Case Study for Performance Portability of GPU Programming Frameworks for Hemodynamic Simulations

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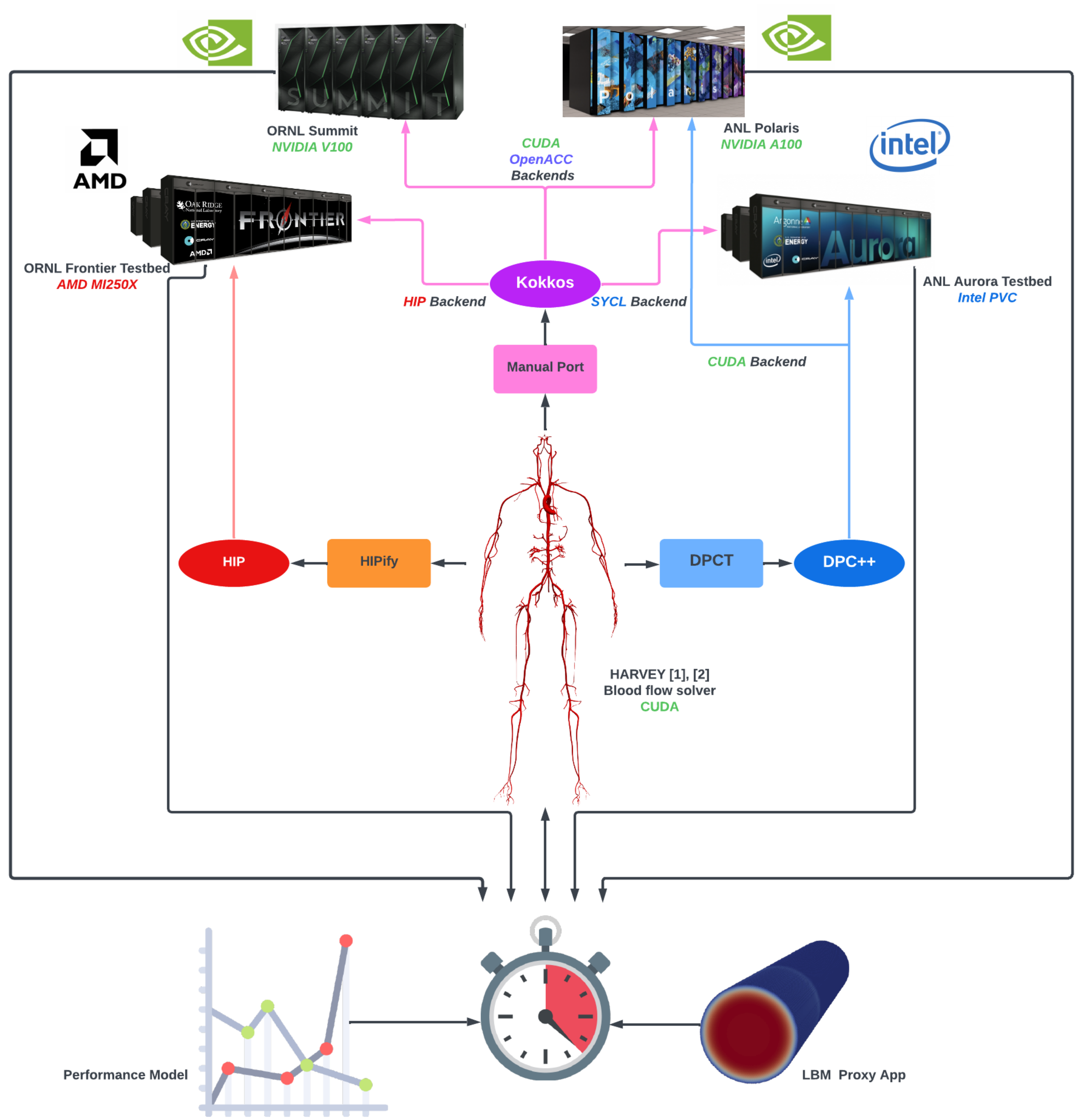
Introduction

- With the advent of GPU-dense node architectures in exascale platforms, achieving vendor-agnostic performance has become critical
- Porting legacy codes to run on current systems can be non-intuitive given the large number of heterogenous programming models available
- Proxy applications and performance models can facilitate rapid prototyping on new systems and help gauge performance bounds of full applications

