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On the Impact of Execution Models: A Case Study in Computational Chemistry

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U.S. DEPARTMENT OF ENERGY

Motivation

- Future extreme scale computing systems will be significantly power constrained
- Current petascale era software & hardware ecosystem:
  - Does it need to evolve?
  - Or be completely replaced?
- Many of these questions relate to the underlying *execution model*
- Execution model:
  - Conceptual framework describing orchestration of computation on parallel hardware & software resources
  - Connects application & algorithms to the underlying architecture & systems software
- How do we keep thousands of compute nodes busy?
  - Load balancing problem
  - Under different execution models

Execution Models

- Communicating Sequential Processes (CSP) as defined in *Hoare'78* [1]
  - Core execution model at the heart of MPI-1 *two-sided* communication
- Bulk Synchronous Processing (BSP) as defined in *Valiant'90* [2]
  - Core execution model for many PGAS environments
  - MPI-RMA, OpenSHMEM, ComEx, GASNet, Global Arrays, etc.
  - MapReduce-like systems
- Load balancing can be implemented under both CSP & BSP
- Shared memory execution models:
  - Considered under a single umbrella in this work (Shared Address Space, SAS)
  - *Key feature:* direct access to a common data store
- Study the **performance impact** of different combinations of **execution models** together with load balancing techniques
  - *Target:* modern multicore clusters

[1]Hoare, C. A. R. (1978). "Communicating sequential processes". Communications of the ACM 21 (8): 666–677
[2]Leslie G. Valiant, "A Bridging Model for Parallel Computation," Communications of the ACM, Volume 33 Issue 8, Aug. 1990

Self-Consistent Field Method (SCF)

- Case study using the Self-Consistent Field (SCF) method
  - Electronic structure calculation in computational chemistry
- Several important challenges for execution models:
  - Irregular work distribution
  - Dependent on structural properties of the input
  - Block-sparse data accesses
  - Tradeoffs between locality & load balance
- Lessons from SCF are broadly applicable
- Explored elements:
  - Execution models
    - CSP, BSP, Hierarchical CSP & BSP with SAS
  - Load balancing
    - Novel semi-matching formulation
    - Hypergraph partitionining
    - Work stealing

Outline

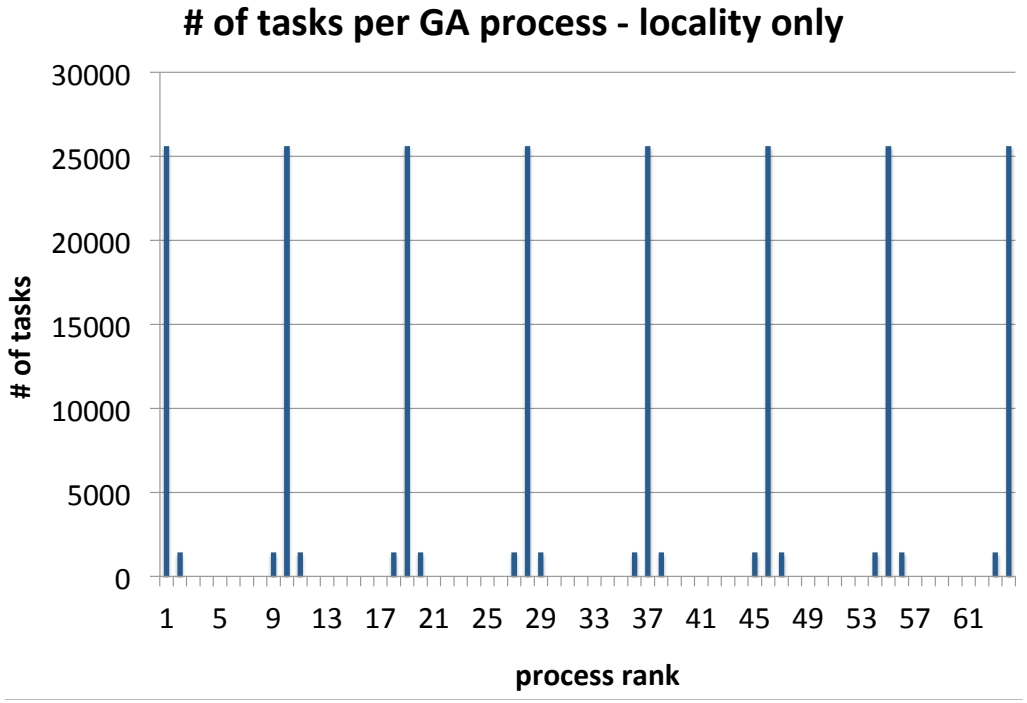
- Motivation
- ☞ Self-Consistent Field method
- Work Partitioners
- Execution Model Variants
  - CSP only: MPI
  - BSP only: Global Arrays
  - CSP + SAS, BSP + SAS
  - Work stealing
  - Work stealing + SAS
- Experimental Results
- Conclusions

