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Developing New Tool Strategies for Scalable HPC Systems

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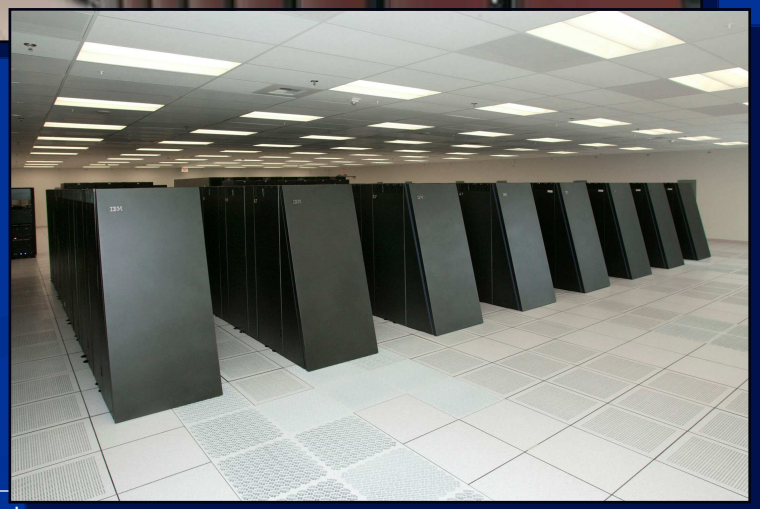
Trend towards Petascale

- Growing HPC Systems
  - *Many system at or above 10,000 cores*
  - *Multi/Many-core chips*
- TOP 500 list
  - *Nov 2005: **140** machines at or above 1024 cores*
  - *Nov 2006: **302** machines at or above 1024 cores*
- Petascale era is coming



Blue Gene/L

(compare this with a 1988 Cray YMP/8 at 2.7 GF/s)

~11mm

Compute Chip

2 processors
700 MHz
2.8/5.6 GF/s
4 MB eDRAM

Compute Card
I/O Card

FRU (field replaceable unit)
25mmx32mm
2 nodes (4 CPUs)
(2x1x1)
5.6/10.2 GF/s
1024 MB Mem

Node Card

16 compute cards
0-2 I/O cards
32 nodes
(64 CPUs)
(4x4x2)
89.6/179.2 GF/s
16 GB Mem

Cabinet

2 midplanes
1024 nodes
(2,048 CPUs)
(8x8x16)
2.9/5.7 TF/s
512 GB Mem
15-20 kW

System

64 cabinets
65,536 nodes
(131,072 CPUs)
(32x32x64)
183.5/367 TF/s
32 TB Mem
1.2 MW
2,500 sq.ft.
MTBF 6.16 Days

#1 of TOP 500 list

Multiscale Simulations

Time Scale

s

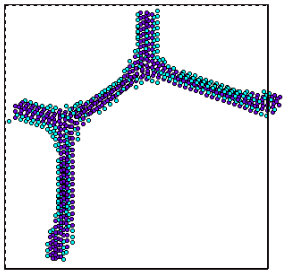
ms

µs

ns

ps

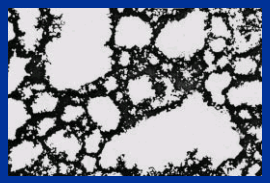
Atomic Scale

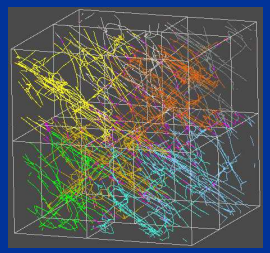


Molecular Dynamics

Unit mechanisms of defect mobility and interaction

Microscale





Dislocation Dynamics

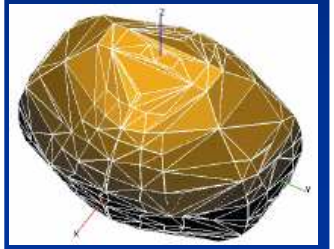
Collective behavior of defects, single crystal plasticity

Mesoscale

Aggregate Materials

Aggregate grain response, poly-crystal plasticity

Continuum



Finite Element

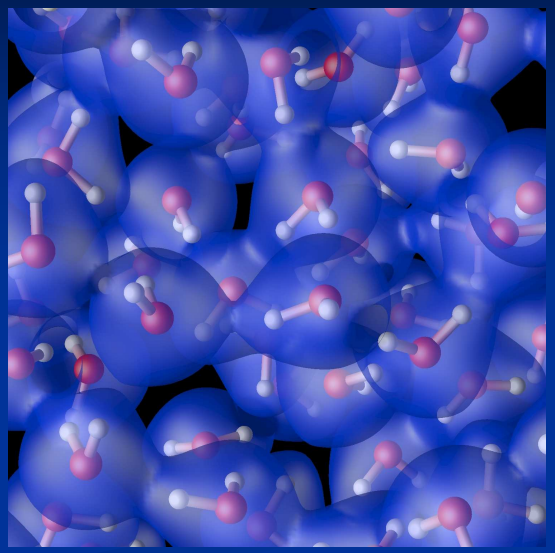
Plasticity of complex shapes

BlueGene/L simulations bring *qualitative* change to ASC material and physics modeling and engineering

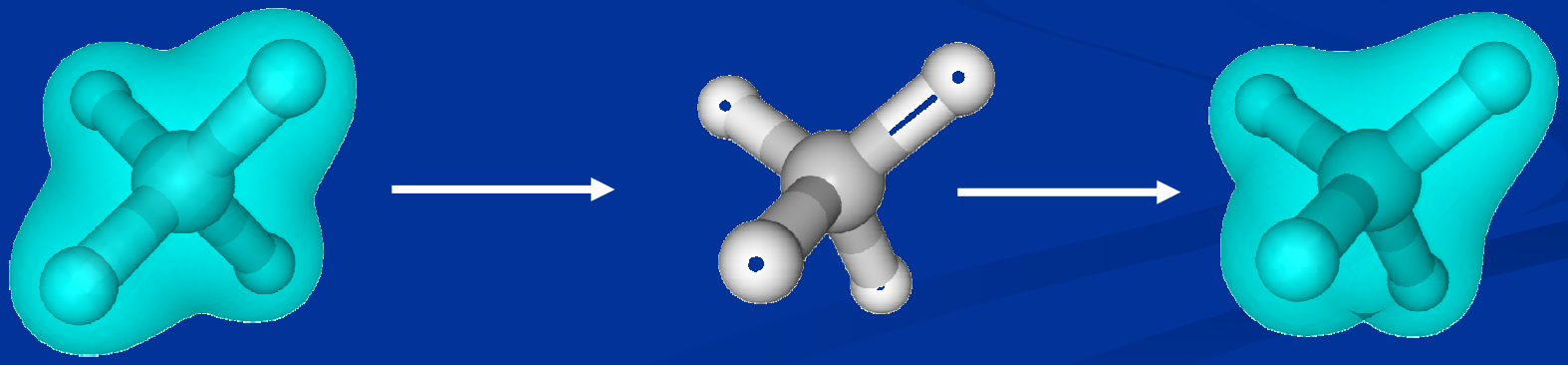
nm µm mm Length Scale

Example: QBox

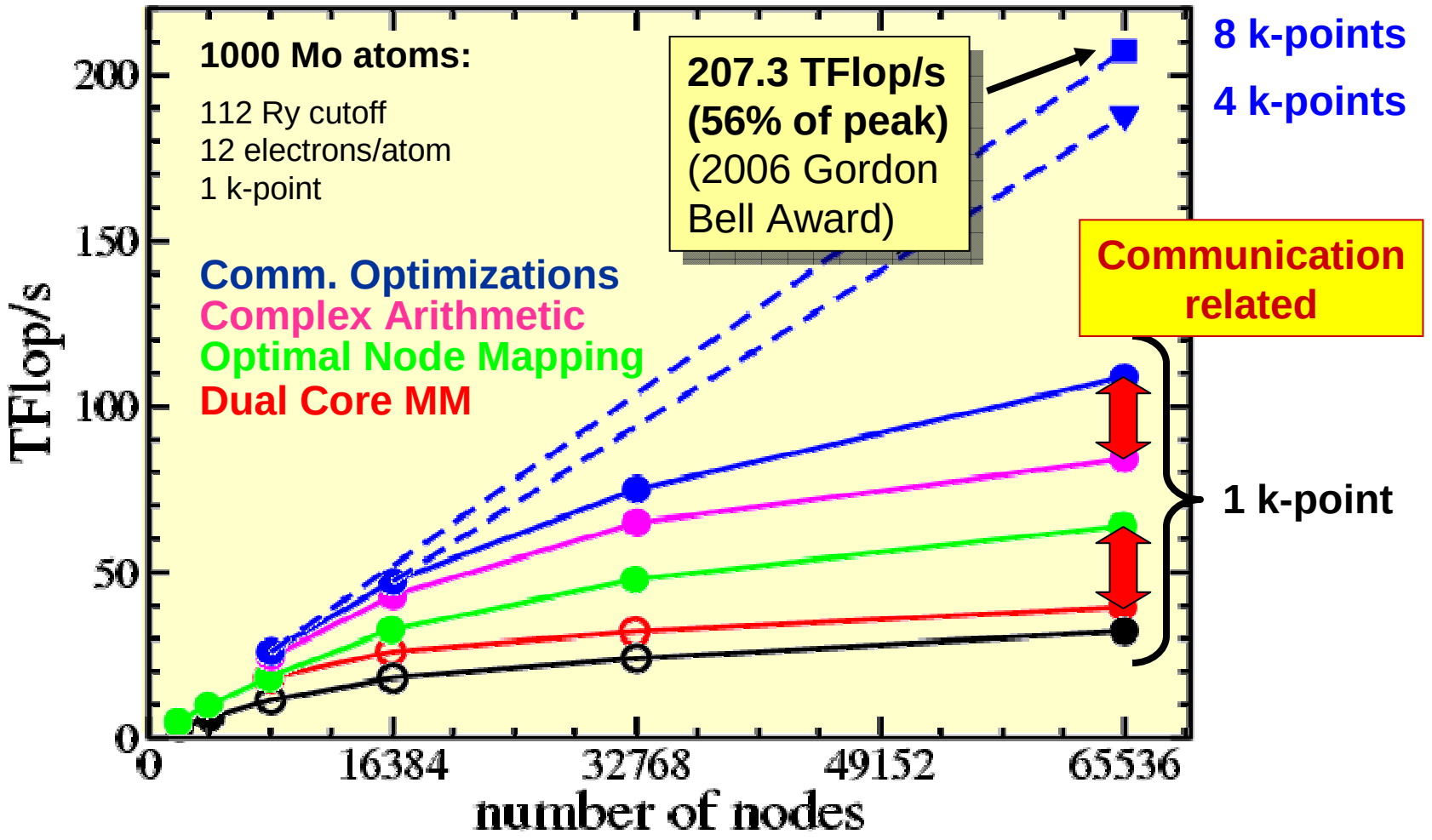
- Material Simulation
- First Principles Method
  - *No empirical parameters*
  - *Chemically dynamic*
    - *Iterative process*
    - *Computationally intensive*



