# a graph algorithm for a new architecture and new algorithms for quantum state evolution

Claire C Ralph

# thank you!


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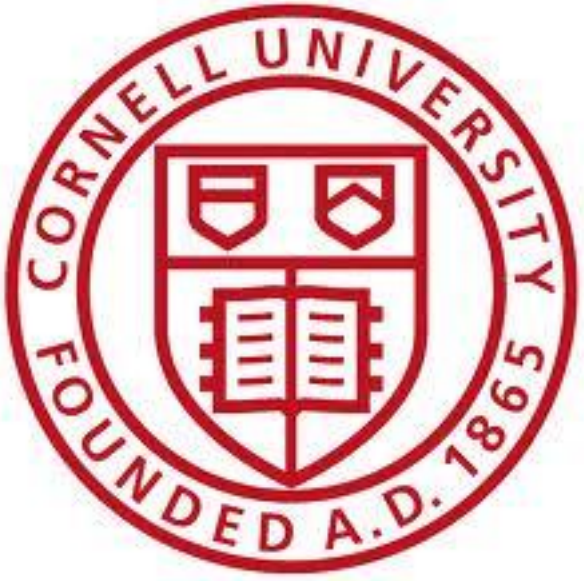
CSGF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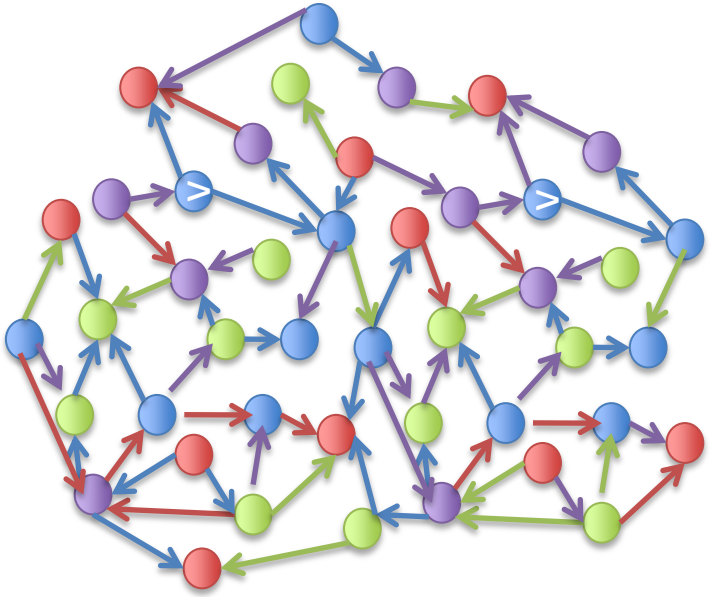
# a graph algorithm for a new architecture

# high performance and graphs

graphs

- Data-driven applications
- Unstructured problems
- Poor locality
- High data access to compute ratio



traditional HP not optimal for graphs

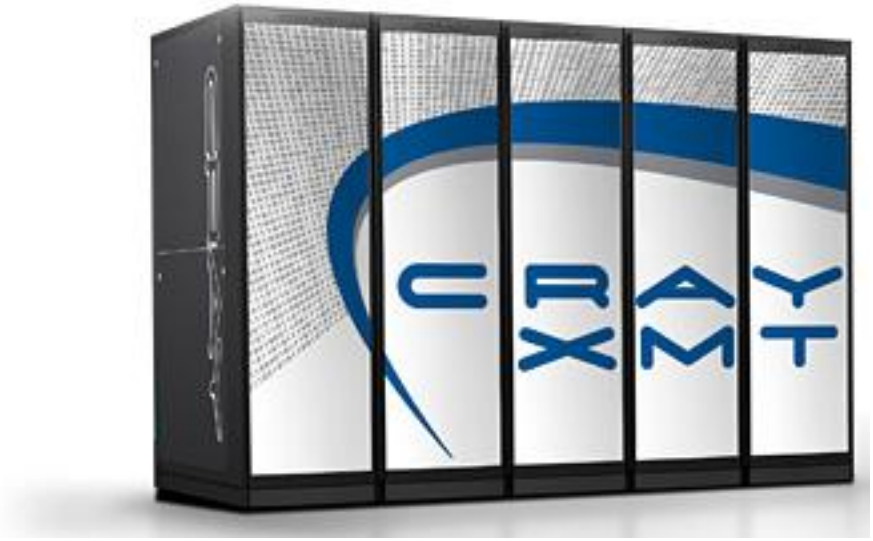
Berry, et. al. IEEE IPDPS, 2007.

