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Building Multi-Petaflop Systems with MVAPICH2 and Global Arrays

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PACIFIC NORTHWEST NATIONAL LABORATORY

MVAPICH2 USER GROUP MEETING, AUGUST' 2013

The Power Barrier

- Power consumption is growing dramatically
  - ~100 MW datacenters are real
  - Facebook, Google, Apple
  - DOE Labs
  - 2% of total US consumption is in datacenters
- 1 M$/ MW-year
  - Significant portion of total cost of ownership
- For the upcoming (2020+) Exascale machine, the power is expected to be between 20MW+
- Many architectural innovations

Our data centers must become immensely more efficient and flexible to meet the need for energy while keeping costs in check as the demand for and price of resources continue to rise.

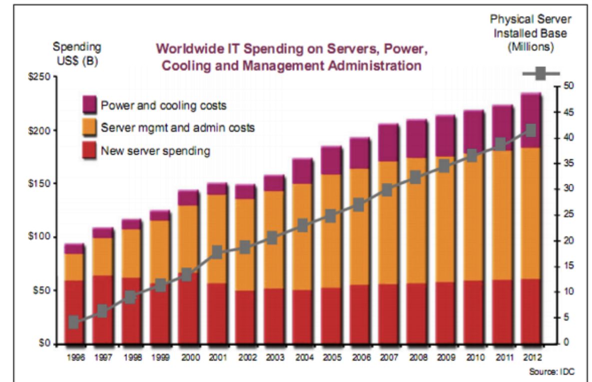
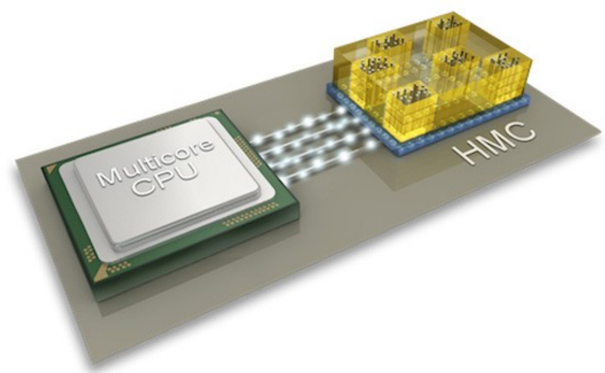
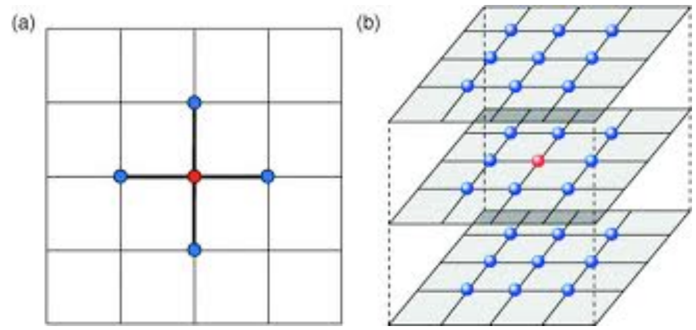


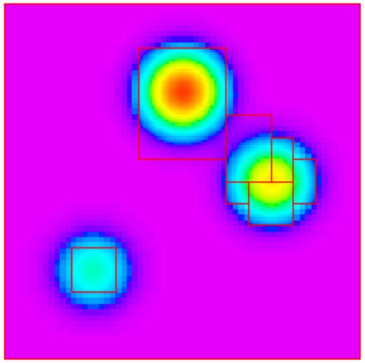
Figure 1 New server spending has plateaued while management and cooling costs continue to climb[3]

