

Diving into NVIDIA Grace Hopper and NVIDIA Grace CPU Superchips: capabilities and performance Filippo Spiga | March 26th, 2024





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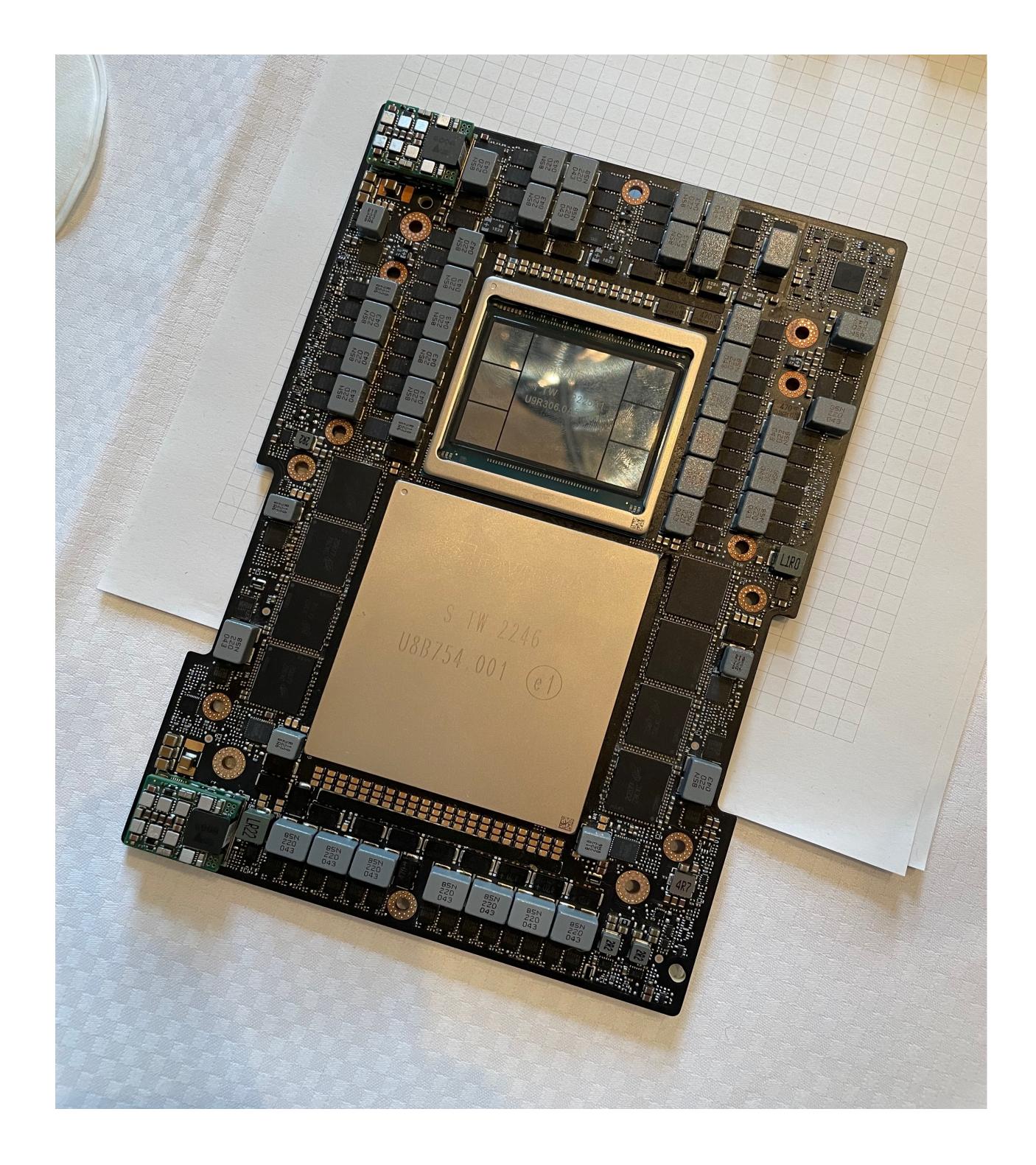


- Products
- Capabilities
- Software
- Use-Cases

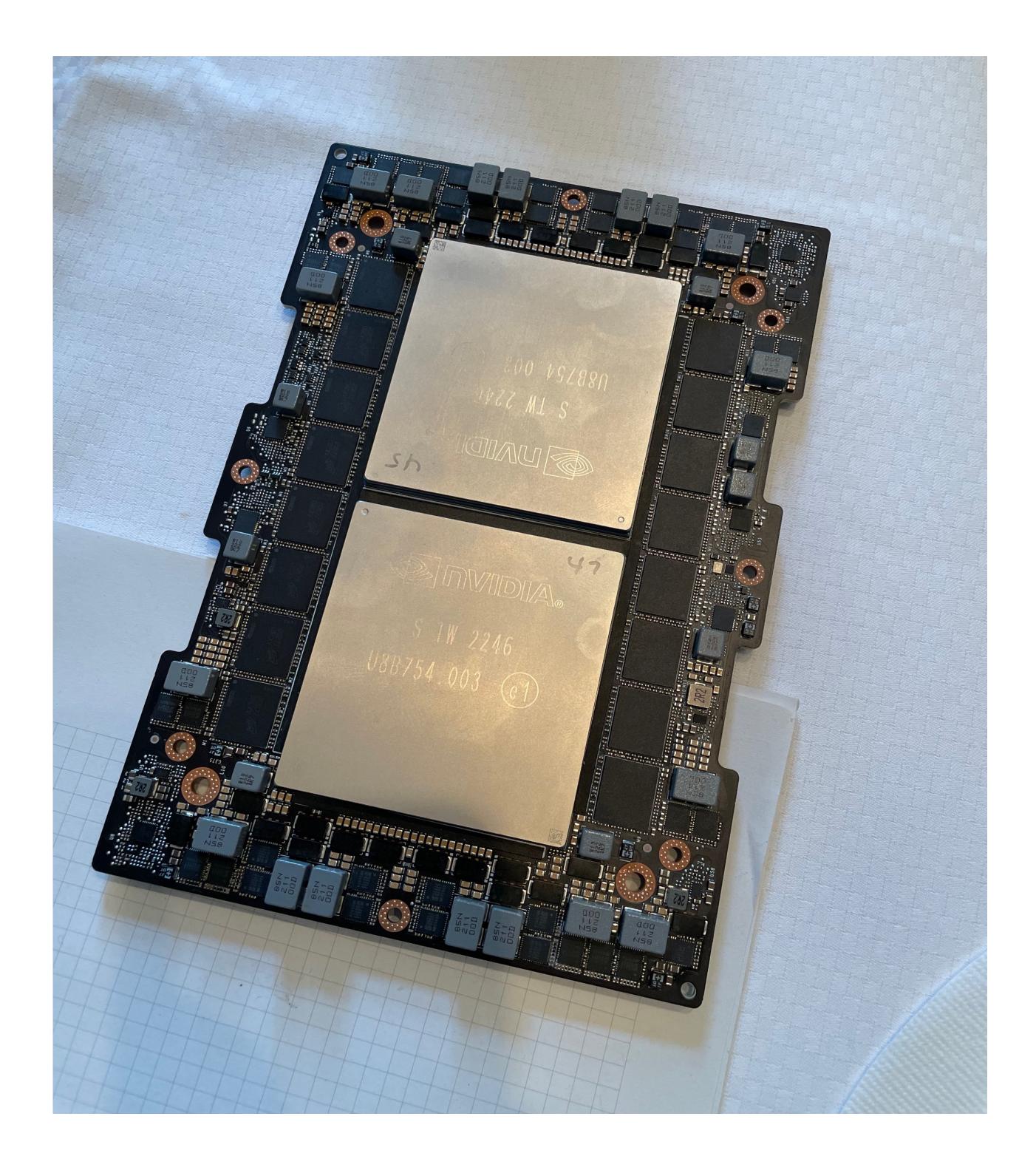


Platforms





NVIDIA Superchip Modules Grace Hopper (GH200) on left || Grace CPU Superchip on right



High Performance Power Efficient Cores

144 flagship Arm Neoverse V2 Cores with SVE2 4x128b SIMD per core

Fast On-Chip Fabric

3.2 TB/s of bi-section bandwidth connects CPU cores, NVLink-C2C, memory, and system IO

High-Bandwidth Low-Power Memory

Up to 960GB of data center enhanced LPDDR5X Memory that delivers up to 1TB/s of memory bandwidth

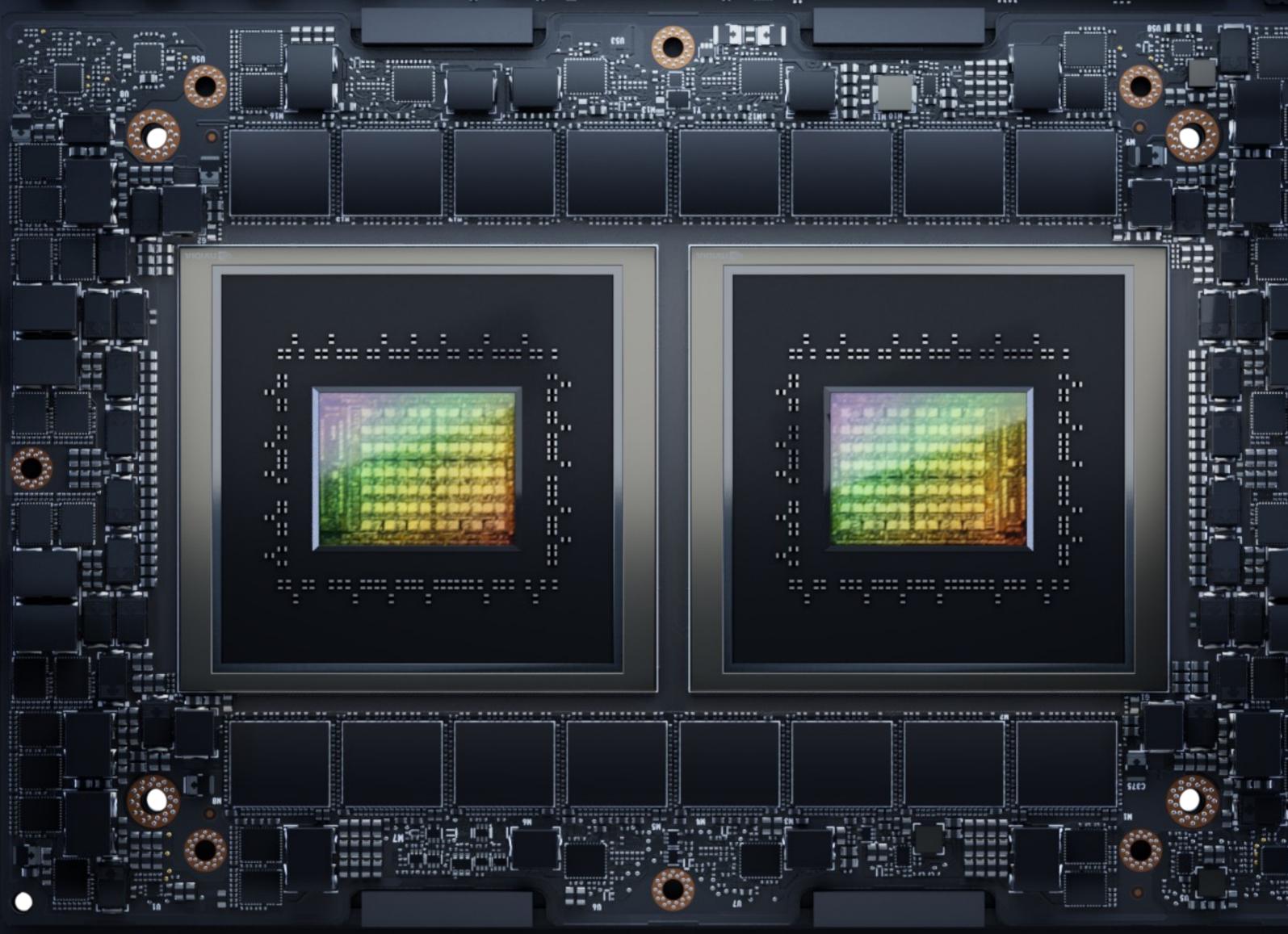
Fast and Flexible CPU IO

Up to 8x PCIe Gen5 x16 interface. PCIe Gen 5 up to 128GB/s 2X more bandwidth compared to PCIe Gen 4

Full NVIDIA Software Stack

Al, Omniverse

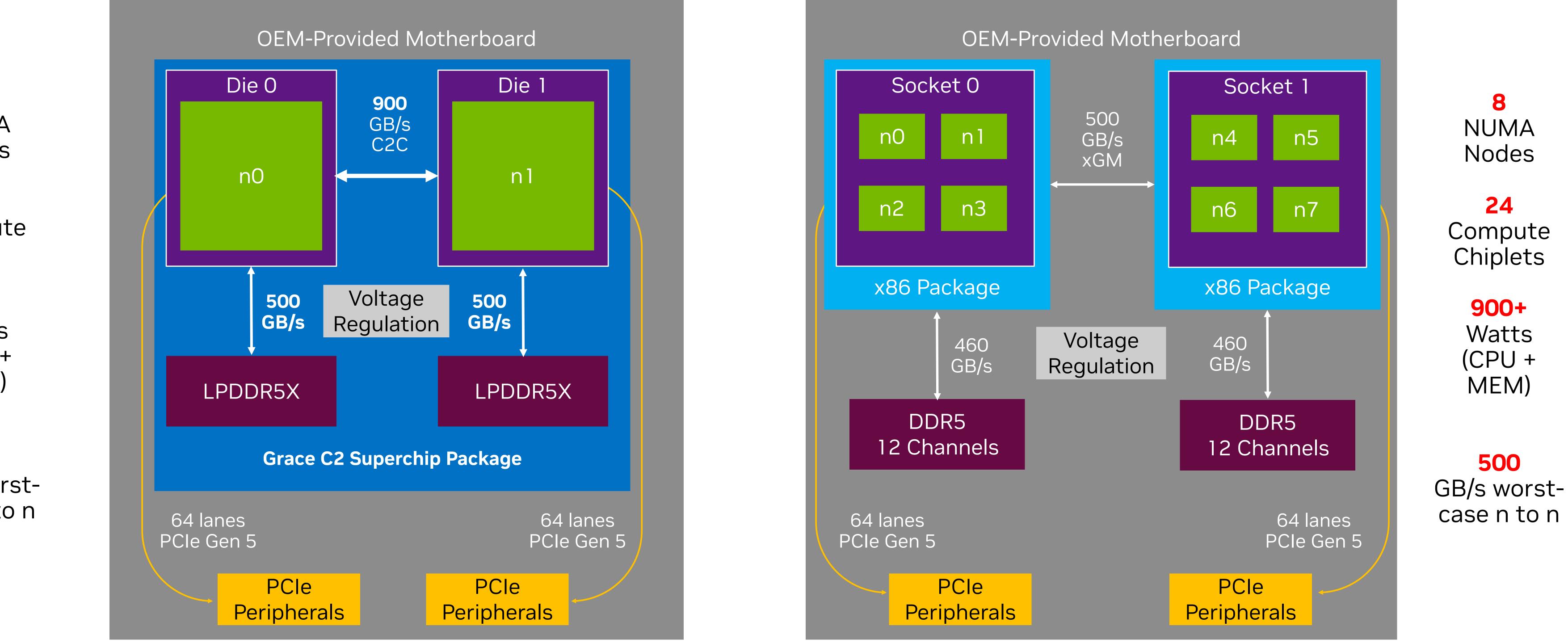
NVIDIA Grace CPU Superchip 2X Performance at the Same Power for the Modern Data Center





