Collaborative Research between DE Labs and Tokyo Tech GSIC of Extreme Scale Computing Success Stories

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> AICS Symposium AICS-Riken, Kobe Japan 20160222

Successful Model of DoE Lab / Tokyo Tech Collaboration

- 1. Initial agreement on collaboration area w/DoE group
 - Funding on both sides not mandated but desirable
- 2. Send a Ph.D. guinea pig student for short-term (2mo) exploratory hard labor internship
- 3. Usually Tokyo Tech student performs extremely well => tangible collaborative research advance
- 4. Student asked back for longer-term (6 mo or greater) more hard labor internship
- 5. Papers published, OSS deliverables, awards, ...
- 6. Student obtains Ph.D. => hired as postdoc at DoE Lab (much higher salary than being hired in Japan!)

Tokyo Tech Collaboration Topics with DoE Labs in the recent years

- Exascale Resiliece (Leonardo Bautista-Gomez@ANL, Kento Sato@LLNL)
- Performance of OpenMP-MPI Hybrid Programming on Many-Core (Abdelhalim Amer@ANL)
- Performance Visualization (Kevin Brown@LLNL)
- Performance Modeling of Tee Code with ASPEN (Keisuke Fukuda@ORNL)
- Large-Scale Graph Store in NVM (Keita Iwabuchi@LLNL)
- OpenACC Data Layout Extensions (Tetsuya Hoshino@ORNL)
- More to come...



FTI: High Performance Fault Tolerance Interface [SC11, EuroPar12 & Cluster12 (Leonardo Bautista-Gomez et al.)] Internship at ANL => PostDoc at ANL

• Diskless checkpoint:

- Create redundant data across local storages on compute nodes using a encoding technique such as Reedsolomon, XOR
 - Scalable by using distributed disks
- Can restore lost checkpoints on a failure caused by small # of nodes like RAID-5

Diskless checkpointing



Diskless checkpoint runtime library using Reed-Solomon encoding



FTI implements a scalable Reed Solomon encoding algorithm by
 utilizing local storages such as SSD

 FTI analyzes the topology of the system and create encoding clusters that increase the resilience



API

FTI (Multilevel checkpointing)

^xFTI is a multilevel checkpointing library with 4 levels of reliability. It has over 8000 lines of c/c++ (with Fortran bindings) under GPL2.1.

Download at http://www.github.com/leobago/fti and you can access the documentation at http://leobago.github.io/fti

^xFTI discovers the location of the processes in the hardware and creates topologyaware virtual rings to enhance reliability.

^xFTI can protect dynamic datasets, where the size, pointers or structure of the dataset changes during the runtime.

^xFTI offers the option to dedicate one process per node for fault tolerance to minimize the checkpoint overhead.

³While using dedicated processes for asynchronous tasks FTI allows the user to do a fine-grained selection about the tasks to offload.

²While using dedicated processes, FTI splits the global communicator and returns a new communicator to isolate the FT-dedicate ranks.

^xFTI monitors the timestep length and can dynamically adapt the checkpointing interval during runtime, keeping a consistent state.

Applications ported: HACC, CESM (ice module), LAMMPS, GYSELA5D, SPECFEM3D (CUDA version), HYDRO.

API and code example

Local Storage: SSD, PCM, NVM. Fastest checkpoint level. Low reliability, transient failures.

Partner Copy: Ckpt. Replication. Fast copy to neighbor node. It tolerates single node crashes.

RS Encoding: Ckpt. Encoding. Slow for large checkppoints. Reliable, multiple node crashes.

File System: Classic Ckpt. Slowest of all levels. The most reliable. Power outage. int main(int argc, char **argv) {

MPI_Init(&argc, &argv);
FTI_Init("conf.fti", MPI_COMM_WORLD);

double *grid; int i, steps=500, size=10000; initialize(grid); FTI_Protect(0, &i, 1, FTI_INTG); FTI_Protect(1, grid, size,FTI_DFLT);

```
for (i=0; i<steps; i++) {
    FTI_Snapshot();
    kernel1(grid);
    kernel2(grid);
    comms(FTI_COMM_WORLD);</pre>
```

}

FTI_Finalize();
MPI_Finalize();
return 0;

FTI scaling

Weak scaling to ~10k proc.
 CURIE supercomputer in France
 SSD on the compute nodes
 HYDRO scientific application
 Checkpointing every ~6 minutes



LAMMPS, Lennard-Jones simulation of 1.3 billion atoms 512 nodes, 64 MPI processes per node (32,678 processes) Power monitoring and checkpoint every ~5 minutes Less than 5% overhead on time to completion





