BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Optimizing Communication on Blue Waters

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GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

"Hottest" Optimizations on Blue Waters

- Serial optimizations (e.g., Vectorization)
- Hybridization (Threads + MPI)
- Communication/Computation Overlap
- Collective Communication (incl. Sparse Colls)
- MPI Derived Datatypes
- Topology Optimized Mapping
- One-Sided (maybe)

In This Talk: Communication Optimization

- Serial optimizations (e.g., Vectorization)
- Hybridization (Threads + MPI)
- Communication/Computation Overlap
- Collective Communication (incl. Sparse Colls)
- MPI Derived Datatypes
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- One-Sided (maybe)

mostly serial (Serial optimizations, Hybridization)

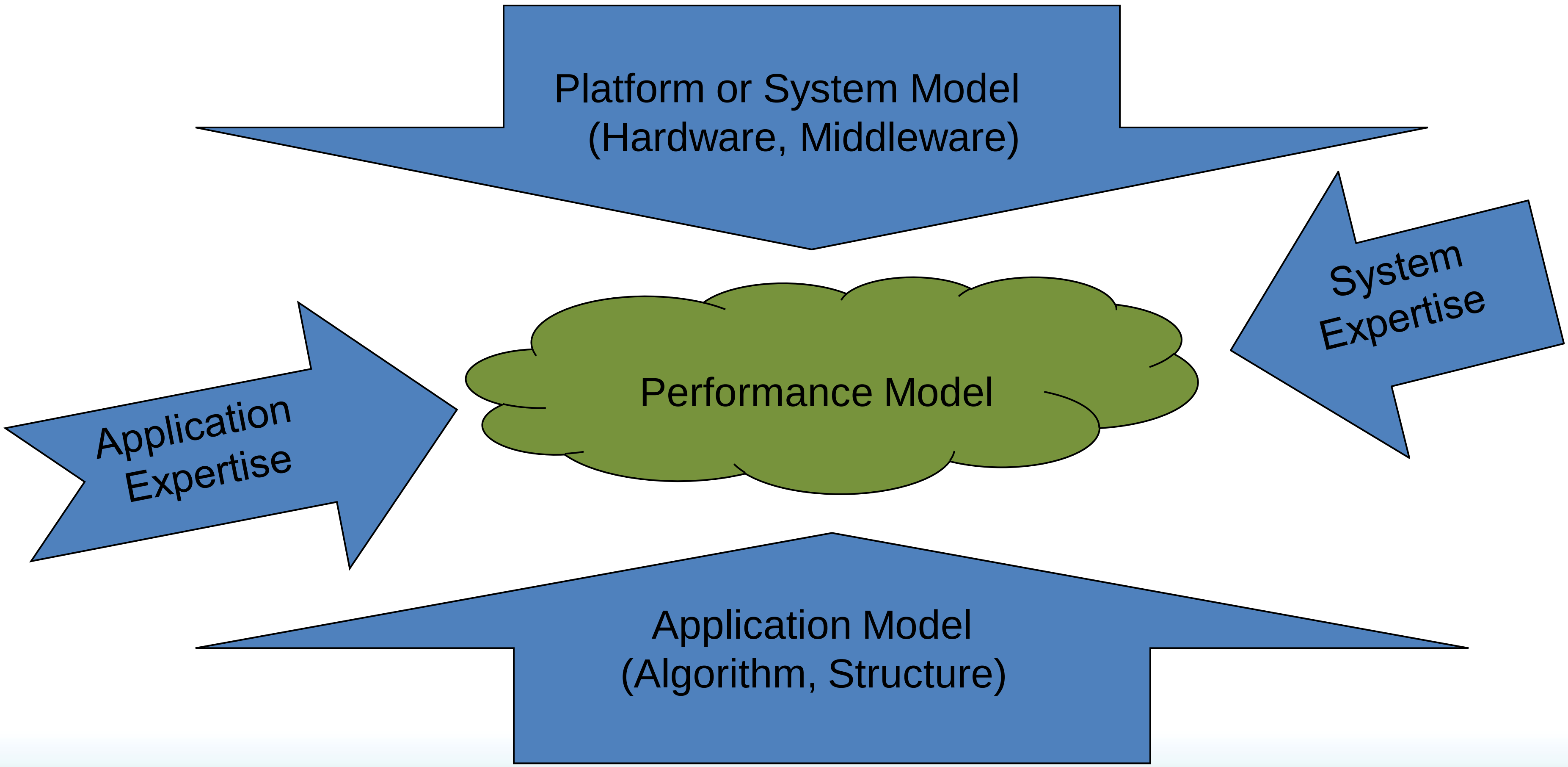
conceptually simple (Communication/Computation Overlap, Collective Communication)

not clearly defined yet (One-Sided)

Is Optimization X Relevant To My Application?

- … at scale? - well, we don't know
  - If you know that it's irrelevant: go, have a coffee now ☺
- Three ways to find out
  - Educated Guessing (based on mental model)
    - Very powerful and often accurate
  - Simulation (problematic, will hear more later today)
    - Very accurate but limited
  - Analytic Performance Modeling
    - Relatively accurate, often relatively simple
    - ➢ Excellent middle ground!

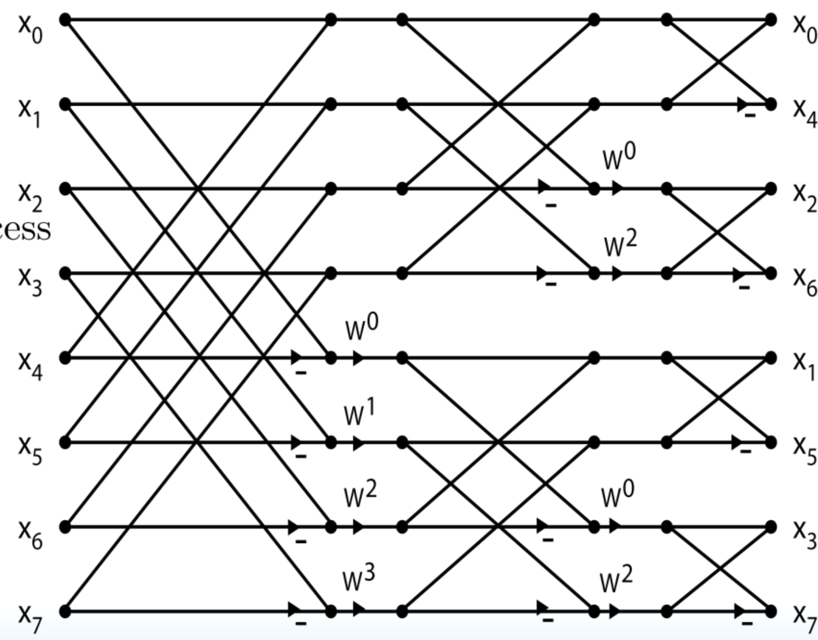
High-level Performance Modeling Overview



Example 1: 2d FFT

- Relatively simple kernel (square box only)
  - dominated by data movement, computation is free

1. perform N_x/P 1-d FFTs in y-dimension (N_y elements each)
2. pack the array into a sendbuffer for the all-to-all (A)
3. perform global all-to-all (B)
4. unpack the array to be contiguous in x-dimension (each process has now N_y/P x-pencils) (C)
5. perform N_y/P 1-d FFTs in x-dimension (N_x elements each)
6. pack the array into a sendbuffer for the all-to-all (D)
7. perform global all-to-all (E)
8. unpack the array to its original layout (F)

