

# High-Performance Computing Research Internship and Appointment Opportunities at Oak Ridge National Laboratory

Dr. Christian Engelmann

Computer Science and Mathematics Division Oak Ridge National Laboratory



U. S. DEPARTMENT OF ENERGY





# **National Center for Computational Sciences**

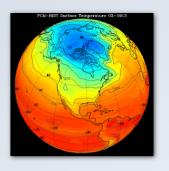
- ◆ 40,000 ft² (3700 m²) computer center:
  - ■36-in (~1 m) raised floor, 18 ft (5.5 m) deck-to-deck
  - 36 MW of power with 6,600 t of redundant cooling
  - High-ceiling area for visualization lab: 35 MPixel PowerWall
- ◆ 5 systems in the Top 500 List of Supercomputer Sites:
  - 1. Jaguar XT5: Cray XT5, with 224,162 processor cores at 2,331 TFlop/s peak
  - 3. Kraken: Cray XT5, with 98,928 processor cores at 1,028 TFlop/s peak
  - 16. Jaguar XT4: Cray XT4, with 30,976 processor cores at 260 TFlop/s peak
  - 30. Athena: Cray XT4, with 17,956 processor cores at 165 TFlop/s peak
  - 370. Eugene: IBM BGP, with 8,192 processor cores at 28 TFlop/s peak

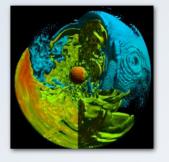


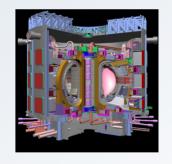


# At Forefront in Scientific Computing and Simulation

- Leading partnership in developing the National Leadership Computing Facility
  - Leadership-class scientific computing capability
  - □Currently planning for 10-20 PFlop/s in 2012
  - **□On the path toward:** 
    - 100 PFlop/s in 2015 ( 10- 100 million cores)
    - 1,000 PFlop/s in 2018 (100-1,000 million cores)
- Attacking key computational challenges
  - □Climate change
  - ■Nuclear astrophysics
  - ■Fusion energy
  - Materials sciences
  - Biology
- Providing access to computational resources through high-speed networking





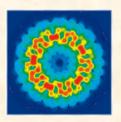


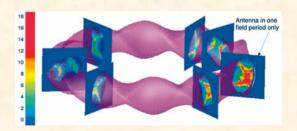


# **Computer Science Research Groups**

- Computer Science and Mathematics (CSM) Division.
  - Applied research focused on computational sciences, intelligent systems, and information technologies.
- CSM Research Groups:
  - Climate Dynamics
  - Complex Systems
  - Computational Chemical Sciences
  - Computational Materials Science
  - Future Technologies
  - Statistics and Data Science
  - Computational Mathematics
  - Computer Science Research (23 researchers & postdocs)







# **Computer Science Research Group Projects**

- Parallel Virtual Machine (PVM)
- PVM





- MPI Specification, FT-MPI and Open MPI
- Common Component Architecture (CCA)
- Open Source Cluster Application Resources (OSCAR)
- Scalable cluster tools (C3)
- Scalable Systems Software (SSS)
- Fault-tolerant metacomputing (HARNESS)



Super-scalable algorithms research



Distributed file and storage systems (Freeloader)



## **MSc Internship Basics**

- 1-2 students (max. 4) for max. 6 months at Oak Ridge National Laboratory in Oak Ridge, Tennessee, USA
- Full-time (40 hours/5 days per week) internship supervised by a research staff member
- Individual leading-edge projects that include background investigation, design, and development
- Includes MSc thesis and draft research paper write-up as part of the final MSc project
- \$1500 per month stipend plus travel costs depending on student qualifications
- Subcontracts through the University of Tennessee, Knoxville, USA

## **MSc Internship Timeline (Spring)**

Early Dec.: Application process

Specify area of interest/project

Submit resume/CV to Vassil

Dec./Jan.: Acceptance notification

**Background Check/Subcontracts** 

J-1 (Student) Visa application

February: Visa issued through U.S. Embassy

1. March: Start of internship

31. August: End of internship

September: Presentation at the University of Reading

#### **MSc Internship Timeline (Fall)**

Early June: Application process

Specify area of interest/project

Submit resume/CV to Vassil

Mid June: Acceptance notification

Background check/subcontracts

J-1 (Student) visa application

August: Visa issued through U.S. Embassy

1. September: Start of internship

28. February: End of internship

March: Presentation at the University of Reading

#### **Further Practical Information**

- Driver license is a must: No public transport to work.
- \$3500 (2500€) in initial min. funds needed for:
  - First rent and various deposits
  - One-week car rental (reimbursed afterwards)
    - Under 25? Car rental & insurance is more expensive
  - Used car, car sales tax, registration, and insurance
- Break-even point:
  - 1 student after 4-5 months, 2 students after 2-3 months
  - Most students leave with a net plus despite extra expenses for: high-speed Internet, cable TV, and weekend trips

