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Performance Analysis of Multi-Containerized MD Simulations for Low-Level Resource Allocation

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Introduction

Container-Based Virtualization

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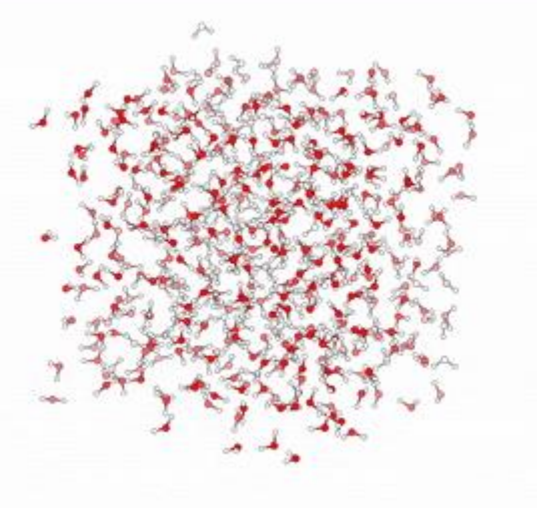
Property	What can we do for drug discovery?
Portability	Distributing applications while maintaining their configurations
Repeatability	Obtaining the same analysis results even on different systems
Low overhead	Running performance-sensitive applications such as molecular dynamics (MD) simulation



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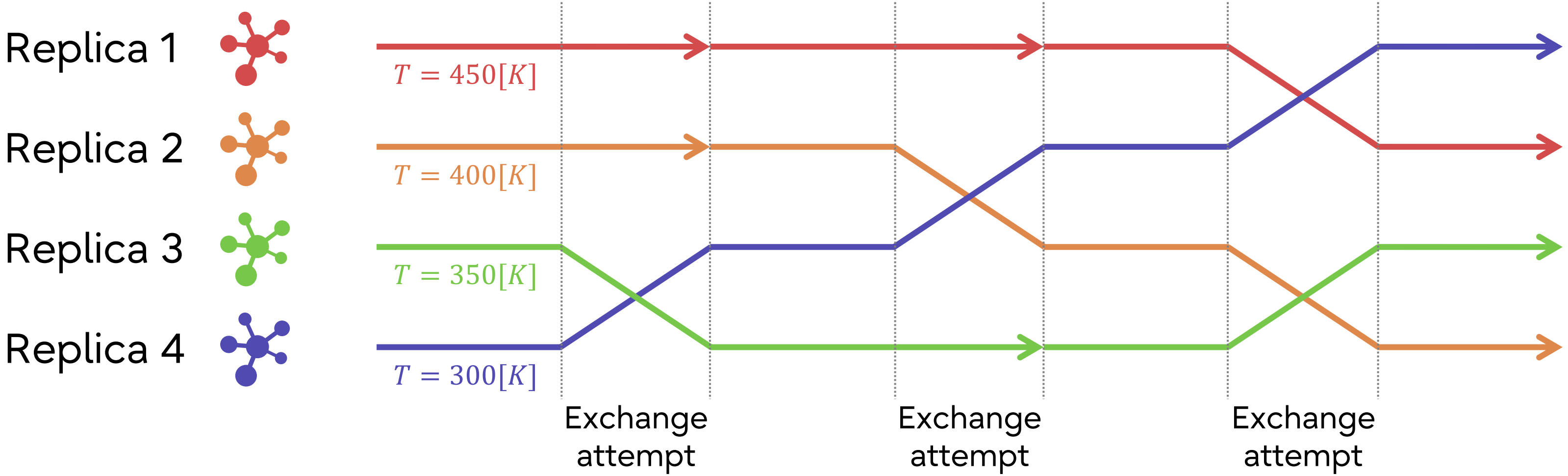
Ensemble Runs of Containers

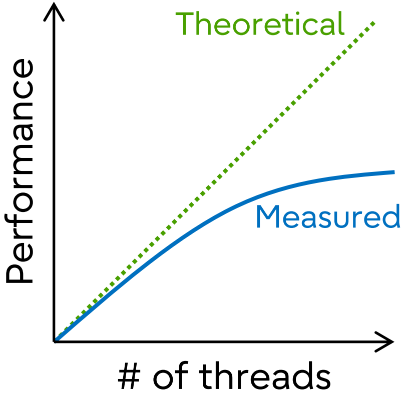
- Increase in # of containers due to microservices
- Other users' containers in multi-tenant cloud environments
- Ensemble simulation with multiple replicas