Extreme-Scale Resilience for Billion-Way Parallelism

Coordinators

- US: Kento Sato, Kathryn Mohror, Adam Moody, Todd Gamblin, Bronis R. de Sipinski (LLNL)
- JP: Satoshi Matsuok (Tokyo Tech), Naoya Maruyama (RIKEN)
- Description
 - The Tokyo Tech group creates resilience APIs for transparent and fast recovery, resilience modeling for optimizing environment, and resilience architecture for scalable and reliable checkpoint/restart, then feeds back to SCR, the production resilience library developed at LLNL. The production library will be deployed in TSUBAME3.0
- How to collaborate
 - Biweekly meeting
 - Student / young researchers exchange
- Deliverables
 - Pre-standardization of Resilience API
 - Production resilience interface, SCR



Kento Sato LLNL Internship Now LLNL PostDoc



Schedule (DRAFT)



LLNL-PRES-665006

FMI: Fault Tolerant Messaging Interface [IPDPS2014, Kento Sato et al.]



Example code & Evaluation

FMI example code





- FMI_Loop enables transparent recovery and rollback on a failure
 - Periodically write a checkpoint
 - Restore the last checkpoint on a failure

P2P communication performance

	1-byte Latency	Bandwidth (8MB)
MPI	3.555 usec	$3.227~\mathrm{GB/s}$
FMI	3.573 usec	3.211 GB/s

FMI directly writes checkpoints via memcpy, and can exploit the bandwidth

Even with the high failure rate, FMI incurs only a 28% overhead

Design and Modeling of Async. Checkpointing [SC12, Kento Sato et al.]



Objective: Minimize checkpoint overhead to PFS

- Minimize CPU usage, memory and network bandwidth
- <u>Proposed method</u>: Implementation and modeling Non-blocking checkpointing
 - Asynchronously write checkpoints to PFS through Staging nodes using RDMA
 - Determine the optimal checkpoint interval on the asynchronous checkpoint scheme



Failure analysis on TSUBAME2.0



LLNL-PRES-665006

Burst Buffers for Resilient Checkpoint/Restart [CCGrid2014 (Best Paper Award), Kento Sato et al.]

API Modeling Architecture

TSUBAME3.0 EBD Prototype mSATA High I/O BW, low power & cost

- Provide POSIX-like I/O interfaces
 - open, read, write and close
 - Client can open any files on any servers
- IBIO use ibverbs for communication between clients and servers
 - Exploit network bandwidth of infiniBand





Burst Buffers for Resilient Checkpoint/Restart [CCGrid2014 (Best Paper Award), Kento Sato et al.]

API Modeling Architecture

Resilience modeling overview

To find out the best checkpoint/restart strategy for systems with burst buffers, we model checkpointing strategies



Publications

IEEE/ACM CCGrid2014 Best Paper Award

 Kento Sato, Kathryn Mohror, Adam Moody, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "A User-level InfiniBand-based File System and Checkpoint Strategy for Burst Buffers", In Proceedings of the 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid2014), Chicago, USA, May, 2014. (Best Paper Award !!)



- Kento Sato, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "FMI: Fault Tolerant Messaging Interface for Fast and Transparent Recovery", In Proceedings of the International Conference on Parallel and Distributed Processing Symposium 2014 (IPDPS2014), Phoenix, USA, May, 2014.
- Kento Sato, Satoshi Matsuoka, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski and Naoya Maruyama, "Burst SSD Buffer: Checkpoint Strategy at Extreme Scale", IPSJ SIG Technical Reports 2013-HPC-141, Okinawa, Sep, 2013
- Kento Sato, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "Design and Modeling of a Non-blocking Checkpointing System", In Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis 2012 (SC12), Salt Lake, USA, Nov, 2012.
- Kento Sato, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "Towards a Light-weight Non-blocking Checkpointing System", In HPC in Asia Workshop in conjunction with the International Supercomputing Conference (ISC'12), Hamburg, Germany, June, 2012 (Poster)
- Kento Sato,Adam Moody,Kathryn Mohror,Todd Gamblin,Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "Design and Modeling of a Non-Blocking Checkpoint System", In ATIP - A*CRC Workshop on Accelerator Technologies in High Performance Computing, Singapore, March, 2012. (Poster)
- Kento Sato, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "Design and Modeling of an Asynchronous Checkpointing System", IPSJ SIG Technical Reports 2012-HPC-135 (SWoPP 2012), Tottori, Aug, 2012.
- Kento Sato, Adam Moody, Kathryn Mohror, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama and Satoshi Matsuoka, "Towards an Asynchronous Checkpointing System", IPSJ SIG Technical Reports 2011-ARC-197 2011-HPC-132 (HOKKE-19), Hokkaido, Nov, 2011.