## Possible Projects (see next slides for details)

- Proactive fault-tolerance
  - Extending the scalable monitoring data aggregation system
  - Integration with the existing fault tolerance framework
- ADDAPT (successor of Harness Workbench)
  - Development of an scientific application execution assistant
  - Development of plug-ins for: job & resource management, data staging tools and/or workflow engines
- IAA simulator
  - Adding enhancements to simulate time-accurate application runs on millions of processors with fault tolerance tests
- Soft Error Resilience
  - Developing diskless checkpoint caching, diskless checkpointng or modular redundancy prototypes



# Proactive Fault Tolerance Using Preemptive Migration

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#### **Motivation**

- Large-scale PFlop/s systems have arrived:
  - #1: ORNL Jaguar with 224,162 processor cores
  - #2: LANL Roadrunner with 129,600 processor cores
- Other large-scale systems exist
  - LLNL @ 212,992, ANL @ 163,840, TACC @ 62,976
- The trend is toward larger-scale systems
  - Up to 1,000,000,000 cores in the next 10 years
- Significant increase in component count and complexity
- Expected matching increase in failure frequency
- Checkpoint/restart is becoming less and less efficient

#### Reactive vs. Proactive Fault Tolerance

- Reactive fault tolerance
  - Keeps parallel applications alive through recovery from experienced failures
  - Employed mechanisms react to failures
  - Examples: Checkpoint/restart, message logging/replay
- Proactive fault tolerance
  - Keeps parallel applications alive by avoiding failures through preventative measures
  - Employed mechanisms anticipate failures
  - Example: Preemptive migration

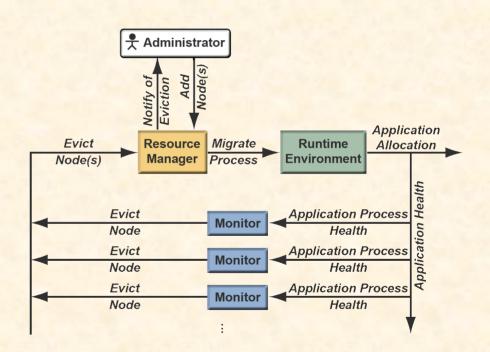
# **Proactive Fault Tolerance using Preemptive Migration**

- Relies on a feedback-loop control mechanism
  - Application health is constantly monitored and analyzed
  - Application is reallocated to improve its health and avoid failures
  - Closed-loop control similar to dynamic load balancing
- Real-time control problem
  - Need to act in time to avoid imminent failures
- No 100% coverage
  - Not all failures can be anticipated, such as random bit flips



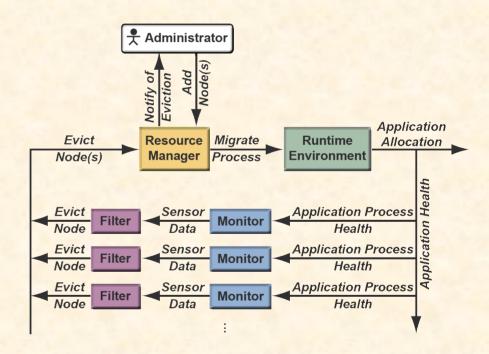
# **Type 1 Feedback-Loop Control Architecture**

- Alert-driven coverage
  - Basic failures
- No evaluation of application health history or context
  - Prone to false positives
  - Prone to false negatives
  - Prone to miss real-time window
  - Prone to decrease application heath through migration
  - No correlation of health context or history



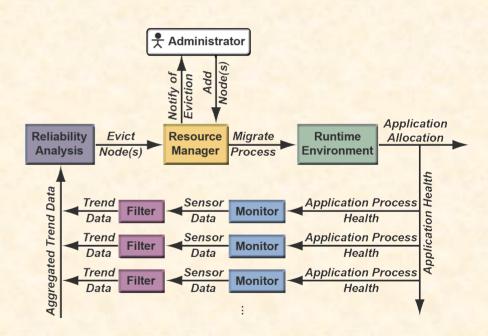
## **Type 2 Feedback-Loop Control Architecture**

- Trend-driven coverage
  - Basic failures
  - Less false positives/negatives
- No evaluation of application reliability
  - Prone to miss real-time window
  - Prone to decrease application heath through migration
  - No correlation of health context or history