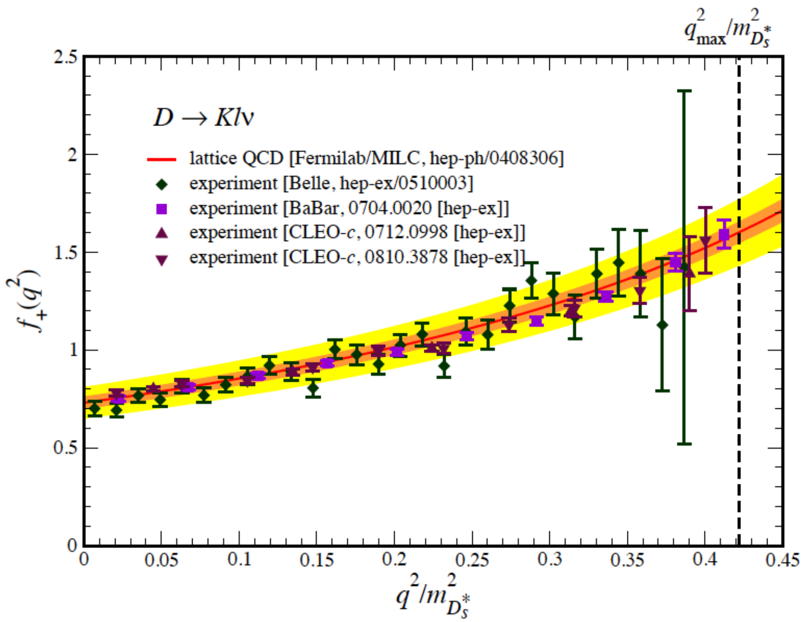


Educated Guess: What Matters for 2D-FFT?

- No detailed model available (yet)!
  - Lots of experience and previous analysis!
- Communication/Computation Overlap
  - Suggestion: Nonblocking Alltoall
    - Outside the scope of this talk!
- MPI Derived Datatypes
  - Eliminate Pack/Unpack Phase (>50%)
- Topology Optimized Mapping
  - Only in higher-dimensional decompositions

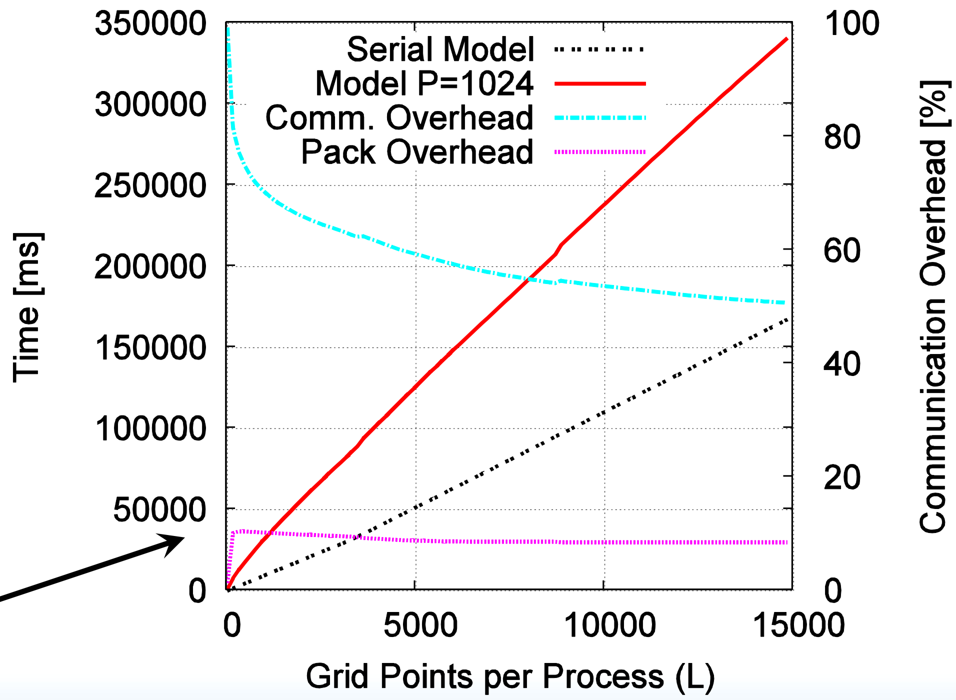
Example 2: MIMD Lattice Computation

- Gain deeper insights in fundamental laws of physics
- Determine the predictions of lattice field theories (QCD & Beyond Standard Model)
- Major NSF application
- Challenge:
  - High accuracy (computationally intensive) required for comparison with results from experimental programs in high energy & nuclear physics



Model-Driven Optimization: What Matters?

- NCSA's MILC Performance Model for Blue Waters
  - Predict performance of 300000+ cores
  - Based on Power7 MR testbed
  - Models manual pack overheads
  - >10% pack time
    - >15% for small L



Chapter 2

MPI Derived Datatypes

Quick MPI Datatype Introduction

- (de)serialize arbitrary data layouts into a message stream
  - Contig., Vector, Indexed, Struct, Subarray, even Darray (HPF-like distributed arrays)
    - Recursive specification possible
  - *Declarative* specification of data-layout
    - "what" and not "how", leaves optimization to implementation (*many unexplored* possibilities!)
  - Arbitrary data permutations (with Indexed)

Datatype Terminology

- Size
  - Size of DDT signature (total occupied bytes)
  - Important for matching (signatures must match)
- Lower Bound
  - Where does the DDT start
    - Allows to specify “holes” at the beginning
- Extent
  - Size of the DDT
    - Allows to interleave DDT, relatively “dangerous”

What is Zero Copy?

