FAST. FLEXIBLE. FREE.
GROMACS

oneAPI Case Study: GROMACS

Andrey Alekseenko

KTH Royal Institute of Technology & SciLifeLab
Stockholm, Sweden

GROMACS

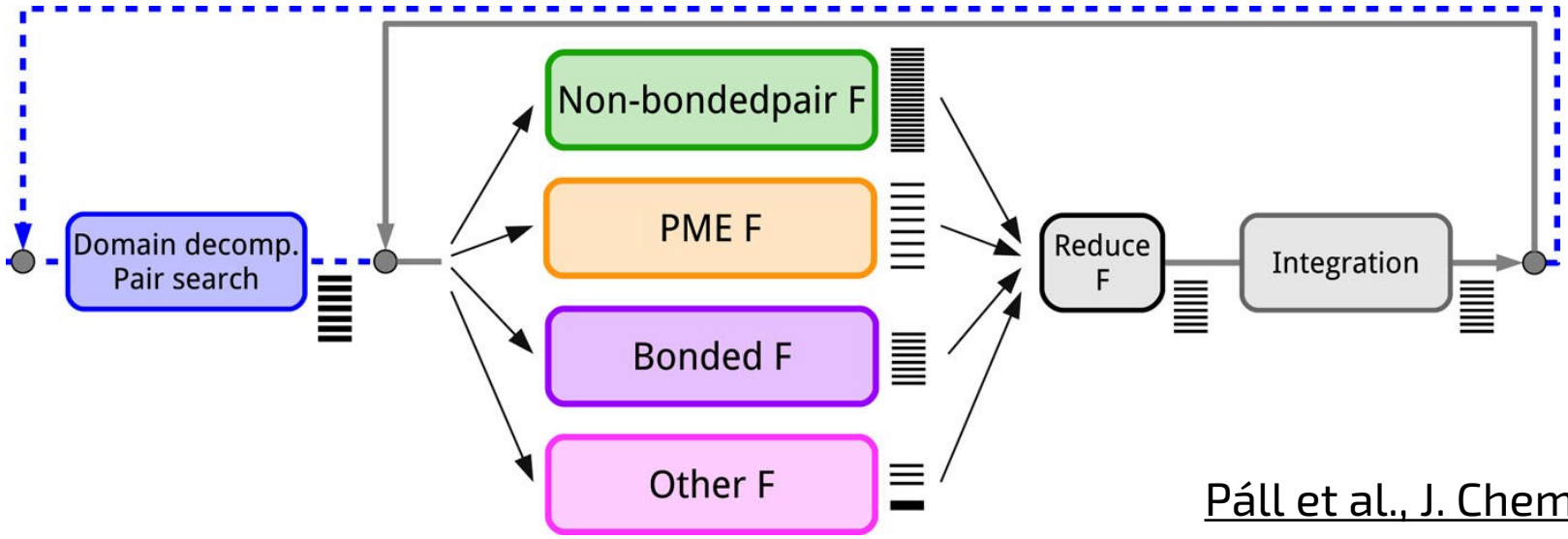
- Open source molecular dynamics engine
- One of the most used HPC codes worldwide
- High-performance for a wide range of modeled systems
- … and on a wide range of platforms:
  - from supercomputers to laptops (Folding@Home)
  - x86, x86-64, ARM, POWER, SPARC, RISC-V
  - 11 SIMD backends
  - NVIDIA, AMD, and Intel GPUs; Intel Xeon Phi
  - Windows, MacOS, included in many Linux distros

GROMACS 2023 (upcoming)

- (Mostly) modern C++17 codebase
  - 449k lines of C++ code
  - With a bit of legacy (first release: 1991)
- MPI for inter-node parallelism
- OpenMP for multithreading
- SIMD for low-latency operations on CPU
- GPU offload for high-throughput operations
  - CUDA: NVIDIA
  - OpenCL: AMD, Apple*, Intel, NVIDIA
  - SYCL: AMD, Intel, NVIDIA

Molecular dynamics

- Iterative problem
  - Like N-body, but with fancier physics
- One step ~1 fs, need to simulate µs to ms
  - 10^9-10^{12} steps



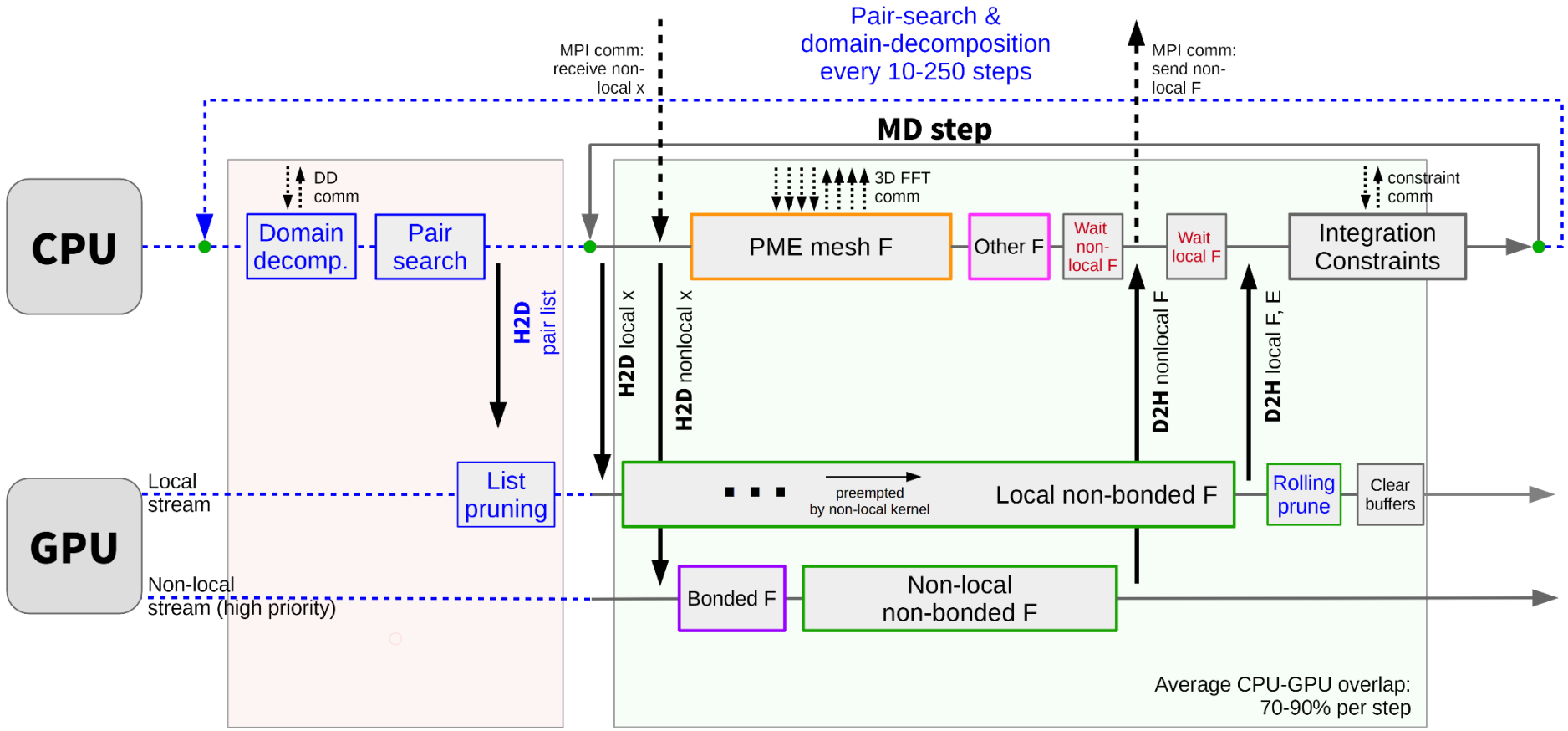
Páll et al., J. Chem. Phys. 153, 134110 (2020)

