2.5D algorithms: from hardware to theory and back

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Outline

A survey of supercomputers

2.5D algorithms
   2.5D matrix multiplication
   2.5D LU factorization

Tensor contractions
   A tensor contraction library implementation

Hardware trends and programming models
Ranger

- TACC, Sun, 2008
- Commodity procs / commodity network
- 16 Opterons/node
  - 147.2 GF/node
Ranger, Cray XT4

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Cray XT4 (Jaguar)

- ORNL, Cray, 2009
- Commodity procs / custom network
- 4 Opterons per node
  - 32.8 GF/node
Ranger, Cray XT4, BG/P

**Ranger**
- TACC, Sun, 2008
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**Cray XT4 (Jaguar)**
- ORNL, Cray, 2009
- Commodity procs / custom network
- 4 Opterons per node
  - 32.8 GF/node

**BG/P (Intrepid)**
- ANL, IBM, 2007
- Custom procs / custom network
- PowerPC 450 (4 cores/node)
  - 13.4 GF/node
Intra-node memory subsystems

<table>
<thead>
<tr>
<th>Supercomputer</th>
<th>Number of Cores</th>
<th>Memory per Node</th>
<th>Memory per Core</th>
<th>L1 Cache</th>
<th>L2 Cache</th>
<th>L3 Cache</th>
<th>Node Bandwidth</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ranger</td>
<td>16</td>
<td>32 GB/node</td>
<td>2 GB/core</td>
<td>128 KB</td>
<td>512 KB</td>
<td>2 MB</td>
<td>21.3 MB/sec</td>
</tr>
<tr>
<td>Cray XT4 (Jaguar)</td>
<td>4</td>
<td>8 GB/node</td>
<td>2 GB/core</td>
<td>128 KB</td>
<td>512 KB</td>
<td>2 MB</td>
<td>10.6 MB/sec</td>
</tr>
<tr>
<td>BG/P (Intrepid)</td>
<td>4</td>
<td>2 GB/node</td>
<td>0.5 GB/core</td>
<td>64 KB</td>
<td>2 KB</td>
<td>8 MB</td>
<td>13.4 MB/sec</td>
</tr>
</tbody>
</table>
Roofline model

![Roofline Model Diagram](image)

- **Ranger**
- **XT4**
- **Blue Gene/P**

- DNANS: Red line
- NAMD: Green line
- MILC: Blue line

**Y-axis:** Gflop/s

**X-axis:** flop per byte
## Network architecture

<table>
<thead>
<tr>
<th>Network</th>
<th>Nodes</th>
<th>Interconnect</th>
<th>Topology</th>
<th>Link Bandwidth</th>
<th>Scheduler</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ranger</strong></td>
<td>3,936</td>
<td>Infiniband</td>
<td>full-CLOS (tree/switched)</td>
<td>1 GB/sec</td>
<td>no topology aware scheduler</td>
</tr>
<tr>
<td><strong>Cray XT4 (Jaguar)</strong></td>
<td>7,832</td>
<td>Seastar</td>
<td>3D torus (not topology-aware)</td>
<td>3.8 GB/sec</td>
<td>no topology aware scheduler</td>
</tr>
<tr>
<td><strong>BG/P</strong></td>
<td>40,960</td>
<td>Custom</td>
<td>3D torus</td>
<td>.425 GB/sec</td>
<td>topology aware scheduler</td>
</tr>
</tbody>
</table>
Point-to-point communication bandwidth

Measured Bandwidth: Without Contention (8K cores)

Measured Bandwidth: With Contention (8K cores)
Collective communication (broadcast)

1 MB multicast on BG/P, Cray XT5, and Cray XE6
Rectangular broadcasts

2D 4X4 Torus

Spanning tree 1

Spanning tree 2

Spanning tree 3

Spanning tree 4

All 4 trees combined
Strong scaling matrix multiplication

Matrix multiplication on BG/P (n=65,536)

Percentage of machine peak

#nodes

2.5D MM

2D MM

2.5D matrix multiplication

教育教学

2.5D algorithms

Tensor contractions

Hardware trends and programming models
Blocking matrix multiplication
2D matrix multiplication

[Cannon 69], [Van De Geijn and Watts 97]
3D matrix multiplication

[Agarwal et al 95], [Aggarwal, Chandra, and Snir 90], [Bernsten 89]
2.5D matrix multiplication

A
B
A
B
A
B
A B
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
CPU CPU CPU CPU
32 CPUs (4x4x2)

2 copies of matrices
2.5D strong scaling

\[ n = \text{dimension}, \quad p = \#\text{processors}, \quad c = \#\text{copies of data} \]

