XDMoD
METRICS ON DEMAND

Are we ready for broader adoption of ARM in the HPC community:

Benchmarks and Applications on High-End ARM Systems with XDMoD Application Kernels

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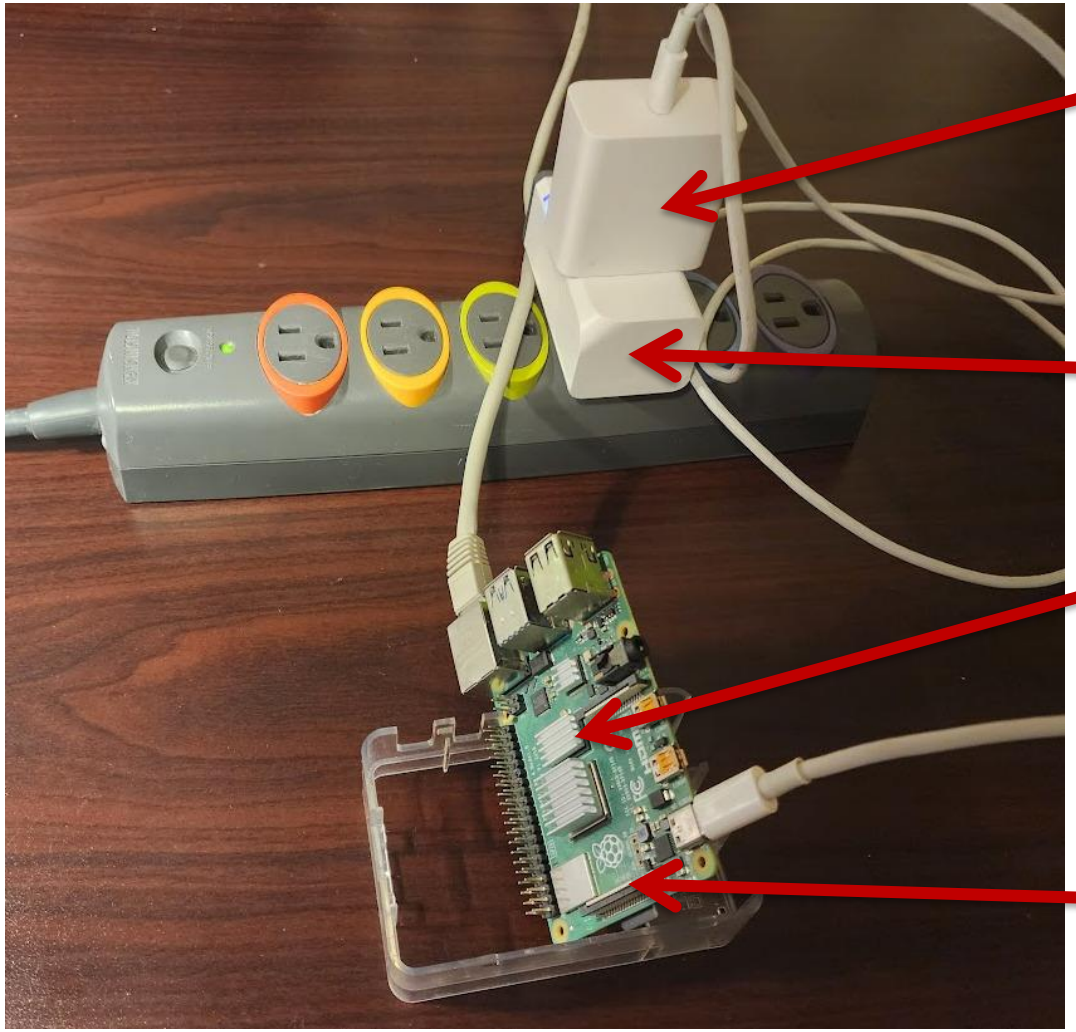
NSF OAC Awards: 2137603 and 1927880

AHUG SC22 Symposium, November 14th, 2022

First Personal Experience with HPC Application on ARM



USB-C interface provides enough power

Smart outlet provides Power measurements

Raspberry Pi 4

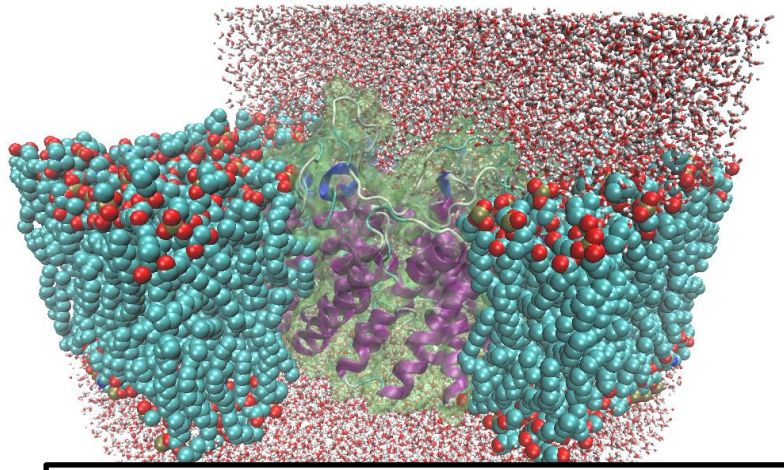
Vertical placement for Efficient cooling

