Overview of open platform programming methods for exascale computing

Dr Tom Deakin University of Bristol

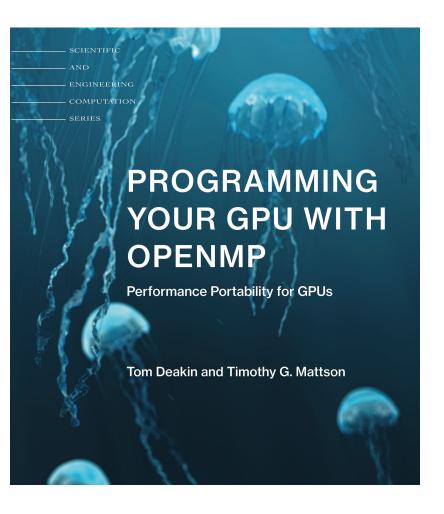
Monday, June 24th 2024



Some bias

- I wrote a book on Programming GPUs with OpenMP
- I am Chair of the SYCL Working Group for The Khronos Group

I am speaking today as an academic based on my research





2020 IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC (P3HPC)

Tracking Performance Portability on the Yellow Brick Road to Exascale

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Abstract-With Exascale machines on our immediate horizon, there is a pressing need for applications to be made ready to best exploit these systems. However, there will be multiple paths to Exascale, with each system relying on processor and accelerator technologies from different vendors. As such, applications will be required to be portable between these different architectures, but it is also critical that they are efficient too. These double requirements for portability and efficiency begets the need for performance portability. In this study we survey the performance portability of different programming models, including the open standards OpenMP and SYCL, across the diverse landscape of Exascale and pre-Exascale processors from Intel, AMD, NVIDIA, Fujitsu, Marvell, and Amazon, together encompassing GPUs and CPUs based on both x86 and Arm architectures. We also take a historical view and analyse how performance portability has changed over the last year.

Index Terms-performance portability, programming models

I. INTRODUCTION

Exascale-class supercomputers are on the immediate horizon,

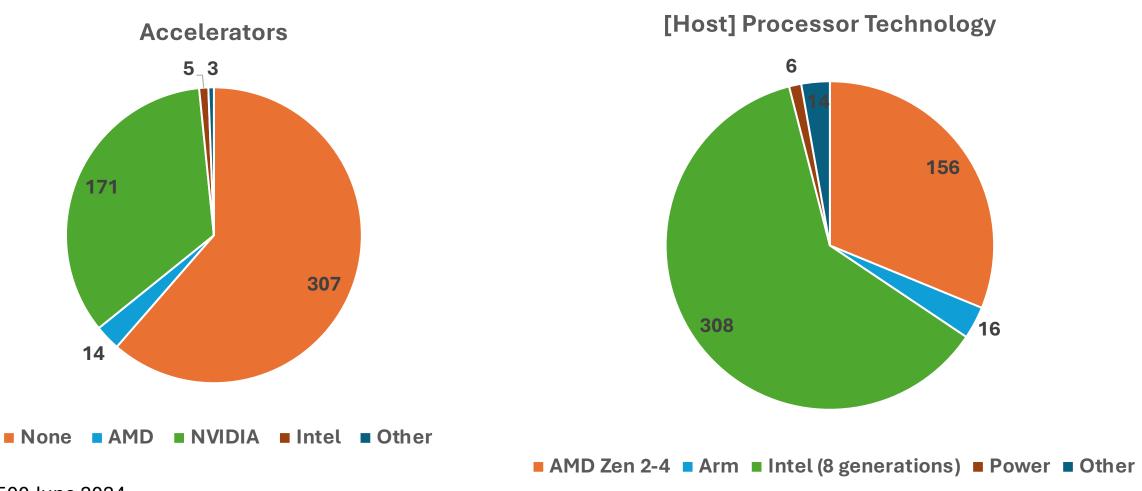
To further enable the development of performance-portable programs, in this study we update and greatly expand our earlier, wide-reaching study on performance portability [1]. We include the latest and greatest architectures, including for the first time the Arm-based Fujitsu A64FX processor, the NVIDIA Ampere GPU, and Intel GPUs. Thus, this study spans the processor architecture design space of the first Exascale machines.