Heterogeneous parallelization

- Minimize latency
- Minimize CPU and GPU stalls
- Minimize data exchange between host and device
  - And between nodes

- Optimal offloading scheme depends on simulated system
  - And on available hardware
- Must be maintainable

Molecular dynamics: real schedule



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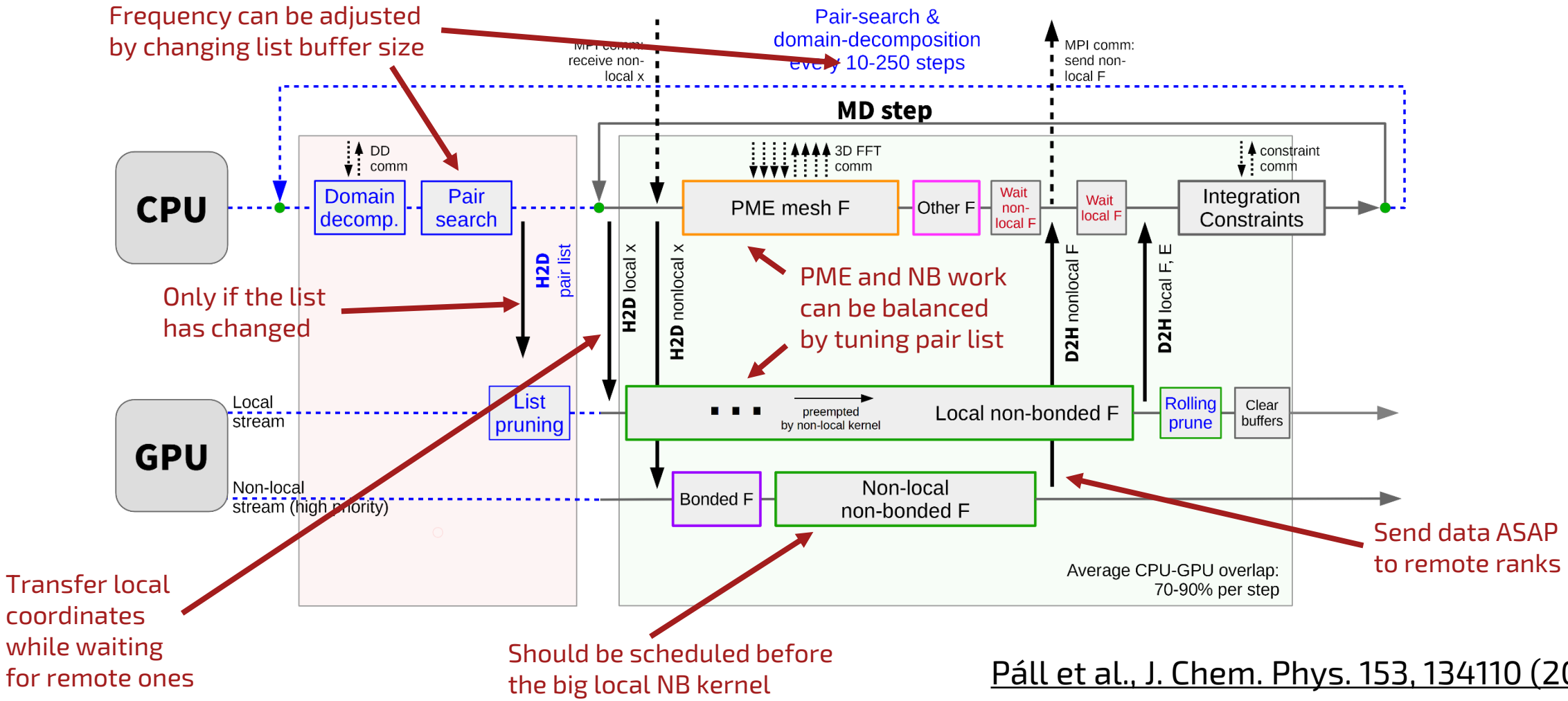

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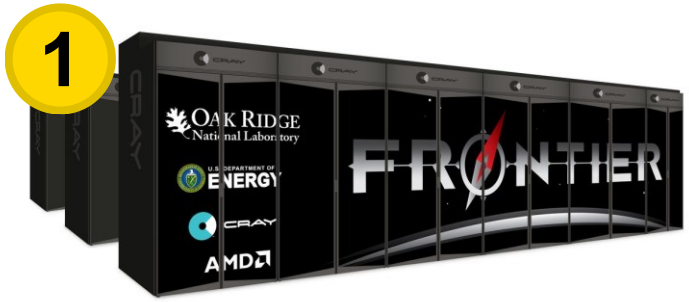
GPU feature support in GROMACS 2020

	NVIDIA CUDA	OpenCL
Non-bonded offload	√	√
PME offload	√	√
Update offload	√	X
Bonded offload	√	X
Direct GPU-GPU comm	√	X
Hardware support	NVIDIA	NVIDIA, AMD, Intel

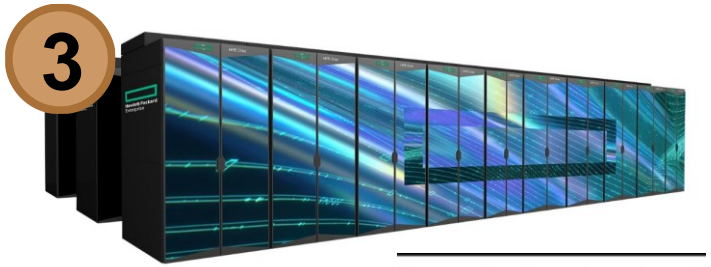
Why another GPU framework?

