Miniapps for Enabling Architecture-Application Co-design for Exascale Supercomputing

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HPCI Application Feasibility Study

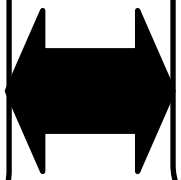
Objective

1. Identify social and scientific challenges for next 5 to 10 years → Computational Science Roadmap
   - Based on the 2011 Computational Science Roadmap
   - Involves a wide range of domains with particular focus on cross-cutting issues
2. Present requirement and tools for evaluating architectures
   - Social and scientific challenges as computational problems
   - Effectiveness to solve the social and scientific challenges

Organization

Roadmap Development:

- Led by major computational science researchers in Japanese universities and national labs



System Evaluation:

- Led by RIKEN AICS and Tokyo Institute of Technology in partnering with major HPC centers in Japan

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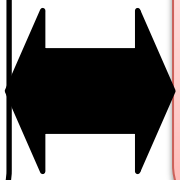

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Miniapp?

A tool for application and architecture codesign

- *Small* applications
  - Lines of code < 1,000
  - Simplified program organization
- *Not too small* applications
  - Retain essential characteristics of the original applications
  - What is essential?
- Simple process to "Download → Compile → Execute"
  - Open-source licenses
  - Easy compilation steps
  - Documentation of program execution input and parameters
  - Packaging of necessary input files

Existing Miniapp Projects

- Mantevo
  - US Sandia NL
  - http://mantevo.org
  - PDE, MD, etc.
- ExaCT
  - US DoE Codesign center
  - http://exactcodesign.org/
  - Combustion miniapp
- LULESH
  - US Lawrence Livermore NL
  - Hydrodynamics
  - Many variants: Serial, MPI, OpenMP, CUDA, OpenACC, Chapel, Charm++, Listz
- New projects at EU

FiBER Mini-App Suite

- A suite of miniapps derived from the full-scale applications for the future computational science challenges
  - Supported by the HPCI Application FS
- Originally developed and used on high-end machines such as the K supercomputers
- Mainly developed at AICS with collaboration with the full-app developers

		処理量 /1PE	処理量 /1チップ	1stepの時間 （演算の時間）	実効効率	性能 /1チップ	性能 /1グループ	ホストへの データ送受信 (双方向の計)
1億原子	構成A （12.3Tflops）	原子数6 （1セル）	原子数24,576 （16x16x16）	0.75ms (0.61ms)	39.7%	4.88 Tflops	20.0 Pflops	0.18ms
	構成B （8.2Tflops）	原子数12 （1セル）	原子数24,576 （16x16x8）	1.02ms (0.86ms)	41.0%	3.36 Tflops	13.8 Pflops	0.18ms
2.5億原子	構成A （12.3Tflops）	原子数15 （1セル）	原子数61,440 （16x16x16）	2.02ms (1.79ms)	43.4%	5.33 Tflops	21.8 Pflops	0.44ms
	構成B （8.2Tflops）	原子数30 （2セル）	原子数61,440 （16x16x16）	3.04ms (2.68ms)	43.2%	3.53 Tflops	14.5 Pflops	0.44ms

E.g., Evaluation results of a MD miniapp at the TSUKUBA FS

Development & Usage

- Call for full-apps
  - 17 full-apps submitted to RIKEN
  - Being converted to mini-apps at RIKEN
- Call for mini-apps
  - 8 mini-app-like small apps submitted to RIKEN
  - Packaged as mini-apps at RIKEN
- Provided to the System Architecture FS for evaluating their systems
  - University of Tohoku, University of Tsukuba, University of Tokyo