Grace Simplifies System Design and Workload Optimization Reduces NUMA & sub-NUMA Bottlenecks

Grace Server Grace C2 Superchip



2 NUMA Nodes

2 Compute Dies

> 500 Watts (CPU +MEM)

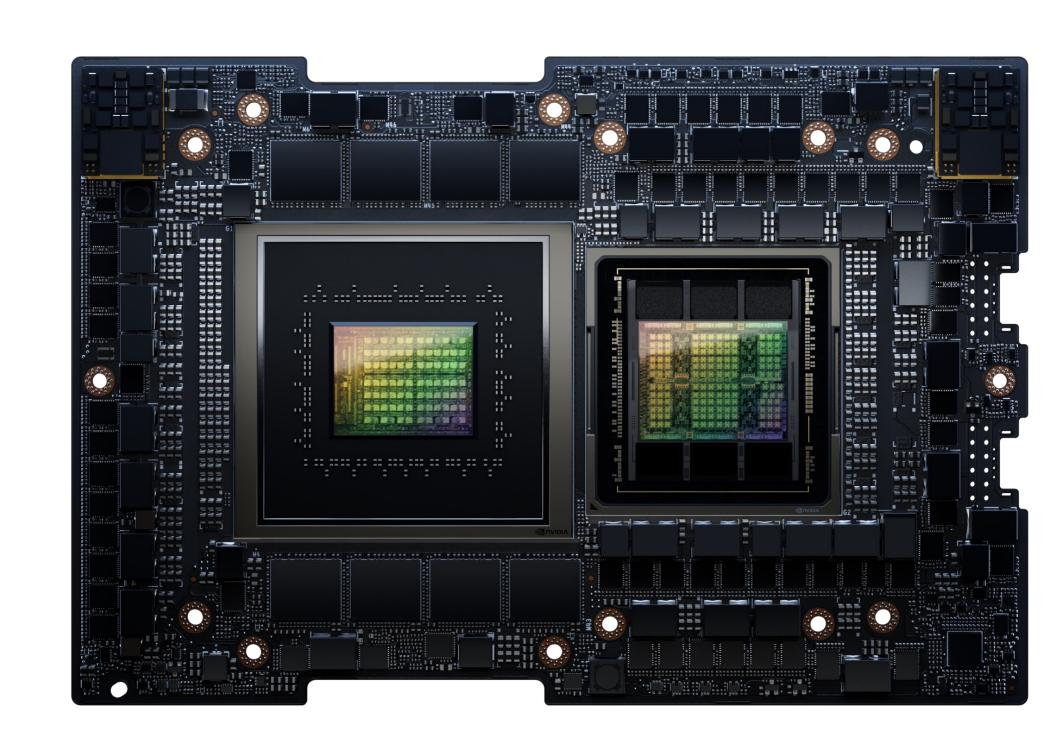
900

GB/s worstcase n to n

Conventional 2-Socket Server Example: 2x AMD Genoa, Native NPS=4



NVIDIA GH200 Grace Hopper Superchip Processor For The Era of Accelerated Computing And Generative AI

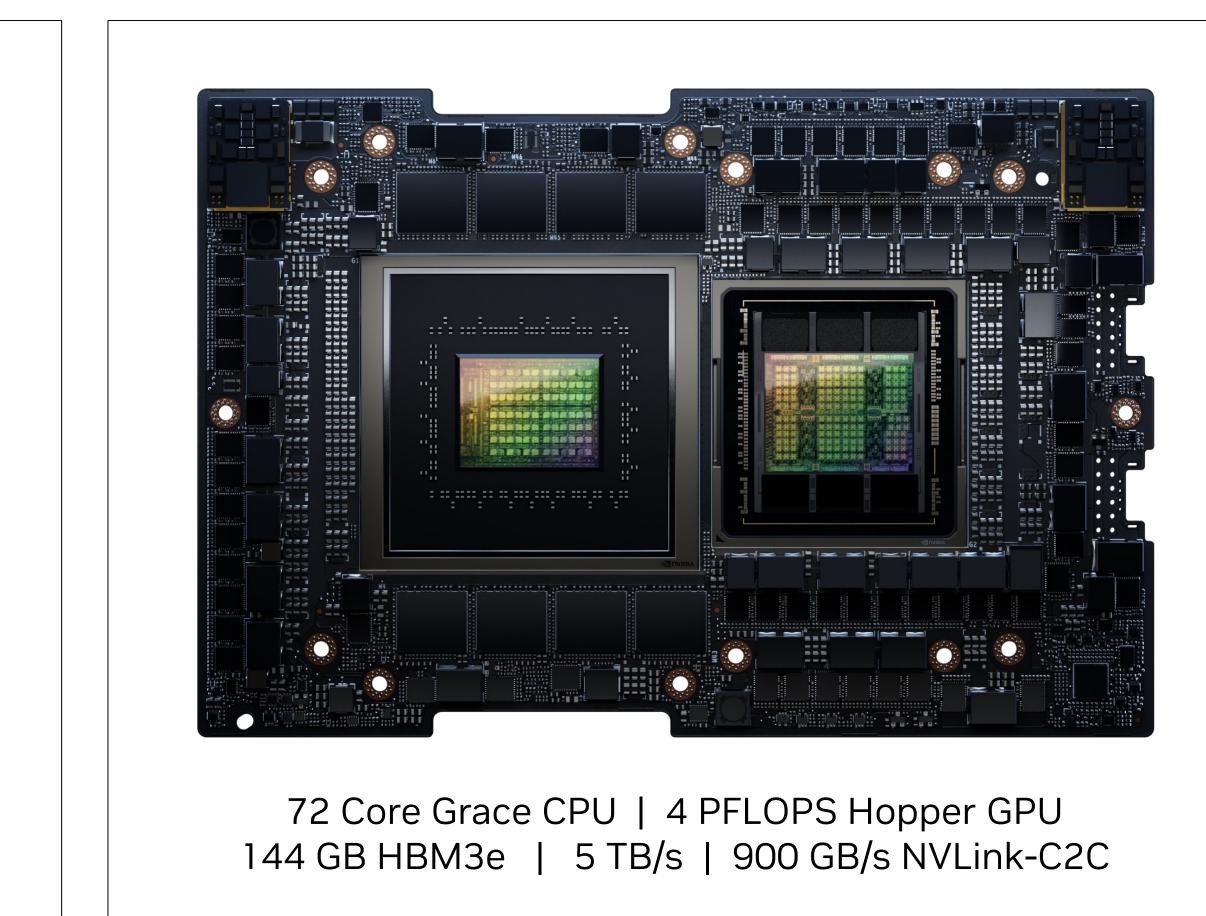


72 Core Grace CPU | 4 PFLOPS Hopper GPU 96 GB HBM3 | 4 TB/s | 900 GB/s NVLink-C2C

- 7X bandwidth to GPU vs PCIe Gen 5
- Combined 576 GB of fast memory
- 1.2x capacity and bandwidth vs H100
- Full NVIDIA Compute Stack

GH200 with HBM3

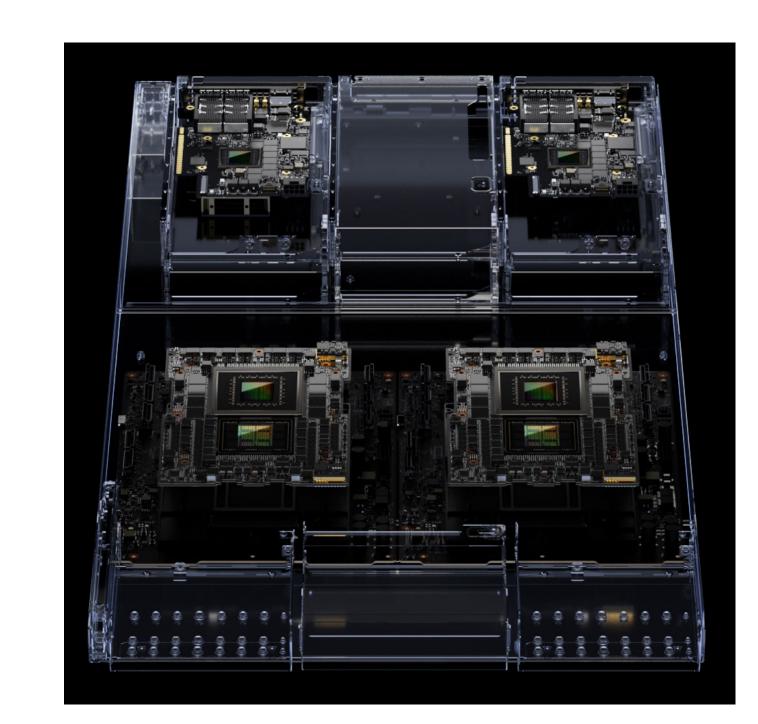
Available for order



- World's first HBM3e GPU
- Combined 624 GB of fast memory
- 1.7x capacity and 1.5x bandwidth vs H100
- Full NVIDIA Compute Stack

GH200 with HBM3e

Available late Q2 2024

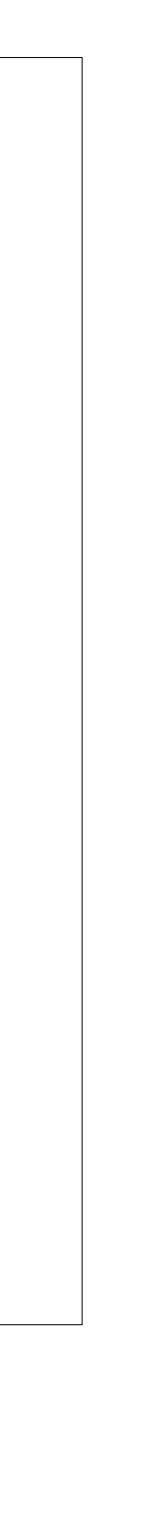


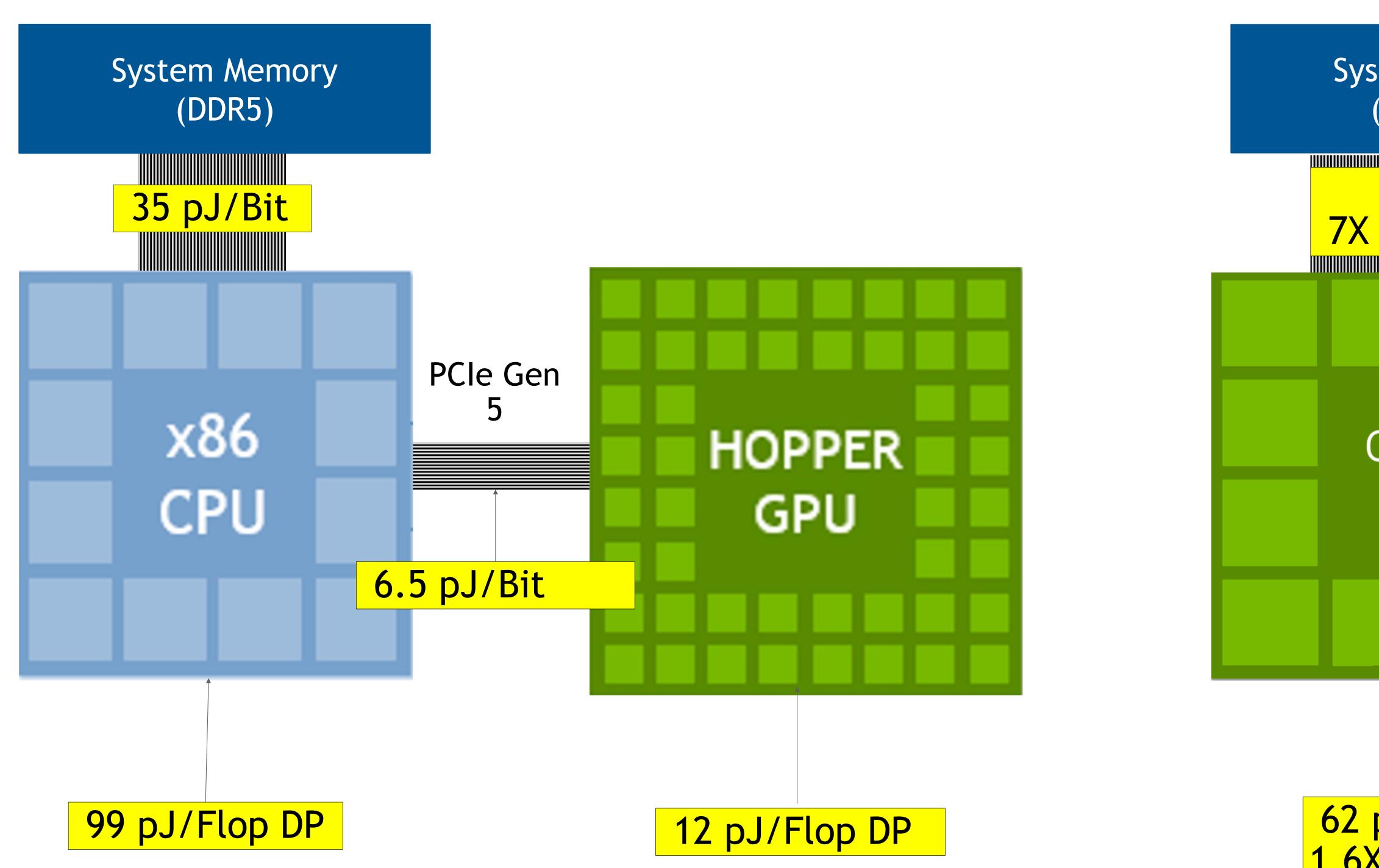
144 Core Grace CPU | 8 PFLOPS Hopper GPU 288 GB HBM3e | 10 TB/s | 900 GB/s NVLink-C2C