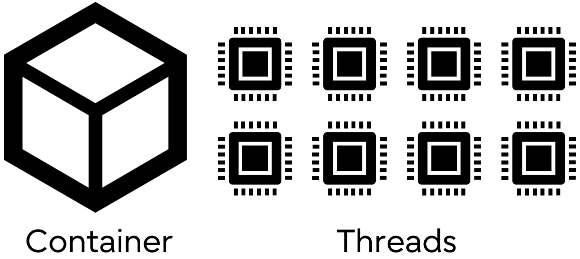
  e.g.) Containerized replica-exchange MD (REMD) simulation



Container Scheduling Problem 1

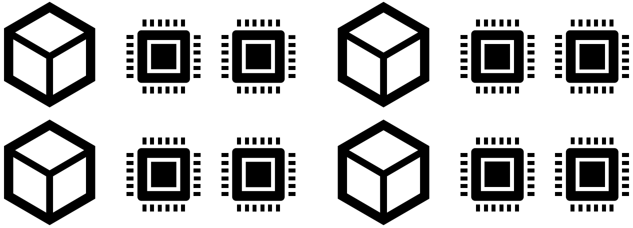
How many containers should we run simultaneously?





Large degree of parallelism

- Good speedup
- Bad throughput

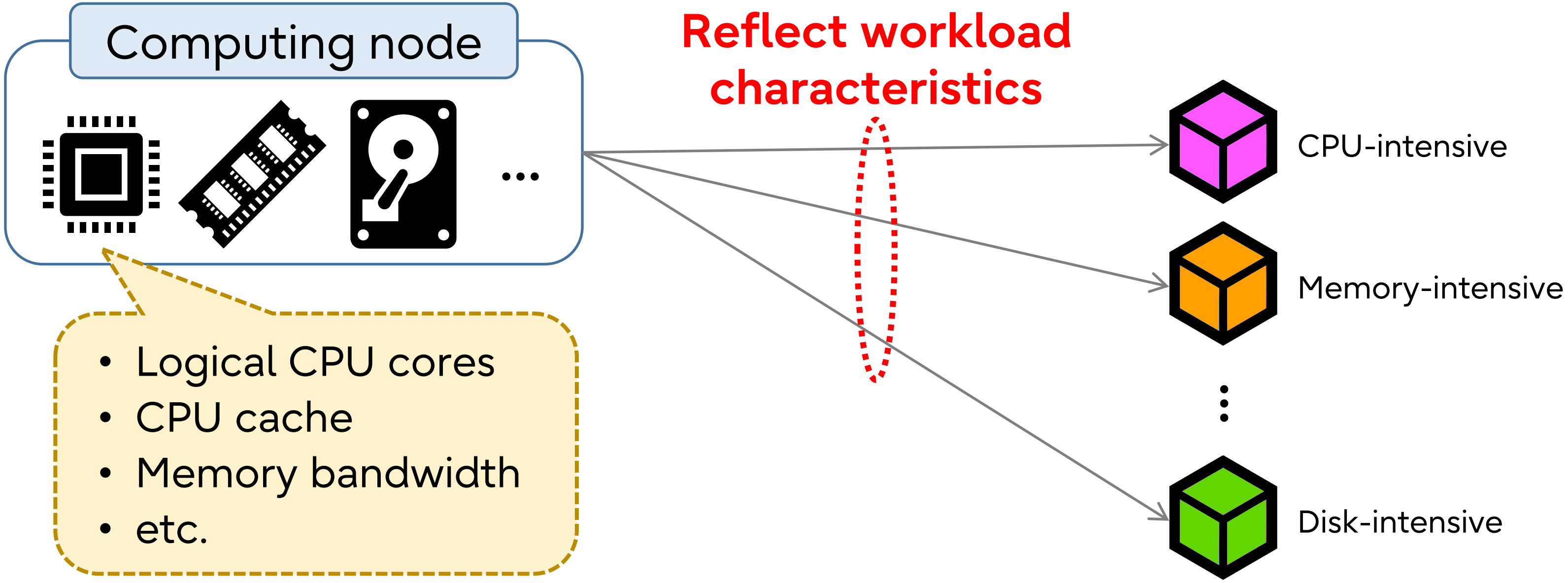


Large number of containers

- Good throughput
- Bad speedup

Container Scheduling Problem 2

How should we allocate resources to each container?