Submitted Applications（1/3）

feram	Nishimatsu	Ferroelectrics MD	OpenMP (with MPI for parameter survey), 3D FFT
MARBLE	Ikekuguchi	MD(PME)	MPI+OpenMP, 3D FFT
SMASH (para-TCCI)	Ishimura	Hartree-Fock	MPI+OpenMP, Sequential diagonalization of dense matrices
FFVC	Ono	Thermal-Fluid Analysis	MPI+OpenMP, SOR or GMRES
pSpatiocyte	Iwamoto	Signal propagation	MPI+OpenMP
NEURON_K+	Kazawa	Neural circuit simulation (Modified NEURON)	MPI+OpenMP, many ALL_GATHER, Translated to C from modeling language
GT5D	Idomura	5D plasma turbulence (5D FDM+2D FEM)	MPI+OpenMP, CG, 1D FFT
MODYLAS	Ando	MD(FMM)	MPI+OpenMP
STATE	Inagaki	First-Principles MD (DFT)	MPI+OpenMP (Replica paralle, k-point parallel, band or plane-wave parallel), FFT, eignevalue problem (RMM)
FrontFlow/blue	Yamade	Thermal-Fluid Analysis (Irregular mesh、FEM)	MPI+auto parallelization, BiCGSTAB
SiGN-L1	Tamada	Neural network (L1 regularization)	MPI+OpenMP, Bottleneck at file output
NTChem/RI-MP2	Katouda	Electron correlation	MPI+OpenMP, DGEMM, Some sequential computation, Memory usage $O(N^3)$

Submitted Applications（2/3）

OpenFMO	Inadomi	Hartree-Fock FMO	MPI+OpenMP, Dynamic load balancing
CONQUEST	Miyazaki	First-principles MD, O(n) method	MPI+OpenMP SpMV, FFT
NGS Analyzer	Tamada	Genome sequence analysis	MPI I/O bound
DCPAM	Nishizawa	Climate model with spectral method	MPI+OpenMP
RSGDX	Hyodo	Earthquake simulation	

Submitted Applications（3/3）

Simplified versions submitted to the RIKEN FS

fft_check, fft_check_mpi	Nishimatsu	3D FFT benchmarking
ALPS/looper	Todo	Quantum monte carlo，linked lists, integer ops MPI+OpenMP
CCS QCD Solver Benchmark test program	Ishikawa	Lattice QCD benchmark，BiCGStab, MPI+OpenMP
ZZ-EFSI	Sugiyama	Fluid Structure Integration MPI+OpenMP
rmcsm bench nocore	Shimizu	Monte Carlo Nuclear Shell Model MPI+OpenMP
GCEED	Nobusada	DFT
NICAM-DC	Yashiro	Climate model (NICAM), dynamics，FVM MPI
mVMC	Imada	Strongly correlated matter

FiBER Mini-App Current Status

CCS QCD	Lattice QCD	→Tokyo FS, Tsukuba FS
MARBLE	MD(PME)	
MODYLAS	MD(FMM)	→Tokyo FS, Tsukuba FS
FFVC	Thermal-Fluid Analysis (Cartesian, FDM)	→Tohoku FS
NGS Analyzer	Genome Sequence Analysis	→Tokyo FS, Tsukuba FS
ALPS/looper	Quantum Monte Carlo	(Almost done)
CONQUEST	First-Principles MD (O(N))	(Almost done)
NICAM-DC	Climate	(Almost done)
FrontFlow/ blue	Thermal-Fluid Analysis (Irregular mesh, FEM)	(Under development)
mVMC	Variational Monte Carlo	(Under development)

Molecular Dynamics

- Two alternative algorithms for solving equivalent problems
  - Particle Mesh Ewald
    - Bottlenecked by all-to-all communications at scale
    - Example implementation: MARBLE (Ikeguchi et al.)
  - Fast Multipole Method
    - Tree-based problem formulation with no all-to-all communications
    - Example implementation: MODYLAS (Okazaki et al.)
- Allows algorithmic comparisons
  - FFT vs. FMM?