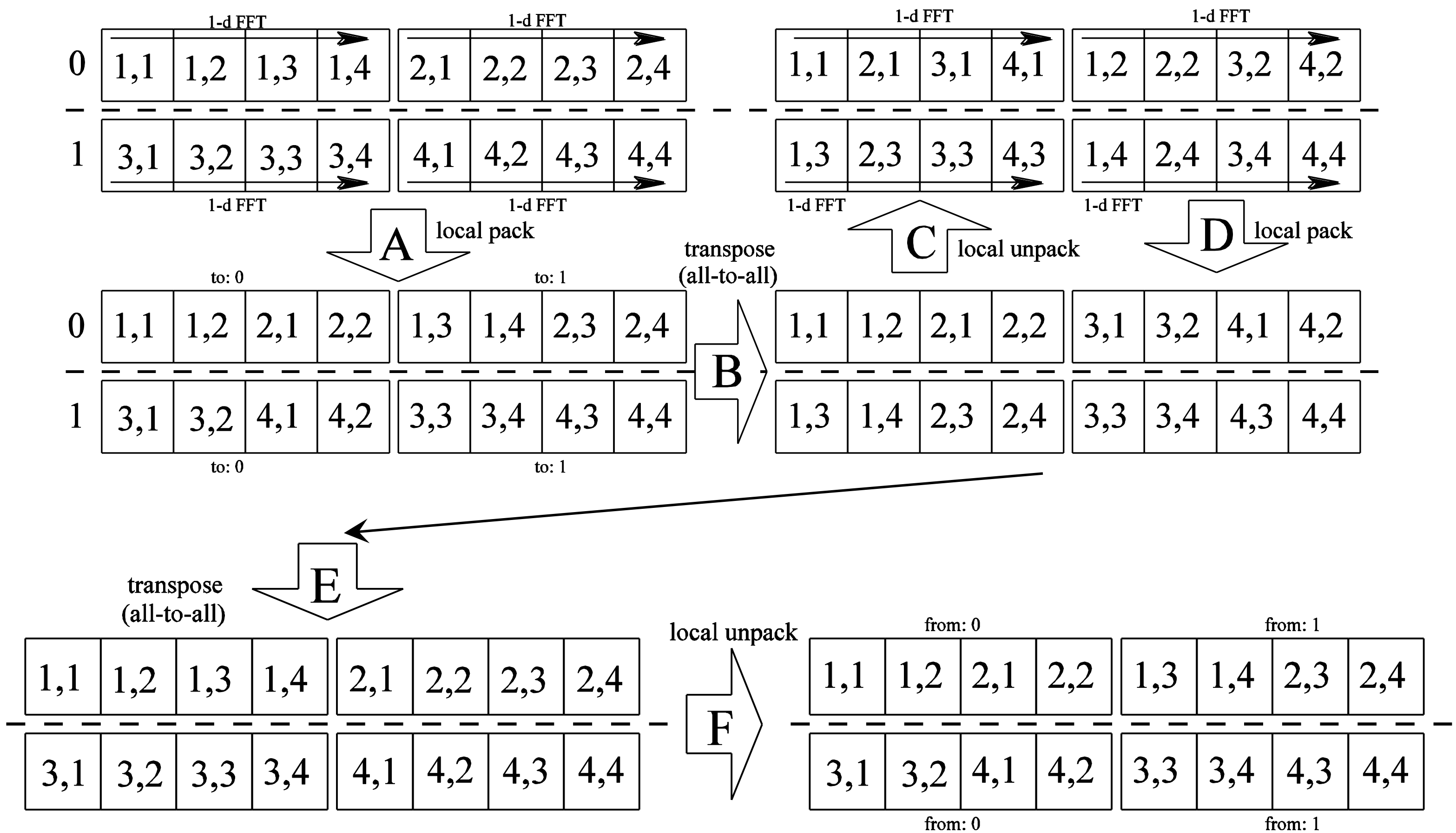
- Somewhat weak terminology
  - MPI forces “remote” copy
- But:
  - MPI implementations copy internally
    - E.g., networking stack (TCP), packing DDTs
    - Zero-copy is possible (RDMA, I/O Vectors)
  - MPI applications copy too often
    - E.g., manual pack, unpack or data rearrangement
    - DDT can do both!

Purpose of this Talk

- Demonstrate utility of DDT in practice
  - Early implementations were bad → folklore
  - Some are still bad → chicken+egg problem
- Show creative use of DDTs
  - Encode local transpose for FFT

- Details in *Hoefler, Gottlieb: "Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes"*

2d-FFT State of the Art



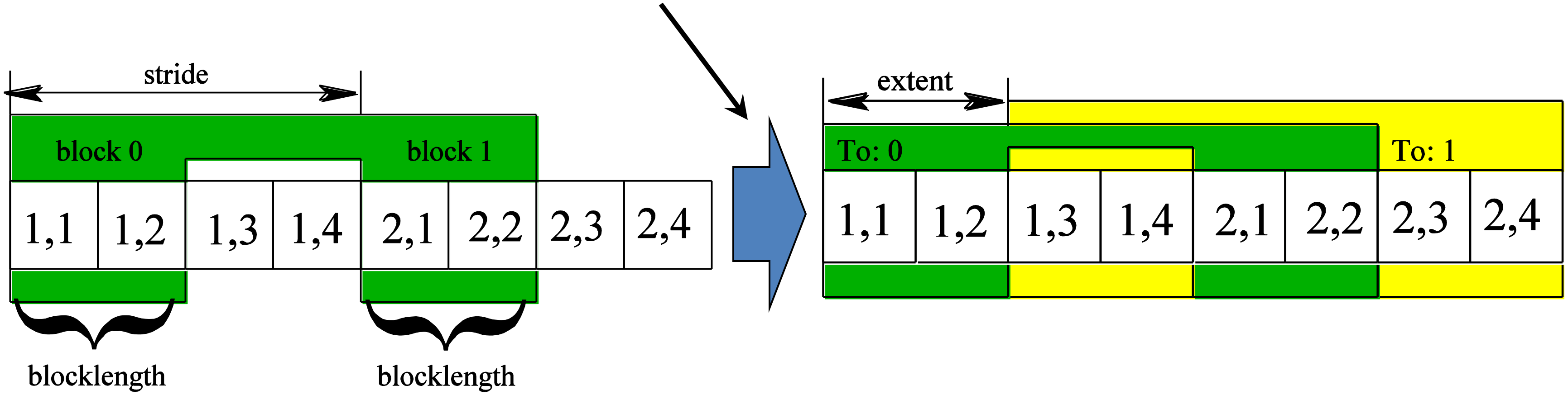
2d-FFT Optimization Possibilities

1. Use DDT for pack/unpack (obvious)
   - Eliminate 4 of 8 steps
     - Introduce local transpose

2. Use DDT for local transpose
   - After unpack
   - Non-intuitive way of using DDTs
     - Eliminate local transpose

The Send Datatype

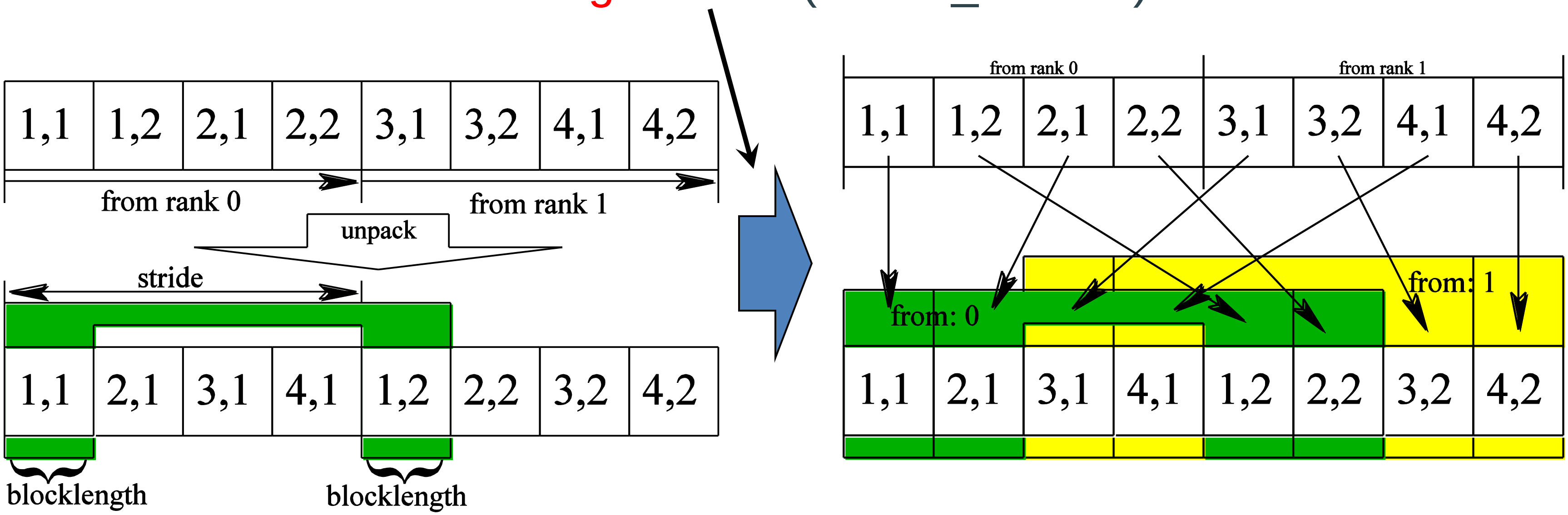
1. Type_struct for complex numbers
2. Type_contiguous for blocks
3. Type_vector for stride
   - Need to change extent to allow overlap (create_resized)