- must satisfy \( 1 \leq c \leq p^{1/3} \)
- special case: \( c = 1 \) yields 2D algorithm
- special case: \( c = p^{1/3} \) yields 3D algorithm

\[
\text{cost}(2.5D \text{ MM}(p, c)) = O(n^3/p) \text{ flops} \\
+ O(n^2/\sqrt{c \cdot p}) \text{ words moved} \\
+ O(\sqrt{p/c^3}) \text{ messages}^* 
\]

*ignoring log(p) factors
2.5D strong scaling

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\[
\begin{align*}
\text{cost}(2D \ MM(p)) &= O(n^3/p) \text{ flops} \\
&\quad + O(n^2/\sqrt{p}) \text{ words moved} \\
&\quad + O(\sqrt{p}) \text{ messages}^* \\
&= \text{cost}(2.5D \ MM(p, 1))
\end{align*}
\]

*ignoring \( \log(p) \) factors
2.5D strong scaling

\[ n = \text{dimension}, \quad p = \#\text{processors}, \quad c = \#\text{copies of data} \]

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- special case: \( c = 1 \) yields 2D algorithm
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\[
\text{cost}(2.5D \text{ MM}(c \cdot p, c)) = O\left(\frac{n^3}{c \cdot p}\right) \text{ flops} \\
+ O\left(\frac{n^2}{c \cdot \sqrt{p}}\right) \text{ words moved} \\
+ O\left(\frac{\sqrt{p}}{c}\right) \text{ messages} \\
= \text{cost}(2D \text{ MM}(p))\frac{1}{c}
\]

perfect strong scaling
2.5D MM on 65,536 cores

Matrix multiplication on 16,384 nodes of BG/P

- 2.5D MM: 12X faster
- 2D MM: 2.7X faster

Using c=16 matrix copies

Percentage of machine peak

Node count: 8192, 131072
Cost breakdown of MM on 65,536 cores

Matrix multiplication on 16,384 nodes of BG/P

- 95% reduction in comm

Execution time normalized by 2D
2.5D LU strong scaling (without pivoting)
2D blocked LU factorization
2D blocked LU factorization

$U_{00}$

$L_{00}$

$U_{00}$

$L_{00}$

$U_{00}$

$L_{00}$
2D blocked LU factorization
2D blocked LU factorization

\[ S = A - LU \]
2D block-cyclic decomposition
2D block-cyclic LU factorization
2D block-cyclic LU factorization
2D block-cyclic LU factorization

\[ S = A - LU \]
2.5D LU factorization
2.5D LU factorization

(A)

(B)

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2.5D LU factorization
2.5D LU factorization

Look at how this update is distributed.

What does it remind you of?
2.5D LU factorization

Look at how this update is distributed.

Same 3D update in multiplication
Communication-avoiding pivoting

Partial pivoting is not communication-optimal on a blocked matrix

- require message/synchronization for each column
- $O(n)$ messages required

Tournament pivoting or Communication-Avoiding (CA) pivoting

- performs a tournament to determine best pivot row candidates
- blocked CA-pivoting algorithm is communication-optimal
Strong scaling of 2.5D LU with tournament pivoting

LU with tournament pivoting on BG/P (n=65,536)

- Ideal scaling
- 2.5D LU
- 2D LU
- ScaLAPACK PDGETRF

Percentage of machine peak

#nodes
2.5D LU factorization with tournament pivoting

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2.5D LU factorization with tournament pivoting
2.5D LU factorization with tournament pivoting
2.5D LU factorization with tournament pivoting
2.5D LU on 65,536 cores

LU on 16,384 nodes of BG/P (n=131,072)

- NO-pivot 2D
- NO-pivot 2.5D
- CA-pivot 2D
- CA-pivot 2.5D

Time (sec)
Towards higher dimensions: tensor contractions

- Tensor contractions are a generalization of matrix multiplication (e.g.)

\[ C_{cdef} = \sum_a \sum_b A_{cdab} \cdot B_{abef} \]

- Tensor contractions can be reduced to regular MM

\[ C_{(cd)(ef)} = \sum_a \sum_b A_{(cd)(ab)} \cdot B_{(ab)(ef)} \]

\[ C_{ij} = \sum_k A_{ik} \cdot B_{kj} \]

- Would like to support tensors up to dimensions 8-12
BLAS 4

Can we save communication by dealing with tensors explicitly rather than reducing to MM?

