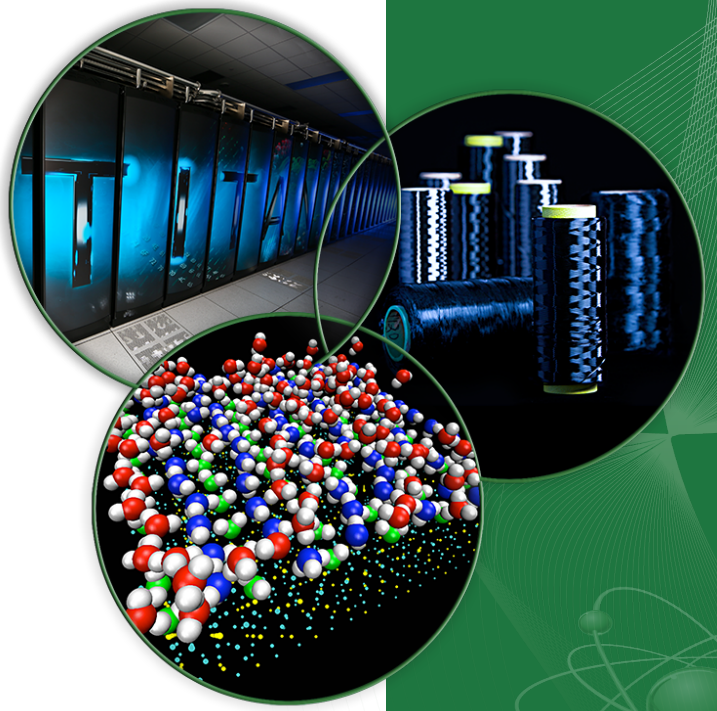
Experiences with using different OpenMP 4.5 programming styles to bring DMRG++ to Exascale



Arghya Chatterjee (ORNL / Georgia Tech.)
Oscar Hernandez (ORNL)
Vivek Sarkar (Georgia Tech.)

Application Support Team
Dr. E. D'Azevedo (CNMS)
Dr. G. Alvarez (CNMS)
Dr. Wael Elwasif (ORNL)

ORNL is managed by UT-Battelle
for the US Department of Energy

OpenMP Con 2017
September 18, 2017

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INTRODUCTION

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- Rapidly changing microprocessor design and heterogeneous architectures

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- Applications must adapt to exploit parallelism

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- Mini-application -- will serve as a foundation for Exascale-ready implementation
- Co-designing with asynchronous programming models (Habanero C++, Kokkos, MAGMA)

OUTLINE

OUTLINE

DMRG++

Target
Application

OUTLINE

Target Application

Physics / Nano-science & Programming Models

OUTLINE

Target Application

Physics / Nano-science & Programming Models

Design, Implementation & Challenges encountered

OUTLINE

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Design, Implementation & Challenges encountered

Programming framework support

OUTLINE

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Adding new Constructs / functionality

DMRG++

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DMRG ++

- DMRG++ → *Density Matrix Renormalization Group*

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DMRG ++

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- DMRG++ algorithm -- deeper understanding of nanoscale material properties
- *Sparse matrix algebra* computational motif
- Actively developed application by Material Applications group @ORNL

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PROFILING : Shared Memory (DMRG++)

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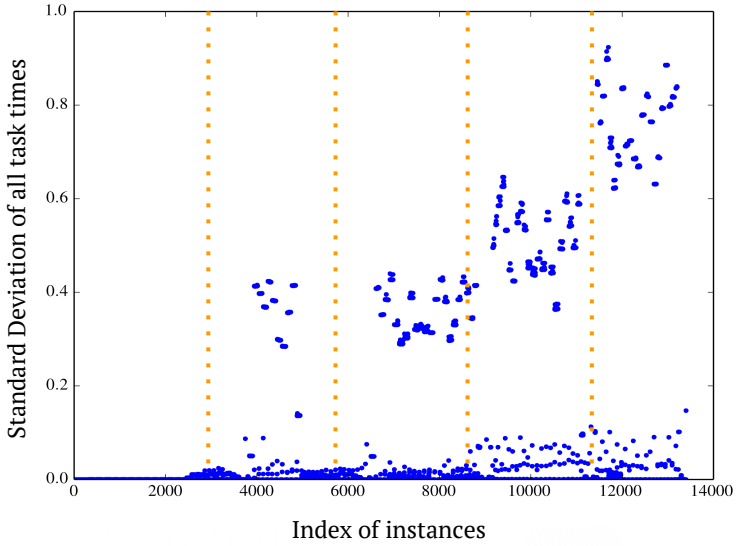
- Profiled on a Bulldozer AMD Opteron processor (TITAN)
- 80% of execution time → calculating the Hamiltonian



Standard deviation of all execution times per parallel region instance over time. Execution uses 8 threads on a single TITAN node (8 blue dots per instance).

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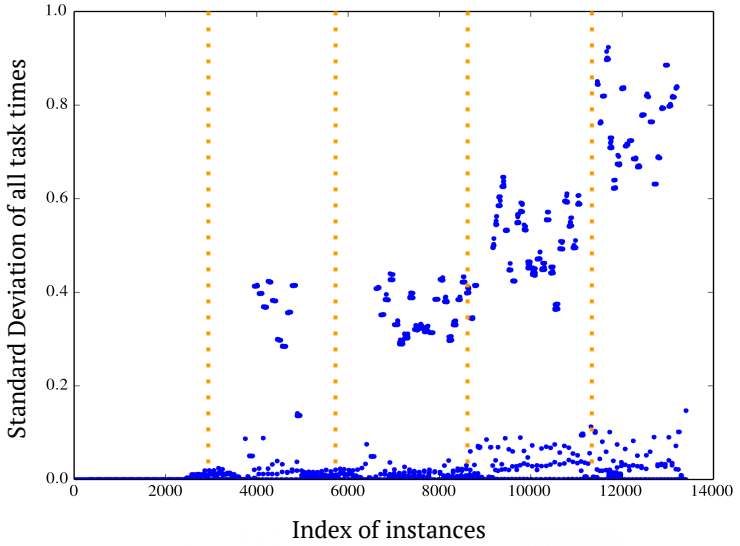

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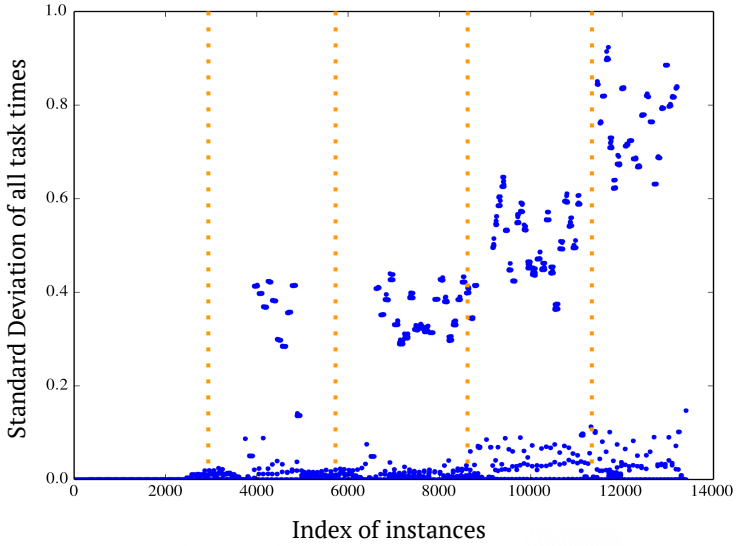

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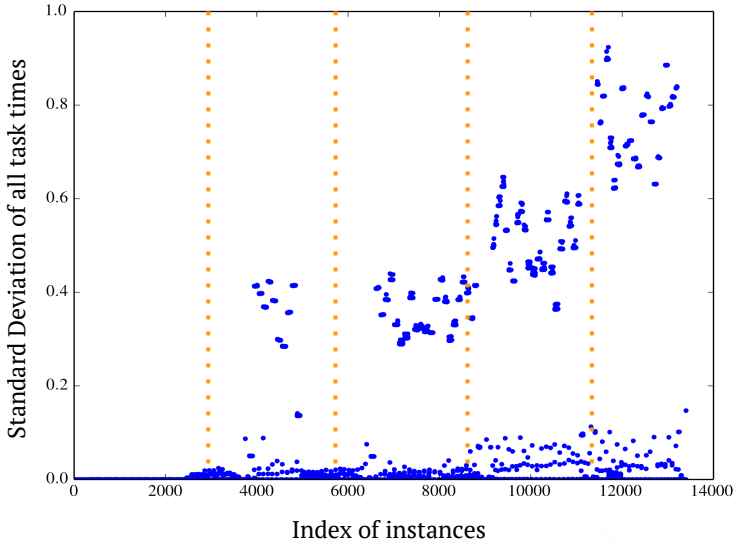
- Dynamic Application → problem size grows → greater load imbalance



