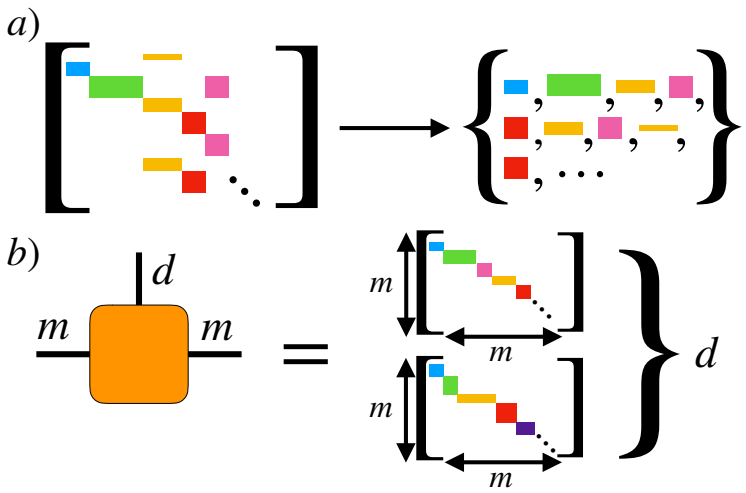
- In the 1D case, H can be represented as a matrix-product operator (MPO) with constant *bond dimension* (rank)

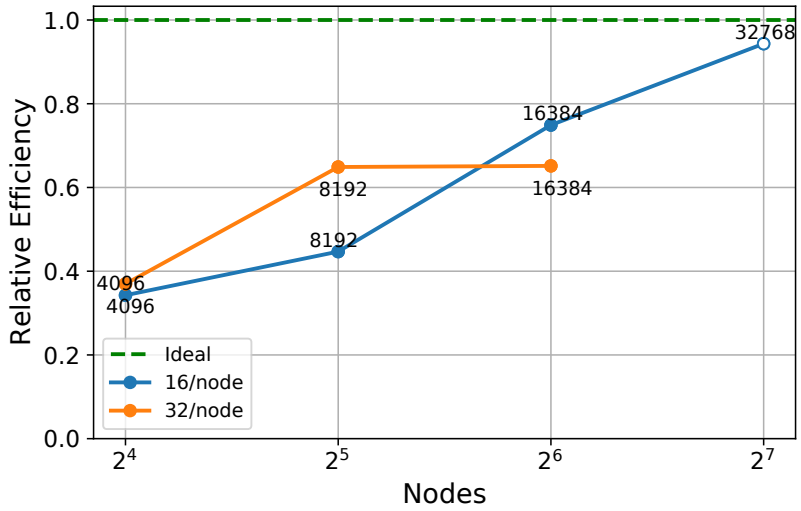


Density Matrix Renormalization Group (DMRG)



Parallel DMRG with Group Symmetry





We have recently developed a parallel DMRG code using Cyclops[1]

- compare two approaches to group symmetry
  - iterate over block-wise contractions
  - use CTF's sparse tensor representation
- match ITensor efficiency at scale for spin-system, but significantly lower efficiency for fermionic system with large number of blocks

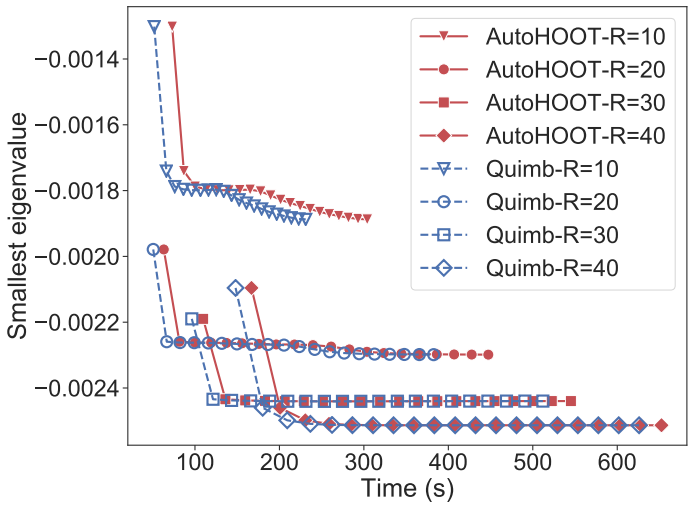
[1] R. Levy, B. Clark, E.S. arXiv:2007.05540