- Three hierarchy-layers

The Receive Datatype

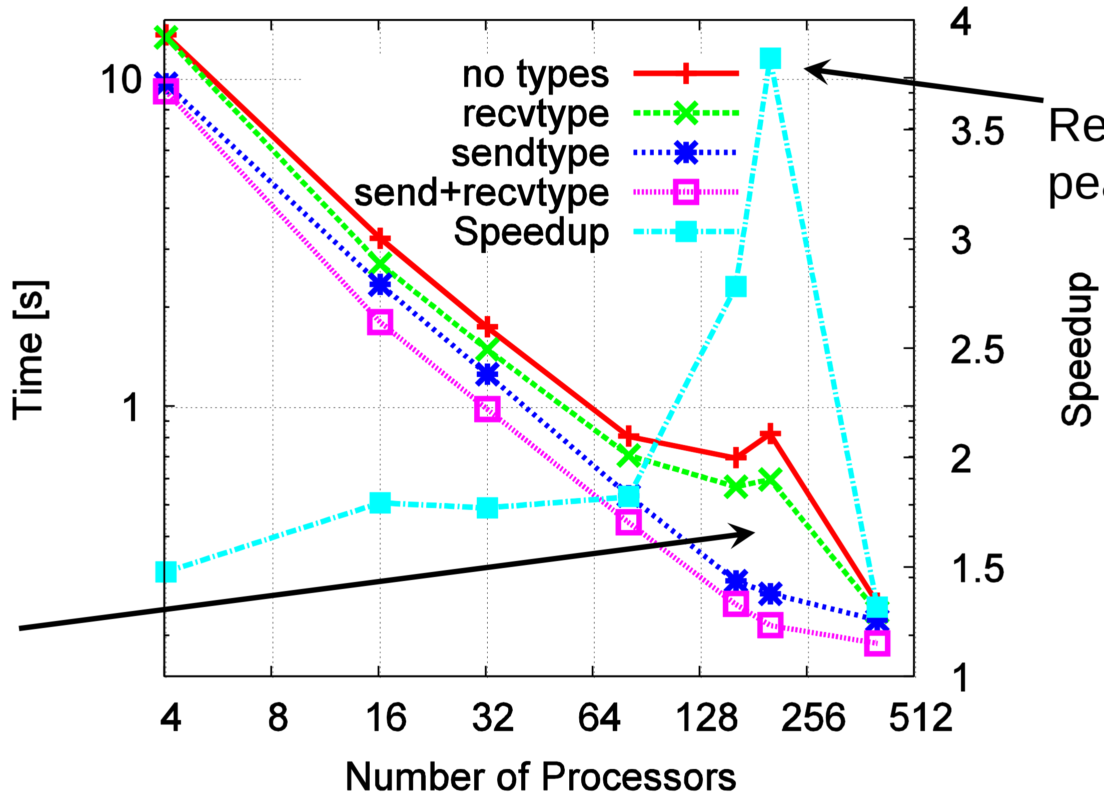
- Type_struct (complex)
- Type_vector (no contiguous, local transpose)
  - Needs to change extent (create_resized)



2D-FFT: Experimental Evaluation

- Odin @ IU
  - 128 compute nodes, 2x2 Opteron 1354 2.1 GHz
  - SDR InfiniBand (OFED 1.3.1).
  - Open MPI 1.4.1 (openib BTL), g++ 4.1.2
- Jaguar @ ORNL
  - 150152 compute nodes, 2.1 GHz Opteron
  - Torus network (SeaStar).
  - CNL 2.1, Cray Message Passing Toolkit 3
- All compiled with “-O3 –mtune=opteron”

Strong Scaling - Odin (8000^2)

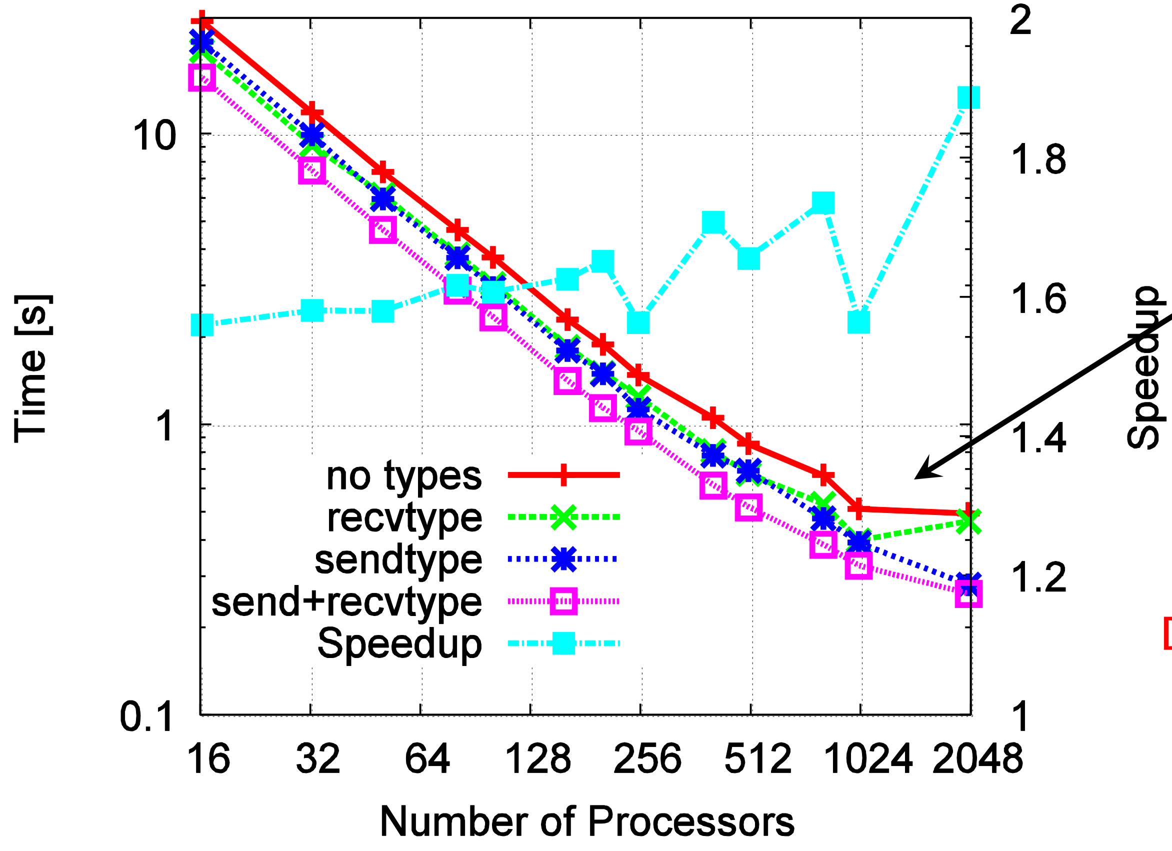


Reproducible peak at P=192

Scaling stops w/o datatypes

- 4 runs, report smallest time, <4% deviation

Strong Scaling – Jaguar ($20k^2$)