Electron density surrounding water molecules, calculated from first-principles

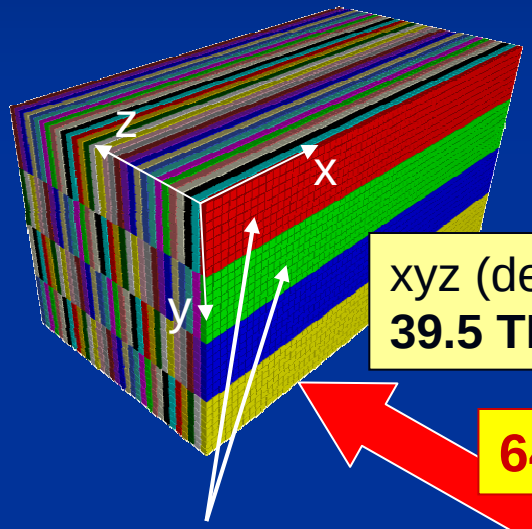


QBox Performance



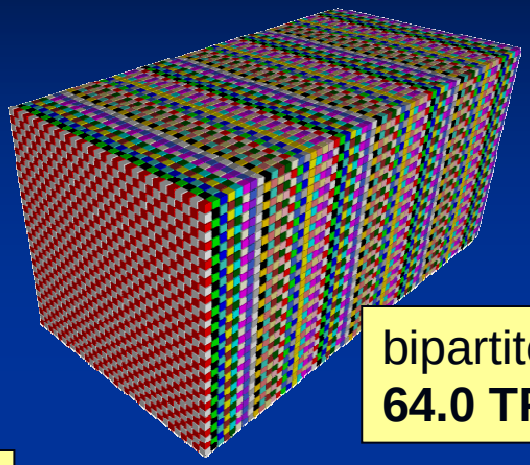
Topology Impact

65536 nodes, in a 64x32x32 torus

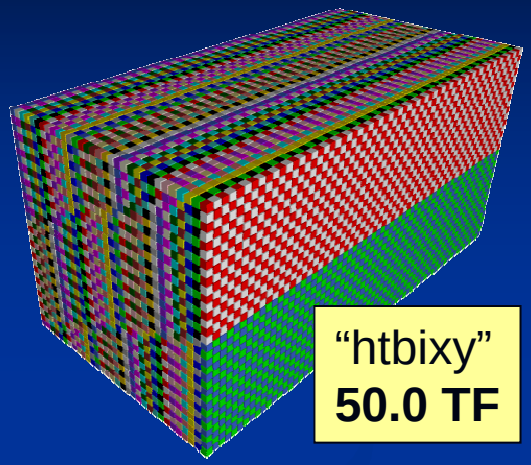


xyz (default)
39.5 TF

512 tasks per MPI subcommunicator

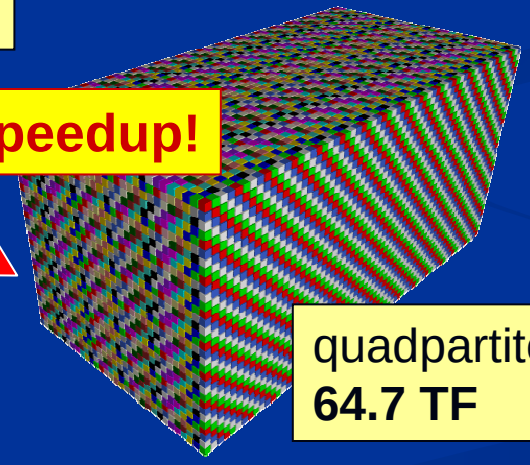


bipartite
64.0 TF

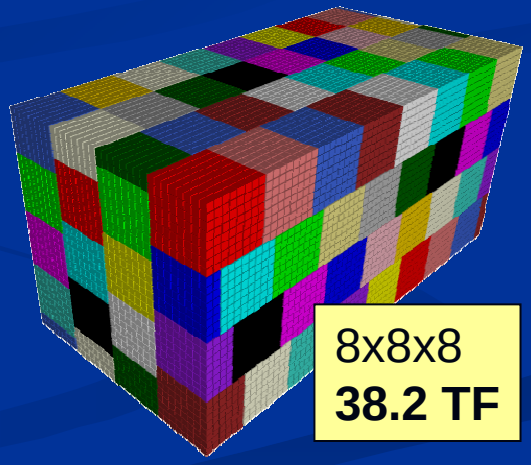


“htbixy”
50.0 TF

64% speedup!



quadpartite
64.7 TF



8x8x8
38.2 TF

Physical task distribution can significantly affect performance

Need for Scalable Tools

- Support complete development cycle
  - *Debugging*
  - *Performance analysis*
  - *Optimization/transformation*
- New challenges with scalability
  - *Large volumes of data to store and analysis*
  - *Central processing/control infeasible*
  - *Light-weight kernel*
- New tool strategies
  - *Scalable infrastructures*
  - *Application specific tool support*
  - *Flexible and interoperable toolboxes*

Outline

- ASC Tools Projects
- Scalable Debugging
  - *Challenges*
  - *Stack Trace Analysis*
- MPI Tool Infrastructure
  - *Layering MPI Tools*
  - *Communicator Specific Profiling*
- Lessons Learned & Future Work
- Conclusions

ASC Tools: Common Thread

- Scalability
  - *Tree-based data collection/processing*
  - *Intelligent data storage & compression*
- Tool components for quick prototyping
  - *Quickly assess new situations*
  - *Application specific tools*
- Ease-of-Use
  - *Little to no code modifications*
  - *Reuse existing, well-known tools*
  - *Keep learning curve low*
- Open source / tool integration

ASC Tool Projects

- Debugging/Correctness
  - *Stack Trace Analysis*
  - *Code Coverage*
  - *MPI Correctness*
  - *TotalView Collaboration*
- Performance Tools
  - *Open|SpeedShop*
  - *Tool Gear*
  - *MPI Profiling*
  - *Extended gprof*
- Static Analysis
  - *ROSE*
- Memory Tools
  - *ValGrind Collaboration*
  - *Memory Tracing*
- Fault Tolerance
  - *(MPI) Checkpointing*
  - *Soft Error Analysis*
- Infrastructures
  - *DPCL successor*
  - *P^NMPI*
  - *Trace Compression*
  - *Open Trace Format*

Debugging Challenges

TotalView on BG/L – 4096 Processes	
Operation	**Latency**
Single step	~15-20 secs.
Breakpoint Insertion	~30 secs.
Stack trace sampling	~120 secs.

Typical debug session includes many interactions

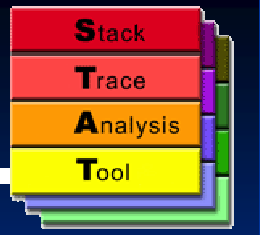
4096 is only 3% of BG/L!