- Simple to deploy MGX-compatible design
- Combined 1.2 TB fast memory
- 3.5x capacity and 3x bandwidth vs H100
- Full NVIDIA Compute Stack

NVLink Dual GH200 System

Available late Q2 2024





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Energy Efficient Design More Efficient Computation and Data Movement



5 pJ/Bit

7X less energy

GRACE HOPPER NVLink-C2C CPU GPU 1.3 pJ/Bit 5X less energy 12 pJ/Flop DP 62 pJ/Flop DP Equal energy 1.6X less energy





Capabilities



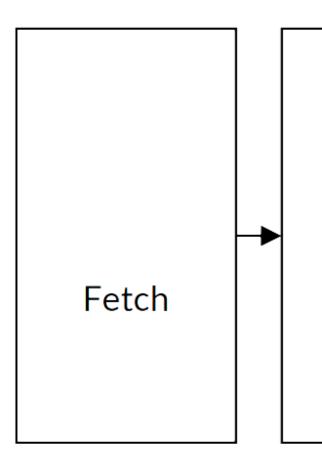
NVIDIA Grace SIMD Highlights

Neoverse V2 Arm IP core

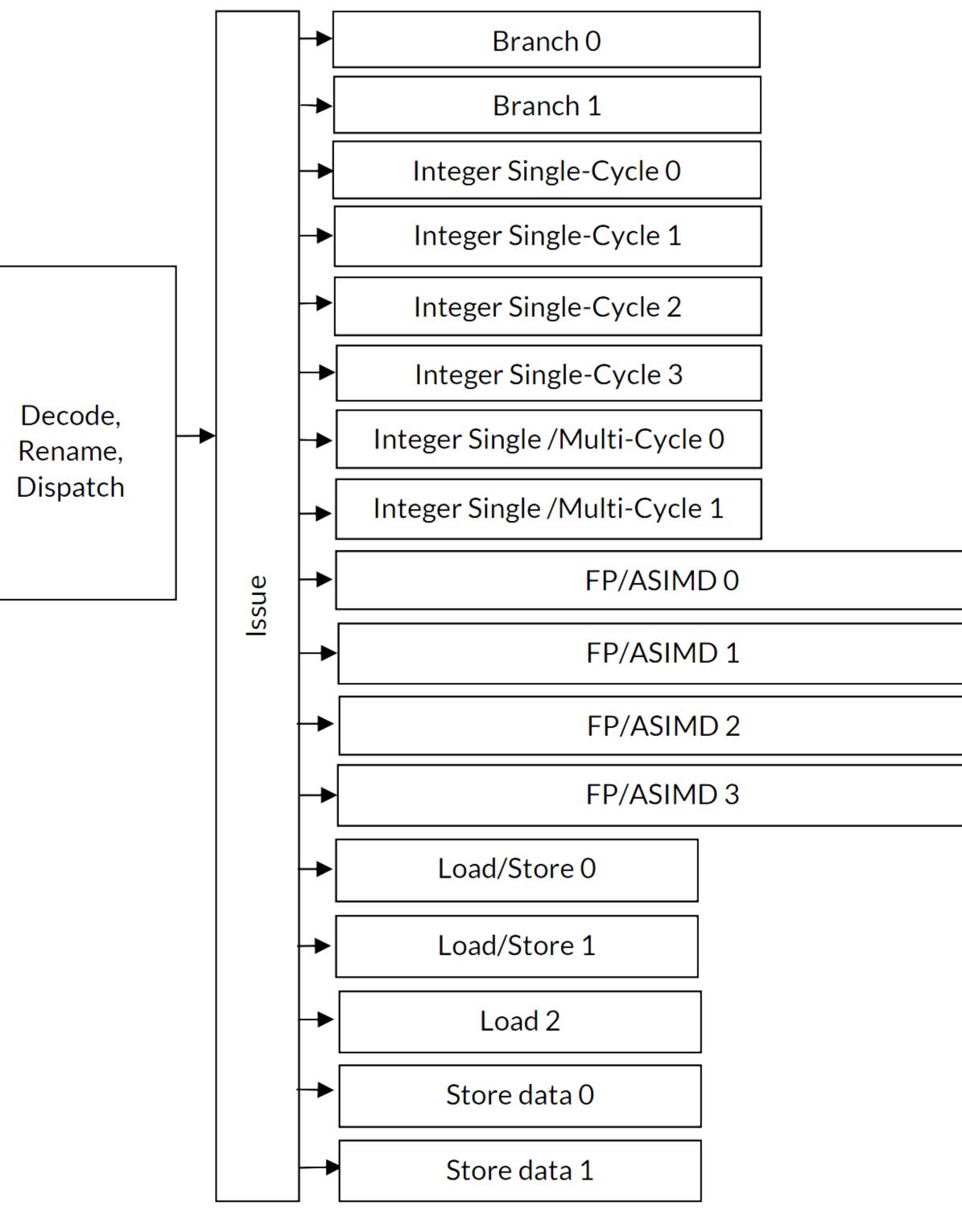
- 4x128b SIMD units = 512b SIMD vector bandwidth total
- Each SIMD unit can retire NEON or SVE2 instructions
- On this architecture, SVE2 and NEON have the same peak performance
- SVE2 can vectorize more complex codes and supports more data types than NEON.
- NEON doesn't require predicate calculation
 - Neither does VLS SVE

For more in-depth core u-arch details: <u>Arm[®] Neoverse™ V2 Core Technical Reference Manual</u>





IN ORDER



OUT OF ORDER



Grace SoC Memory Subsystem Compute and Data-mover Architecture

- Separate L1 data and instruction caches per core
 - L1 64KB, 4-way set associative, 64B cache line
- Private, unified data and instruction L2 cache per core
 - 1MB, 8-way set associative
- Scalable Coherency Fabric
 - Shared, uniform 117MB of L3 cache for entire chip.

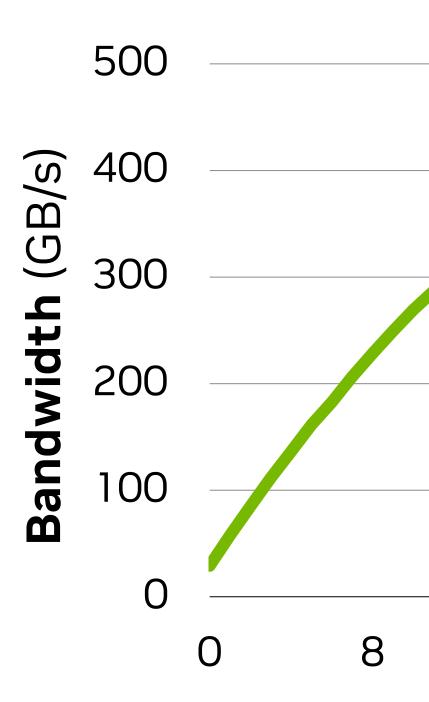
Superchip	Capacity (GB)	OMP_NUM_THREADS	Expected TRIAD Bandwidth
Grace-Hopper	120	72	450+
Grace-Hopper	480	72	340+
Grace CPU	240	144	900+
Grace CPU	480	144	900+
Grace CPU	960	144	680+

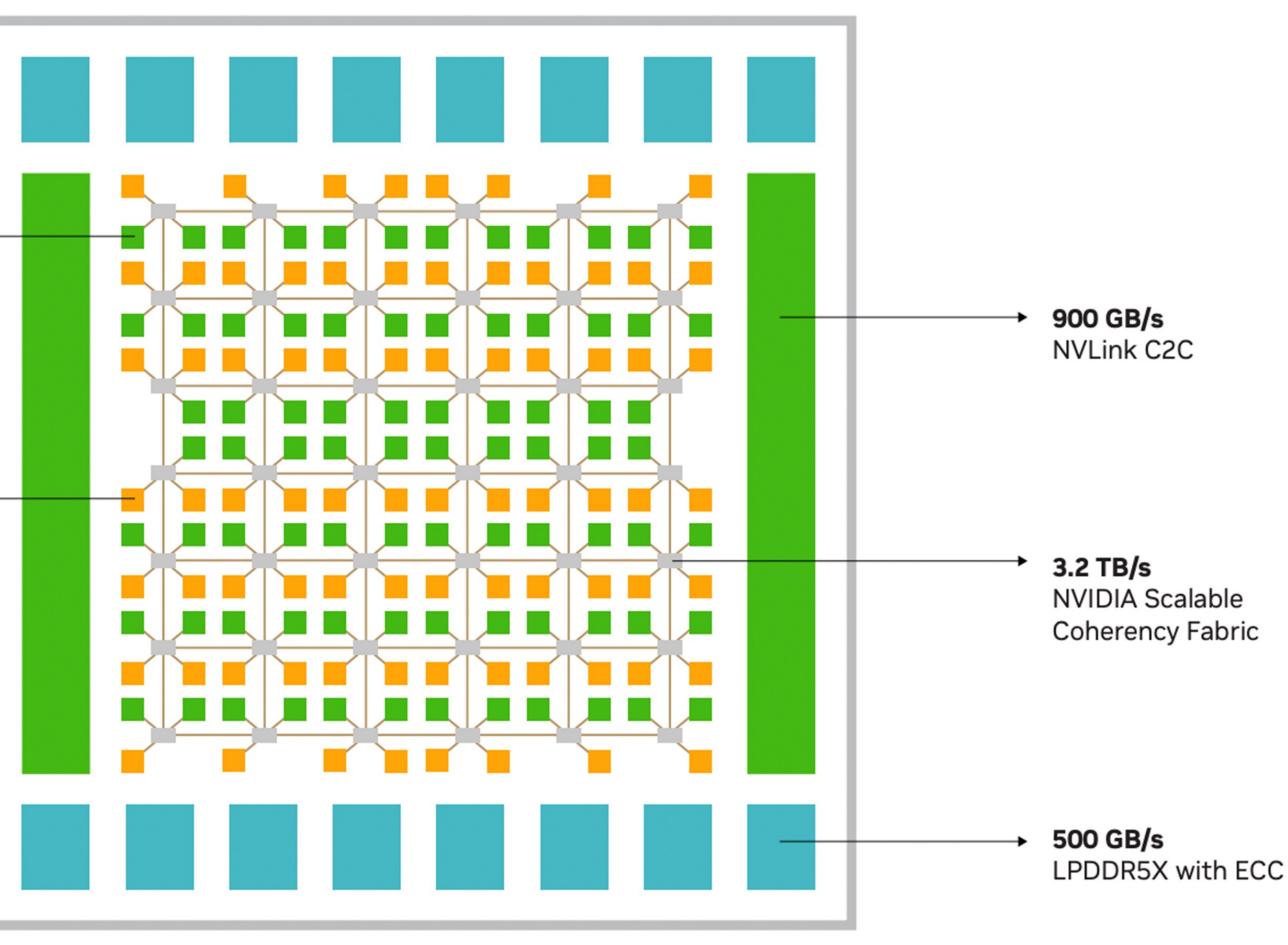
Source: https://docs.nvidia.com/grace-performance-tuning-guide.pdf