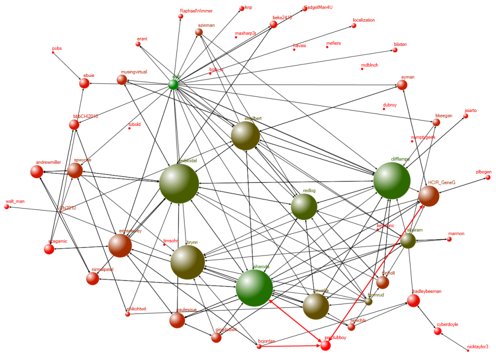


Workloads and Programming Models

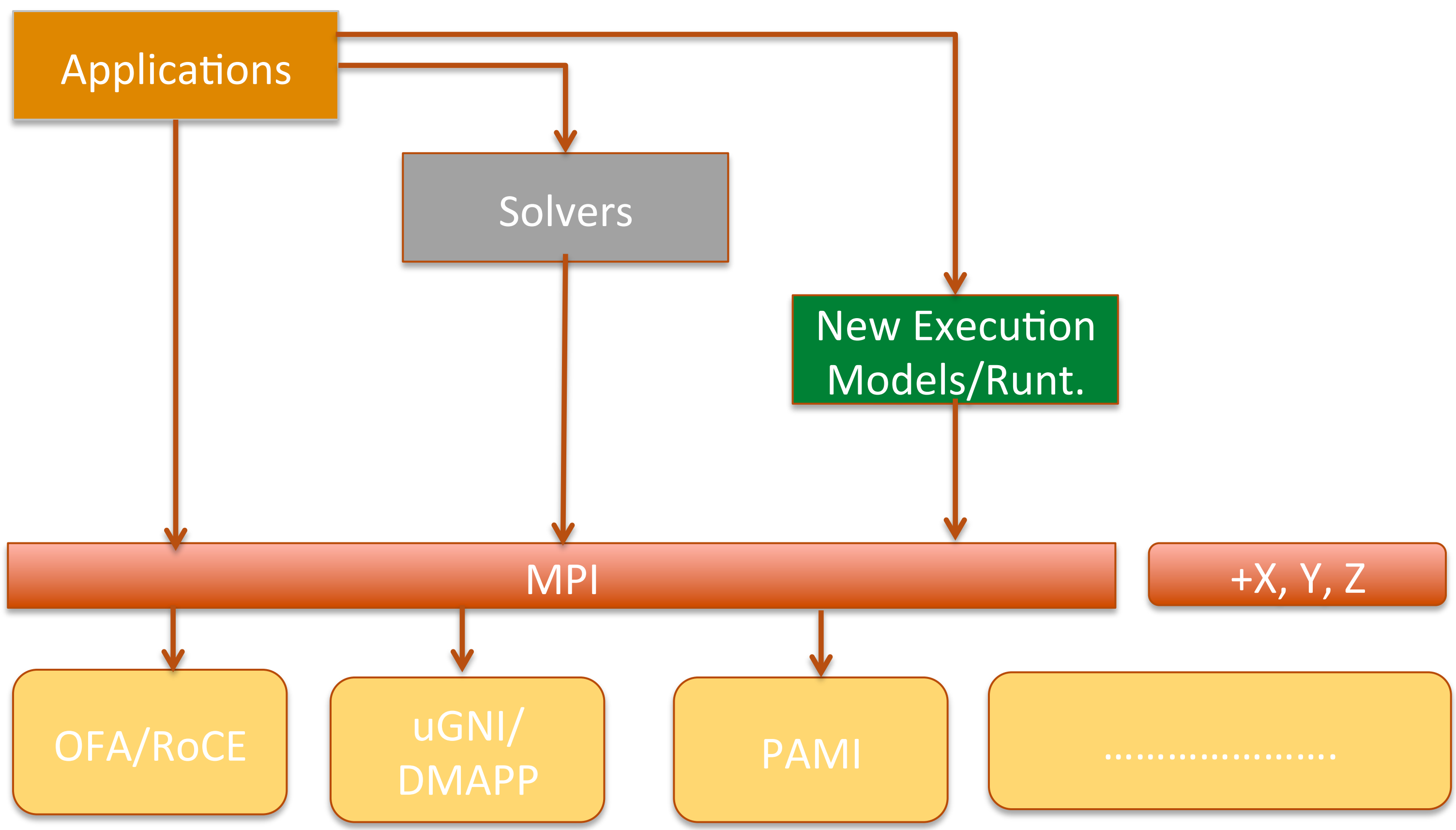
- Program in multiple programming models
  - MPI + X+ Y …
  - Evolve the existing application to “newer architecture”
- Evolution of newer execution models
  - Task models (PLASMA, MAGMA, DaGuE)
  - With possible MPI runtime backend
- Workloads are changing dramatically
  - Examples: Graph500