# New Architecture → New Techniques → New Algorithms

'Tolerate' not 'reduce' latency.

Load balancing not an issue.

Hotspotting still a problem!

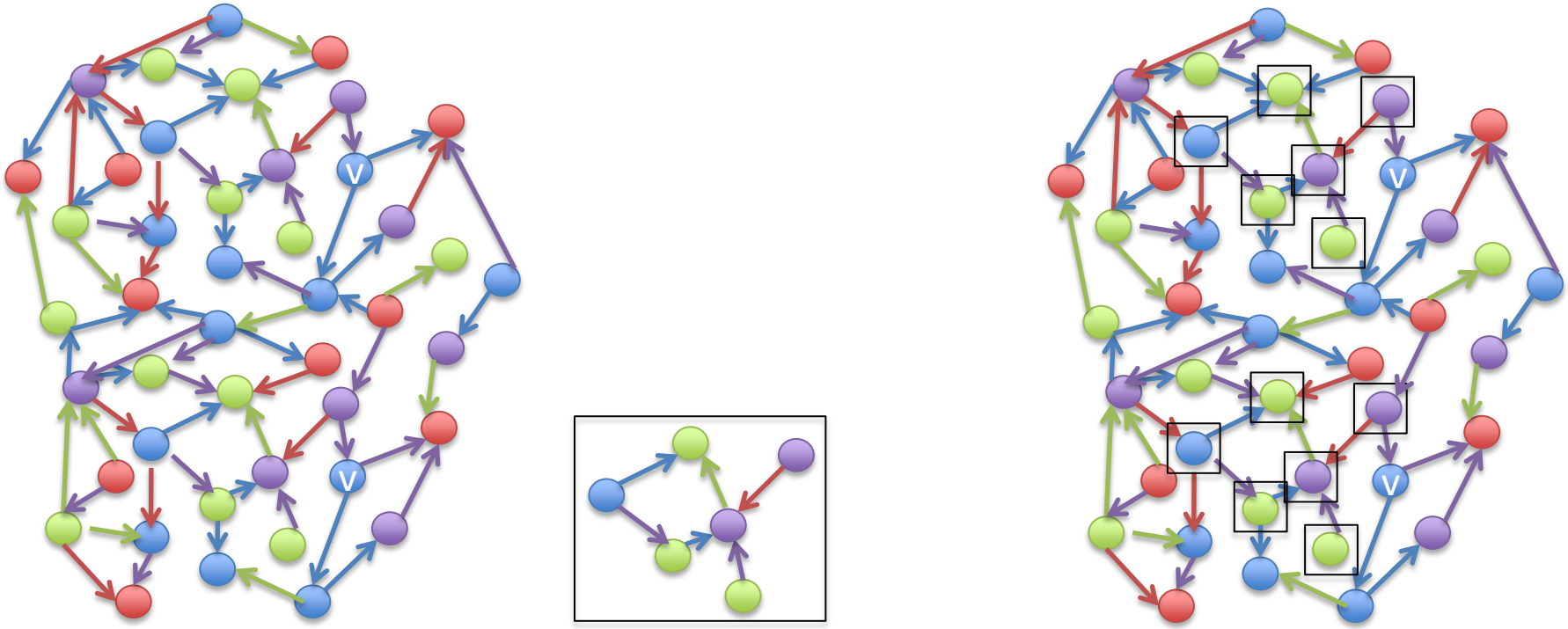



## The Cray XMT

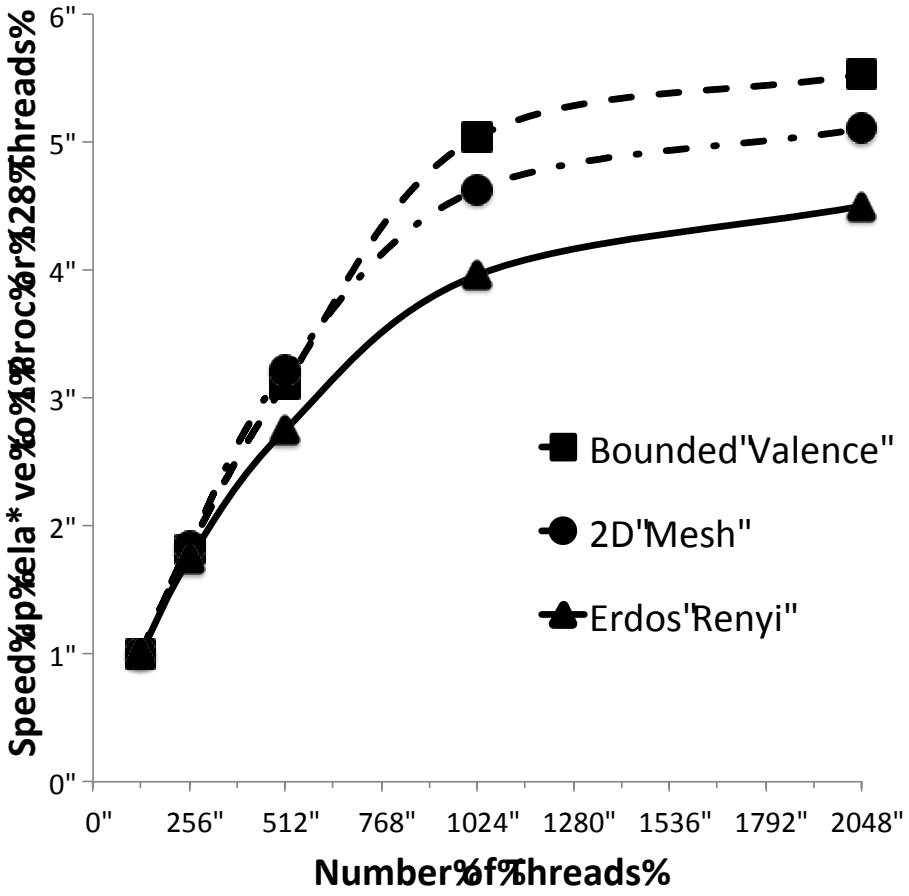
- 500 MHz single 64 bit Cray Threadstorm Processor
- 128 threads per processor
  - Single cycle switching
- 8GB shared memory/processor
- Automated dynamic scheduling
- Largest is 512 processors
  - 65,536 threads
- Largest SMP has 2560 cores
  - 4096 threads

Konecny. CUG 2007.

# Subgraph Isomorphism



# Speed up of Final Algorithm




Scales to 1000 threads.