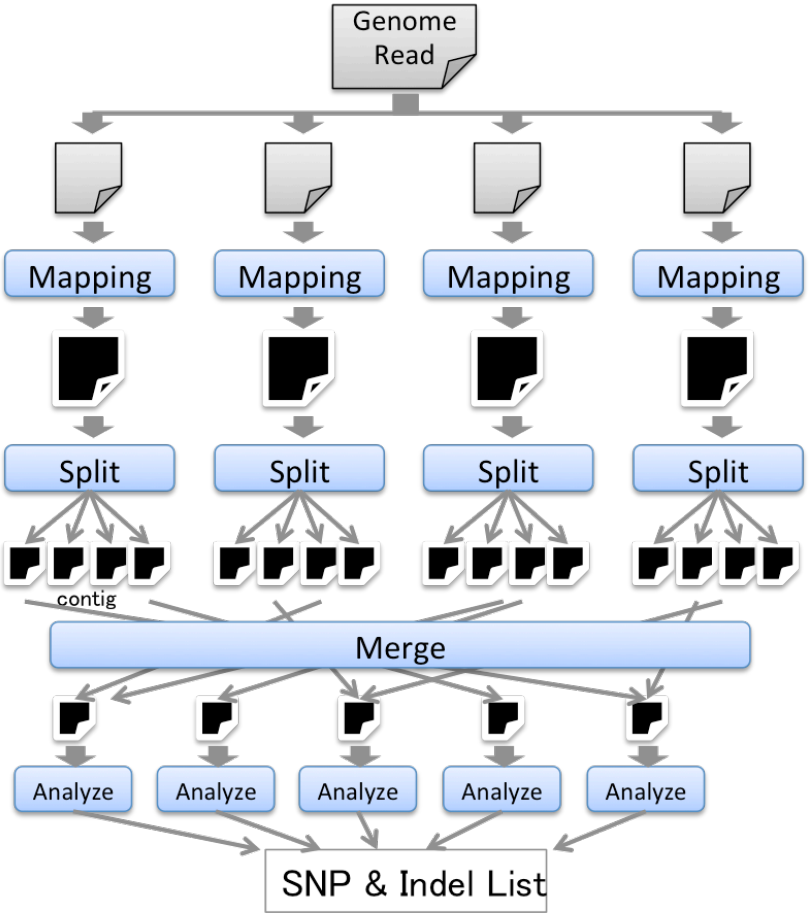
Molecular Dynamics

- Simplified problem settings
  - Only simulates water molecules in the NVE setting
  - Can reduce the codebase significantly
  - Easier to create input data sets of different scales
  - Whether it's sufficient is still under discussions
- Kernels: Pairwise force calculation + Long-range updates (FFT or FMM)
- Two reference implementations to study performance implications by algorithmic differences
  - MARBLE (12K SLOC)
  - MODYLAS (11K SLOC)

NGS Analyzer

- Genome analysis tool for cancer cell's mutation detection
  - Read the output genome data generated by a next-generation genome sequencer
    - Current: 500GB/human
    - In 2020: 100TB/human
  - The analysis pipeline consists of widely used genome analysis software, and performs sequence mapping, genotyping, etc.
    - BWA sequence mapping
    - SAM/BAM formatting software
  - Runs on K computer in parallel