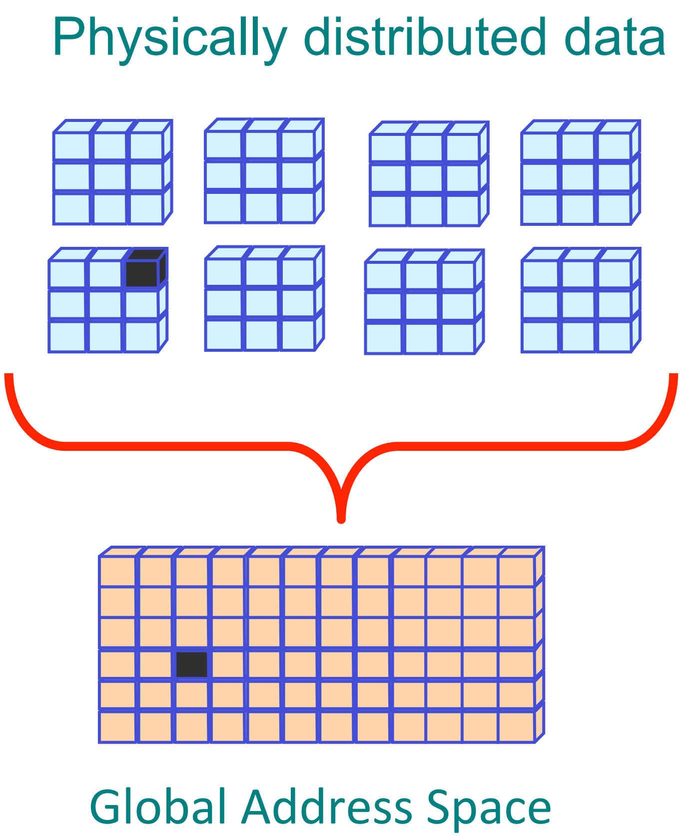




The Role of MPI Moving Forward: Least Common Denominator



Examples for X: Global Arrays, UPC, CAF



- A distributed-shared object programming model
  - Shared data view
  - One-sided communication models
  - Used in wide variety of applications
  - Global Arrays - Computational Chemistry
    - NWChem, molcas, molpro …
  - Bioinformatics
    - ScalaBLAST
  - Machine Learning
    - Extreme Scale Data Analysis Library (xDAL)

Global Arrays and MVAPICH2 at PNNL

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- PNNL Institutional Computing (PIC) cluster
- PIC:
  - 604 AMD Barcelona, IB QDR systems
  - MVAPICH2 default MPI in many cases
  - Global Arrays uses Verbs for Put/Get and MPI for collectives
  - Continuously updated with stable and beta releases
- Primary Workloads
  - NWChem
  - WRF
  - Climate (CCSM)

