JUWELS BOOSTER – EARLY USER EXPERIENCES
PERMAVOST WORKSHOP

25 June 2021 | Andreas Herten | Jülich Supercomputing Centre, Forschungszentrum Jülich

JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

Overview

Jülich Supercomputing Centre

Forschungszentrum Jülich Germany, near Cologne, interdisciplinary research, 6400 employees

Jülich Supercomputing Centre

- Operation of supercomputers
- Education, training
- Application Support, Domain Science Support
- Research & Development

Accelerating Devices Lab Support, research, education for GPUs et al.; NVIDIA Application Lab at Jülich

Supercomputers

Production JUWELS, JURECA DC, JUSUF

Prototypes JUMAX, DEEP, …

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JUWELS Booster System

JUWELS Overall Architecture

JUWELS Cluster (2018)

- 2511 compute nodes (2× Skylake)
- 48 GPU nodes (4× V100 w/ NVLink2)
- Mellanox EDR 100 Gbit/s network, fat-tree topology (1:2@L1)
- 12 PFLOP/s

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JUWELS Booster (2020)

- 936 compute nodes (2× AMD Rome, 4× A100 w/ NVLink3)
- Mellanox HDR 200 Gbit/s network, DragonFly+ topology
- 73 PFLOP/s

JUWELS Overall Architecture

JUWELS Cluster (2018)

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- 48 nk2)
- Me rk,
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Top500 Nov-2020:

- #1 Europe
- #7 World
- #1* Green500

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JUWELS Booster Overview

Node Configuration

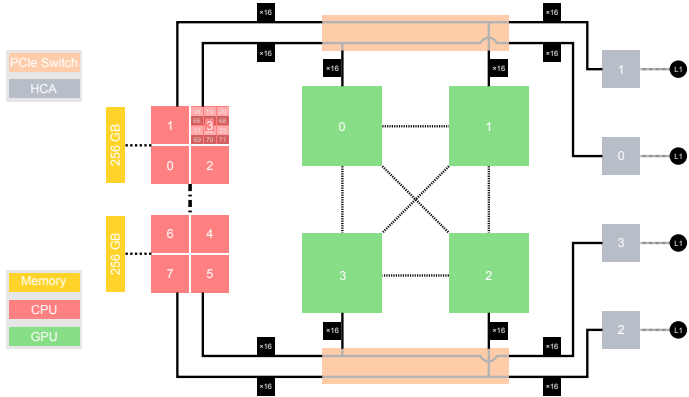
Arch Atos Bull Sequana XH2000

CPU 2 × AMD EPYC 7402:
$2_{\text{Socket}} \times 24_{\text{Core}} \times 2_{\text{SMT}}$,
2 × 256 GB DDR4-3200 RAM;
NPS-4

GPU 4 × NVIDIA A100 40 GB, NVLink3

HCA 4 × Mellanox HDR200
(200 Gbit/s) InfiniBand
ConnectX 6

etc 2 × PCIe Gen 4 switch



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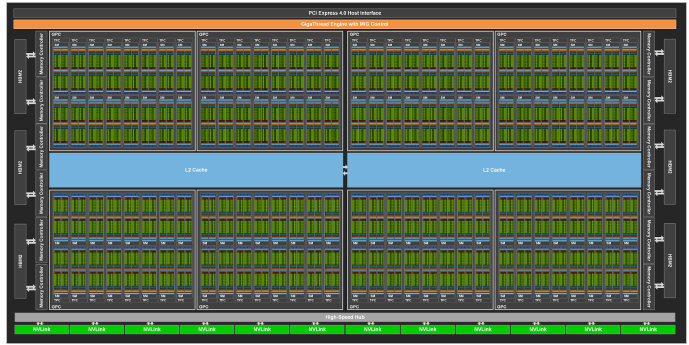
NVIDIA A100 Tensor Core GPU

- JUWELS Booster:
  3744 A100 GPUs
- Vs. V100: More SMs, larger/faster L1, larger/faster L2, faster memory, faster NVLink, faster PCIe, …
- New features: MIG, async copy to/barrier in shared mem



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- New Tensor Cores

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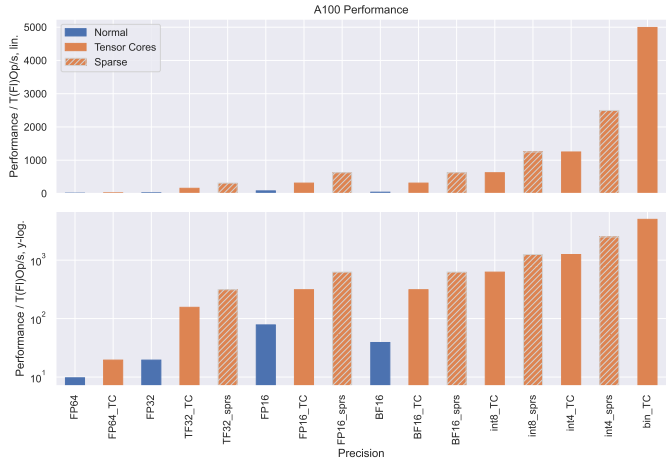
- New features: MIG, async copy to/barrier in shared mem
- New Tensor Cores, new performances:

  73 PFLOP/s_{FP64TC} 584 PFLOP/s_{FP32TC}
  1.16 EFLOP/s_{FP16TC} 18.7 EOP/s_{BinTC}



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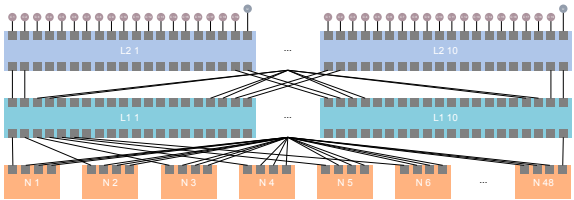
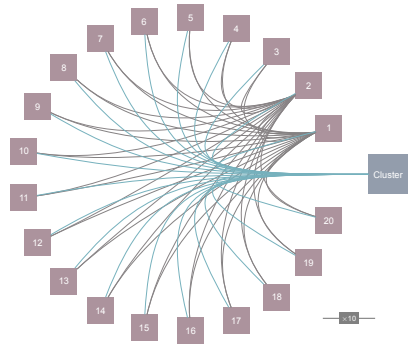
JUWELS Booster Overview

Network Configuration: DragonFly+ Network





In-Cell (48 nodes): Full fat-tree in 2 levels

Inter-Cell (20 cells): 10 links between each pair of cells

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JUWELS

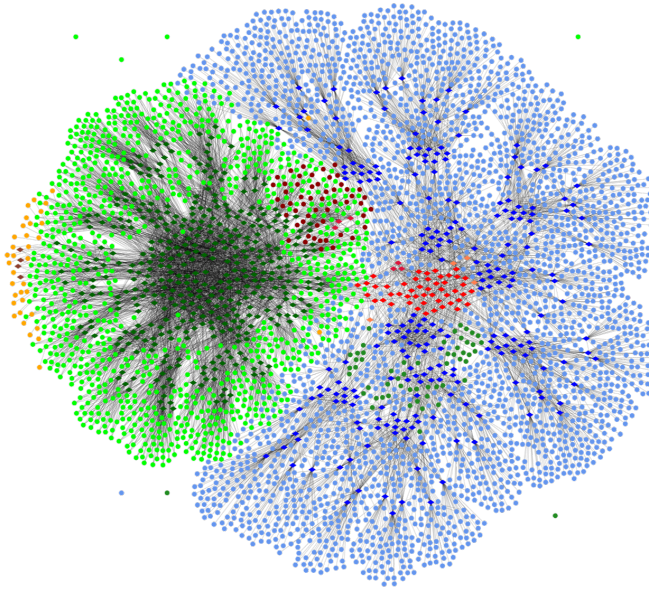
Cluster Booster Integration

Fully integrated system: **JUWELS** with Cluster and Booster modules

- File system: GPFS
- Network: InfiniBand
- Workload management: Slurm
- Resource management: ParaStation / ParaStation Slurm

Picture legend:

- Cluster CPU node
- Cluster GPU node
- Cluster switch
- Cluster gateway
- Top-level switch
- Booster node
- Booster switch
- Booster gateway
- JUST
- Service node



Graphic provided by D. Alvarez

JUWELS Software Stack

- Software
  - Software management: EasyBuild, LMod
  - Compilers: GCC, Intel, NVHPC
  - GPU-aware MPIs (ParaStationMPI, OpenMPI; via UCX)

  → https://apps.fz-juelich.de/jsc/llview/juwels_modules_booster/
- Operation
  - Operation System: CentOS 8
  - Provisioning: Ansible

JUWELS Timeline

JUWELS Milestones

2018	JUWELS Cluster production start
2018 Jun	JUWELS Cluster Top500: #23
2019	JUWELS Booster kick-off
2020 Apr	JUWELS Booster installation start
2020 May	JUWELS Booster Early Access Program first job
2020 Nov	JUWELS Booster: production start, first compute-time period; Top500 #7
2021 May	JUWELS Booster second compute-time period

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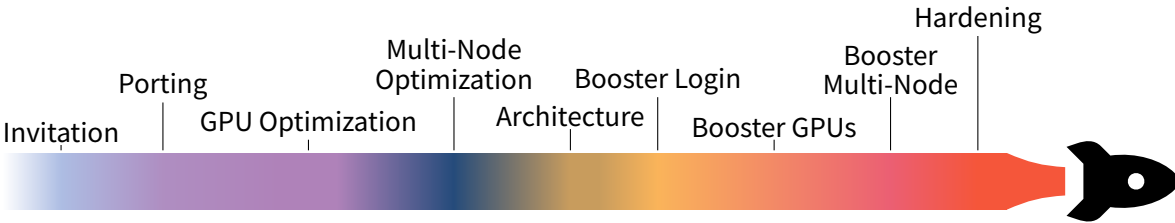
Early Access Program

- Key program for early science and early feedback
- Started in early 2020
- Invited 14 applications from various scientific domains
  - Aimed for applications that could use JUWELS Booster at scale
  - Some teams already use JUWELS Cluster, others new
- **Offer**: Use JUWELS Booster before general access; **Request**: Help improve system, compute-time allocation
- Endeavor of many parts in **JSC** and beyond
  - NVIDIA Application Lab: Steering, GPU optimization, application support, system support
  - Application support, Simulation Labs
  - Performance Optimisation and Productivity team
  - System operations team
  - Vendors: NVIDIA, ParTec, Atos