Scalable Debugging

- Large volumes of debug data
- Single frontend for all node connections
- Centralized data analysis
- Vendor licensing limitations

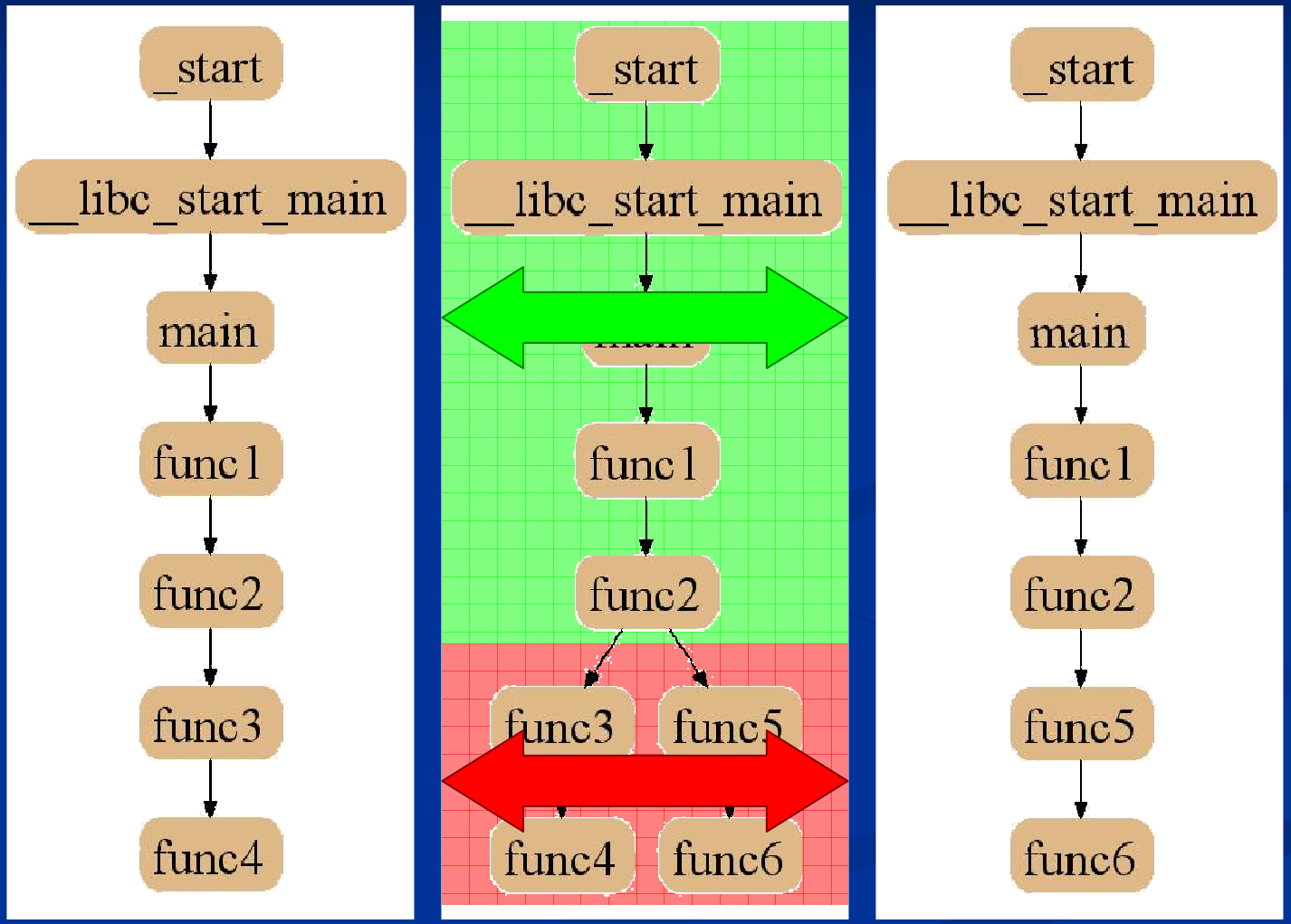
- Approach: scalable, lightweight debugger
  - *Discover equivalent process behavior*
  - *Reduce exploration space to small subset*
  - *Full-featured debugger for deeper digging*
  - *Analysis in tree-based reduction network*

STAT Approach

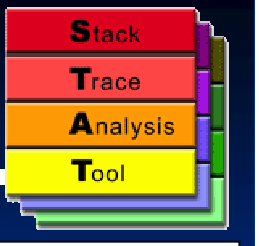


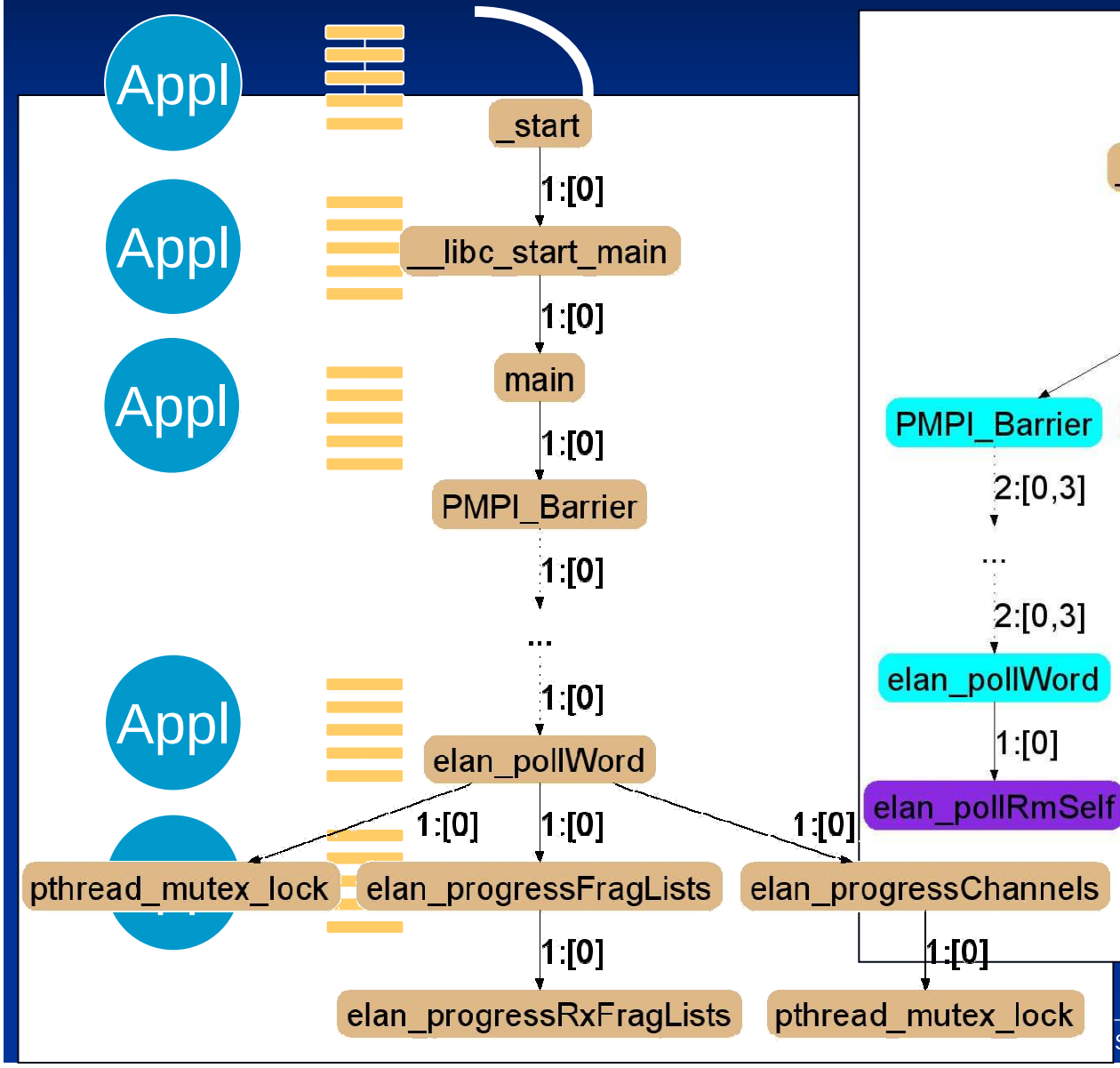
- Sample application stack traces
  - *Multiple snapshots across time and space*
  - *Through third party (DynInst) interface*
  - *Stored in graph representation*
- Create call graph prefix tree
  - *Only merge nodes with identical stack backtrace*
  - *Retains context information*
  - *First merge per node, then across nodes*
- Export in widely used graph formats
  - *Use existing viewer*