# in summary

- developed a new graph algorithm
- got to work with a cool new architecture
- pretended to be a computer scientist for a couple of months

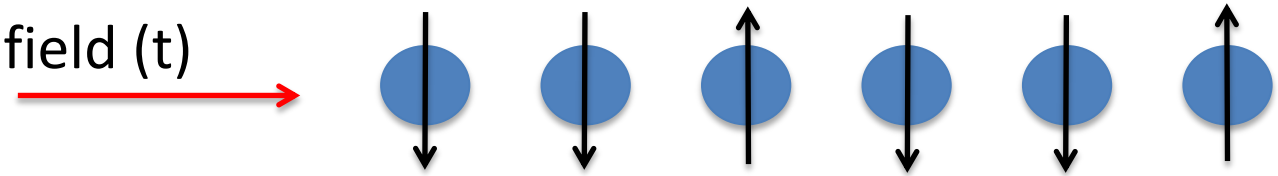
ACM SPAA (2012).

# new algorithms for quantum state evolution

# time dependent Schrodinger Equation for a system of n spins

$$i\frac{\partial}{\partial t}\Psi(\sigma_1,\ldots,\sigma_n) = \hat{H}\Psi(\sigma_1,\ldots,\sigma_n)$$

magnetic field (t)



$$\Psi_t = e^{-iH\Delta t}\Psi_o$$

# a technical detail

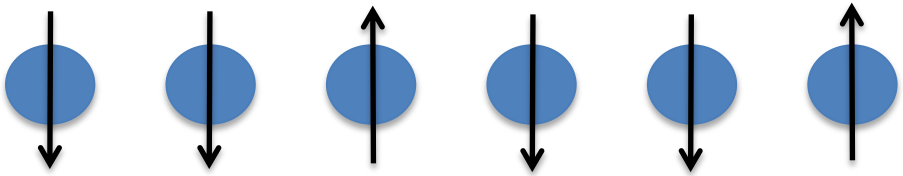
For a closed system:

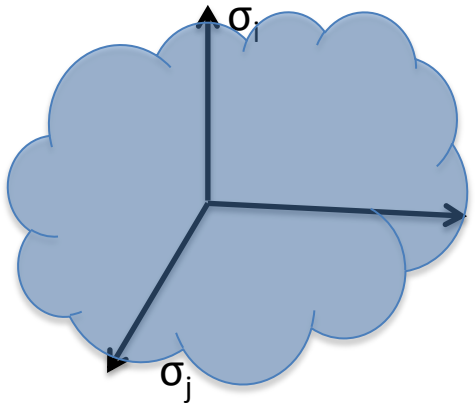
$$\Psi_t = e^{-iH\Delta t}\Psi_o$$

For an open system:

$$\Gamma_t = e^{-iL\Delta t}\Gamma_o$$

# why so complicated?

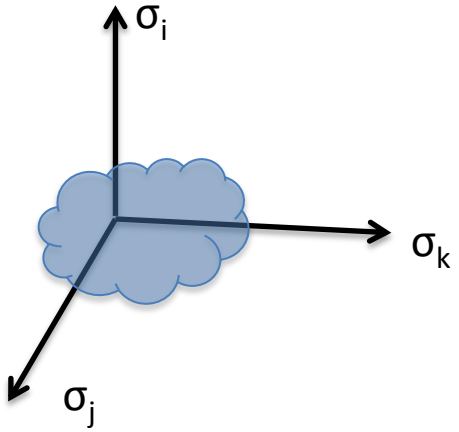




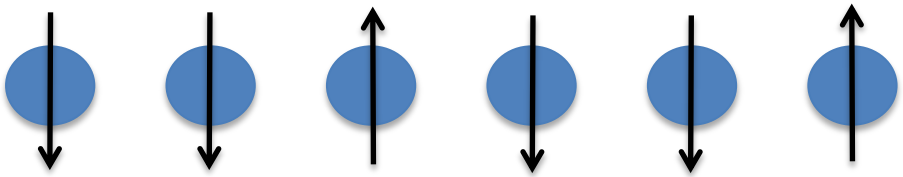

$$|\Psi\rangle = \sum_{\sigma} c_{\sigma_1 \ldots \sigma_n} |\sigma_1 \ldots \sigma_n\rangle$$

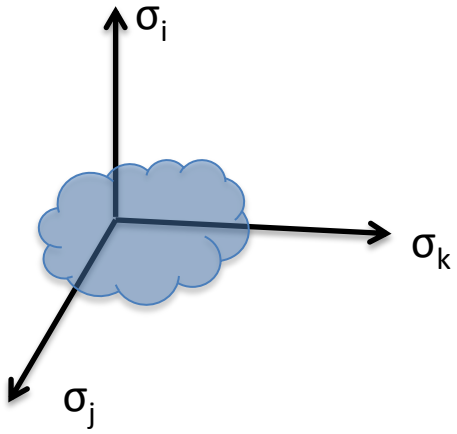
n spins → tensor of dim $2^n$

$$c^{\sigma_1 \ldots \sigma_n}$$



# strategies for approximation






1. state space restriction.

$$C^{\sigma_1 \ldots \sigma_n}$$

tensor of dim $2^n$ is mostly zero

2. quantum monte carlo

not promising for this problem

3. low dimensional factorization

$$C^{\sigma_1 \ldots \sigma_n} \longrightarrow A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_n}$$

# the matrix product state

$$A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_n}$$

We have a form, so:

yes for time independence

?? for dynamics

1. how do we find the elements that make up the ‘best’ product?

2. can we calculate properties (take expectation values) directly from this form?