72 Cores Arm Neoverse V2 Cores with 2X Perf/W Over Today's Server

> 117 MB L3 Cache

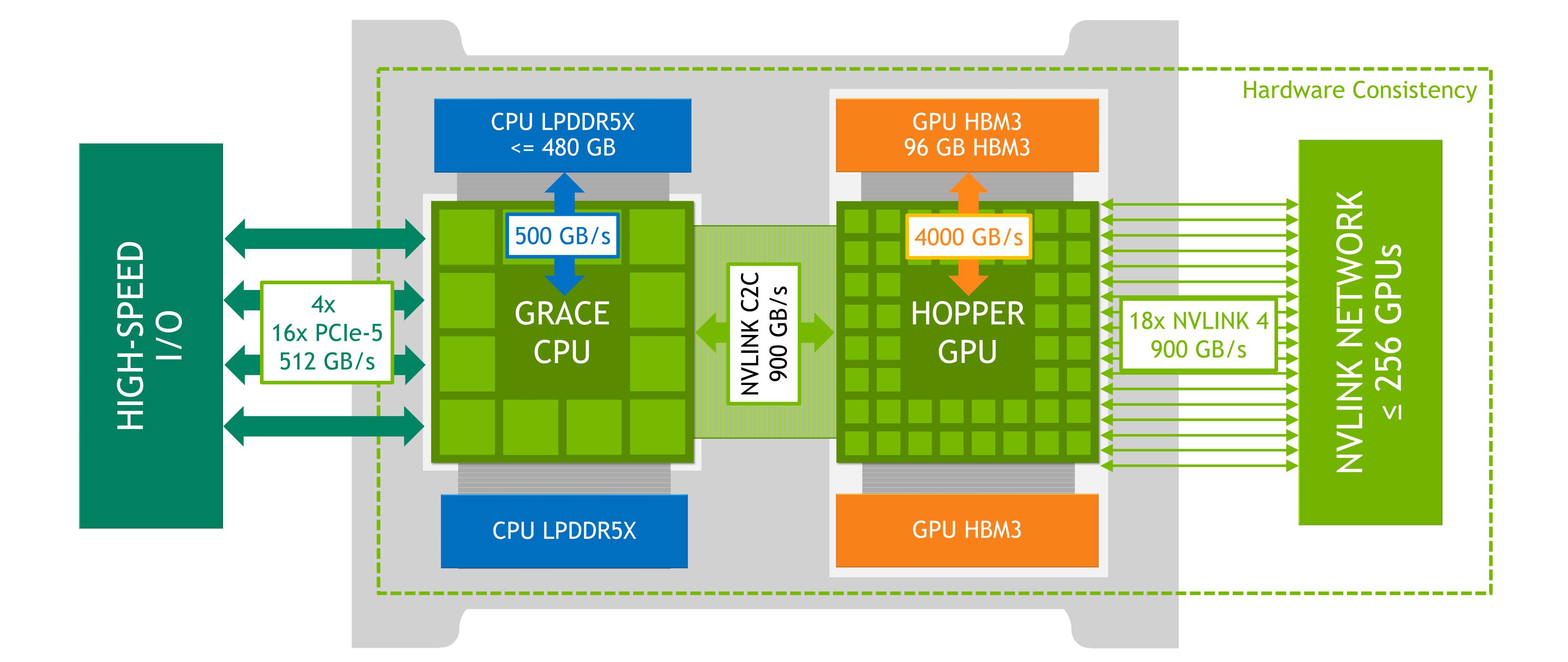




Grace SoC STREAM Triad

16	24	32	40	48	56	64	
Threads							



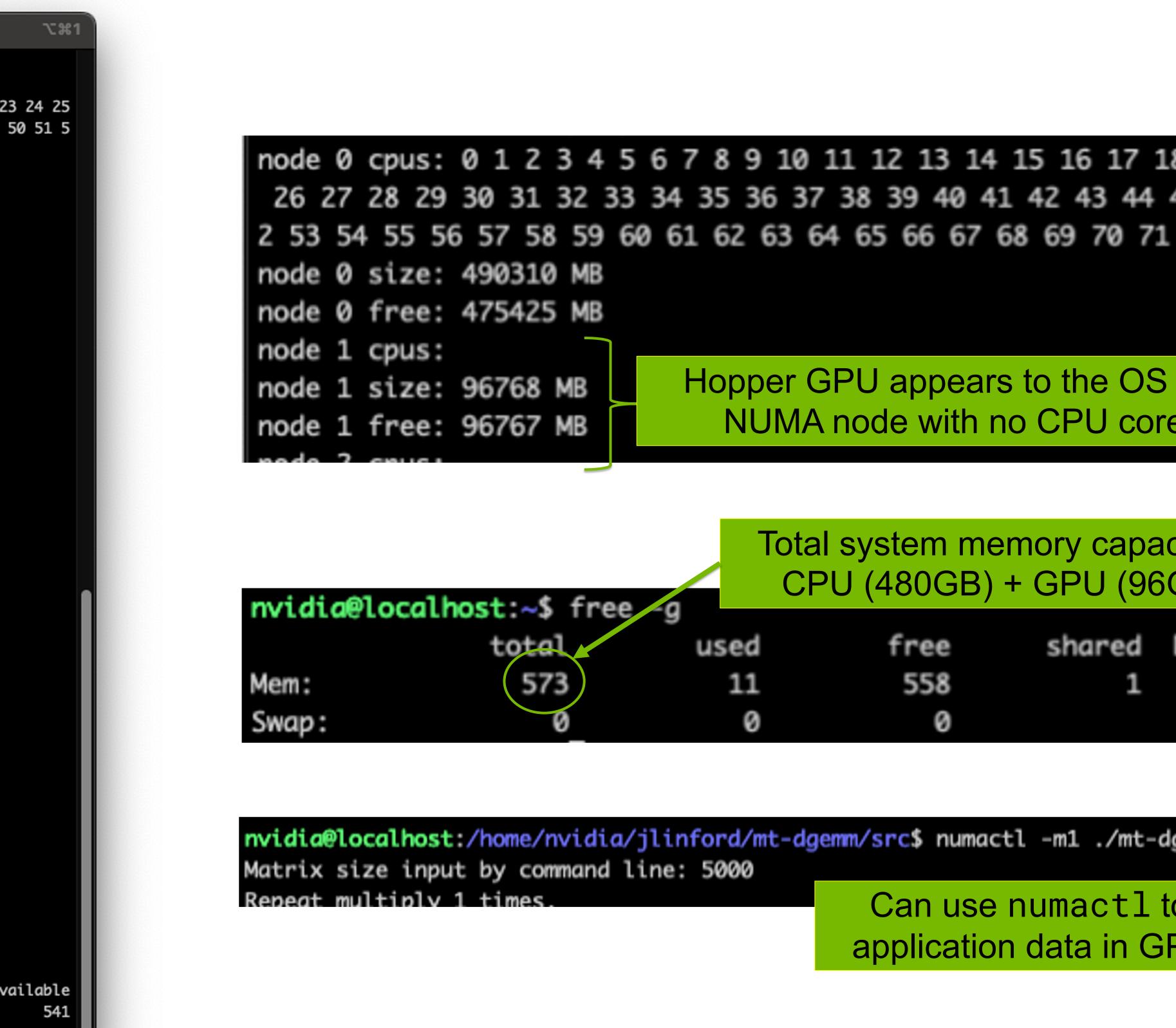


Grace Hopper Superchip GPU can access CPU memory at CPU memory speeds



GPU Memory is Visible to the Operating System Standard operating system commands work on the GPU

•••		n	vidia@locall	host: ~		
nvidia@loc	alhost:~\$	numactl -H				
available:						
	~	-	0 11 12 13	14 15 16	17 18 19 20 21	22 2
· · · · · ·					44 45 46 47 4	
		59 60 61 62 63				• • • •
node 0 size		AD .				
node 0 free			U I			
node 1 cpus						
node 1 size						
node 1 free			U			
node 2 cpus						
node 2 size						
node 2 free						
node 3 cpus						
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node 6 cpus						
node 6 size						
node 6 free						
node 7 cpus						
node 7 size						
node 7 free						
node 8 cpus						
node 8 size						
node 8 free						
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	1 2 3	4 5 6	78			
	80 80 80	4 5 6 80 80 80	7 8 80 80			
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		255 255 255		255		
		255 255 255		255		
		255 255 255	255 255	10		
nvidia@loc		· .	6	-1	ad bucc/aast	
Mome	total	used	free			av
Mem:	573	11	558		1 3	
Swap:	0	0	0			
nvidia@loc	alnost:~\$					



node 0 cpus: 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 5

> Hopper GPU appears to the OS as a NUMA node with no CPU cores

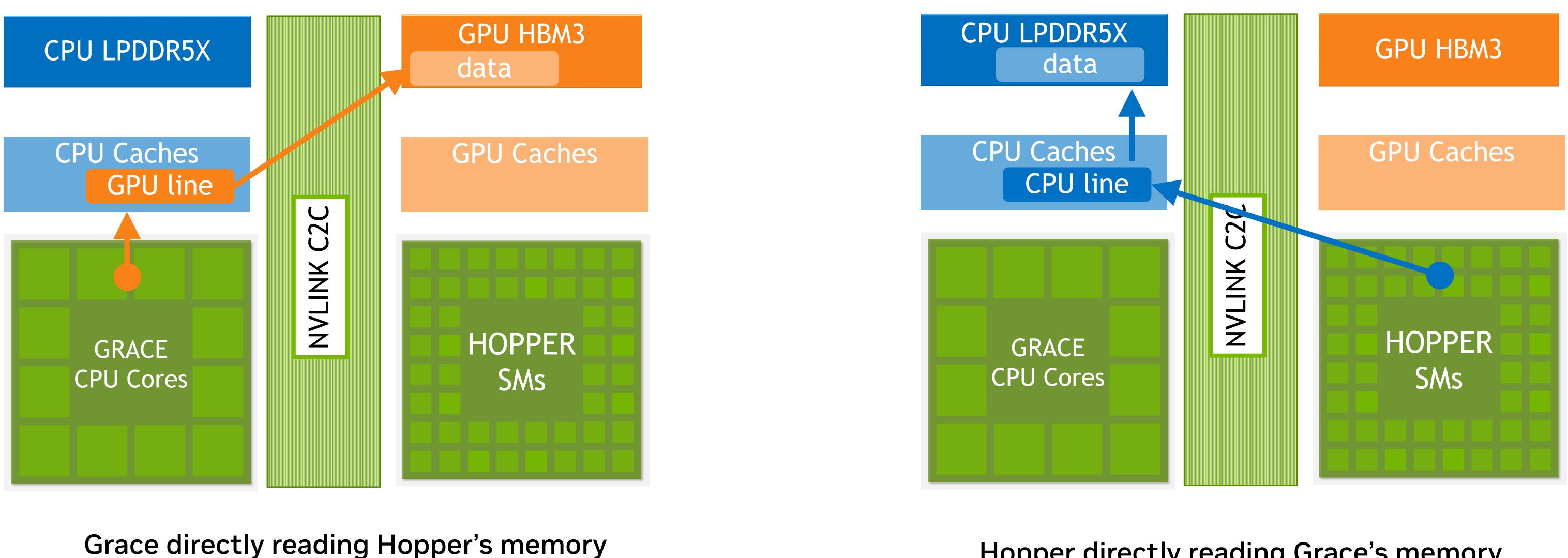
> > Total system memory capacity is CPU (480GB) + GPU (96GB)

free	shared	buff/cache	available
558	1	3	541
0			

nvidia@localhost:/home/nvidia/jlinford/mt-dgemm/src\$ numactl -m1 ./mt-dgemm.nvpl 5000 1 1 1 0 1 1

Can use numactl to put CPU application data in GPU memory





CPU fetches GPU data into CPU L3 cache Cache remains **coherent** with GPU memory Changes to GPU memory **evict** cache line

Global Access to All Data Cache-coherent access via NVLink C2C from either processor to either physical memory

GPU loads CPU data via CPU L3 cache CPU and GPU can both hit on cached data Changes to CPU memory **update** cache line

Hopper directly reading Grace's memory



Software



- Use a compiler that supports Neoverse V2
- Check and update your compiler flags
- Use -mcpu=native
- If possible use -Ofast
- Use -flto to enable link-time optimization
- Fortran may benefit from -fno-stack-arrays
- Remember to check your dependencies

Compilers

Can also use -mcpu=neoverse-v2, but -mcpu=native will "port forward"

 If fast math optimizations are not acceptable, use -03 -ffp-contract=fast • For even more accuracy, use -ffp-contract=off to disable floating point operation contraction (e.g. FMA)

• The benefits of link-time optimization vary from code to code, but can be significant • See e.g. <u>https://gcc.gnu.org/onlinedocs/gcc/Optimize-Options.html</u> for details

• Apps may need -fsigned-char or -funsigned-char depending on the developer's assumption

• This is also a good opportunity to check for newer version with improved Arm Neoverse V2 / Grace support

Compiler	Version ≧
GCC	12.2
LLVM (Clang)	16
NVIDIA HPC	23.3
Arm Compiler	23.04



Porting Applications that use Math Libraries (MKL, OpenBLAS, etc.) Several library options to choose from

 Prefer Netlib BLAS/LAPACK and FFTW interfaces Building on these interfaces enables compatibility

NVPL

-I/PATH/TO/nvpl/include \ -L/PATH/TO/nvpl/lib \ -o mt-dgemm.nvpl mt-dgemm.c \ -lnvpl_blas_lp64_gomp

ArmPL

 gcc -DUSE_CBLAS -ffast-math -mcpu=native -03 -o mt-dgemm.armpl mt-dgemm.c \ -larmpl_lp64

```
• gcc -DUSE_CBLAS -ffast-math -mcpu=native -03 \
```

```
-I/opt/arm/armpl-23.10.0_Ubuntu-22.04_gcc/include \
-L/opt/arm/armpl-23.10.0_Ubuntu-22.04_gcc/lib '
```

• ATLAS, OpenBLAS, BLIS, ... Community supported with some optimizations for Neoverse V2. Works on Grace, but unlikely to outperform NVPL and ArmPL. A good compatibility option.

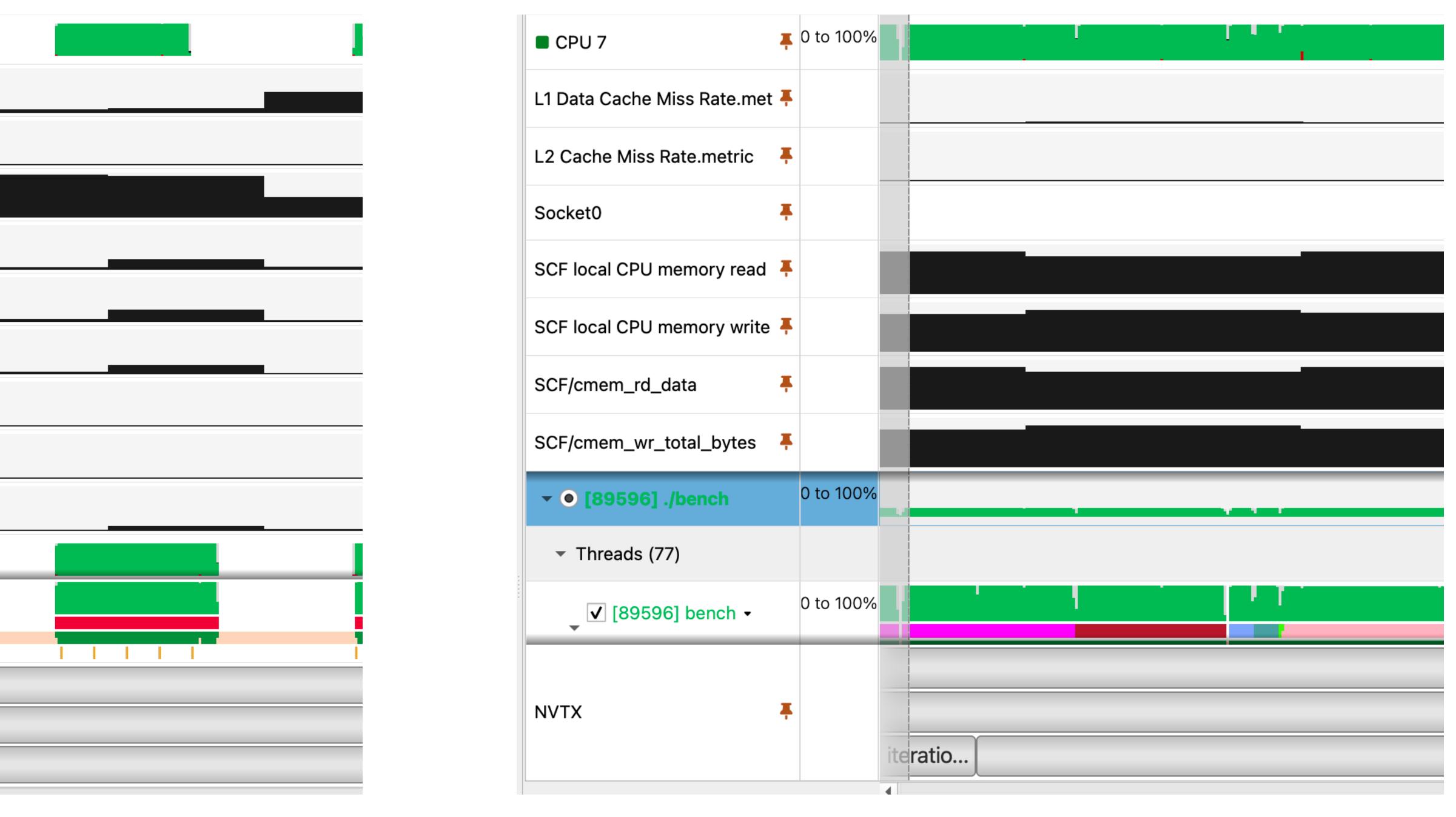
libnvpl_blas_ilp64_gomp.so libnvpl_blas_ilp64_seq.so libnvpl_blas_lp64_gomp.so libnvpl_blas_lp64_seq.so libnvpl_fftw.so libnvpl_lapack_ilp64_gomp.so libnvpl_lapack_ilp64_seq.so libnvpl_lapack_lp64_gomp.so libnvpl_lapack_lp64_seq.so libnvpl_rand_mt.so libnvpl_rand.so libnvpl_scalapack_ilp64.so libnvpl_scalapack_lp64.so libnvpl_sparse.so libnvpl_tensor.so