Methodology

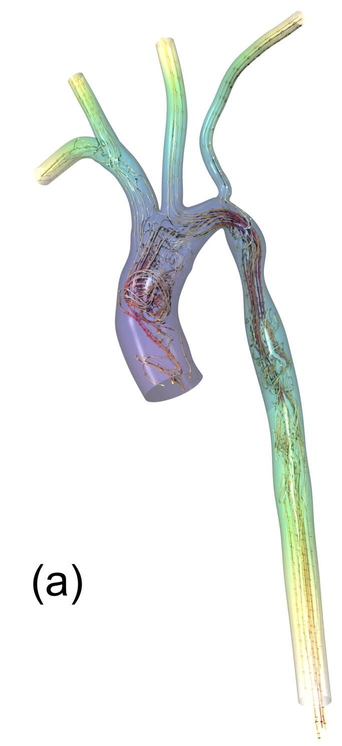
- Ported a massively parallel fluid dynamics application, HARVEY [1], as well as a proxy app, from CUDA to SYCL/DPC++, HIP, Kokkos + backends using manual handtuning and automated assist tools
- Runs conducted on Summit (ORNL/NVIDIA V100), Polaris (ALCF/NVIDIA A100), Crusher (ORNL/AMD MI250X) and Sunspot (ALCF/Intel PVC)
- Compared performance (millions of fluid lattice updates per second) of HARVEY against LBM proxy app and GPU performance model



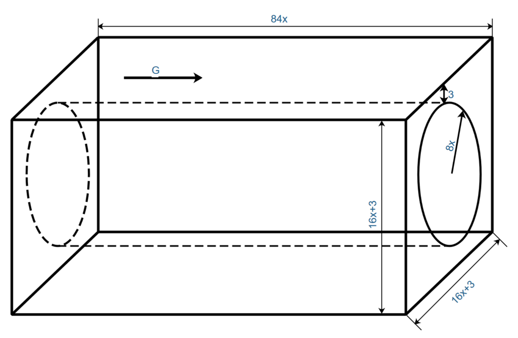
Applications Overview

- HARVEY is an LBM-based, computational fluid dynamics code capable of simulating blood flow in image-derived vasculature at cellular resolution, like the aorta shown in (a)
- We developed an open-source proxy app based on the LBM that can solve fluid flows in simple geometries as shown in (b)

(a)



(b)



Lattice Boltzmann Method

- The lattice Boltzmann method is used to model fluid flow
- Nearest-neighbor communication pattern lends LBM to parallelization

$$f_i(x + c_i, t+1) = \left(1 - \frac{1}{\tau}\right) f_i(x,t) + \frac{1}{\tau} f_i^{eq}(x,t) + F_i(x,t)$$

GPU Performance Model

- We extend a forecast model we previously developed for CPUs [2] to predict scaling performance on GPU nodes
- Time is estimated from memory bandwidth measured with BabelStream [4] and communication times collected from custom pingpong benchmark:

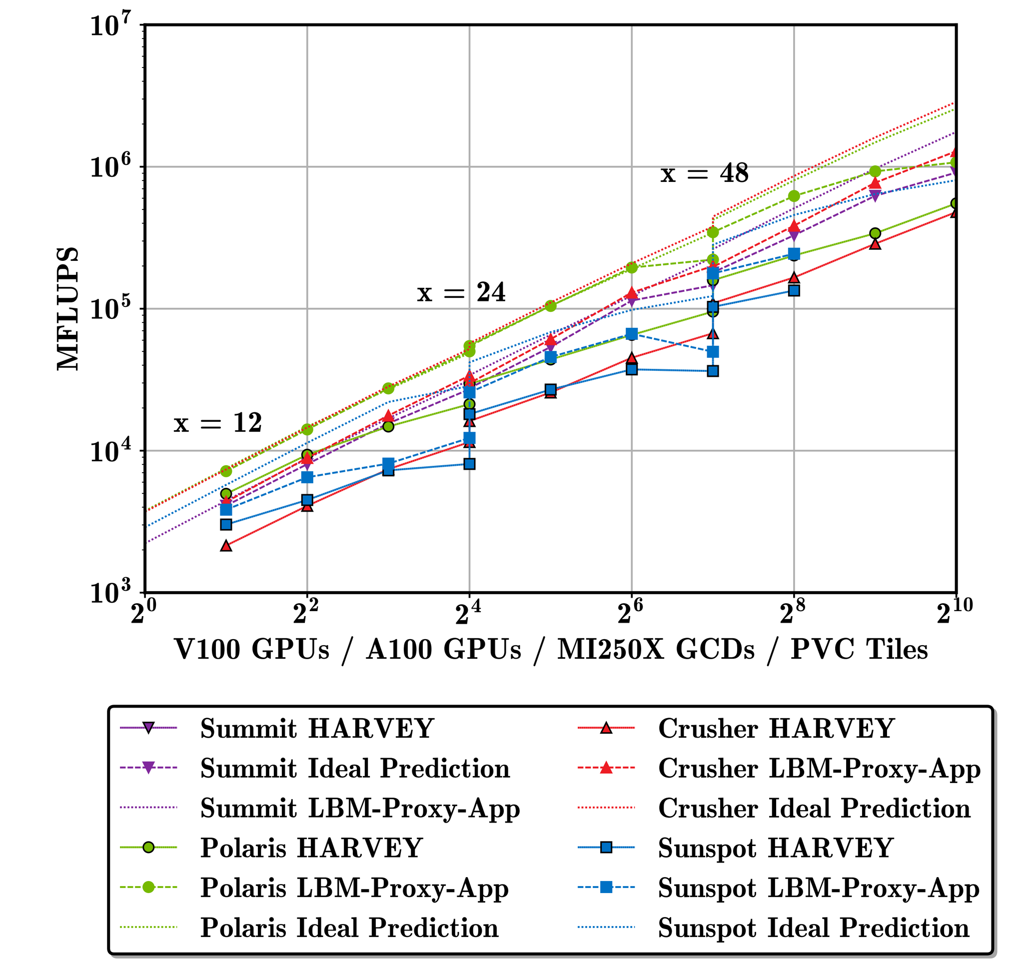
$$t = t_{streamcollide} + \sum_{j}^{n_{events}} t_{comm_j}$$