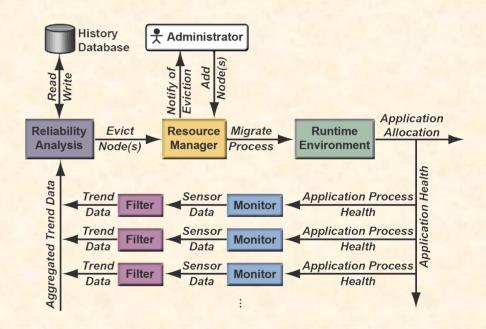
## **Type 3 Feedback-Loop Control Architecture**

- Reliability-driven coverage
  - Basic and correlated failures
  - Less false positives/negatives
  - Able to maintain real-time window
  - Does not decrease application heath through migration
  - Correlation of short-term health context and history
- No correlation of long-term health context or history
  - Unable to match system and application reliability patterns



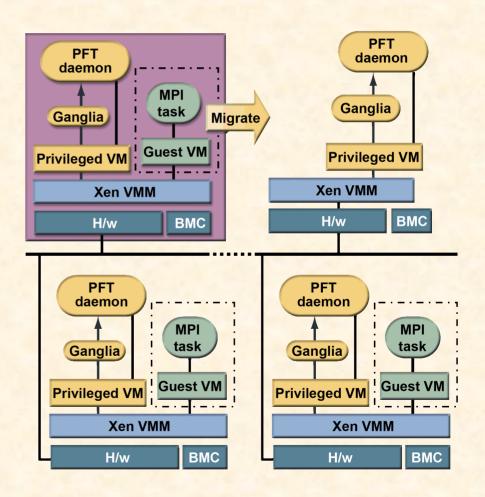
## **Type 4 Feedback-Loop Control Architecture**

- Reliability-driven coverage of failures and anomalies
  - Basic and correlated failures, anomaly detection
  - Less prone to false positives
  - Less prone to false negatives
  - Able to maintain real-time window
  - Does not decrease application heath through migration
  - Correlation of short and longterm health context & history



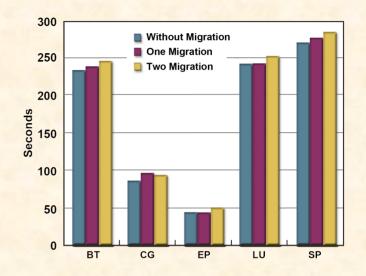
## **VM-level Preemptive Migration using Xen**

- Type 1 system setup
  - Xen VMM on entire system
  - Host OS for management
  - Guest OS for computation
  - Spare nodes without Guest OS
  - System monitoring in Host OS
  - Decentralized scheduler/load balancer using Ganglia
- Deteriorating node health
  - Ganglia threshold trigger
  - Migrate guest OS to spare
  - Utilize Xen's migration facility



## **VM-level Migration Performance Impact**

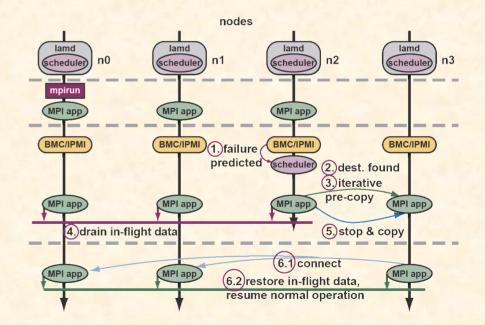
- Single node migration
  - 0.5-5% longer run time
- Double node migration
  - 2-8% longer run time
- Migration duration
  - Stop & copy : 13-14s
  - Live : 14-24s
- Application downtime
  - Stop & copy > Live



16-node Linux cluster at NCSU with dual core, dual-processor AMD Opteron and Gigabit Ethernet

## **Process-Level Preemptive Migration w/ BLCR**

- Type 1 system setup
  - LAM/MPI with Berkeley Lab Checkpoint/Restart (BLCR)
  - Per-node health monitoring
    - Baseboard management controller (BMC)
    - Intelligent platform management interface (IPMI)
  - New decentralized scheduler/ load balancer in LAM
  - New process migration facility in BLCR (stop&copy and live)
- Deteriorating node health
  - Simple threshold trigger
  - Migrate process to spare



#### **Process-Level Migration Performance Impact**

Single node migration overhead

- Stop & copy: 0.09-6 %

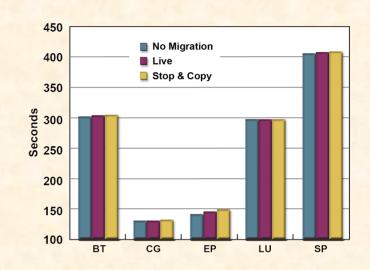
- Live : 0.08-2.98%

Single node migration duration

- Stop & copy: 1.0-1.9s

- Live : 2.6-6.5s

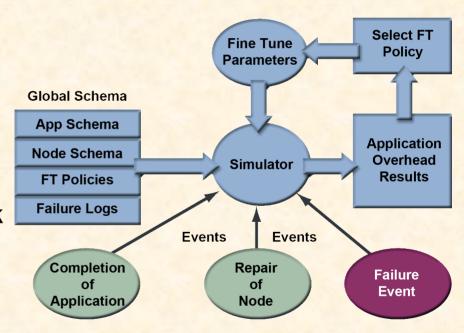
- Application downtime
  - Stop & copy > Live
- Node eviction time
  - Stop & copy < Live</li>