🕶 📕 CPU 21	Ŧ	0 to 100%	
Backend Stalls.metric			
Frontend Stalls.metric			
Retiring.metric			
CPU_CYCLES			
OP_RETIRED			
OP_SPEC			
STALL_BACKEND			
STALL_FRONTEND			
STALL_SLOT			
CPU 23		0 to 100%	
✓ [89166] bench -	Ŧ	0 to 100%	
NVTX	Ŧ		
			it er

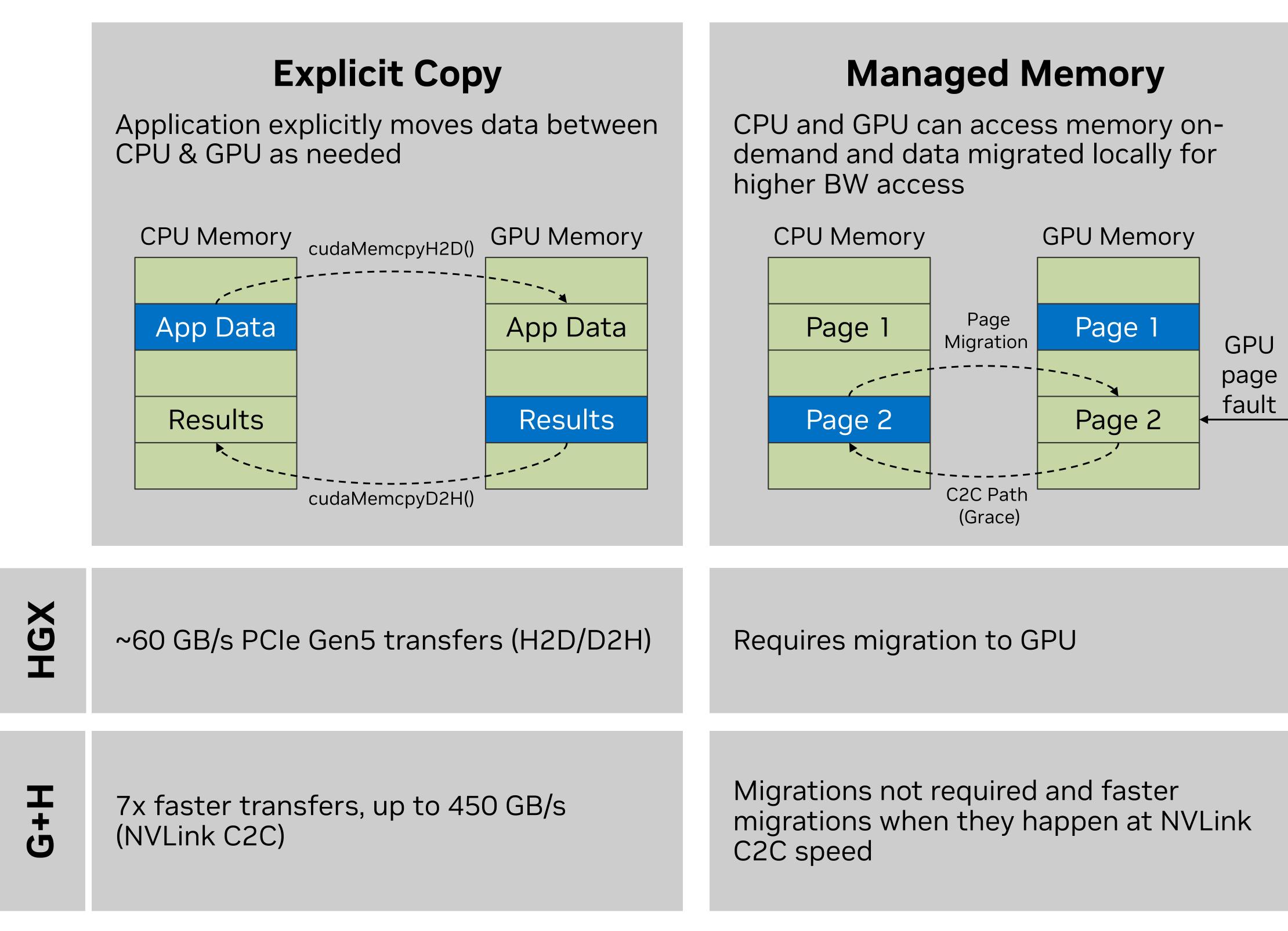
nsys profile --cpu-core-metrics=help

Nsight Systems – Core/Uncore metrics Collect core/uncore performance metrics



nsys profile --cpu-socket-metrics=help





The Grace Hopper Advantage Full CUDA support with additional Grace memory extensions

System Allocated					
GPU can access memory allocated from malloc(), mmap(), etc.					
CPU Memory GPU Memory App Data App Data GPU access to malloc() memory Image: State of the state of t					

Access possible with explicit call to cudaHostRegister() at PCle speeds Requires HMM patch in Linux Kernel

cudaHostRegister() not needed; access at NVLink C2C speeds



Use-cases: NEMO on GH200

(Presented at GTC24 - S62337)



A partially accelerated case utilizing unified memory on Grace-Hopper

The "Nucleus for European Modelling of the Ocean" (NEMO) is a state-of-the-art modelling framework, used for research activities and forecasting services in ocean and climate sciences.

• Setup (NEMO v4.2.0)

- **GYRE_PISCES** benchmark
 - Scaling factor for grid resolution: **nn_GYRE = 25**
 - ~ORCA ½ grid
 - ~80 GB RAM, fits on single GPU
- **MPI-only**, single core to every MPI process for CPU runs
- Incremental porting on Grace-Hopper (480GB) using unified memory and access-counter based migrations
 - Memory management left to runtime **system-allocated memory** with automatic migrations
 - compile with -gpu=unified, nomanaged
 - Simply offloading loops to GPU using **OpenACC**, in 3 steps:
 - Horizontal (lateral) diffusion,
 - Advection,
 - Vertical diffusion and time-filtering,

for both "active" (TRA) and "passive" (TRC) tracer transport

NEMO Ocean Model

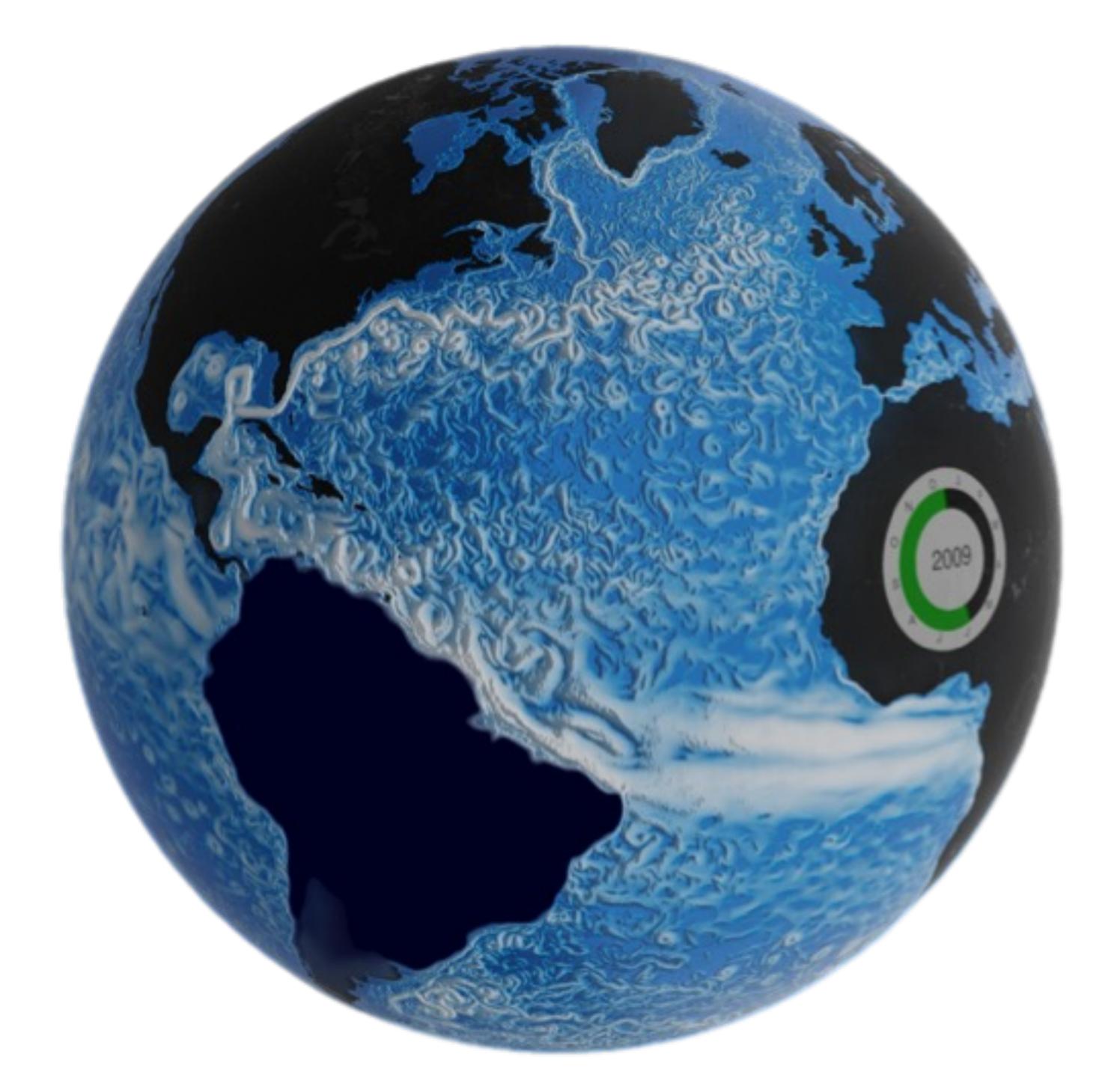
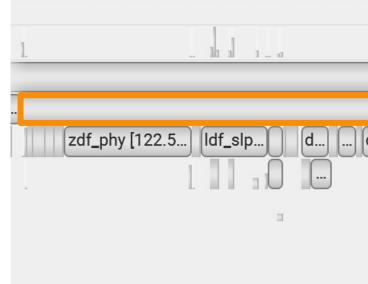




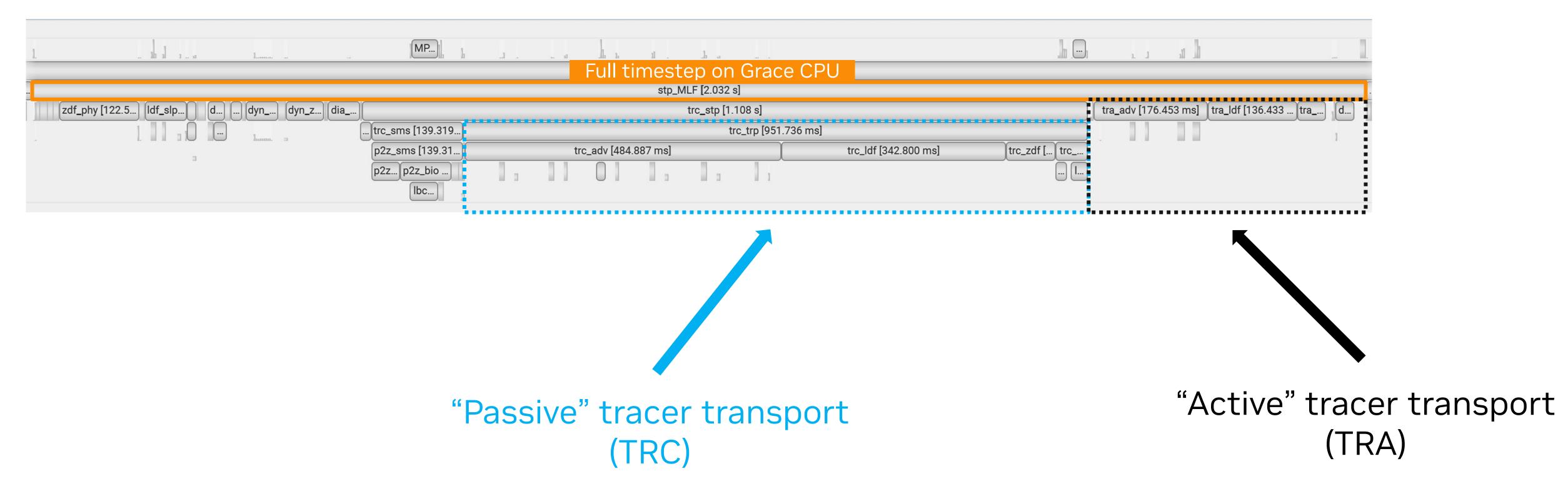
Image source: NEMO User Guide — NEMO release-4.2.2 documentation (nemo-ocean.io)



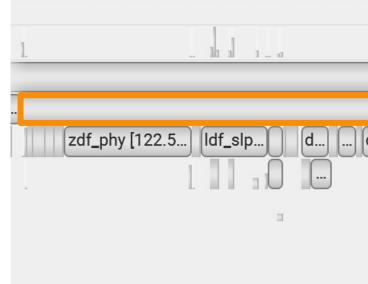


Lomo	MP	Full timestep on Grace	e CPU			
		stp_MLF [2.032 s]				
.) [dyn] [dyn_z] [dia]		trc_stp [1.108 s]			tra_adv [176.453 ms] tra_ldf [1	136.433 tra d
hann. 3	trc_sms [139.319	trc_trp [951.]	736 ms]			
	p2z_sms [139.31]	trc_adv [484.887 ms]	trc_ldf [342.800 ms]	trc_zdf [trc		
	p2z p2z_bio			[]		









Lomo	MP	Full timestep on Grace	e CPU			
		stp_MLF [2.032 s]				
.) [dyn] [dyn_z] [dia]		trc_stp [1.108 s]			tra_adv [176.453 ms] tra_ldf [1	136.433 tra d
hann. 3	trc_sms [139.319	trc_trp [951.]	736 ms]			
	p2z_sms [139.31]	trc_adv [484.887 ms]	trc_ldf [342.800 ms]	trc_zdf [trc		
	p2z p2z_bio			[]		





Ported to GPU: Horizontal diffusion

We run multiple (i.e. 40) MPI processes on **CPU** and GPU using MPS, and use **"migratable"** system allocated memory

	1 1			
trc_zdf [trc		I53 ms] tra_ldf [1	136.433 tra d	
			1.9x	1.3x
ene en		 		
zdf [6 trc	tra_adv [162.74	18 ms] tra_ldf traldf_is traldf_is	so_t	1.65x