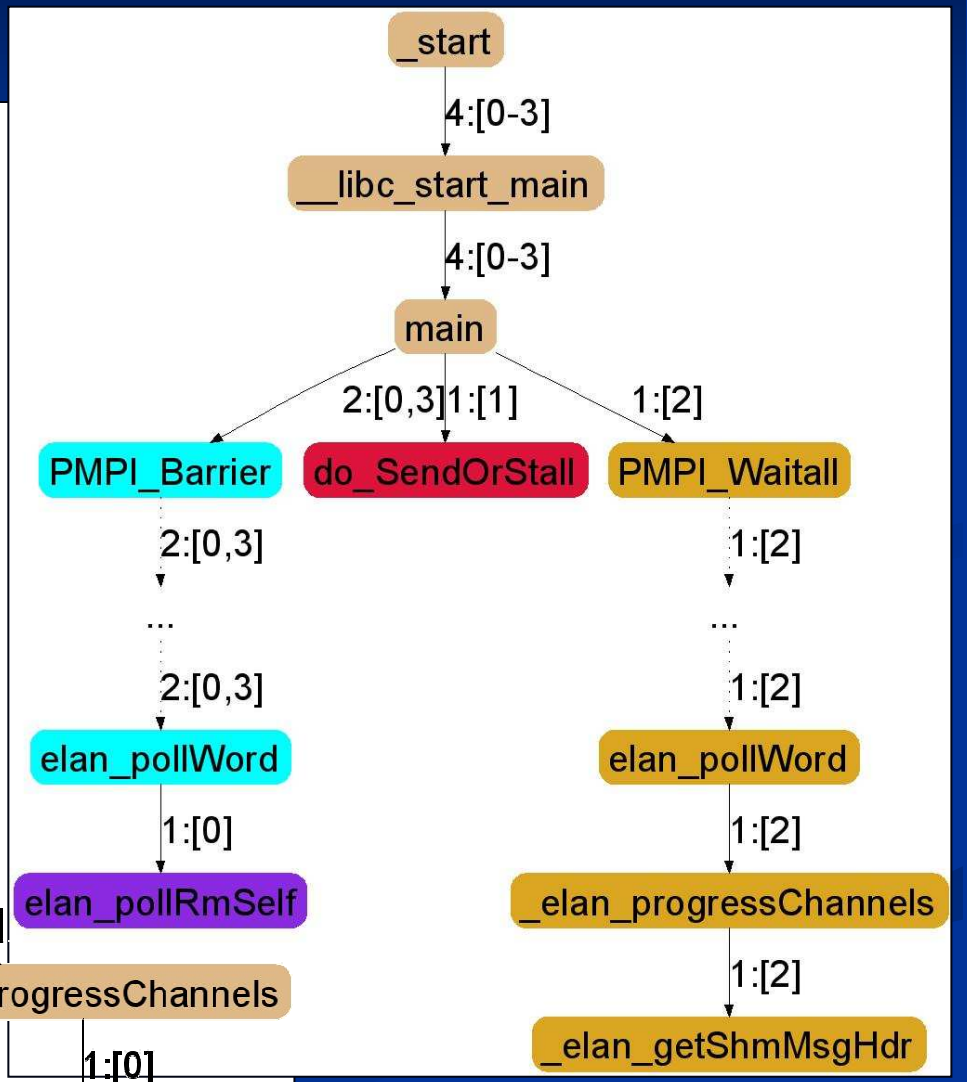
Stack Prefix Trees



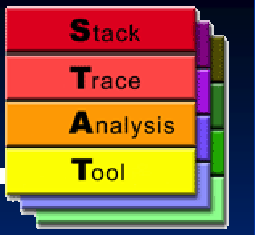
2D Trace Analysis







3D-Trace/Space/Time Analysis



Appl

Appl

Appl

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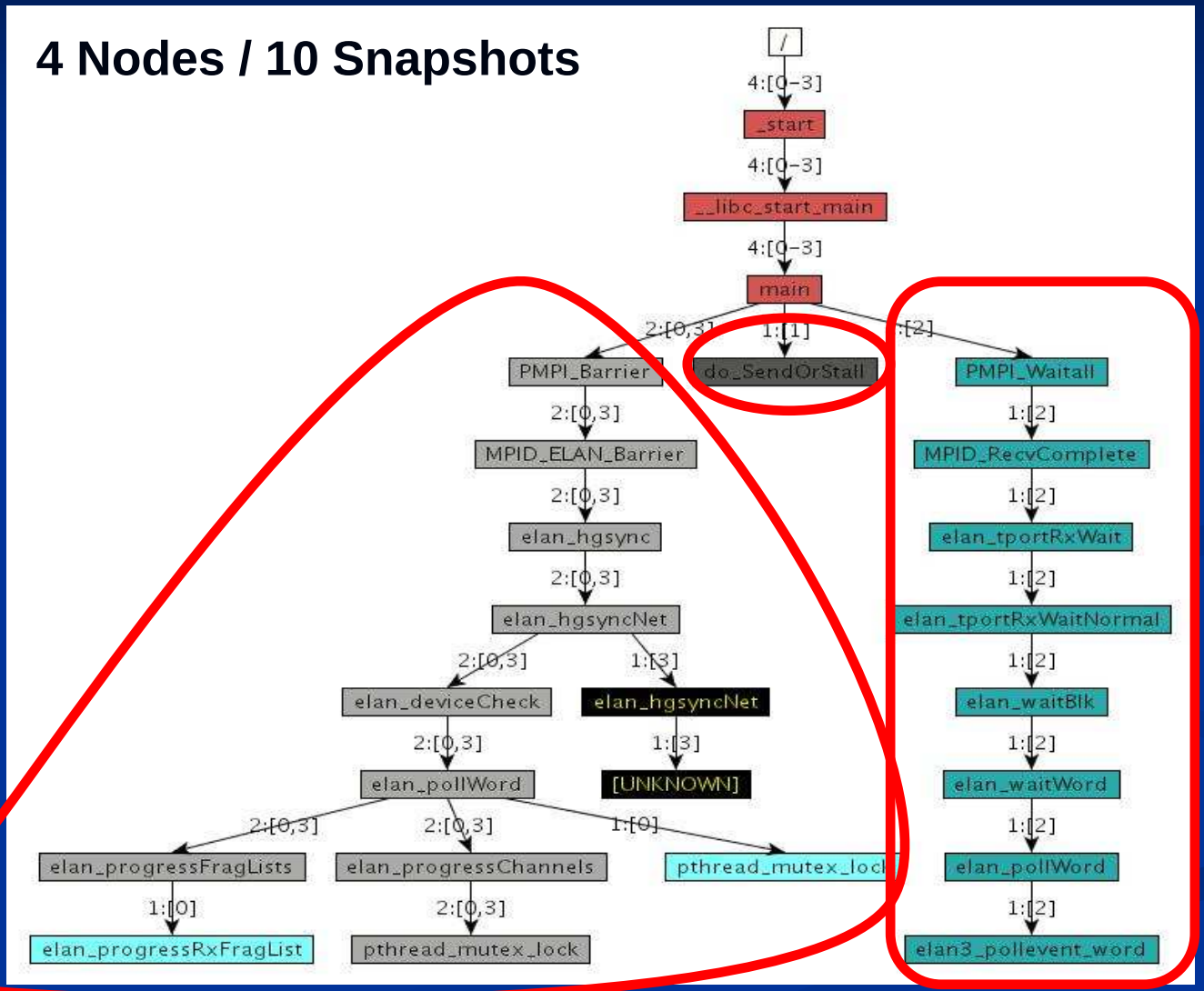
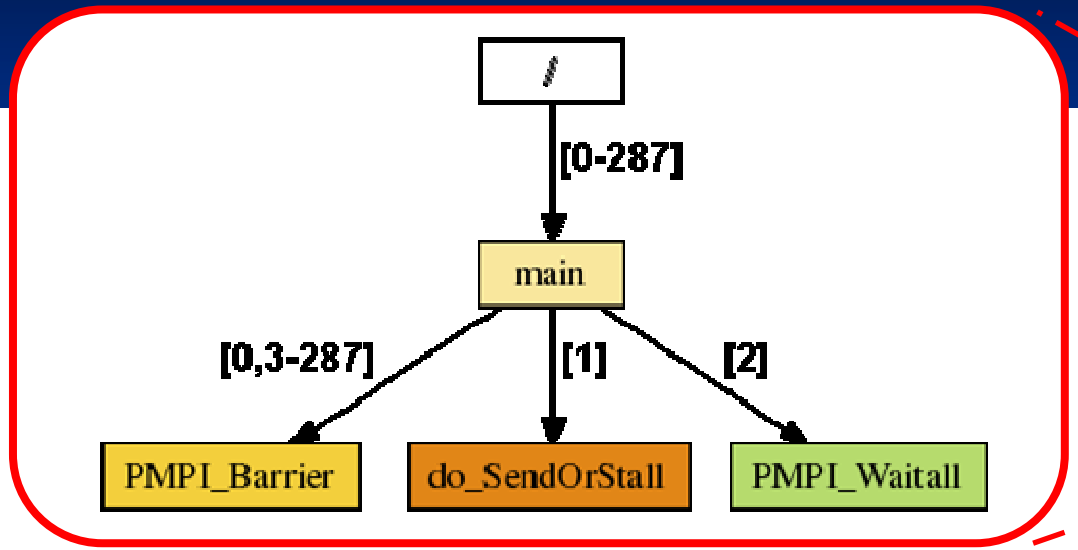
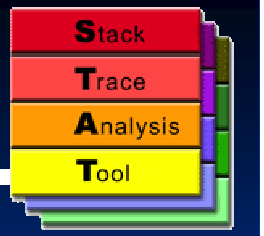


3D-Trace/Space/Time Analysis

Stack Trace Analysis Tool

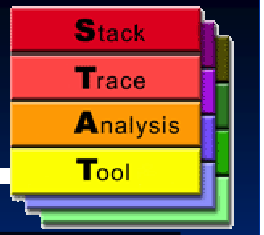


Achieving Scalability

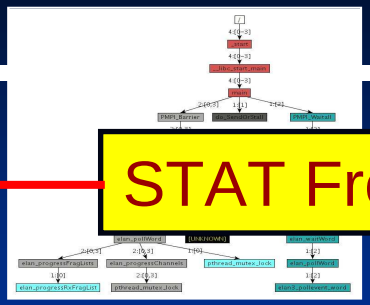


- Lower overhead than full debugger, but …
  - *Need to aggregate across all nodes*
  - *Bottleneck on tool front end*
  - *Traditional designs will not scale*
- Tree based reduction
  - *Merge partial trees on the fly*
  - *Implementation using MRNet*
- STAT components
  - *Backend (BE) daemons gathering traces*
  - *Communication processes merging prefix trees*
  - *Frontend (FE) tool storing the final graph*

Work and Data Flow



trace(count, freq.)



FE

STAT Frontend

Tree Merge

CP

CP

MRNet Communication Process

CP

CP

STAT Tool Daemon

BE

M M M MPI

BE

M M M MPI

. . .