As this work is an expansion and update of the 2019 study, we are able to begin to explore the historical perspective for how performance portability changes over time. The ecosystems surrounding each of the processors have had time to expand and mature, and therefore by refreshing many of the results from the original study in 2019 we can track the progress of support, performance, and performance portability.

In this update, for the first time we include results from applications written in SYCL. The applications we include are all open source and were ported for the purposes of this study thus representing a contribution to the community in



Homogeneous-heterogenenous world of Top 500



Data: TOP500 June 2024

Updated version of chart from: Deakin, Cownie, Lin, McIntosh-Smith, Heterogeneous Programming for the Homogeneous Majority

https://doi.org/10.1109/P3HPC56579.2022.00006



Bristol definition of performance portability

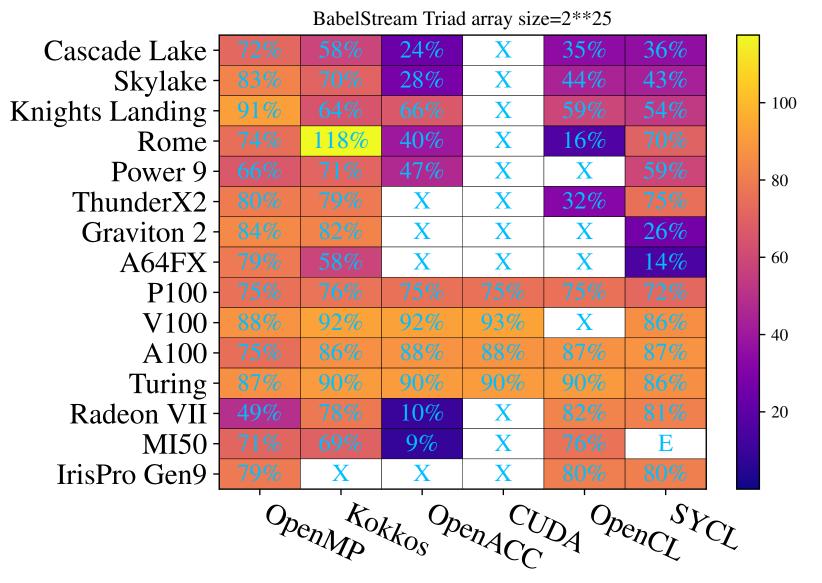
"A code is performance portable if it can achieve a similar fraction of peak hardware performance on a range of different target architectures".

- Needs to be a good fraction of best achievable (i.e., hand optimised).
- Range of architectures depends on your goal, but important to allow for future developments.
- Most interested in consistency of distribution of performance across systems
- Aligns with PP metric from Pennycook, et al.



From Pennycook, Sewall, Jacobsen, Deakin, McIntosh-Smith Navigating Performance, Portability, and Productivity <u>https://doi.org/10.1109/MCSE.2021.3097276</u>⁸

Back to the beginning of the yellow brick road



https://doi.org/10.1109/P3HPC51967.2020.00006

Heterogeneous programming model abstractions

Device discovery and control

Data location and movement in discrete memory spaces

Expressing concurrent and parallel work

OpenMP = OpenMP 1 + OpenMP 4/5 (+tasks)?

```
#pragma omp parallel for
for (int i = 0; i < N; ++i) { map(alloc: C[:N]) \
   C[i] = A[i] + B[i];
```

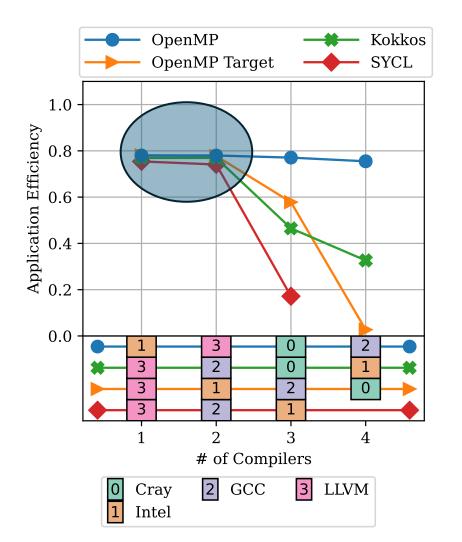
```
#pragma omp target enter data \
map(to: A[:N], B[:N])
```