16-node Linux cluster at NCSU with dual core, dual-processor AMD Opteron and Gigabit Ethernet

#### **Simulation of Fault Tolerance Policies**

- Evaluation of fault tolerance policies
  - Reactive only
  - Proactive only
  - Reactive/proactive combination
- Evaluation of fault tolerance parameters
  - Checkpoint interval
  - Prediction accuracy
- Event-based simulation framework using actual HPC system logs
- Customizable simulated environment
  - Number of active and spare nodes
  - Checkpoint and migration overheads



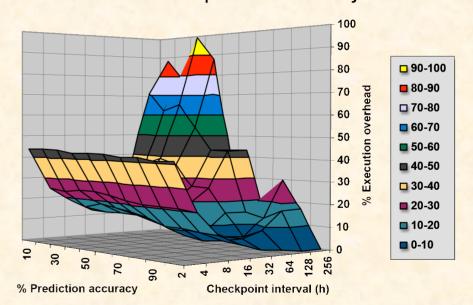
# **Combining Proactive & Reactive Approaches**

- Best: Prediction accuracy >60% and checkpoint interval 16-32h
- Better than only proactive or only reactive
- Results for higher accuracies and very low intervals are worse than only proactive or only reactive

Number of processes	125
Active/Spare nodes	125/12
Checkpoint overhead	50min
Migration overhead	1 min

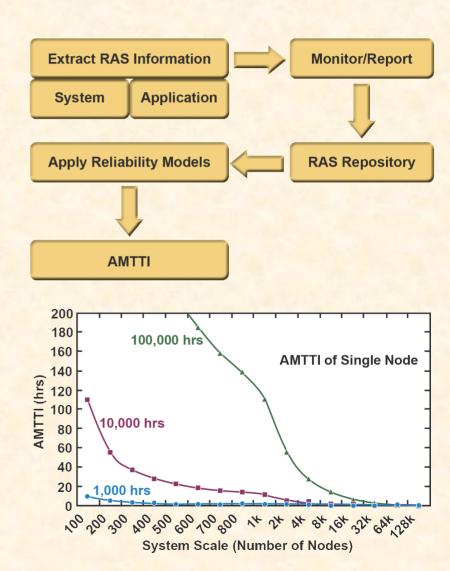
Simulation based on ASCI White system logs (nodes 1-125 and 500-512)

Execution overhead for various checkpoint intervals and different prediction accuracy



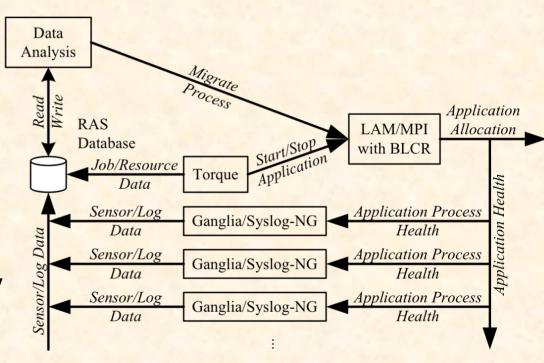
## **Research in Reliability Modeling**

- Type 3 system setup
  - Monitoring of application and system health
  - Recording of application and system health monitoring data
  - Reliability analysis on recorded data
  - Application mean-time to interrupt (AMTTI) estimation
- Type 4 system setup
  - Additional recording of application interrupts
  - Reliability analysis on recent and historical data



#### **Proactive Fault Tolerance Framework**

- Unified interfaces between components
- Extendable RAS engine core interfacing with
  - Monitoring data aggregation/filtering component
  - Job and resource management service
  - Process/VM migration mechanism
  - Online/offline reliability modeling
- Previous Reading MSc student (A. Litvinova)



## **Ongoing and Future Work**

- Research in scalable monitoring data aggregation/filtering
  - Scalable, fault tolerant overlay reduction networks
  - In-flight monitoring data aggregation
  - Current MSc student (Swen Boehm)
- Research in scalable monitoring data filtering
  - Extend the current prototype with in-flight data filtering
  - Enhance filters with statistical analysis techniques
- Research in scalable syslog data aggregation/filtering
  - Extend the current prototype with log message aggregation
- Integrate scalable monitoring prototype with proactive fault tolerance framework