BE

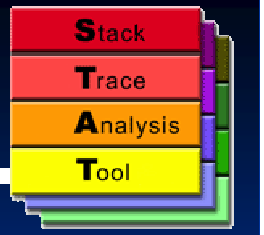
M M M MPI

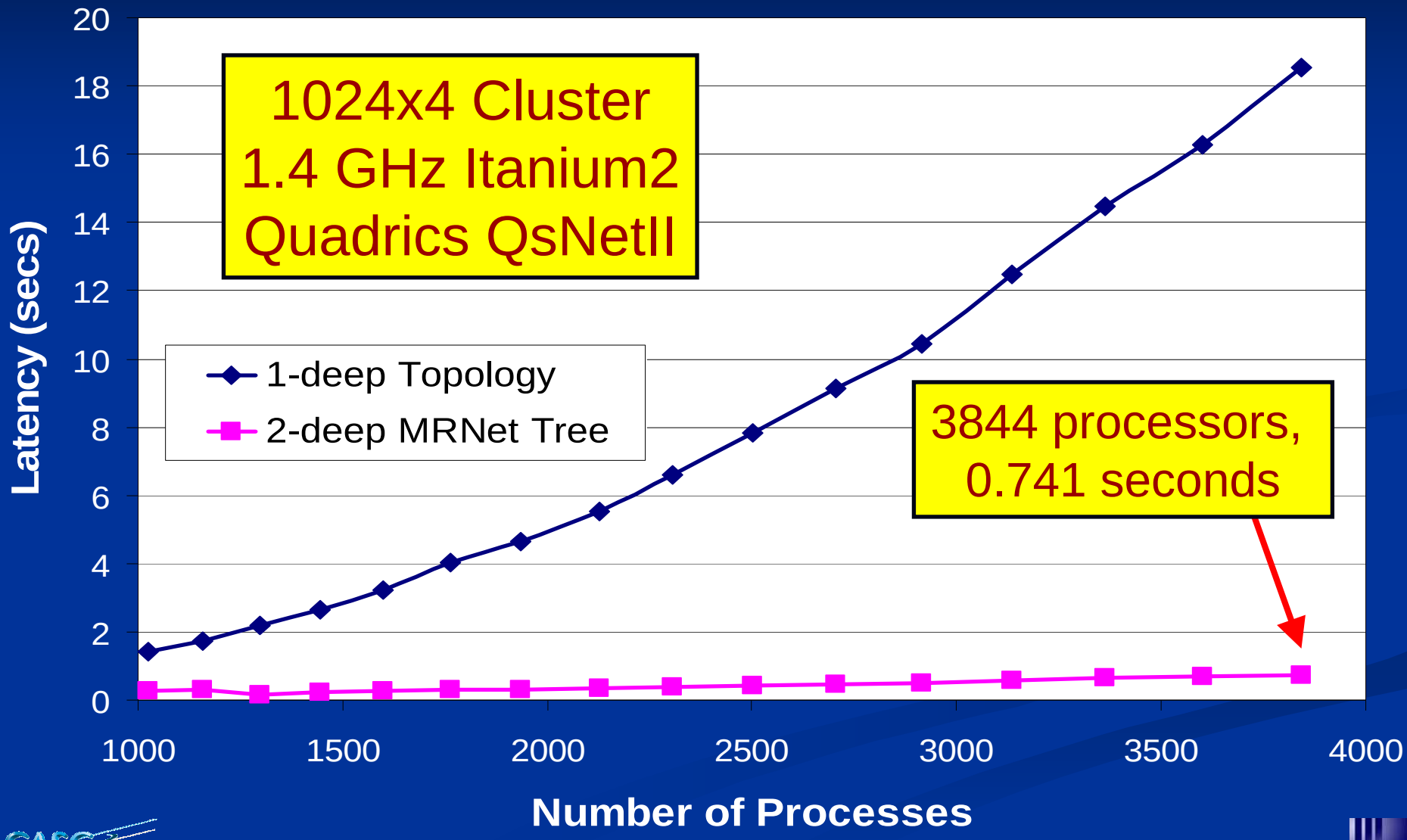
BE

M M M MPI

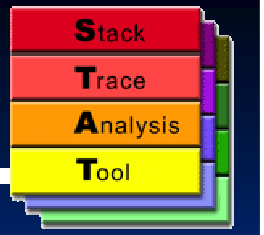
Application Processes

STAT Performance





STAT Summary



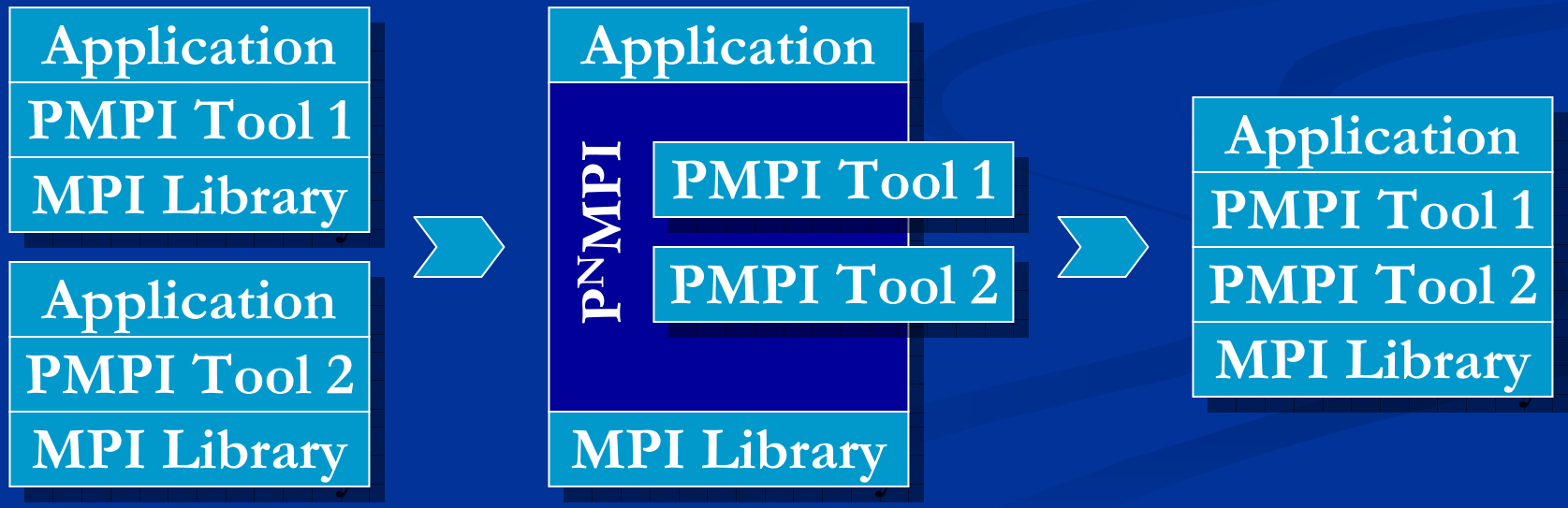
- Scalable Stacktrace Analysis
  - *Lightweight tool to identify process classes*
  - *Aggregation in Time and Space*
  - *Guide the use of full featured debuggers*
- Reduction network
  - *Based on merged callgraph prefix trees*
  - *Process merge operation inside the tree*
- *More Information:*
  - Stack Trace Analysis for Large Scale Debugging *Arnold, Ahn, de Supinski, Lee, Miller, Schulz IPDPS 2007*
  - *http://www.paradyn.org/STAT*

General Tool Infrastructures

- Application Specific Tools
  - *Adjust to special scenarios*
  - *Analyze and Optimize one target code*
  - *Prototypes for more general tools*
- Need the ability for quick prototypes
  - *Reuse existing components*
  - *Dynamically assemble tools*
  - *Specialize existing tools*
- MPI Tools
  - *Successful interface: PMPI*
  - *No support for cooperation or integration*
  - *All tools have a global scope*

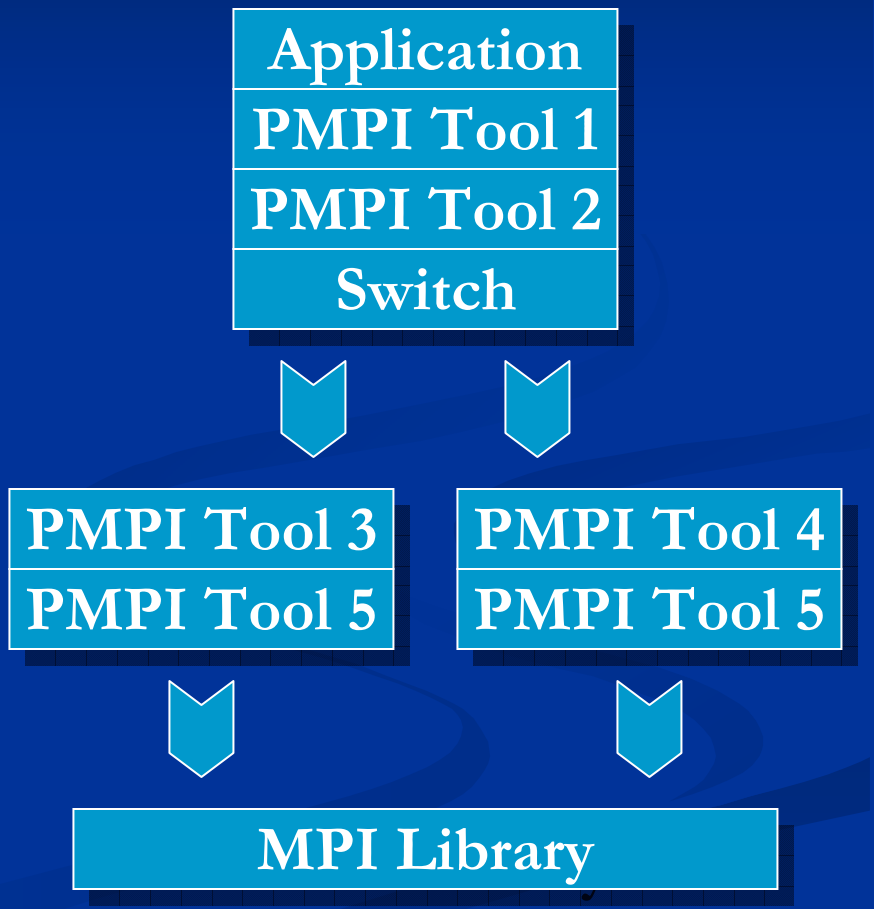
PNMPI Infrastructure

- MPI Tool Infrastructure
  - *Maintain compatibility with PMPI interface*
  - *Dynamic creation of tool stacks*
  - *Transparent to end & tool user*
  - *Plug-ins binary compatible with PMPI tools*