# a new algorithm: aMPS

1. how do we find the elements that make up the 'best' product?

   derived EofM for individual matrices

   linearize these using special structure

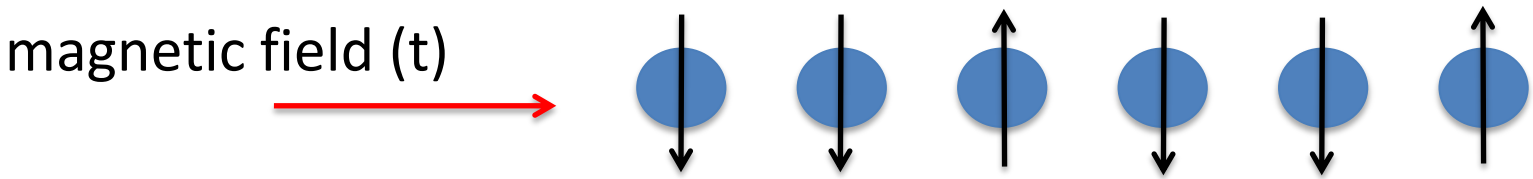
   Fast and Accurate

1. can we calculate useful properties from this form?

   response functions and excitations

Adv. Chem. Phys. (2012)
arXiv:1103.2155v1 [cond-mat.str-el]

# so we can use the MPS, but is it useful?

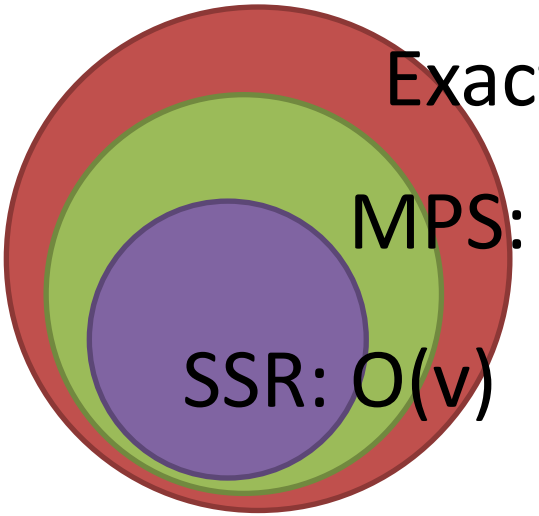



| | NMR | ESR |
|---|---|---|
| high temp limit | ✔ | ✖ |
| SSR | ✔ | ✖ |
| MPS | ? | ? |

aMPS ‘automatically’ gives optimal basis

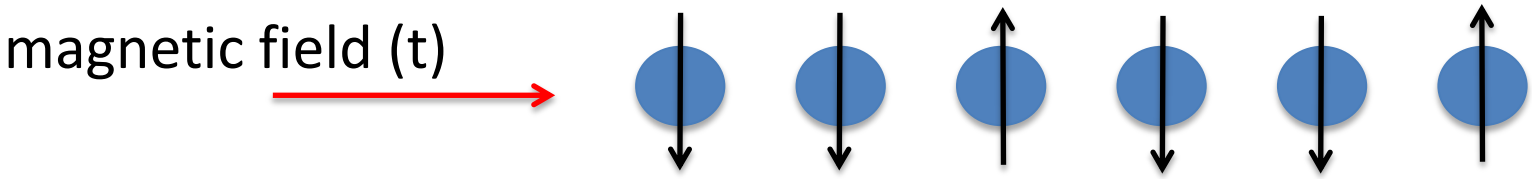
relationship between SSR and MPS: MPS covesr the space of the SSR basis with $O(n^3)$ storage.

# storage of SSR to MPS




MPS guaranteed to do better than SSR with polynomial increase in storage cost.