Scaling stops w/o datatypes

DDT increase scalability

Negative Results

- Blue Print - Power5+ system
  - POE/IBM MPI Version 5.1
  - Slowdown of 10%
  - Did not pass correctness checks ☹
- Eugene - BG/P at ORNL
  - Up to 40% slowdown
  - Passed correctness check ☺

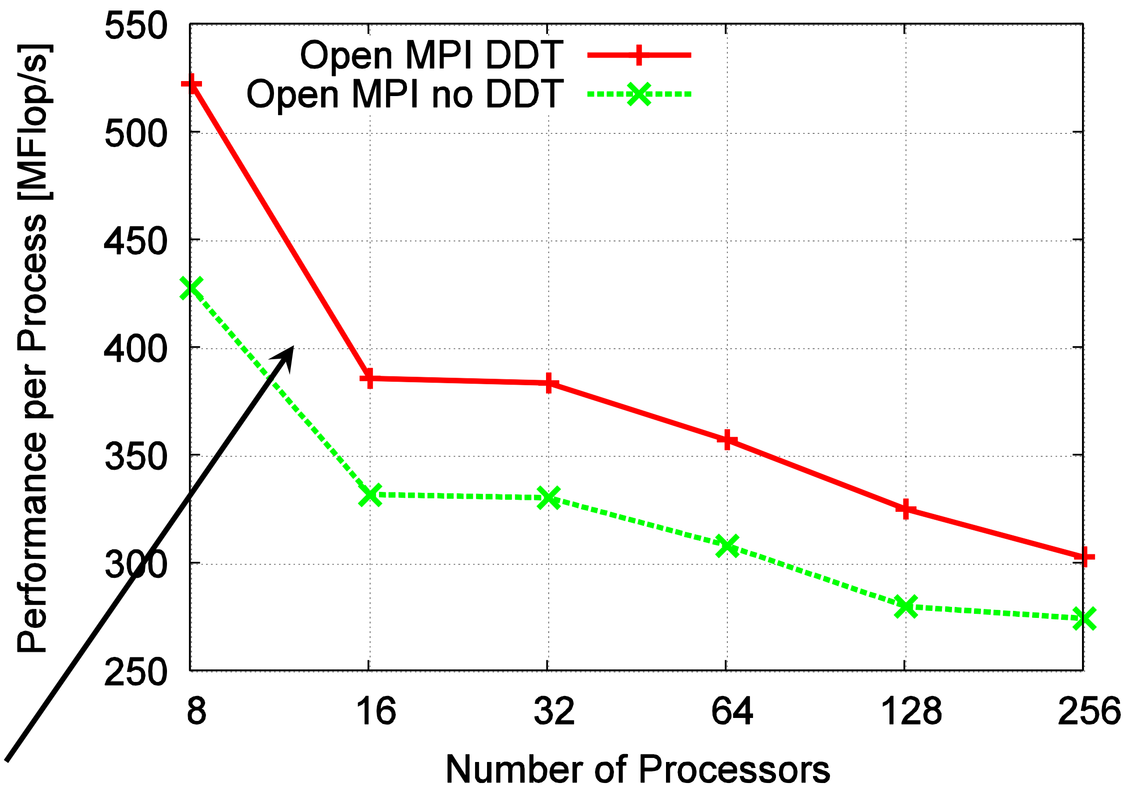
MILC Communication Structure

- Nearest neighbor communication
  - 4d array → 8 directions
  - State of the art: manual pack on send side
    - Index list for each element (very expensive)
  - In-situ computation on receive side
- Multiple different data access patterns ☹
  - su3_vector, half_wilson_vector, and su3_matrix
  - Even and odd (checkerboard layout)
  - Eight directions
  - 48 contig/hvector DDTs total (stored in 3d array)
- Allreduce (no DDTs, nonblocking alreduce is investigated!)

MILC: Experimental Evaluation

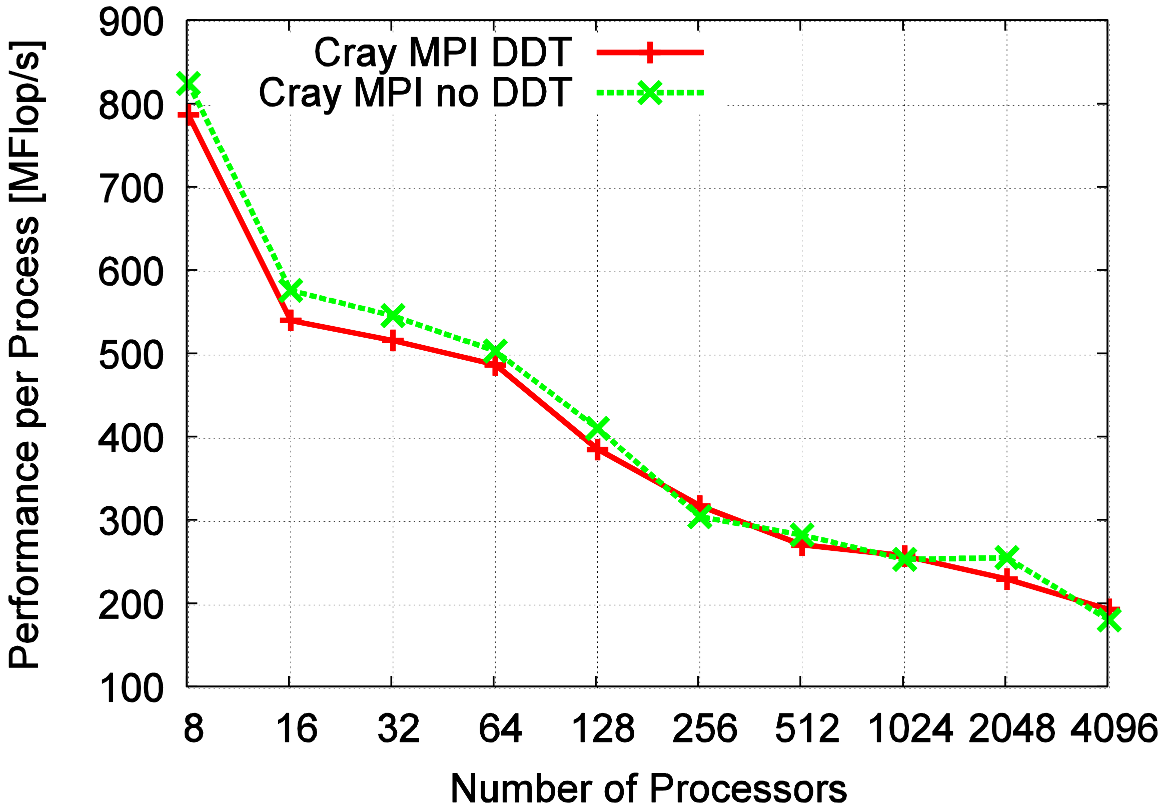
- Weak scaling with $L=4^4$ per process
  - Equivalent to NSF Petascale Benchmark on Blue Waters
- Investigate Conjugate Gradient phase
  - Is the dominant phase in large systems
- Performance measured in MFlop/s
  - Higher is better ☺

MILC Results - Odin



- 18% speedup!