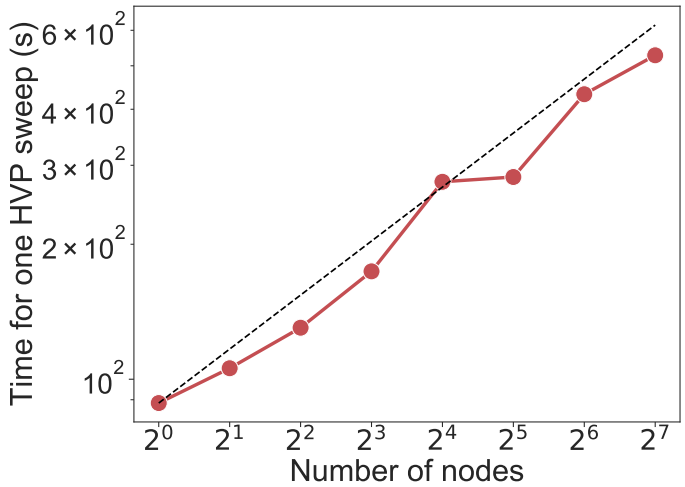
Automatic Generation of Tensor Network Methods

- Automatic differentiation (AD) in principle enables automatic generation of methods such as ALS and DMRG
- Both apply Newton's method on a sequence of subsets of variables
- However, existing AD tools such as Jax (used by TensorFlow) are designed for deep learning and are ineffective for more complex tensor computations
  - focus purely on first order optimization via Jacobian-vector products
  - unable to propagate tensor algebra identities such as $(\boldsymbol{A} \otimes \boldsymbol{B})^{-1} = \boldsymbol{A}^{-1} \otimes \boldsymbol{B}^{-1}$ to generate efficient code

AutoHOOT: Automatic High-Order Optimization for Tensors

- AutoHOOT[1] provides a tensor-algebra centric AD engine
- Designed for `einsum` expressions and alternating minimization common in tensor decomposition and tensor network methods
- Python-level AD is coupled with optimization of contraction order and caching of intermediates
- Generates code for CPU/GPU/supercomputers using high-level back-end interface to tensor contractions





[1] Linjian Ma, Jiayu Ye, and E.S. arXiv:2005.04540, 2020

Tensor Network State Evolution

- We can evolve a tensor network state by Trotterization of a Hamiltonian with m local terms

$$e^{-iH\tau} = \prod_{j=1}^{m} e^{-iH_j\tau} + O(\tau^2)$$

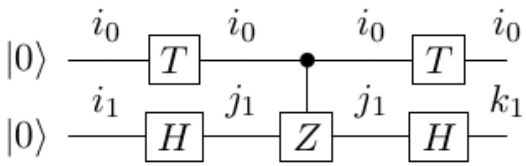
- Dynamics may be simulated by time-evolution $|\psi^{t+\tau}\rangle = e^{-iH\tau}|\psi^t\rangle$
- Ground state calculation can be done via imaginary time evolution, $|\psi^{i(t+\tau)}\rangle = e^{-H\tau}|\psi^{it}\rangle$, maximizing as follows

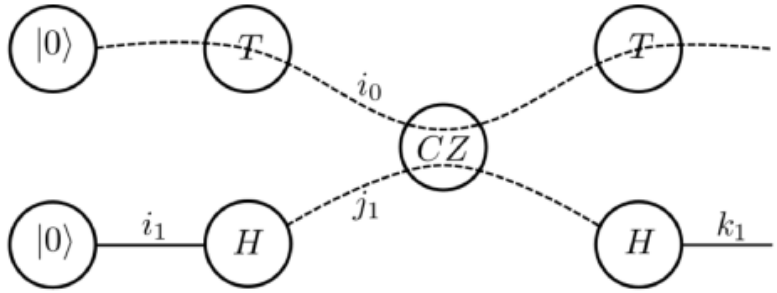
$$e^{-E\tau} = \max_{\|\psi\|_2} \langle\psi|e^{-H\tau}|\psi\rangle$$

  which is equivalent to minimizing E and leads to the same maximizer/minimizer ψ
- If H_j is a local (e.g., one/two-site) operator, so is $e^{-iH_j\tau}$