HPCS4: Upcoming Multi-Petaflop System@PNNL

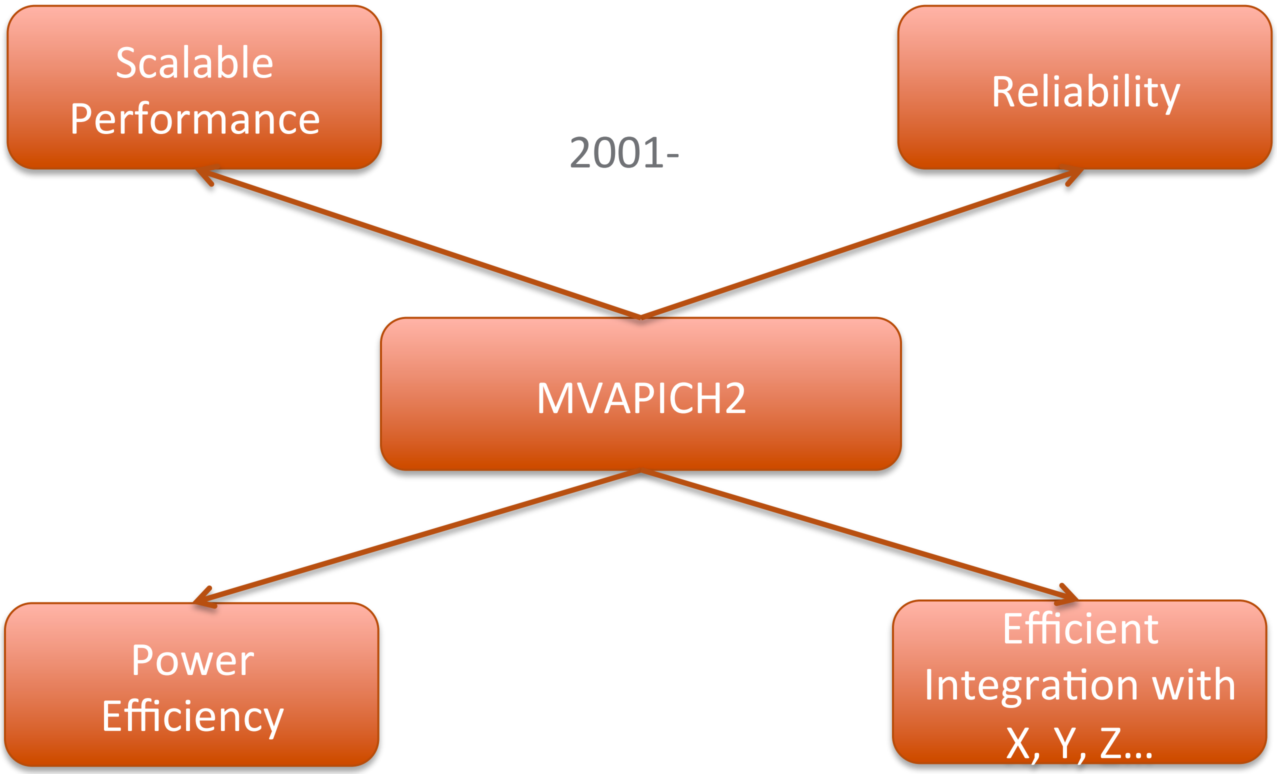
- 1440 Dual socket Intel Sandybridge @ 2.6 Ghz
- 128 GB memory/node
  - Requirements from compute intensive/data intensive applications such as NWChem
- 2 Xeon Phi / node, and 8 GB / Xeon Phi
- Mellanox InfiniBand FDR
- Theoretical peak / node : 2.35 TF
- 3.4 PF/s peak performance
- Expected efficiency on LINPACK : > 70%
- Power consumption < 1.5 MW
- Software Ecosystem:
  - MVAPICH2, Global Arrays, Intel-MPI
- Applications
  - NWChem, WRF

As a User of MVAPICH2, What I Like (with Feedback from Others at the Lab)!

- Job startup time
  - Very important at large scale
  - Consistent improvement over the releases
- Collective communication performance
  - Allreduce scales very well
  - Primary collective operation in many applications
- Low memory footprint
  - Numerous optimizations over the years

- A remark on collectives:
  - Collective performance with OS noise
  - Problems with a non-customized kernel
  - Liu-IPDPS'04, Mamidala-Cluster'05
    - The theme was collectives with process skew
    - OS noise introduces similar issues

As a User of MVAPICH2, What would I like ..