MILC Results - Jaguar

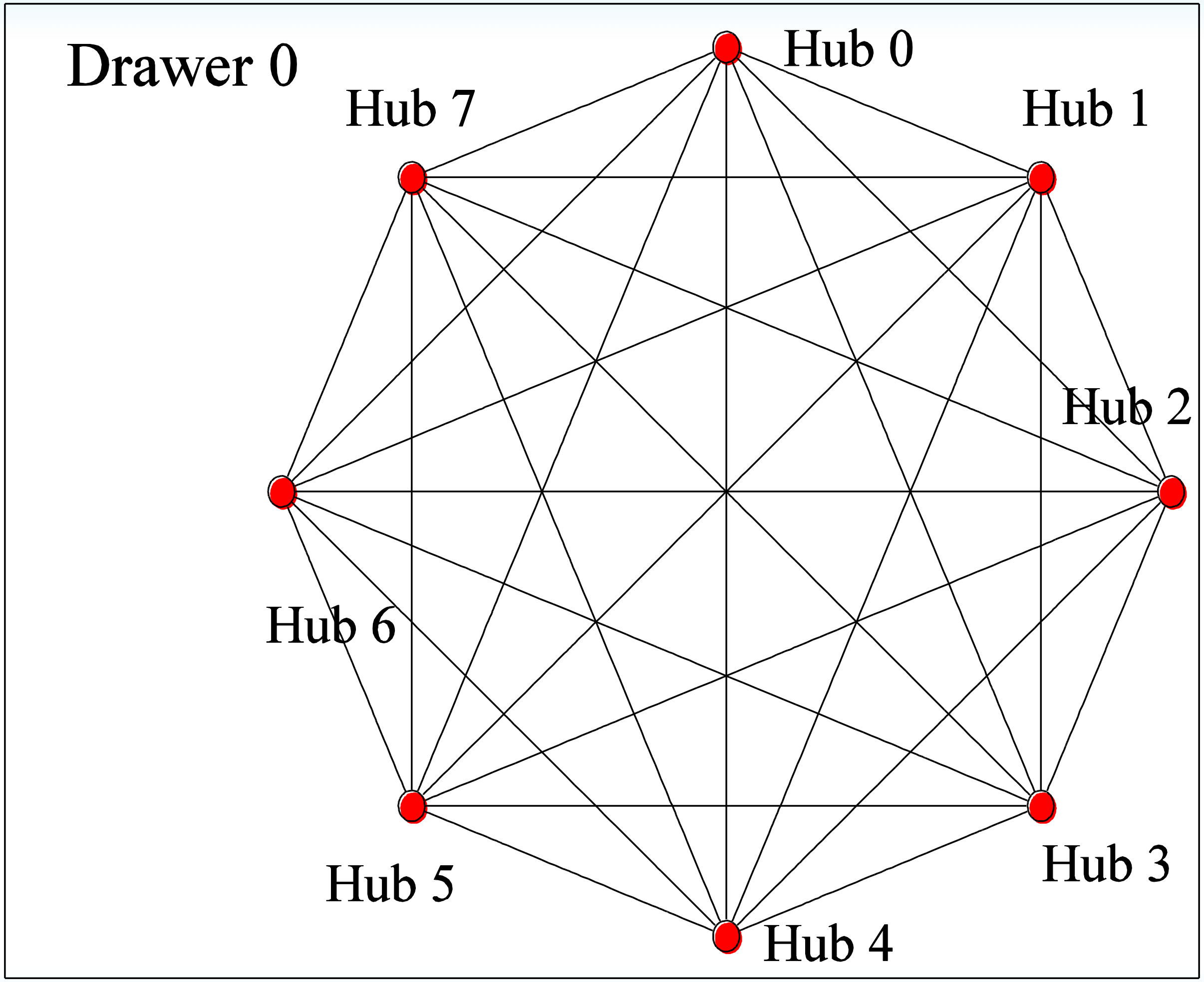


- Nearly no speedup (even 3% decrease) ☹

Chapter 3

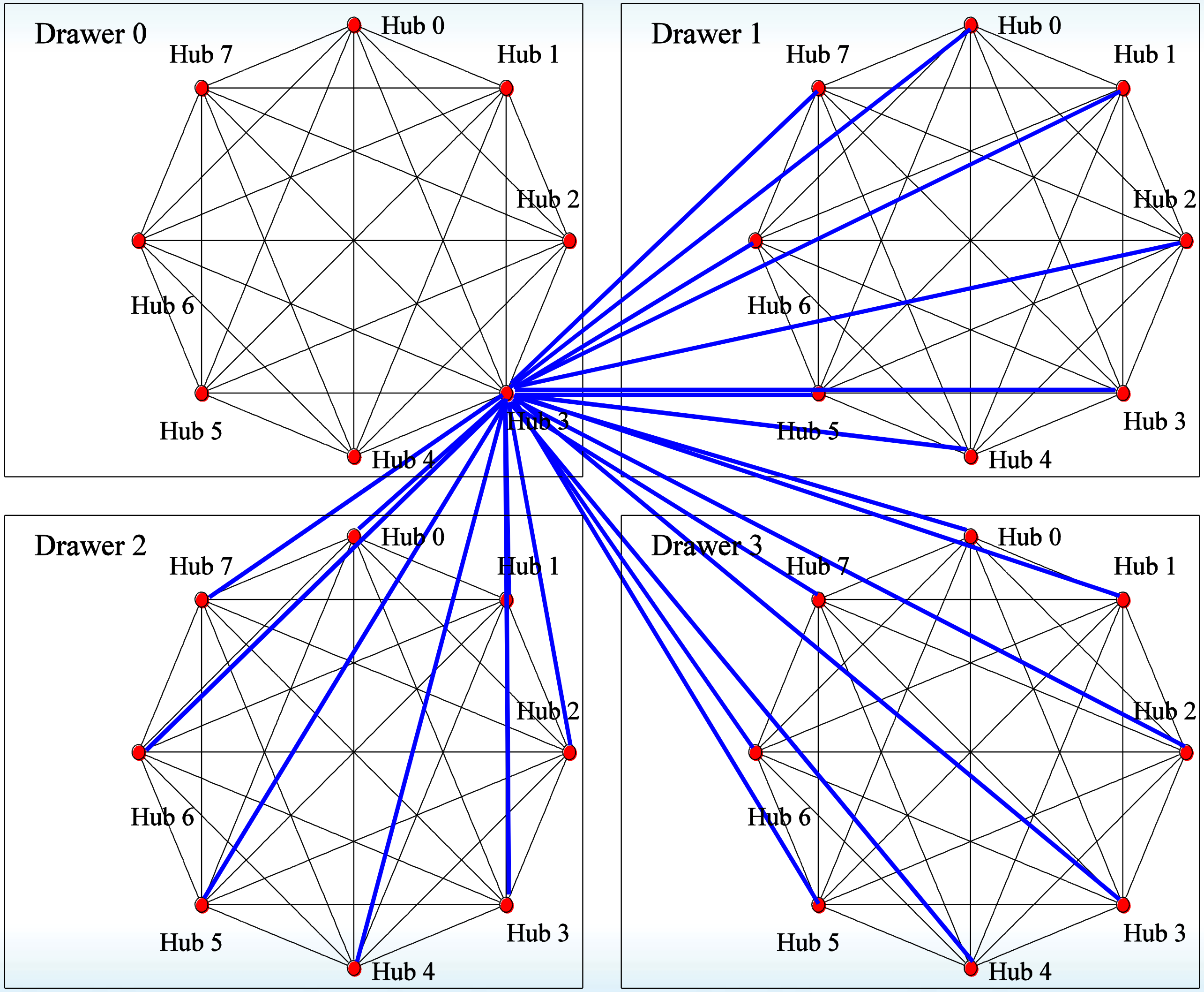
Topology Mapping

- LL Topology
  - 24 GB/s
  - 7 links/Hub
  - Fully connected
  - 8 Hubs



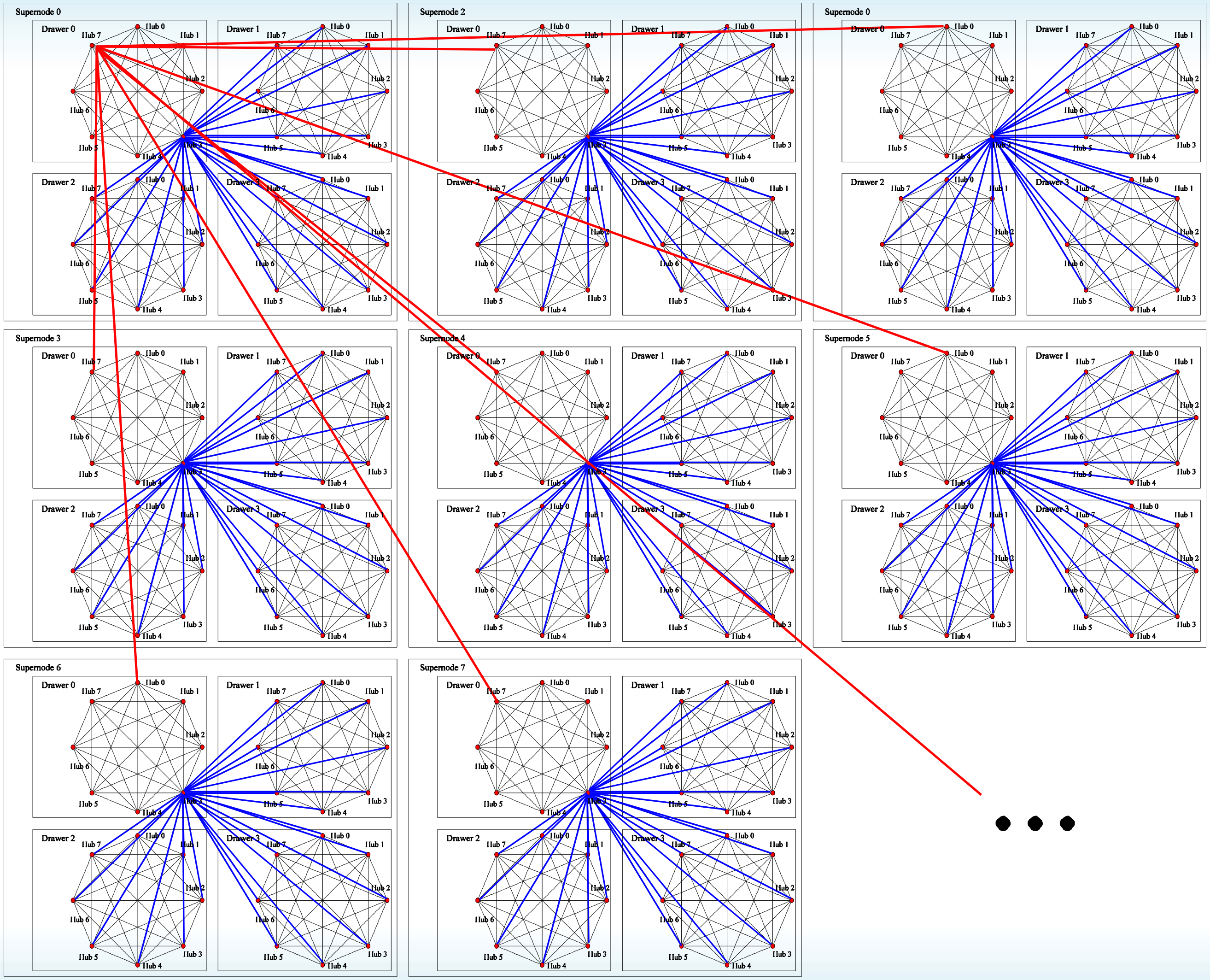
Source: B. Arimilli et al. *"The PERCS High-Performance Interconnect"*

- LR Topology