- Logical CPU cores
- CPU cache
- Memory bandwidth
- etc.

Allocate low-level resources

Solution to Container Scheduling Problem

	How many containers should we run simultaneously?	How should we allocate resources to each container?
Existing schedulers	Heuristics approach	No support for low-level resources
Our scheduler	**Automatic adjustment**	**Low-level resource allocation based on workload characteristics**

What We Did in This Research

- Discussion about low-level hardware resources for container scheduling

- Evaluation with multi-containerized MD simulations
  - Examining the effect of CPU resource allocation with simultaneous multi-threading (SMT)

Concept of Our Scheduler

Low-Level Hardware Resource Allocation

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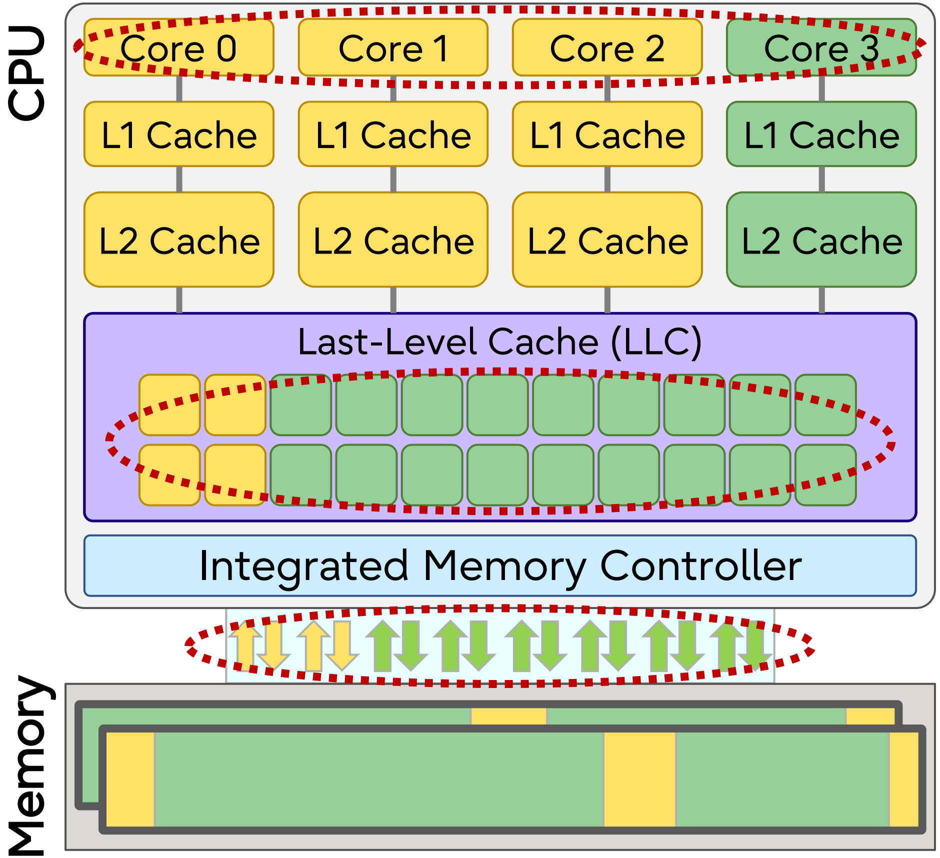

1. CPU core control

- Increasing CPU frequency for parallel applications with poor speedup
- Enabling simultaneous multi-threading (SMT) for applications with low resource contention