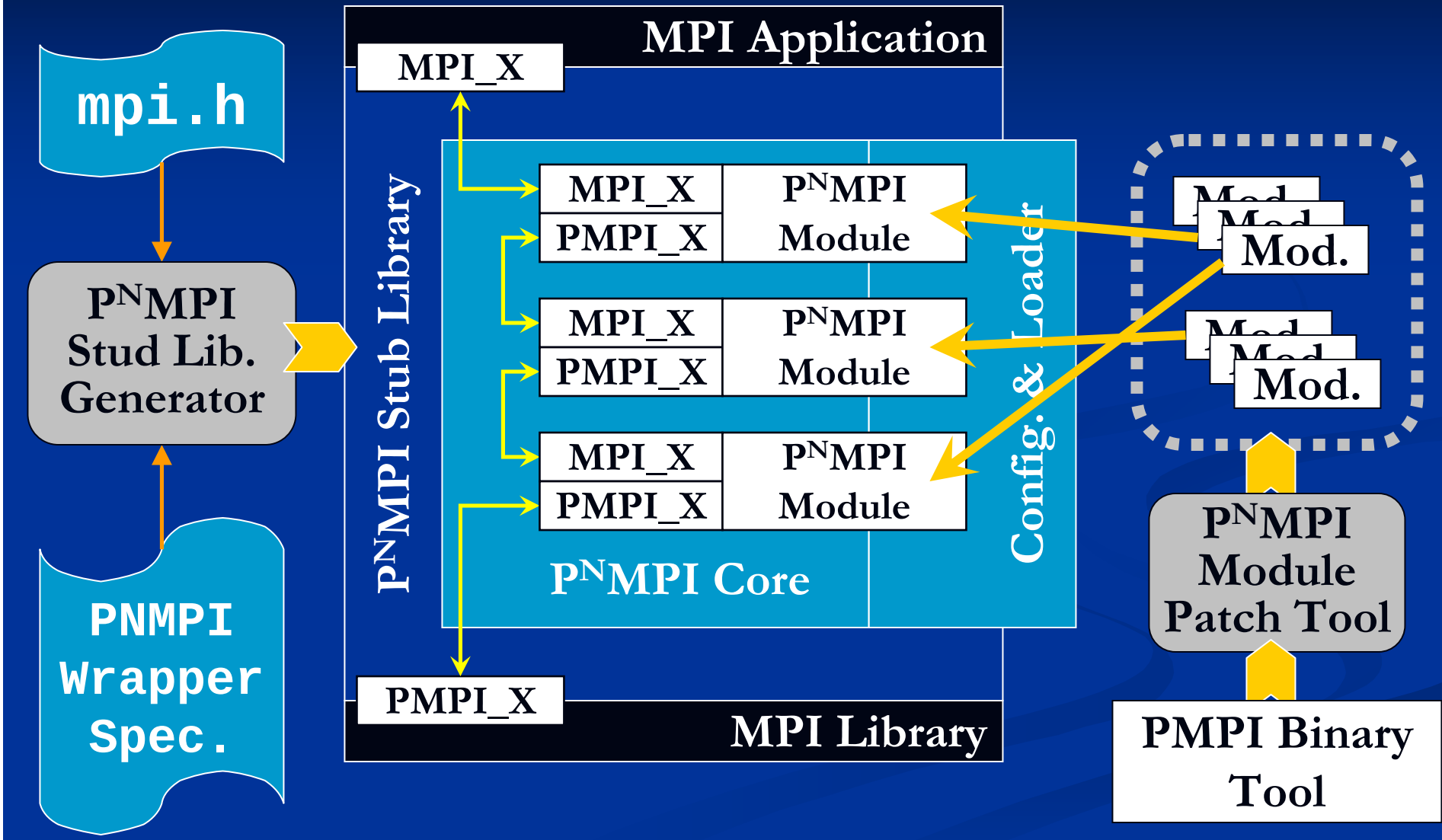


PNMPI Switch Modules

- Multiple tool stacks
  - *Defined independently*
  - *Initial tool stack called by application*
- Switch modules
  - *Dynamic stack choice*
  - *Based on arguments or dynamic steering*
- Duplication of tools
  - *Multiple contexts*
  - *Separate global state*

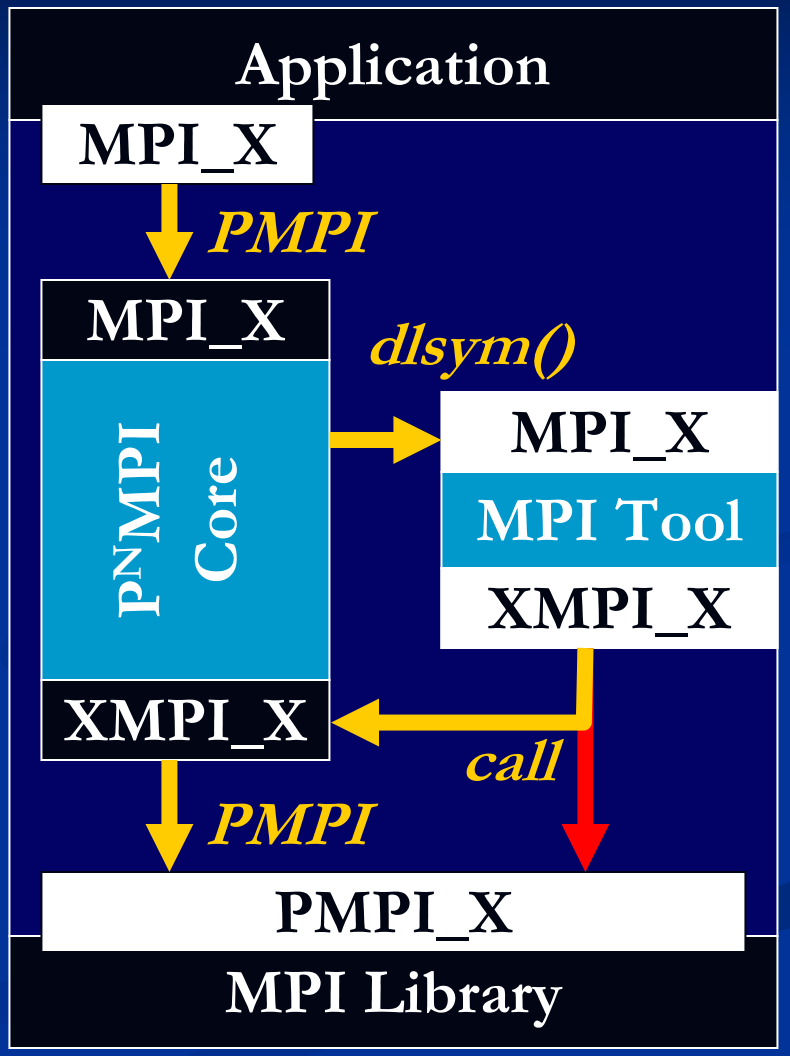


Architecture



Module Creation

- Reuse existing tools
  - *PMPI binaries*
  - *Transparency*
- Prevent PMPI calls
  - *Patch binary to rename all PMPI calls*
  - *Provide routine with patched name in P^{N}MPI*
- Core gains control after module invocation



