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The 12th International Workshop on OpenCL and SYCL

Unlocking Performance Portability on LUMI-G Supercomputer: A Virtual Screening Case Study

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Dompé

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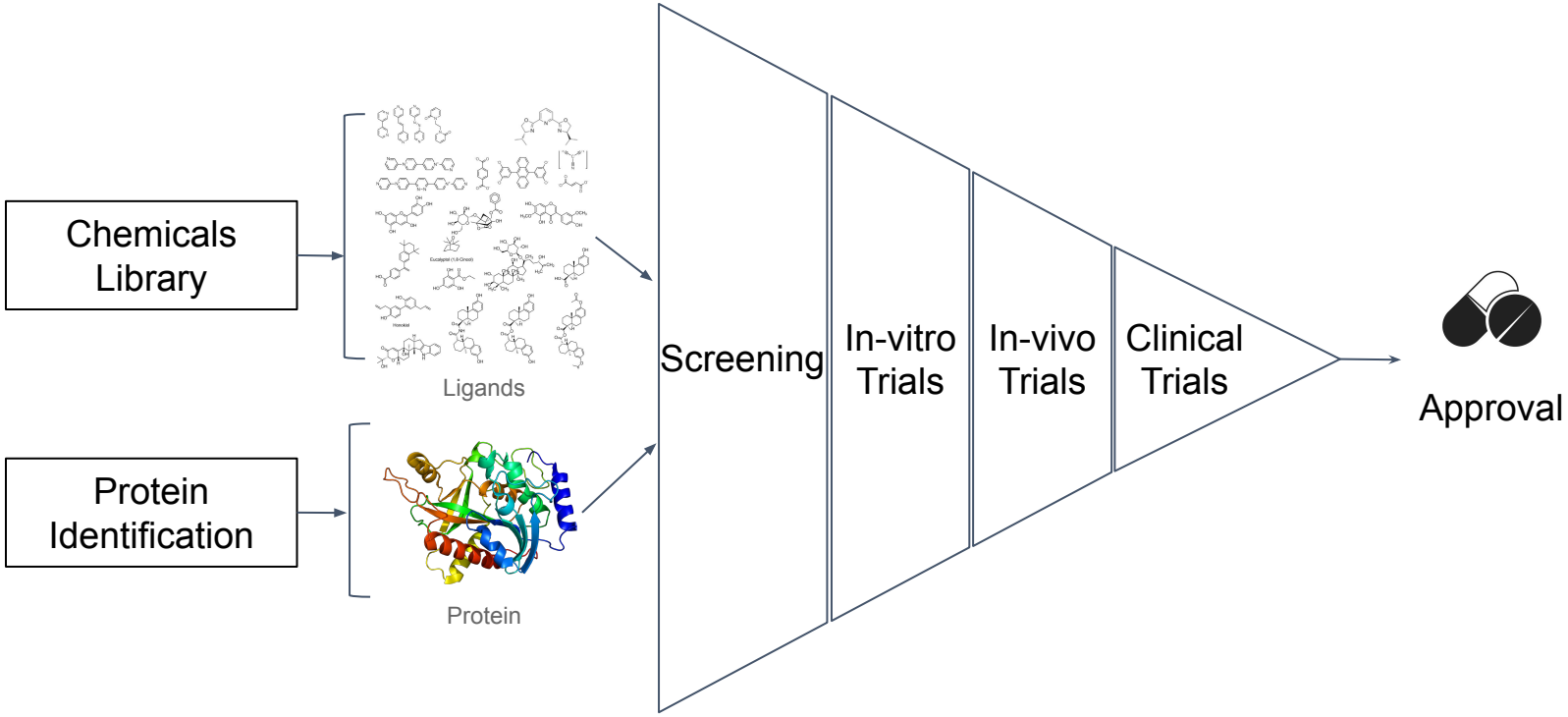
Overview

1. **Drug Discovery and Virtual Screening**
2. HPC for Urgent Computing
3. LiGen Batched GPU Acceleration
4. SYCL Porting
5. LUMI Benchmark Access
6. Results and Conclusions

Drug Discovery

- Identify chemicals that yield potential therapeutic effects
- It is a very long and costly process
  - Due to failure while finding drug candidates