2. Cache block control

3. Memory bandwidth control

Implementation using Kubernetes Scheduler

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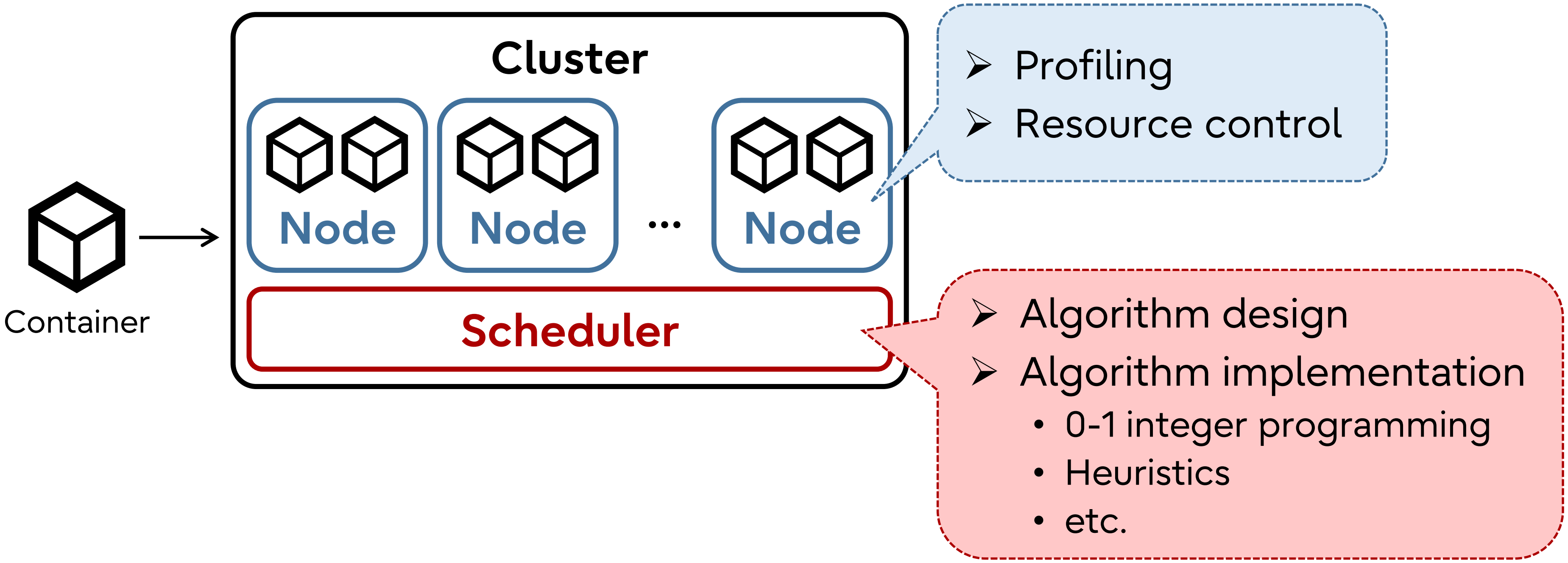
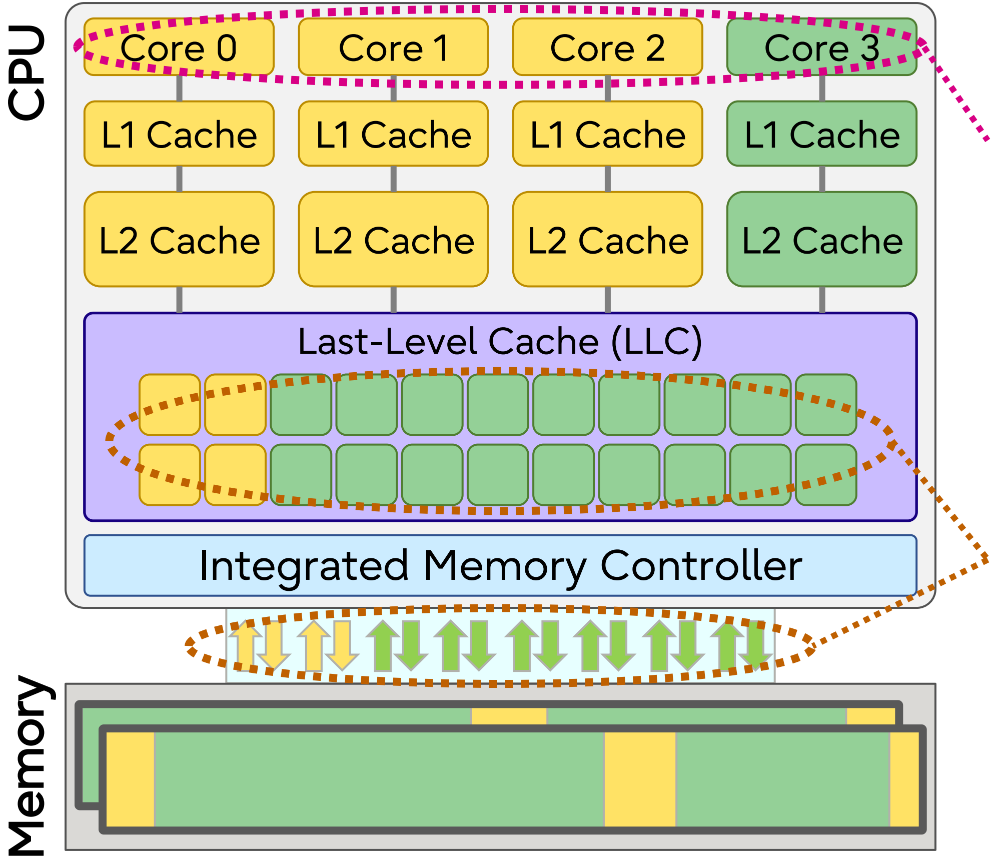
- Default resource types
  - CPU (in number of cores)
  - Memory (in bytes)
- Bin packing along with extended resources
  - 😊 Improvement in container aggregation rate
  - 😟 Difficult to consider workload characteristics