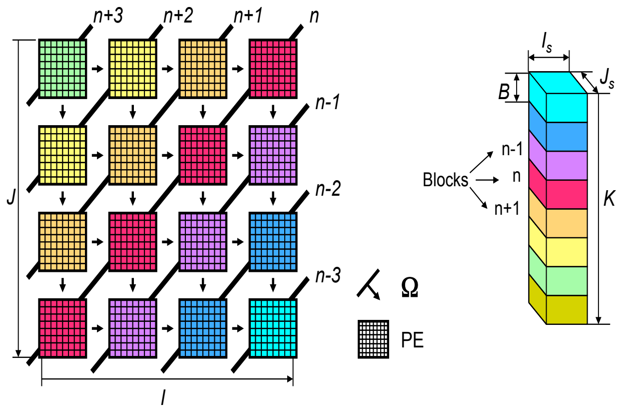


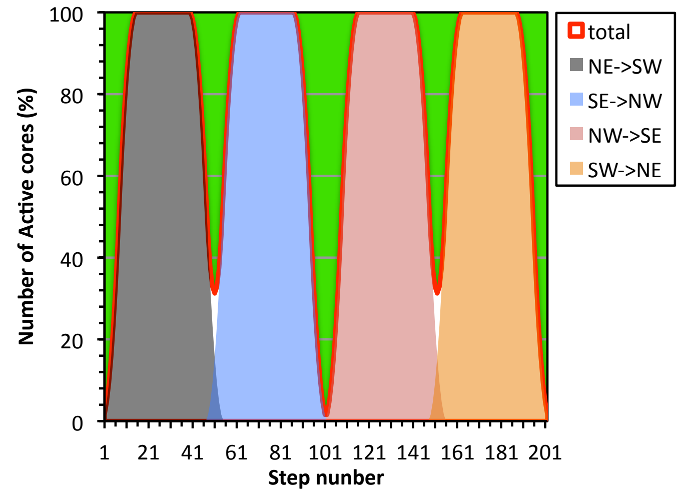
Position Statement 1: Power

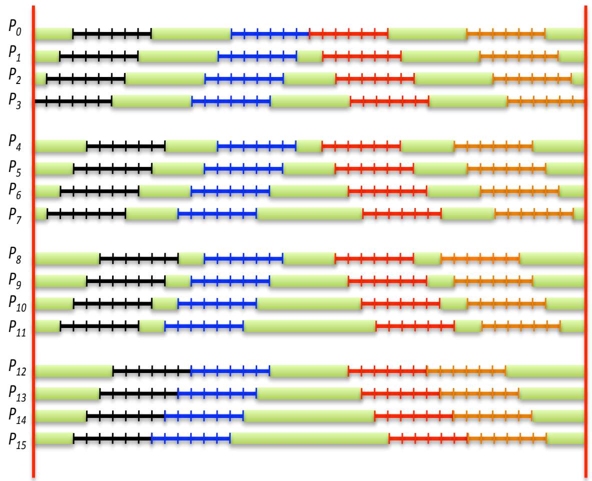
- Why should software do it?
  - Amdahl’s law: Once power optimized hardware is available, the relative power inefficiency of software grows proportionally
- Why should MPI do it (as well)?
  - It knows a lot about application indirectly!
  - The key is to automatically discover patterns
- Previous work is an important step, albeit with limitations
  - *Kandalla et al. – ICPP’09*
  - Efficiency for the size of data movement
    - Most collectives are small size
    - Some applications work on state transitions using pt-to-pt messages