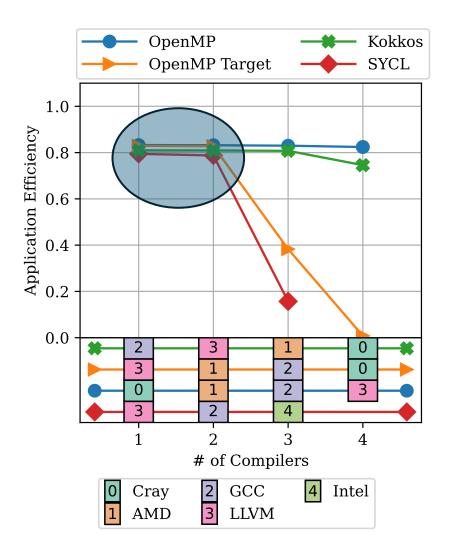
```
#pragma omp target
#pragma omp loop
for (int i = 0; i < N; ++i) {</pre>
    C[i] = A[i] + B[i];
}
```

#pragma omp target exit data \ map(from: C[:N])

Can you just write the target version and get good performance? https://doi.org/10.1109/P3HPC56579.2022.00006







Heterogeneous Programming for the Homogeneous Majority https://doi.org/10.1109/P3HPC56579.2022.00006

"Then, if you don't mind, I'll go with you," said the Lion, "for my life is simply unbearable without a bit of courage." from The Wonderful Wizard of Oz by L. Frank Baum



		C++17 StdPar	SYCL.	OpenMP target		OpenCL OpenCL	Kokkos Kokkos	^{Julia}	
	Code portability	Compiler/ Compiler flags	Compiler/ Compiler flags	Compiler/ Compiler flags	Not portable	Runtime	Compiler/ Compiler flags	Partial* * library dependent	
	Device portability	CPU,GPU	CPU,GPU,FPGA	CPU,GPU	GPU (CPU via third-party impl.)	CPU,GPU, FPGA	CPU,GPU	CPU,GPU	
	Supported platform	Intel/AMD/NVIDIA	Intel/AMD/NVIDIA	Intel/AMD/NVIDIA	Vendor-only	Intel/AMD/NVIDIA	Intel/AMD/NVIDIA	Intel/AMD/NVIDIA	
	Format	Single-source	Single-source	Single-source	Single-source	Multi-source	Single-source	Single-source	
"How" { data access {	Data movement	Implicit: USM	Explicit: accessors Implicit: USM	Explicit: pragmas Implicit: USM	Explicit: vendor API Implicit: USM	Explicit: buffers Implicit: SVM	Explicit: views	Explicit: library API	
"How/What" / parallel	Traversal	std::for_each std::for_each_n std::transform	queue.submit([&](auto &h) { h.parallel_for(); });	# OpenMP >= 5.0 omp loop omp target teams distributed \ parallel for	global void kernel() {} // kernel<< <n>>>()</n>	(> 10 lines, in two files)	Kokkos::parallel_for	Yes* *library dependent	
	Reduction	std::transform_reduce std::reduce std::accumulate	queue.submit([&](sycl::handler &h) { h.parallel_for(sycl::reduction(),) });	omp reduction(inscan,) { omp scan inclusive() omp scan exclusive() }	(> 10 lines, "roll your own")	(> 10 lines, "roll your own")	Kokkos::parallel_reduce	Yes* *library dependent	
"When" { parallel	Task asynchrony/ scheduling		Command queues	#pragma omp nowait/depends() (Blocking by default)	Streams	Command queues	Futures (C++ like)	Yes* *library dependent	
"Where" { parallel	Affinity	No control (Ongoing proposals)	Device API	#pragma omp device() (Host is also a device)	Vendor API	Device API	Device API	Yes* *library dependent	