AMD Instinct GPU

Intel Ponte Vecchio GPU



First exascale systems



LUMI

Why not OpenCL?

- OpenCL kernels are C99, the rest of GROMACS is C++17
  - C++ kernels are not widely supported
- Separate-source model
- Hard to maintain
- Supported by all vendors, preferred by none

Why SYCL?

- Open standard, free (libre) implementations
- Implemented on top of existing backend
  - Intel® oneAPI DPC++: OpenCL and LevelZero; CUDA; HIP
  - hipSYCL: CUDA, HIP; LevelZero (via DPC++)
  - Leverage existing profiling and debugging tools
  - And device compilers
- Standard C++ with a custom library
  - No need for extra support in linters, IDEs, etc.
- Logically similar to OpenCL
  - (Almost) no need to deeply modify existing code

SYCL enablement plan (late 2020)

- Step 1:
  - Target oneAPI DPC++ / Intel GPUs, but stay standard-compliant
  - Device detection and initialization
  - Remove code specific to CUDA/OpenCL
- Step 2:
  - Port kernels accounting for majority of run time
- Step 3:
  - Expand support to AMD GPUs
  - Port the rest of the kernels
  - Add support for GPU-aware MPI
  - Optimize kernels and runtime

SYCL enablement plan

- Step 1:
  - Target oneAPI DPC++ / Intel GPUs, but stay mostly standard-compliant
  - Device detection and initialization
  - Remove code specific to CUDA/OpenCL: still ongoing…
- Step 2:
  - Port kernels accounting for majority of run time
- Step 3:
  - Expand support to hipSYCL; AMD and NVIDIA GPUs
  - Port the rest of the kernels
  - Add support for GPU-aware MPI
  - Optimize kernels and runtime: we're here

Automatic conversion?

- We want to have both CUDA and SYCL in the same codebase
- Already have abstraction layer for Device, Queue, etc
  - Supports CUDA and OpenCL
  - CUDA kernels heavily optimized for NVIDIA
  - OpenCL kernels have Intel-optimized code paths
  - Rewriting kernels is ~trivial

- Conclusion: manual porting

GPU framework comparison

	NVIDIA CUDA	OpenCL	SYCL
Scheduling	in-order queue or explicit DAG	in-order and out-of-order queues	implicit DAG and in-order queues
Synchronization event	separate pseudo-task	associated with a task or a pseudo-task	associated with a task
Timing measurement	regions	of a single event	of a single event
Timing enablement	at event creation	at queue creation	at queue creation
Device selection	stateful per-thread	explicit in each call	explicit in each call
Native float3 size	12 bytes	16 bytes	16 bytes

GPU framework comparison

We already had an abstraction layer

Scheduling	in-order queue or explicit DAG	in-order and out-of-order queues	implicit DAG and in-order queues
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DAG-based scheduling

- Good: Prevent bugs and improve performance
- Bad: GROMACS is built around for in-order queues, with explicit barrier synchronizations:
  - Performance: synchronizing twice
  - Correctness: device-to-host copies
- Bad: Runtime must be smart
- Ugly: Additional divergence between backends

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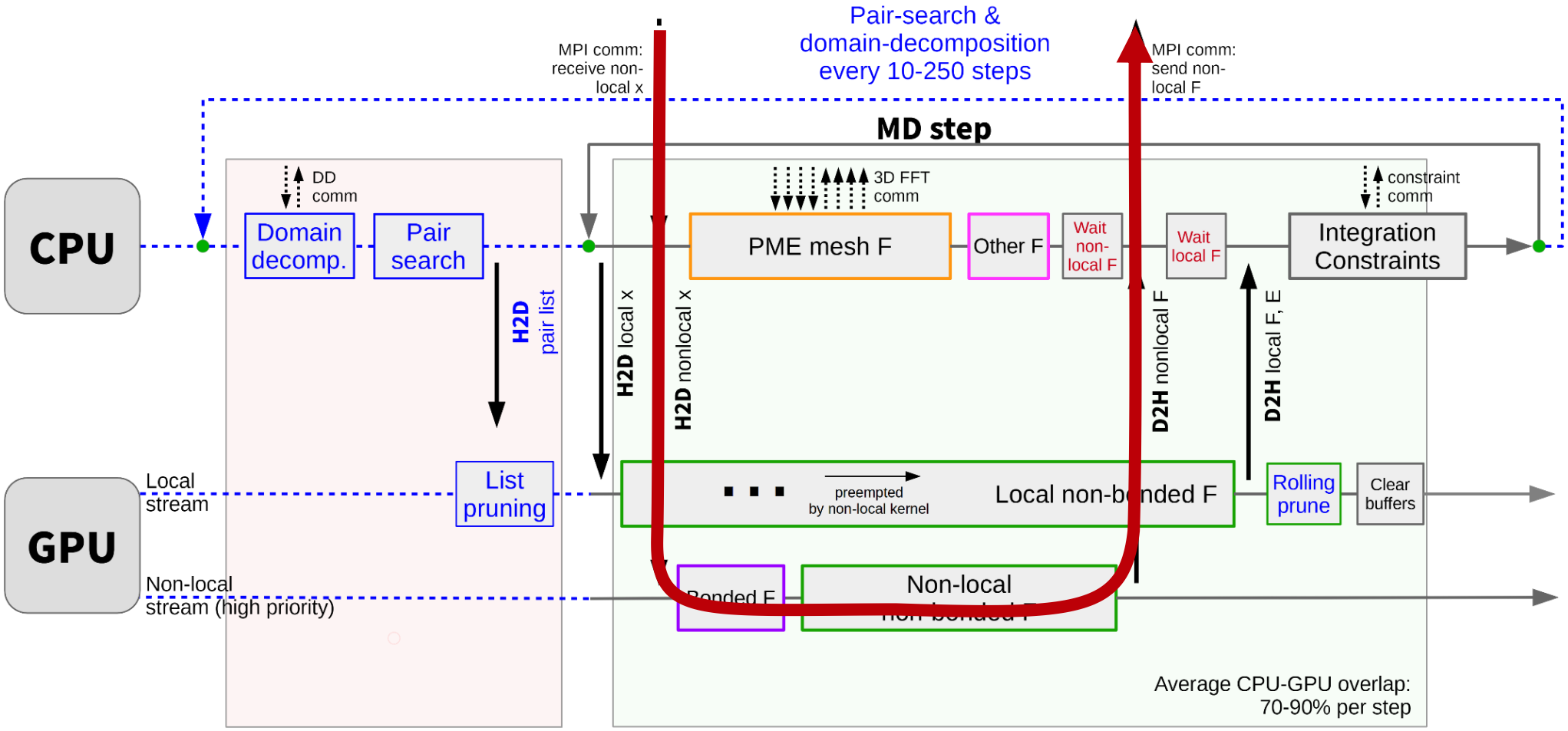