First Personal Experience with HPC Application on ARM

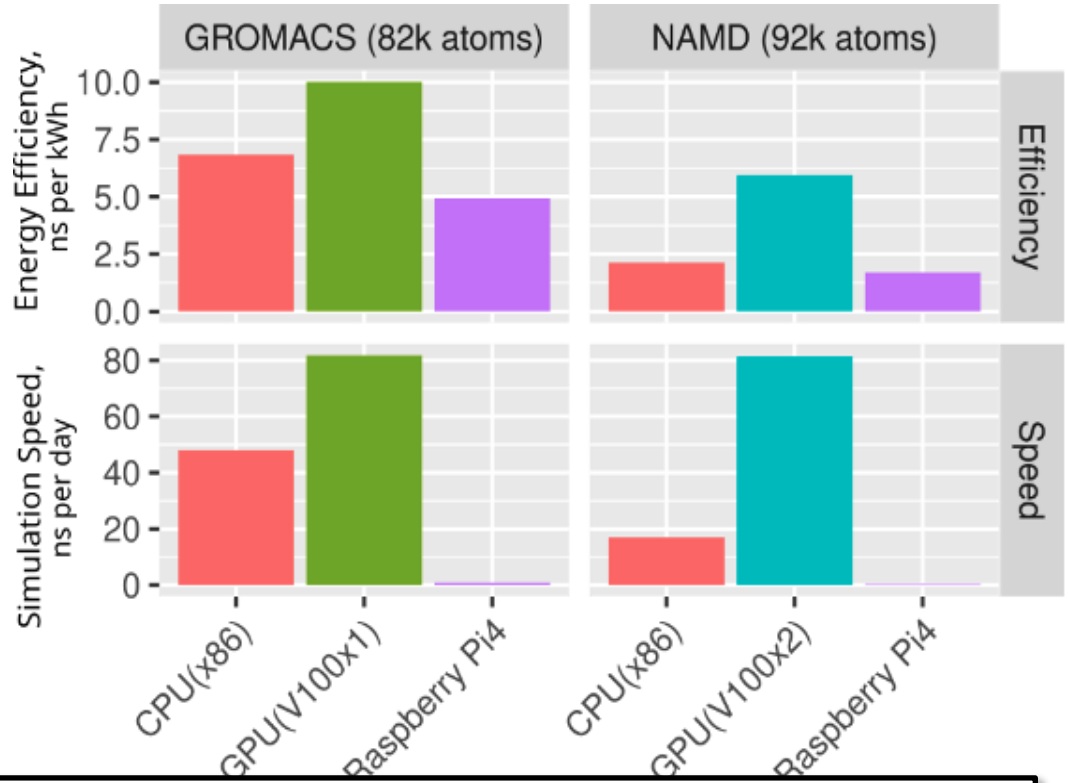
Gromacs

Membrane protein system

~82k atoms



Performance



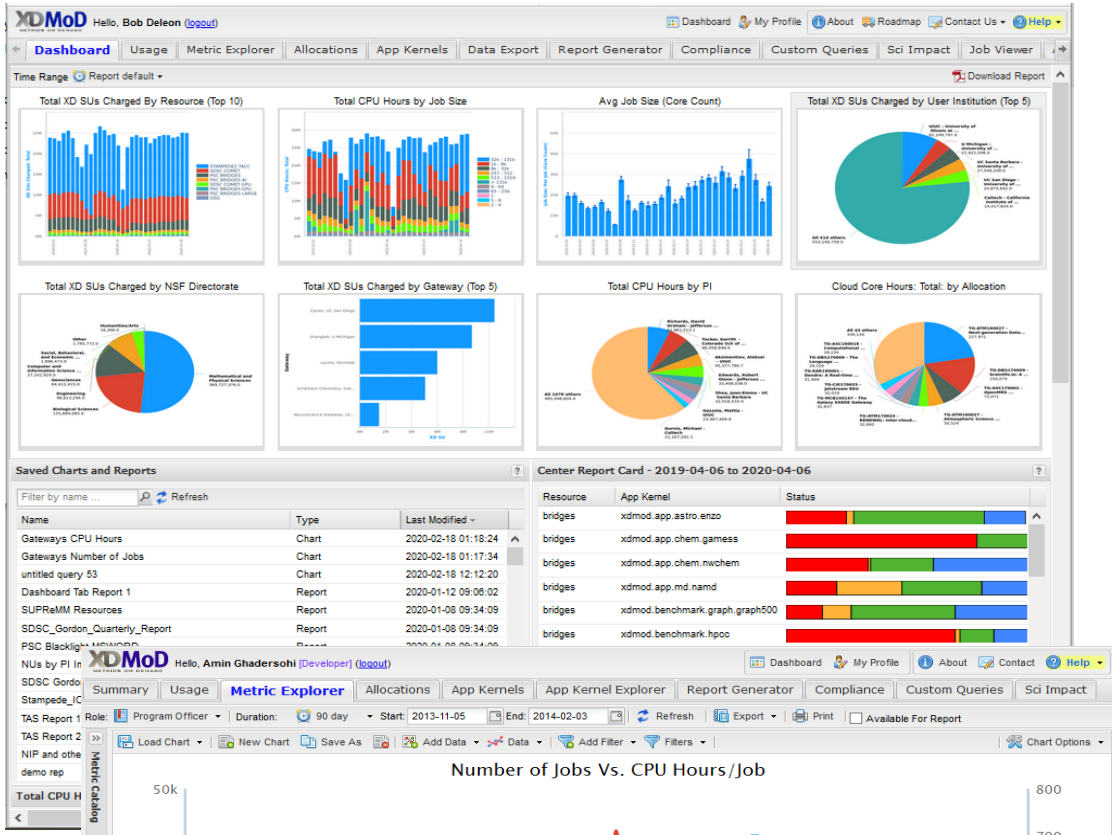
Results:

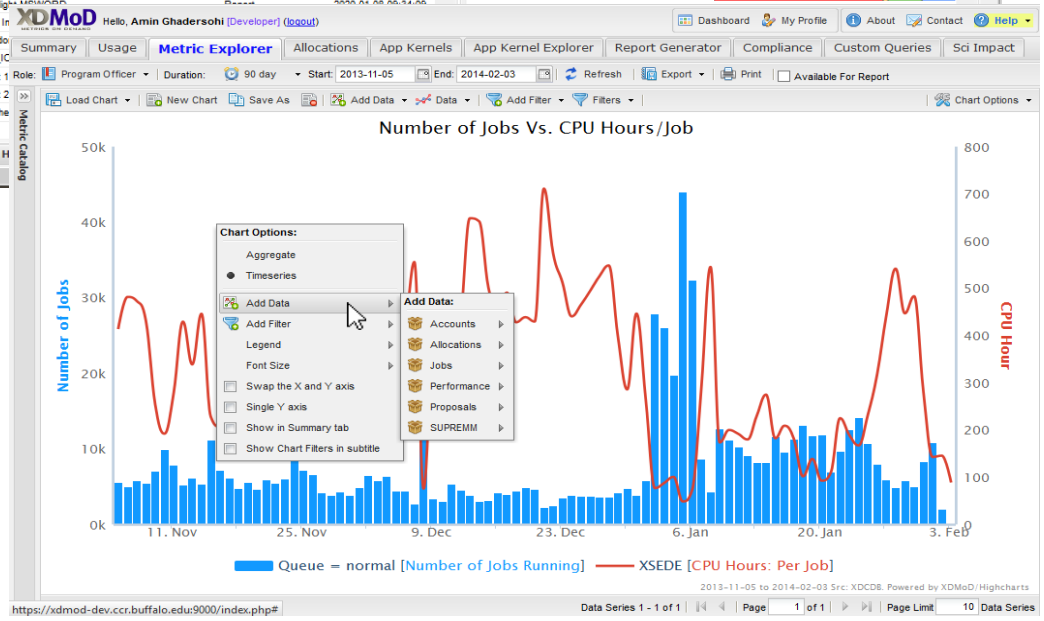
Good: everything compiled and run

Bad: Raspberry Pie 4 is neither fast nor energy efficient in compute intensive application like molecular dynamics

What is the performance state of modern high end ARM CPUs?

XDMoD: A Comprehensive Tool for HPC System Management





- **NSF ACCESS Measurement and Metrics Service (MMS),**
  - Following XD Net Metrics Service (XMS) and prior 5 year TAS award
  - Develop & deploy **XDMoD** (**XD M**etrics **o**n **D**emand) Tool
- **Open XDMoD: Open Source version for Data Centers**
  - Used to measure and optimize performance of HPC centers
  - 300+ academic & industrial installations worldwide
- **Goal: Optimize Resource Utilization and Performance**
  - Provide detailed information on utilization
  - Measure Quality of Service
  - Enable data driven upgrades and procurements
  - Measure and improve job and system level performance