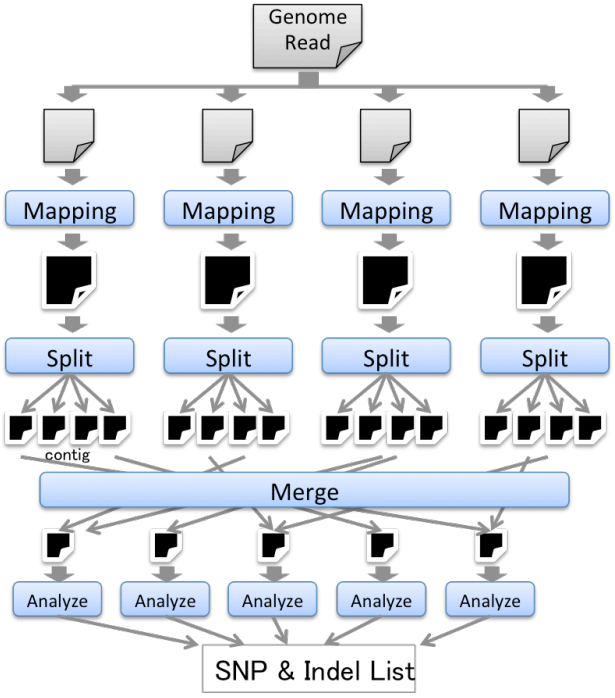
Work Flow of NGS Analyzer



- Workflow
  - Split the input genome read, perform mapping on each of them and then split the results based on contigs
  - Merge mapping results of each contig and run analysis process on each merged data
- The original NGS Analyzer runs this workflow by executing five separated jobs in turn

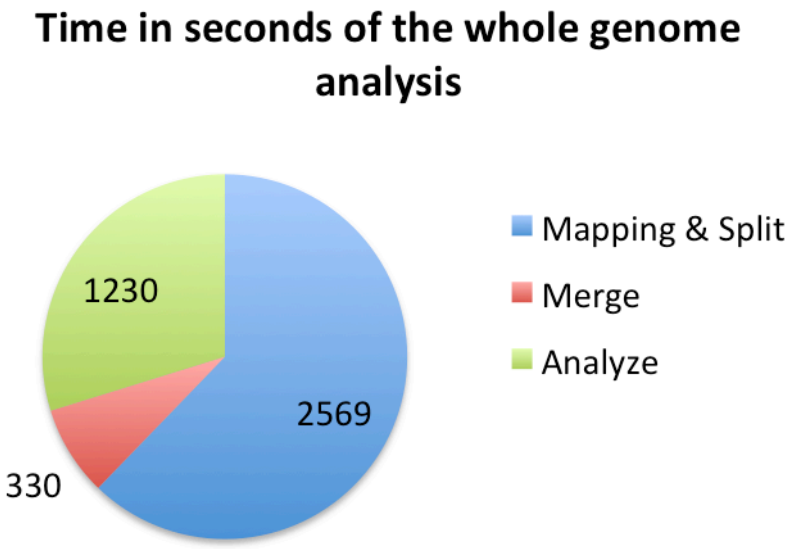
NGS Analyzer IO

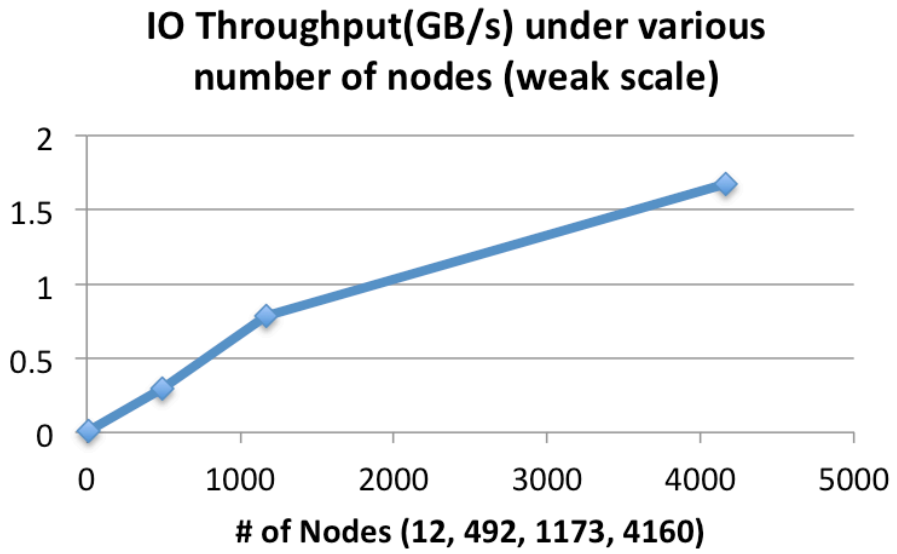
- Input
  - Output of a next-generation sequencer
  - Reference genome
  - e.g.) whole genome of a Japanese individual
    - 490 GB of genome read,
      6.3GB of reference genome
- Output
  - Analysis results of each config
  - e.g.) Output of the above input: 874 MB
- Intermediate output
  - unsplit mapping results, results that contain duplicate sequence, etc.
  - e.g.) Intermediate output of the above input: 6 TB
- Though IO of “Mapping”, “Split” and “Analyze” can be local, IO of “Merge” is global where all nodes exchange data
  - e.g.) Exchanged data of the above input: 617 GB