Example: Neutron Transport @ Los Alamos

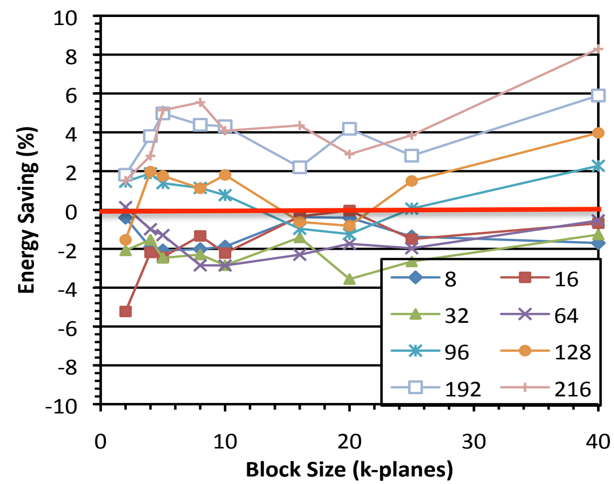
Sweep 3D – Neutron transport



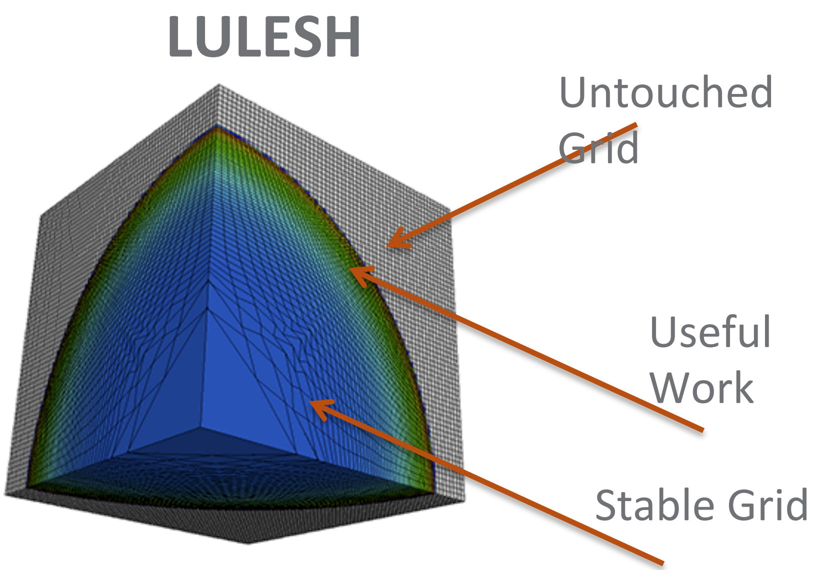




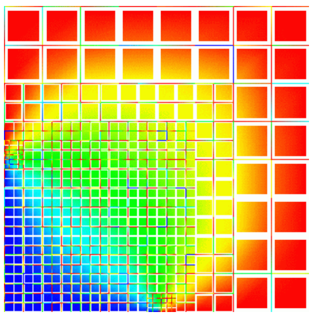
The “Slack”

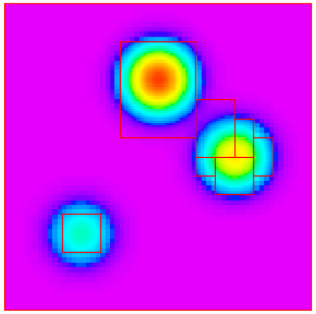


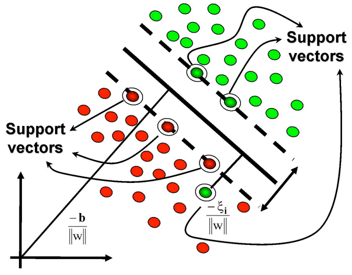
Shock Hydrodynamics @ LLNL



- Sedov blast problem
- Deposit Force at origin, and see the impact on material
- A small subset of processes perform useful work
- Difficult to define a static model for deformation
- Significant potential for Power efficiency
- Very different from Sweep3D problem





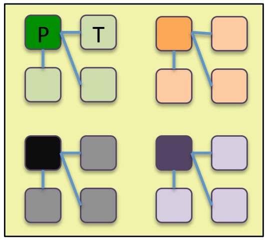


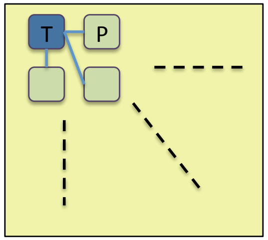
+ non-determinism

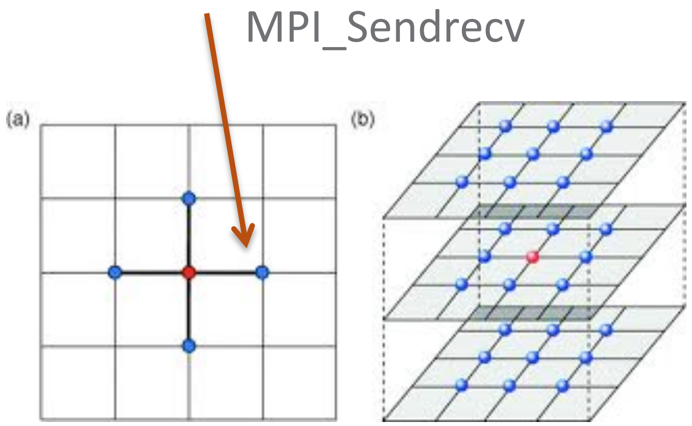
- Hardware
  - Lots of dynamism/uncertainty due to near threshold voltage execution
    - The dark silicon effect
  - Different chips perform varied levels of bit-correction
    - Difficult to capture on a static performance model
- Software
  - MPI + X, X is expected to be an adaptive programming model
  - Implication is that MPI needs to handle non-temporal patterns in communication
  - OS Noise
- Possible R&D
  - There are clear examples
  - The key is to automatically discover communication patterns
  - Potential for significant energy savings without one-off solution for a single application