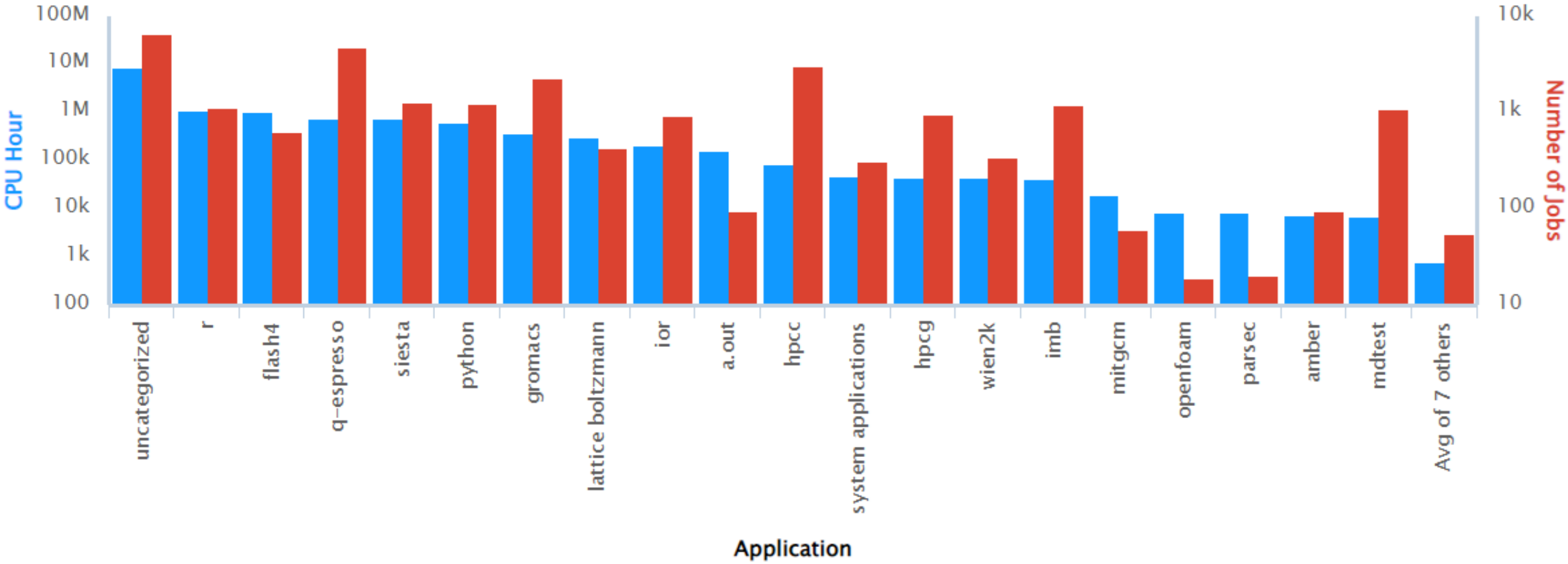
XDMoD METRICS ON DEMAND

University at Buffalo
Center for Computational Research

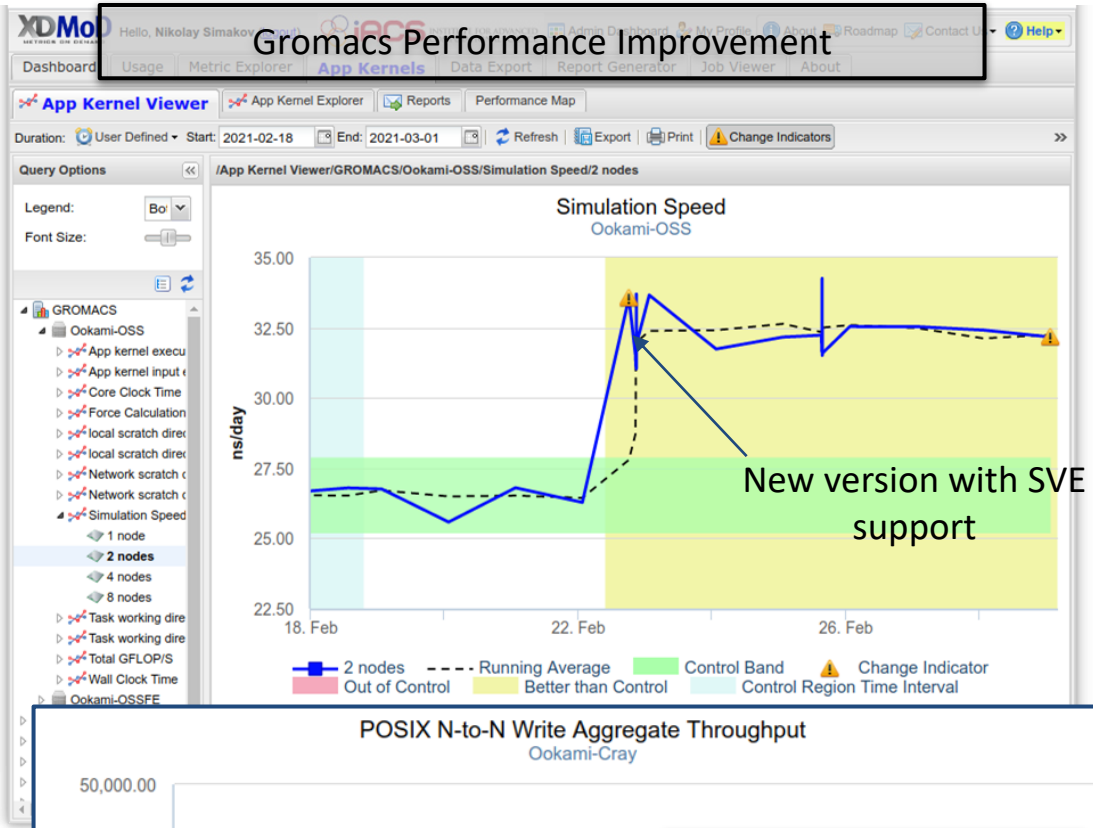
Application usage on Ookami (Fujitsu A64FX)

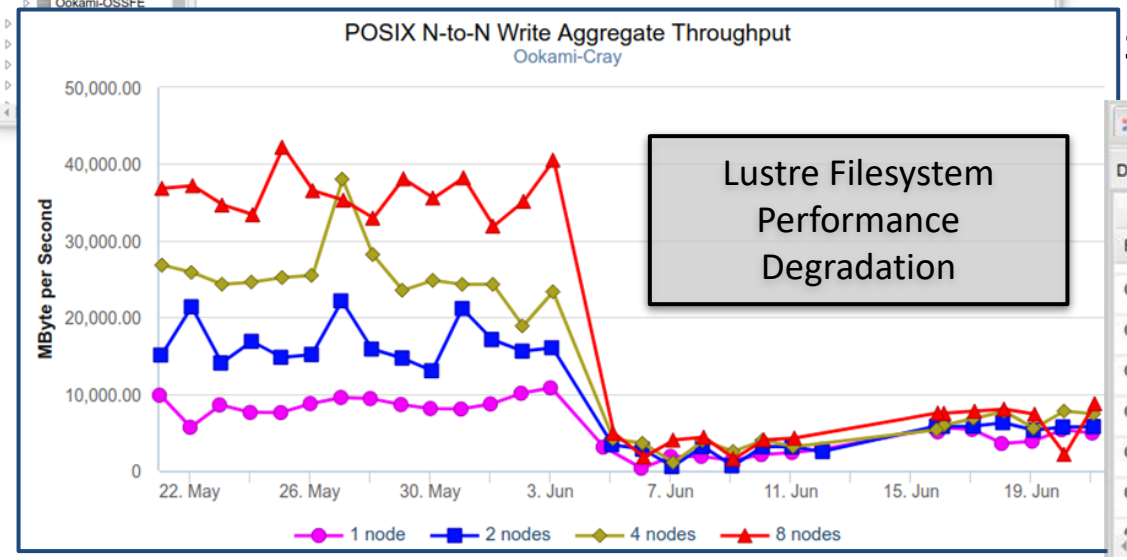
Ookami – an ARM Fujitsu A64FX machine with SVE support (512 bit wide)

Determine what are the mostly widely used applications (2021-01 application usage to 2022-09-30 shown)



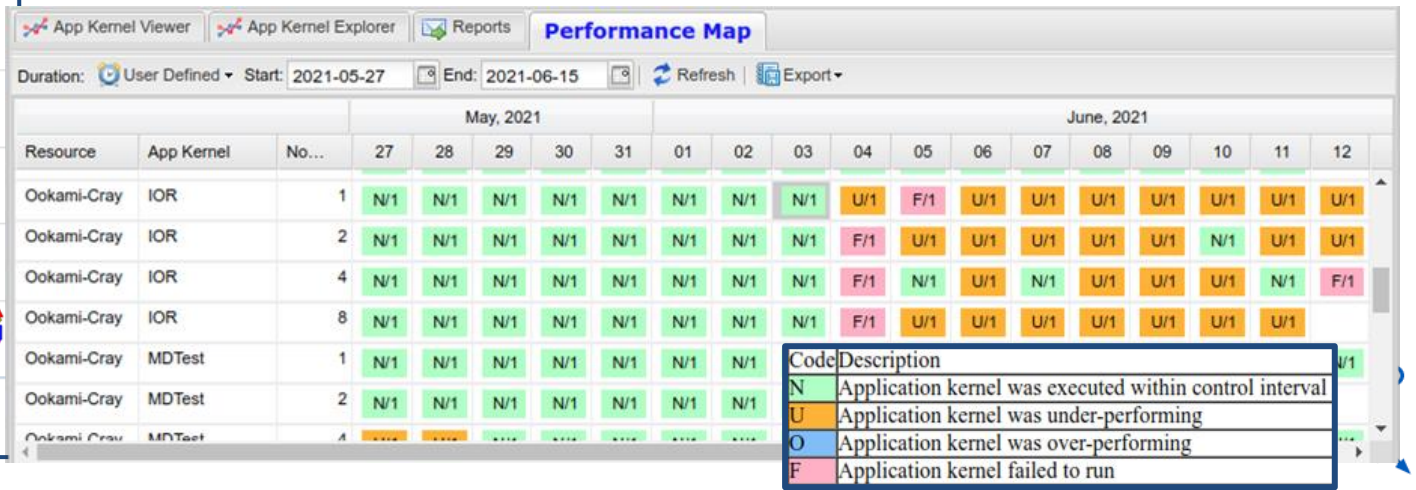
QoS and Performance Monitoring with Application Kernels





- Computationally lightweight benchmarks or applications
  - Run periodically or on demand to actively measure performance
- Measure system performance from User's perspective

  Local scratch, global filesystem performance, local processor-memory bandwidth, allocatable shared memory, processing speed, network latency and bandwidth
- Proactively identify underperforming hardware and software