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MOTIVATION — Physics

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- Current DMRG++ — limited to 1-Dimensional Problems

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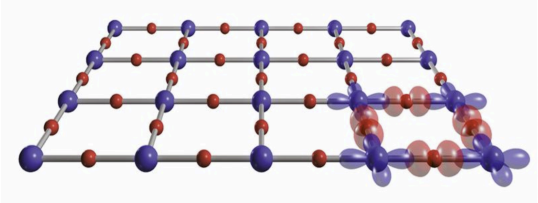
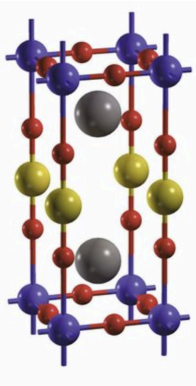


2-D model



3-D model

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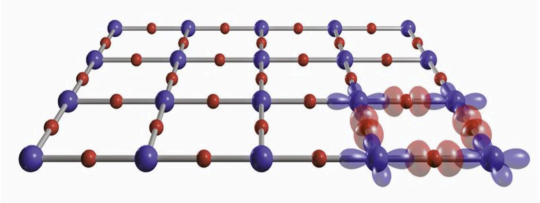
  - ✤ First principle (almost) models without approximating electron-electron interaction



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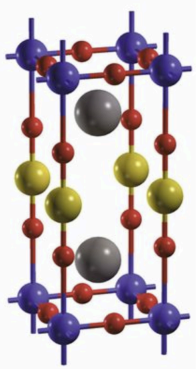

3-D model

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MOTIVATION — Programming Models

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↑ Productivity ↑ Performance

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KRONECKER PRODUCT (y = H*x)

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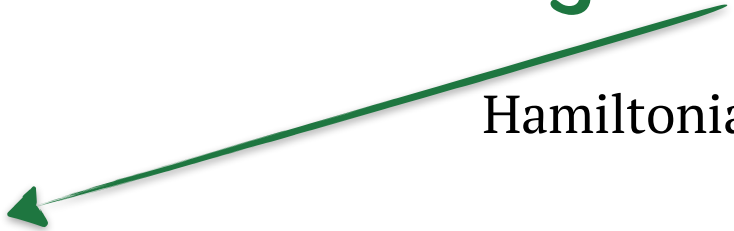

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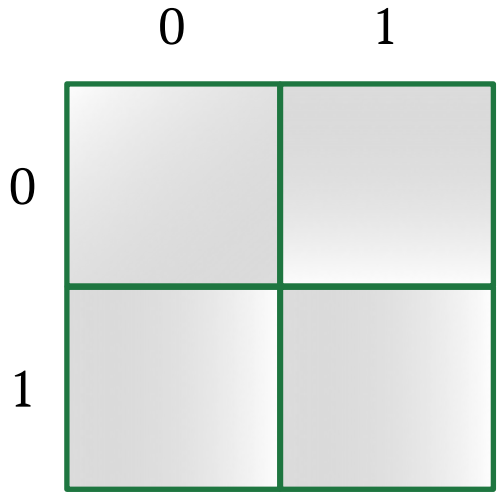
KRONECKER PRODUCT (y = H*x)

Hamiltonian Matrix



CIJ [npatches : npatches]

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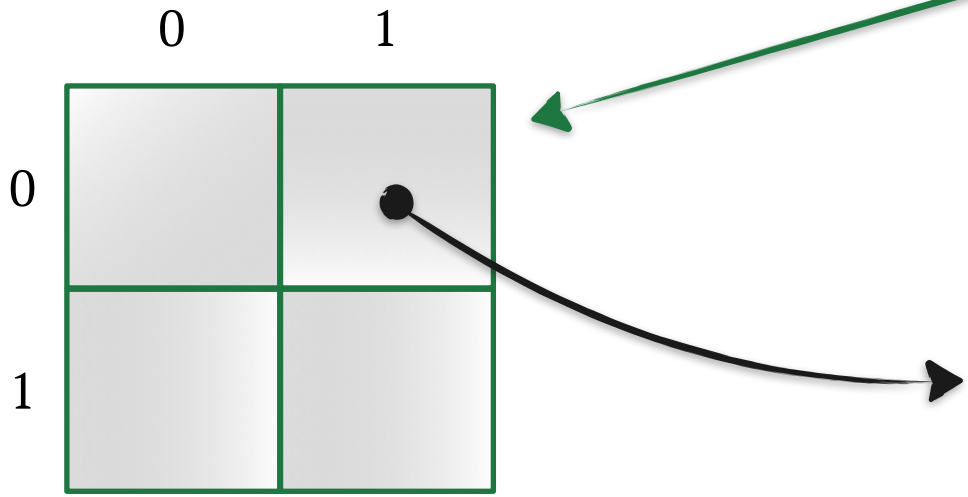

Hamiltonian Matrix

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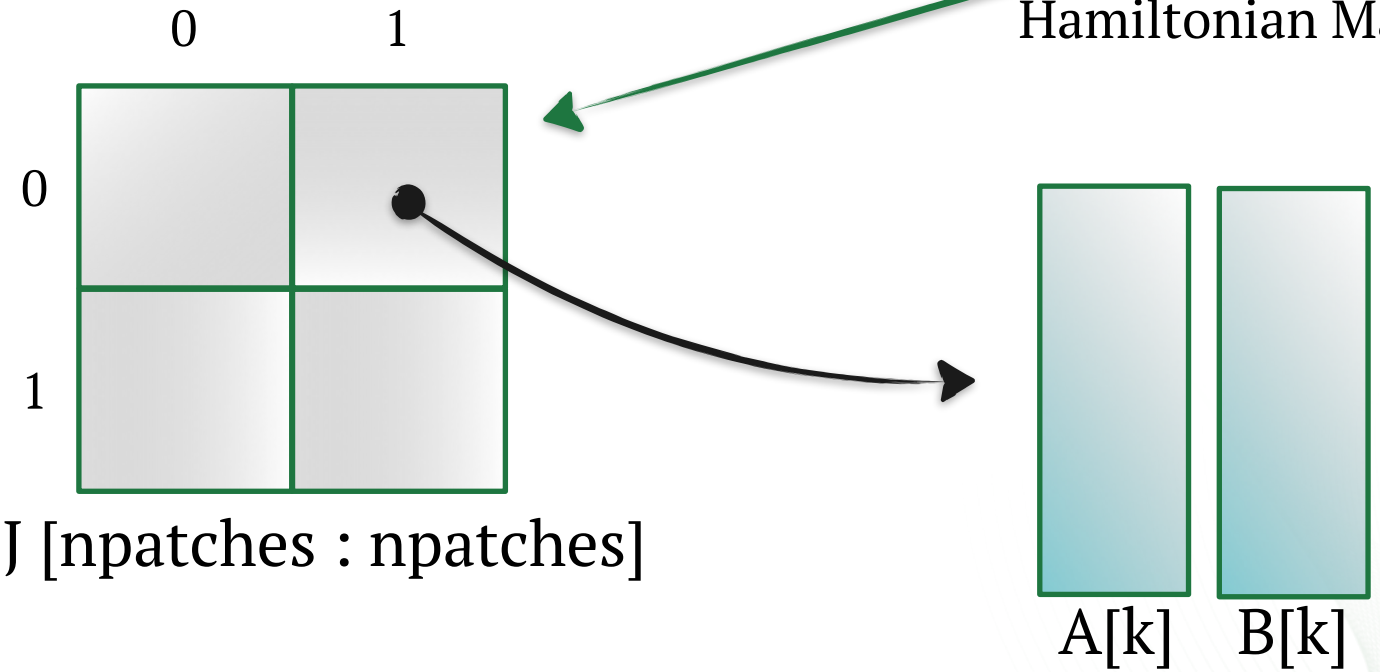

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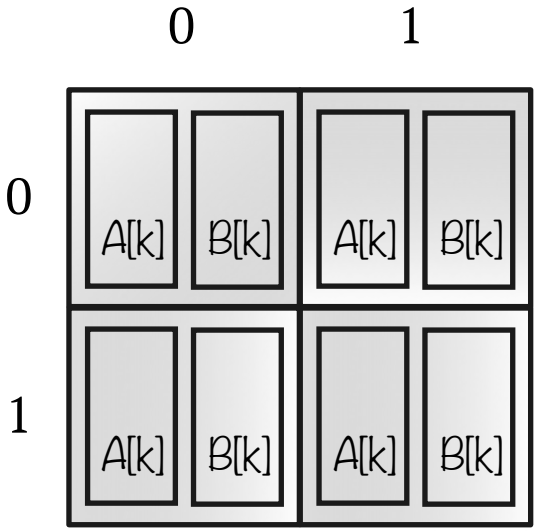