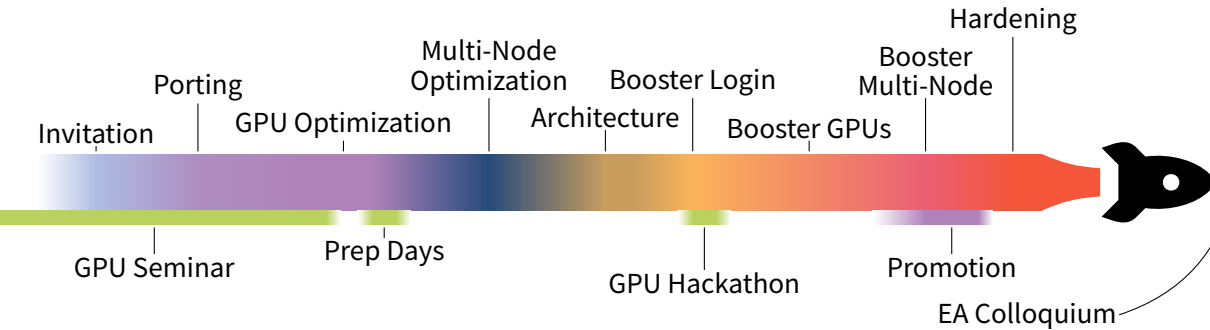
Timeline to Booster

- Preparation Timeline



Timeline to Booster

- Preparation Timeline
- Additionally: events



Applications I

Climate/Meteo/Hydro (*ESM*)

DeepACF High-resolution Weather Forecast Based on Deep Learning </> Lib:DL
JSC: Bing Gong, Michael Langguth, Amirpasha Mozaffari, Martin Schultz, Scarlet Stadtler

ICON Next-Generation Physical Weather and Climate Models </> OpenACC
MPI Met: Luis Kornblueh; NVIDIA: Dmitry Alexeev

MPTRAC Massive Parallel Trajectory Calculations of Volcanic Emissions </> OpenACC
JSC: Sabine Grießbach, Lars Hoffmann

ParFlow Surface, Soil, Ground Water Flow </> CUDA C
IBG-3: Jaro Hokkanen, Stefan Kollet

Biological Matter

Amber Drug Binding over Biologically Relevant Timescales (MD) </> Lib
JSC/HHU: Holger Gohlke, Christopher Pfleger, Michele Bonus

SOMA Kinetics of Nanomaterial Formation (Soft Matter) </> OpenACC
U Göttingen: Ludwig Schneider, Niklas Blagojevic

Applications II

PIConGPU Plasma Simulations for Next Generation Particle Accelerators (Plasma) </> CUDA C++
HZDR: Alexander Debus, Anton Lebedev, Rene Widera, Michael Bussmann

JUQCS-G Simulating Universal Quantum Computer (Quantum) </> CUDA Fortarn
JSC: Hans De Raedt, Kristel Michielsen, Dennis Willsch

E-train Understanding Learning Processes in Brain (Neuro) </> Lib:DL
U Graz: Franz Scherr, Wolfgang Maass; U Sussex: James Knight; INM-6: Sacha van Albada

NBODY6++GPU Dense Star Clusters and Gravitational Waves (Astro) </> CUDA Fortran
U Heidelberg: Rainer Spurzem

Lattice QCD

Bonn Flavour Singlet Structure of Hadrons </> Lib:QUDA
U Bonn: Simone Bacchio, Bartosz Kostrzewa, Carsten Urbach

Wuppertal SignQCD – Studying the Hottest Man-made Liquid </> Lib:QUDA
U Wuppertal: Szabolcs Borsányi, Kalman Szabo

Bielefeld HotQCD – Studying Extreme States of Matter </> CUDA C++
U Bielefeld: Christian Schmit, Dennis Bollweg, Frithjof Karsch

Regensburg Baryons with Charm </> Lib:Grid
Peter Boyle, Christoph Lehner, Gunnar Bali, Sara Collins

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→ Details on each app online

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Early Experiences

System-Related

Feedback during EA Program

Issues

- Performance fluctuations (GPU, node, network)
- OpenMPI segmentation violations
- NCCL hangs
- NVHPC Fortran compiler bugs
- UCX configuration (caches)
- PCIe switch bi-directional bandwidth
- PCIe device crashes
- I/O subsystem maturity

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Peculiarities

- Software versions
- AMD CPUs / NUMA domains
- PCIe switch
- GPU device affinity
- Network design (DragonFly+)

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AMD EPYC Rome

Some Processor Basics

- JUWELS Booster: AMD EPYC Rome 7402 (24 core (SMT-2) $\times$ 2 sockets)
- EPYC processor: Built as Multi-Chip Module
  $\rightarrow$ Many building blocks, hierarchies

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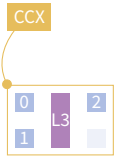

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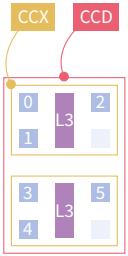

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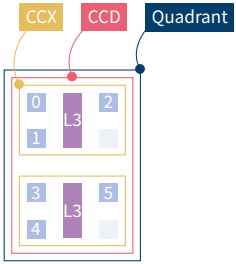

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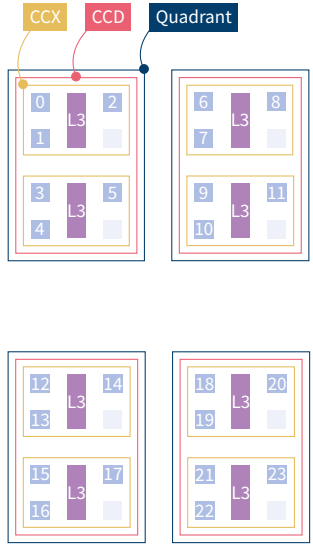

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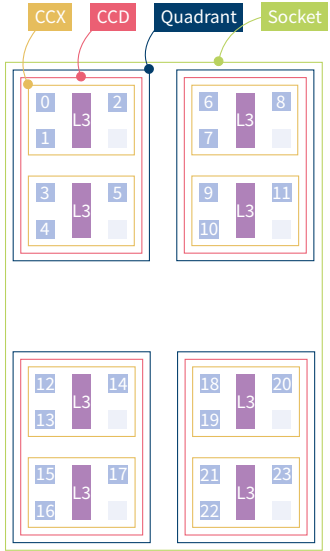

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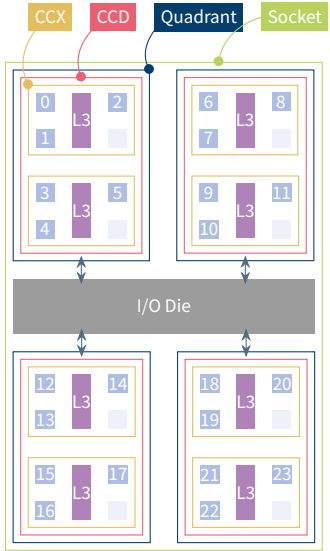

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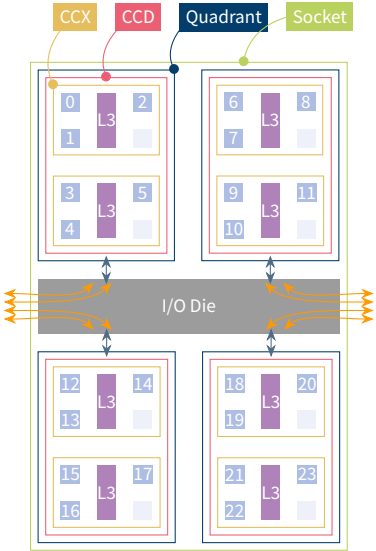
RAM	8 memory channels, 2 per quadrant



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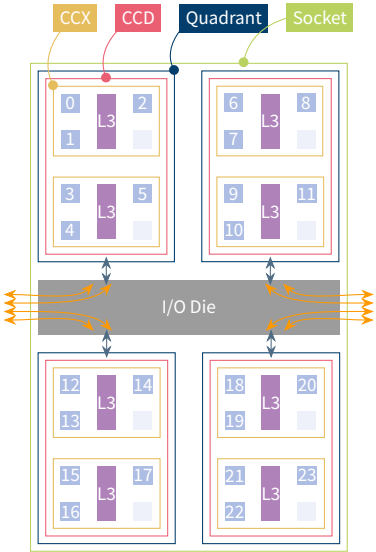
$\Rightarrow$ **Complex topology!**



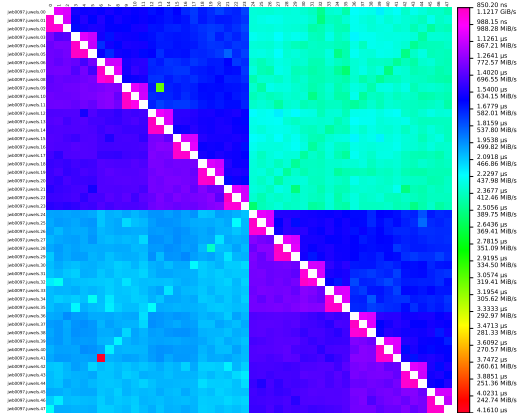
EYPC Core-to-Core

Linktest

- Test core-to-core connections with JSC's Linktest
- Linktest: MPI Ping Pong usually for large machines
- Here: Within a node
- EPYC structure clearly visible

⇒ Thread placement very important, especially for L3-using application
We saw 30 % performance increase by proper placement

- *Configuration: GCC, ParaStationMPI, serial*



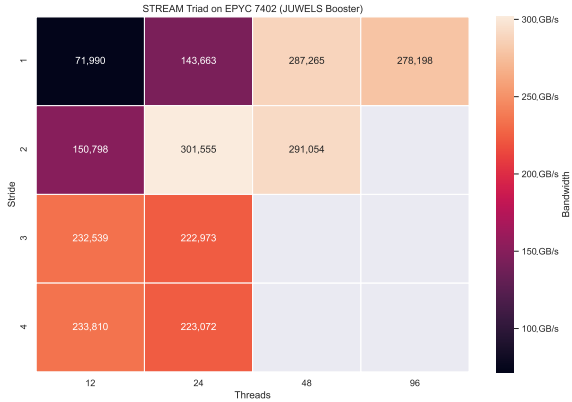
Graphic provided by M. Holicki

Memory

STREAM

- EPYC Rome: 8 memory channels, 2 per quadrant
- Thread placement important for memory performance
- STREAM benchmark! *all in Appendix*