Need to develop own container scheduler

What We Need to Implement Our Scheduler



Resource Control by CRI Resource Manager*



Intel Speed Select Technology

- Power management control

Intel Resource Director Technology

- LLC control
- Memory bandwidth control

* https://github.com/intel/cri-resource-manager

Towards Algorithm Design/Implementation

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Workload analysis → Design → Implemen-tation → Evaluation → Refinement

Conducted preliminary experiments!

- Application
  - Multi-containerized MD simulation
- Low-level hardware resource
  - Simultaneous multi-threading (SMT)

Experiment

Evaluation Setup

- CPU: Intel Xeon Gold 6148 2.4GHz 20-core × 2 sockets
  - Hyper-Threading Technology enabled (80 logical cores in total)
  - Turbo Boost Technology enabled (1.00–3.70GHz)
  - CPU scaling governor: powersave
- Memory: DDR4-2666 16GB × 12 (96GB / socket)
- Software
  - Container: Docker 20.10.8 with `--cpuset-cpus --cpuset-mems`
  - Compiler: GCC 9.3.0 with `-O3 -march=skylake-avx512`
  - Application: OpenMM 7.6.0 and GROMACS 2021.4
  - Input: Amber20 Benchmark Suite (DHFR and STMV)

Performance of Single Container (OpenMM)