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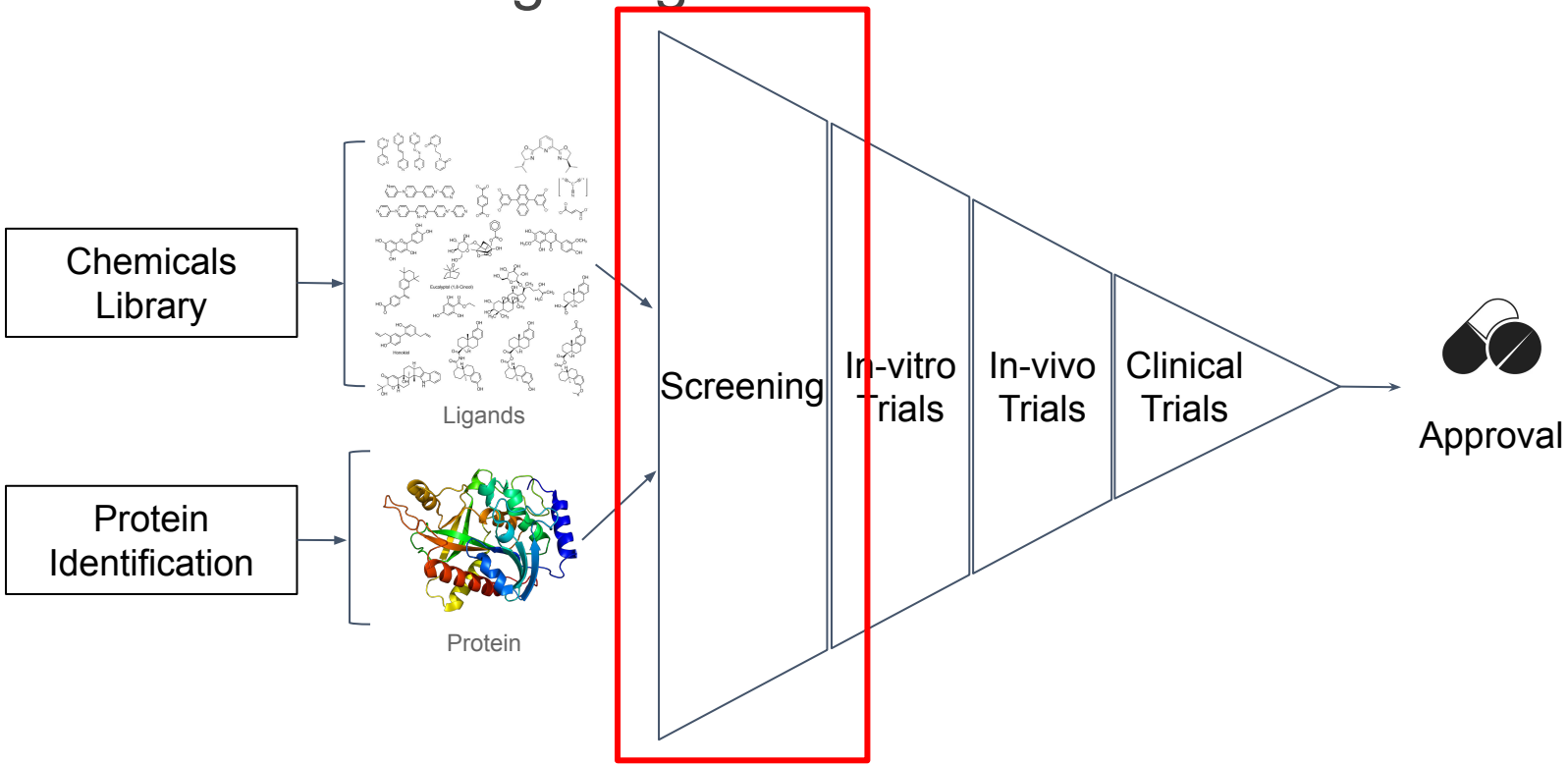
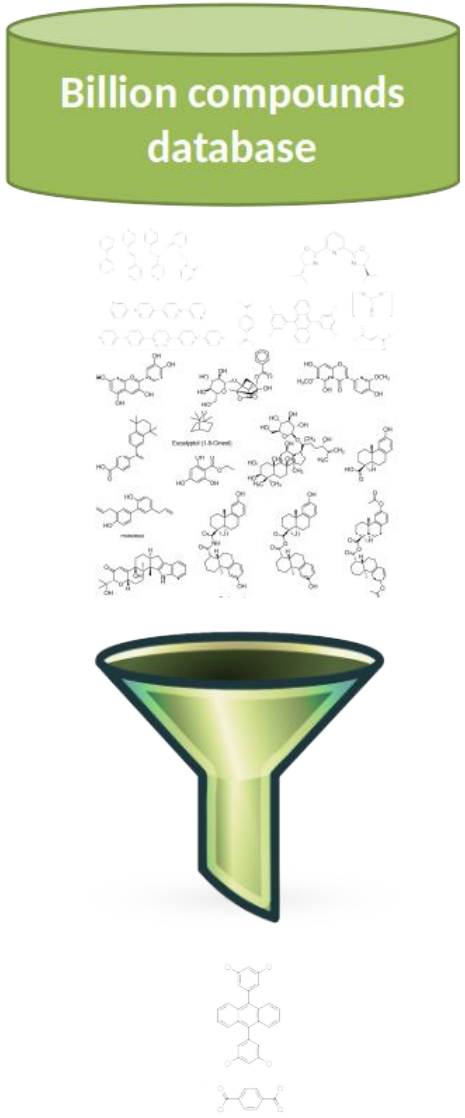


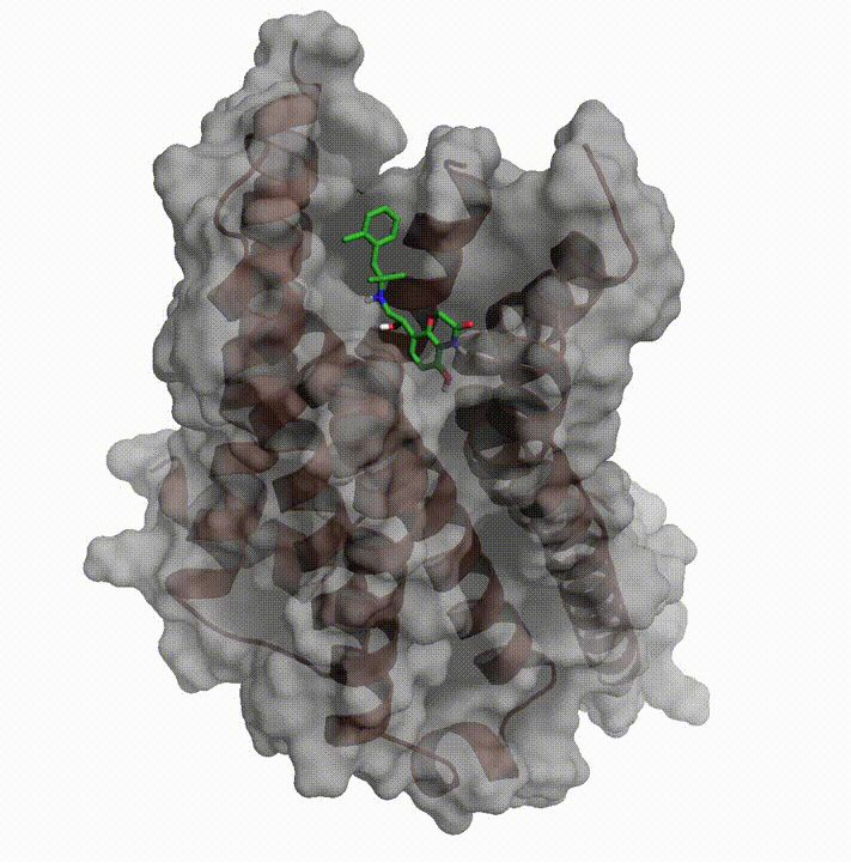
Virtual Screening



- It's an early stage of the drug discovery process
- It screens a large database of known compounds
  - Looking for the most promising drug candidates
- *In-silico* filter of compounds
  - Generate feasible compounds poses
  - Evaluate each pose-protein interaction strength