NGS Analyzer Performance

- Execution time for analyzing the whole genome of a Japanese individual : 4,129 sec
  - IO throughput is 1.6 GB/s
    (490GB + 874MB + 6TB) / 4129
  - Measured on the K computer using 4,160 nodes





NGS Analyzer Mini App

- Three serial programs that run individual steps of the workflow to measure both computational and IO performance of each step
  - Sequence mapping
  - Duplicate removal of the mapping results
  - Mutation detection
- Single program that runs the entire workflow in parallel to measure the overall performance

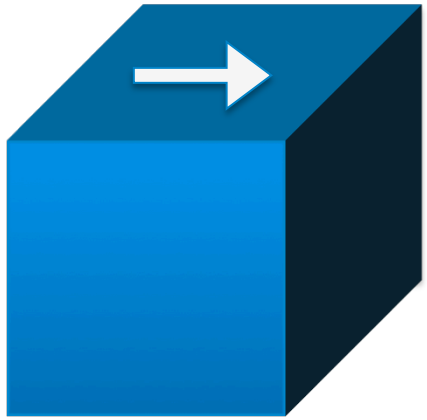
FFVC (FrontFlow/Violet Cartesian)

- 3D unsteady incompressible thermal fluid solver developed at University of Tokyo
- Regular Cartesian grids, Finite volume, Fractional Step method
- Mini-app version
  - 3D cavity flow cavity flow model
    - Outer boundary condition
    - Retain the original control flow

FFVC mini

- Algorithm (fixed)
  - Time step: Euler explicit method
  - Pressure Poisson: Red-black SOR
- Simplified program execution
  - No configuration nor input file necessary
- Code size