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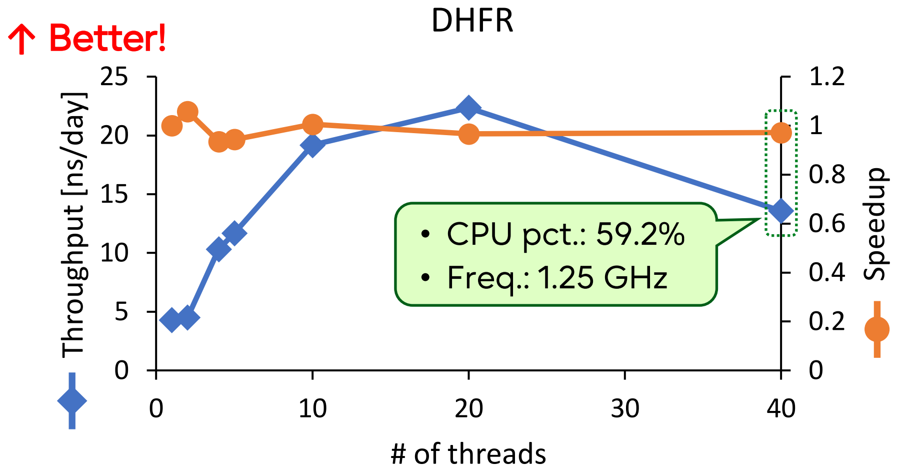
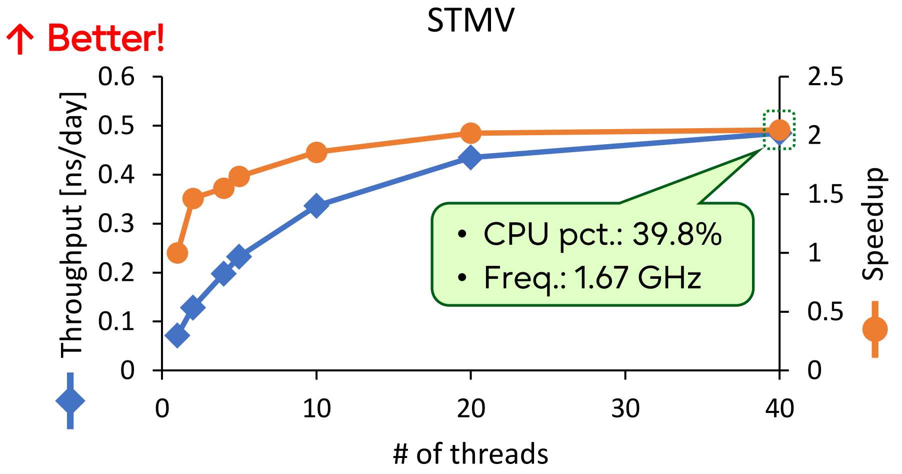
- Lower CPU percentage in parallel executions
  - Many sequential processes
  - Functions with high memory access (executed only in parallel exec.)
  - Inter-socket memory accesses (# of threads > 20)





Performance of Single Container (GROMACS)

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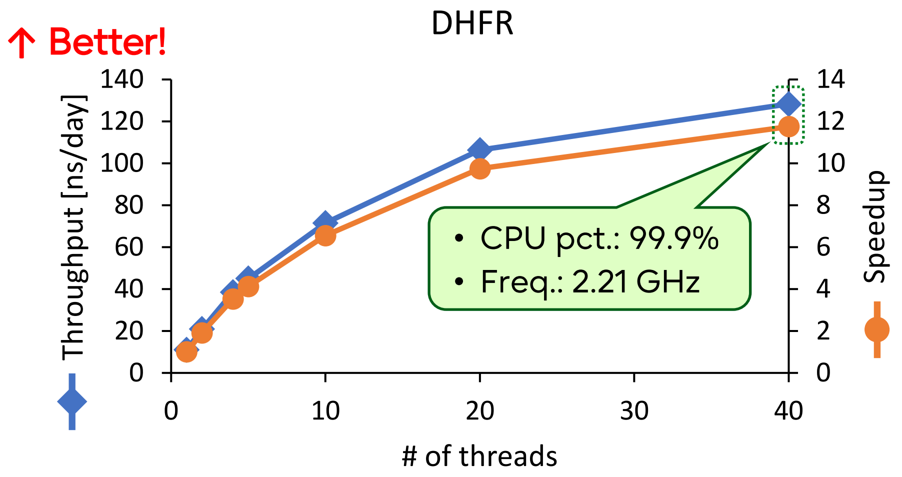
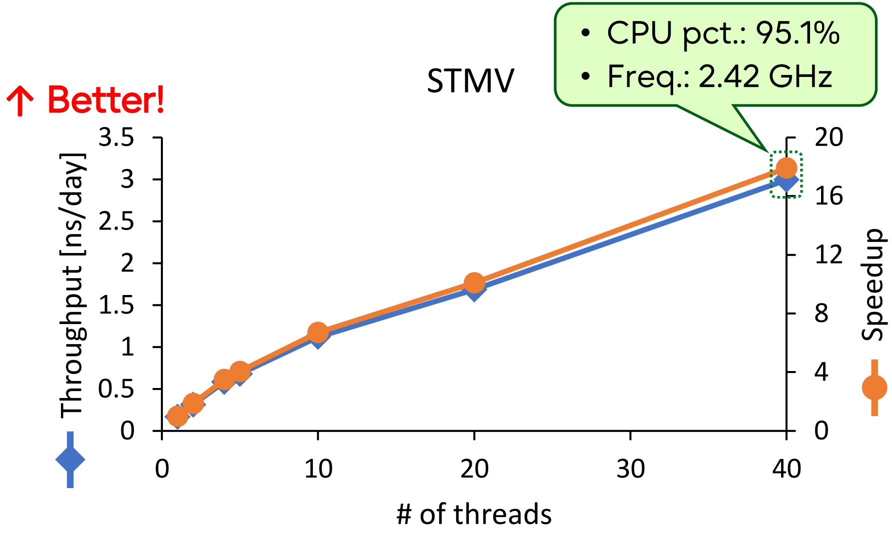
- Decrease in CPU frequency with increase in # of threads
  - Turbo Boost Technology
  - AVX-512 (Max 2.20GHz with 20 active cores per socket)