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Hamiltonian Matrix

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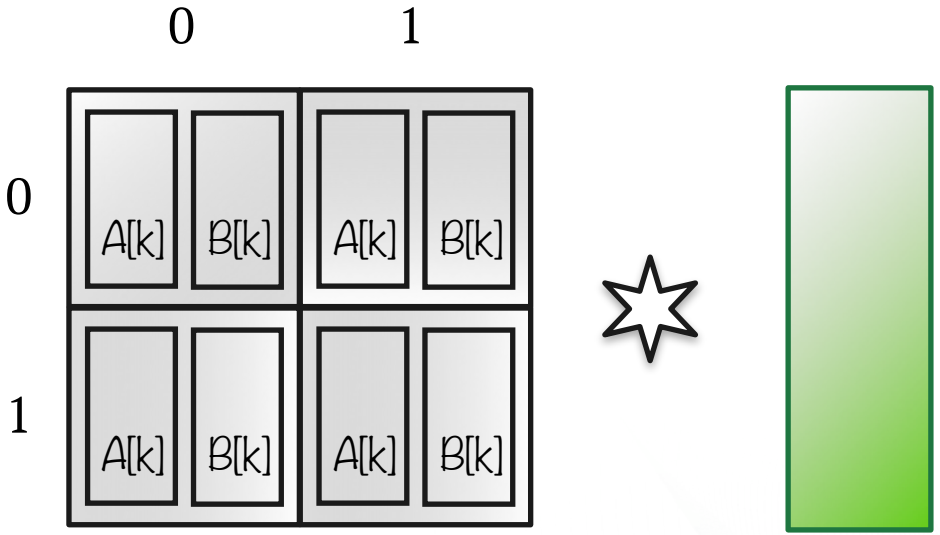

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Hamiltonian Matrix

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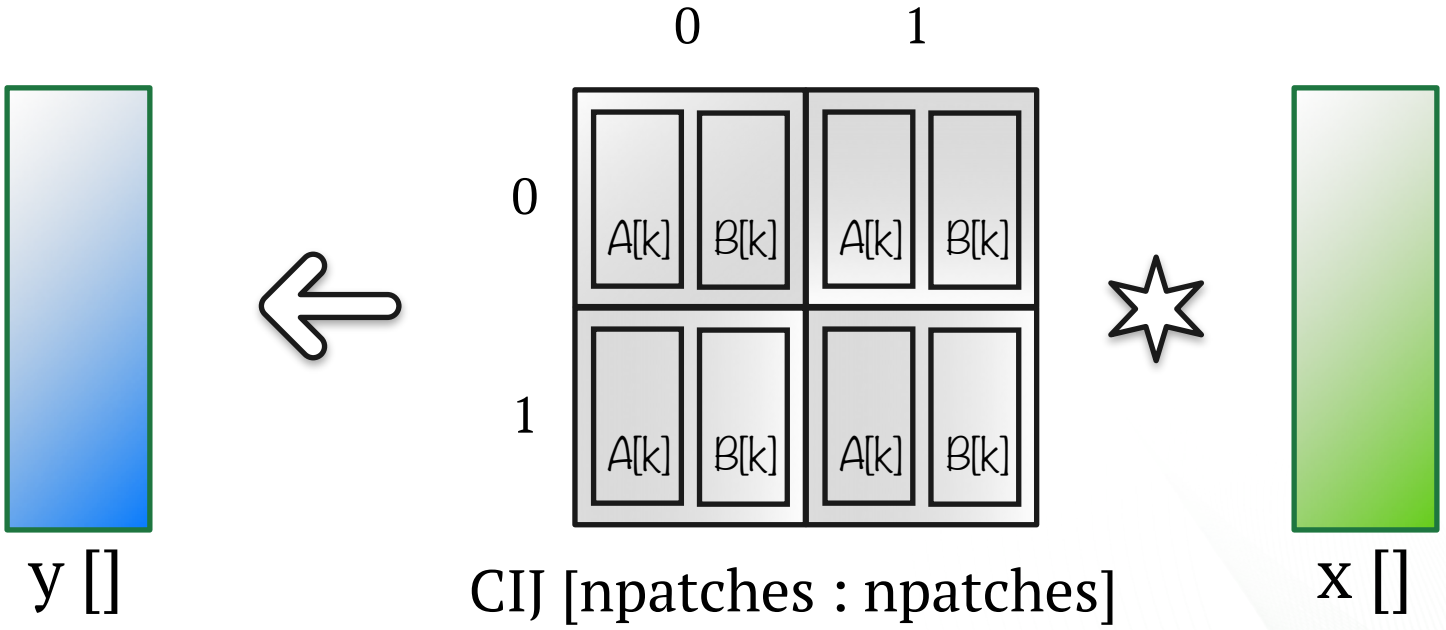

Hamiltonian Matrix

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PSEUDO CODE — (y = H*x) : Sequential

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```
for ( i in C_Rows )
    Y[i] = 0.0;
    for ( j in C_Cols )
        for ( k in C [i][j].list() )
            Y[i] + = C[i][j]. A[k] * C[i][j]. B[k] * X[i]
                    (dgemm call — IBM ESSL)
```


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PSEUDO CODE — (y = H*x) : Parallel

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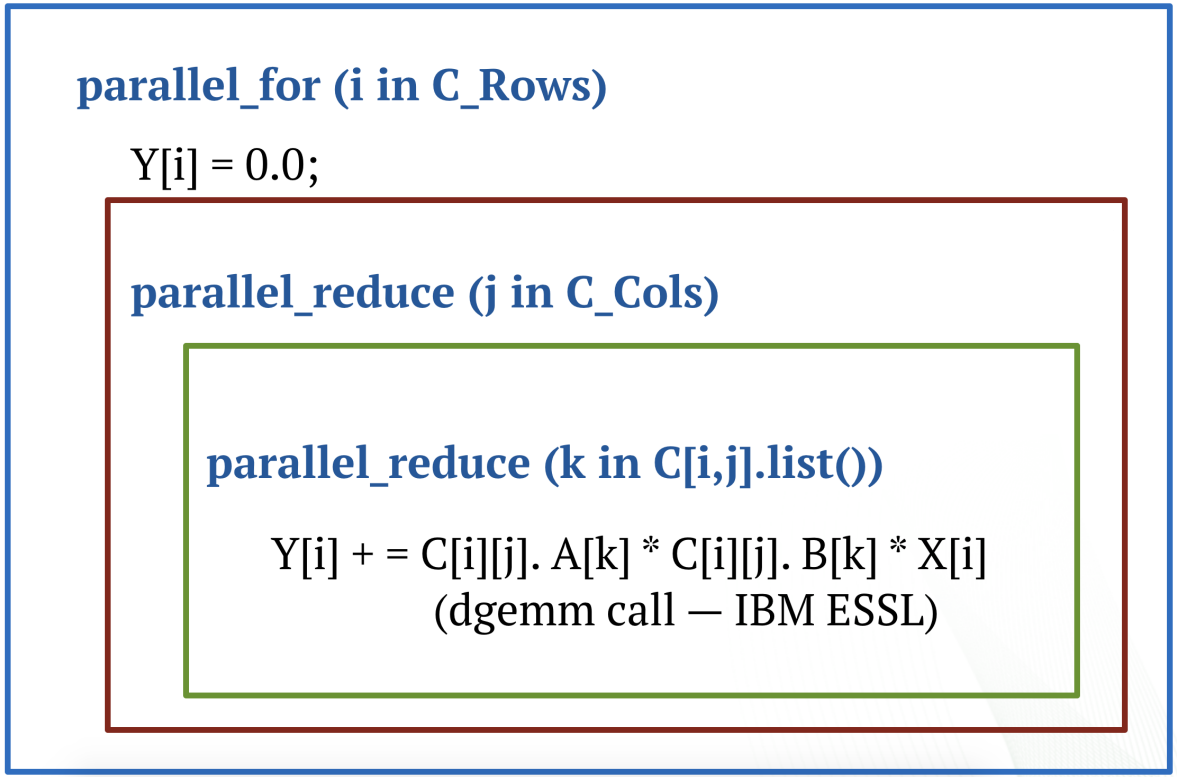

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PROGRAMMING STYLES

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PROGRAMMING STYLES

- Nested Parallelism

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PROGRAMMING STYLES

- Nested Parallelism
- Multi-Level Tasking

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PROGRAMMING STYLES

- Nested Parallelism
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- Multi-Level Tasking with Nested Parallelism

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1. Nested Parallelism

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1: **INPUT:** C Matrix, X Vector
2: **OUTPUT:** Y Vector
3: Enumerate over the entire C Matrix
4: **omp parallel for:** i in C_Rows
5: Reduction Variable: YI[i]= 0.0
6: **omp parallel for w/ reduction(YI):** j in C_Cols
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8: **omp parallel for w/ reduction(YIJ):** k in C[i,j].list()
9: **Update YIJ:** += C[i][j].A[k] ⊗ C[i][j].B[k] * X[]
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User-defined Reductions

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1. Nested Parallelism : Challenges

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- Lack of support for nested work-sharing loops (Spec. Restriction)

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  - ✤ omp single / *omp master / omp critical*
- Thread affinity (using OpenMP Places / proc-bind) — depth 3

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2. Multi-level Tasking : using taskloop

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- No support for OpenMP constructs within task-loops
  - ✤ omp single / *omp master* / *omp critical*
- Task-elasticity — no support for dynamic resource allocation
  - grain-size — thread to task-mapping

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3. Multi-level Tasking with Nested Parallelism

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User-defined Reductions

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3. Multi-level Tasking with Nested Parallelism