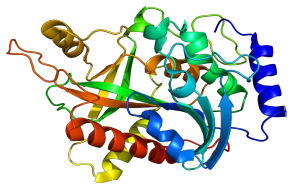
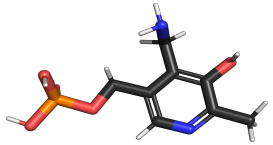
Molecular Docking

- Structural-based virtual screening
- Given two molecules, it searches for feasible ligands poses
  - It binds ligands onto a target protein



Scoring Functions

- Predicts the interaction strength of each pose-protein pair
  - The output **SCORE** is a numerical value
  - It is used for ranking
- Consider different chemical interactions
  - Hydrogen bonding
  - Solvent
  - Buried surface
  - Van der Waals forces

$f\{$  ,  $\} = SCORE$

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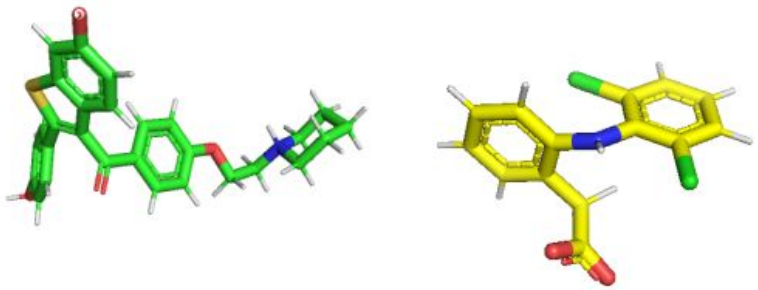
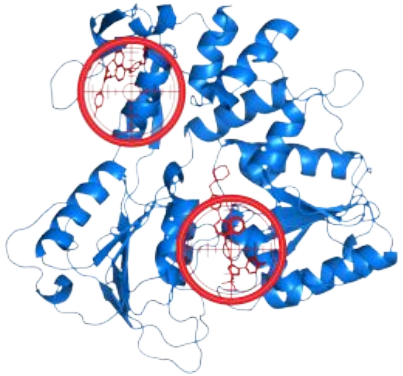
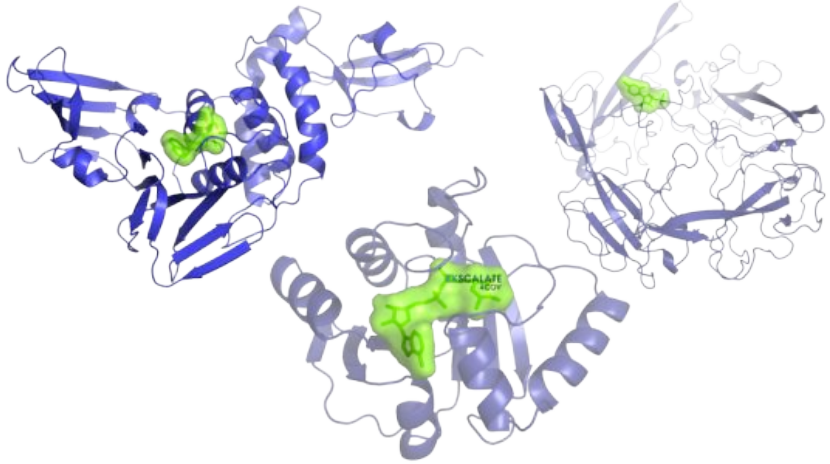
Virtual Screening and HPC



- Virtual screening is complex
  - Virtual compound libraries are very large
- Each ligand-protein evaluation is independent
  - Embarrassing parallel problem
- Supercomputers are leveraged to perform virtual screening campaign





LiGen

- Virtual screening application owned by Dompé
- It is a component of the EXSCALATE drug discovery platform
- Design to hinge the modern supercomputer nodes
- Used to perform extreme-scale virtual screening campaign

References:
D. Gadioli et al., “EXSCALATE: An Extreme-Scale Virtual Screening Platform for Drug Discovery Targeting Polypharmacology to Fight SARS-CoV-2”, TETC, 2022

Urgent Computing

- Virtual screening campaign to fight back against pandemics
  - ANTAREX 4ZIKA CPU only version
  - EXSCALATE 4COV GPU support (CUDA)
- The LIGATE European is developing a CADD workflow
  - Support for several EuroHPC supercomputers
  - LUMI deployment showed a new challenge

References:
G. Palermo et al., “Tunable and Portable Extreme-Scale Drug Discovery Platform at Exascale: the LIGATE Approach”, CF, 2023