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DAG-based scheduling

- No, just use in-order queues and USM

- Bonus:
  - Accessors hard to optimize for compiler
  - Easier interop with GPU-aware MPI

GPU framework comparison

			
Scheduling	in-order queue or explicit DAG	in-order and out-of-order queues	implicit DAG and in-order queues
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Device selection	by special function	explicit in each call	explicit in each call
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Synchronization Events

- Event can be recorded far from the last submission
  - Not easy to tell which operation should be used for synchronization

- Custom extensions to mark events:
  - oneAPI DPC++: `SYCL_EXT_ONEAPI_ENQUEUE_BARRIER`
  - hipSYCL: `hipSYCL_enqueue_custom_operation` to submit empty jobs acting as barriers

- hipSYCL's coarse-grained events

GPU framework comparison

			
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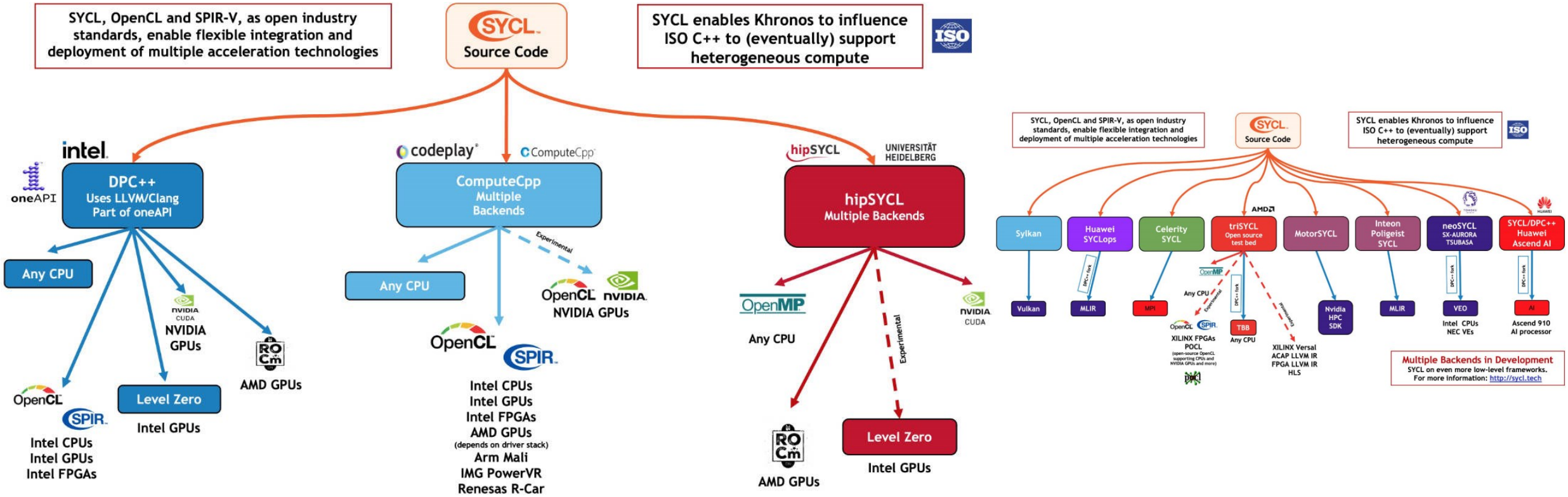
Other differences to keep in mind

- Exceptions vs return codes
- Different and variable (for Intel) sub-group sizes
- Thread indexing order:
  - CUDA and OpenCL: thread (x, y, z) is adjacent to (x+1, y, z)
  - SYCL: thread (x, y, z) is adjacent to (x, y, z+1)
- No SYCL implementation is fully standard-compliant yet
  - Some standardized features still implemented as extensions
  - It's getting better
- No SYCL implementation is fully optimized
  - Less of an issue for compilers, more of an issue for the runtime

SYCL beyond oneAPI



https://www.khronos.org/sycl/

Portability in practice: FFT

- 3D real-to-complex, forward and backward FFT

- Intel GPUs: oneMKL
- AMD GPUs: rocFFT/vkFFT via `HIPSYCL_EXT_ENQUEUE_CUSTOM_OPERATION`
- NVIDIA GPUs: vkFFT via `HIPSYCL_EXT_ENQUEUE_CUSTOM_OPERATION`

- Future: HeFFTe to decompose FFT over multiple nodes?