# a model system

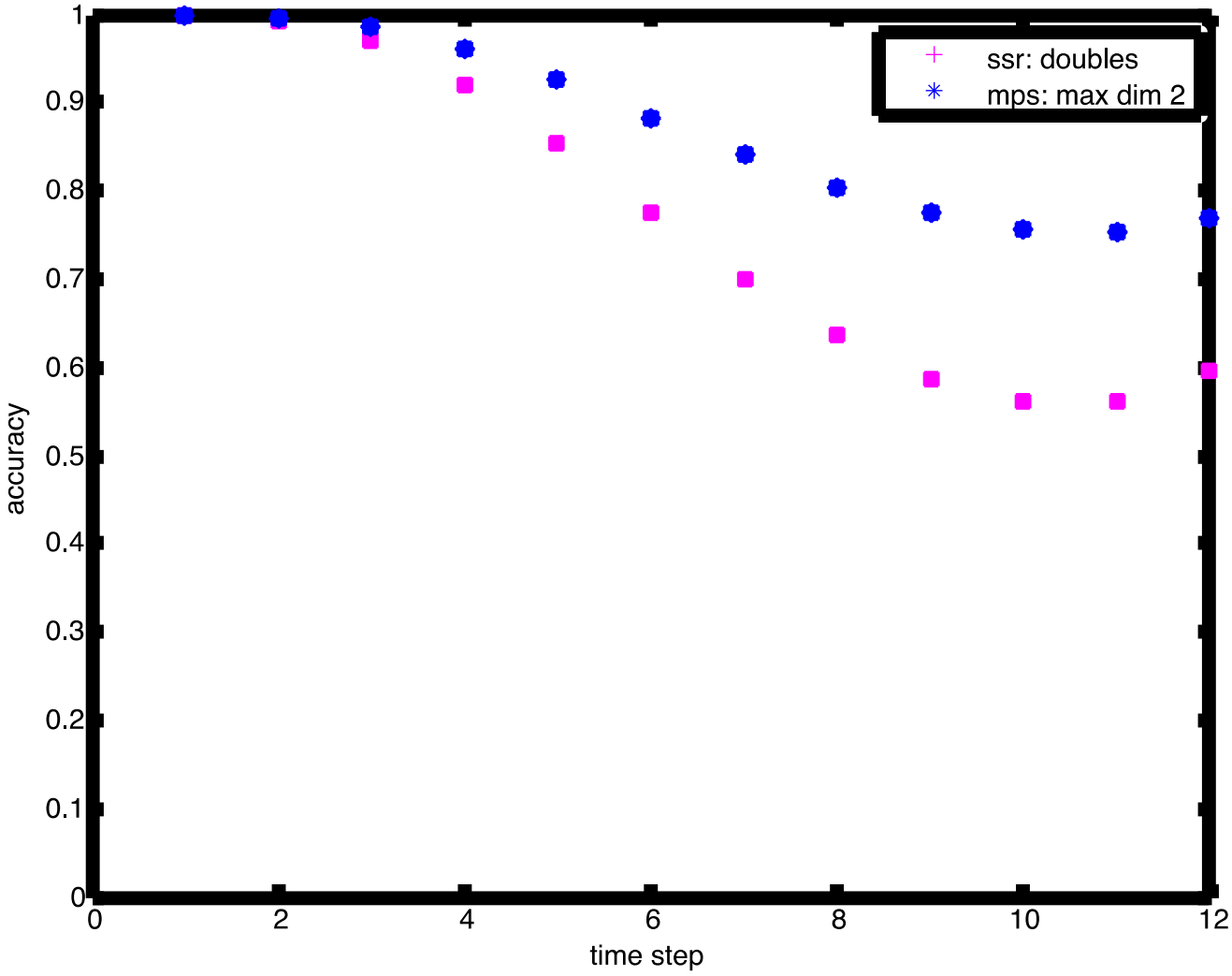



$$e^{-iH\Delta t}$$

$$\Psi_o \rightarrow \Psi_1 \rightarrow \Psi_2 \rightarrow \Psi_3$$

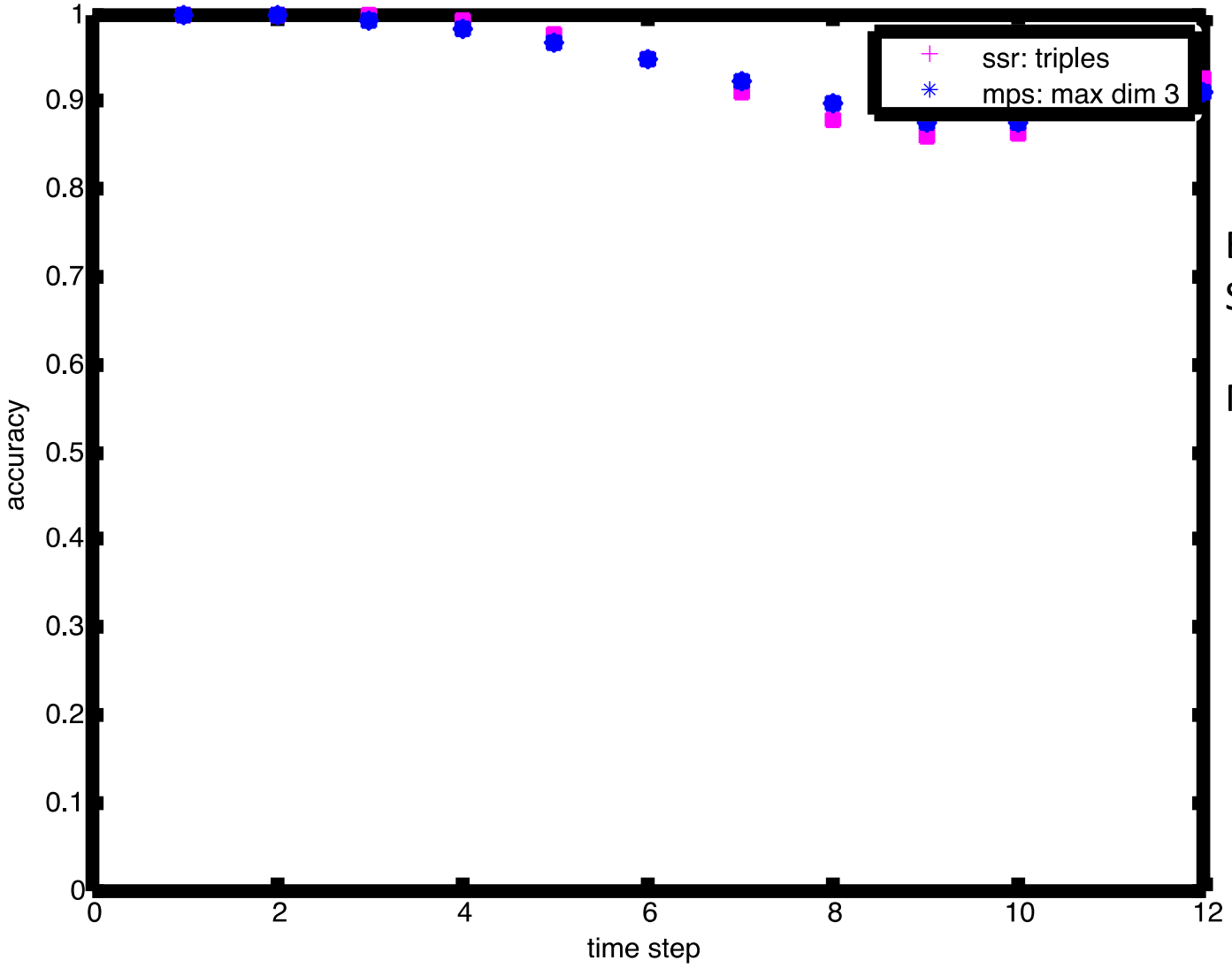
mps ssr | mps ssr | mps ssr | mps ssr

# numerical comparison of SSR vs MPS



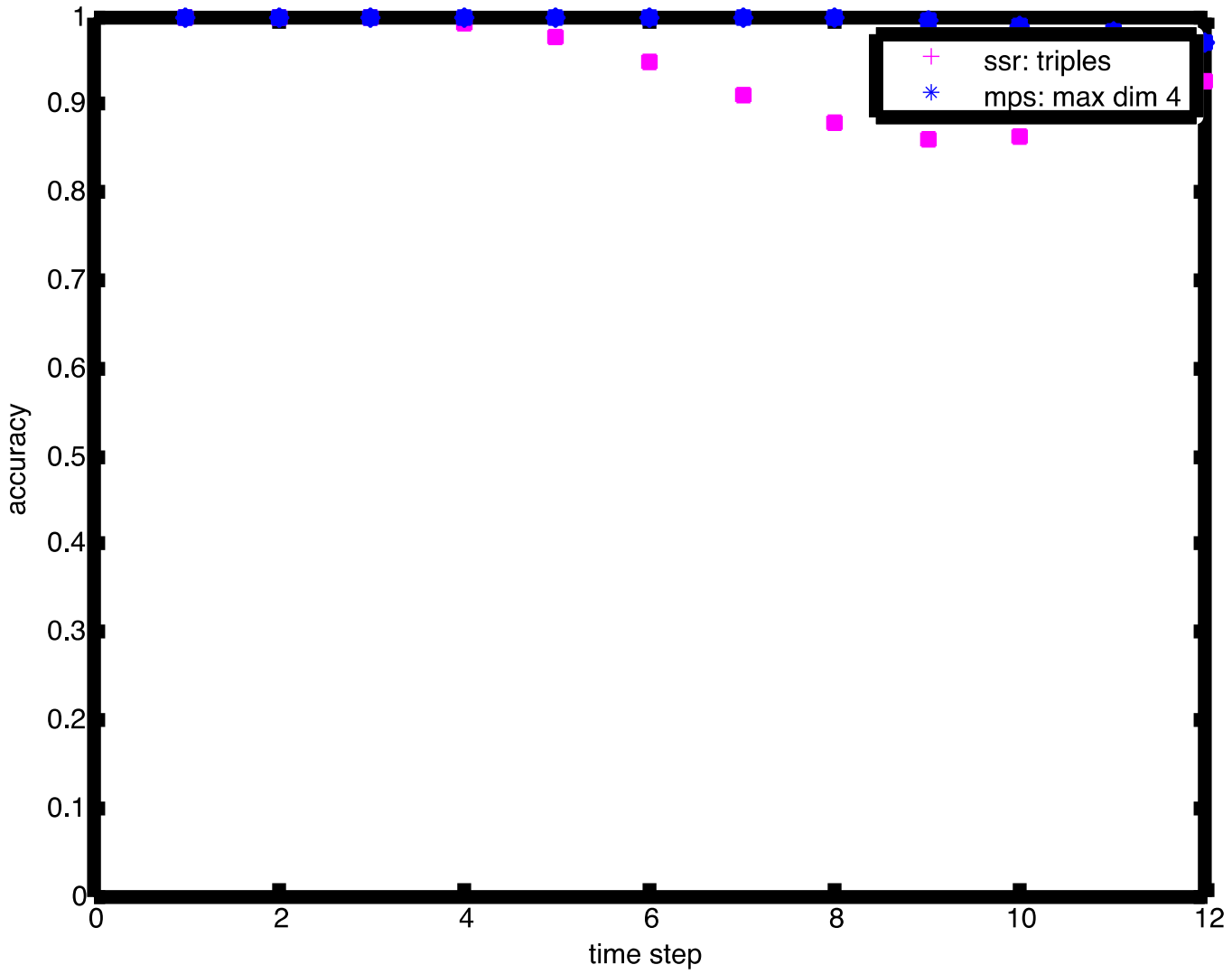

| | | |
|---|---|---|
| Ext | nelem | 256 |
| SSR | nelem | 67 |
| | nnz | 16 |
| MPS | nelem | 48 |