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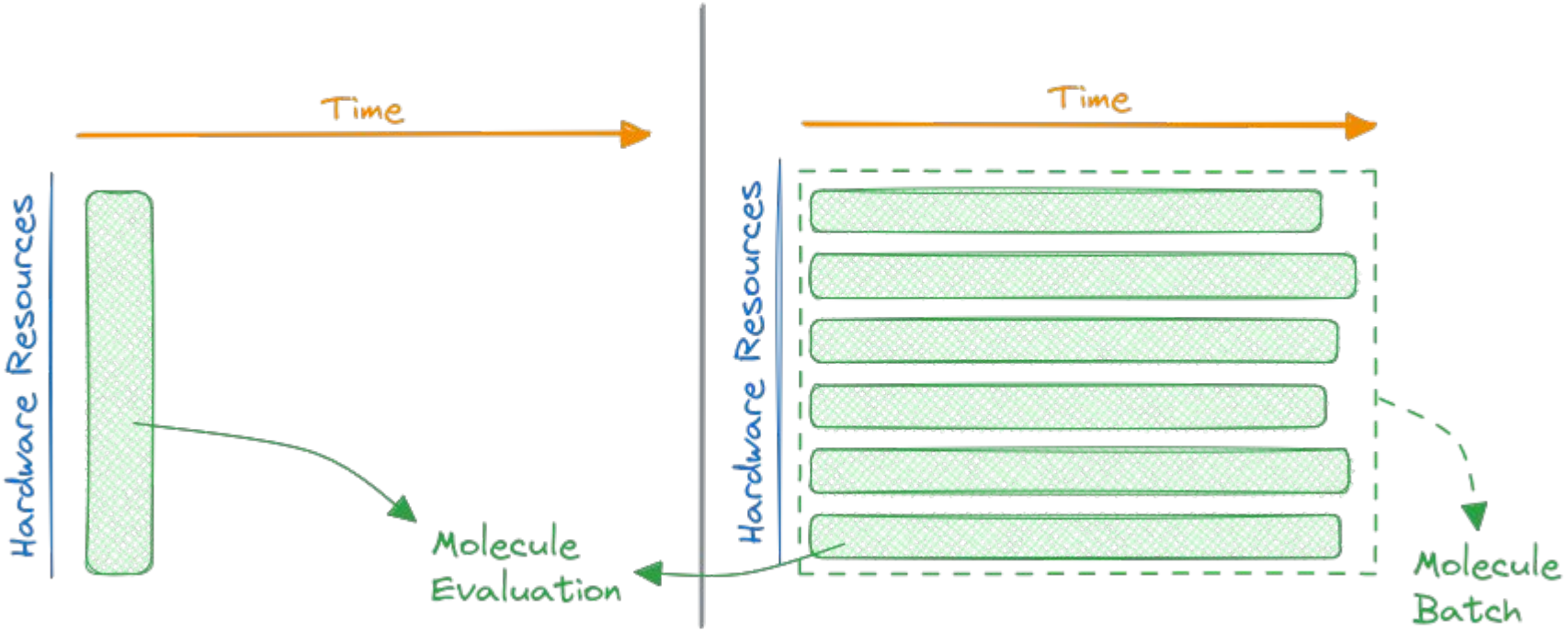
LiGen GPU Approach

- LiGen deploys a highly optimized CUDA version
  - GPU computational approach shifted from a latency to a throughput one
  - Thanks to a collaboration with NVIDIA's engineers



NVIDIA CUDA

References:
E. Vitali et al., “GPU-optimized approaches to molecular docking-based virtual screening in drug discovery: A comparative analysis”, JPDC, 2024

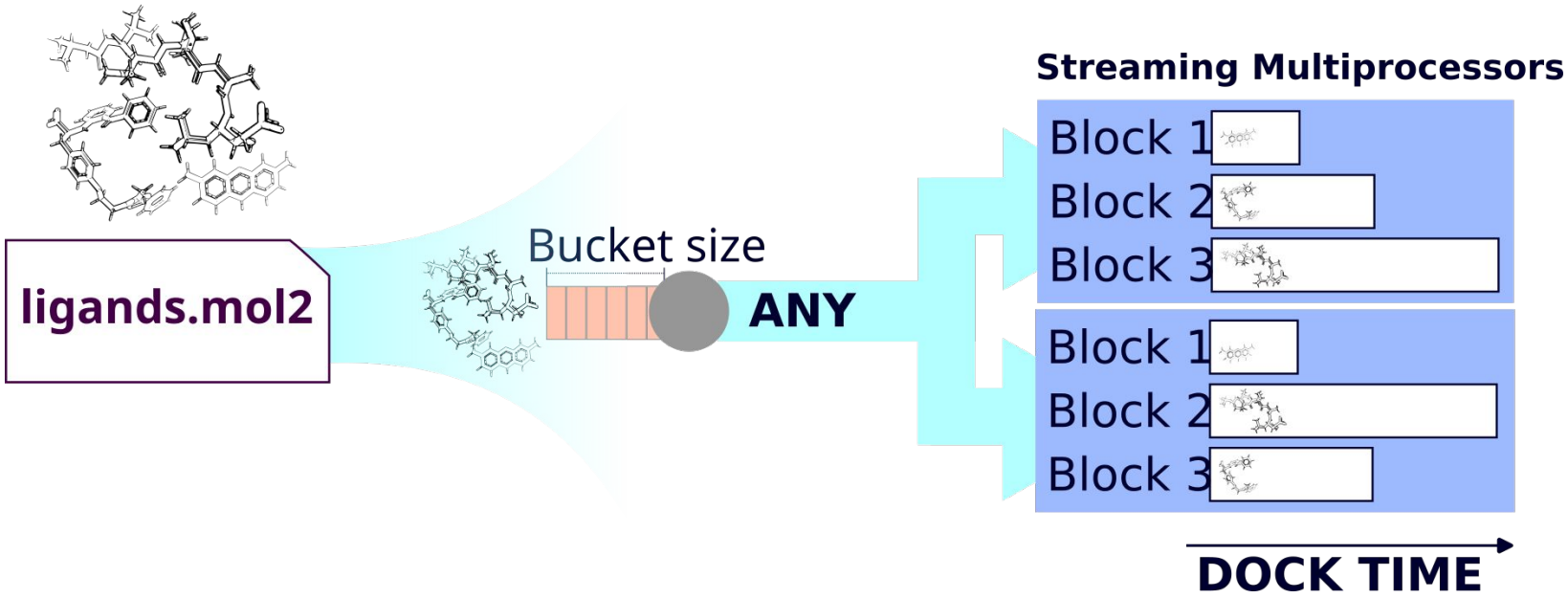
LiGen Batched Approach - 1

- LiGen code makes extensive use of template meta-programming
  - Influence kernel's registers pressure
  - Batch's ligands properties are used to select a kernel implementation
- Batches can be tuned
  - Total number of batches used
  - Each batch dimension
    - Influenced by the hardware characteristics
    - Auto-tuning using CUDA runtime API

References:
G. Accordi et al., “Out of kernel tuning and optimizations for portable large-scale docking experiments on GPUs”, JoS, 2024