```
1:  INPUT: C Matrix, X Vector
2:  OUTPUT: Y Vector
3:  Enumerate over the entire C Matrix
4:  OpenMP Parallel region
5:      for i in C_Rows
6:          Create OpenMP Tasks: adjust granularity
7:          OpenMP Parallel region w/ Reduction (YI)
8:              Reduction Variable: YI[i]= 0.0
9:              for j in C_Cols
10:                 Create OpenMP Tasks: adjust granularity
11:                 OpenMP Parallel region w/ Reduction (YIJ)
12:                     Reduction Variable: YIJ[i]= 0.0
13:                     for k in C[i,j].list()
14:                         YIJ += C[i][j].A[k] ⊗ C[i][j].B[k] * X[]
15:                     Reducing YIJ in Parallel region
16:             Reducing YI in parallel region: YI += YIJ
17:         Update Y: Y = YI
18: Return vector Y
```

User-defined Reductions

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3. Tasking with Nested Parallelism: Challenges

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3. Tasking with Nested Parallelism: Challenges

- Creating / destroying parallel regions — affects scalability

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3. Tasking with Nested Parallelism: Challenges

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- Task-loops — variable are *first private* and **NOT** *thread private*
  - ✤ reduction becomes complicated

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3. Tasking with Nested Parallelism: Challenges

- Creating / destroying parallel regions — affects scalability

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  - ✤ reduction becomes complicated

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3. Tasking with Nested Parallelism: Challenges

- Creating / destroying parallel regions — affects scalability

- Task-loops — variable are *first private* and **NOT** *thread private*
  - ✤ reduction becomes complicated

- Task-affinity — within OpenMP nested parallel region
  - ✤ extensions to *tied-tasks* (depth 3)

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EXPERIMENTAL SETUP

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EXPERIMENTAL SETUP