Self-Consistent Field Method (SCF)

- Fundamental quantum chemistry calculation
  - Used to build the Hartree-Fock matrix
  - Building block for higher-order methods: Coupled Cluster, Density Functional Theory
- Dominant computational kernel in SCF:
  - Two-electron contribution to the Fock matrix
- Principal data structures: Schwarz, density & Fock matrices
  - 2D block distribution amongst processes on a cluster
- Computationally sparse n^4 calculation over n^2 data space
  - *n* is number of basis sets in input
  - Set of n^4 tasks over the data space
  - Each task: reads tiles from Schwarz & density matrices, accumulate results onto tiles of the Fock matrix
  - Most tasks ***do not*** contribute significantly to the result
  - < 1% of tasks do contribute, for large inputs

SCF method (cont.)

- Pure locality-based schedule:



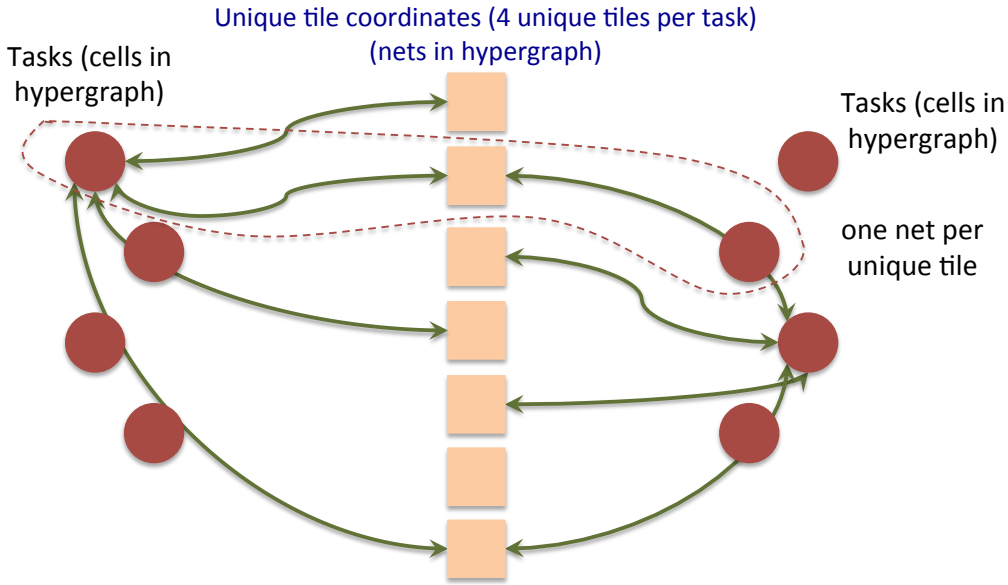
- Maximizing locality with respect to data tile access produces severe load imbalance
- Computational cost of each task varies (roughly proportional to number of non-zeroes in data tiles)