  - 5 GB/s
  - 24 links/Hub
  - Fully connected
  - 4 Drawers
  - 32 Hubs



Source: B. Arimilli et al. *"The PERCS High-Performance Interconnect"*

- D Topology
  - 10 GB/s
  - 16 links/Hub
  - Fully connected
  - 512 SNs
  - 2048 Drawers
  - 16384 Hubs



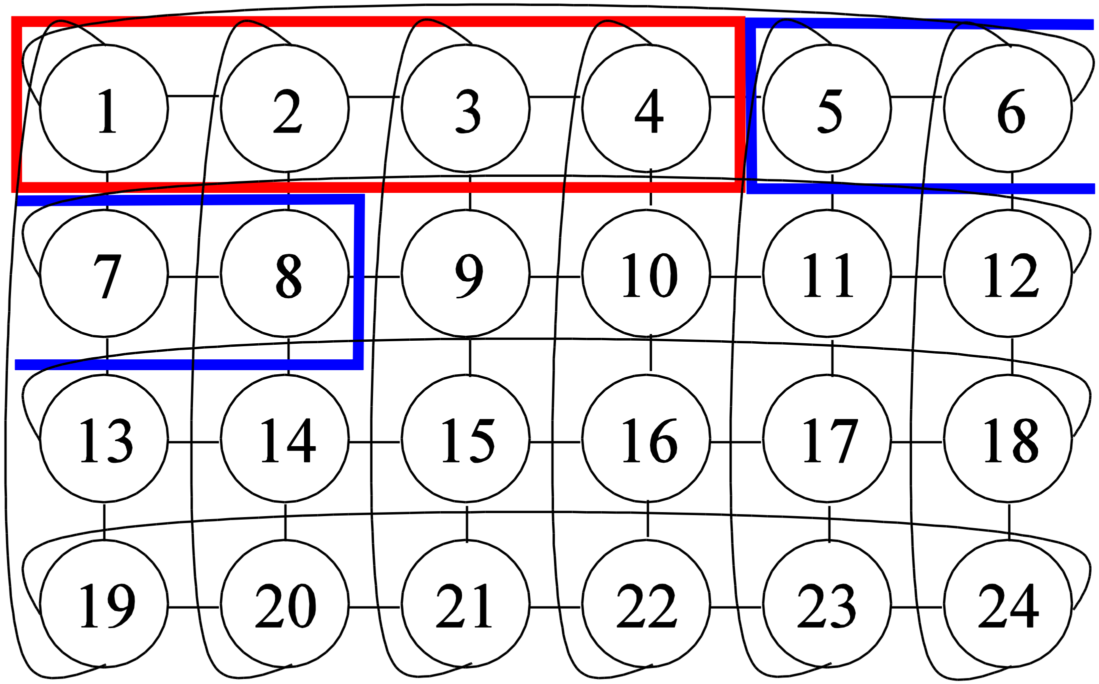
Source: B. Arimilli et al. *"The PERCS High-Performance Interconnect"*