Portability in practice: hipSYCL

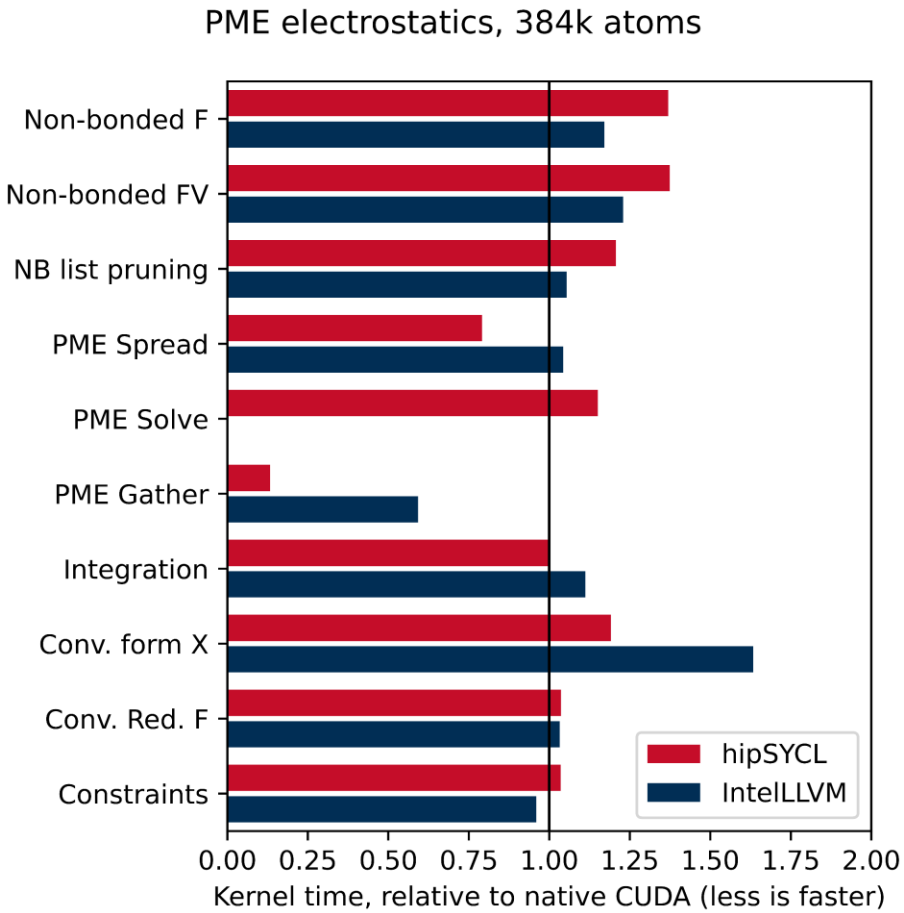
- At start, only Intel oneAPI DPC++ and Intel GPUs supported
  - hipSYCL added later to target AMD devices
- Effort:
  - Workarounds due to backend / compiler issues
    - Different parts of SYCL 2020 implemented
  - Fix a few bugs not triggered with oneAPI
  - CMake scripting
  - Kernel optimizations mostly ported from OpenCL
    - Still, some time with profiler was required
  - Runtime profiling/tuning
    - When the GPU FLOPS are not the bottleneck

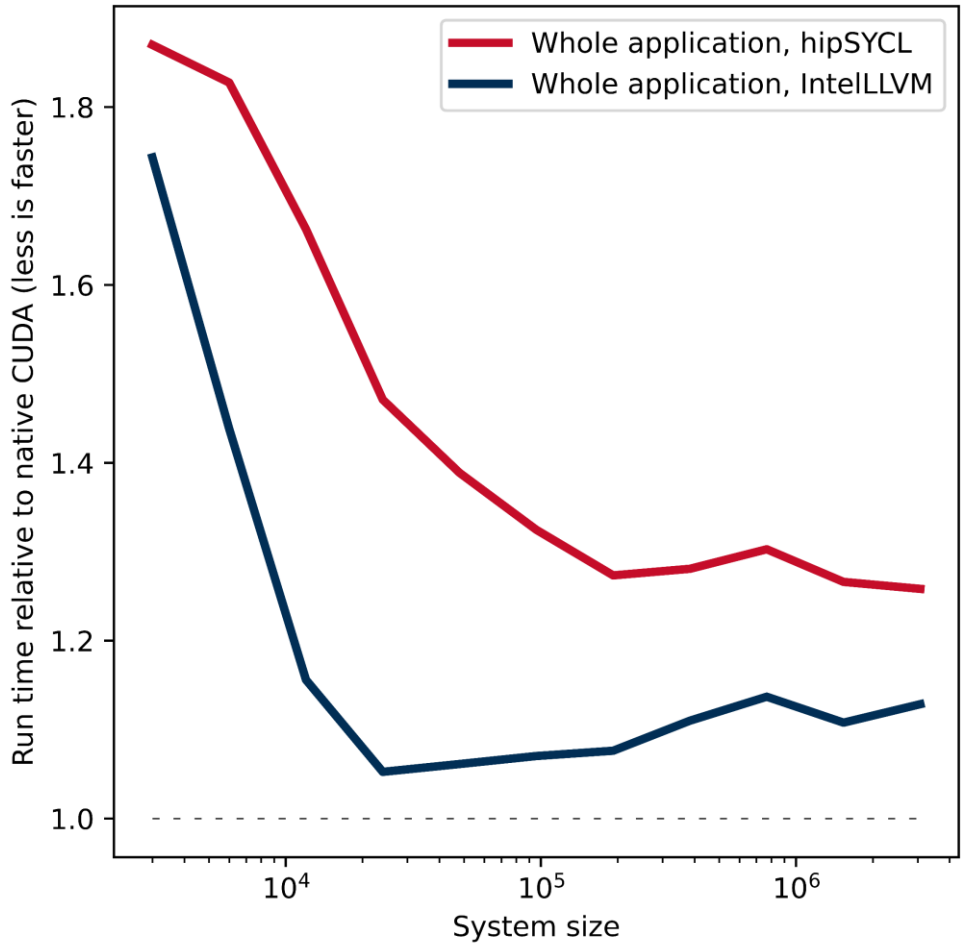
Portability in practice: results

- GROMACS can use SYCL to run on:
  - Intel GPUs via oneAPI,
  - AMD and NVIDIA GPUs via oneAPI and hipSYCL
- Performance, compared to native CUDA/HIP/OpenCL:
  - Complex kernels are slower
  - Less complex kernels on par, sometimes faster
  - Extra runtime overhead
- Relatively little vendor-specific code
  - Sub-group-size-dependent algorithms
  - Workarounds for compiler issues
  - FFT invocation