Work Partitioners

- Given these challenges from the SCF application
  - Explore best options for mapping it efficiently onto a cluster
- Deal with load imbalance first
- Task weights:
  - Each task accesses two distinct data tiles from Schwarz matrix
  - Examine all elements in the Cartesian product of the tiles
  - Weight corresponds to number of non-zeroes in the product
- Map tasks to processes on the cluster:
  - Such that the sum of the task weights per process is approximately equal
- Two static approaches:
  - Hypergraph partitioning
  - Weighted semi-matching over bipartite graph

Hypergraph Partitioning

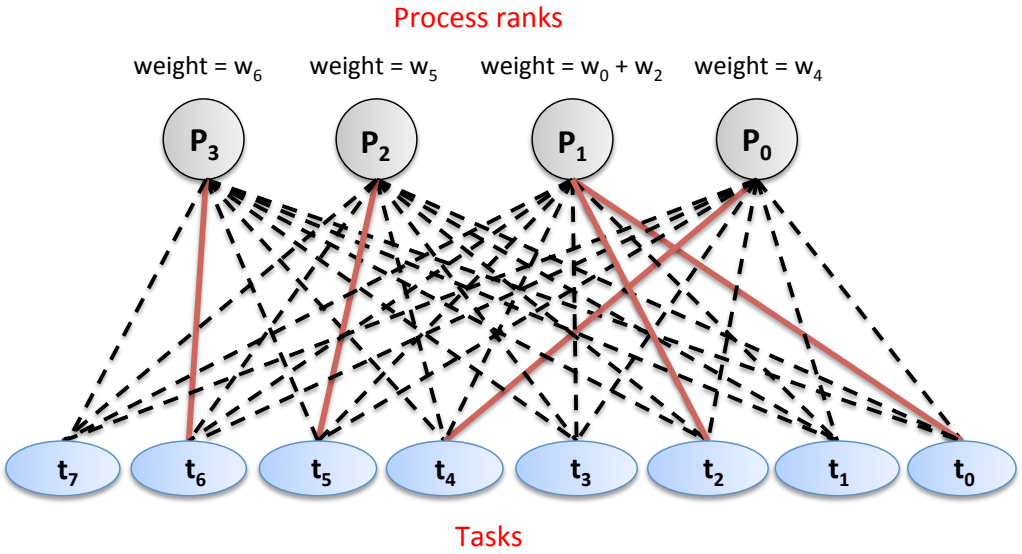
- PaToH hypergraph formulation:



- Each task accesses six different tiles (read 4 tiles of Schwarz & density, write 2 tiles of Fock)
  - However, only four unique sets of coordinates
- Multi-constraint formulation:
  - Equalize weight and number of tasks per process
  - Larger number of lighter tasks is not equivalent to a few heavy tasks

Semi-matching Partitioning

- Weighted semi-matching formulation:



- Bi-partite graph with tasks & processes
- Single-constraint formulation:
  - Equalize sum of task weights per process