LiGen Latency Approach

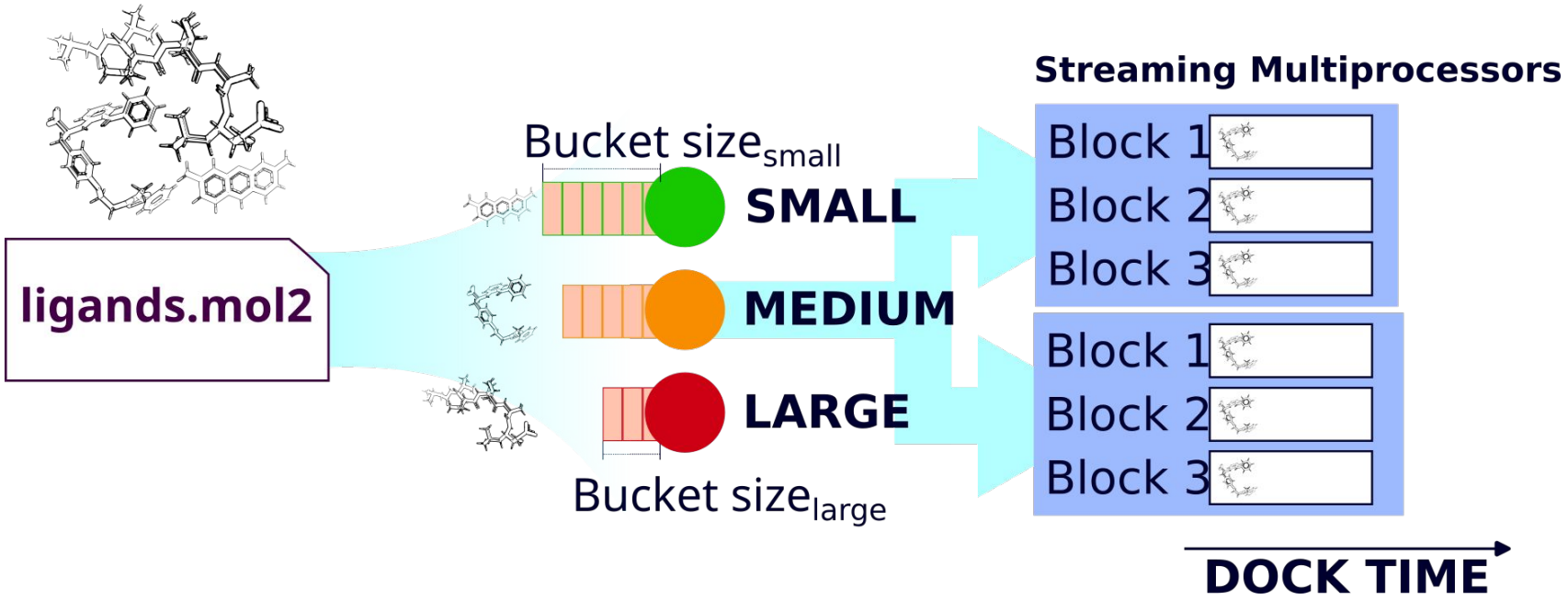
- LiGen latency version process ligand in-order



References:
G. Accordi et al., “Out of kernel tuning and optimizations for portable large-scale docking experiments on GPUs”

LiGen Batched Approach - 2

- LiGen throughput version process ligand out-of-order
  - It packs ligands with the same expected execution time in batches



References:
G. Accordi et al., “Out of kernel tuning and optimizations for portable large-scale docking experiments on GPUs”, JoS, 2024

API Query & Formulas

CUDA

$$l = b \times SM \times \frac{t}{ws}$$

- CUDA b obtained with
  - `cudaOccupancyMaxActiveBlocksPerMultiprocessor`

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LiGen SYCL porting

- SYCL porting has initially been focused on NVIDIA GPUs
  - We focused on maintaining LiGen functionality end-to-end
- Then, the LiGen SYCL version was extended to run on multi-GPU and multi-node architectures
  - The batched approach has been ported into SYCL

References:
L. Crisci et al., “Enabling Performance Portability on the LiGen Drug Discovery Pipeline”, FGCS, 2024

API Query & Formulas

CUDA

$$l = b \times SM \times \frac{t}{ws}$$

SYCL

$$l = \frac{wgs}{t} \times CU \times \frac{t}{sgs}$$

- CUDA b obtained with
  - `cudaOccupancyMaxActiveBlocksPerMultiprocessor`
- SYCL wgs obtained with
  - `kernel_device_specific::work_group_size`
  - Part of the `kernel_bundle` API

LiGen Number of Batches

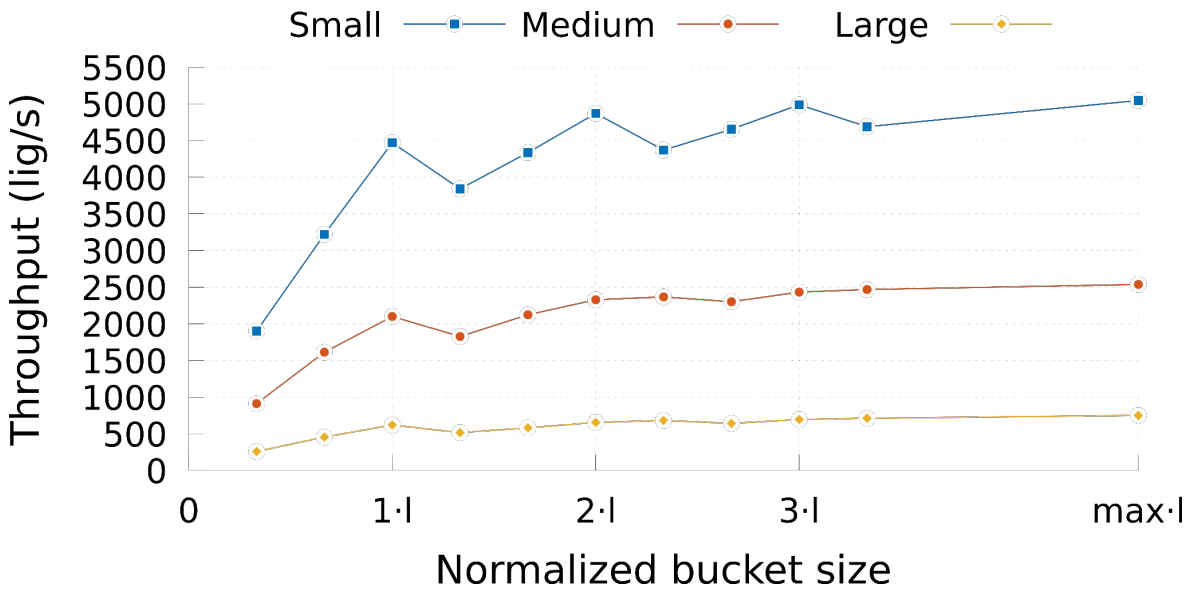
Number of atoms cluster \ Number of rotamers cluster	1	4	6	9	23
6	1.48475	1.72236	1.96128	2.07905	2.19256
4	1.46474	1.70132	1.93353	2.04994	2.17648
2	1.3416	1.56971	1.82724	1.94081	2.02947
1	1	1.13429	1.34559	1.37753	1.44393