⇒ Thread placement very important, also for memory-intensive application

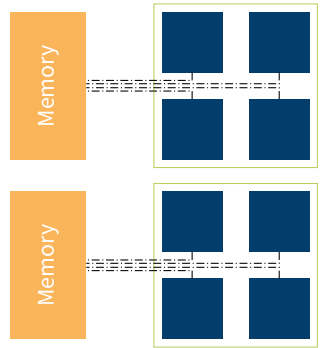


Stride: `OMP_PLACES={0}:24:2` → stride 2

STREAM config: AOCC 3.0.0, `-O3 -mcmodel=large -ffp-contract=fast -fnt-store`, array size: 2500000000, best of 200

PCIe Affinity

- PCIe via I/O die → also hierarchy
- GPUs connected via PCIe (through PCIe switch)



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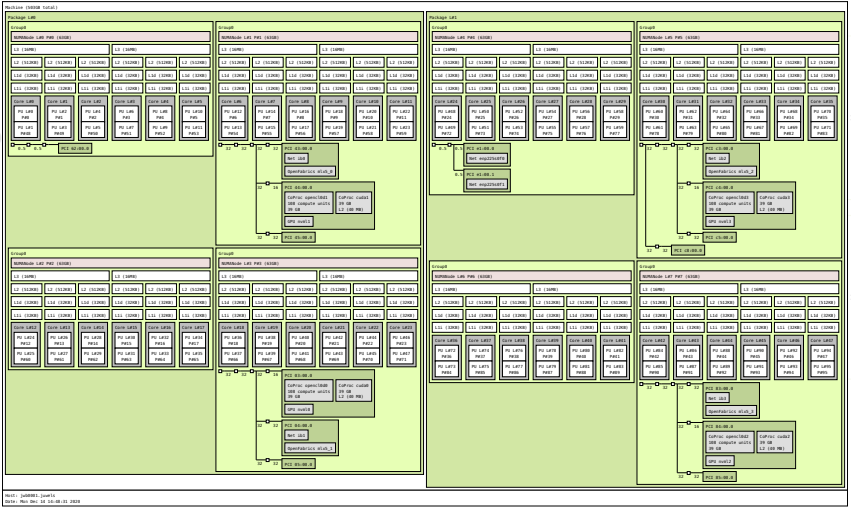

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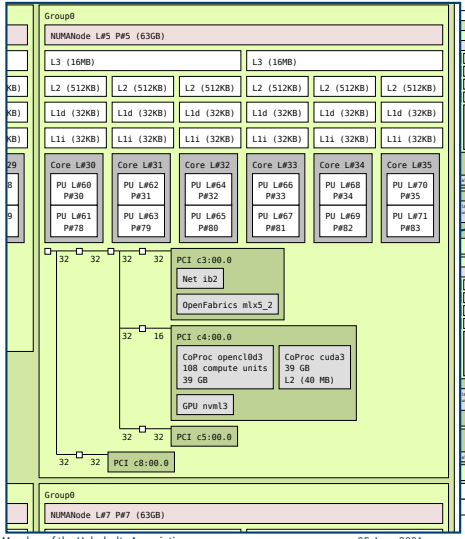
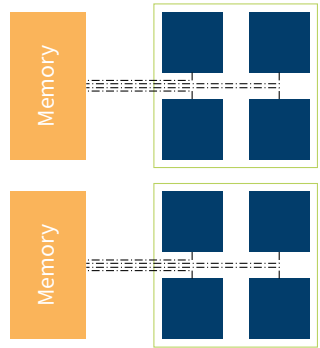


PCIe Affinity

- PCIe via I/O die $\rightarrow$ also hierarchy
- GPUs connected via PCIe (through PCIe switch)
- PCIe 4.0 lanes: 2×16, each 16 connected to 1 quadrant



PCIe Affinity

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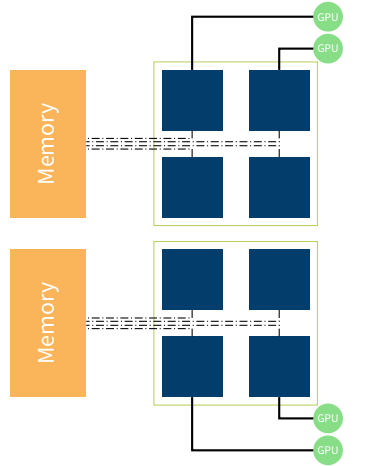
$\rightarrow$ *True* GPU affinity only by half of chiplets

But impact application-dependent and possibly quite low



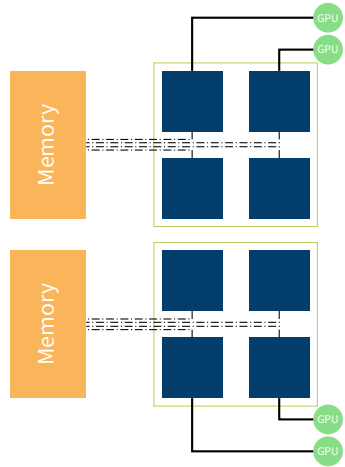
PCIe Affinity

- PCIe via I/O die → also hierarchy
- GPUs connected via PCIe (through PCIe switch)
- PCIe 4.0 lanes: 2 × 16, each 16 connected to 1 quadrant

→ *True* GPU affinity only by half of chiplets

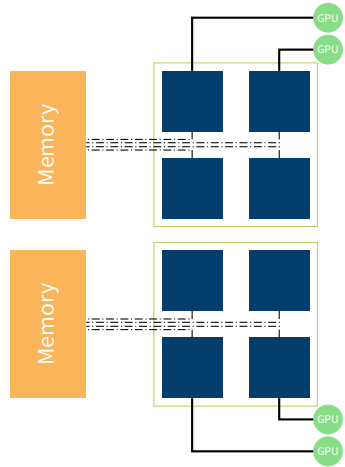
But impact application-dependent and possibly quite low

- InfiniBand HCA adapters also via PCIe switch
  - Same affinity considerations
  - 1:1 relation between HCA and GPU



NUMA Numbering

- NUMA domains (= quadrants) are numbered
- Not all domains have GPU/HCA affinity
- Guess numbers of domains with affinity!



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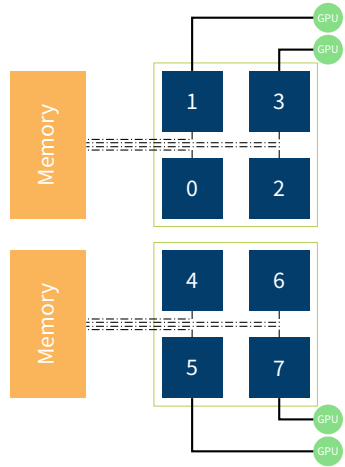

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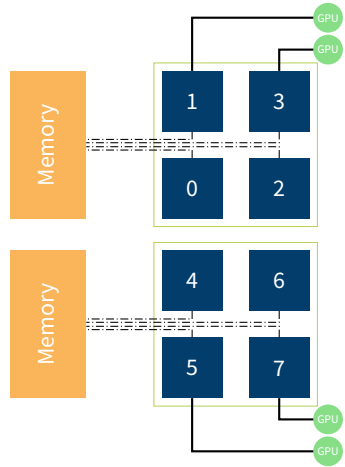

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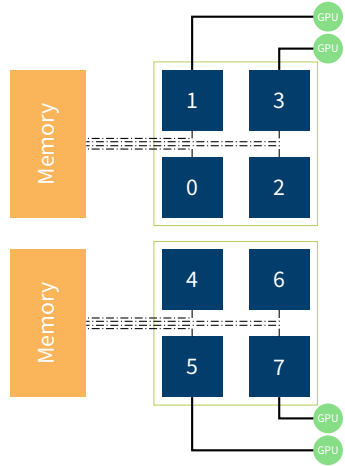

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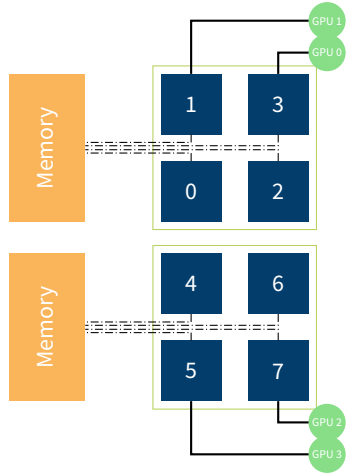

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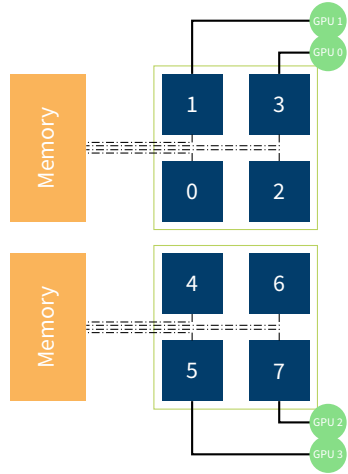
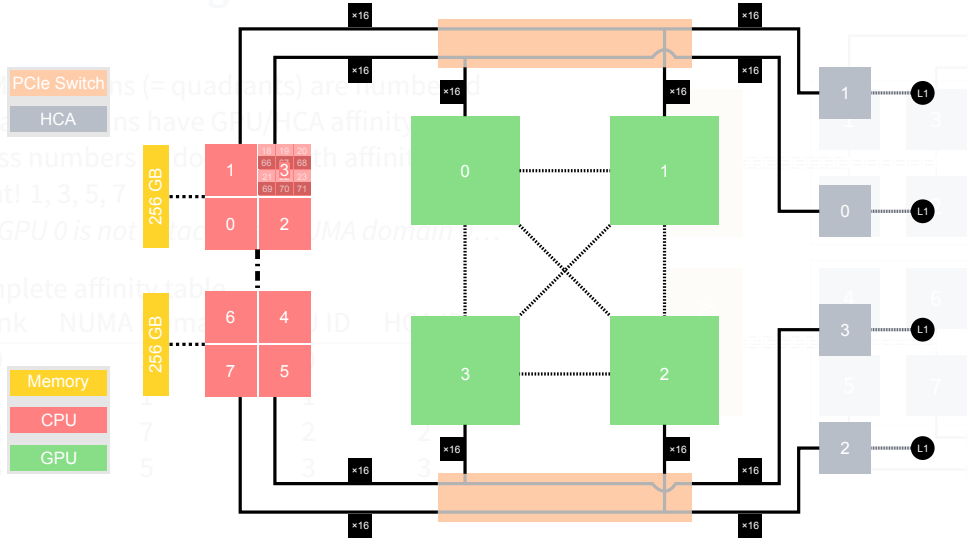
- Complete affinity table