- Compilers used: **GCC**, XLC++, CLANG++

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EXPERIMENTAL SETUP

- Compilers used: **GCC**, XLC++, CLANG++
- Evaluated on Summit-dev (OLCF):
  - **2, 10-core IBM Power8 CPUs (8 h/w threads per core)**
  - 4 NVIDIA Tesla P100 GPUs

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EXPERIMENTAL SETUP

- Compilers used: **GCC**, XLC++, CLANG++
- Evaluated on Summit-dev (OLCF):
  - **2, 10-core IBM Power8 CPUs (8 h/w threads per core)**
  - 4 NVIDIA Tesla P100 GPUs
- DGEMM call: IBM ESSL (and ESSL-smp)

EXPERIMENTAL DATASET

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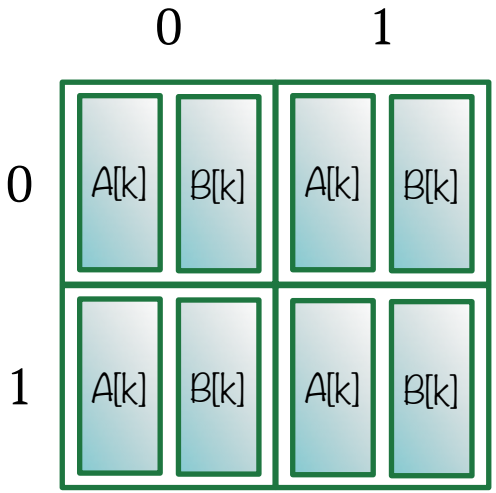
EXPERIMENTAL DATASET



CIJ [npatches : npatches]

Hamiltonian Matrix

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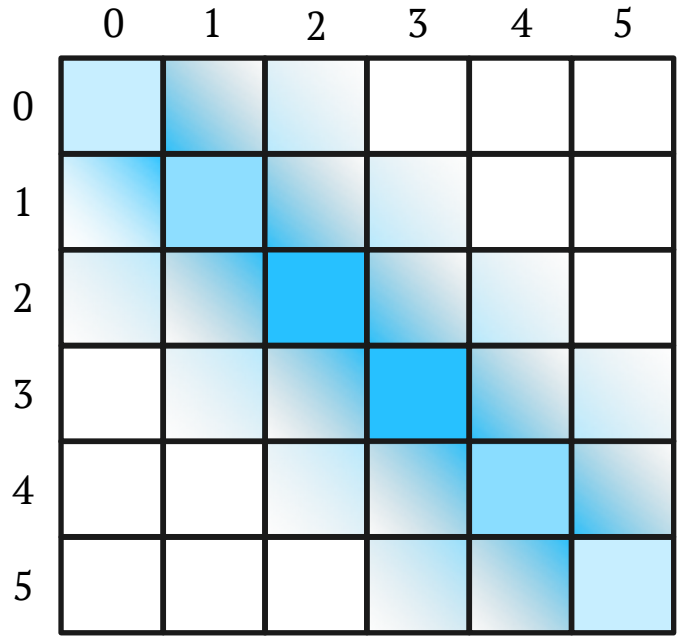
EXPERIMENTAL DATASET



Sparsity of the Hamiltonian Matrix

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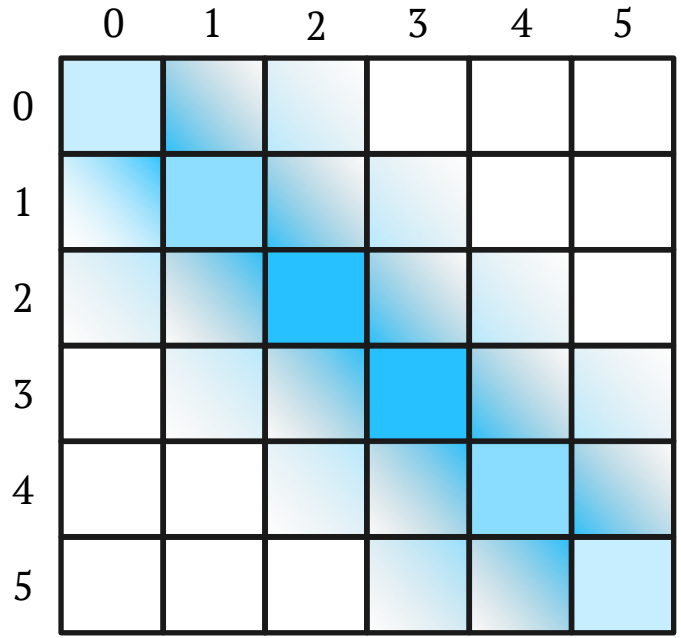
EXPERIMENTAL DATASET



Sparsity of the Hamiltonian Matrix

- Data (A[k]'s and B[k]'s)
  → mostly principal diagonal

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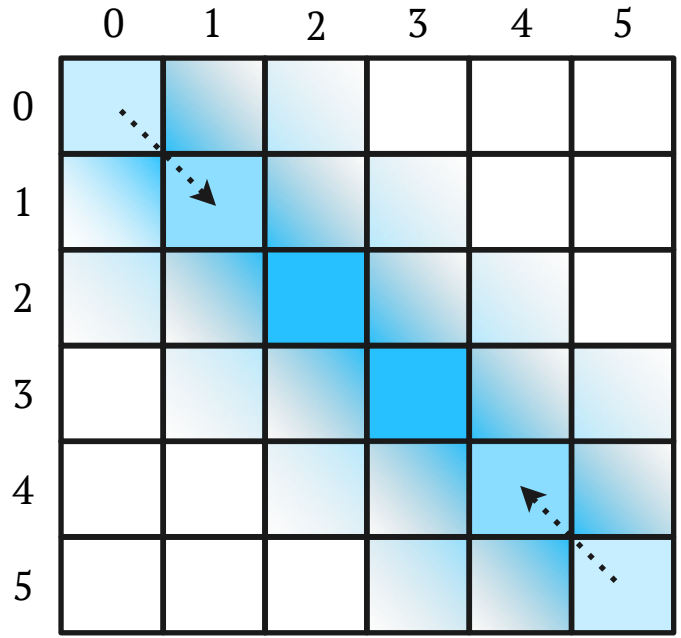
EXPERIMENTAL DATASET



Sparsity of the Hamiltonian Matrix

- Data (A[k]'s and B[k]'s)
  → mostly principal diagonal
- Density increases
  → towards the center

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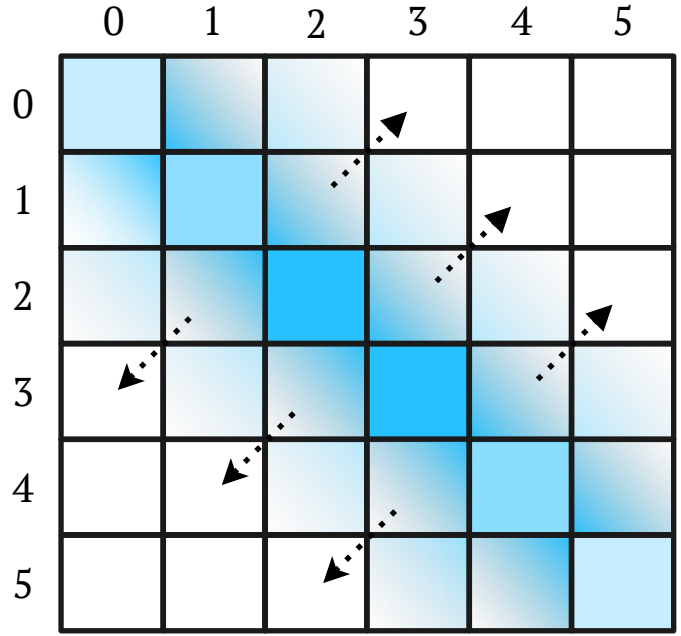
EXPERIMENTAL DATASET



Sparsity of the Hamiltonian Matrix

- Data (A[k]'s and B[k]'s)
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- Density increases
  → towards the center
- Sparsity increases
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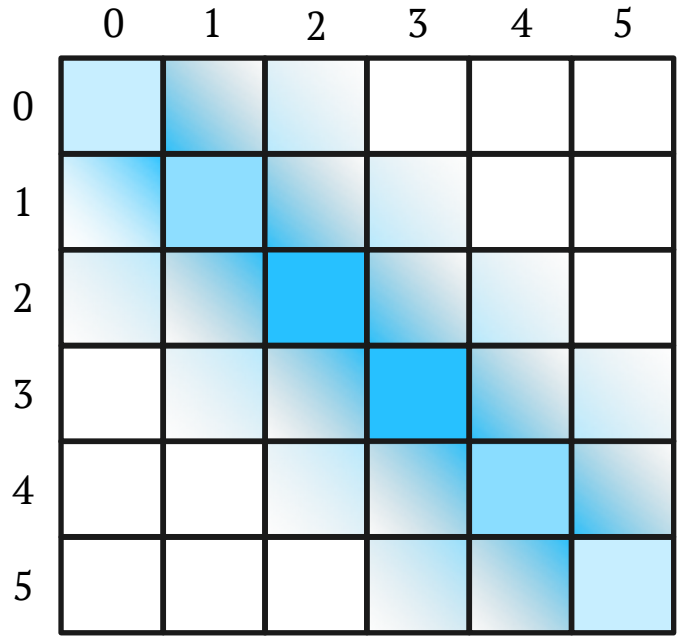
EXPERIMENTAL DATASET



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EXPERIMENTAL EVALUATION

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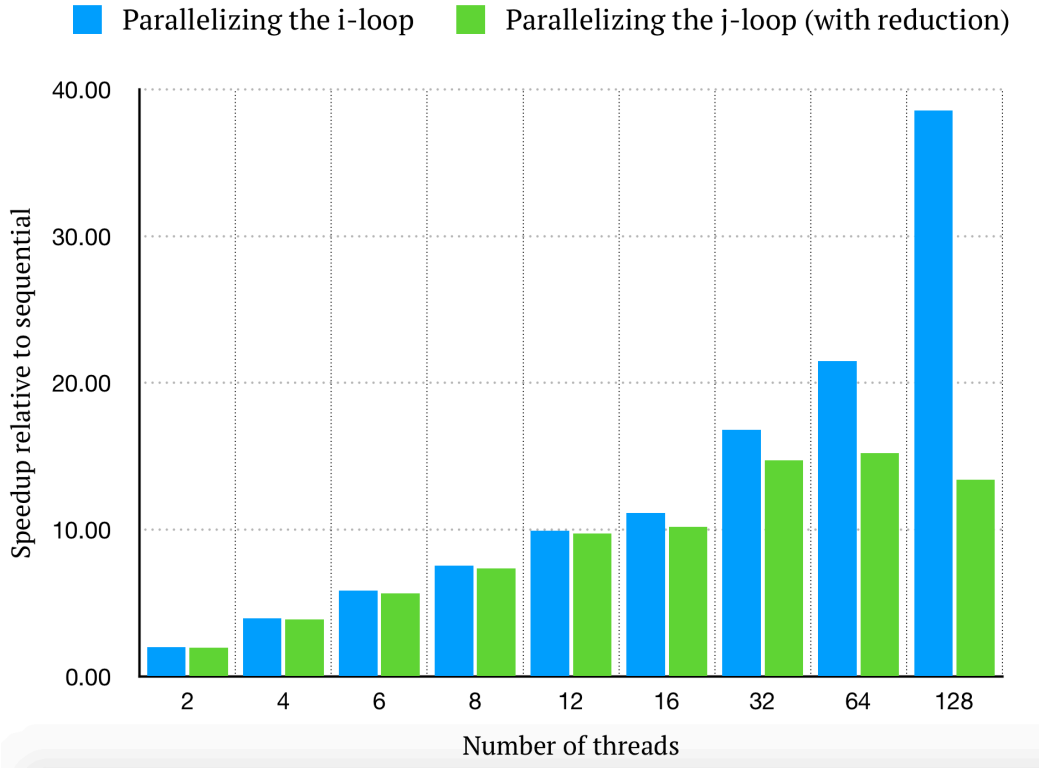
EXPERIMENTAL EVALUATION



- Each loop is parallelized separately

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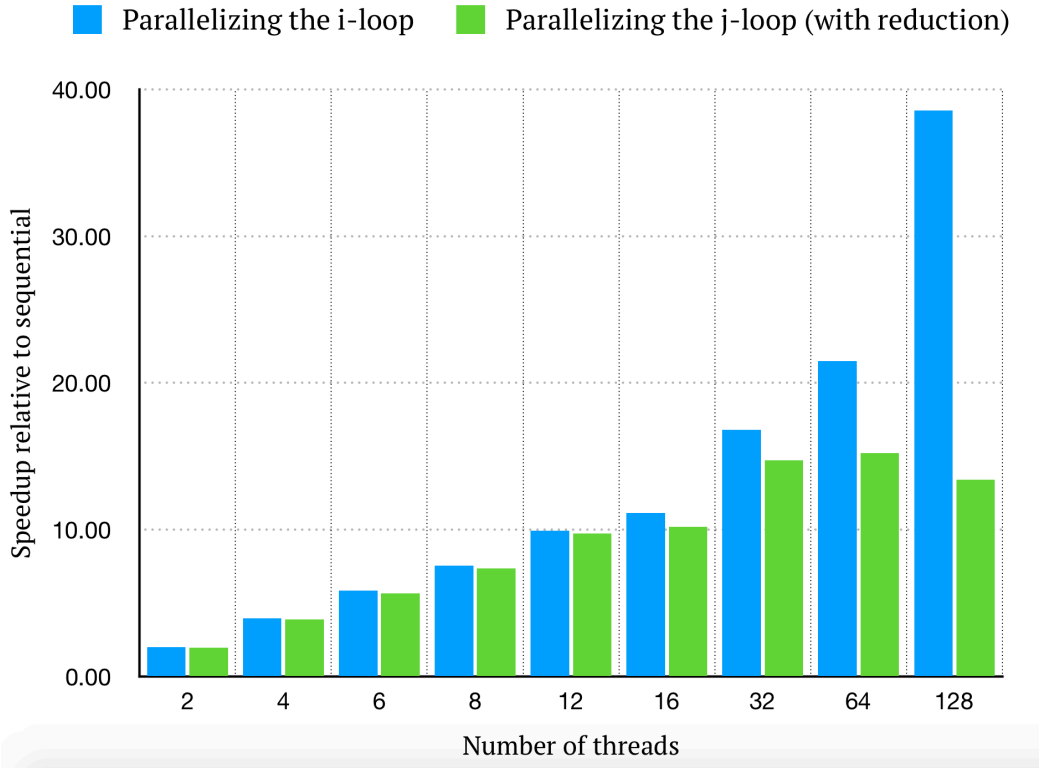