From my PhD student: Wei-Chen Lin

ISO C++ parallel algorithms on x86 CPUs

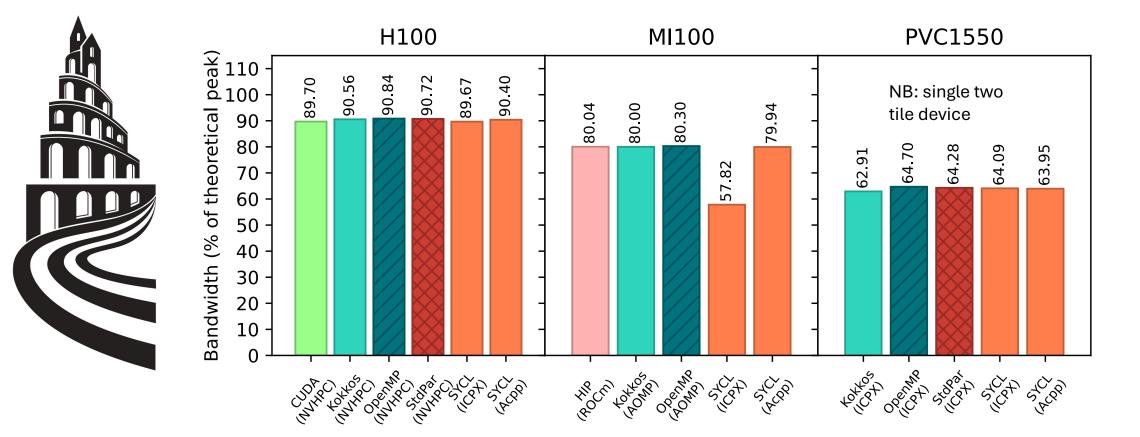
	Architectural efficiency																		
0			20			40				н 60			8	D		100			
Copy	72	71	77	71	70	65	16	35	33	35	54	15	25	54	88	44	39	39	
bbA	75	75	65	75	75	65	16	38	36	38	67	17	28	65	41	47	41	45	Xe
Mul	72	71	58	71	70	58	18	37	34	37	53	13	15	52	39	45	38	44	Xeon 6338
Triad	76	75	65	75	75	64	18	38	36	38	65	23	20	65	40	45	42	44	338
Dot	85	84	84	81	81	80	22	44	42	44	80	25	30	80	46	50	46	51	
Copy	54	54	80	54	54	54	27	32	28	29	54	29	28	54	31	36	31	38	
Add	59	59	59	59	59	59	28	33	32	33	59	30	31	59	34	38	33	42	ΕP
Mul	52	52	54	52	52	52	26	31	31	29	52	26	26	52	31	38	30	37	EPYC 7713
Triad	59	59	59	59	59	59	27	34	26	31	59	28	28	59	33	39	33	40	713
Dot	83	82	83	80	82	81	33	38	34	37	82	35	35	82	38	47	37	44	
	- Clang*	- GCC	- NVHPC	- Clang*	- GCC	- NVHPC	- Clang*	- GCC	- Clang*	- GCC	- NVHPC	- Clang*	- GCC	- NVHPC	- Clang*	- GCC	- Clang*	- GCC	
	Oj	OpenMP		K	TBB Kokkos		3B	C++17 (data)				C++17 (index)			C++17 (data) oneDPL w/OMP		C++17 (index) oneDPL w/OMP		

Lin, Deakin, McIntosh-Smith

Evaluating ISO C++ Parallel Algorithms on Heterogeneous HPC Systems

https://doi.org/10.1109/PMBS56514.2022.00009

The University of Bristol is an Intel oneAPI Center of Excellence helped support this work.



On latest GPUs from NVIDIA, AMD, and Intel, performance portability for BabelStream possible in most mainstream performance portable programming models:

- ISO C++ stdpar, OpenMP, SYCL, Kokkos
- Same performance as "native" CUDA/HIP

FORTRAN

- We also looked at parallelism in Fortran (DO CONCURRENT)
- Lots of recent progress in this space, and more to explore.
- See Hammond, Deakin, Cownie, McIntosh-Smith, *Benchmarking Fortran DO CONCURRENT on CPUs and GPUs Using BabelStream*, https://doi.org/10.1109/PMBS56514.2022.00013

Same conclusion as C++ paper.



"I shall take the heart," returned the Tin Woodman; "for brains do not make one happy, and happiness is the best thing in the world."

from The Wonderful Wizard of Oz by L. Frank Baum



"I am everywhere," answered the Voice, "but to the eyes of common mortals I am invisible."

