Experiences with Mixed MPI and Threaded Programming Models

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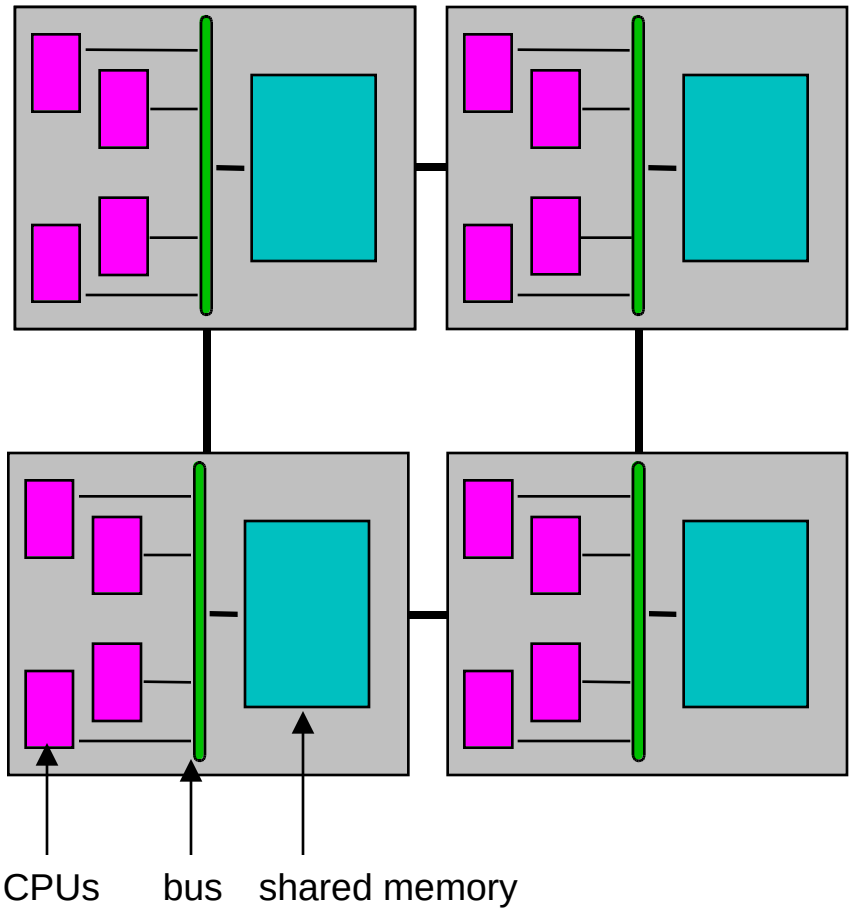
What is the best programming model for shared memory clusters?



- How do different programming models affect application performance?
- How do hardware characteristics affect application performance?
- How much work does it take to move to a new programming model?

Outline

- Hardware environment
- Mixed programming models
- Three mixed-model codes
  - Ares: regular-grid hydrodynamics
  - Ardra: neutral particle transport
  - JEEP: molecular dynamics
- Observations on mixed models

Hardware environment

- IBM “Tech Refresh” system
  - 168 four-way SMP nodes
  - Message passing can use “User Space” or “IP”
  - No global shared memory
- DEC cluster
  - Typical configuration has 80 CPUs divided (not equally) among 8 nodes
  - Message passing can span all CPUs, although most runs are not over the full system (capacity, not capability)

Programming models: Pure MPI

- Each CPU runs a separate MPI job
- Requires no changes for existing MPI codes
- Does not take advantage of shared memory
- Message passing is theoretically less efficient than shared memory
- Until recently, IBM didn’t support multiple user-space tasks on the same node

Programming models: Threads

- Explicit thread libraries (pthreads)
  - Maximum control
  - Most difficult threading model
- Parallelization directives
  - Examples include OpenMP and IBM SMP
  - Implies loop-level parallelization
  - Works best when loop iterations are large and independent
- Threaded libraries
  - If code spends substantial time in standard function (e.g. Fourier transform), can look for threaded version
  - Easiest to use
  - Performance depends on time spent in library

Mixed programming models

- Use MPI for internode communication and a threaded model within nodes
- Requires a thread-safe MPI library
  - Not all threads may communicate, but MPI may call non-thread-safe functions (e.g. malloc)
- Allows (one hopes) efficient use of shared memory
- Other models for multilevel parallelism exist (e.g. KeLP) but they aren't used in our codes

- Three examples from LLNL: Ares, Ardra, JEEP

Ares: Regular grid hydrodynamics

- Domain overloading
  - Decomposes problem space into more domains than processes
  - Improves load balance and cache use
  - Makes threading straightforward
  - One thread handles all MPI communication
- Initial threading used pthreads
  - Thread pool kept threads alive between phases
  - Complicated to program
- Switched to parallelization directives when available
  - Much easier to manage
  - No significant performance difference

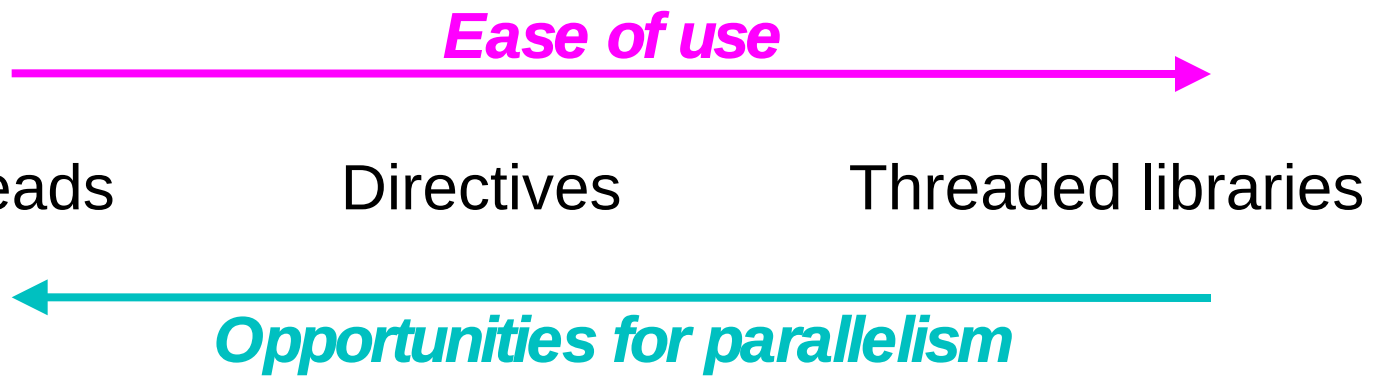
Ardra: Neutral particle transport

- Block-structured mesh
- About half the time spent in a “sweep” phase
- Programming model is data-driven for both message passing and threads
- Explicit threads scan work queue; compute each data point when its input dependencies are satisfied
- Initially used a thread pool; now spawn threads as needed
- Code is not well-suited for loop-based parallelism

JEEP: Molecular dynamics

- Computes molecular interactions at quantum-mechanical level
- Solves Schrödinger equation at each time step
- Message passing code is parallelized over electronic states
- Each state requires Fourier transform computations
- Fourier transform done with IBM's multithreaded ESSL code
- Easy way to get multithreading; speedup is limited

Conclusions



- **For loop-level parallelism, it's better to parallelize one outer loop than many inner loops, if possible**
- **Directive-based compilers are maturing**
- **No hard data yet on performance of threads vs. pure MPI; initial results are mixed**

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