Performance of Multiple Containers (STMV)

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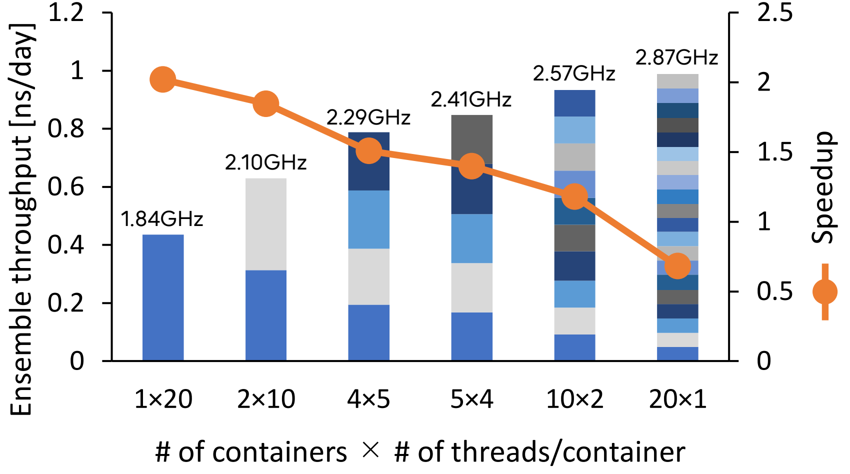
OpenMM

😊 Throughput: 0.435 → 0.987 (× 2.27)
😟 Speedup: 2.02 → 0.682 (× 0.338)

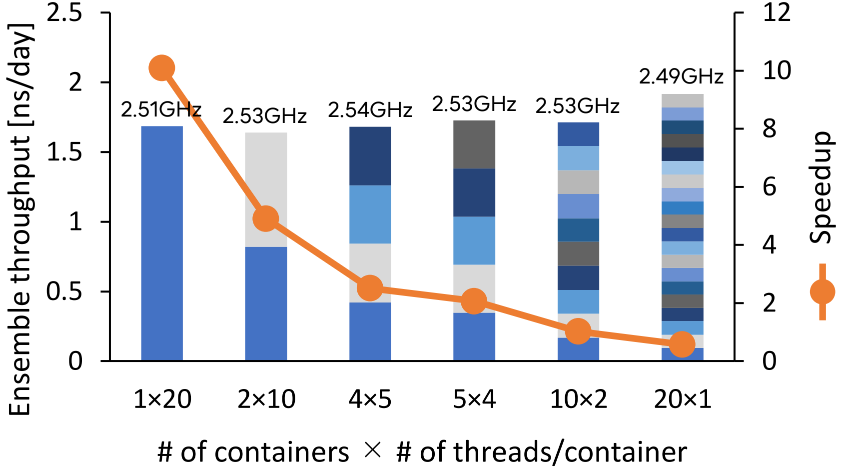
GROMACS

🙂 Throughput: 1.69 → 1.92 (× 1.14)
😱 Speedup: 10.1 → 0.573 (× 0.0568)

↑ Better!