OpenMP-MPI Performance collaboration w/ANL -Abdelhalim Amer

- Visits
 - Abdelhalim Amer, PhD. Student at Tokyo Institute of Technology
 - − Sept 2013 Nov 2013 (Tokyo Tech \rightarrow ANL)
 - Characterizing lock contention in multithreaded
 MPI applications
 - Nov 2013 Apr 2013 (ANL → Tokyo Tech)
 - Develop hybrid MPI kernels relying on multithreaded communication
 - − Apr 2014 Sep2014 (Tokyo Tech \rightarrow ANL)

Abdelhalim Amer (Halim) Postdoctoral Researcher, ANL

- Large scale analysis of hybrid MPI graph traversal kernels
- Characterize and mitigate thread arbitration issues to enhance communication progress
- Apr 2015 ~: Postdoc at ANL. Planning for future collaborations/visits
- Outcome
 - Two publications (PPoPP'15 and PPMM')
 - Software contribution to the MPICH library
 - Ongoing collaboration

Research and Achievements Summary

- Characterizing state-of-the-art MPI+Threads runtimes
 - Application and runtime perspectives
 - Large scale analysis (512K cores on Mira)
- Exposing thread-synchronization issues the MPI-runtime
- Develop MPI-aware thread-synchronization to improve runtime performance

[ACM PPOPP'15] Abdelhalim Amer, Huiwei Lu, Yanjie Wei, Pavan Balaji and Satoshi Matsuoka. MPI+Threads: Runtime Contention and Remedies. ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP) [PPMM'15] Abdelhalim Amer, Huiwei Lu, Pavan Balaji, and Satoshi Matsuoka. Characterizing MPI and Hybrid MPI+Threads Applications at Scale: Case Study with BFS. Workshop on Parallel Programming Model for the Masses (PPMM)

Large-Scale MPI+Threads Graph Analytics Characterization on BG/Q [PPMM'15]

ΤΟΚΥΟ ΤΕΕΗ

Pursuina Excellence

Communication Progress and Thread-Synchronization: Beware of Unbounded-Unfairness [PPoPP'15]

Adapt arbitration to maximize work

- FIFO locks overcome the shortcomings of mutexes
- Polling for progress can be wasteful (waiting does not generate work!)
- Prioritizing issuing operations
 - Feed the communication pipeline
 - Reduce chances of wasteful internal process (e.g. more requests on the fly
 - ➔ higher chances of making

Message Rate between two 36 Haswell cores nodes

SWAP-Assembler Genome assembly application

Insightful Analysis of Performance Metrics on Fat-tree Networks[Kevin Brown, ICPADS15]

Non-intrusive collection of performance metrics w/

our **ibprof** profiler

- Low overhead
- Captures links traffic

Insightful Analysis of Performance Metrics on Fat-tree Networks

Each element represents a link

- No occlusion of data
- ✓ Space efficient design
- ✓ More link design options

Data (traffic, load, etc.) is encoded in the size, shape, color, and/or hue of the links

ibprof's Profiling Overhead

NAS Parallel Benchmarks

- All NPB apps averaged < 1%
- Peak overhead occurred with MPI_Bcast when Open MPI switched from send/recv to RDMA
- All other collectives averaged < 5%

Process-centric Visualizations vs. Boxfish Fat Tree Visualization

Samplesort on 128 nodes of TSUBAME2.5

<u>Paraver</u>

Does not show network traffic hotspots

<u>Boxfish</u>

Capable of highlighting network hotspots and traffic patterns

Visualizing the Traffic Patterns of Different Open MPI Library version

Open MPI v1.82 uses a single subnet per operation with the default configurations on TSUBAME2.5

Open MPI v1.65 balances traffic over both subnets ofTSUBAME2.5 with the default configuration

Publications

Poster (Prior to internship but using LLNL's work):

Kevin A. Brown, Jens Domke, and Satoshi Matsuoka. *"Tracing Data Movements within MPI Collectives"*. In Proceedings of the 21st European MPI Users' Group Meeting (EuroMPI/ASIA '14).