Rank	NUMA Domain	GPU ID	HCA ID
0	3	0	0
1	1	1	1
2	7	2	2
3	5	3	3




PCIe Switch
HCA
Memory
CPU
GPU
256 GB
256 GB
×16
1
0
2
6
4
7
5
0
1
3
2
L3
18 19 20
66 67 68
21 22 23
69 70 71
1
0
3
2
L1
L1
L1
L1

Affinity

- Changes to environment/Slurm to match node topology
- Recipe: GPU first, CPU second

Affinity

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- Example Slurm task distribution for 5 tasks, each 1 core:

  Task 1 First core of NUMA domain 3
  Task 2 First core of NUMA domain 1
  Task 3 First core of NUMA domain 7
  Task 4 First core of NUMA domain 5
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- Fill up NUMA domain with `--cpus-per-task N`

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Affinity

CPU Affinity Mask I

- *PS*Slurm sets CPU affinity masks with *GPU first*

Affinity

CPU Affinity Mask I

- *PS*Slurm sets CPU affinity masks with *GPU first*
- CPU mask example for 5 tasks, each 1 core:

```
$ srun --cpu-bind=verbose -n 5 bash -c "" |& sort
cpu_bind=THREADS - jwb0001, task  0  0 [18049]: mask 0x40000 set
cpu_bind=THREADS - jwb0001, task  1  1 [18050]: mask 0x40 set
cpu_bind=THREADS - jwb0001, task  2  2 [18055]: mask 0x40000000000 set
cpu_bind=THREADS - jwb0001, task  3  3 [18059]: mask 0x40000000 set
cpu_bind=THREADS - jwb0001, task  4  4 [18061]: mask 0x1000 set
```

Affinity

CPU Affinity Mask I

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cpu_bind=THREADS - jwb0001, task  3  3 [18059]: mask 0x40000000 set
cpu_bind=THREADS - jwb0001, task  4  4 [18061]: mask 0x1000 set
```

- Visualize masks in binary representation *(SMT-2 omitted)*

hex2bin

```
000000 000000 000000 100000 000000 000000 000000 000000  # 0x40000, GPU 0
000000 100000 000000 000000 000000 000000 000000 000000  # 0x40, GPU 1
000000 000000 000000 000000 000000 000000 000000 100000  # 0x40000000000, GPU 2
000000 000000 000000 000000 000000 100000 000000 000000  # 0x40000000, GPU 3
000000 000000 100000 000000 000000 000000 000000 000000  # 0x1000, no GPU
```

Affinity

CPU Affinity Mask II

- *PS*Slurm sets CPU affinity masks with *GPU first*
- CPU mask example for 2 tasks, each 2 cores:

```
$ srun --cpu-bind=verbose -n 2 --cpus-per-task 2 bash -c "" |& sort
cpu_bind=THREADS - jwb0001, task  0  0 [18402]: mask 0xc0000 set
cpu_bind=THREADS - jwb0001, task  1  1 [18403]: mask 0xc0 set
```

hex2bin

```
000000 000000 000000 110000 000000 000000 000000 000000  # 0xc0000, GPU 0
000000 110000 000000 000000 000000 000000 000000 000000  # 0xc0, GPU 1
```

Affinity

GPU Affinity

- *PS*Slurm sets `$CUDA_VISIBLE_DEVICES` to associated GPU

Affinity

GPU Affinity

- *PS*Slurm sets `$CUDA_VISIBLE_DEVICES` to associated GPU
- GPU affinity for 2 tasks:

```
$ srun -n 2 --cpu-bind=verbose env | grep 'PMI_RANK\|CUDA_VIS'
cpu_bind=THREADS - jwb0001, task  0  0 [18307]: mask 0x40000 set
cpu_bind=THREADS - jwb0001, task  1  1 [18309]: mask 0x40 set
PMI_RANK=0
CUDA_VISIBLE_DEVICES=0
PMI_RANK=1
CUDA_VISIBLE_DEVICES=1
```

Affinity

GPU Affinity

- *PS*Slurm sets `$CUDA_VISIBLE_DEVICES` to associated GPU
- GPU affinity for 2 tasks:

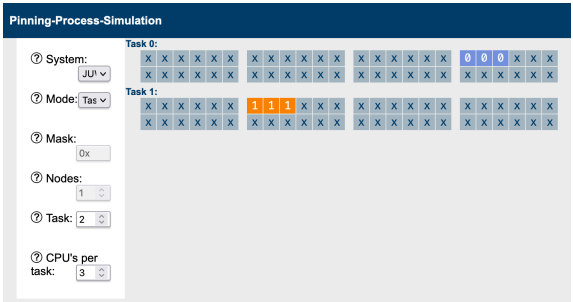
```
$ srun -n 2 --cpu-bind=verbose env | grep 'PMI_RANK\|CUDA_VIS'
cpu_bind=THREADS - jwb0001, task  0  0 [18307]: mask 0x40000 set
cpu_bind=THREADS - jwb0001, task  1  1 [18309]: mask 0x40 set
PMI_RANK=0
CUDA_VISIBLE_DEVICES=0
PMI_RANK=1
CUDA_VISIBLE_DEVICES=1
```

- Special case: GPU affinity for exactly 1 task:

```
$ srun -n 1 env | grep 'PMI_RANK\|CUDA_VIS'
PMI_RANK=0
CUDA_VISIBLE_DEVICES=0,1,2,3
```

Handling Affinity Handling

- Node affinity now more important than ever! *(maybe…)*
- JSC provides tools and documentation as first-level support!
- Mask generator
- CLI mask tool
- **Extensive system documentation**



apps.fz-juelich.de/jsc/llview/pinning/

DragonFly+ Topology

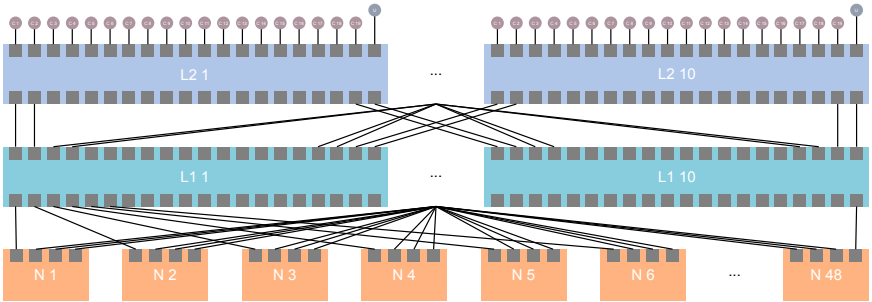
Overview

- 3744 end points; adaptive routing
- HDR200: 200 Gbit/s per link per direction
- Dragonfly+ Topology selected as good way to balance factors (space, investment, performance)
- Two-level topology: local (in-cell), non-local (inter-cell)
- Still learning practical implications of topology

DragonFly+ Topology

In-Cell Topology

- In-cell: full fat-tree in 2 levels
  - 48 nodes, each 4 links *(strided to 4 L1 switches)*
  - 10 L1 switches, 48 port *(each L1 switch: 2 links to L2, strided to 10 L2 switches)*
  - 10 L2 switches, 48 port *(each L2 switch: 1 link to L2 switch of all other cells, 1 link to cluster)*

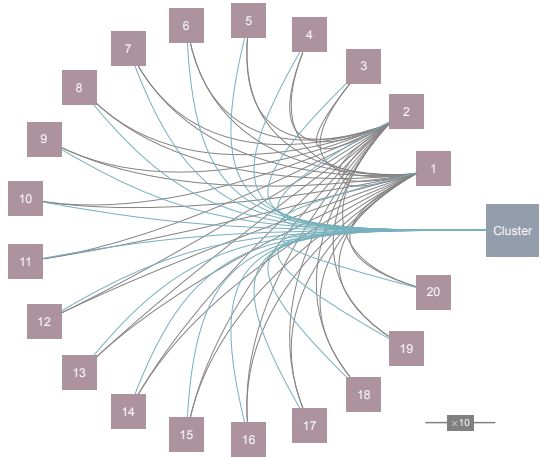


DragonFly+ Topology

Intra-Cell Topology

- Inter-cell: 20 cells
  - 10 links between each pair of cells
  - 10 links per cell to JUWELS Cluster
  - Filesystem access via cell 20
  - Bi-section bandwidth between N cells:

$$\mathcal{B}(N) = \lfloor (N/2)^2 \rfloor \times (10 \times \mathrm{bw}_1)$$

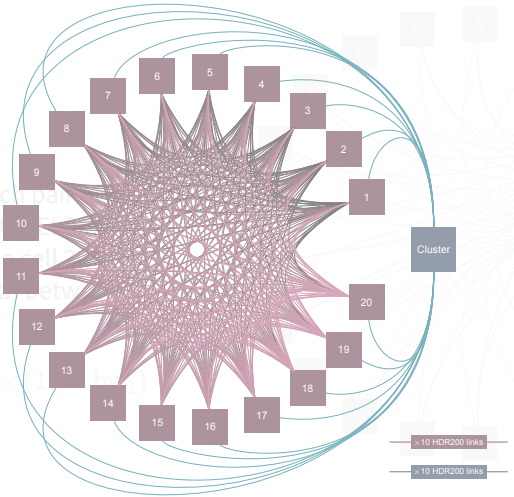


DragonFly+ Topology

Intra-Cell Topology

- Inter-cell: 20 cells
  - 10 links between each pa
  - 10 links per cell to J
  - Filesystem access via all
  - Bi-section bandwid
    cells:

$$B(N) = \lfloor (N/2)^2 \rfloor$$



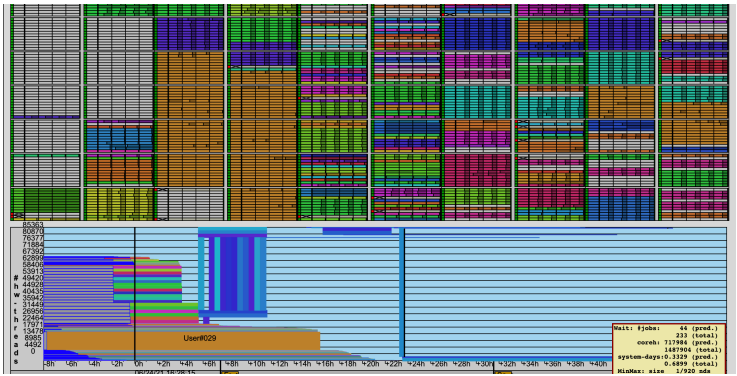
Interactive Job Reporting

LLview

- LLview: JSC's online tool for scheduler statistics
- Already around for some time, now extended with GPU-related info
- System overview (nodes, GPUs; timeline)

→ `llview.fz-juelich.de`

- JSC: Access via JuDoor



JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

Interactive Job Reporting

LLview

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- Job focus (many metrics)

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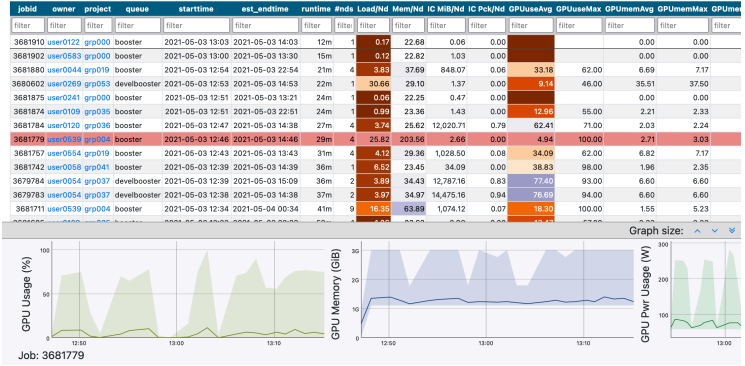

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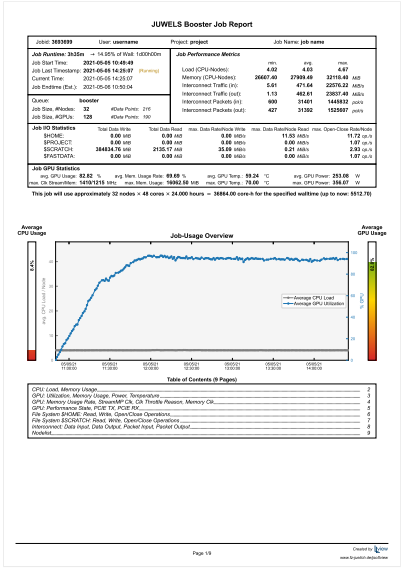
PDF Job Reports

From LLview

- **New:** Detailed PDF job reports
- Automatically generated
- Many metrics, graphs
- v2.0 live since yesterday
- Via LLview job view



JUWELS Booster Job Report

Job Name: job name

Job Runtime: 3h35m — 14.58% of Wall: 1d20h00m

Job Start Time: 2021-05-05 10:49:49
Job Last Timestamp: 2021-05-05 14:25:07 (Running)
Current Time: 2021-05-05 14:25:07
Job Endtime (Est.): 2021-05-06 10:53:04

Queue: booster
Job Size, #Nodes: 32
Job Size, #CPUs: 128
#Data Points: 216
#Data Points: 100

Job /Performance Metrics

	min.	avg.	max.	
Load (CPU-Nodes):	4.02	4.05	4.07	
Memory (CPU-Nodes):	26607.40	27909.49	32116.40	MiB
Interconnect. Traffic (in):	5.01	471.64	22576.22	MiB/s
Interconnect. Traffic (out):	1.13	462.61	23837.40	MiB/s
Interconnect. Packets (in):	600	31401	1445832	pckt/s
Interconnect. Packets (out):	427	31302	1525697	pckt/s

Job I/O Statistics

	Total Data Write	Total Data Read	max. Data Rate/Node Write	max. Data Rate/Node Read	max. Open+Close Rate/Node
$HOME:	0.00 MiB	0.00 MiB	0.00 MiB/s	11.53 MiB/s	11.72 op/s
$PROJECT:	0.00 MiB	0.00 MiB	0.00 MiB/s	0.00 MiB/s	1.07 op/s
$SCRATCH:	38434.76 MiB	2135.17 MiB	35.09 MiB/s	0.21 MiB/s	2.93 op/s
$FASTDATA:	0.00 MiB	0.00 MiB	0.00 MiB/s	0.00 MiB/s	1.07 op/s

Job GPU Statistics

avg. GPU Usage:	62.82 %	avg. Mem. Usage Rate:	69.69 %	avg. GPU Temp.:	59.24 °C	avg. GPU Power:	253.08 W
max. Clk Streamfilters:	1410/1215 MHz	max. Mem. Usage:	38092.50 MiB	max. GPU Temp.:	70.00 °C	max. GPU Power:	338.07 W

This job will use approximately 32 nodes × 48 cores × 24.000 hours ≈ 36864.00 core-h for the specified walltime (up to now: 5512.76)

Average CPU Usage

Job-Usage Overview

Average GPU Usage

Average CPU Load
Average GPU Utilization

Table of Contents (9 Pages)

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Jobid: **3693699** User: **username** Project: **project** Job Name: **job name**

Job Runtime: **3h35m** → 14.95% of Wall: 1d00h00m

Job Start Time: **2021-05-05 10:49:49**

Job Last Timestamp: **2021-05-05 14:25:07** (Running)

Current Time: 2021-05-05 14:25:07

Job Endtime (Est.): 2021-05-06 10:50:04

Queue: **booster**

Job Size, #Nodes: **32** *#Data Points: 216*

Job Size, #GPUs: **128** *#Data Points: 190*

Job Performance Metrics

	min.	avg.	max.	
Load (CPU-Nodes):	**4.02**	**4.03**	**4.67**	
Memory (CPU-Nodes):	**26607.40**	**27909.49**	**32118.40**	*MiB*
Interconnect Traffic (in):	**5.61**	**471.64**	**22576.22**	*MiB/s*