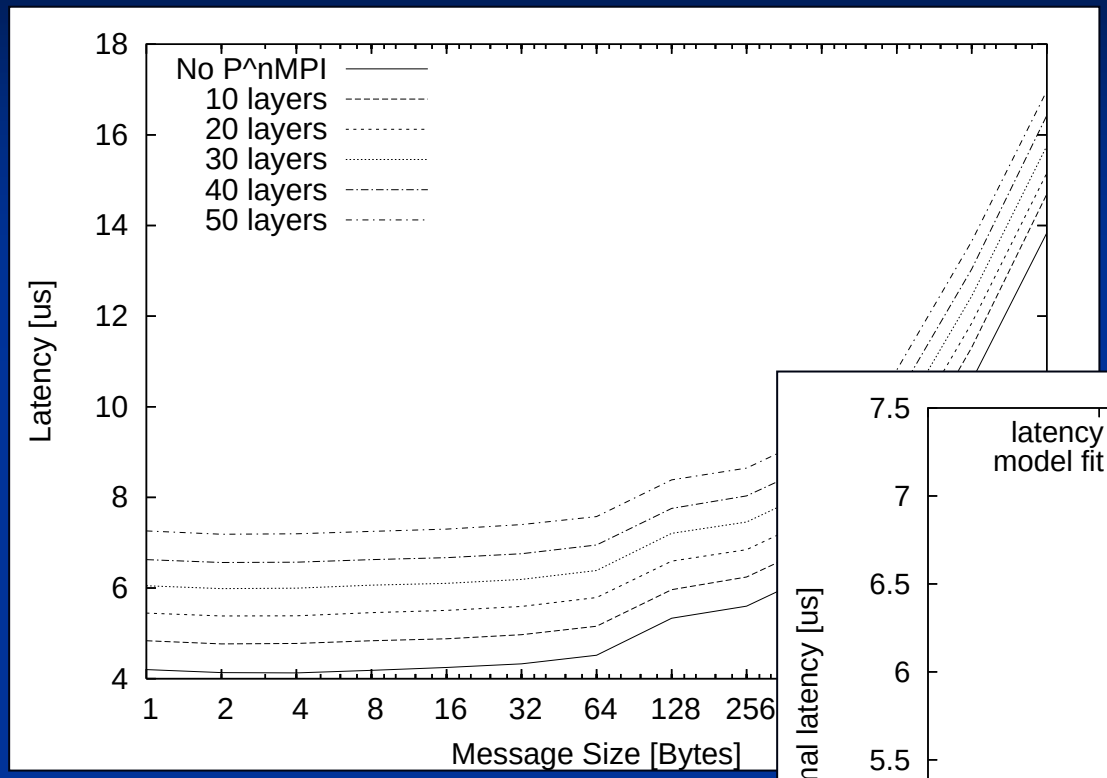
PNMPI Services

- Registration
  - *Make tool module visible to other tools*
  - *Process module arguments*
- Publish/Subscribe Services
  - *Offer callbacks to services*
  - *Query services in other modules*
  - *Type signatures*
- Pcontrol
  - *Control selected modules*
  - *PNMPI specific Pcontrol syntax*

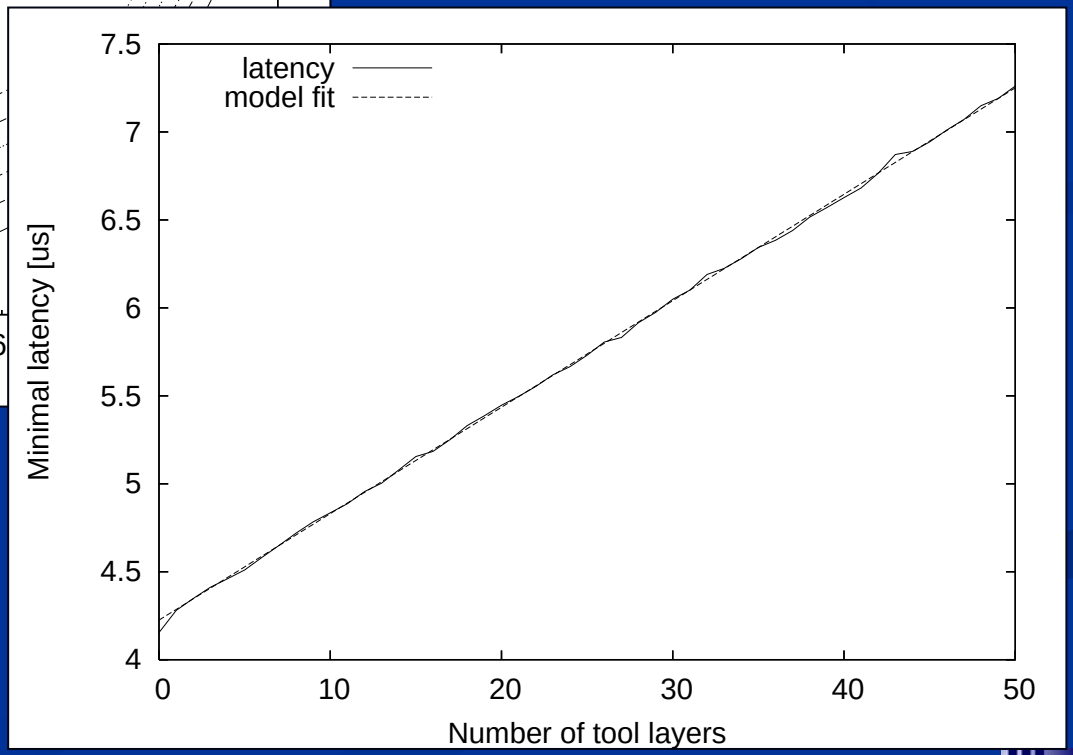
Setup & Configuration

- P^{N}MPI configuration file
  - *Define tool stacks*
  - *Set tool arguments*
  - *Evaluated at program start*
- Static version available
  - *Prelink configuration of tool stack*
  - *Support for machines like BG/L*
- Experimental Setup
  - *Atlas cluster: 44 TFlop/s cluster at LLNL*
  - *1152 nodes with 8 Opteron cores each*
  - *Mellanox Infiniband Interconnect*

Overhead



Stacking Empty Tool Layers



Overhead ~ # tools

Independent of # tasks

Usage Scenarios

- Concurrent Execution of Transparent Tools
  - *Tracing and Profiling*
  - *Message Perturbation and MPI Checker*
- Tool Cooperation
  - *Encapsulate common tool operations*
  - *Examples: datatype walking, request tracking*
  - *Application level MPI checkpointing*
- Tool Multiplexing
  - *Apply tools to subsets of applications*
  - *Run concurrent copies of the same tool*
- MPI job virtualization

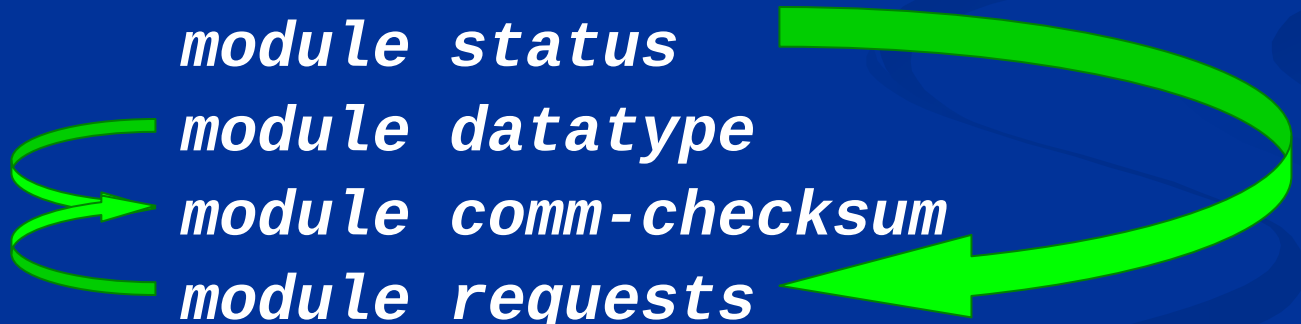
Checksums

- Goal: checksums for each message
  - *Compute at SEND*
  - *Piggyback checksum*
  - *Check at RECV*
- Detects message corruptions
  - *Message buffer corruptions*
  - *Incorrect MPI implementations*
- Requires many typical tasks
  - *Walk arbitrary datatypes*
  - *Track requests for asynchronous messages*
  - *Intercept all communication events*

Implementation

- Encapsulate each task in one module
  - *Module to capture all MPI datatypes*
  - *Replace MPI Request and Status objects*
  - *Extend generic communication callback module*
- Configuration file

```
module status
module datatype
module comm-checksum
module requests
```



- Test application: SMG 2000

Checksum Performance

Active Modules	16 tasks / 4 nodes Exec. Time	Overhead	64 tasks / 16 nodes Exec. Time	Overhead	256 tasks / 64 nodes Exec. Time	Overhead
No P^NMPI	29.18	—	31.35	—	34.84	—
Status	29.28	0.3%	31.45	0.3%	34.98	0.4%
Requests	29.37	0.6%	31.59	0.8%	35.18	1.0%
Datatype	29.25	0.2%	31.42	0.2%	34.98	0.4%
Comm	29.47	1.0%	31.75	1.3%	35.30	1.3%
Piggyback	29.85	2.3%	32.48	3.6%	36.77	5.5%
Checksum	34.39	17.8%	37.11	18.4%	42.67	22.5%