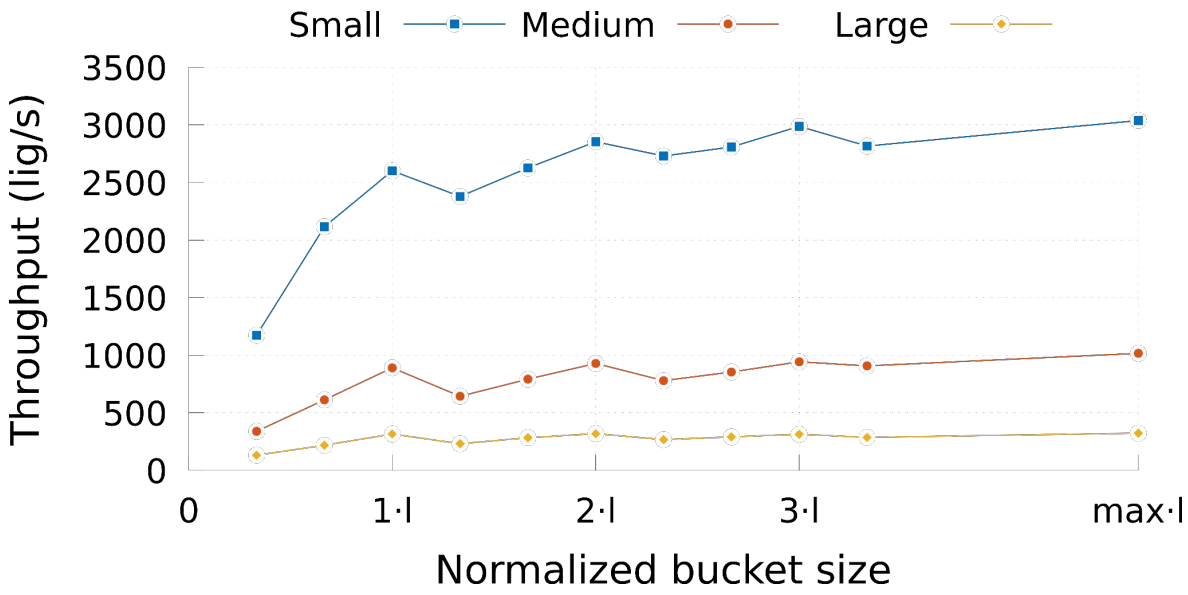
(a) CUDA implementation

Number of atoms cluster \ Number of rotamers cluster	1	4	6	9	23
6	1.28707	1.51416	1.65884	1.82244	1.93901
4	1.24815	1.47157	1.6077	1.76181	1.86973
2	1.14244	1.35158	1.48027	1.62752	1.71154
1	1	1.13143	1.19798	1.2902	1.32217

(b) SYCL implementation

LiGen Batch Dimension





- Batching showed a similar performance improvement

References:
G. Accordi et al., “Out of kernel tuning and optimizations for portable large-scale docking experiments on GPUs”

Batching Registers Pressure

- Ligands' sizes used as typed template parameter
- Template parameters impact loop unrolling
  - Increased register pressure
- Fix register number does not help
  - Slower kernel

Num Atoms	**CUDA** Registers	**SYCL**(oneAPI) Registers
32	102	158
64	103	176
96	98	176
128	102	178
160	112	176
192	124	182

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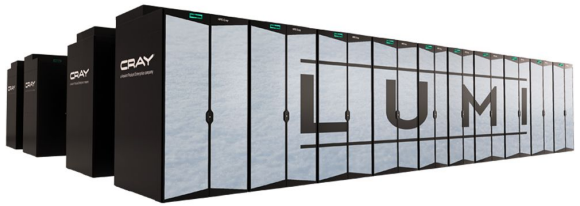
Benchmark Access