| | nnz | 45 |

# numerical comparison of SSR vs MPS




| | | |
|---|---|---|
| Ext | nelem | 256 |
| SSR | nelem | 175 |
| | nnz | 40 |
| MPS | nelem | 96 |
| | nnz | 92 |

# numerical comparison of SSR vs MPS




| | | |
|---|---|---|
| Ext | nelem | 256 |
| SSR | nelem | 175 |
| | nnz | 40 |
| MPS | nelem | 160 |
| | nnz | 148 |

# in summary

- derived a new time propagation scheme for a beloved wavefunction ansatz, MPS
- derived methods for computing important physical properties such as response functions
- analyzed relationship between MPS and SSR
- initial numerical results are promising

next step:

implementation of time propagation algorithm

# thank you!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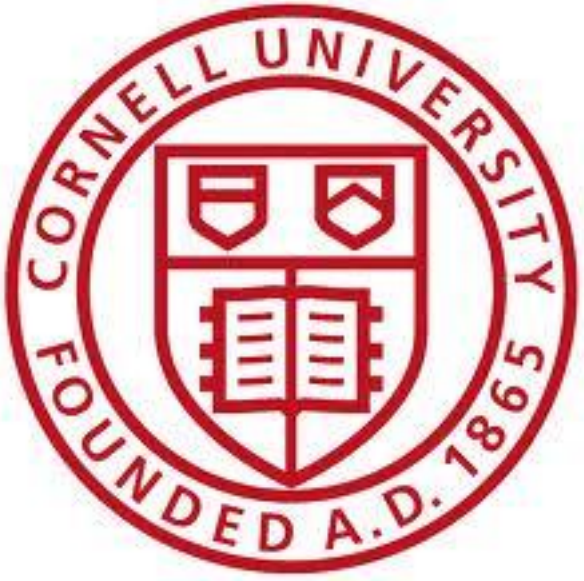
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