Quantum Circuit Simulation with Tensor Networks

- Evolution of tensor network states can also simulate quantum circuits
- In fact, a quantum circuit is a direct description of a tensor network[1]





- Why use HPC to (approximately) simulate quantum circuits?
  - enable development/testing/tuning of larger quantum circuits
  - understand approximability of different quantum algorithms
  - quantify sensitivity of algorithms to noise/error
  - potentially enable new hybrid quantum-classical algorithms
- Tensor network states (e.g., MPS/PEPS) provide robust tools for approximate simulation

[1] Markov and Shi SIAM JC 2007

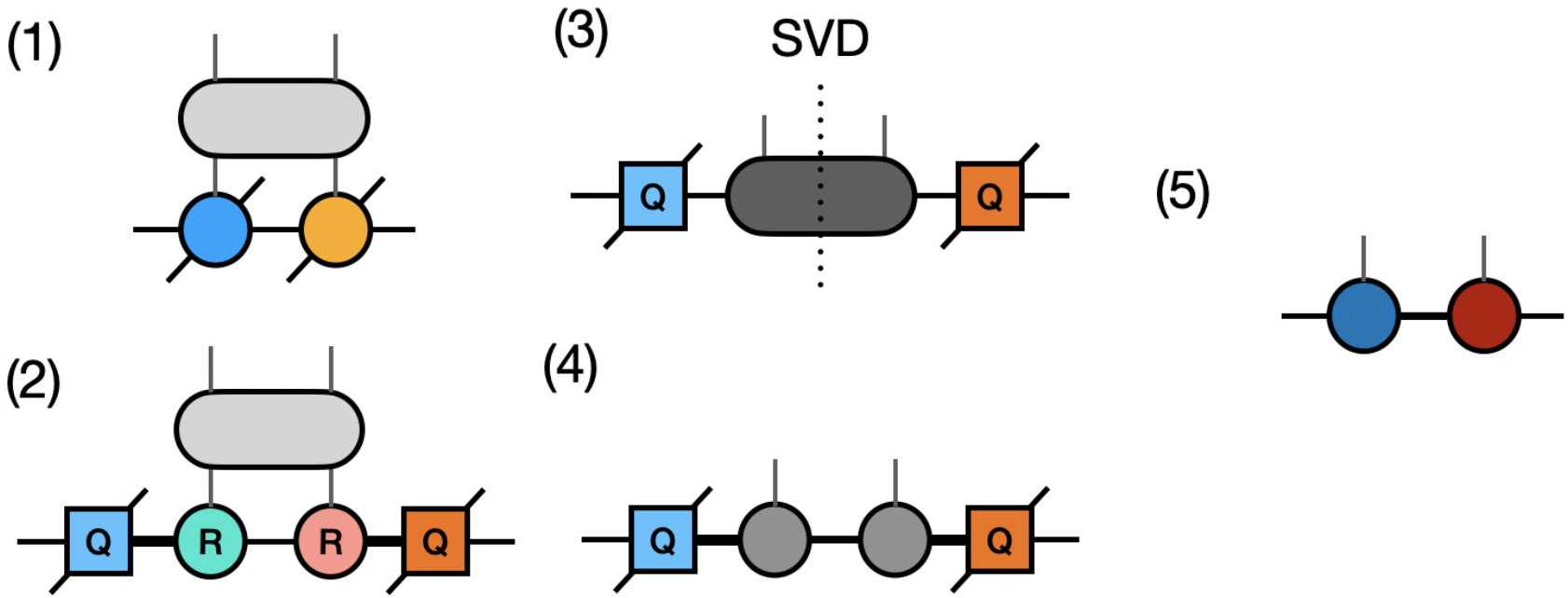
Quantum Circuit Simulation using PEPS[1]

- Near-term quantum architectures mostly connect qubits in a 2D fashion
- Non-local gates can be applied via the use of swap gates (with corresponding overhead)
- 2D tensor networks (projected entangles pair states (PEPS)) provide a natural way to simulate 2D quantum circuits
- Same software/algorithms infrastructure is also effective for (imaginary) time evolution with many Hamiltonians of interest
- Gate application and contraction of PEPS can both have exponential cost in the size of the circuit, so desire effective approximation

[1] Yuchen Pang, Tianyi Hao, Annika Dugad, Yiqing Zhou, and E.S., arXiv:2006.15234.