# **Challenges Ahead**

- Health monitoring
  - Identifying deteriorating applications and OS conditions
  - Coverage of application failures: Bugs, resource exhaustion
- Reliability analysis
  - Performability analysis to provide extended coverage
- Scalable data aggregation and processing
  - Key to timeliness in the feedback control loop
- Need for standardized metrics and interfaces
  - System MTTF/MTTR != Application MTTF/MTTR
  - System availability != Application efficiency
  - Monitoring and logging is system/vendor dependent

#### **Acknowledgements**

- Investigators at Oak Ridge National Laboratory:
  - Stephen L. Scott [Lead PI], Christian Engelmann, Geoffroy Vallée, Thomas Naughton, Anand Tikotekar, George Ostrouchov
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- Investigators at North Carolina State University:
  - -Frank Mueller [Lead PI], Chao Wang, Arun Nagarajan, Jyothish Varma
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# ADDAPT: Assisting Application Development, Deployment, and Execution

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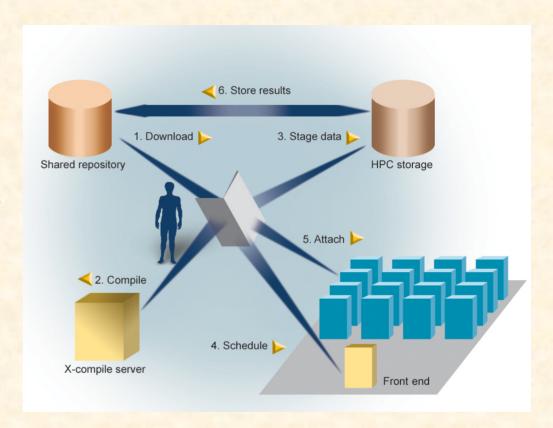
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#### **Research and Development Goals**

- Increasing the overall productivity of developing and executing computational codes
- Optimizing the development and deployment processes of scientific applications
- Simplifying the activities of application scientists, using uniform and adaptive solutions
- "Automagically" supporting the diversity of existing and emerging high—performance computing architectures



Typical scientific application development, deployment, and execution activities

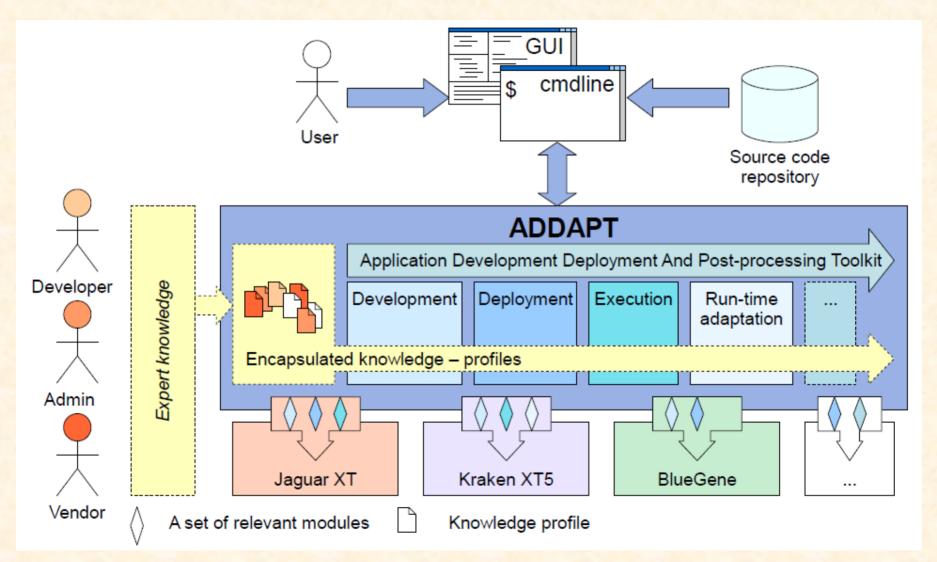








#### **ADDAPT Architecture**



## **ADDAPT Components**

#### Porting assistant

- to help port new libraries and kernels into legacy codes,
- to identify incompatibilities with the system software stack,
- do automatic source-to-source translation, and
- identify areas to improve performance or fault tolerance.

#### Build assistant

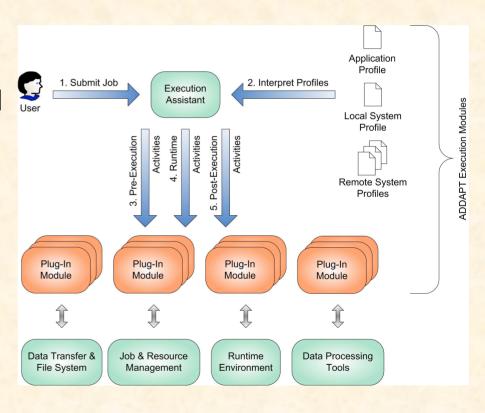
- to adapt the application's build script to the site-specific versions of compilers, libraries, and flags, and
- to help resolve problems at the link stage.