EXPERIMENTAL EVALUATION



- Each loop is parallelized separately
- Inner loop (jPatch) performs *vector reduction*

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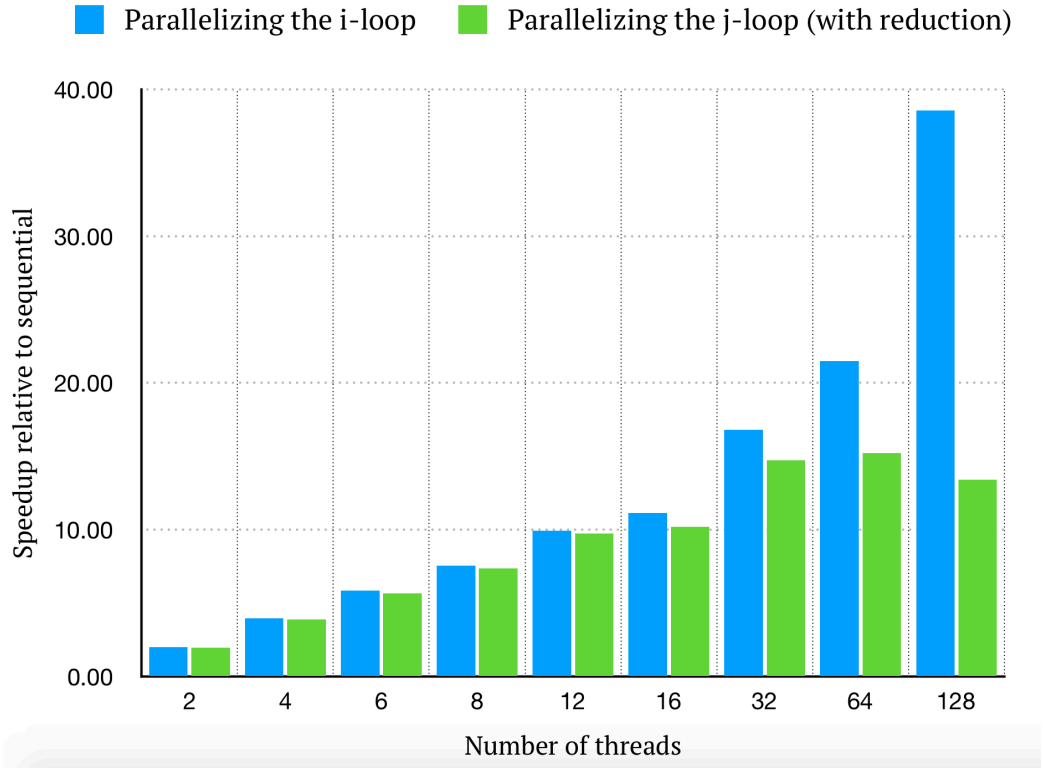
EXPERIMENTAL EVALUATION



- Each loop is parallelized separately
- Inner loop (jPatch) performs *vector reduction*
- Parallelizing k-loop → *threaded DGEMM (IBM ESSL)*

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EXPERIMENTAL EVALUATION: Projection

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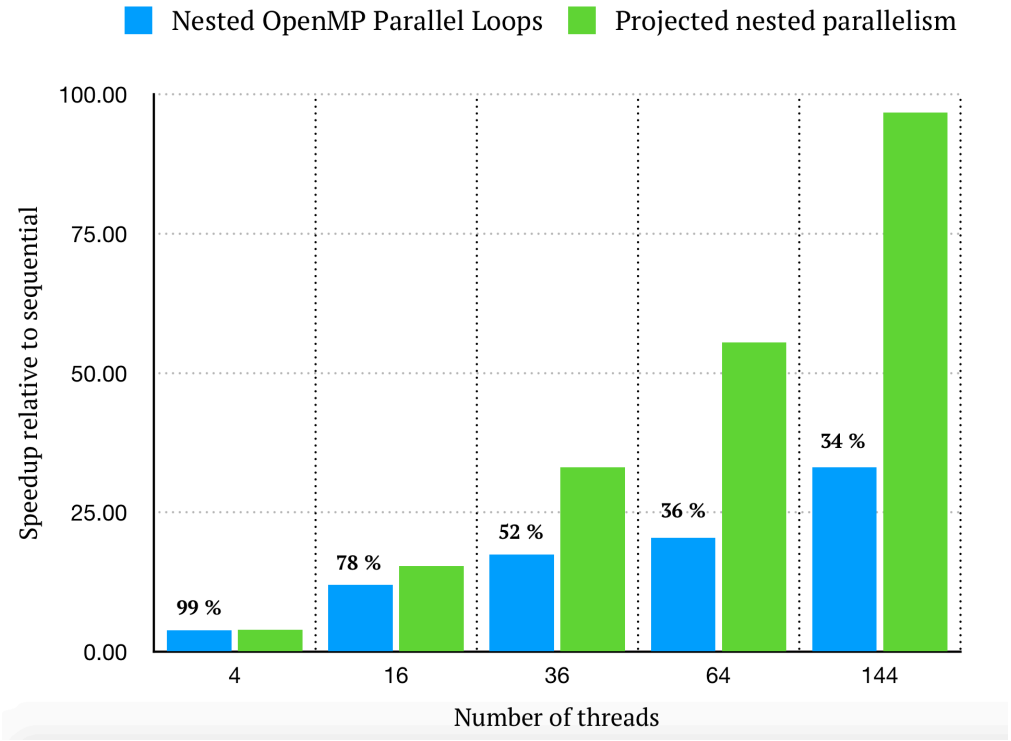
EXPERIMENTAL EVALUATION: Projection



- Nested parallel-for's
  → iPatch and jPatch
- Processor bindings
  - ✤ *Outer*: Spread
  - ✤ *Inner*: Close

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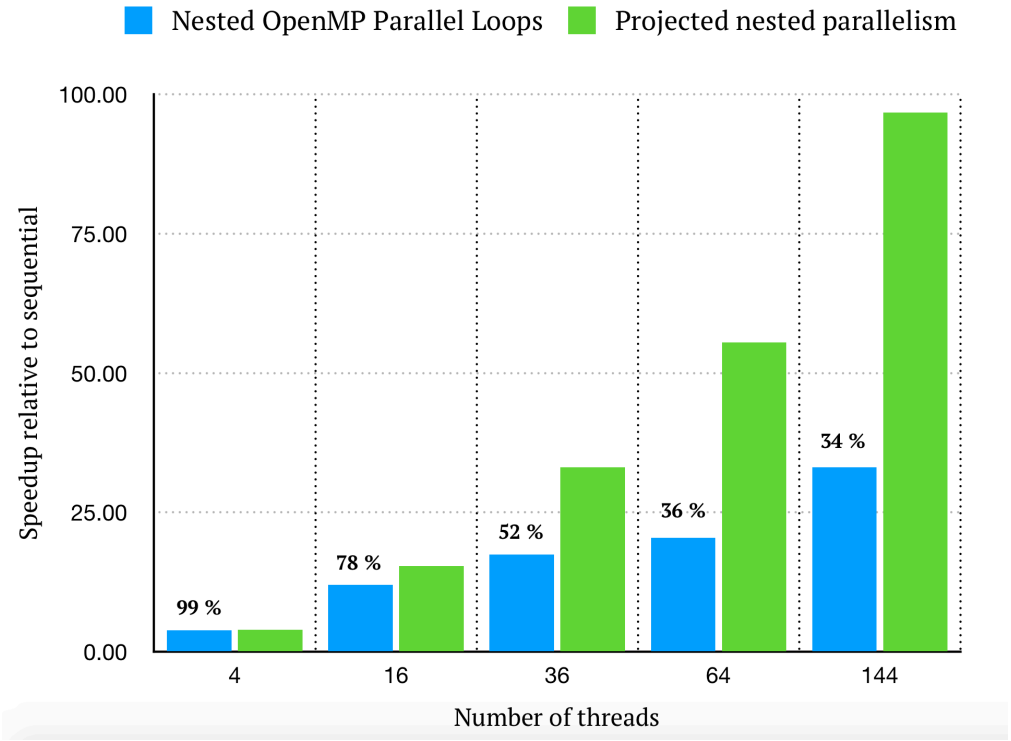
EXPERIMENTAL EVALUATION: Projection



- Nested parallel-for's
  → iPatch and jPatch
- Processor bindings
  - *Outer*: Spread
  - *Inner*: Close
- Dynamic scheduling

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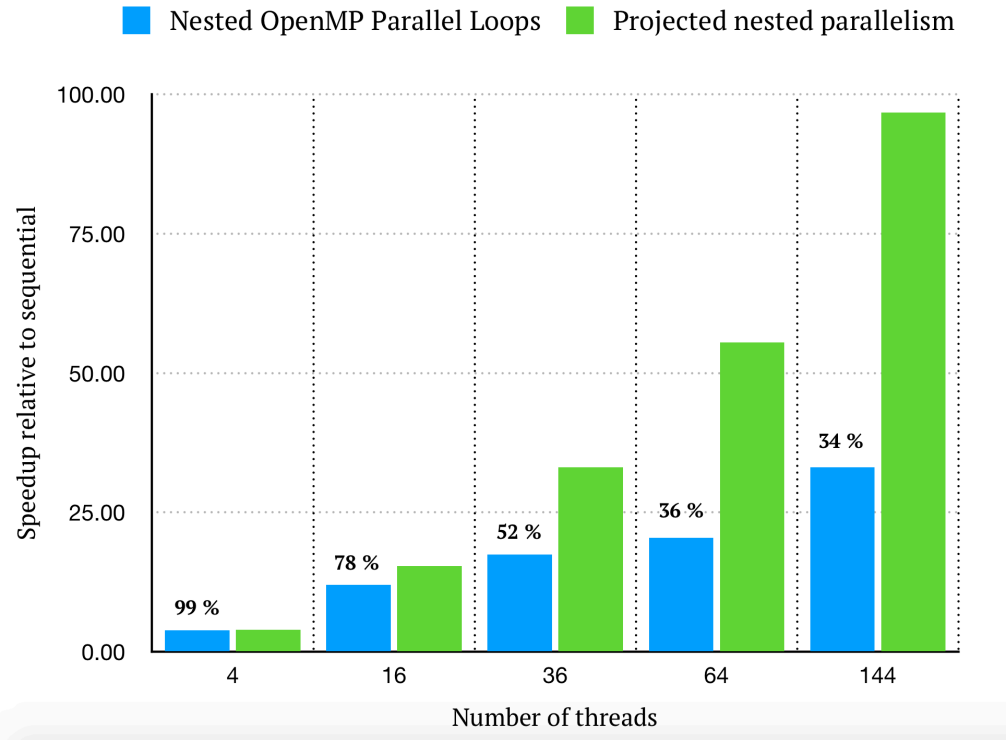
EXPERIMENTAL EVALUATION: Projection



- Nested parallel-for's
  → iPatch and jPatch
- Processor bindings
  - ✤ *Outer*: Spread
  - ✤ *Inner*: Close
- Dynamic scheduling
- Significant overhead
  →creating / destroying || regions

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USING OpenMP WITH LIBRARIES

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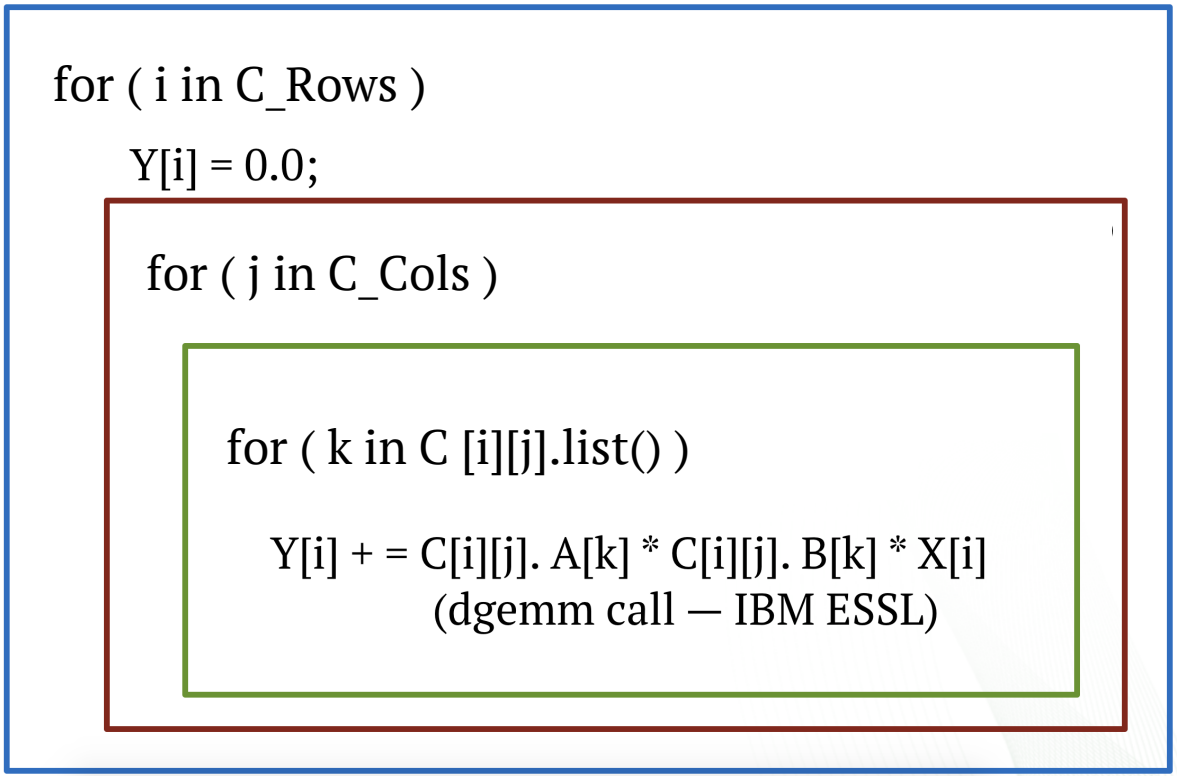
USING OpenMP WITH LIBRARIES



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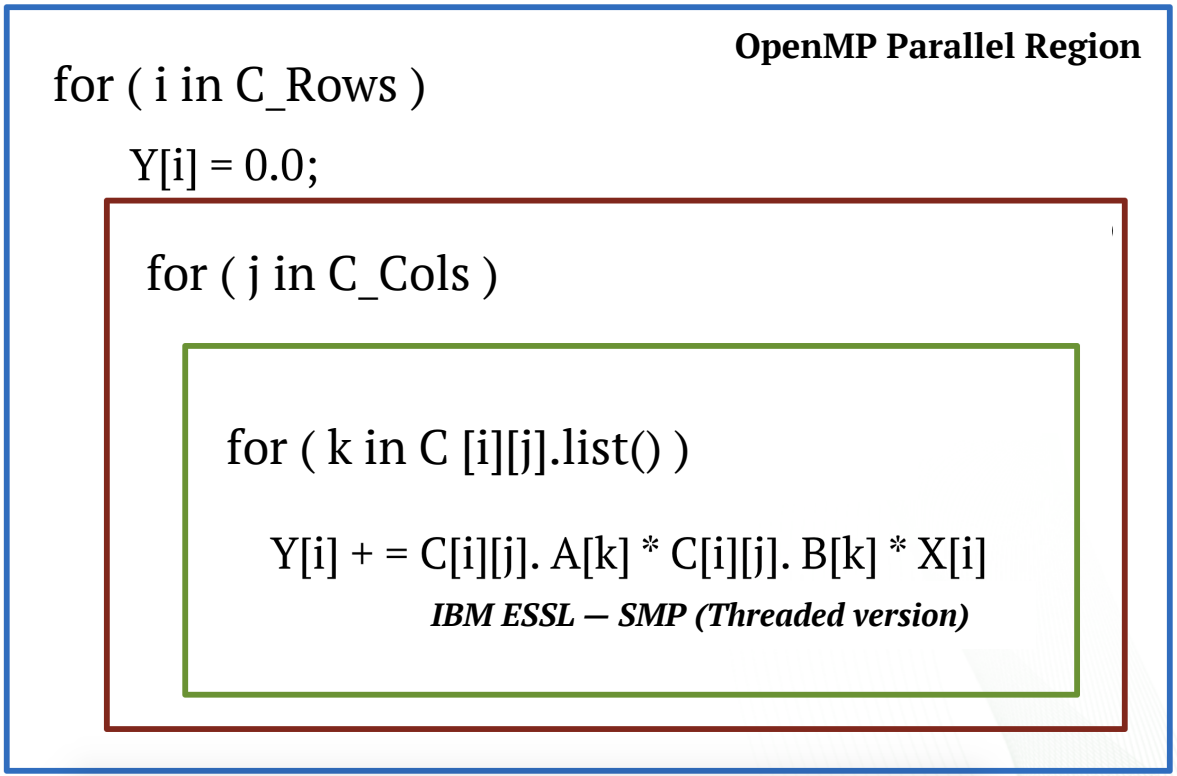
USING OpenMP WITH LIBRARIES



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OpenMP WITH LIBRARIES: Challenges

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- Current thread support:
  - OMP_SET_NUM_THREADS <num of threads>

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OpenMP WITH LIBRARIES: Challenges

- Current thread support:
  - OMP_SET_NUM_THREADS <num of threads>
- Lack of support for dynamic thread assignment
- Interoperability with external libraries:
  - Support to extract task-level/thread-level information
  - Within nested parallel region — undefined behavior

HABANERO C/C++ LIBRARY (HCLib)

HabaneroUPC++: a Compiler-free PGAS Library. *V. Kumar, Y. Zheng, V. Cavé, Z. Budimlić, and V. Sarkar, PGAS 2014*

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- HCLib — path to Exascale programming system
  → intra-node: resource management & scheduling
  → inter-node: integration w/ communication models (MPI, UPC++ or OpenSHMEM)

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FINISH ACCUMULATORS

Finish Accumulators: a Deterministic Reduction Construct for Dynamic Task Parallelism*. J. Shirako, V. Cavé, J. Zhao, & V. Sarkar. WODET 2013*

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FINISH ACCUMULATORS

- Construct for pre-defined / user-defined reductions

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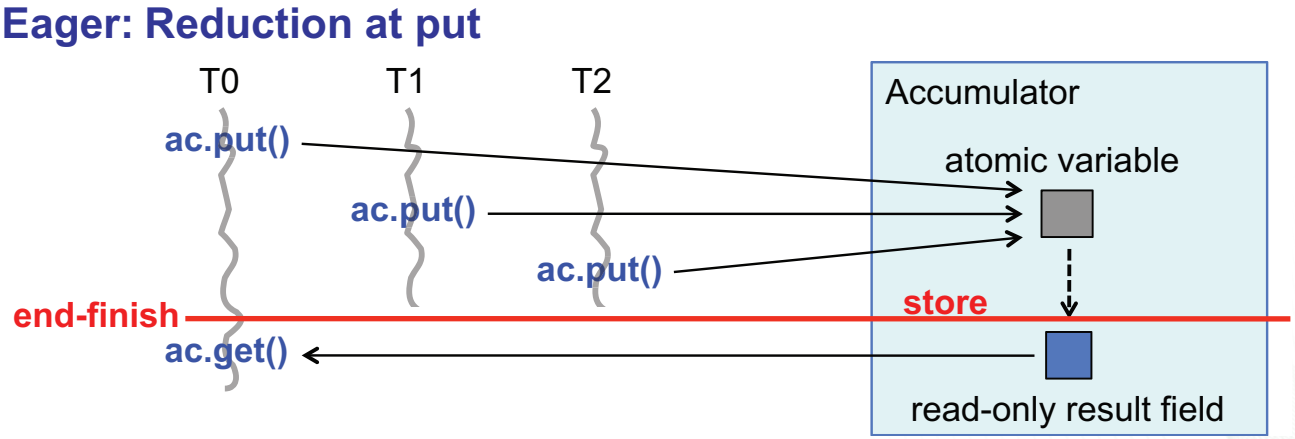
FINISH ACCUMULATORS

- Construct for pre-defined / user-defined reductions
- Large flexibility for implementations:
  - Eager reduction policy — portable implementation



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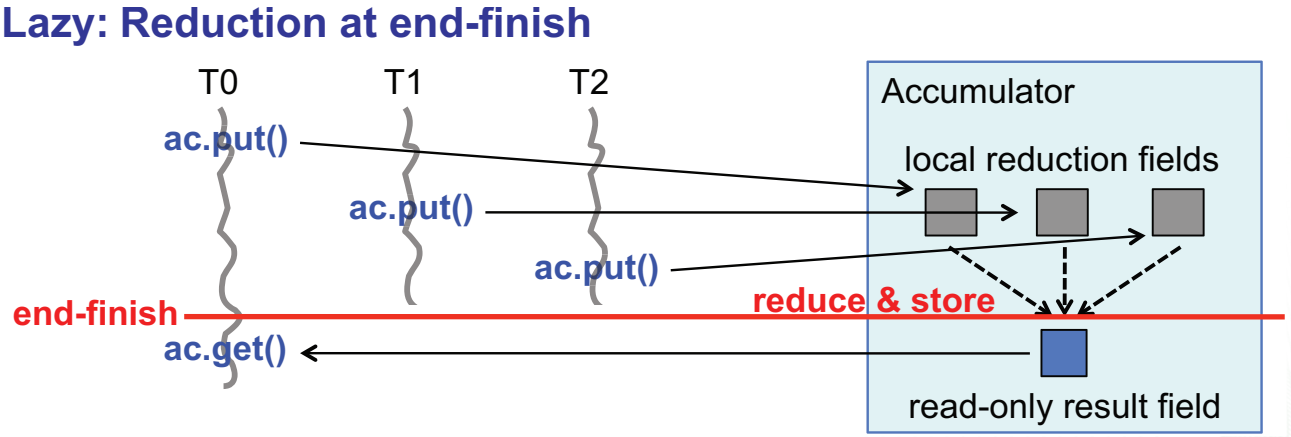
FINISH ACCUMULATORS

- Construct for pre-defined / user-defined reductions
- Large flexibility for implementations:
  - Lazy reduction policy — customized for target runtime task scheduler



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PSEUDO CODE: HABANERO C++

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```
1:  INPUT: C Matrix, X Vector
2:  OUTPUT: Y Vector
3:  Create array of Accumulators: accs <SUM> (npatches)
4:  Create OpenMP Parallel region
5:  Create OpenMP Single region
6:     for i in C_Rows do
7:        Create OpenMP Tasks
8:        for For: j in C_Cols do
9:           Create OpenMP Tasks
10:          YIJ[i]= 0.0
11:          for k in C[i,j].list() do
12:             Update YIJ: YIJ+ = C[i][j].A[k] ⊗ C[i][j].B[k] ∗ X[]

13:             Update Accumulator: accs[ipatch]->put(YIJ)
14:          end for
15:       end for
16:    end for
17: Retrieve Accumulator: accs[...]->get()
18: Return vector Y
```