Interconnect Traffic (out):	**1.13**	**462.61**	**23837.40**	*MiB/s*
Interconnect Packets (in):	**600**	**31401**	**1445832**	*pck/s*
Interconnect Packets (out):	**427**	**31392**	**1525607**	*pck/s*

Job I/O Statistics

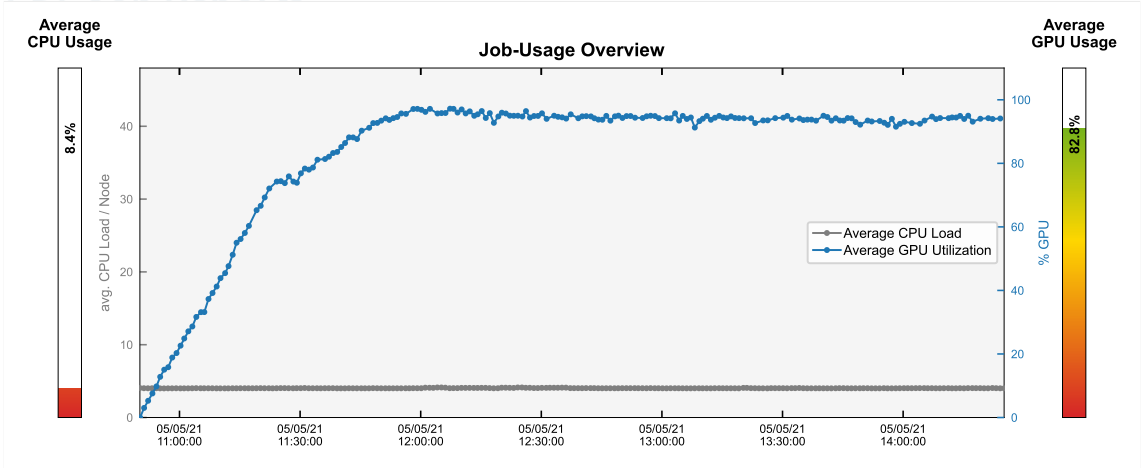
	Total Data Write	Total Data Read	max. Data Rate/Node Write	max. Data Rate/Node Read	max. Open-Close Rate/Node
$HOME:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**11.53** *MiB/s*	**11.72** *op./s*
$PROJECT:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**1.07** *op./s*
$SCRATCH:	**384834.76** *MiB*	**2135.17** *MiB*	**35.09** *MiB/s*	**0.21** *MiB/s*	**2.93** *op./s*
$FASTDATA:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**1.07** *op./s*

Job GPU Statistics

avg. GPU Usage:	**82.82** %	avg. Mem. Usage Rate:	**69.69** %	avg. GPU Temp.:	**59.24** °C	avg. GPU Power:	**253.08** W
max. Clk Stream/Mem:	**1410/1215** MHz	max. Mem. Usage:	**16062.50** MiB	max. GPU Temp.:	**70.00** °C	max. GPU Power:	**356.07** W

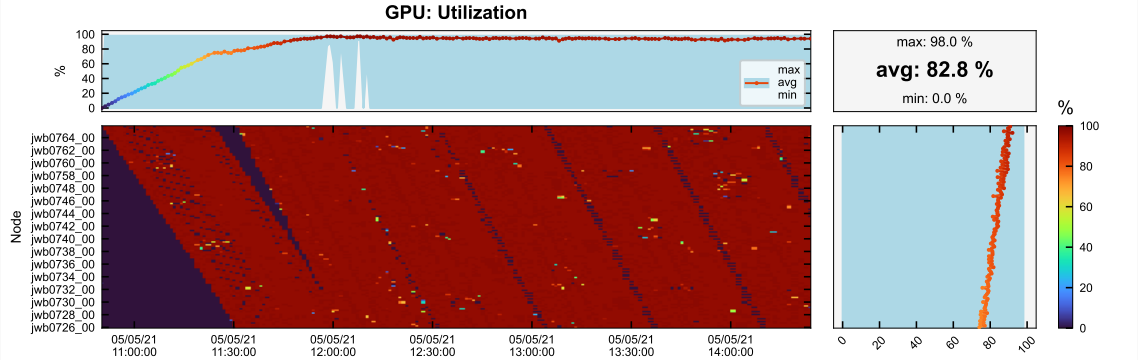
This job will use approximately 32 nodes × 48 cores × 24.000 hours = 36864.00 core-h for the specified walltime (up to now: 5512.70)

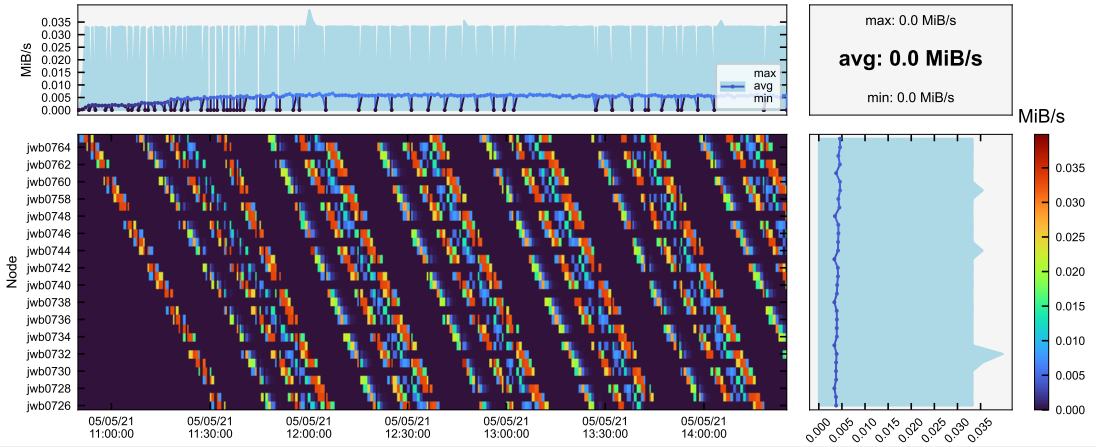
PDF Job Reports



PDF Job Reports

From LLview





Nodelist

1 **jwb0726** 1 **GPU0:** 74.1% 14.5GiB 1332MHz 2 **GPU1:** 77.1% 14.5GiB 1341MHz 3 **GPU2:** 74.5% 14.5GiB 1334MHz 4 **GPU3:** 76.5% 14.5GiB 1339MHz Interconnect group: 11	2 **jwb0727** 5 **GPU0:** 74.5% 14.5GiB 1332MHz 6 **GPU1:** 76.8% 14.5GiB 1344MHz 7 **GPU2:** 75.2% 14.5GiB 1339MHz 8 **GPU3:** 77.1% 14.5GiB 1345MHz Interconnect group: 11	3 **jwb0728** 9 **GPU0:** 74.8% 14.5GiB 1336MHz 10 **GPU1:** 78.3% 14.5GiB 1346MHz 11 **GPU2:** 75.0% 14.5GiB 1336MHz 12 **GPU3:** 77.4% 14.5GiB 1344MHz Interconnect group: 11	4 **jwb0729** 13 **GPU0:** 76.9% 14.5GiB 1347MHz 14 **GPU1:** 77.3% 14.5GiB 1346MHz 15 **GPU2:** 77.6% 14.5GiB 1346MHz 16 **GPU3:** 77.8% 14.5GiB 1346MHz Interconnect group: 11	5 **jwb0730** 17 **GPU0:** 76.1% 14.5GiB 1342MHz 18 **GPU1:** 78.2% 14.5GiB 1346MHz 19 **GPU2:** 78.7% 14.5GiB 1347MHz 20 **GPU3:** 77.0% 14.5GiB 1342MHz Interconnect group: 11	6 **jwb0731** 21 **GPU0:** 77.5% 14.5GiB 1342MHz 22 **GPU1:** 78.2% 14.5GiB 1346MHz 23 **GPU2:** 78.8% 14.5GiB 1347MHz 24 **GPU3:** 79.1% 14.5GiB 1349MHz Interconnect group: 11
7 **jwb0732** 25 **GPU0:** 78.6% 14.5GiB 1349MHz 26 **GPU1:** 75.8% 14.5GiB 1342MHz 27 **GPU2:** 79.1% 14.5GiB 1349MHz 28 **GPU3:** 78.9% 14.5GiB 1349MHz Interconnect group: 11	8 **jwb0733** 29 **GPU0:** 78.7% 14.5GiB 1350MHz 30 **GPU1:** 78.1% 14.5GiB 1344MHz 31 **GPU2:** 79.4% 14.5GiB 1351MHz 32 **GPU3:** 79.8% 14.5GiB 1349MHz Interconnect group: 11	9 **jwb0734** 33 **GPU0:** 78.4% 14.5GiB 1346MHz 34 **GPU1:** 79.3% 14.5GiB 1347MHz 35 **GPU2:** 80.8% 14.5GiB 1352MHz 36 **GPU3:** 80.4% 14.5GiB 1352MHz Interconnect group: 11	10 **jwb0735** 37 **GPU0:** 79.7% 14.5GiB 1351MHz 38 **GPU1:** 79.3% 14.5GiB 1347MHz 39 **GPU2:** 81.8% 14.5GiB 1356MHz 40 **GPU3:** 80.4% 14.5GiB 1351MHz Interconnect group: 11	11 **jwb0736** 41 **GPU0:** 80.9% 14.5GiB 1354MHz 42 **GPU1:** 79.3% 14.5GiB 1347MHz 43 **GPU2:** 80.8% 14.5GiB 1352MHz 44 **GPU3:** 79.2% 14.5GiB 1349MHz Interconnect group: 11	12 **jwb0737** 45 **GPU0:** 80.8% 14.5GiB 1354MHz 46 **GPU1:** 79.3% 14.5GiB 1347MHz 47 **GPU2:** 81.3% 14.5GiB 1354MHz 48 **GPU3:** 81.3% 14.5GiB 1354MHz Interconnect group: 12
13 **jwb0738** 49 **GPU0:** 81.2% 14.5GiB 1356MHz 50 **GPU1:** 79.2% 14.5GiB 1354MHz 51 **GPU2:** 80.9% 14.5GiB 1361MHz 52 **GPU3:** 82.2% 14.5GiB 1361MHz Interconnect group: 12	14 **jwb0739** 53 **GPU0:** 81.6% 14.5GiB 1359MHz 54 **GPU1:** 80.3% 14.5GiB 1359MHz 55 **GPU2:** 81.3% 14.5GiB 1361MHz 56 **GPU3:** 82.4% 14.5GiB 1362MHz Interconnect group: 12	15 **jwb0740** 57 **GPU0:** 81.6% 14.6GiB 1356MHz 58 **GPU1:** 81.1% 14.6GiB 1357MHz 59 **GPU2:** 81.8% 14.6GiB 1357MHz 60 **GPU3:** 82.4% 14.6GiB 1361MHz Interconnect group: 12	16 **jwb0741** 61 **GPU0:** 82.1% 14.6GiB 1359MHz 62 **GPU1:** 83.0% 14.6GiB 1359MHz 63 **GPU2:** 82.3% 14.6GiB 1362MHz 64 **GPU3:** 83.6% 14.6GiB 1364MHz Interconnect group: 12	17 **jwb0742** 65 **GPU0:** 84.3% 14.6GiB 1364MHz 66 **GPU1:** 83.7% 14.6GiB 1362MHz 67 **GPU2:** 83.9% 14.6GiB 1362MHz 68 **GPU3:** 84.4% 14.6GiB 1364MHz Interconnect group: 12	18 **jwb0743** 69 **GPU0:** 82.1% 14.6GiB 1359MHz 70 **GPU1:** 83.6% 14.6GiB 1362MHz 71 **GPU2:** 81.4% 14.6GiB 1362MHz 72 **GPU3:** 84.4% 14.6GiB 1369MHz Interconnect group: 12