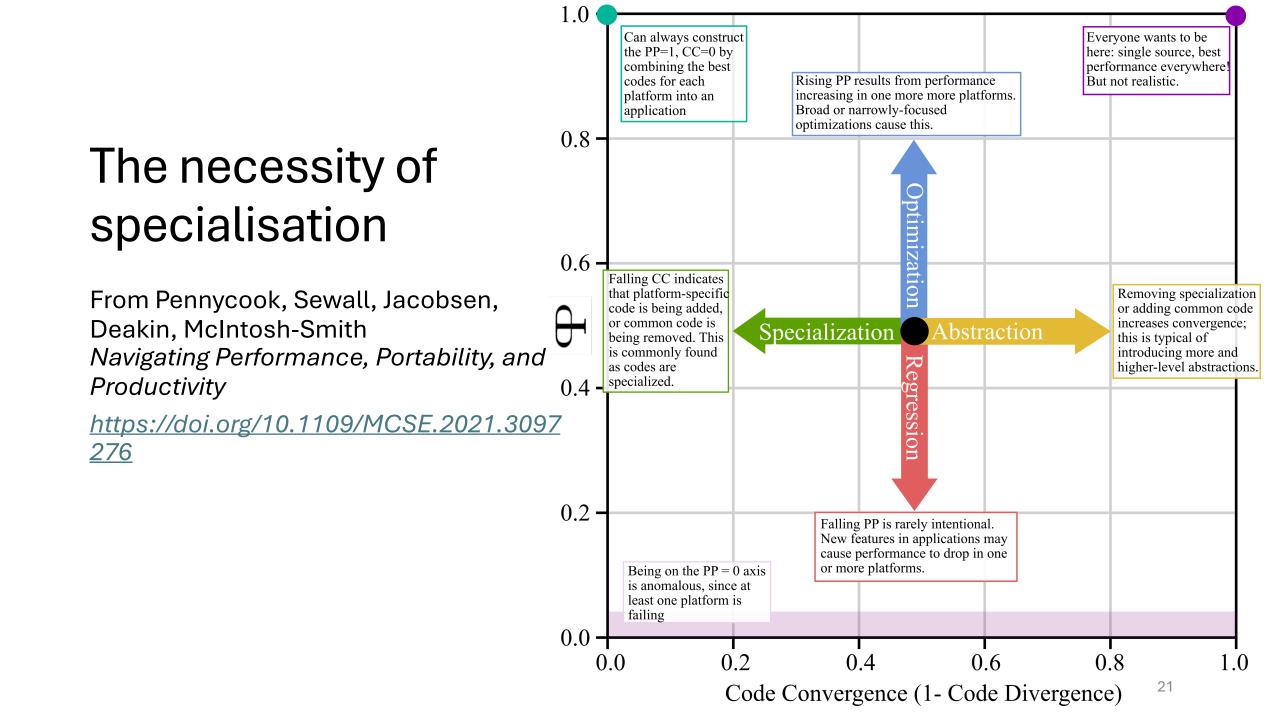
from The Wonderful Wizard of Oz by L. Frank Baum

See Doerfert, et al. *Breaking the Vendor Lock: Performance Portable Programming through OpenMP as Target Independent Runtime Layer,* <u>https://doi.org/10.1145/3559009.3569687</u>



"But I do not want people to call me a fool, and if my head stays stuffed with straw instead of with brains, as yours is, how am I ever to know anything?"

from The Wonderful Wizard of Oz by L. Frank Baum



The Yellow Brick Road to Productive Performance Portability is paved with OpenMP and SYCL

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OPENMP

Shared-memory Paralilling Road

SYCL

Single-source Hetoreup proverming

Related performance portability papers

Tuomas, Christidi, Giordano, Dubrovska, Quinn, Maynard, Case, Olgu, and Deakin. "Principles for Automated and Reproducible Benchmarking." In First International Workshop on HPC Testing and Evaluation of Systems, Tools, and Software. IEEE, 2023.

https://doi.org/10.1145/3624062.3624133

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Hammond, J.R., Deakin, T, Cownie, J. and McIntosh-Smith, S. "Benchmarking Fortran DO CONCURRENT on CPUs and GPUs Using BabelStream." In International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS), 2022. https://doi.org/10.1109/PMBS56514.2022.00013 Lin, W.C, Deakin T, and McIntosh-Smith S. "Evaluating ISO C++ Parallel Algorithms on Heterogeneous HPC Systems." In International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS), 2022. https://doi.org/10.1109/PMBS56514.2022.00009

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Pennycook, S. J., Sewall, J. D., Jacobsen, D. W., Deakin, T and McIntosh-Smith, S. "Navigating Performance, Portability and Productivity." Computing in Science and Engineering, 2021. <u>https://doi.org/10.1109/MCSE.2021.3097276</u>

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