QoS and Performance Monitoring with Application Kernels

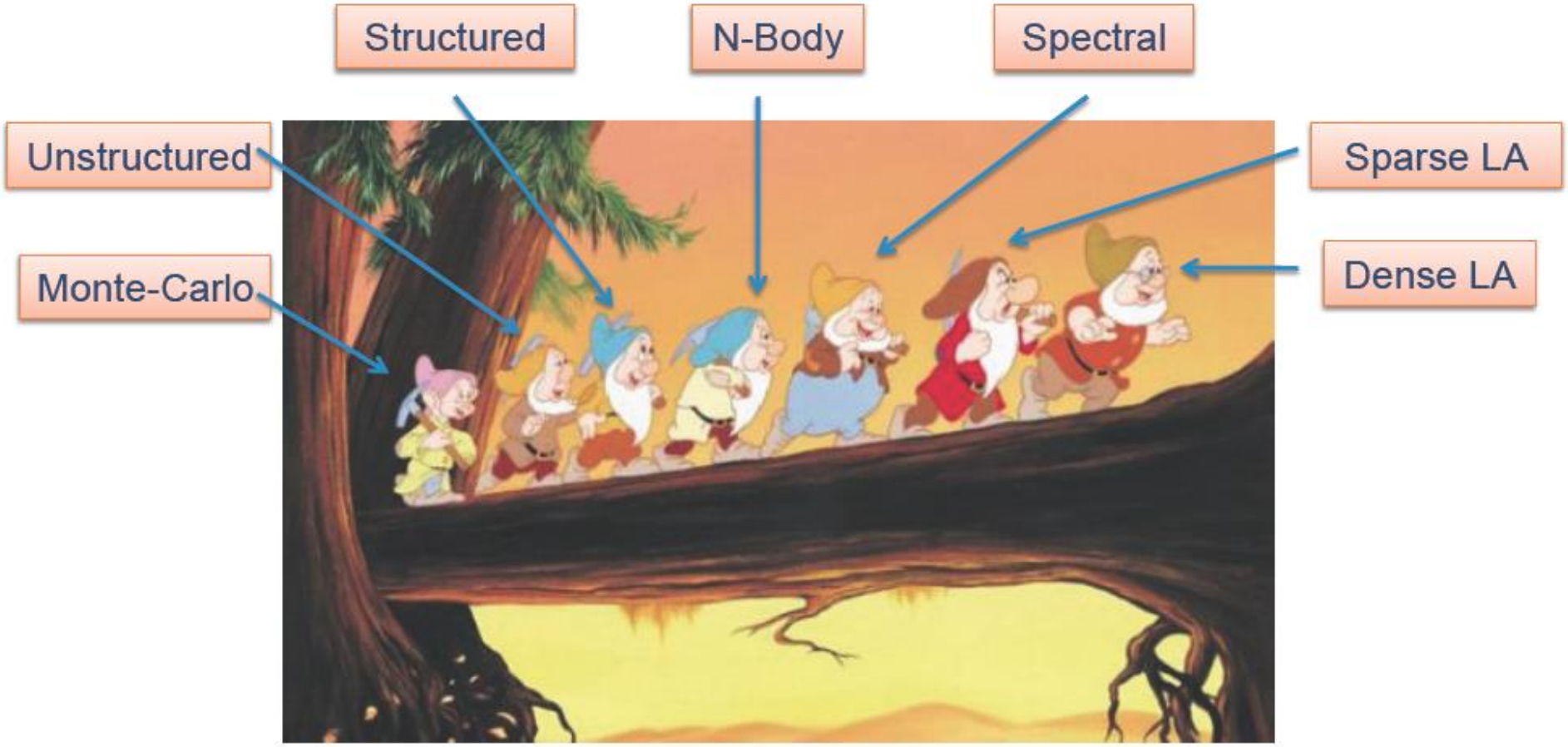
- Application kernels are based on benchmarks and real applications:
  - **HPCC**, HPCG, Graph500,IMB, IOR, MDTest, **AI-Benchmark-Alpha**
  - **Gromacs**, NAMD, **NWChem**, **Enzo**, **OpenFoam**

- We run benchmarks and application on multiple systems:
  - Ookami – an ARM Fujitsu A64FX machinve with SVE support (512 bit wide)
  - ACCESS/XSEDE
    - TACC Stampede 2 (Intel Sky Lake/Ice lake)
    - PSC Bridges 2 (AMD Rome)
    - SDSC Expanse (AMD Rome)
    - Purdue University Anvil (AMD Millan)
  - Our center (Intel Sky Lake, Ice lake and older)
  - Got access to public cloud through CloudBank and can run on

Can we compare systems using our appkernels?

Colella's 7 Dwarfs

- "Seven Dwarfs" of algorithms for simulation in the physical sciences.
- "Dwarfs" mine compute cycles for golden results



http://www.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.pdf

Tested Applications and Compute Resources

Application kernels used in this study:

- **HPCC**
- **Gromacs, NWChem, Enzo, OpenFOAM, AI-Benchmark-Alpha (Tensorflow)**

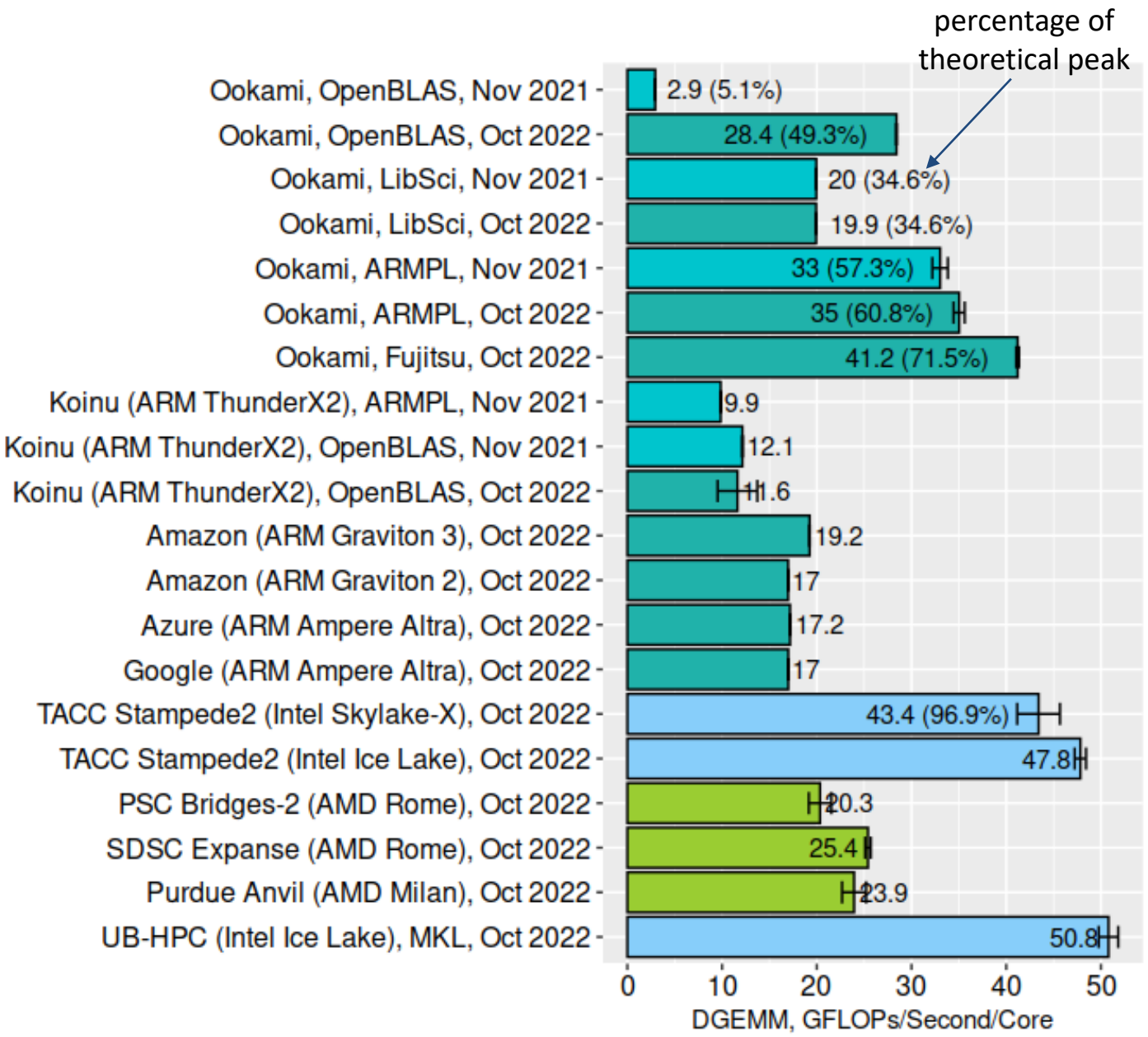
Resource	CPU	Release Date	Cores per Node	Freq, GHZ
Stony Brook Ookami	ARM Futjitsu A64FX, SVE 512bit	~2019	48	1.8
ThunderX2	ARM Cavium ThunderX2	2018	64	2.0-2.5?
Amazon-Graviton3-48	ARM Amazon Graviton 3, Neoverse V1, SVE 256bit	Nov-21	48	2.5
Amazon-Graviton2-48	ARM Amazon Graviton 2, Neoverse N1	Nov-19	48	2.6
Azure Cloud	ARM Ampere Altra, Neoverse N1	Mar-21	48	Up to 3.0
Google Cloud	ARM Ampere Altra, Neoverse N1	Mar-21	48	Up to 3.0
PSC Bridges-2	x86 AMD EPYC 7742 Zen2(Rome), AVX2	Mid-2019	128	2.25
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	Mid-2019	128	2.25
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	Mar-21	128	2.45
TACC-Stampede 2 KNL	x86 Intel Xeon Phi 7250, Knights Landing, AVX512	Q2 2016	68	1.4
TACC-Stampede 2 SKX	x86 Intel Xeon Platinum 8160, Skylake-X, AVX512	Q3 2017	48	2.1
TACC-Stampede 2 ICX	x86 Intel Xeon Platinum 8380, Ice Lake, AVX512	Q2 2021	80	2.3
UBHPC_56core	x86 Intel Xeon Gold 6330, Ice Lake, AVX512	Q2 2021	56	2