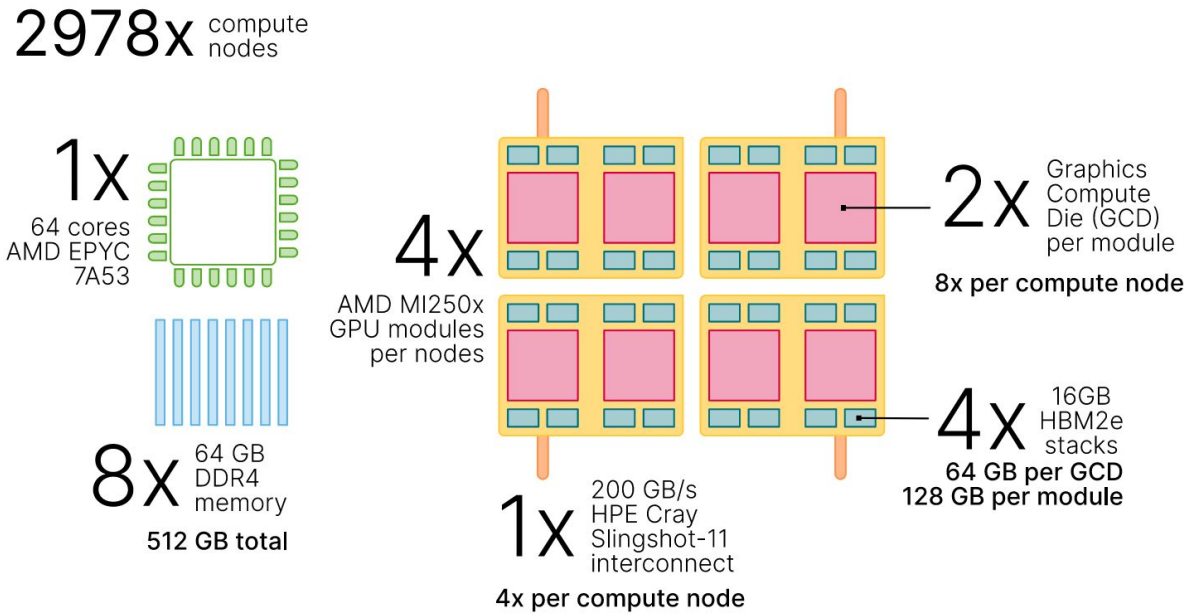
- SYCL support has been extended to AMD GPUs
  - Thanks to a Benchmark Access on the LUMI-G partition
- SYCL Porting tested and tuned for AMD architecture
- On AMD GPUs, no LiGen reference is available
  - HIP porting using HIPIFY
  - The HIP version has been tested but not tuned

AMD ROCm

LUMI

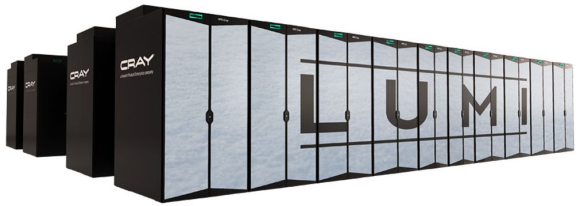
- Located at CSC Data Center in Finland, co-founded by EuroHPC
- It has a speed of 550 petaFLOPS
  - 5th supercomputer in the world, according to November 2023 Top500
  - 1st supercomputer in Europe, according to the same ranking
- Based on HPE Cray EX architecture





LUMI

- No official SYCL support when we started collecting data
  - We have been in contact with the CSC support team
  - We preferred to compile everything from scratch
  - Some technical problems to get a working SYCL toolchain



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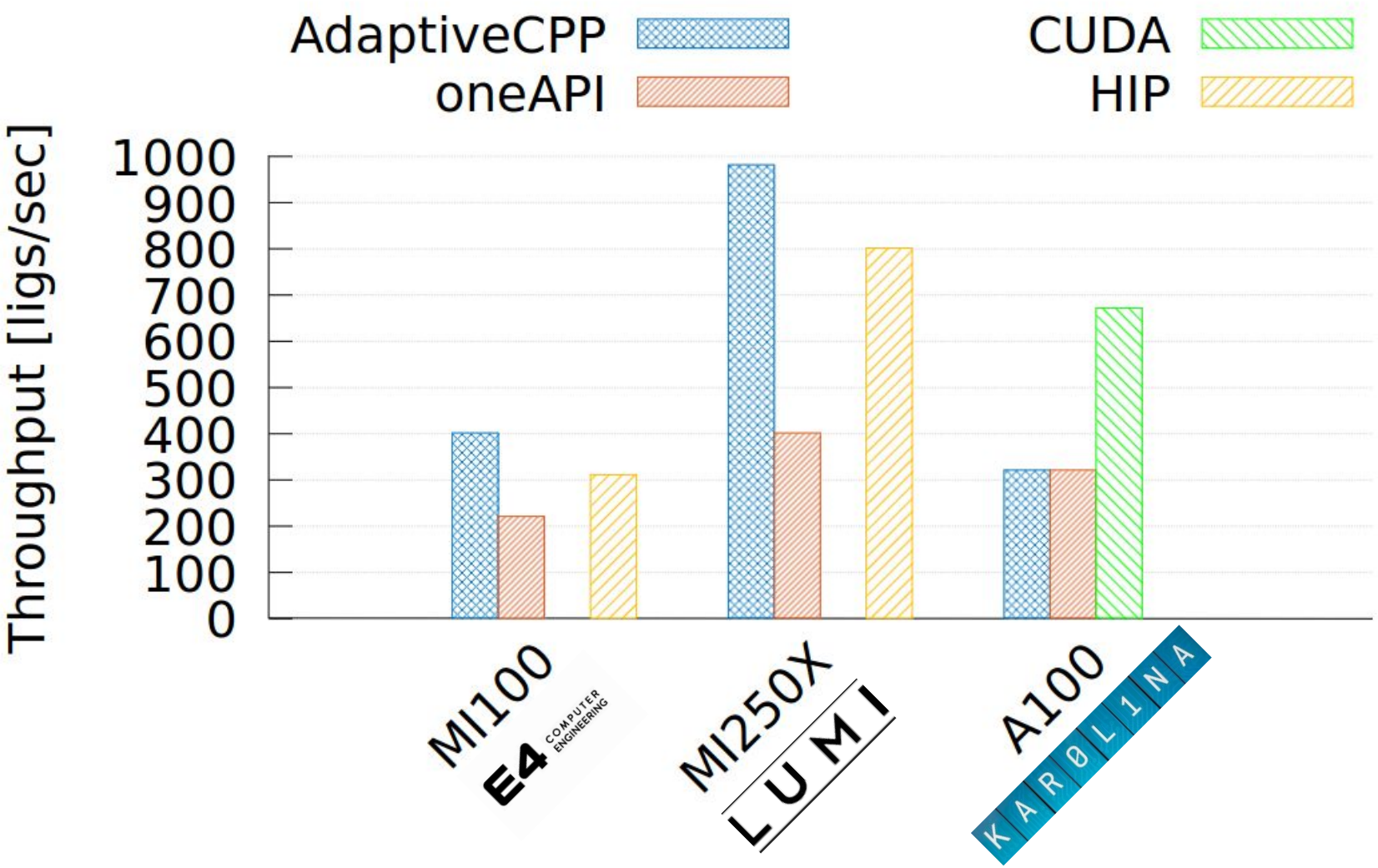
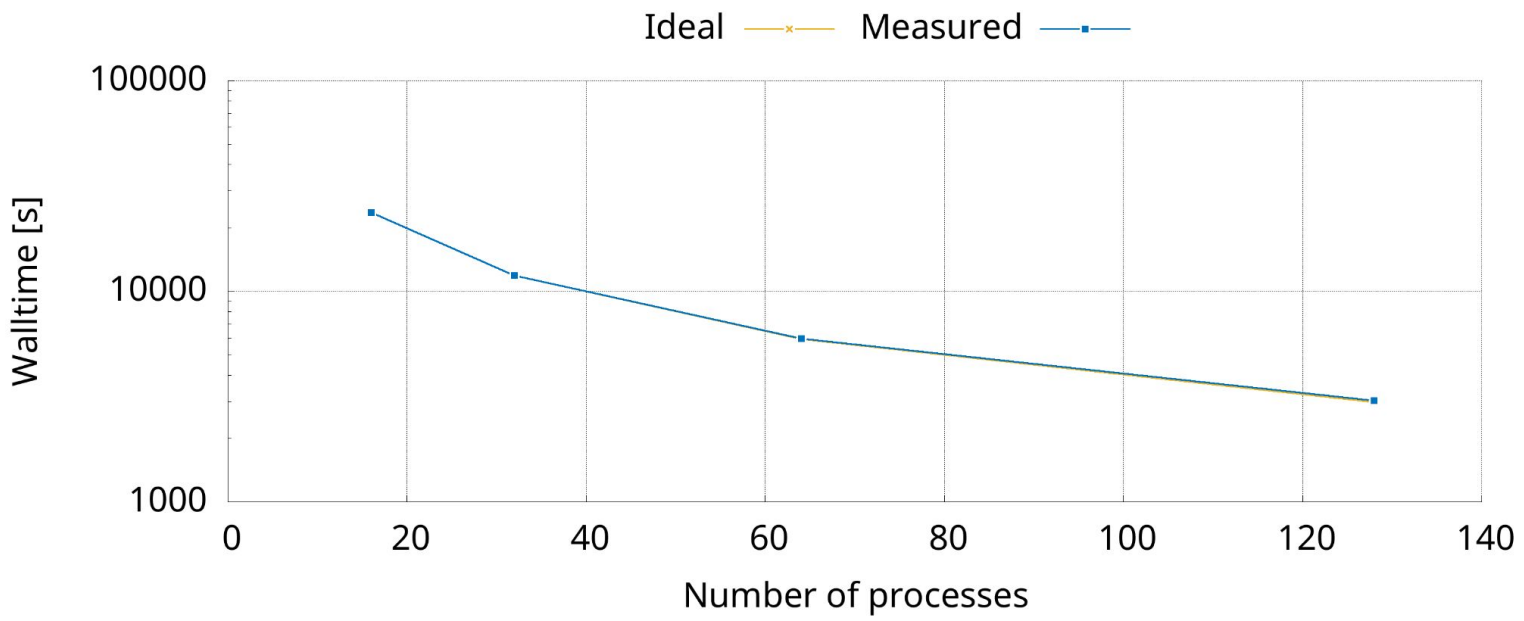
Experimental Setup