Topology Mapping

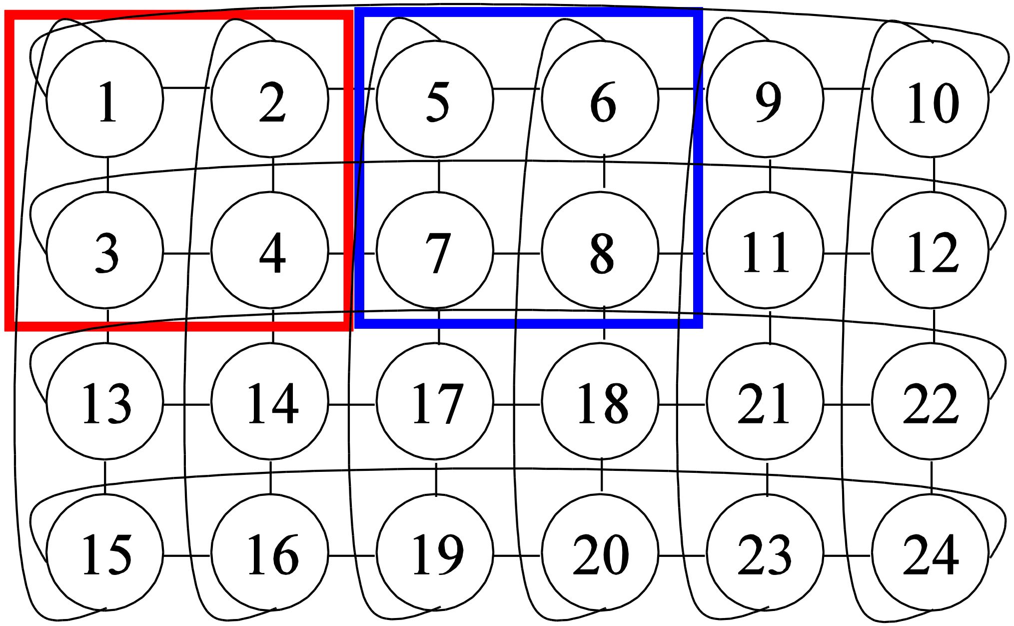
- Some simple observations
  1. A node is a clique with 48 GiB/s
  2. A drawer is a clique with 24 GiB/s
  3. D is faster than LR, but there are more LR links!
  4. Everything else is complicated ☺
- If I were you, I'd let others deal with this mess
  - Specify communication topology to the runtime
    - MPI-2.2 Cartesian or scalable graph communicator
      - Hoefler et. al: "The Scalable Process Topology Interface of MPI 2.2"
    - This is safe, talking with IBM about more options

2D Example: Process-to-Clique Mapping

- Trivial linear default mapping
- With 4 processes per node:
  - 6 internal edges
  - 10 remote edges
- Wrap-around
  - Looses two internal edges
  - Unbalanced communication



Optimized 2D Process-to-Clique Mapping



- Optimal mapping
  - cf. Lagrange multiplier
  - 8 internal edges
  - 8 remote edges
- Similar for 4d mapping
  - 16 cores, linear: 30 internal, 98 remote edges ($L_z > 16$)
  - optimal sub-block: $\sqrt[4]{16} = 2 \cdot 2 \cdot 2 \cdot 2$
    - ½ remote edges

FFT Topology Mapping

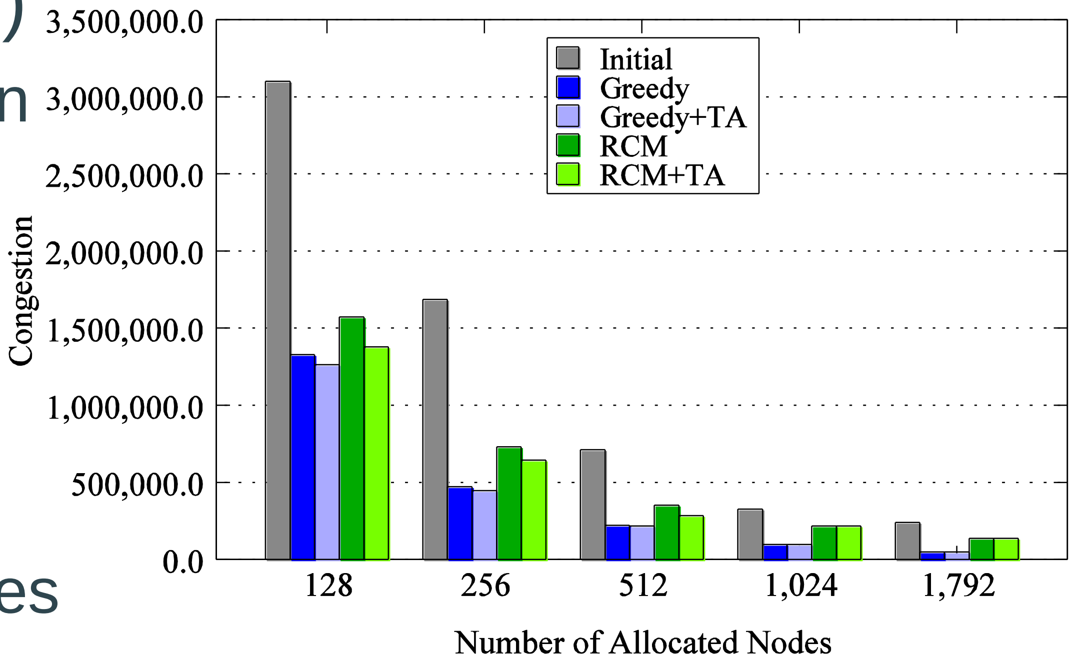
- Only useful in 2D (or higher) decomposition
- Map all-to-all communicators onto cliques
  - Node, Drawer, (D-clique?), … not trivial
  - Could specify a fully connected graph topology
    - Not sure if this would work too well (needs experiments)
- Maybe adapt decomposition to network structure
  - Square might not be always optimal
  - Needs information about topology
    - We’re working on this …

Map Irregular Structures

- Both MILC and FFT are very regular
- Many codes (AMR, etc.) are not!
  - Only beneficial if communication pattern is somewhat persistent!
  - The scalable graph topology interface provides opportunities for irregular applications!
  - Helps even more if communication is unbalanced
    - Will map heavy communication to fast links!

Encouraging Simulation Results

- Simulate mapping of Sparse MatVec from UFL collection (nlpkkt240)
  - Heuristic Optimization Technique
  - Reduces Congestion up to 80%
  - Greedy strategy computes mapping in ~0.8s for 1024 cores



Takeaways, Questions & Discussion

- Performance Modeling can guide optimizations!
- Serial optimizations & Overlap are most important
- Derived Datatypes and Topology Mapping are often neglected!
  - They have high potential!
  - But implementations need to improve
  - We're working on this with IBM

Datatype benchmarks: http://www.unixer.de/research/datatypes/

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