HPCC: HPC challenge benchmark

HPC Challenge Benchmark combine multiple benchmarks together

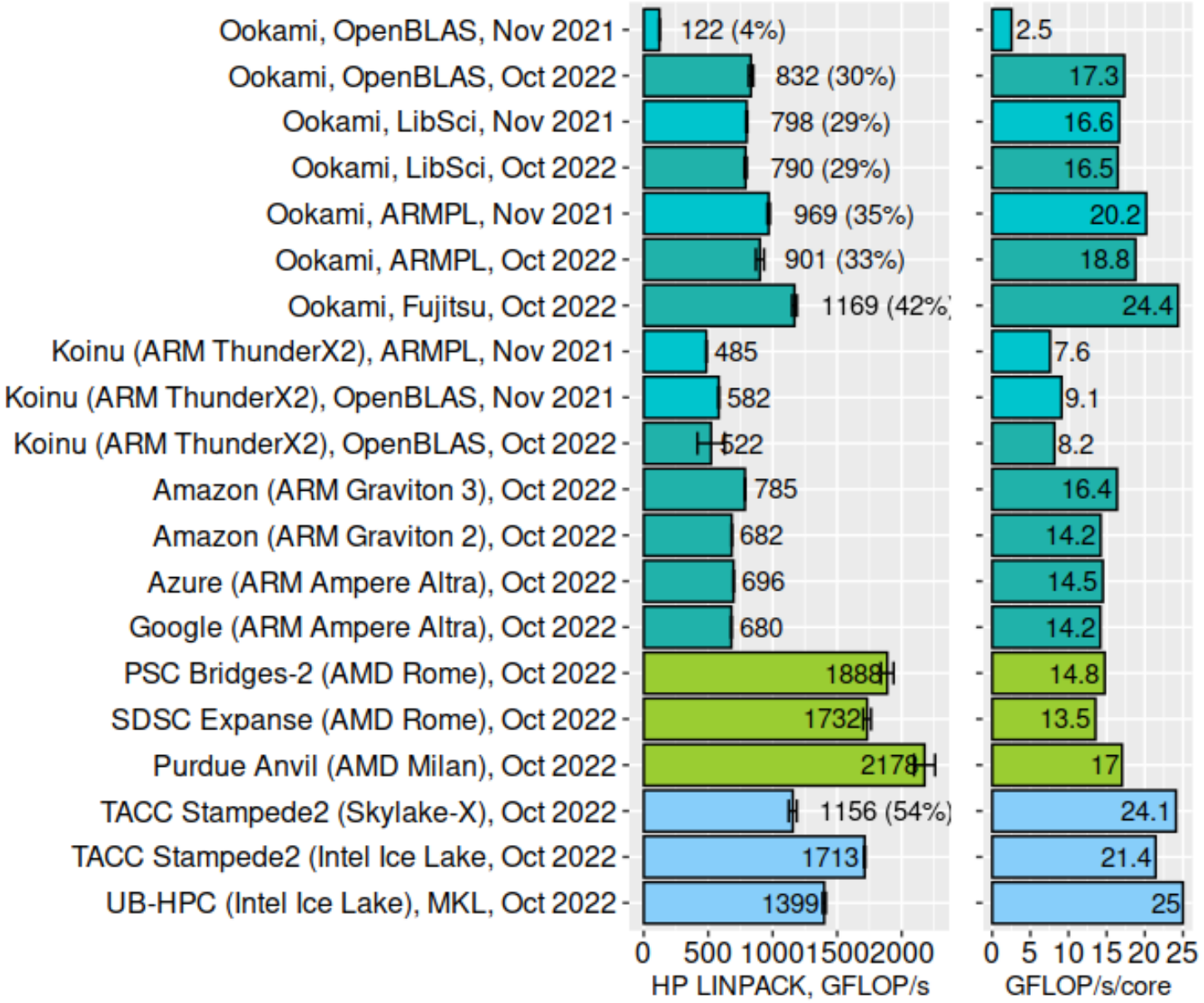
- High Performance LINPACK, which solves a linear system of equations and measures the floating-point performance
- Matrix-matrix multiplication
- Fast Fourier Transform
- Stream: memory bandwidth
- Parallel Matrix Transpose
- MPI Random Access

HPCC: DGEMM: Matrix-Matrix Multiplication



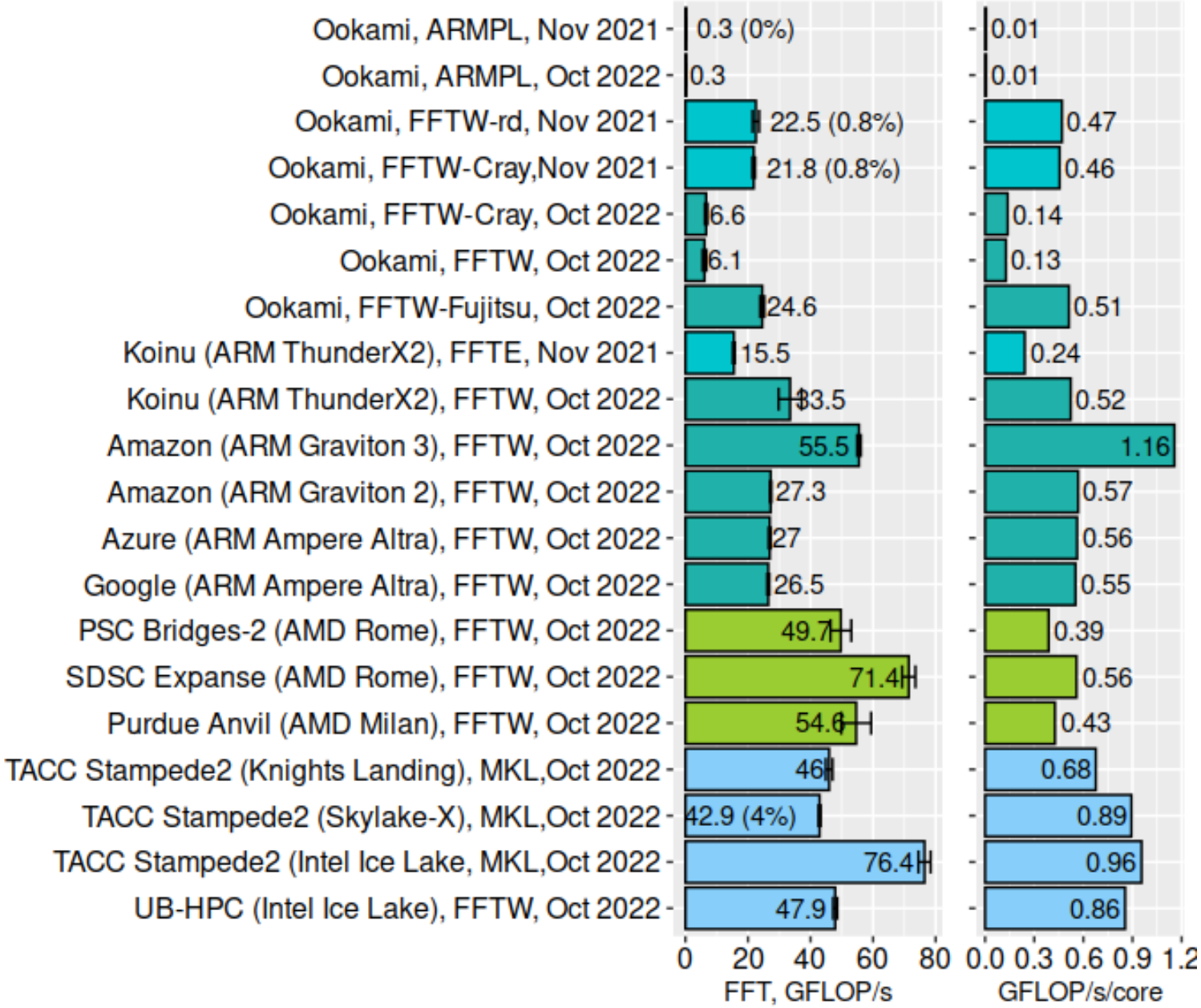
- Dual modality: 512 bit SIMD offer best performance
- Fujitsu A64FX has highest performance in ARM camp
- Overall ARM performance is comparable to x86 counterparts