Performance: NVIDIA

V100, CUDA 11.5, hipSYCL develop and IntelLLVM vs CUDA





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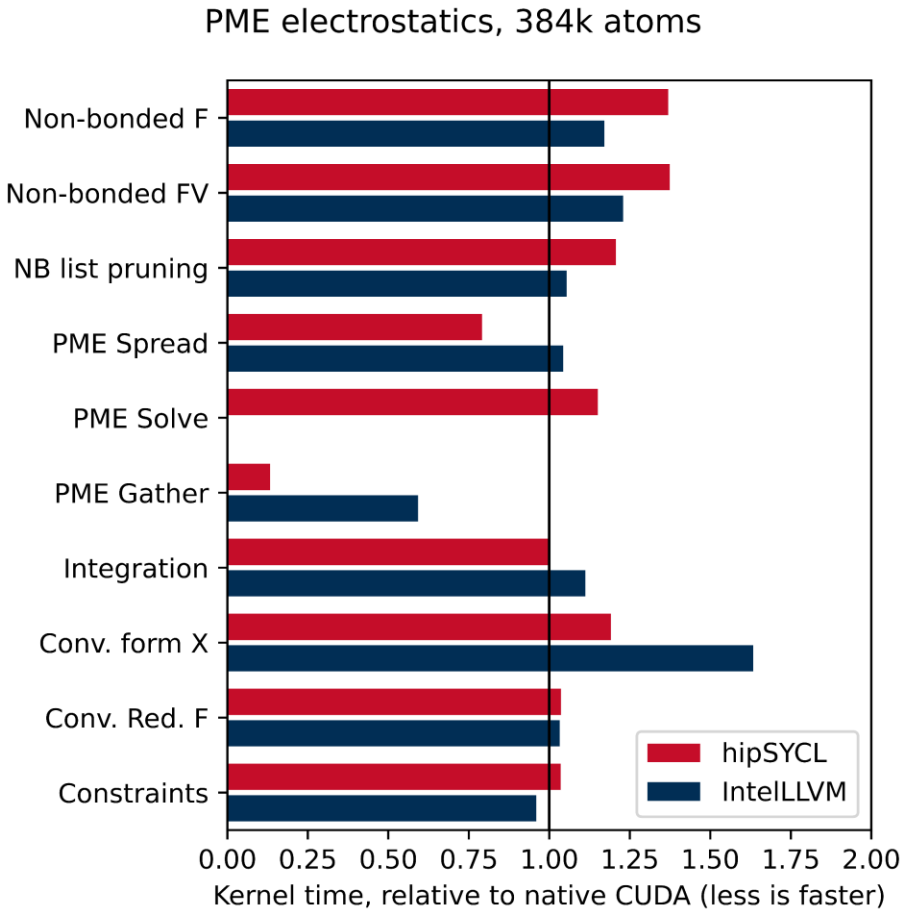
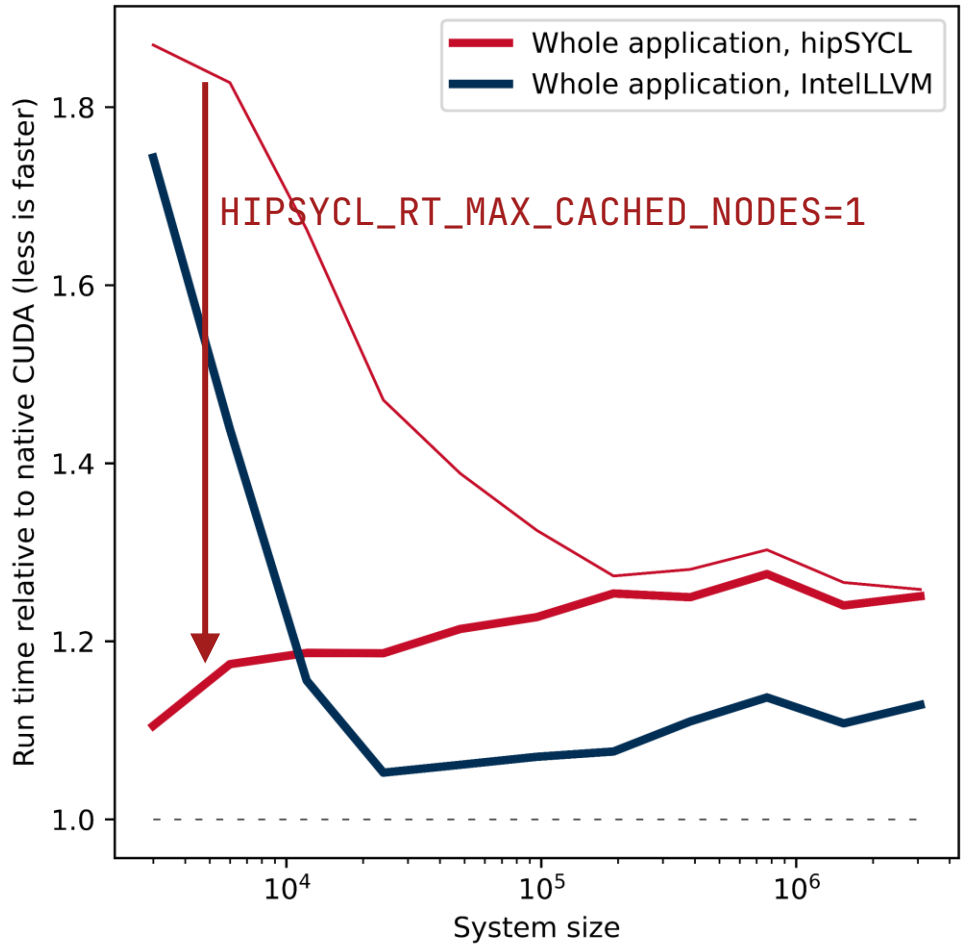
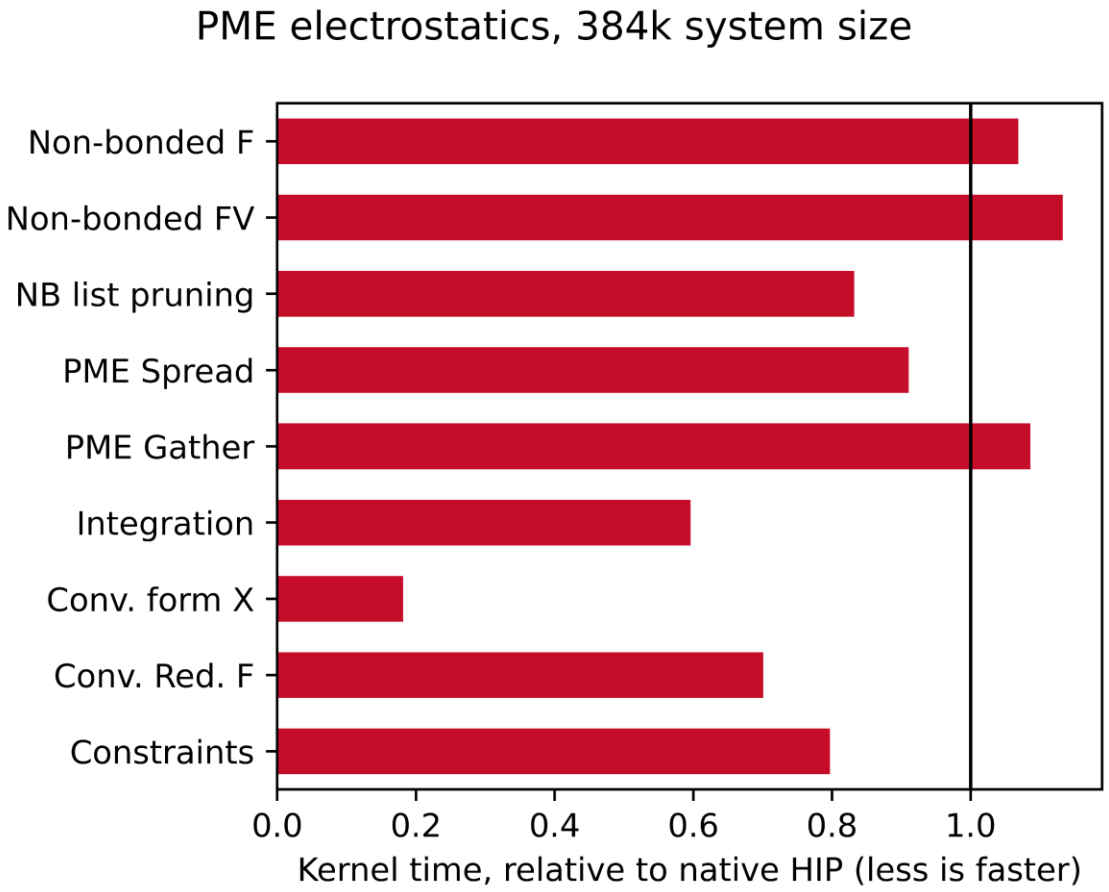