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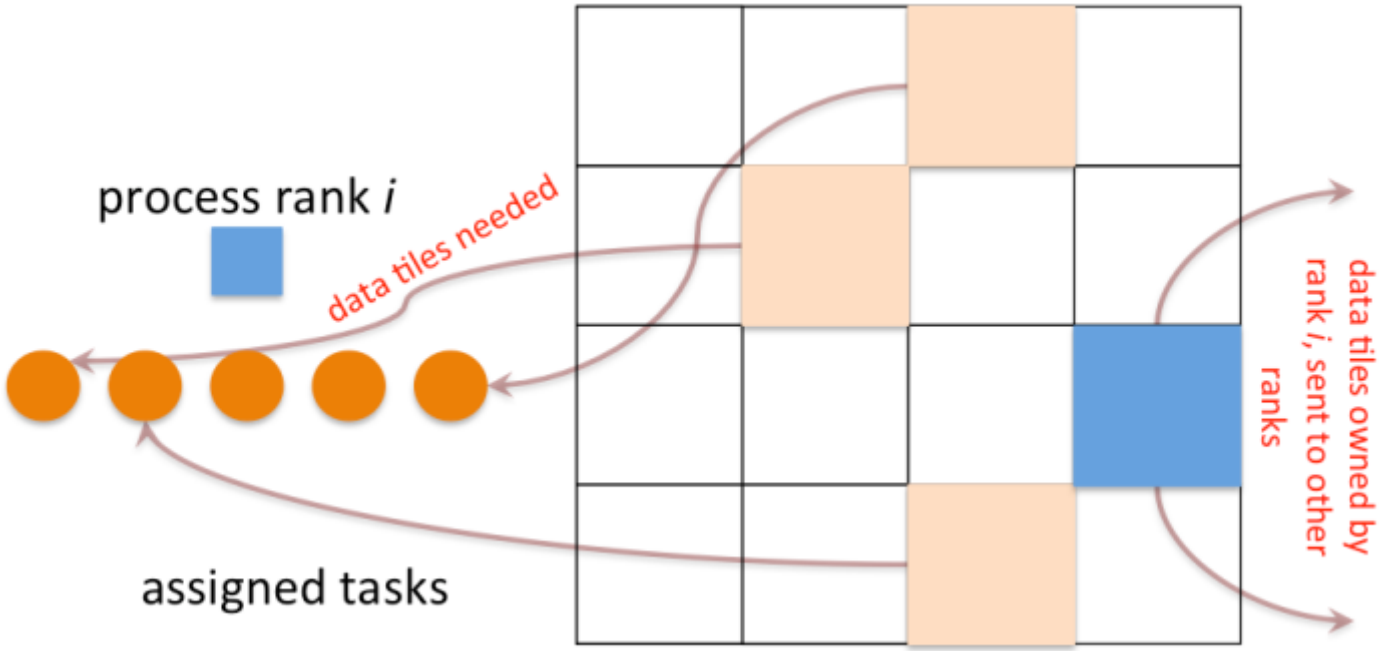
CSP only: MPI

- MPI is the de facto programming model for clusters
  - Core execution model is CSP
- Basic concept: need a two-sided communication schedule
  - What does each rank need to send and receive?
  - Use static work partitioners and 2D data decomposition to create schedule
- Computation & communication macro-steps



BSP Only: Global Arrays

- Main difference with CSP:
  - One sided communication enables “position-independent” representation of tasks
  - Can execute on any process since data accesses are specified in absolute/ global terms
  - No need to build communication schedule
- Key concept to enable *work stealing* across processes

CSP + SAS, BSP + SAS

- Couple CSP & BSP implementations with SAS execution model
  - As realized in the OpenMP programming model
- Two-level load balancing:
  - Inter-node using CSP or BSP
  - Intra-node load balancing across threads
- CSP + SAS
  - Implemented on top of the hypergraph partitioning approach
  - Master thread performs communication
  - All threads access communicated data from shared buffers
  - Synchronization to prepare write-back (Fock) buffer
- BSP + SAS
  - Communication is done inline by all threads (synchronized by locks)
  - Not much overhead due to large computational load

Work Stealing

- Distributed work stealing across processes on a cluster
- Dynamic adaptivity in the presence of load imbalance
- Two variants:
  - Per-core work stealing
  - Work stealing + SAS
- Both use one-sided communication to access task queues on remote compute nodes
- Persistence-based approach:
  - Initial seeding of task queues based on pure locality approach
  - Keep track of which actual tasks were executed by the process to seed queues for following iterations
- Work stealing + SAS
  - Steal tasks at a coarser granularity
  - Execute them using OpenMP work sharing constructs

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Experimental Results

- Ran on up to 2048 cores of PNNL's Olympus cluster
  - Dual-socket AMD Interlagos processors (16 cores per sockets), 64GB RAM per node
  - Use every other core for runs due to shared floating point units (Bulldozer)
  - QDR Infiniband interconnect
- 16 processes per node or 16 threads w/single process for OpenMP runs
- Two input decks:
  - 256 atoms of Beryllium (Be), 356 atoms of Be
- Work stealing granularities:
  - Process-based: 1 task
  - SAS-based: 1024 tasks
    - To reduce steal overhead and keep threads busy

	BSP			CSP
Intra-node/Inter-node	**WS**	**SM**	**HG**	**HG**
Process-centric	•	•	•	•
OpenMP guided (MT)	•		•	•

Table I: SCF two-electron kernel versions where WS is Work Stealing, SM is Semi-Matching, and HG is Hypergraph.