HPCC: High Performance LINPACK



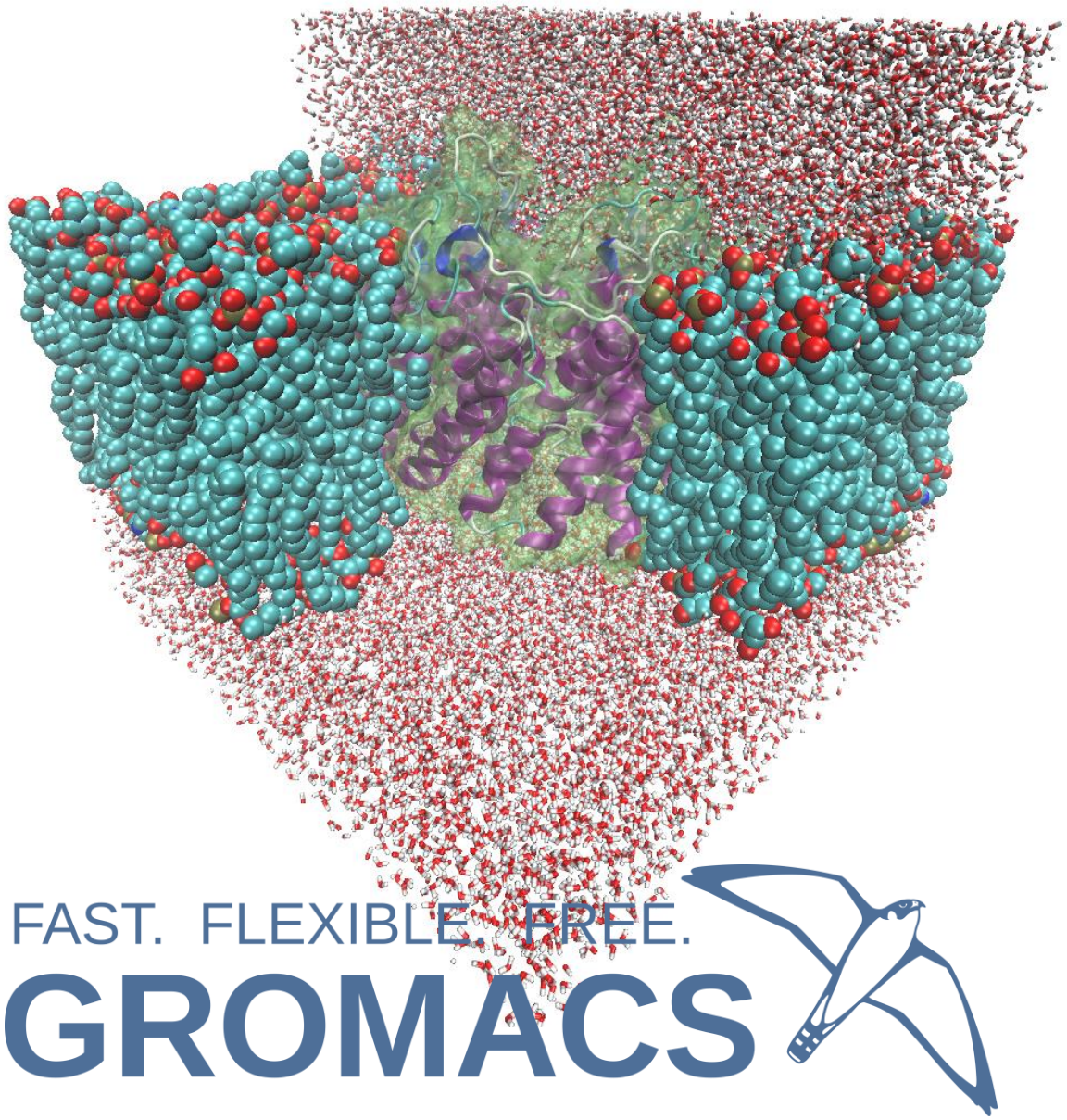
- Similar to DGEMM there is dual mode behaiviour
- Fujitsu A64FX is fastest in ARM camp
- Per core performance is competitive with x86 counterpart with similar SIMD widths

HPCC: Fast Fourier Transform (FFT)



- Graviton 3 is fastest in ARM camp. It is also has highest per core performance overall.
- Overall performance is competitive with x86 counterpart with similar SIMD widths

GROMACS: Molecular Dynamics of Biomolecular Systems



GROMACS is molecular dynamics simulation of biomolecular systems

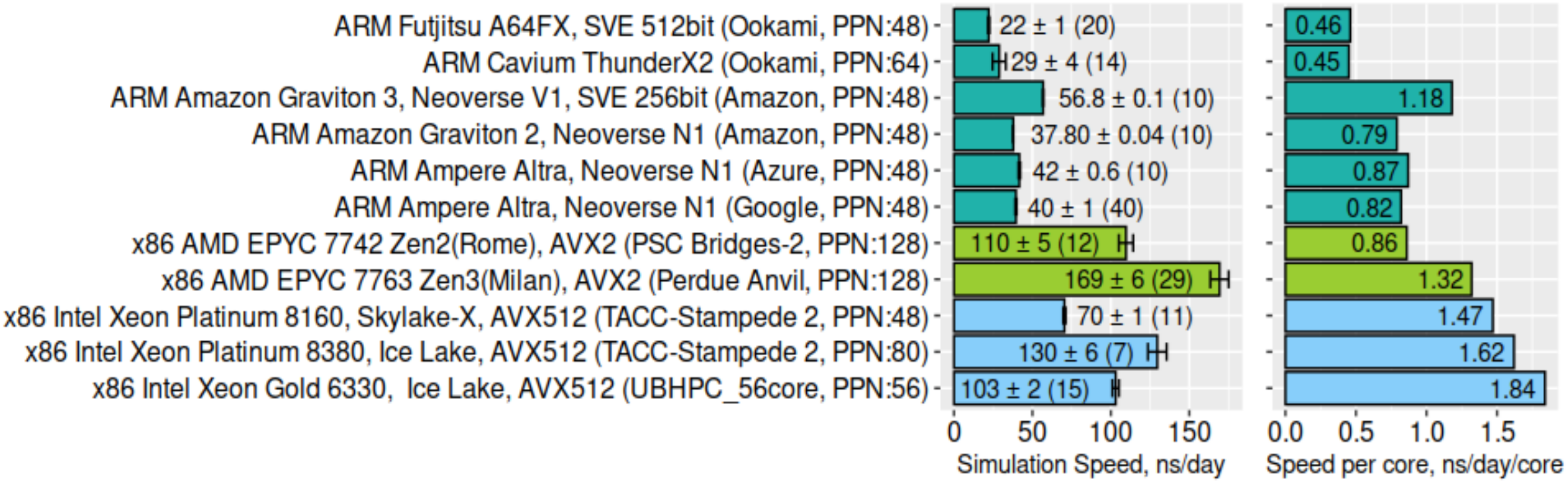
Application computational characteristics:

- Solve ODE (second Newton law)
- Particle interactions
  - Short range/long range
- FFT

Test case:

- Membrane protein
- 82k atoms system

GROMACS: Molecular Dynamics of Biomolecular Systems



- Graviton 3 is the fastest in ARM camp
- Per core performance of Graviton 2 and Ampere Alta is similar to Zen 2 (Rome) and Graviton 3 is approaching zen3 (Millan) and Skylake-X.