- Cannot improve flops/byte asymptotically over MM
- But *can* exploit higher-dimensional structure in tensors
- Higher-dimensional representation contains 'more information'
Symmetric tensor contractions

- A fully symmetric tensor of dimension $d$ requires only $n^d/d!$ storage.
- Memory reduction also translates to communication reduction via 2.5D.
- Blocked or block-cyclic virtual processor decompositions give irregular or imbalanced virtual grids.
Solving the symmetry problem

- A **cyclic decomposition** allows balanced and regular blocking of symmetric tensors
- If the cyclic-phase is the same in each symmetric dimension, each sub-tensor retains the symmetry of the whole tensor
A generalized cyclic layout

- In order to retain partial symmetry, all symmetric dimensions of a tensor must be mapped with the same cyclic phase.
- The contracted dimensions of $A$ and $B$ must be mapped with the same phase.
- And yet the virtual mapping, needs to be mapped to a physical topology, which can be any shape.
Virtual processor grid dimensions

- Our virtual cyclic topology is somewhat restrictive and the physical topology is very restricted
- Virtual processor grid dimensions serve as a new level of indirection
  - If a tensor dimension must have a certain cyclic phase, adjust physical mapping by creating a virtual processor dimension
  - Allows physical processor grid to be ‘stretchable’
Constructing a virtual processor grid for MM

Matrix multiply on 2x3 processor grid. Red lines represent virtualized part of processor grid. Elements assigned to blocks by cyclic phase.
Unfolding the processor grid

- Higher-dimensional fully-symmetric tensors can be mapped onto a lower-dimensional processor grid via creation of new virtual dimensions.
- Lower-dimensional tensors can be mapped onto a higher-dimensional processor grid via by unfolding (serializing) pairs of processor dimensions.
- However, when possible, replication is better than unfolding, since unfolded processor grids can lead to an unbalanced mapping.
A basic parallel algorithm for symmetric tensor contractions

1. Arrange processor grid in any $k$-ary $n$-cube shape
2. Define and input (via unfold & virt) both $A$ and $B$ into cyclic layouts
3. Remap (via unfold & virt) both $A$ and $B$ cyclically along the dimensions being contracted
4. Remap (via unfold & virt) the remaining dimensions of $A$ and $B$ cyclically
5. For each tensor dimension contracted over, recursively multiply the tensors along the mapping
   - Each contraction dimension is represented with a nested call to a local multiply or a parallel algorithm (e.g. Cannon)
Tensor library structure

The library supports arbitrary-dimensional parallel tensor contractions with any symmetries on n-cuboid processor torus partitions

1. Load and map tensor data by (global rank, value) pairs
2. Once a contraction is defined, remap participating tensors
3. Distribute or reshuffle tensor data/pairs
4. Construct contraction algorithm with recursive function/args pointers
5. Contract the sub-tensors with a user-defined sequential contract function
6. Output (global rank, value) pairs on request
Current tensor library status

- Dense and symmetric remapping/repadding/contractions implemented
- Currently tuning an efficient symmetric transpose kernel
- Can perform automatic mapping with physical and virtual dimensions, but cannot unfold processor dimensions yet
- Complete library interface implemented, including basic auxiliary functions (e.g. map/reduce, sum, etc.)
Next implementation steps

- Currently integrating library with a SCF method code that uses dense contractions
- Automatic unfolding of processor dimensions
- Implement mapping by replication to enable 2.5D algorithms
- Integrate with a sequential symmetric contraction library
Very preliminary contraction library results

Contracts tensors of size 64x64x256x256 in 1 second on 2K nodes

Strong scaling of dense contraction on BG/P 64x64x256x256

- no rephase
- rephase every contraction
- repad every contraction

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Potential benefit of unfolding

Unfolding smallest two BG/P torus dimensions improves performance.
A new generation of machines: BlueWaters

BlueWaters

- NCSA, IBM, (scheduled 2011)
- Power 7 processors
- Hierarchical network
- 10 PF installation
  Cancelled
A new generation of machines: Cray XE6

Cray XE6 (Hopper)

- NERSC, Cray, 2011
- 2 twelve-core AMD MagnyCours/node
- 6,384 nodes
- 2.9/5.8 GB/sec per link
- 3D Torus (Gemini)
A new generation of machines: Cray XE6, K computer

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**K computer**
- RIKEN, Japan, Fujitsu, 2011
- 68,544 2 GHz 8-core SPARC64 nodes
- 5 GB/sec per link
- **6D Torus** (Tofu)
### Cray XE6, K computer, BG/Q

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**BG/Q**
- IBM, 2012
- 16 cores (205 GF/s)
- 98,304 nodes (20 PF)
- 2 GB/sec per link
- **5D Torus**
More supercomputers...