#### Execution assistant

 to assist in data staging, fast application launch, runtime support, and post-execution data off loading.

# Ongoing and Future Work: ADDAPT Execution Assistant Component

- Combine knowledge from application and site profiles
  - Match application properties with system needs using ontologies and reasoning
- Assist the scientist in running his/her application
  - Adapt system configuration to application needs
- Automate data staging and pre-/post-processing activities
  - Interface with respective tools through plug-ins





# Institute for advanced Architectures and Algorithms (IAA): Simulation Efforts at ORNL

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#### **Objectives**

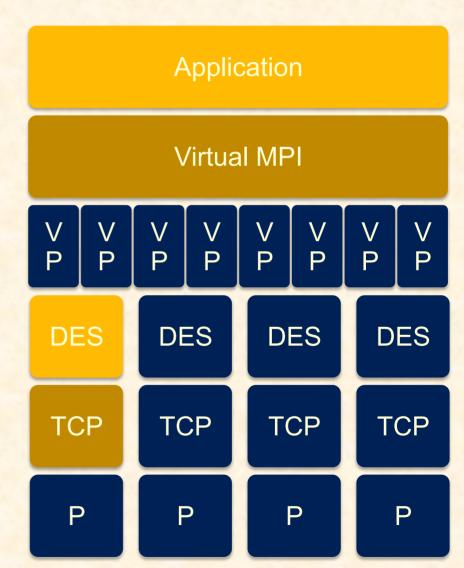
- Simulation of system architectures at scale
- To investigate scalability, performance, and fault tolerance of algorithms at extreme scale
- ORNL's earlier work was already able to run up to 1,000,000 simulated processes (JCAS)

### Java Cellular Architecture Simulator (JCAS)

- Developed at ORNL in Java
- Native C and Fortran application support using JNI
- Runs as standalone or distributed application
- Lightweight framework simulates up to 1,000,000 lightweight virtual processes on 9 real processors
- Standard and experimental network interconnects:
  - Multi-dimensional mesh/torus
  - Nearest/Random neighbors
- Message driven simulation without notion of time
  - Not in real-time, no time-accurate discrete event simulation
- Primitive fault-tolerant MPI support
  - No collectives, no MPI 2