where

$$t_{streamcollide} = \frac{n_{bytes}}{B_{mem}}$$

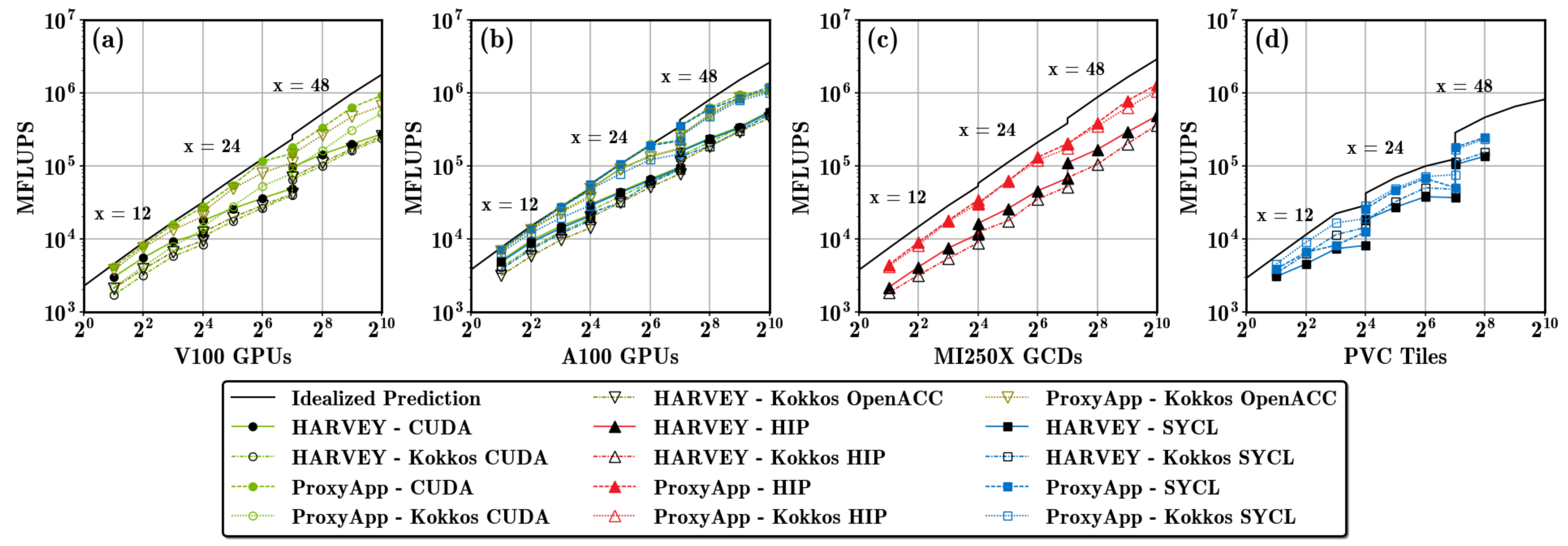
Results: Hardware Comparison

- Compared native programming models on each system for HARVEY, LBM proxy app, and performance model through strong-weak scaling



Results: Backend Comparison

- Compared programming model backends against native language on Summit (a), Polaris (b), Crusher (c), and Sunspot (d)



Lessons Learned

- With backends for CUDA, SYCL, HIP, and OpenACC, the Kokkos version of the HARVEY application was most portable but required the most porting effort
- The HIP codes required the least porting effort but were the most limited in portability
- Out-of-the-box machine-generated SYCL and HIP ports were competitive as informed by performance predictions and proxy application
- Native programming models generally outperformed off-brand models
- Performance predictions and proxy applications proved invaluable tools for navigating porting process and facilitating manual tuning efforts

References:

[1] Randles, Amanda Peters, et al. "Performance analysis of the lattice Boltzmann model beyond Navier-Stokes." *2013 IEEE 27th International Symposium on Parallel and Distributed Processing*. IEEE, 2013.
[2] Ladd, William, et al. "Optimizing Cloud Computing Resource Usage for Hemodynamic Simulation." *2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, 2023.

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