Paper:

Brown, K.A.; Domke, J.; Matsuoka, S., "Hardware-Centric Analysis of Network Performance for MPI Applications". In 2015 IEEE 21st International Conference on Parallel and Distributed Systems (ICPADS)

Challenges to model a tree-based irregular applications with Aspen

Keisuke Fukuda (Ph.D Student) Research Internship @ORNL

- 2013 Sep-Nov
- 2014 Oct-Nov
- Now long-term intern at AICS 2015 Oct-2016 Sep

Challenges in modeling irregular applications

- Performance modeling of application is used to:
 - Runtime (power, memory) estimation
 - Hardware/machine design
- Conventional, ad-hoc mathematical modeling is not suitable if irregular data structure (e.g. tree) and control flows affect the performance
- How to model such applications?
 - We focus on the Fast Multipole Method

- Applied Aspen modeling language to FMM
 - Runtime estimation for lattice, sphere, plummer distribution, Ncrit = 16∼512
- Estimation errror was 7-13% error in avg.
- Room for optimization for find-grained kernels and in deriving constants
- Aspen requires large time and memory to evaluate the models

Whole-app model of ExaFMM

Error: avg 7.7%, max 33.2%, min 3.7%

Whole-app model of ExaFMM

Distributed Large-Scale Dynamic Graph Data Store

Keita Iwabuchi^{1, 2}, Scott Sallinen³, Roger Pearce², Brian Van Essen², Maya Gokhale², Satoshi Matsuoka¹

- 1. Tokyo Institute of Technology (Tokyo Tech)
- 2. Lawrence Livermore National Laboratory (LLNL)3. University of British Columbia

a place of mind The UNIVERSITY OF BRITISH COLUMBIA

Dynamic Graphs (temporal graph)

- the structure of a graph changes dynamically over time
- many real-world graphs are classified into dynamic graph

Source: Jakob Enemark and Kim Sneppen, "Gene duplication models for directed networks with limits on growth", Journal of Statistical Mechanics: Theory and Experiment 2007

n) Sparse Large Scale-free

- social network, genome analysis, WWW, etc.
 - e.g., Facebook manages
 1.39 billion active users
 as of 2014, with more
 than 400 billion edges

UBC

- Most studies for large graphs have not focused on a dynamic graph data structure, but rather a static one, such as Graph 500
- Even with the large memory capacities of HPC systems, many graph applications require additional out-of-core memory (this part is still at an early stage)

Developing a distributed dynamic graph store for data intensive supercomputers equipped with locally attached NVRAM

Degree Aware Dynamic Graph Data Store

- Degree aware data structures, while RHH degree vertices are compactly represented
- Use Robin Hood Hashing^[1] because of its locality properties to minimize the number of accesses to NVRAM, reducing page misses.

[2] R. Pearce, et al, "Scaling techniques for massive scale-free graphs in distributed (external) memory," IPDPS' 13

Dynamic Large-Scale Graph Construction (on-memory)

- **STINGER**: a state-of-the-art shared-memory dynamic graph processing framework developing at Georgia Tech
- **Baseline**: a baseline model using *Boost.Interprocess*
- DegAwareRHH: our proposed dynamic graph store

Due to a skewness of the data set (RMAT graph), DegAwareRHH overperforms the both implementations significantly

Publication list

- Keita Iwabuchi, Roger A. Pearce, Brian Van Essen, Maya Gokhale, Satoshi Matsuoka, "Design of a NVRAM Specialized Degree Aware Dynamic Graph Data Structure", SC 2015 Regular, Electronic, and Educational Poster, International Conference for High Performance Computing, Networking, Storage and Analysis 2015 (SC '15), Nov. 2015
- Keita Iwabuchi, Roger A. Pearce, Brian Van Essen, Maya Gokhale, Satoshi Matsuoka, "Design of a NVRAM Specialized Degree Aware Dynamic Graph Data Structure", 7th Annual Non-Volatile Memories Workshop 2016, Mar. 2016

An OpenACC Extension for Data Layout Transformation w/ORNL

Tetsuya Hoshino(Ph.D Student) Research Internship @ORNL 2014 Sep-Nov

Now: Assistant Professor @ Supercomputing Center, The University of Tokyo

Why the extension is needed?

The graph shows the result of manual data layout transformation for the viscosity and convection phases of a real-world CFD application UPACS (Hoshino et al. "CUDA vs OpenACC: Performance Case Studies with Kernel Benchmarks and a Memory-Bound CFD Application", CCGrid13)

- An OpenACC program can be executed on any devices
 - multi-core CPU, Xeon Phi, GPUs
- OpenACC target devices have different performance characteristics especially about memory access
 - ex. SoA and AoS
- Data layout of real-world applications is complicated and is shared in the whole program
 - Auto-tuning is required