↑ Better!



Performance with SMT (STMV)

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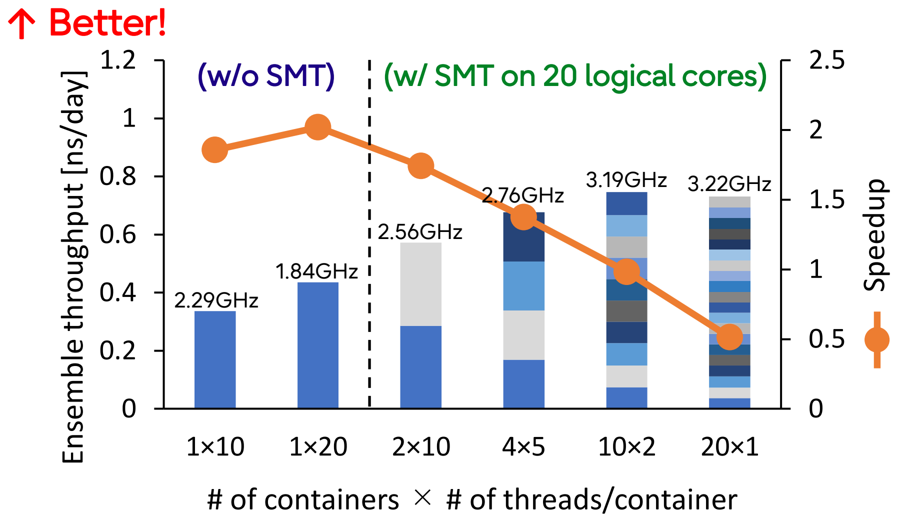
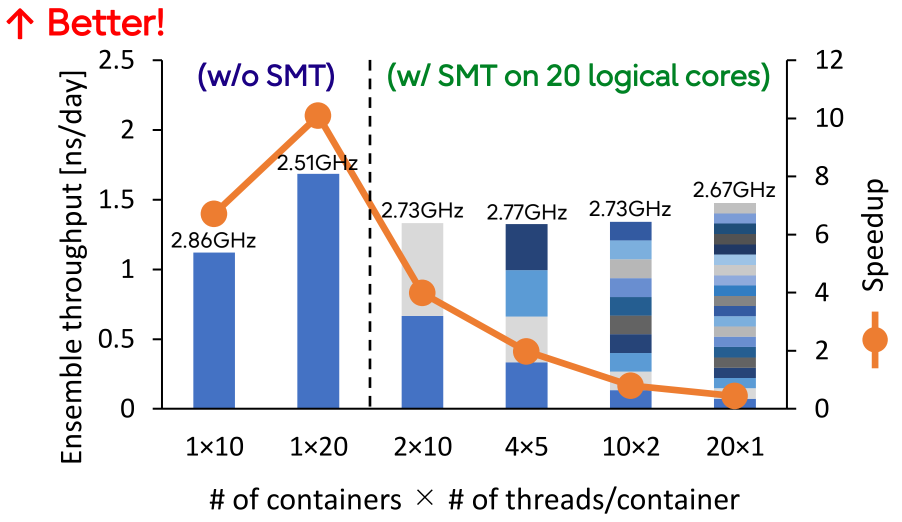
OpenMM (10 containers × 2 threads)

	Throughput	Speedup
vs. 1 cont. × 10 th.	× 2.22	× 0.530
vs. 1 cont. × 20 th.	× 1.71	× 0.487

GROMACS (20 containers × 1 thread)

	Throughput	Speedup
vs. 1 cont. × 10 th.	× 1.32	× 0.0659
vs. 1 cont. × 20 th.	× 0.875	× 0.0438





Conclusion

Conclusion

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Container scheduling problem

- How many containers and how many threads per container should we allocate?
- Which low-level resources should we allocate to reflect workload characteristics?

- Scheduling strategies in multi-containerized MD simulations
  - Large number of containers with fewer threads
    - Improving ensemble throughput while decreasing speedup
  - CPU core allocation considering SMT
    - OpenMM: 2.22-fold ensemble throughput with 0.530-fold speedup
  - Variable CPU frequency
- Implementing our scheduler…

Thank you