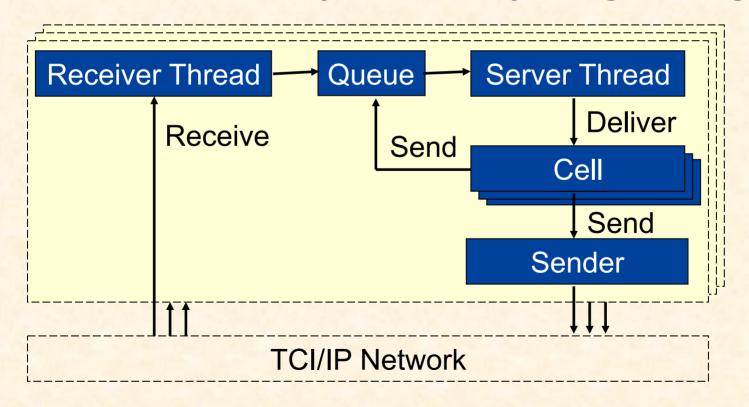
#### **Technical Approach**

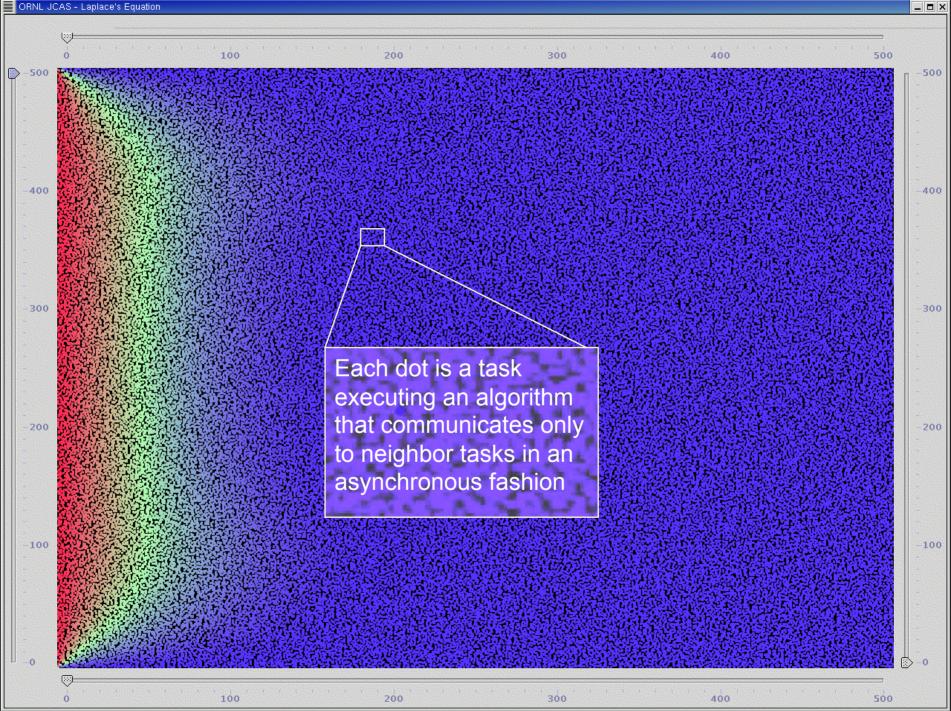
- Distributed set of discrete event simulators with nodelocal message queues
- Simulation of virtual MPI processes for parallel app.
- Virtual processes run on real hardware with virtual MPI
- No virtual process time
- Fault injection capability
- Interactive graphical user interface as front-end
- TCP servers as back-ends

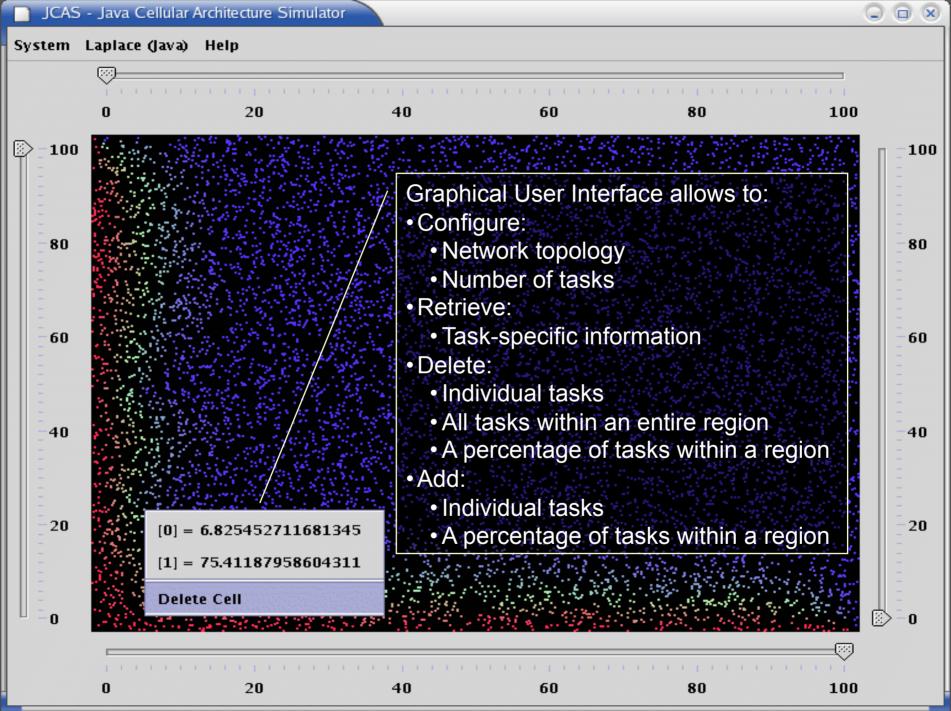


#### **Implementation**

- Every cell has own code, memory and neighbors list
- Server hosts cells and initiates the context switch
- Cells communicate asynchronously using messages





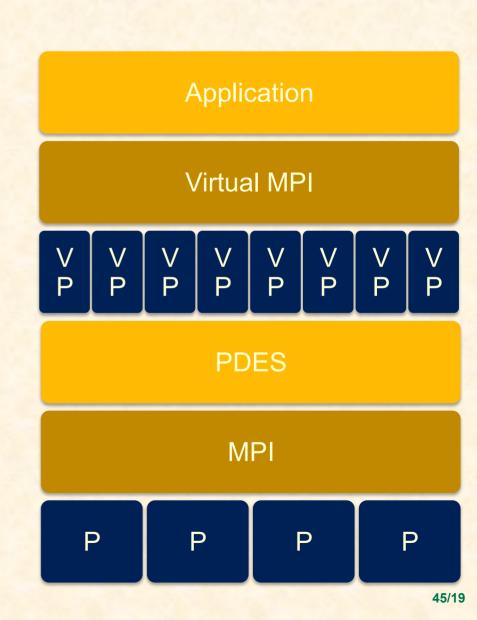


#### **IAA Simulation Efforts at ORNL**

- Investigate scalability, performance and fault tolerance of algorithms at extreme scale through simulation
- Extending the JCAS simulation capabilities
  - Simulating more processes (~10,000,000)
  - Running more complex and resource-hungry algorithms
  - Support for unmodified MPI applications
- Evaluation of algorithms at extreme scale
  - Notion of global virtual time and virtual process clocks
  - Accounting for resource usage, such as processor and network
  - Gathering of scalability, performance & fault tolerance metrics
  - Parameter studies at scale