NWChem: Quantum Chemistry

- NWChem is an ab initio computational chemistry software package developed by Pacific Northwest National Laboratory.
- The input to the benchmark runs is the Hartree-Fock energy calculation of Au+ with MP2 and Coupled Cluster corrections

NWChem: Open Source High-Performance Computational Chemistry

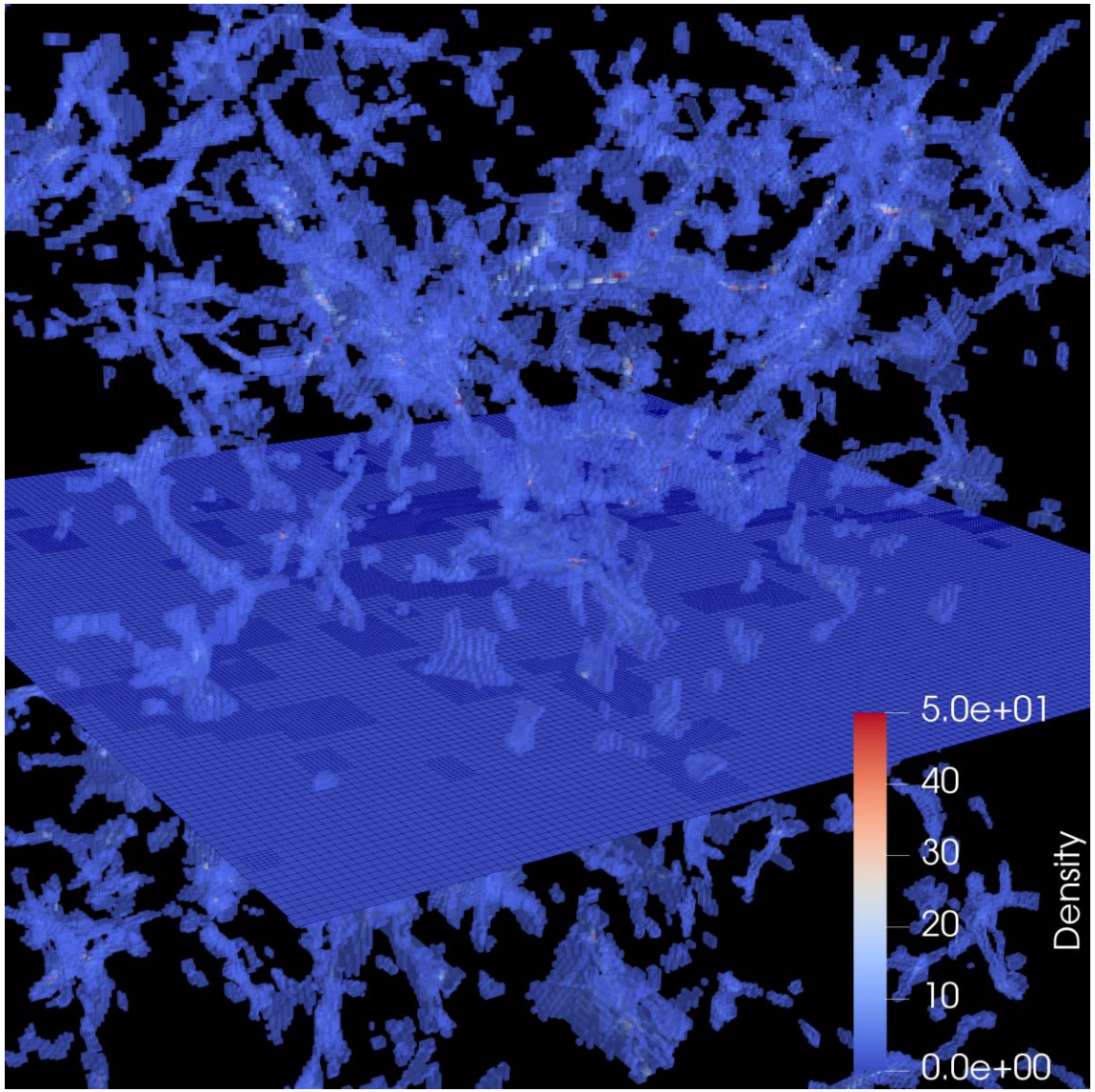
EMSL

NWChem: Quantum Chemistry

Resource	cpu	cores per node	Freq., GHz	Walltime, s [lower better]
Ookami-OSS	ARM Futjitsu A64FX, SVE 512bit	48	1.8	62.9
Amazon-Graviton3-48	ARM Amazon Graviton 3, Neoverse V1, SVE 256bit	48	2.5	36.6
Amazon-Graviton2-48	ARM Amazon Graviton 2, Neoverse N1	48	2.6	61.1
Google-T2A-48	ARM Ampere Altra, Neoverse N1	48	<=3.0	56.5
TACC-Stampede 2 KNL	x86 Intel Xeon Phi 7250, Knights Landing, AVX512	68	1.4	262.1
TACC-Stampede 2 SKX	x86 Intel Xeon Platinum 8160, Skylake-X, AVX512	48	2.1	31.2
TACC-Stampede 2 ICX	x86 Intel Xeon Platinum 8380, Ice Lake, AVX512	80	2.3	19.2
PSC Bridges-2	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	32.4
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	28.6
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	128	2.45	26.7

- We need bigger input
- Graviton 3 is fastest in ARM Camp, 18% slower than Stampede 2 (Skylake-X)

Enzo: Astrophysics and Cosmology

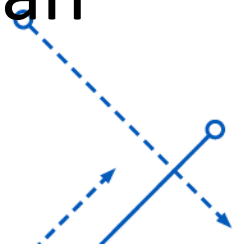


- Enzo is an Adaptive Mesh Refinement Code for Astrophysics
- Application computational characteristics:
  - Unstructured grid
  - Adaptive Mesh Refinement
- Test case: cosmology simulation that simulates reionization using the ray tracing radiation transfer method with radiating star particles and a Haardt & Madau background.

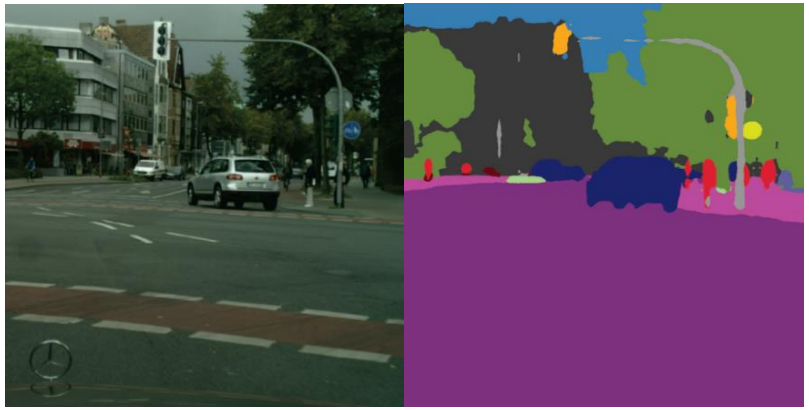
Enzo: Astrophysics and Cosmology

Resource	cpu	cores per node	Freq., GHz	Walltime, min [lower better]
Ookami-OSS	ARM Futjitsu A64FX, SVE 512bit	48	1.8	115.7
Amazon-Graviton3-48	ARM Amazon Graviton 3, Neoverse V1, SVE 256bit	48	2.5	17.0
Amazon-Graviton2-48	ARM Amazon Graviton 2, Neoverse N1	48	2.6	23.6
Google-T2A-48	ARM Ampere Altra, Neoverse N1	48	Up to 3.0	21.0
TACC-Stampede 2 KNL	x86 Intel Xeon Phi 7250, Knights Landing, AVX512	68	1.4	14.7
TACC-Stampede 2 SKX	x86 Intel Xeon Platinum 8160, Skylake-X, AVX512	48	2.1	4.2
PSC Bridges-2	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	7.2
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	6.6
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	128	2.45	7.0

- Failed to compile enzo on intel Ice Lake, Skylake binary also failed.
- Graviton 3 is fastest in ARM Camp, still significantly slower than x86 counterparts (2.5 to 4.0 times)



AI-Benchmark-Alpha (Tensorflow)



- AI-Benchmark-Alpha includes multiple machine learning tasks utilizing deep neuron networks. Tests includes classification, image to image mapping, image segmentation, image inpainting, sentence sentiment analysis and text translation.
- It is relatively light-weight
- Utilize Tensorflow for computation

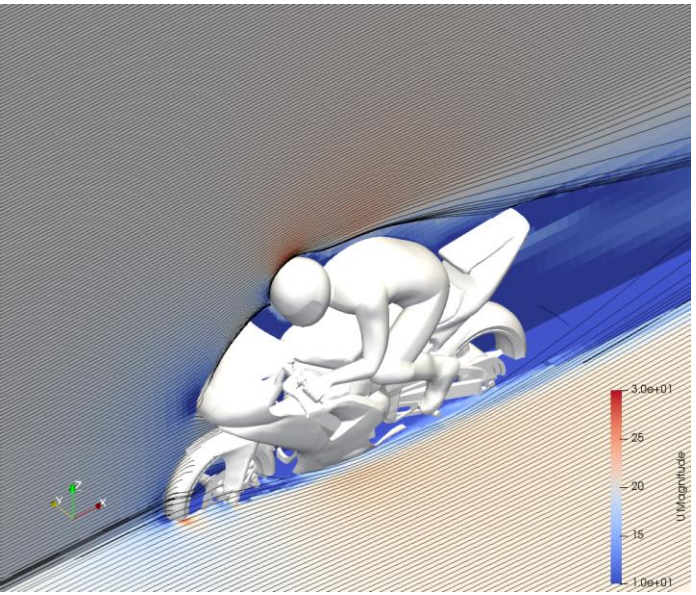
Images are taken from https://ai-benchmark.com/alpha