An OpenACC extension #pragma acc transform

• Specification

#pragma acc transform [clause [[,] clause] ...] new-line
 structured block

- Clause list
 - transpose(array_name::transpose_rule)
 - for multi-dimensional array
 - A[Z][Y][X][3] → A'[3][Z][Y][X] (transpose rule :: [4,1,2,3])
 - redim(array_name::redim_rule)
 - for 1 dimensional array
 - $B[Z^*Y^*X^*3] \rightarrow B'[Z][Y][X][3] \rightarrow B''[3][Z][Y][X]$ (by transpose clause)
 - expand(derived_type_array_name)
 - for array of structures
 - $C[Z][Y][X].c[3] \rightarrow C'[Z][Y][X][3] \rightarrow C''[3][Z][Y][X]$ (by transpose clause)

Collaborate with ORNL

- Implement the directive top on OpenARC that is an Open-source OpenACC compiler developed by ORNL
 - Source-to-Source translator
 - Input : Extended OpenACC program
 - Output : OpenACC program
 - It is on going work

Evaluate with Himeno benchmark (27-point stencil program)

- Apply *transpose* to coefficient arrays of Himeno benchmark
 - But the transformation is applied by hands
 - Transformed program is same as the output program that OpenARC should output
- Performance evaluation
 - CPU : Original is the best
 - GPU : 24% up
 - MIC : more than 60% down
 - Translator change the coefficient multidimensional array to 1-dimensional array, it disturbs prefetching

Lessons Learned

- Sending actual Ph.D. students to DoE labs extremely productive for both sides for tangible collabration
- Tokyo Tech Ph.D. students are extremely good and well trained by global standards – they usually survive the filtering of summer interns and produce tangible results
- Many students end up being hired by DoE labs. Others go to Japanese univ. & labs, etc. => great talent pool
- Some administrative obstacles, esp. travel and funding from both ends – need more flexibility in purpose, airlines, gaps in travel itinerary, etc.

Tokyo Tech Research on Big Data Convergence JST-CREST "Extreme Big Data" Project (2013-2018) Future Extreme Big Data Scientific Apps

Cloud IDC Very low BW & Efficiency Highly available, resilient

Supercomputers Compute&Batch-Oriented More fragile

The Graph500 – June 2014 and June/Nov 2015 K Computer #1 Tokyo Tech[EBD CREST] Univ. Kyushu [Fujisawa Graph CREST], Riken AICS, Fujitsu

2017 Q1 TSUBAME3.0+2.5 Towards Exa & Big Data

- 1. "Everybody's Supercomputer" High Performance (15~20 Petaflops, ~4PB/s Mem, ~1Pbit/s NW), innovative high cost/performance packaging & design, in mere 100m²...
- 2. "Extreme Green" 9~10GFlops/W power-efficient architecture, system-wide power control, advanced cooling, future energy reservoir load leveling & energy recovery
- 3. "Big Data Convergence" Extreme high BW &capacity, deep memory hierarchy, extreme I/O acceleration, Big Data SW Stack 2013 TSUBAME2.5 for machine learning /DNN, graph processing, ... upgrade
- 4. "Cloud SC" dynamic deployment, container-based node co-location & dynamic configuration, resource elasticity, assimilation of public clouds...
- 5. "Transparency" full monitoring & user visibility of machine & job state, accountability via reproducibility

2006 TSUBAME1.0 80 Teraflops, #1 Asia #7 World "Everybody's Supercomputer"

2010 TSUBAME2.0 2.4 Petaflops #4 World "Greenest Production SC" A A A A A A

2011 ACM Gordon Bell Prize

Big Data and HPC Convergent Infrastructure => "Big Data & Supercomputing Convergent Center"

- "Big Data" currently processed managed by domain laboratories => No longer scalable
- HPCI HPC Center => Converged HPC and Big Data Science Center
- People convergence: domain scientists + <u>data scientists</u> + CS/Infrastructure => Big data science center
- Data services including large data handling, big data structures e.g. graphs, ML/DNN/AI services...

New collaborations under consideration

- Fault tolerance towards exascale
 - Modeling & analyzing soft errors with "realistic" machine fault models (Kobayashi)
- To be presented @ DoE/MEXT workshop)
- General system-level GPU checkpointing (Suzuki)
- Big Data / IoT / Machine Learning-AI & HPC Convergence
 - Modeling deep learning algorithms performance (Ooyama)
 - Counterpart to Tokyo Tech Extreme Big Data (EBD) Project w/DENSO
- Post-Moore computing
 - Programming / Performance modeling future FPGAs (also w/Riken AICS Naoya Maruyama (Hamid)
 - FLOPS to BYTES from compute intensive to bandwidth/capacity intensive computing (w/Kengo Nakajima, Toshio Endo et. al.)
- ADAC (Accelerated Data Analytics and Computing) Institute ORNL – ETH/CSCS – Tokyo Tech GSIC