19 **jwb0744** 73 **GPU0:** 83.9% 14.6GiB 1362MHz 74 **GPU1:** 83.9% 14.6GiB 1364MHz 75 **GPU2:** 83.4% 14.6GiB 1362MHz 76 **GPU3:** 84.1% 14.6GiB 1366MHz Interconnect group: 12	20 **jwb0745** 77 **GPU0:** 84.3% 14.6GiB 1366MHz 78 **GPU1:** 84.9% 14.6GiB 1366MHz 79 **GPU2:** 83.6% 14.6GiB 1367MHz 80 **GPU3:** 84.6% 14.6GiB 1367MHz Interconnect group: 12	21 **jwb0746** 81 **GPU0:** 84.3% 14.6GiB 1367MHz 82 **GPU1:** 84.3% 14.6GiB 1366MHz 83 **GPU2:** 85.8% 14.6GiB 1372MHz 84 **GPU3:** 81.6% 14.6GiB 1361MHz Interconnect group: 12	22 **jwb0747** 85 **GPU0:** 86.4% 14.6GiB 1371MHz 86 **GPU1:** 86.0% 14.6GiB 1369MHz 87 **GPU2:** 85.5% 14.6GiB 1367MHz 88 **GPU3:** 84.2% 14.6GiB 1366MHz Interconnect group: 12	23 **jwb0748** 89 **GPU0:** 87.5% 14.6GiB 1374MHz 90 **GPU1:** 85.3% 14.6GiB 1369MHz 91 **GPU2:** 86.8% 14.6GiB 1371MHz 92 **GPU3:** 84.4% 14.6GiB 1369MHz Interconnect group: 12	24 **jwb0757** 93 **GPU0:** 87.4% 14.6GiB 1374MHz 94 **GPU1:** 85.7% 14.6GiB 1371MHz 95 **GPU2:** 87.2% 14.6GiB 1376MHz 96 **GPU3:** 84.0% 14.6GiB 1372MHz Interconnect group: 12
25 **jwb0758** 97 **GPU0:** 87.8% 14.6GiB 1376MHz 98 **GPU1:** 86.0% 14.6GiB 1372MHz 99 **GPU2:** 88.7% 14.6GiB 1383MHz 100 **GPU3:** 83.8% 14.6GiB 1375MHz Interconnect group: 12	26 **jwb0759** 101 **GPU0:** 89.6% 14.6GiB 1380MHz 102 **GPU1:** 85.6% 14.6GiB 1372MHz 103 **GPU2:** 89.3% 14.6GiB 1384MHz 104 **GPU3:** 86.6% 14.6GiB 1376MHz Interconnect group: 12	27 **jwb0760** 105 **GPU0:** 89.4% 14.6GiB 1382MHz 106 **GPU1:** 85.9% 14.6GiB 1374MHz 107 **GPU2:** 88.7% 14.6GiB 1382MHz 108 **GPU3:** 87.7% 14.6GiB 1376MHz Interconnect group: 12	28 **jwb0761** 109 **GPU0:** 89.5% 14.6GiB 1385MHz 110 **GPU1:** 86.6% 14.6GiB 1374MHz 111 **GPU2:** 90.1% 14.6GiB 1385MHz 112 **GPU3:** 86.8% 14.6GiB 1376MHz Interconnect group: 12	29 **jwb0762** 113 **GPU0:** 88.8% 14.6GiB 1382MHz 114 **GPU1:** 86.9% 14.6GiB 1376MHz 115 **GPU2:** 87.6% 14.6GiB 1380MHz 116 **GPU3:** 90.0% 14.6GiB 1382MHz Interconnect group: 12	30 **jwb0763** 117 **GPU0:** 88.6% 14.6GiB 1382MHz 118 **GPU1:** 89.5% 14.6GiB 1380MHz 119 **GPU2:** 88.3% 14.6GiB 1382MHz 120 **GPU3:** 90.6% 14.6GiB 1387MHz Interconnect group: 12
		31 **jwb0764** 121 **GPU0:** 89.4% 14.6GiB 1384MHz 122 **GPU1:** 89.8% 14.6GiB 1382MHz 123 **GPU2:** 89.3% 14.6GiB 1383MHz 124 **GPU3:** 92.1% 14.6GiB 1389MHz Interconnect group: 12	32 **jwb0765** 125 **GPU0:** 87.4% 14.6GiB 1380MHz 126 **GPU1:** 90.2% 14.6GiB 1385MHz 127 **GPU2:** 89.6% 14.6GiB 1385MHz 128 **GPU3:** 90.8% 15.6GiB 1387MHz Interconnect group: 12		

Early Experiences

Early Experiences: Application-Related

Overview

- Some first results by users
- Mainly EA participants
- Most results preliminary
- Results partly on machine under construction

Early Experiences

Application-Related: *Soft Matter: SOMA*

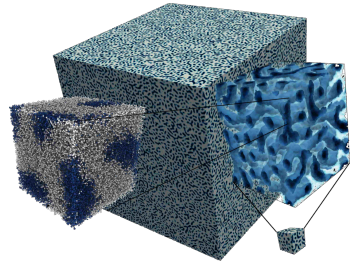
Soft Matter: SOMA

- **SOMA**: Soft, coarse-grained Monte-Carlo Acceleration
  L. Schneider and M. Müller, Comput. Phys. Commun. 235C 463–476 (2019) and GPU Seminar Talk
- Kinetics of nanomaterial formation; multi-component polymer systems (battery materials, membranes, …)
- Unique: Resolve details of polymer, but study lengths relevant to engineering

Team: L. Schneider, N. Blagojevic, L. Pigard, M. Müller, et al

→ `gitlab.com/InnocentBug/SOMA/`

- C, OpenACC, MPI
- Frequent JUWELS user



GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

SOMA
yes, soft matters

JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

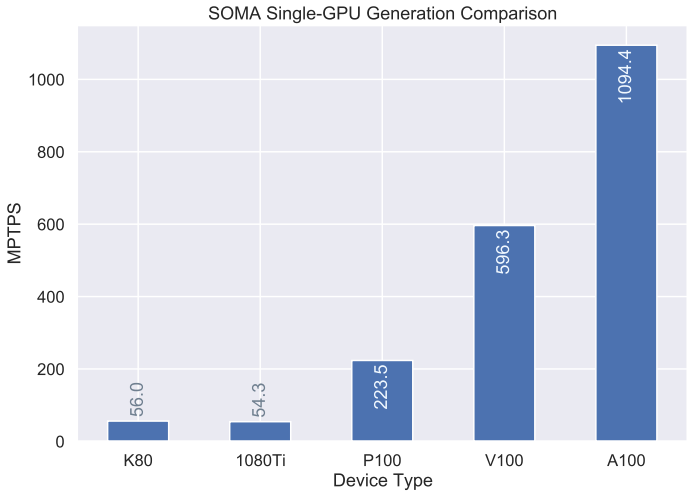
Soft Matter: SOMA

Comparison of GPU Generations

- Long experience with various GPU architectures

→ **Update to new generations early!**

- Some algorithmic changes between generations; also feature additions
- *PTPS: Particle Timesteps Per Second*



Data provided by SOMA / L. Schneider

Soft Matter: SOMA

Kernel Comparison: Memory Chart

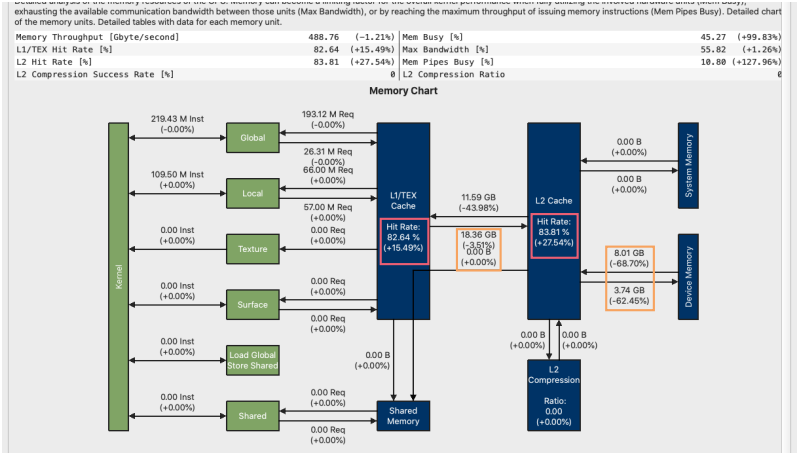
- Many random accesses

→ Benefit from larger L1, L2 caches

→ More FP64 throughput

- Knock-on effect: less memory traffic
- **Kernel runtime:**

V100	25.8 ms
A100	21.5 ms
A100*	18.9 ms

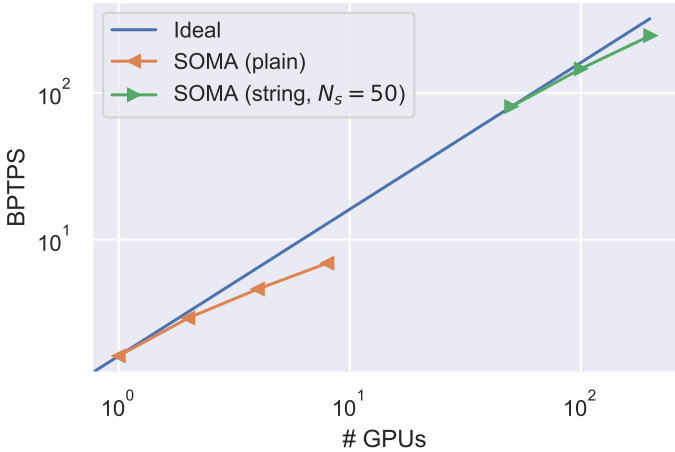


Nsight Compute profile provided by SOMA

Soft Matter: SOMA

New Method for Scaling

- **Scale of Booster: New algorithms, implementations with more scalability!**
- New project for Booster: *String* Method
- String-coupled SOMA ensemble simulation
- Master thesis of N. Blagojevic



Data provided by SOMA / N. Blagojevic

Early Experiences

Application-Related: *JUQMES*

Quantum Computing: JUQMES

- **JUQMES**: Jülich Quantum Master Equation Simulator
  D. Willsch, et al.
- Simulation of physical realizations of quantum computers
- Compute-intensive

Team: Research group Quantum Information Processing

- C++, OpenACC, CUDA C
- Frequent JUWELS user

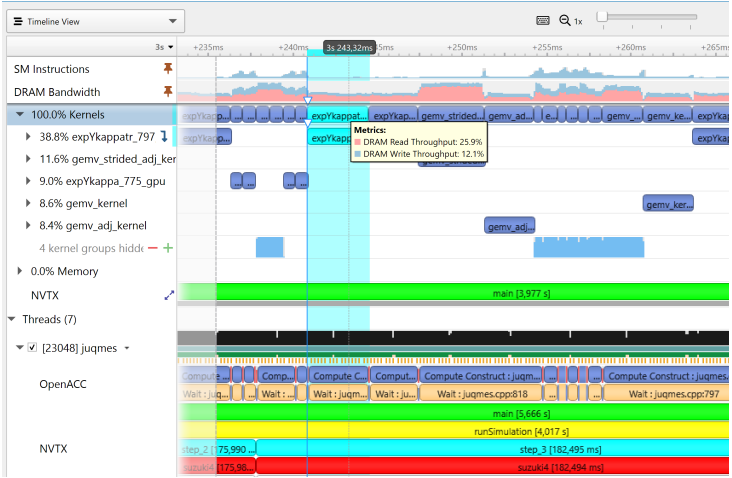
JÜLICH SUPERCOMPUTING CENTRE

JUQMES

Nsight Systems

- Start of analysis with Nsight Systems
- Instrumented with **NVTX** ranges (`main`, `runSimulation`, ...)
- Focus: Kernel `expYkappatr`
- Low Streaming Multiprocessor (SM) utilization
- Low memory utilization

→ What is limiter?