Experimental Results (cont.)

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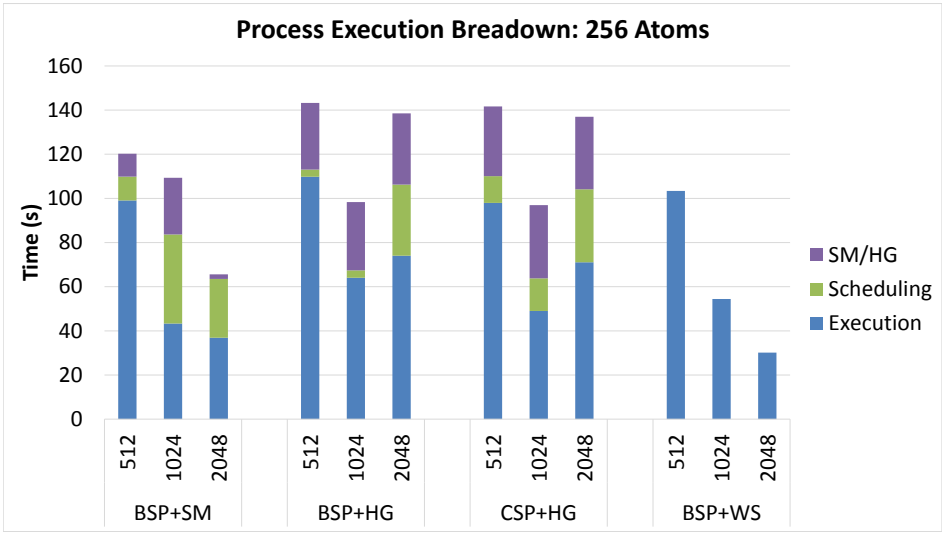