1	
 zdf_phy [122	2.5 Idf_slp d
2.	
zdf_phy [88	3.2 Idf_slp [69 d
zdf_phy [91.718 ms] [ldf_slp [68.48

Ported to GPU: Horizontal diffusion

Advection

We run multiple (i.e. 40) MPI processes on **CPU** and GPU using MPS, and use **"migratable"** system allocated memory



tra_adv [176.453 ms] tra_ldf [136.433 tra d	
1.9x	1.3x
tra_adv [162.748 ms] tra_ldf [72 tra_zdf [_zdf [6 trc] traldf_iso_t	1.65x
2.5x	
	1.92x

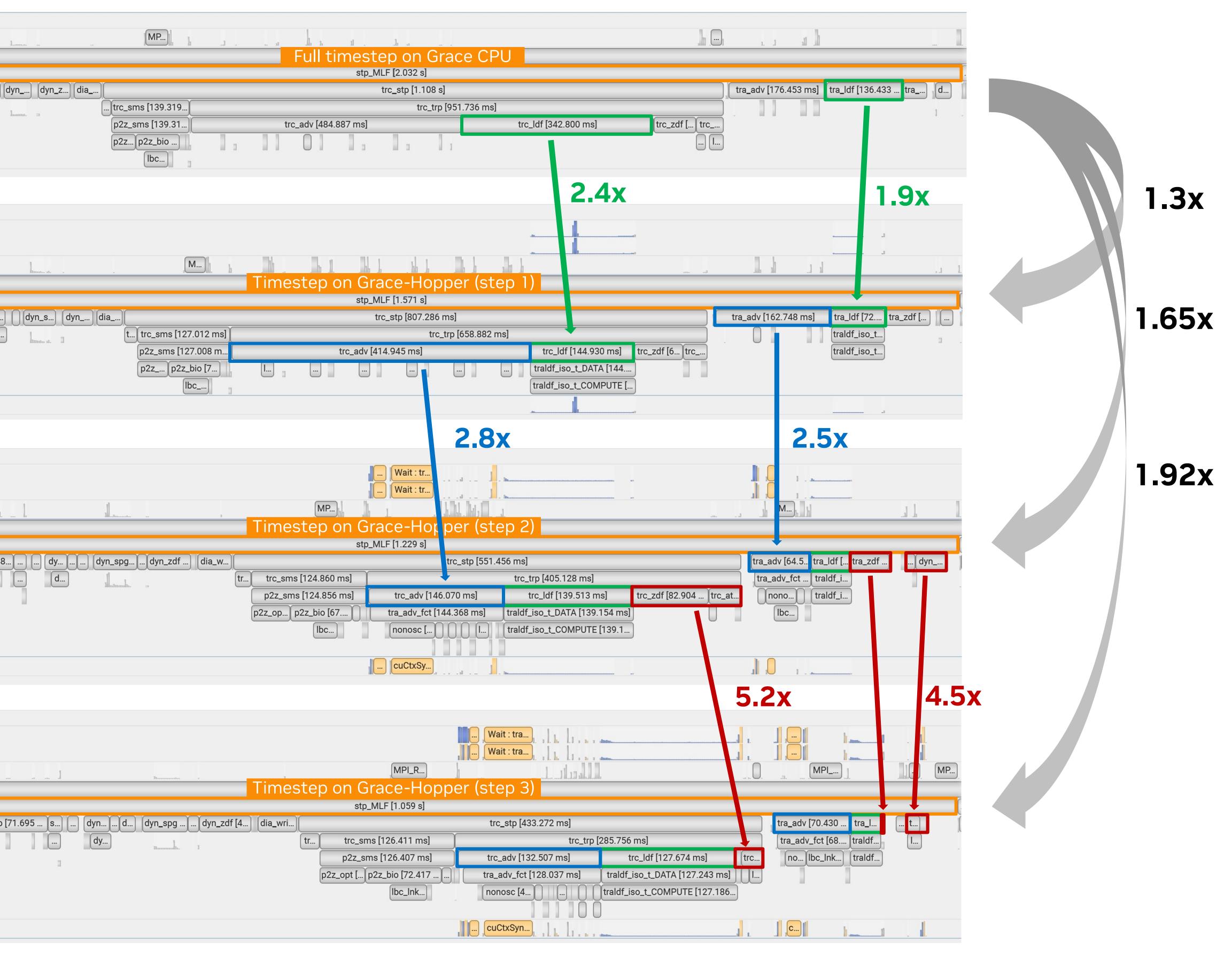


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		1		1	Ŀ
	18 m	 s]) (df_s	Ip [68	3.4
)zdf_phy [9:	3.052	? ms]		ldf_	slt

Ported to GPU:

- Horizontal diffusion
- Advection
- Vertical diffusion and time-filtering

We run multiple (i.e. 40) MPI processes on **CPU and GPU** using **MPS**, and use **"migratable"** system allocated memory

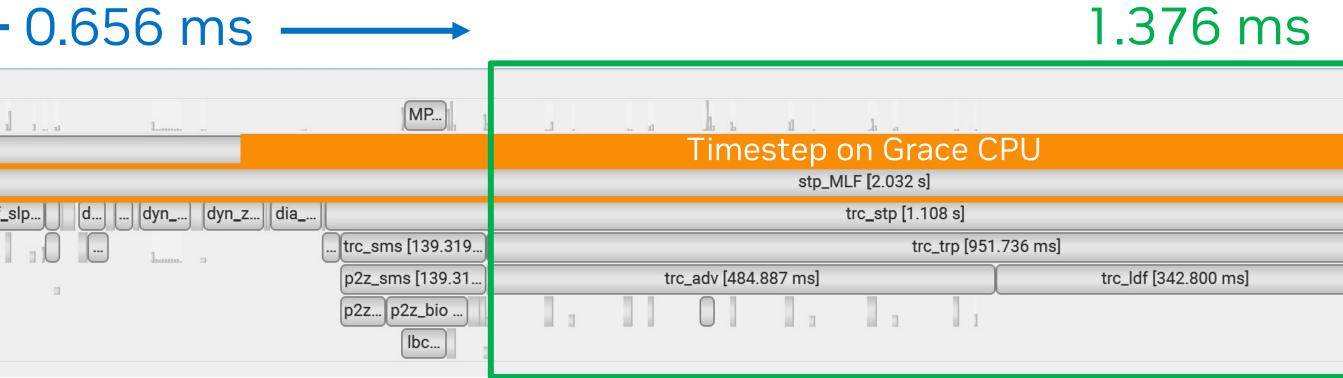




Porting NEMO to Grace-Hopper using Unified Memory A deeper look into the effect of access-counter based migrations on the partially accelerated port

10 1 1 zdf_phy [122.5...] ldf_slp...] d...] dyn_...] dyn_z...] dia_...]

CPU only run

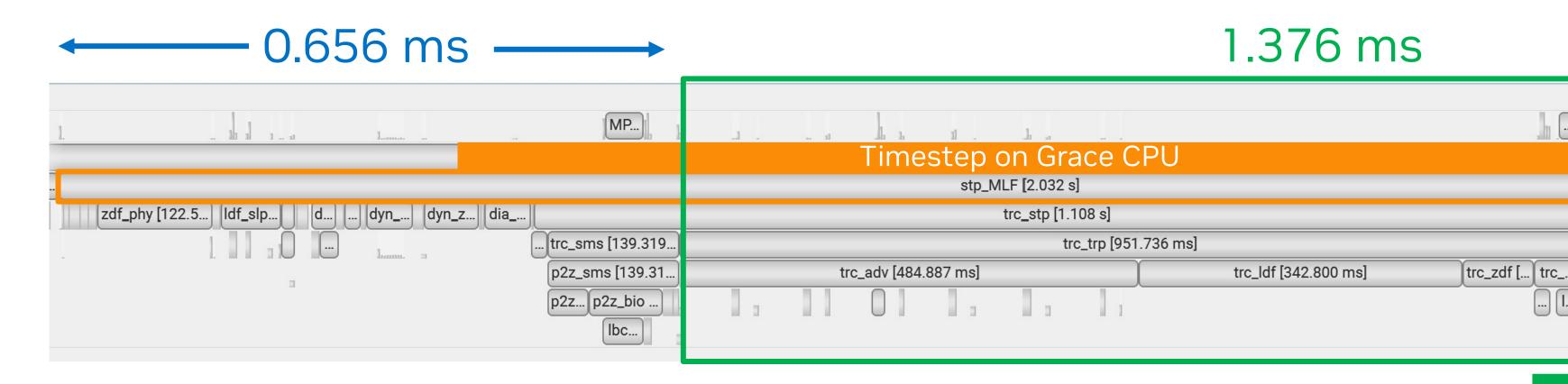


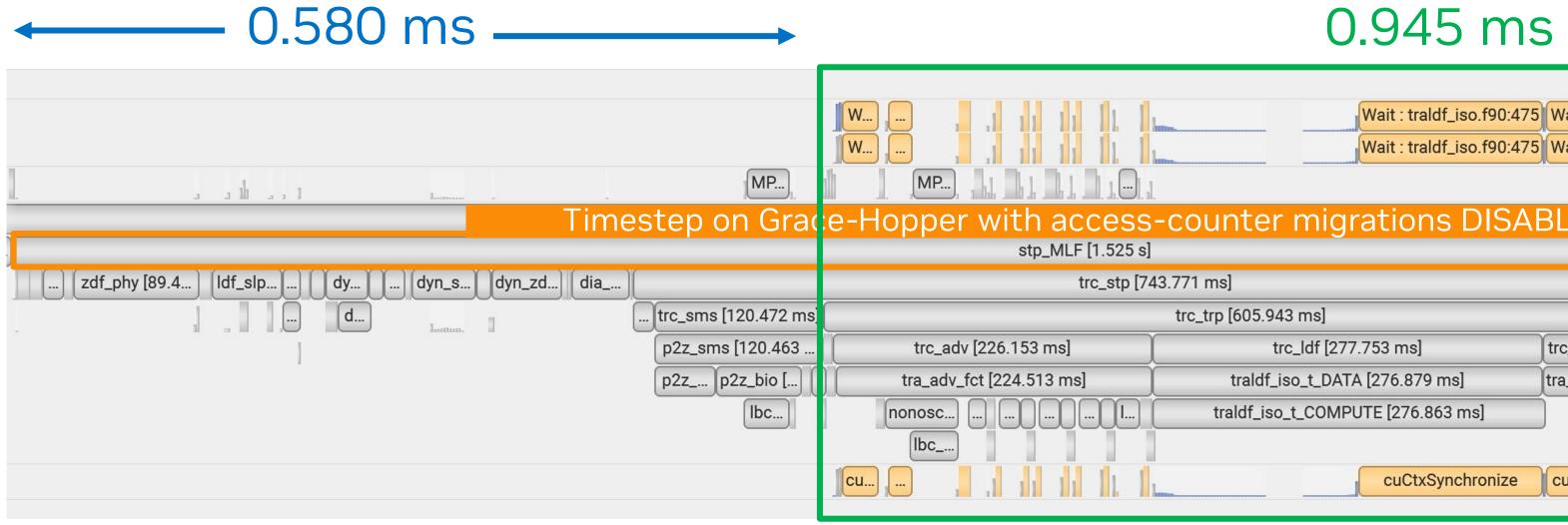
	1.]	1 J		
trc_zdf [trc	tra_adv [176.4	453 ms] tr	a_ldf [136.433	tra d



Porting NEMO to Grace-Hopper using Unified Memory A deeper look into the effect of access-counter based migrations on the partially accelerated port

CPU only run





Tracer transport on GPU with migrations disabled

(buffers with first-touch on CPU will never migrate to GPU memory)



1.46x GPU kernels pull data first-touched by CPU directly from **CPU memory**

/ait : tr	Wa	Wait : traldf Wait : traldf	Wa	Wait : Wait
	alle a she	3		<u> </u>
LED				6
				ŀ
	tra_adv [96.436	tra_ldf [114.705 ms]	tra	dyn_at
	tra_adv_fct [9	traldf_iso_t_DATA []	tra	
c_zdf trc_a	n	traldf_iso_t_COMP		
a_zdf I I				
u Otu O		au ChuChur a h		
uCtxS	Cu	cuCtxSynch	cu	cuCt

LL L.

11 11

tra_adv [176.453 ms] tra_ldf [136.433 ... tra_... d...

1.44x



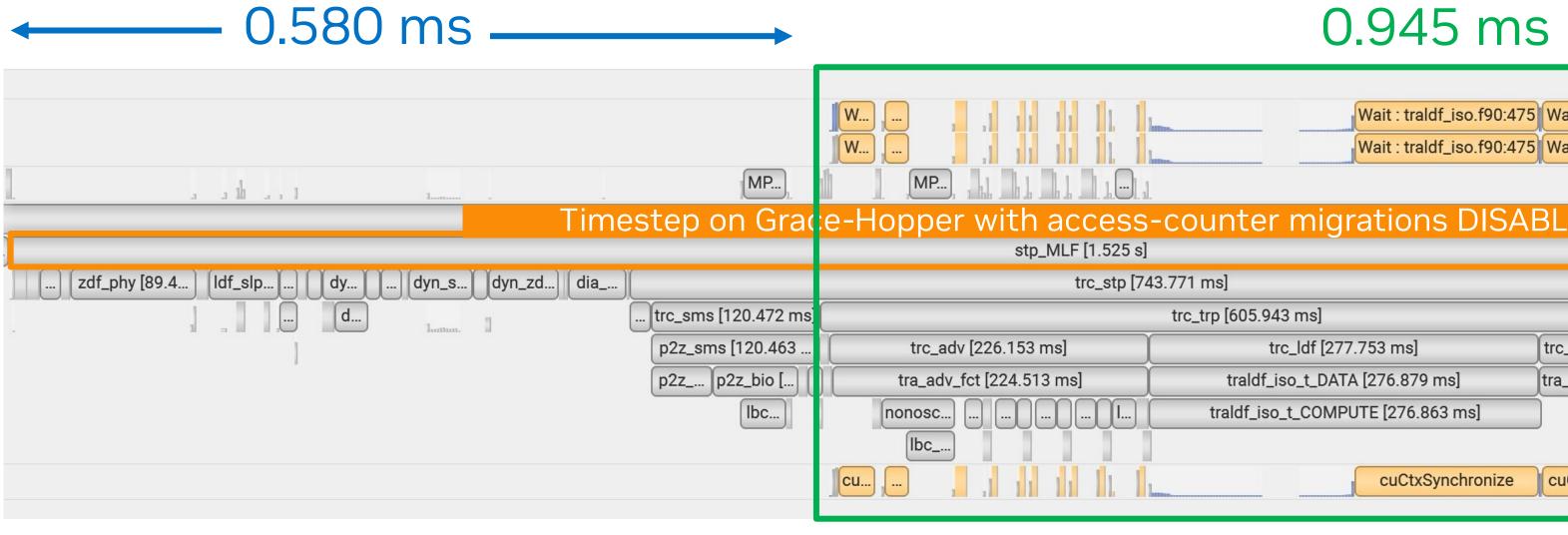
Porting NEMO to Grace-Hopper using Unified Memory A deeper look into the effect of access-counter based migrations on the partially accelerated port