#### **Technical Approach**

- Parallel discrete event simulation (PDES) atop MPI
- Simulation of virtual MPI processes for parallel app.
- Virtual processes run on real hardware with virtual MPI
- Consistent virtual process clock from PDES
- Virtual process clock can be scaled by PDES via model
- Virtual interconnect latency is set by PDES via model



#### **Ongoing and Future Work**

- Ported JCAS to C/C++ to improve scalability/performance
- Replaced TCP/IP with (native) MPI communication
- Replaced distributed set of DESs with PDES
  - Conservative synchronization only, need optimistic and timewarp synchronization
- Extend virtual MPI capabilities
  - Asynchronous, collectives, process control (spawn), ...
- Extend fault injection and notification mechanisms
  - Injection based on failure distributions and application state
- Add simulated machine model (for network)
- Gather scalability, performance & fault tolerance metrics



### Soft-Error Resilience for Future-Generation High-Performance Computing Systems

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#### **Motivation**

- Next-generation HPC systems will have
  - More frequent failures in general
  - More frequent soft errors in particular
  - Less efficient parallel file system checkpoint/restart
- Existing fault tolerance approaches an ongoing research efforts do not cover soft error resilience
  - ECC double-bit errors require node/process restart
  - Silent data corruption remains undetected
- Lack of soft error resilience strategy is preventing deployment of GPUs and FPGAs at scale

#### **Technical approach**

- Compute-node in-memory checkpoint caching
  - Short-term solution
  - Improving parallel file system checkpoint/restart
- Compute-node in-memory checkpoint/restart
  - Near-term solution
  - Replacing parallel file system checkpoint/restart
- Dual-modular redundancy (DMR)
  - Long-term solution
  - Replacing rollback recovery schemes in HPC

## Comparison of traditional and proposed technologies (1/2)

	Dual- Modular Redundancy	In-Memory Checkpoint/ Restart	In-Memory Checkpoint Caching	Traditional Checkpoint/ Restart
<ul><li>Resilience</li></ul>	++++	+++	++	+
← Efficiency	++	+		
Application	Application Application	Application Frequent Checkpointing	Application Frequent Checkpointing	Application
In-Memory		Storage	Cache	
Storage		Storage		
	Infrequent	Infrequent	Frequent	Frequent
Parallel	Checkpointing	Checkpointing	Checkpointing	Checkpointing
File System	Storage	Storage	Storage	Storage
<b>Storage</b>	Storage	Storage	Storage	Storage
8				

# Comparison of traditional and proposed technologies (2/2)

Solution	Processor	Memory	Price	Power
Current: Lustre	1xAMD Opteron 2356		\$500	75W
checkpoint/restart		2x4GB Micron DDR2-800	+\$750	+2W
			=\$1250	=77W
Short-term: Compute-	1xAMD Opteron 2356		\$500	75W
node in-memory		4x4GB Micron DDR2-800	+\$1500	+4W
checkpoint caching			=\$2000	=79W
Near-term: Compute-	1xAMD Opteron 2356		\$500	75W
node in-memory		2x4GB Micron DDR2-800	+\$750	+2W
checkpoint/restart with		4x4GB Kingston DDR2-800	+\$600	+4W
possibly new boards			> \$1700	> 81W
Long-term: DMR with	2xAMD Opteron 2356		\$1000	150W
possibly new boards		4x4GB Kingston DDR2-800	+\$600	+4W
and/or more racks			> \$1600	> 154W

#### **Ongoing and Future Work**

- Develop compute-node in-memory checkpoint caching
  - User-space (FUSE) front-end for storage virtualization
  - User-space (FUSE) backend for seamless integration
  - Asynchronous draining of cache to parallel file system
- Develop compute-node in-memory checkpoint/restart
  - Checkpoint data replication for fault tolerance
  - Integration with application- and system-level C/R solutions
- Develop dual-modular redundancy
  - Design modular redundancy models and algorithms
  - Implement static modular computation redundancy prototype
  - Experiment with I/O & file system access under redundancy
  - Implement dynamicmodular computation redundancy prototype
- Create trade-off models



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