- Software-stack
  - GCC 11.3 and LLVM 15.0.6
  - AdaptiveCpp 0.9.4
  - oneAPI DPC++ 2022-12
  - NVCC 11.7
  - HIP 5.3
- Hardware
  - AMD MI250X on LUMI-G nodes
  - AMD MI100 on E4 cluster
  - NVIDIA A100 on Karolina nodes

LiGen LUMI GPUs Performance



LiGen Scaling on LUMI

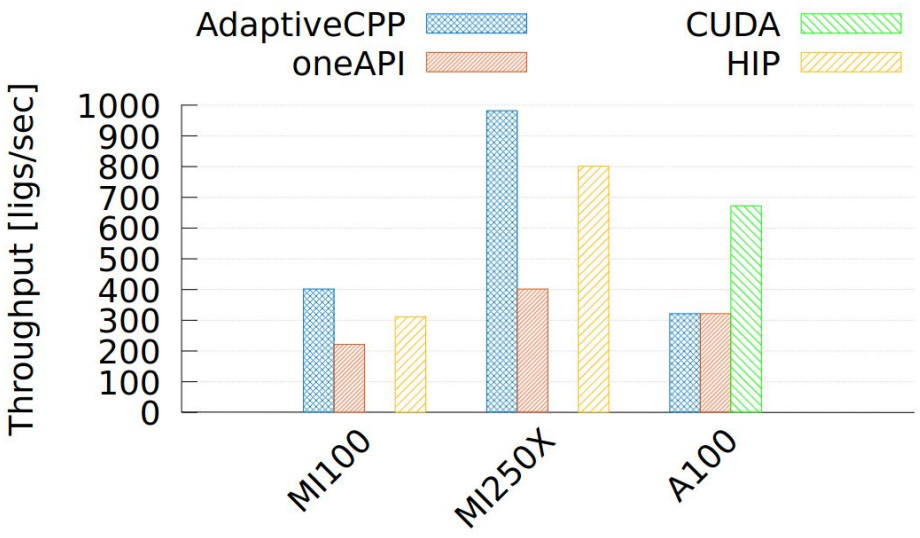


Num GPUs/node	Speed-up
1	1
8	7.756

NOTE: due to a technical problem with the FS, we used only 1 GPU per node

Conclusions

- We are now able to support several EuroHPC supercomputers
  - Performance portability unlocked
- There is still room for improvement
  - On NVIDIA, we cannot go fully SYCL
    - High register pressure
  - Support now for AMD systems
    - SYCL compiler performs differently
    - HIP requires some tuning



<u>Urgent computing scenarios can perform future virtual screening campaigns on more supercomputing architectures</u>

Thank you for your attention!

- Acknowledgment
  - EuroHPC JU for awarding this project access to
    - LUMI under project EHPC-BEN-2022B12-001
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  - European Union’s Horizon 2020 research and innovation program
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