Approximate Application of Two-Site Operators

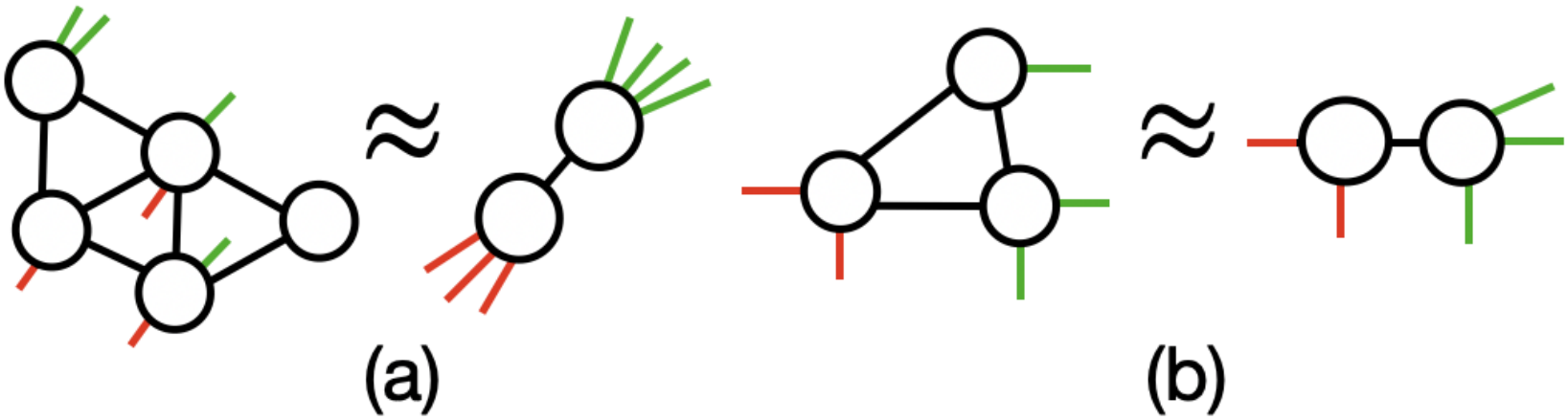
- Consider application of a two-site operator on neighboring PEPS sites
- *Simple update (QR-SVD)* algorithm:



- We provide an efficient distributed implementation of QR-SVD
- This operation is an instance of what we'll refer to as `einsumsvd` and QR-SVD is one algorithm/implementation

Implicit Randomized `einsumsvd`

- The `einsumsvd` primitive will also enable effective algorithms for PEPS contraction

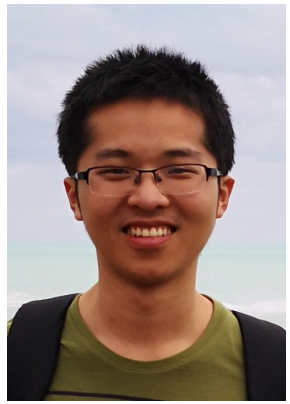


- An efficient general implementation is to leverage randomized SVD / orthogonal iteration, which iteratively computes a low-rank SVD by a matrix–matrix product that can be done implicitly via tensor contractions
- This approach improves complexity for PEPS boundary contraction method