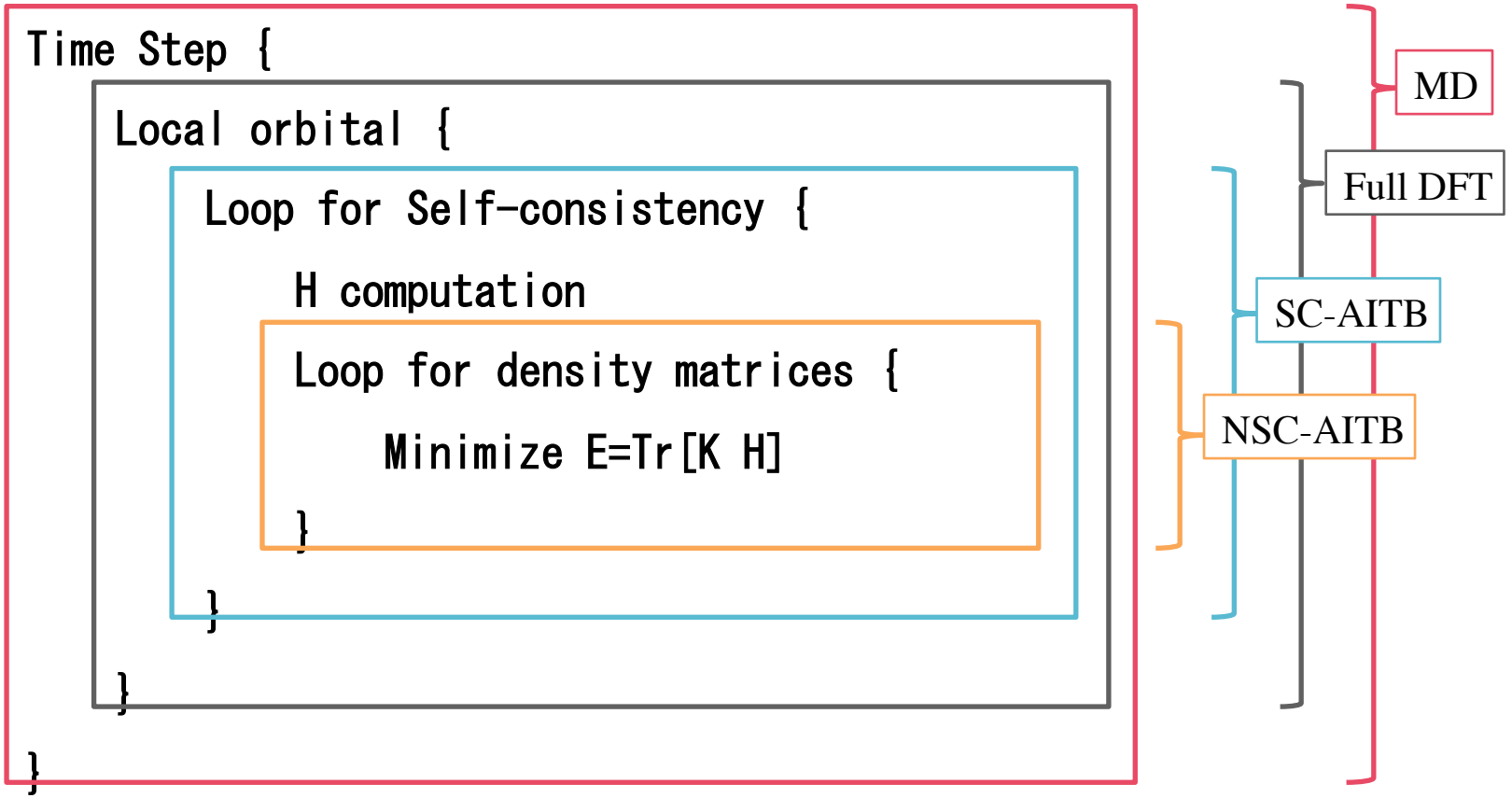
  100K SLOC → 10K SLOC (sloccount)



CONQUEST

- Domain and method:
  - First-Principles computation with O(n) method
  - Structural optimization, molecular dynamics
- Author:
  - Tsuyoshi Miyazaki（National Institute for Materials Science）, et al.
  - URL: http://www.order-n.org/
- Programming language:
  - Fortran90
- Program size:
  - 115K SLOC
- Target problem size:
  - Ensemble simulations with 100K to 1M atoms
  - Simulation of 100M atoms