AI-Benchmark-Alpha (Tensorflow)

Resource	cpu	cores per node	Freq., GHz	Larger Better Training Score	Larger Better Inference Score	Larger Better AI Score
Ookami-Bin	ARM Futjitsu A64FX, SVE 512bit	48	1.8	484	533	1017
Amazon-Graviton3-48	ARM Amazon Graviton 3, Neoverse V1, SVE	48	2.5	2174	2407	4581
Amazon-Graviton2-48	ARM Amazon Graviton 2, Neoverse N1	48	2.6	1355	1676	3030
Google-T2A-48	ARM Ampere Altra, Neoverse N1	48	Up to 3.0	1375	1803	3177
TACC-Stampede 2 SKX	x86 Intel Xeon Platinum 8160, Skylake-X, A	48	2.1	1314	2292	3606
TACC-Stampede 2 ICX	x86 Intel Xeon Platinum 8380, Ice Lake, AV	80	2.3	5081	3725	8805
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	936	1761	2696
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	128	2.45	1087	1992	3079

- For a reference NVIDIA V100 performance is:
  - Training score: 18’528
  - Inference score: 18’618
  - AI score: 37’146
- Intel Ice Lake show fastest performance among CPUs and 4.2 times slower than V100 GPU
- ARM Graviton 3 is second fastest CPU outperformed only by Intel Icelake X
- ARM Graviton 2 and Ampre Alta show results comparable to older x86

OpenFOAM: Toolbox for numerical solvers (CFD)



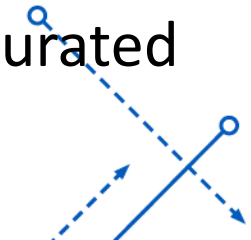
- OpenFOAM is a library and collection of application for numerical solution of PDE. Used often in computation fluid dynamics.
- Test case incompressible airflow around motorcycle
- Application computational characteristics:
  - Unstructured grid

OpenFOAM®

OpenFOAM

Resource	cpu	cores per node	Freq., GHz	Runtime, min	Mashing, min	Solver, min
Ookami-Fujitsu	ARM Futjitsu A64FX, SVE 512bit	48	1.8	22.42	8.47	10.88
Amazon-Graviton3-48	ARM Amazon Graviton 3, Neoverse V1, SVE 256bit	48	2.5	7.16	2.23	4.68
Amazon-Graviton2-48	ARM Amazon Graviton 2, Neoverse N1	48	2.6	11.94	3.54	8.02
Google-T2A-48	ARM Ampere Altra, Neoverse N1	48	Up to 3.0	11.08	3.22	7.63
TACC-Stampede 2 SKX	x86 Intel Xeon Platinum 8160, Skylake-X, AVX512	48	2.1	10.67	3.74	6.41
TACC-Stampede 2 ICX	x86 Intel Xeon Platinum 8380, Ice Lake, AVX512	48	2.3	6.98	2.57	3.99
TACC-Stampede 2 ICX	x86 Intel Xeon Platinum 8380, Ice Lake, AVX512	80	2.3	6.65	2.70	3.44
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	128	2.45	6.65	3.52	2.44
Purdue Anvil	x86 AMD EPYC 7763 Zen3(Milan), AVX2	48	2.45	6.55	2.74	3.40
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	128	2.25	10.99	6.84	3.31
SDSC Expanse	x86 AMD EPYC 7742 Zen2(Rome), AVX2	48	2.25	8.05	4.38	3.00

- Graviton 3 is fastest in ARM Camp, comparable to modern x86 and faster than older generations
- Mashing is fastest in Graviton 3
- OpenFOAM doesn’t scale well within node. Possibly saturated memory bandwidth earlier.



Conclusions

- Building/compiling is same as for traditional HPC systems
- BLAS and FFT libraries has good performance on ARM machines.
- Gromacs, OpenFOAM, Tensorflow and NWChem show performance comparable to x86 counterparts, sometimes outperforming previous generation of x86 CPUs (largely Amazon Graviton3)
- ENZO performance on any ARM system is significantly slower that on x86 systems
- Although not tested here but based on available specs ARM might offer lower power consumption.
- Among tested ARM CPUs only Ampere Alta is currently available for purchase to wider audience and it is priced lower than similar x86 system.

- From the performance point of view as of now for several application ARM provides a viable alternative to x86 counterpart and not only as a cheaper option for GPU gateway.
  - Intel Skylake-X is very robust architecture for scientific calculations

Acknowledgements

- This work is supported by the National Science Foundation under awards OAC 2137603 and 1927880.
- This work used compute resources at SUNY UB CCR, the XSEDE/ACCESS (CCR120014), CloudBank and SUNY Stony Brook University.

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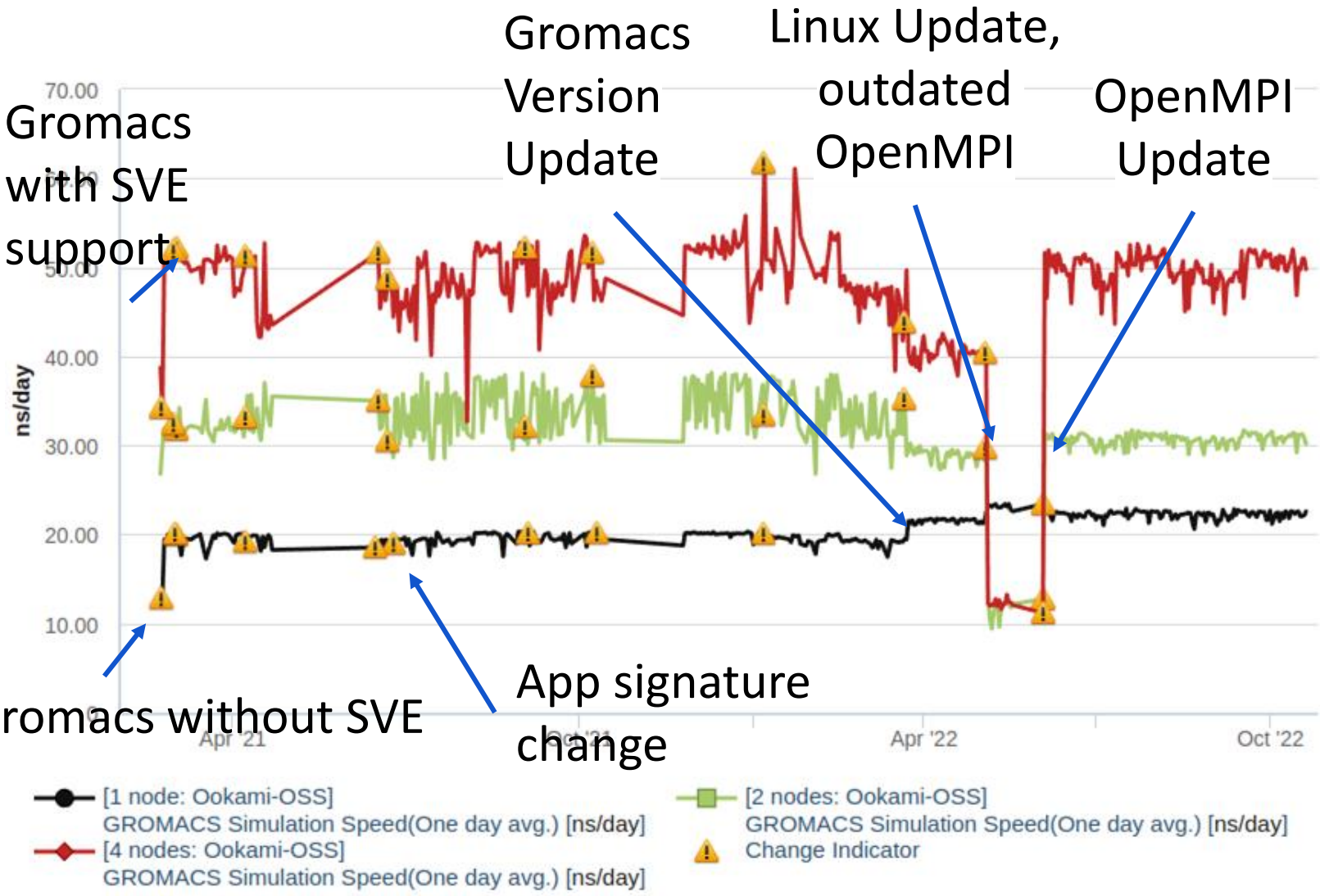
Performance over Time: GROMACS on Ookami (ARM Fujitsu A64FX)



Ookami XDMoD Application Kernels

Time based tracking of quality of service from user's perspective

Track progress and performance of Ookami software development (compliers, etc.) and usability/speed