CPU only run

Tracer transport on GPU with migrations disabled

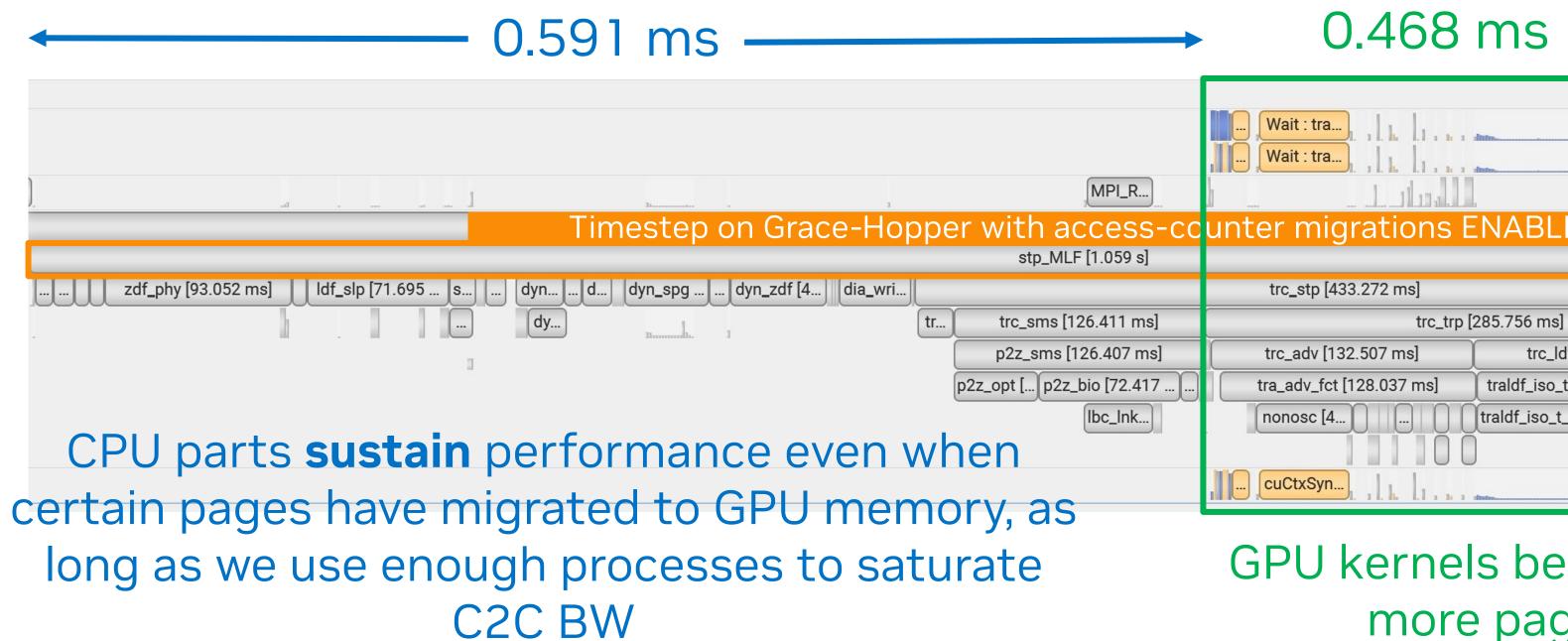
(buffers with first-touch on CPU will never migrate to GPU memory)

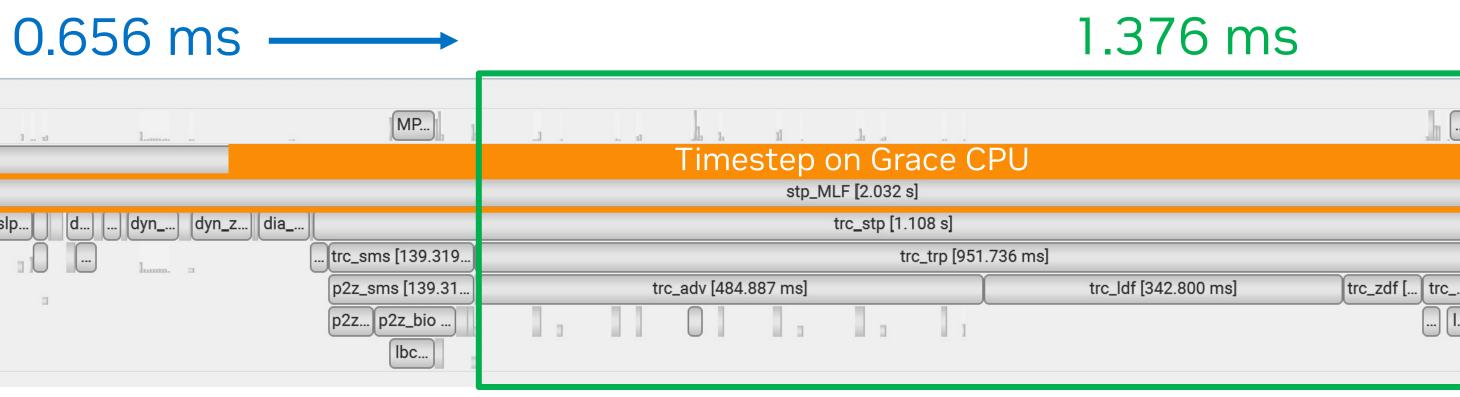
zdf_phy [122.5... | ldf_slp... | d... | dyn_... | dyn_z... | dia_..



Enabling automatic page migrations from CPU to GPU

("hot" pages migrate to GPU)







1.46x GPU kernels pull data first-touched by CPU directly from CPU memory

	Wa Wait : traldf Wa Wait : Wa Wait : traldf Wa Wait
_ED	
tra_adv [9 tra_adv_ c_zdf trc_a a_zdf l l	6.436 tra_ldf [114.705 ms] tra dyn_at fct [9 traldf_iso_t_DATA [tra traldf_iso_t_COMP
uCtxS	cu cuCtxSynch cu cuCt
2	.02x
FD	
s] df [127.674 ms] trc. _t_DATA [127.243 ms] I. t_COMPUTE [127.186	tra_adv [70.430 tra_l tra_adv_fct [68 traldf I no lbc_lnk traldf I

LL L.

tra_adv [176.453 ms] tra_ldf [136.433 ... tra_... d...

GPU kernels become faster as more and more pages migrate to GPU

C...

1.44x



Use-cases: Petrobras SolverBR

(Presented at GTC24 - S62529)





SolverBR



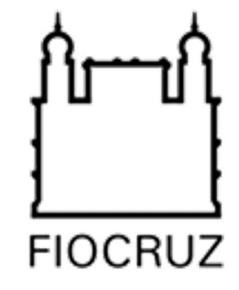










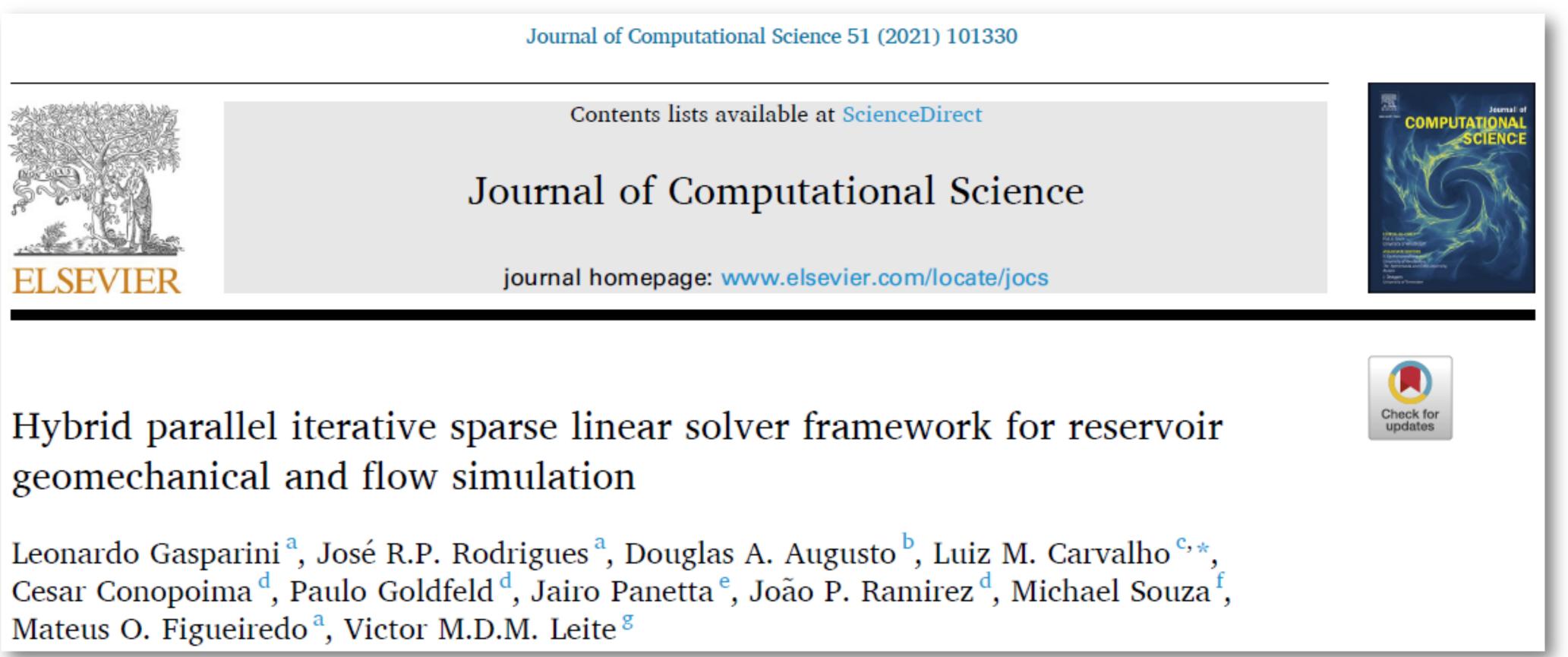






• The SolverBR is a high-performance CPU sparse linear solver specialized for reservoir simulation applications developed in collaboration with academic institutions.

• It combines excellence in parallel computing with the most advanced algorithms of sparse linear algebra for flow and geomechanics problems.





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Porting to Arm

- Build systems adjustments
 - Added a new compile target for aarch64 architecture
 - Mapped compatible compile variables
 - Initially used gcc for a "fair" and easier comparison
- Code porting adjustment
 - Removed Intel Intrinsics
 - Evaluated the usage of SIMDe and SSE2NEON libraries as replacement
 - Addressed synchronization issues that led to precision errors in floating-point calculation
 - Follow best practices

35	ALWAYS_INLINE void
36	{
37	<pre>#ifdefaarch64</pre>
38	OPENMP (omp flu:
39	OPENMP (omp ato
40	#endif
41	taskFinished[tas
42	3

14	ALWAYS INLINE void
15	const int * parer
16	{
17	for (int tIdx =
18	{
19	<pre>#ifdefaarch64</pre>
20	const int t =
21	int finished;
22	do
23	
24	OPENMP (on
25	OPENMP (on
26	finished =
27	<pre>} while (fini</pre>
28	#else
29	const int t =
30	while (taskFi
31	#endif
32	}
33	}



```
#ifndef __aarch64_
#include <xmmintrin.h>
#else
#include <utils/simd/sse2neon.h>
#endif
```

P2PNotify(const int task, volatile int * taskFinished)

```
nic write)
```

```
sk] = 1;
```

```
P2PWait( const int threadTask, const int * parentIndex,
nts, const volatile int * taskFinished )
```

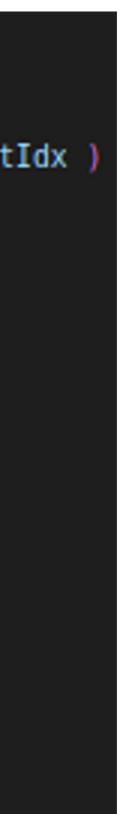
parentIndex[threadTask]; tIdx < parentIndex[threadTask + 1]; ++tIdx]</pre>

```
parents[ tIdx ];
```

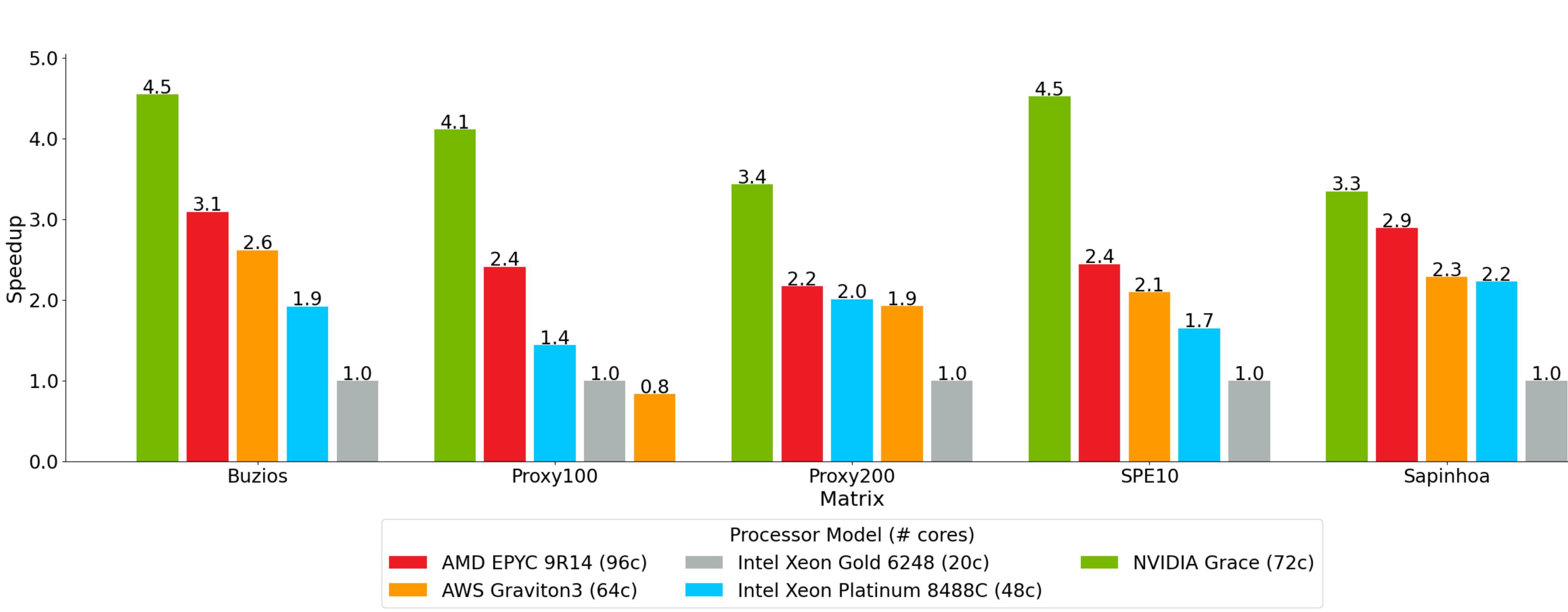
```
p flush)
p atomic read)
taskFinished[ t ];
ished == 0);
```