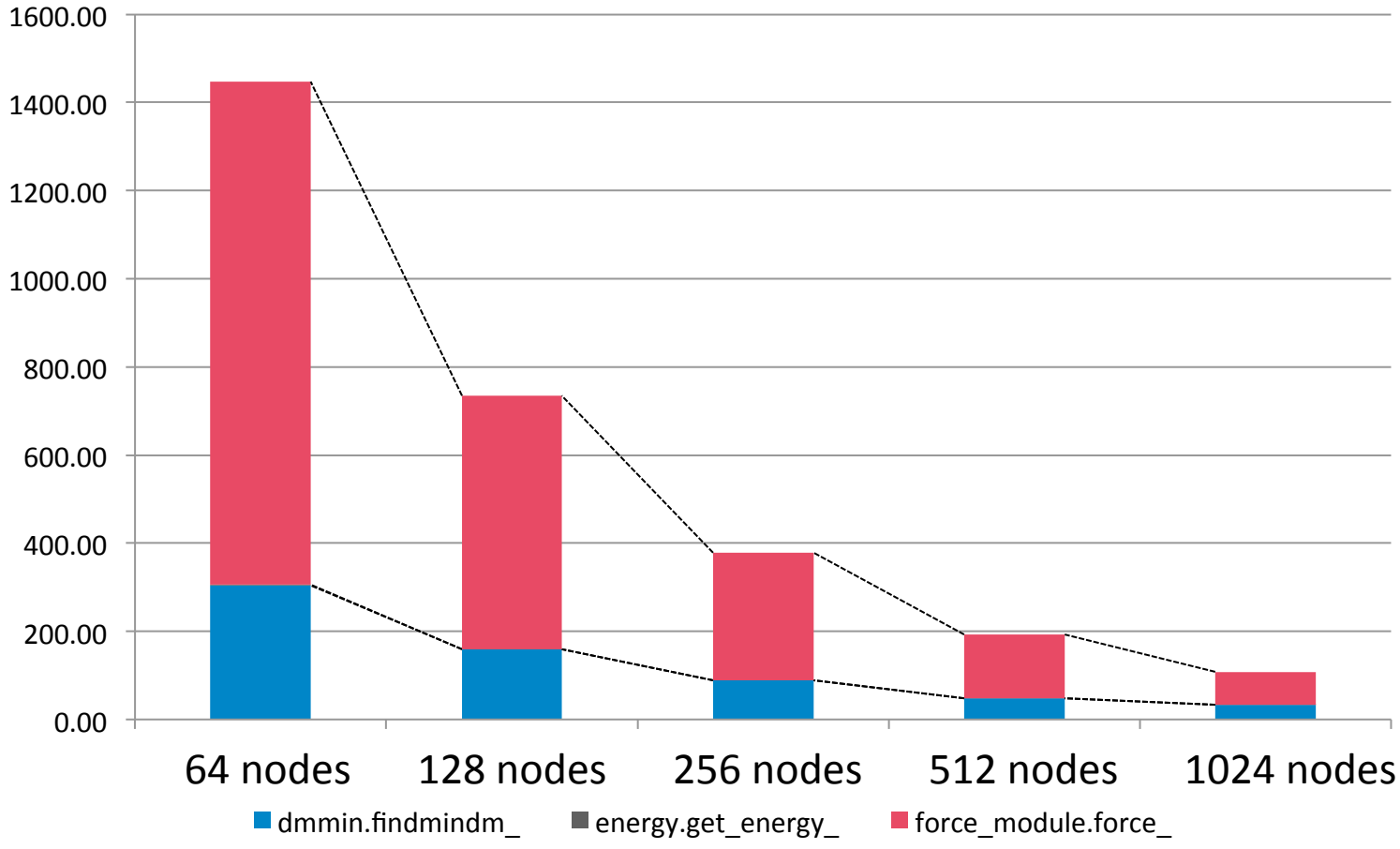
Program Loop Structure and Mini-App



- Compute NSC-AITB only as benchmark mode
  - The time for full DFT can be easily estimated from the time for NSC-AITB
- Approximately 25K SLOC

Strong Scaling (Atom Si32768)

- FX10 (Oakleaf @ U-Tokyo)



Future Plan

- Need to be continuously developed and maintained as the Application Roadmap progresses
- Will be continued as part of the Exa-scale project at RIKEN AICS
  - Positions available! http://bit.ly/1nxI22L
- Wider coverage of application domains
- Optimization, porting, performance modeling
- First release
  - http://github.com/fiber-miniapp
  - miniapp at riken.jp
- Usage of miniapps
  - M. Kondo et al., “Evaluation of power dissipation of HPC systems using miniapps,” SDHPC10