- Titan (ORNL) 2012?
  - Gemini 3D torus interconnect
  - GPUs
  - 20 PF

- Tianhe 1 (China) 2010
  - GPU accelerated
  - fat-tree network
  - 2.5 PF

- Stampede (TACC) 2011?
  - Intel MIC (Many Integrated Core)
  - Infiniband cluster
  - 10 PF
Supercomputing in higher-dimensionality

- Higher-dimensional interconnects
  - 3D Torus networks wide-spread
  - 5D/6D next-gen machines (BG/Q, K-computer)
  - higher bisection bandwidth and scalability

- Higher-dimensional algorithms
  - avoid communication with higher-dimensional blocking
    - 2.5D algorithms
  - avoid communication by exploiting higher-dimensional structure
    - tensor symmetry
    - conjecture: tensor sparsity
Current HPC programming models

- PGAS models are 1D
  - flat memory
  - weak notion of spacial locality

- Hierarchical models
  - cache-oblivious algorithms, recursive algorithms
  - express hierarchical spacial locality
  - natural for tree networks, not torus networks
A higher-dimensional programming model

- Decompose problem dimensionally
  - communicate along dimensions
  - maintain dimensionality of original problem
- Efficient dimensional communication primitives
  - reductions/broadcasts (rectangular algorithms)
  - replication (2.5D algorithms)
  - reconfiguration/transposition (convert tensor mappings)
  - virtualization (map to architecture)
- Advantages
  - use higher-dimensional blocking to reduce communication
  - use higher-dimensional structure to conserve memory/communication
  - maps communication directly to torus networks to reduce contention
Backup slides
Conclusion

Our contributions:

- 2.5D mapping of matrix multiplication
  - Optimal according to lower bounds in [Irony, Tiskin, Toledo 04] and [Aggarwal, Chandra, and Snir 90]
- A new latency lower bound for LU
- Communication-optimal 2.5D LU
  - Bandwidth-optimal according to general lower bound [Ballard, Demmel, Holtz, Schwartz 10]
  - Latency-optimal according to new lower bound

Open questions:

- 2.5D Householder QR

Reflections:

- Replication allows better strong scaling
- Topology-aware mapping cuts communication costs
A new latency lower bound for LU

LU with $O(\sqrt{P/c^3})$ messages?

- For block size $n/d$ LU does
  - $\Omega(n^3/d^2)$ flops
  - $\Omega(n^2/d)$ words
  - $\Omega(d)$ msgs
- Now pick $d$ (=latency cost)
  - $d = \Omega(\sqrt{P})$ to minimize flops
  - $d = \Omega(\sqrt{c \cdot P})$ to minimize words

No dice. Lets minimize bandwidth.
Performance of multicast (BG/P vs Cray)

1 MB multicast on BG/P, Cray XT5, and Cray XE6

Bandwidth (MB/sec) vs #nodes for different systems:
- BG/P
- XE6
- XT5
Why the performance discrepancy in multicasts?

- Cray machines use **binomial multicasts**
  - Form spanning tree from a list of nodes
  - Route copies of message down each branch
  - Network contention degrades utilization on a 3D torus

- BG/P uses **rectangular multicasts**
  - Require network topology to be a $k$-ary $n$-cube
  - Form $2n$ edge-disjoint spanning trees
    - Route in different dimensional order
    - Use both directions of bidirectional network
Model verification: one dimension

DCMF Broadcast on a ring of 8 nodes of BG/P

Bandwidth (MB/sec) vs. msg size (KB)

- $t_{\text{rect}}$ model
- DCMF rectangle dput
- $t_{\text{bnm}}$ model
- DCMF binomial

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2.5D algorithms
Model verification: two dimensions

![Graph showing bandwidth vs. message size for DCMF Broadcast on 64 (8x8) nodes of BG/P. The graph compares models t_{rect} and t_{bnm} with DCMF rectangle dput and DCMF binomial.]
Model verification: three dimensions

DCMF Broadcast on 512 (8x8x8) nodes of BG/P

Bandwidth (MB/sec) vs. msg size (KB)

- $t_{\text{rect}}$ model
- Faraj et al data
- DCMF rectangle dput
- $t_{\text{bnm}}$ model
- DCMF binomial

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Another look at that first plot

Just how much better are rectangular algorithms on $P = 4096$ nodes?

- Binomial collectives on XE6
  - $1/30$th of link bandwidth
- Rectangular collectives on BG/P
  - $4.3X$ the link bandwidth
- Over $120X$ improvement in efficiency!

How can we apply this?
Decoupling memory usage and topology-awareness

- 2.5D algorithms couple memory usage and virtual topology
  - $c$ copies of a matrix implies $c$ processor layers
- Instead, we can nest 2D and/or 2.5D algorithms
- Higher-dimensional algorithms allow smarter topology aware mapping
4D SUMMA-Cannon

How do we map to a 3D partition without using more memory

- SUMMA (bcast-based) on 2D layers
- Cannon (send-based) along third dimension
- Cannon calls SUMMA as sub-routine
  - Minimize inefficient (non-rectangular) communication
  - Allow better overlap
- Treats MM as a 4D tensor contraction