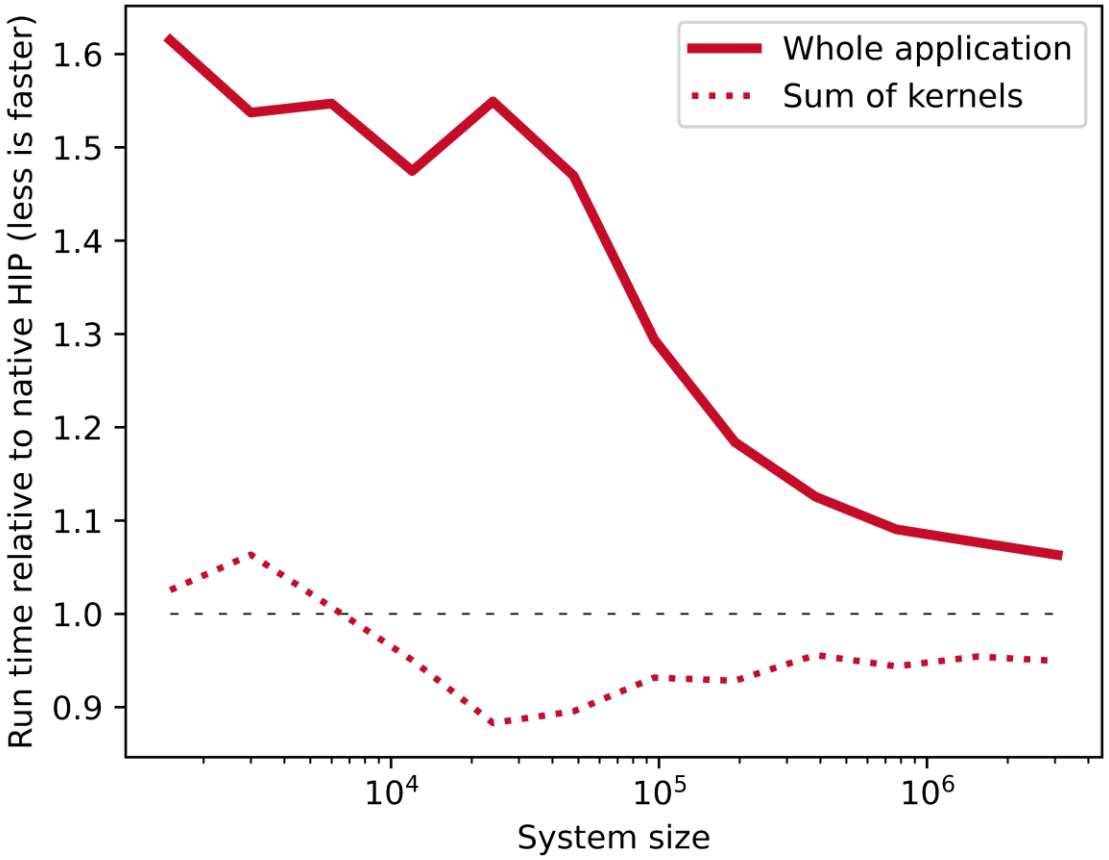


Performance: AMD

older GROMACS version

MI100, ROCm 4.5.2, hipSYCL 0.9.2 vs experimental HIP port by AMD/StreamHPC

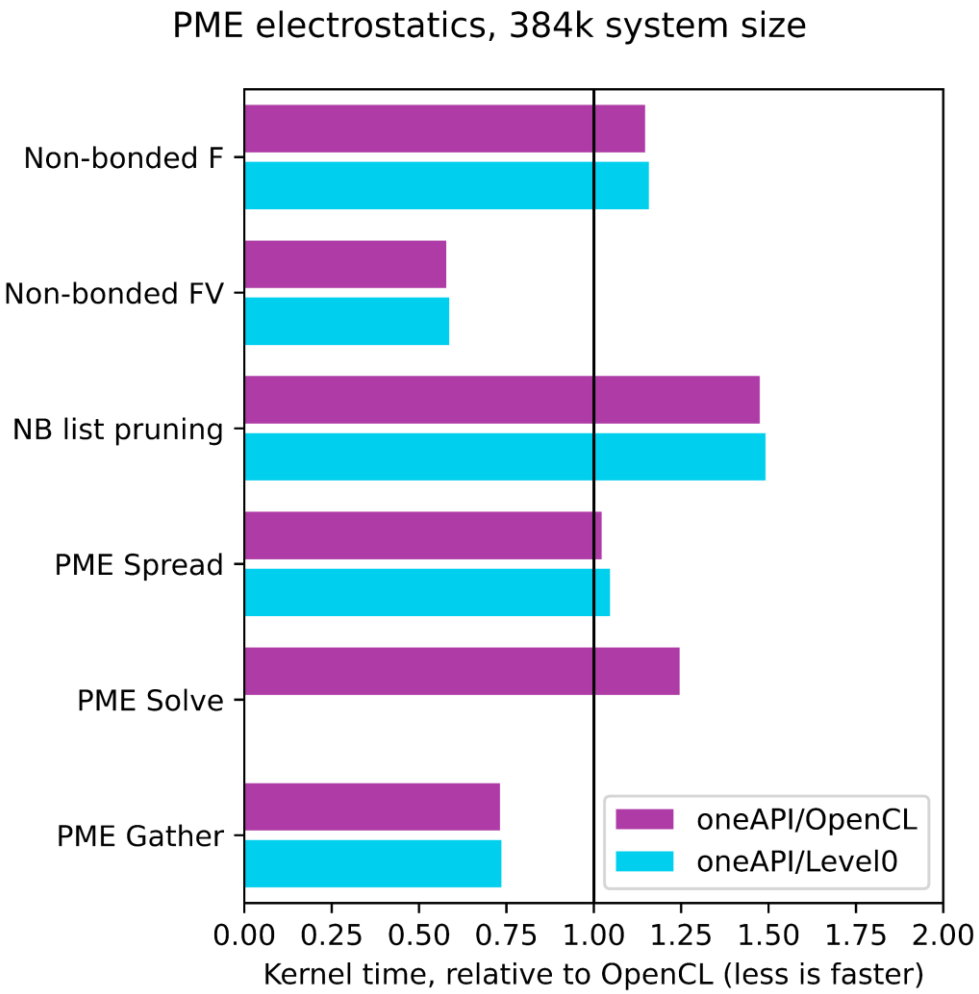


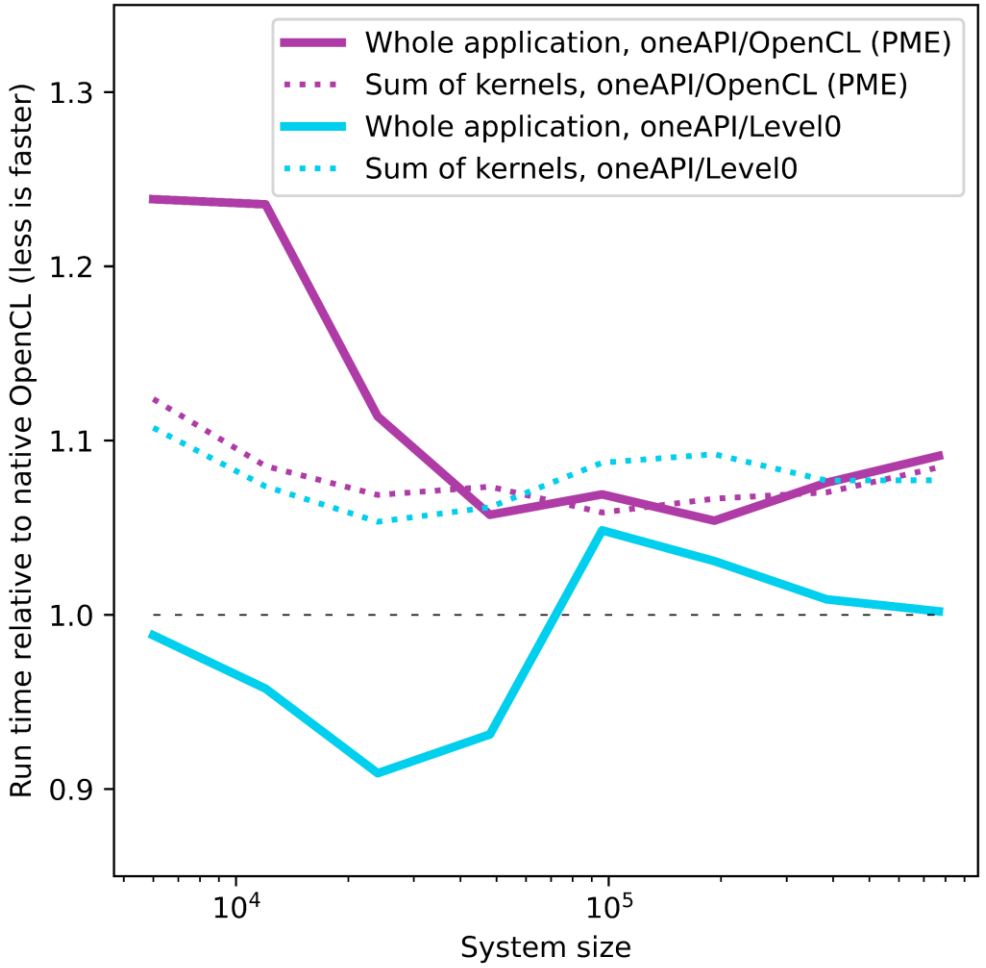


Performance: Intel

older GROMACS version, low-end GPU

Xe MAX (DG1), oneAPI 2022.1, oneAPI (LevelZero, OpenCL) vs OpenCL





Missing features / Wishlist

- Queue/task priorities
- Fine control of host scheduling
- Hardware topology information
- Inter-node communication: Celerity?
- Libraries: oneMKL?
- Robustness: installation, error messages, …

GPU feature support in GROMACS 2023

	NVIDIA CUDA	OpenCL	SYCL
Non-bonded offload	√	√	√
PME offload	√	√	√
Update offload	√	X	√
Bonded offload	√	X	√
Direct GPU-GPU comm	√	X	√*
Hardware support	NVIDIA	AMD, Intel, NVIDIA	AMD, Intel, NVIDIA

Conclusions

- “Write once, run anywhere” mostly works
  - Trivial changes to support all three major vendors with oneAPI and hipSYCL
- But running fast is not easy
  - Still need vendor-specific code branches to get high performance
  - Runtime might behave sub-optimally by default
- API is similar to OpenCL in spirit, but usually nicer
- The whole ecosystem is rapidly evolving

Acknowledgements

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- Heinrich Bockhorst and Roland Schulz (Intel)
- Aksel Alpay (Heidelberg University Computing Centre)
- GROMACS dev team, in particular Mark Abraham, Paul Bauer, Szilárd Páll, and Artem Zhmurov

Learn more

- https://gromacs.org/
- https://www.gromacs.org/Support/GMX-Developers_List
- https://gitlab.com/gromacs/gromacs/
- https://manual.gromacs.org/documentation/2022-rc1/index.html

- Páll *et al.*, J. Chem. Phys. 153, 134110 (2020)

- **If you have questions: andrey.alekseenko@scilifelab.se**