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Parallel Region

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Parallel Region

User-defined Reduction

Candidates for Future OpenMP Support

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Candidates for Future OpenMP Support

- Support for Task-level reductions

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Candidates for Future OpenMP Support

- Support for Task-level reductions
- Task-inflation: dynamic resource allocation to tasks

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Candidates for Future OpenMP Support

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- Task-affinity: binding tasks to cores (extending tied-tasks)

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Candidates for Future OpenMP Support

- Support for Task-level reductions
- Task-inflation: dynamic resource allocation to tasks
- Task-affinity: binding tasks to cores (extending tied-tasks)
- Thread persistence in nested parallelism (Depth 3)

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Candidates for Future OpenMP Support

- Support for Task-level reductions
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- Task-affinity: binding tasks to cores (extending tied-tasks)
- Thread persistence in nested parallelism (Depth 3)
- Dynamic OpenMP Places
- Addressing debugging Challenges

ONGOING WORK: DMRG++

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ONGOING WORK: DMRG++

- OpenMP target directives — GPUs on Summit-dev

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ONGOING WORK: DMRG++

- OpenMP target directives — GPUs on Summit-dev
- OpenMP parallel regions — create abstractions on CPUs

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ONGOING WORK: DMRG++

- OpenMP target directives — GPUs on Summit-dev
- OpenMP parallel regions — create abstractions on CPUs
- Co-designing:
  - Using Kokkos (Sandia National Lab)
  - Using MAGMA — DGEMM batched kernel (Univ. of Tennessee, Knoxville)
  - Habanero C/C++ Accumulators (Georgia Tech. / Rice University)
    - Original implementation of finish accumulators was done in Habanero-Java

ACKNOWLEDGEMENTS

- We would like to thank our collaborators:
  - ORNL: Dr. Wael Elwasif (CSMD)
    Dr. E. D'Azevedo (CNMS)
    Dr. G. Alvarez (CNMS)
  - Rice University : Dr. Jun Shirako

- *This research used resources of the **O**ak Ridge **L**eadership **C**omputing **F**acility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.*

Bringing the DMRG++ Scientific Application to Exascale

...

Arghya “Ronnie” Chatterjee
Research Collaborator, CSMD, ORNL
Ph.D. Student, Georgia Tech
arghya@gatech.edu
September 18th, 2017