Koala

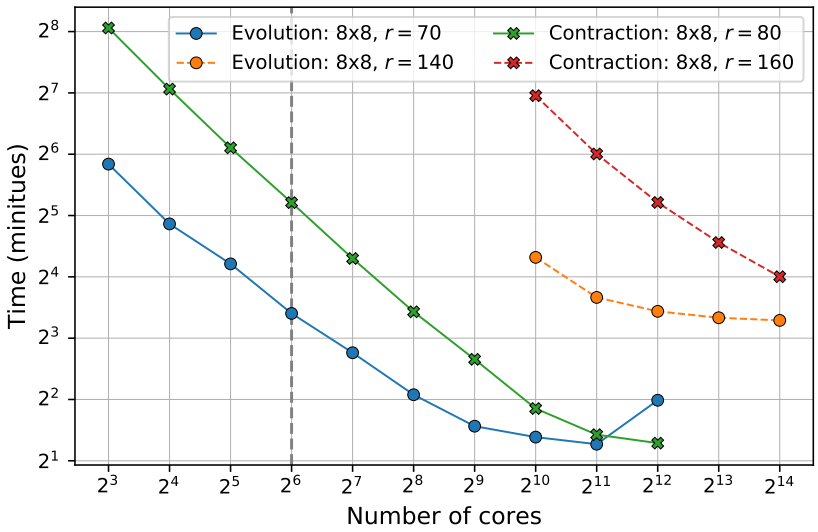
- We introduce a new library, Koala[1], for high-performance simulation of quantum circuits and time evolution with PEPS

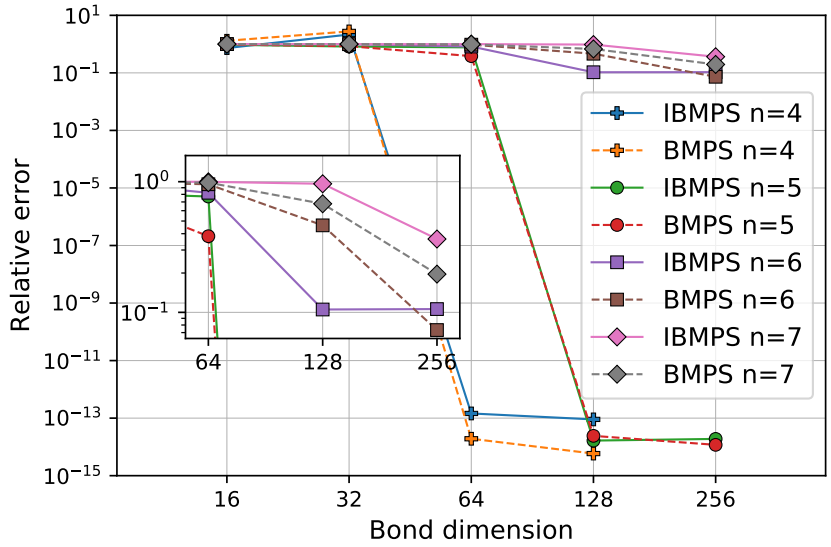
```python
from koala import peps, Observable
from tensorbackends.interface import ImplicitRandomizedSVD

# Create a 2-by-3 PEPS in distributed memory using CTF
qstate = peps.computational_zeros(nrow=2, ncol=3, backend='ctf')

# Construct operators and apply them to the quantum state
Y = qstate.backend.astensor([0,-1j,1j,0]).reshape(2,2)
CX = qstate.backend.astensor([1,0,0,0,0,1,0,0,0,0,0,1,0,0,1,0,])
CX = CX.reshape(2,2,2,2)

qstate.apply_operator(Y, [1])
qstate.apply_operator(CX, [1,4], update_option=peps.QRUpdate(rank=2))

# Construct an observable and calculate the expectation with IBMPS
observable = Observable.ZZ(3, 4) + 0.2 * Observable.X(1)
result = qstate.expectation(
    observable, use_cache=True,
    contract_option=peps.BMPS(ImplicitRandomizedSVD(rank=4)),
)
```