Position 2: Effective Integration with "Other" Programming Models

- MPI + X (+ Y + ..)
- Shared Address Space examples of X
  - OpenMP, Pthreads, Intel TBB ..
- Classical data and Work decomposition
  - MPI_THREAD_MULTIPLE is not required, lower level models would do
- When multiple threads make MPI calls
  - Symmetric communication
- For MPI runtime, the challenge is MPI progress on multiple threads
  - Handling the critical section







Multi-threaded MVAPICH2 Performance

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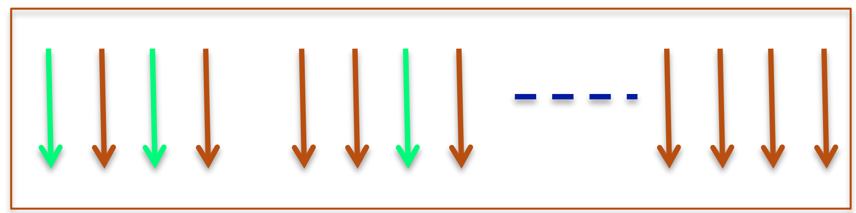
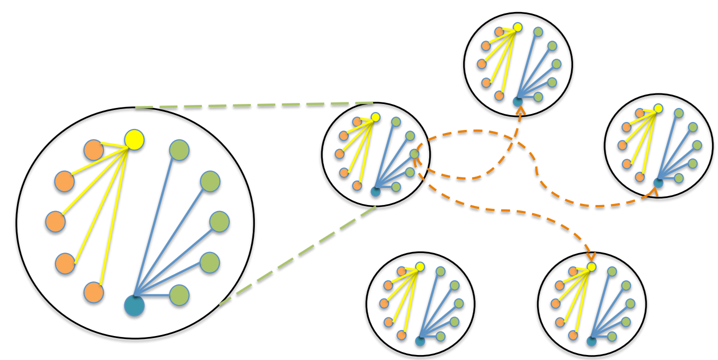
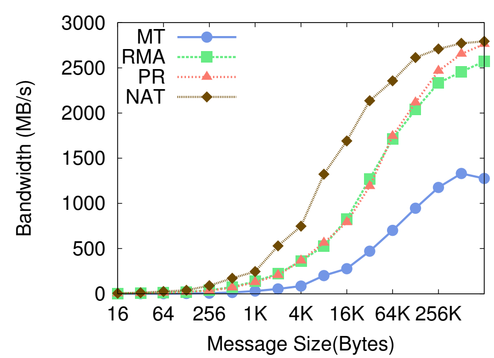
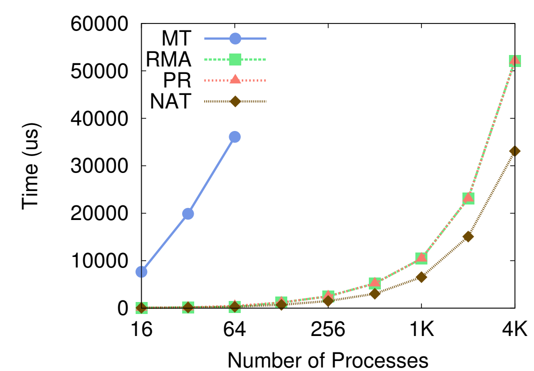
- Dinan et al. – EuroMPI’13
- Provide an endpoint to each thread
- Separate communicators for each thread
  - Prevents Thread Local Storage (TLS) conflicts between threads
- Problem:
  - Space complexity
  - Even harder with over-subscription (Charm++)
- Possible solution partly in specification, and other in runtime

Compute Node









Conclusions and Future Directions

- MPI will continue to be the least common denominator
  - Significant investment in applications
  - Newer execution models are adapting MPI for designing their runtimes
- MVAPICH2 has many features for scalable performance
- Larger scale systems would need MPI to be Power Efficient
  - The algorithms are different from each other
  - The architecture is expected to be radically different
  - Perfect recipe for advanced research and development
- Efficient support in MPI + X model would be critical
  - New execution models are looking forward to using MPI runtime with "revolutionary approaches"
  - The research space is very open

Thanks for Listening

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