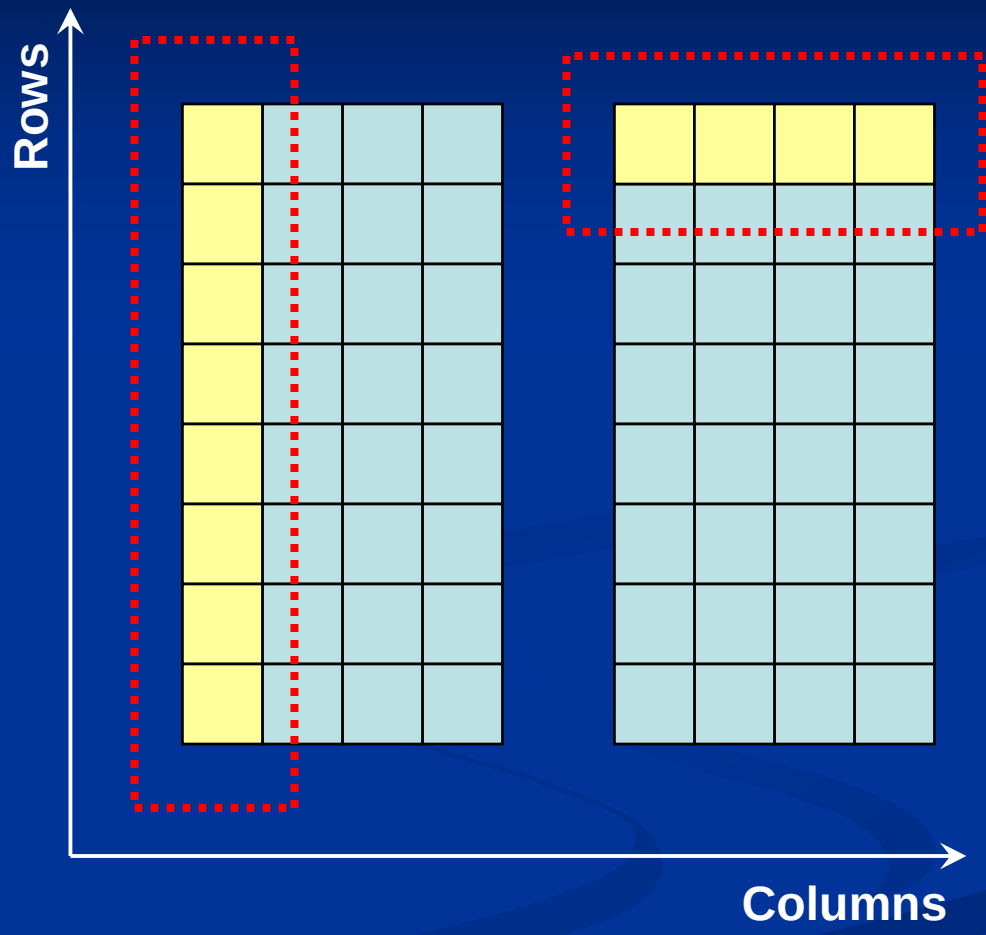
- Observations:
  - *Support modules cause only minimal overhead*
  - *Scalability*
  - *Actual overhead comes from tool itself*

Selective Profiling

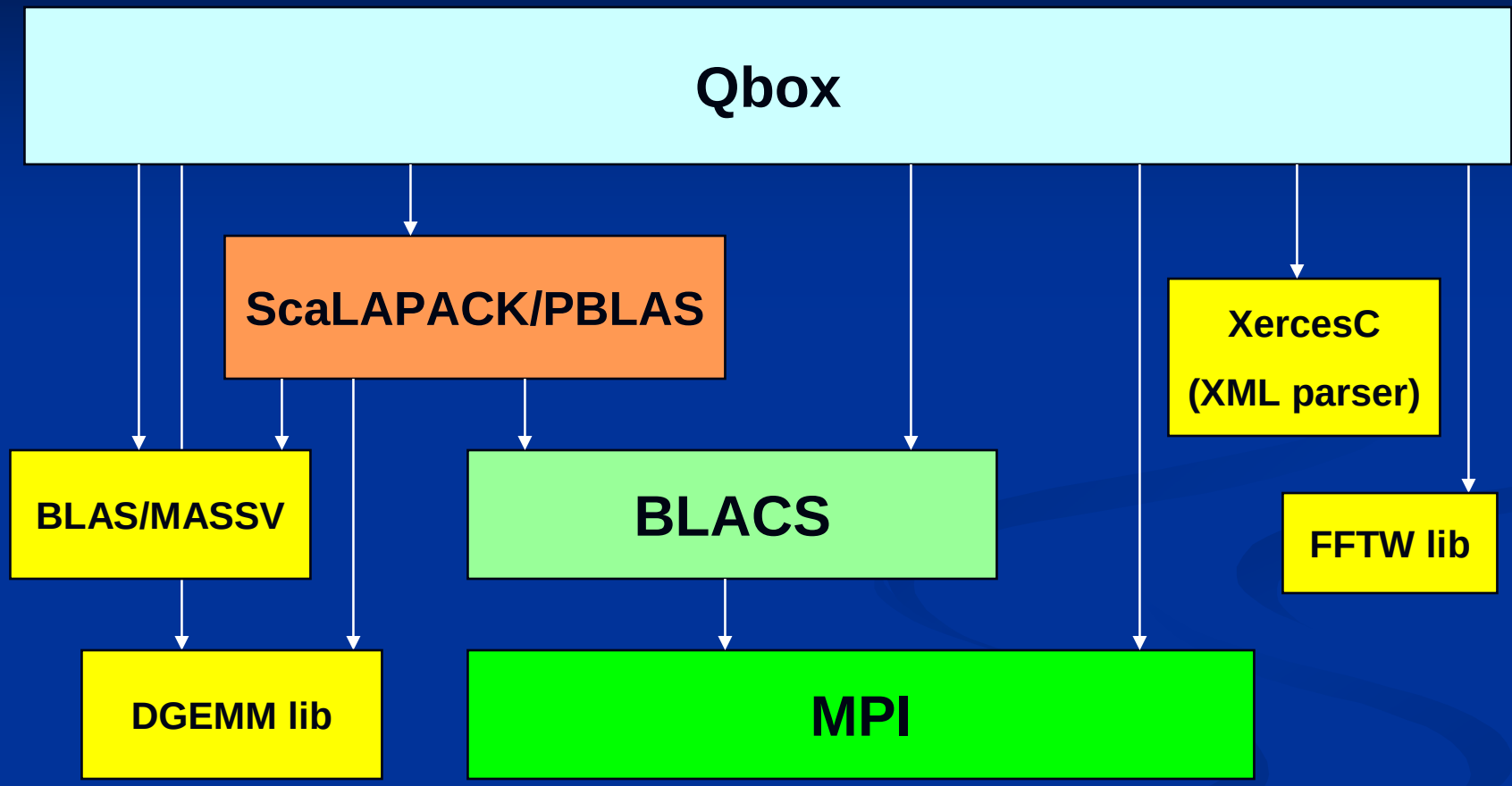
- MPI Profiling
  - *Provide aggregated view of MPI performance*
  - *Example: mpiP library*
- Disadvantage
  - *Global view of whole application*
  - *Can't distinguish communicators or groups*
- Approach with P^{N}MPI
  - *Replicate instances of unmodified profiler*
  - *Switch module to determine context*
  - *Forward MPI call to matching profiler instance*

Example: QBox

- Dense matrix
  - *Row and column communicators*
  - *Global operations*
- Communication patterns
  - *Depends on the communicator*
  - *Need to profile separately*



QBox Code Structure



- *Implicit generation of communicators*
- *Frequent creation and destruction*

Profiling Setup

- Configuration file:

Default Stack

```
module commsize-switch
argument sizes 8 4
argument stacks column row
module mpiP
```

Target Stack 1

```
stack row
module mpiP1
```

Target Stack 1

```
stack column
module mpiP2
```

Switch Module

Arguments controlling switch module

Multiple profiling instances

Results

Count	Global	Sum	COMM_WOLRD	Row	Column
Send	317365	317245	31014	202972	83259
Allreduce	319028	319028	269876	49152	0
All2allv	471488	471488	471488	0	0
Recv	379355	379265	93034	202972	83259
Bcast	401312	401042	11168	331698	58176

- Information helpful for …
  - *Evaluating interactions of libraries and MPI*
  - *Understanding impact on the network*
  - *Optimization of collectives*
  - *Node mapping*

Summary PnMPI

- PNMPI tool infrastructure
  - *Keep PMPI interface*
  - *Specify any number of tools at runtime*
  - *Dynamic creation of tool chains*
- Optional services
  - *Publish/Subscribe services*
  - *Dynamic tool stack selection*
- Extend/Specialize/Assemble tools
  - *New functionality using existing building blocks*
  - *Change tools without relinking*
  - *Fast prototyping using generic tool services*

Lessons for Petascale Tools

- Tools are essential in Petascale efforts
  - *Need to debug at large scale*
  - *Performance optimization to exploit machines*
- Centralized infrastructures will not work
  - *Tree-based aggregation schemes*
  - *Distributed storage and analysis*
  - *Node count independent infrastructures*
- Need for flexible and scalable toolboxes
  - *Integration and interoperability*
  - *Comprehensive infrastructures*
  - *Community effort necessary*

Future Work

- Scalable performance tools
  - *Utilization of tree-based communication (MRNet)*
  - *Platform: Open|SpeedShop*
- Tool integration & infrastructures
  - *Leverage or establish community standards*
  - *Encapsulate common tasks (e.g., MPI launcher)*
- New capabilities
  - *Automatic MPI pattern extraction*
  - *Memory scalability analysis*
  - *"Performance Cook Books"*

Conclusions

- System size growing towards Petascale
  - *Tools must scale with systems and codes*
  - *New concepts and infrastructures necessary*
- Scalable debugging with STAT
  - *Lightweight tool to narrow search space*
  - *Tree-based stack trace aggregation*
- Dynamic MPI tool creation with P^NMPI
  - *Ability to quickly create application specific tools*
  - *Transparently reuse and extend existing tools*
- Tool interoperability increasingly important