[1] https://github.com/cyclops-community/koala

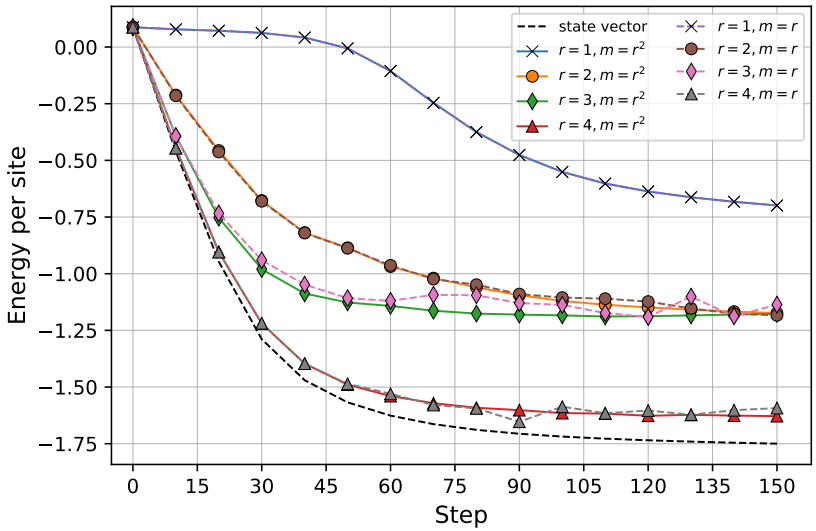
PEPS Benchmark Performance

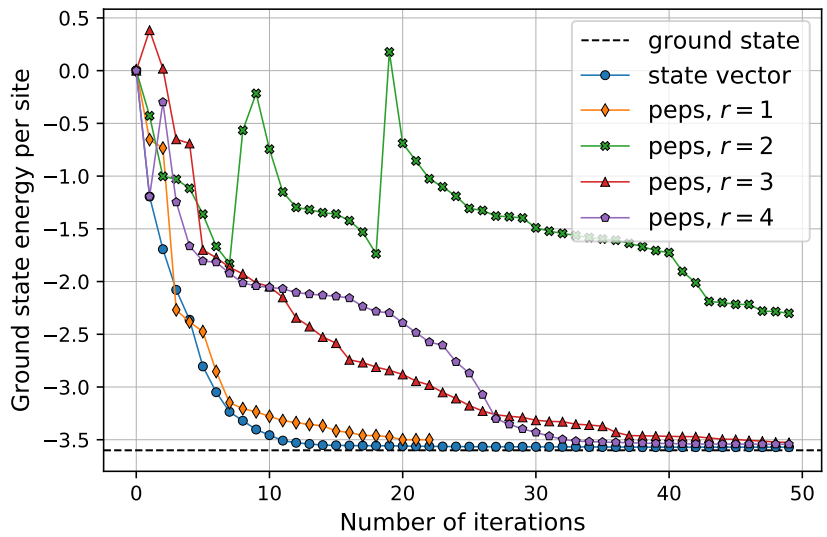




- Koala achieves good parallel scalability for approximate gate application (evolution) and contraction
- Approximation can be effective even for adversarially-designed circuits such as Google's random quantum circuit model (figure on right)

PEPS Accuracy for Quantum Simulation





- ITE code achieves improvable accuracy with increased PEPS bond dimension, but approximation in PEPS contraction is not variational
- Variational quantum eigensolver (VQE), which represents a wavefunction using a parameterized circuit $U(\theta)$ and minimizes

$$\langle U(\theta)| H |U(\theta)\rangle ,$$

also achieves improvable accuracy with higher PEPS bond dimension

Conclusion

- We have presented innovations to numerical algorithms and software libraries for tensor contractions, decompositions, and tensor networks
- Our research group is developing an ecosystem of algorithms and software for simulation of quantum systems
- This work is relevant to both classical methods for quantum chemistry and physics, as well as quantum computation
- See our website[1] and github pages for access to high performance software for tensor methods

[1] http://lpna.cs.illinois.edu

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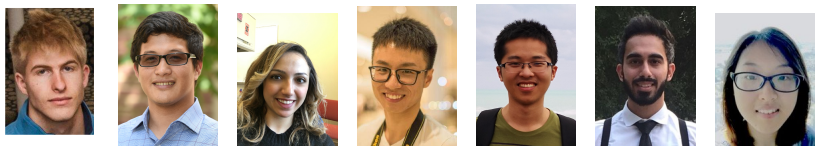

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