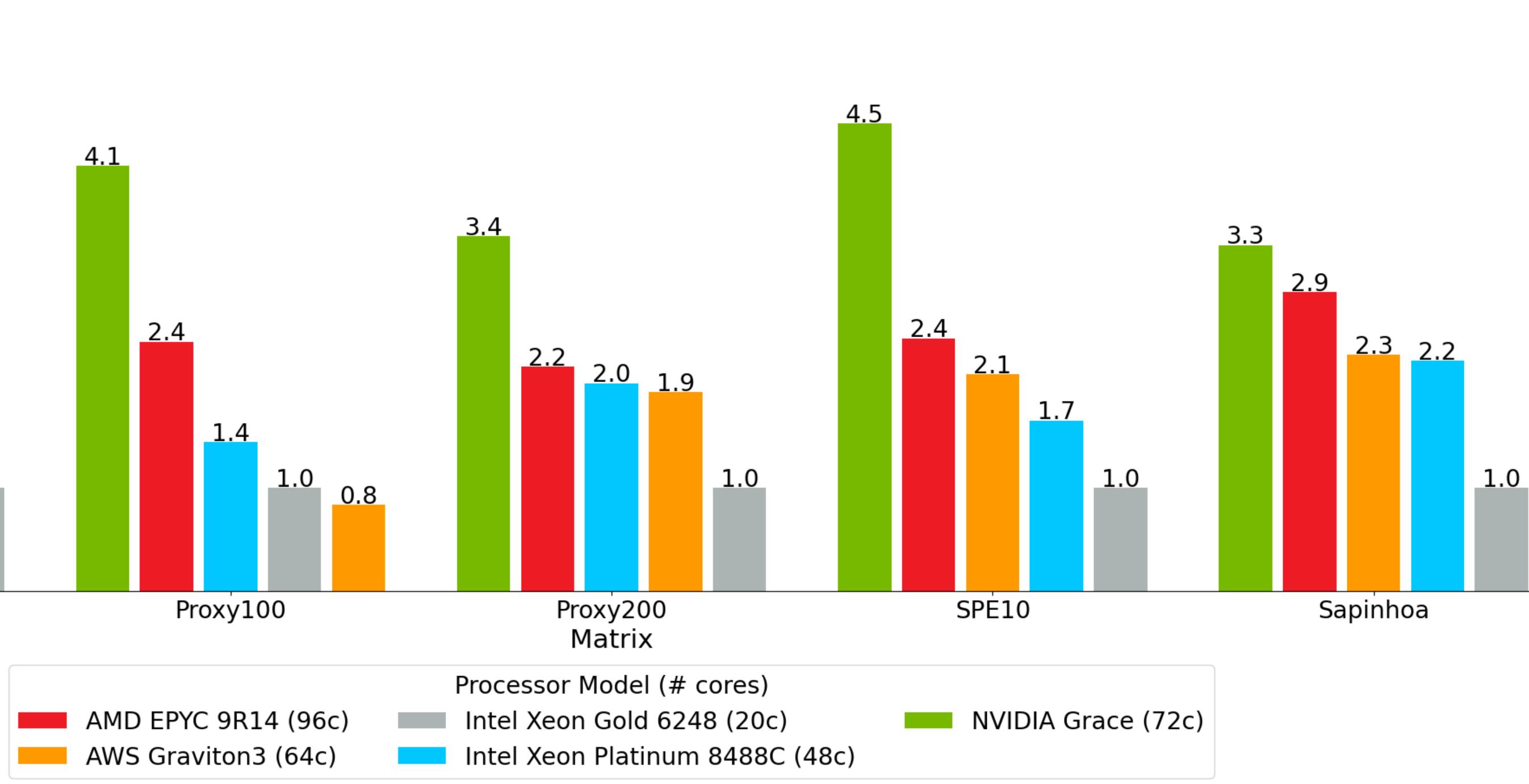
```
parents[ tIdx ];
inished[ t ] == 0 ) PAUSE;
```





Single-socket Speedups (max core-count)





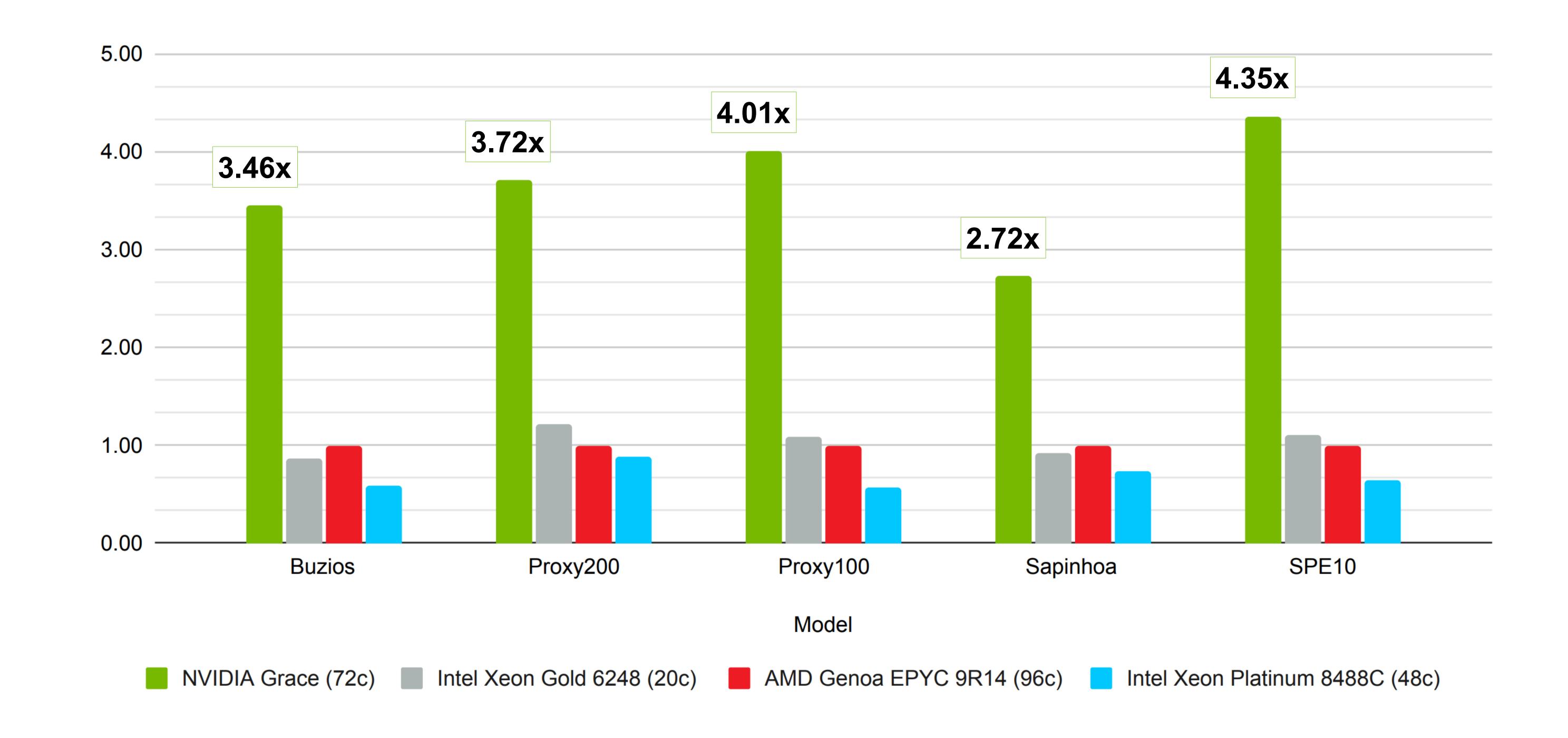
Average of 150 executions per matrix (considering 3 different timesteps)







Estimated Energy Efficiency at max load



Estimated are computed considering CPU max TDP at full load plus estimated memory consumption based on capacity and technology. We assume an average of 3W per 8 GB for DDR4 and 4.75W per 16 GB for DDR5. For Grace SoC, CPU plus memory is ~250W. Speed-ups are computed using AMD EPYC 9R14 as baseline.





To conclude...



E4 and NVIDIA Partnership Relentless pursue of innovation and added value

- Remote access to GH200 and Grace Superchip • CHIRON LAB: <u>https://www.e4company.com/en/chiron-lab/</u>
- Systems from various OEM/ODM
 - Ability to run comparison across architectures
 - Ability to measure server power consumption
- E4 long-standing experience in Arm-based systems
- E4 expertise in system configuration and bring-up
- NVIDIA expertise in GPU application tuning

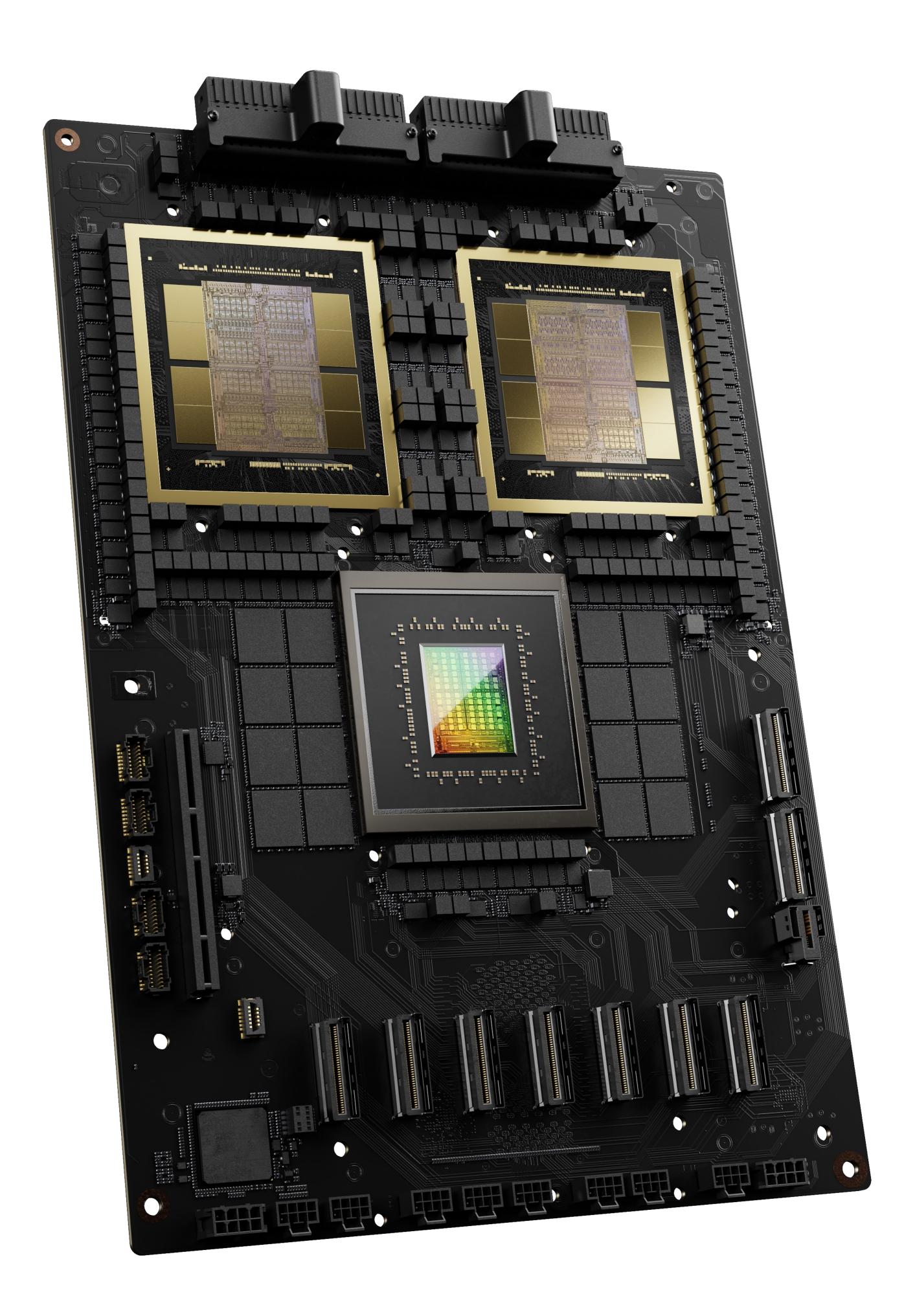
<u>Contact</u>: Marco Cicala (<u>marco.cicala@e4company.com</u>)





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5th GENERATION NVLINK Scales to 576 GPUs



SECURE AI Full Performance Encryption & TEE



DECOMPRESSION ENGINE 800 GB/sec







Further Resources for Grace CPU and Grace Hopper

Grace CPU Superchip

- Grace CPU Customer Deck
- Grace CPU Superchip Architecture Whitepaper
- Grace CPU Architecture In-Depth Blog
- Grace CPU Superchip Data Sheet
- Grace CPU Energy Efficiency Blog
- <u>A Demonstration of AI and HPC Applications for NVIDIA Grace CPU [S51880]</u>
- Grace CPU Power Efficiency Video
- Unlock the Power of NVIDIA Grace and Hopper with Foundational HPC Software

GH200 Grace Hopper Superchip

- GH200 Grace Hopper Customer Deck
- <u>Grace Hopper Superchip Architecture Whitepaper</u>
- <u>Grace Hopper Architecture In-Depth Blog</u>
- Grace Hopper Superchip Architecture Data Sheet
- Grace Hopper Recommender System Blog
- Programming Model and Applications for the Grace Hopper Superchip [S51120]
- Accelerating HPC applications with ISO C++ on Grace Hopper [S51054]
- Deploying RAG Applications on NVIDIA GH200