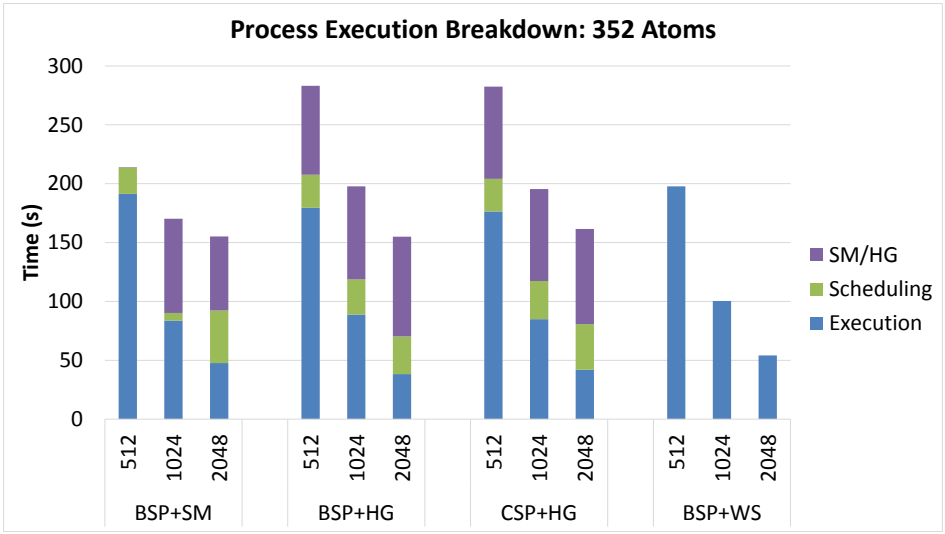

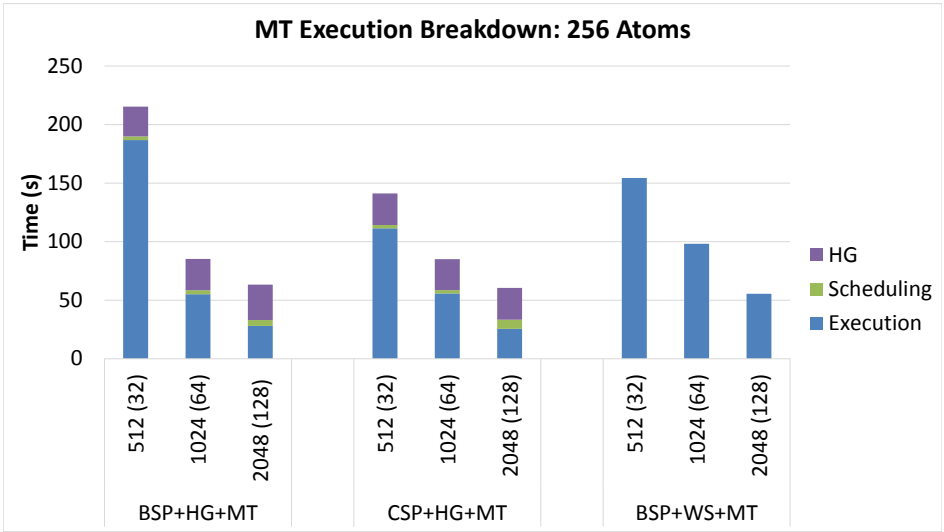

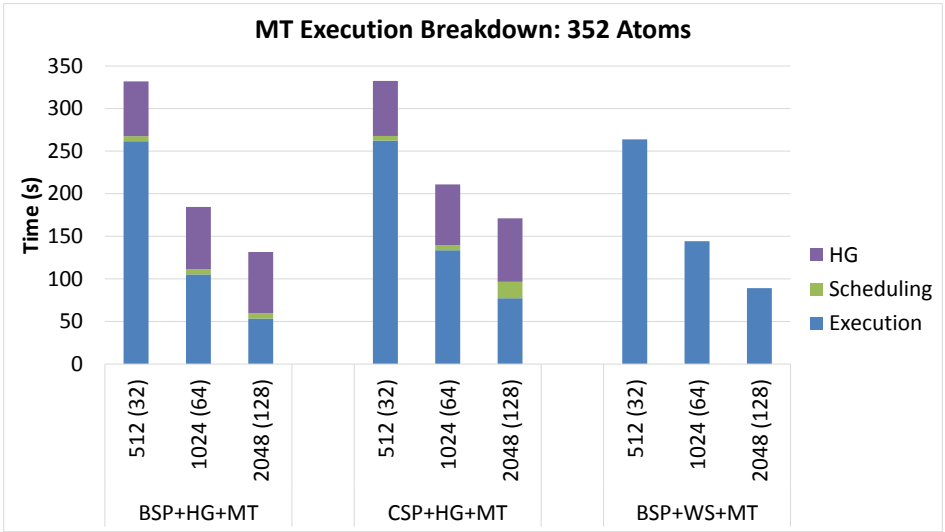

Analysis & Conclusions

- Studied a large number of execution model variants for SCF benchmark
  - Different communication primitives, task scheduling, concurrency
- Statically scheduled versions can match and sometimes exceed work stealing-based version
- Semi-matching executes fast for a static partitioning
  - Can produce lower quality partitionings
- Hypergraph is better but very slow
- System wide dynamic adaptation
  - Requires the right kind of communication & concurrency primitives
- Execution model design choices & assumptions can limit critical optimizations
  - Such as global, dynamic load balancing
- Future work: consider other execution & programming models, improve accuracy of static partitioning formulations