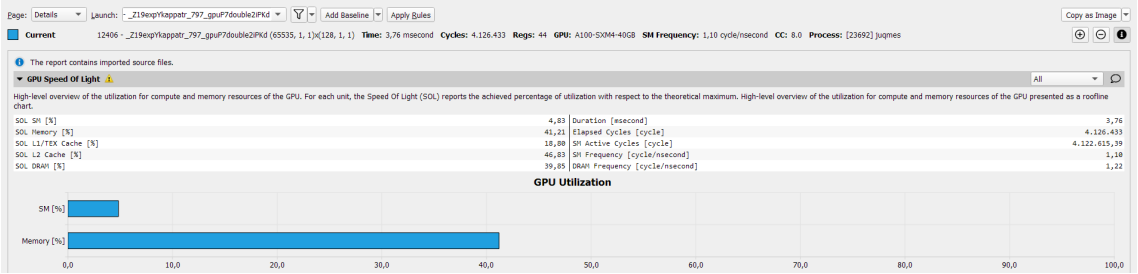
JUQMES

Nsight Compute

- Focus analysis with Nsight Compute
- Important metric: **GPU Utilization** as *Speed-of-Light*

- Low SM utilization
- Low memory utilization

→ Latency bound? (stalls? parallelism)



JUQMES

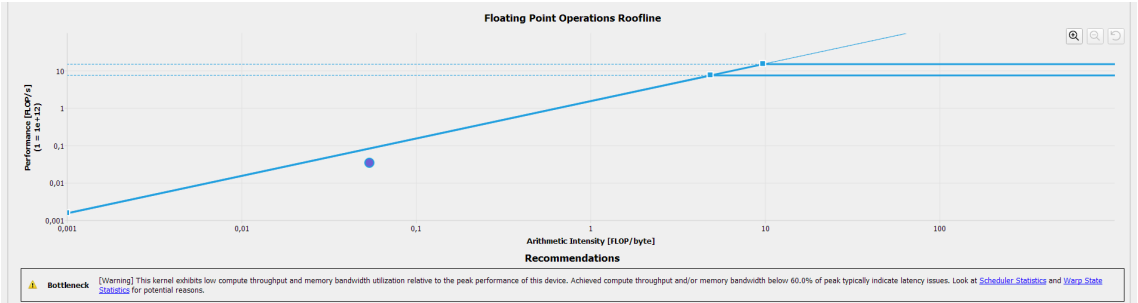
Nsight Compute

- **Roofline Model**: Performance (FLOP/s) vs. Arithmetic Intensity (FLOP/B)

- 60 % below roofline!

→ Latency bound!

- Further tip available



Bottleneck: This kernel exhibits low compute throughput and memory bandwidth utilization relative to the peak performance of this device. Achieved compute throughput and/or memory bandwidth below 60 % of peak typically indicate latency issues. Look at Scheduler Statistics and Warp State Statistics for potential reasons.

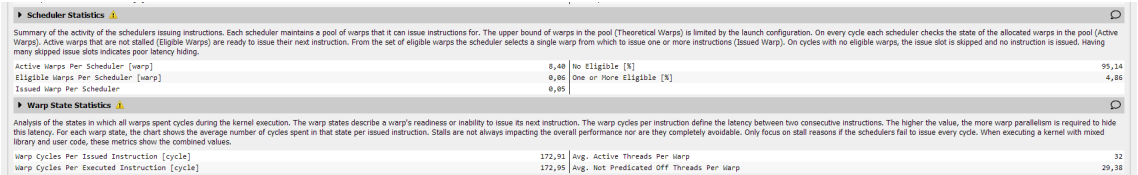
JUQMES

Nsight Compute

- See statistics for scheduler and warp state
- Many non-eligible warps, many cycles per instructions

- Many *LG Throttles* and *Long Scoreboard Stalls* *(not shown)*

→ See source view!



Scheduler Statistics

Summary of the activity of the schedulers issuing instructions. Each scheduler maintains a pool of warps that it can issue instructions for. The upper bound of warps in the pool (Theoretical Warps) is limited by the launch configuration. On every cycle each scheduler checks the state of the allocated warps in the pool (Active Warps). Active warps that are not stalled (Eligible Warps) are ready to issue their next instruction. From the set of eligible warps the scheduler selects a single warp from which to issue one or more instructions (Issued Warp). On cycles with no eligible warps, the issue slot is skipped and no instruction is issued. Having many skipped issue slots indicates poor latency hiding.

Active Warps Per Scheduler [warp]	8,40	No Eligible [%]	95,14
Eligible Warps Per Scheduler [warp]	0,06	One or More Eligible [%]	4,86
Issued Warp Per Scheduler	0,05		

Warp State Statistics

Analysis of the states in which all warps spent cycles during the kernel execution. The warp states describe a warp's readiness or inability to issue its next instruction. The warp cycles per instruction define the latency between two consecutive instructions. The higher the value, the more warp parallelism is required to hide this latency. For each warp state, the chart shows the average number of cycles spent in that state per issued instruction. Stalls are not always impacting the overall performance nor are they completely avoidable. Only focus on stall reasons if the schedulers fail to issue every cycle. When executing a kernel with mixed library and user code, these metrics show the combined values.

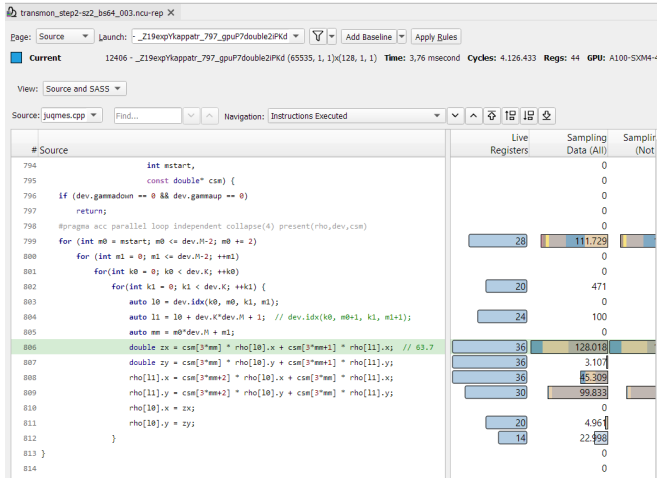
Warp Cycles Per Issued Instruction [cycle]	172,91	Avg. Active Threads Per Warp	32
Warp Cycles Per Executed Instruction [cycle]	172,95	Avg. Not Predicated Off Threads Per Warp	29,38

JUQMES

Nsight Compute

- Source view: Source vs. SASS
- With register sampling
- Pin-point stalls in source
- Non-optimal data access

⇒ Loop re-order!

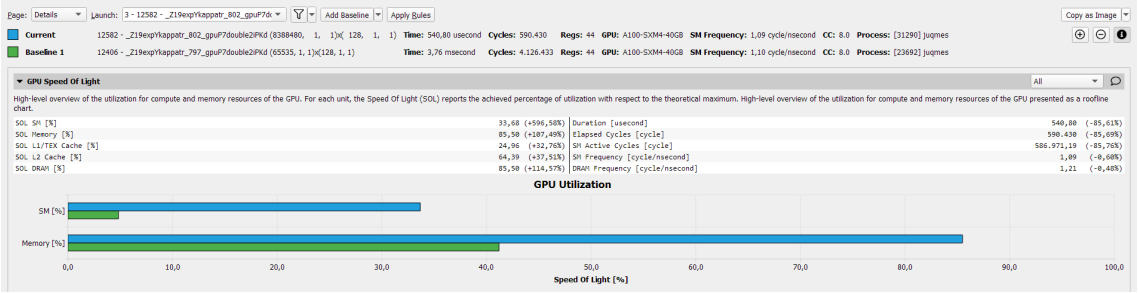


JUQMES

Nsight Compute

- Compare view Nsight Compute (compare previous baseline with optimized version)

- Improve GPU utilization

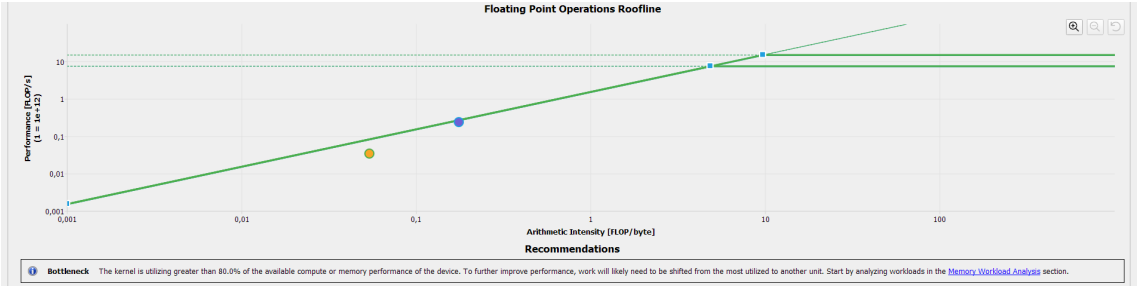


JUQMES

Nsight Compute

- Compare view Nsight Compute (compare previous baseline with optimized version)

- Improve GPU utilization
- Improve Roofline

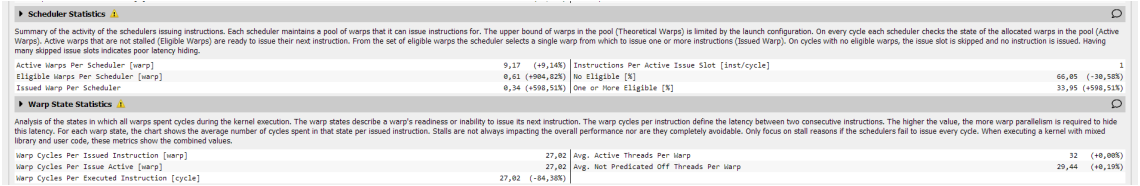


JUQMES

Nsight Compute

- Compare view Nsight Compute (compare previous baseline with optimized version)

- Improve GPU utilization
- Improve Roofline
- Improve scheduler statistics



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Active Warps Per Scheduler [warp]	9,17	(+9,14%)	Instructions Per Active Issue Slot [inst/cycle]	1	
Eligible Warps Per Scheduler [warp]	0,61	(+904,82%)	No Eligible [%]	66,05	(-30,58%)
Issued Warp Per Scheduler	0,34	(+598,51%)	One or More Eligible [%]	33,95	(+598,51%)

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Warp Cycles Per Issue Active [warp]	27,02		Avg. Not Predicated Off Threads Per Warp	29,44	(+0,19%)
Warp Cycles Per Executed Instruction [cycle]	27,02	(-84,38%)			

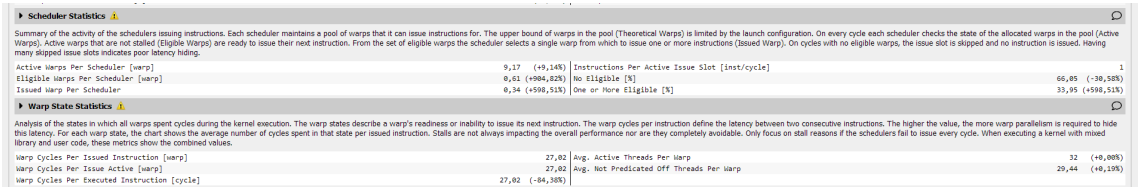
JUQMES

Nsight Compute

- Compare view Nsight Compute (compare previous baseline with optimized version)

- Improve GPU utilization
- Improve Roofline
- Improve scheduler statistics

$\Rightarrow$ 35 % runtime improvement for benchmark, 6$\times$ for kernel



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Warp Cycles Per Executed Instruction [cycle]	27,02	(-84,38%)			

Early Experiences

Application-Related: *Earth-System Modeling: ParFlow*

Earth-System Modeling: ParFlow

- **ParFlow**: Numerical model for groundwater and surface water flow

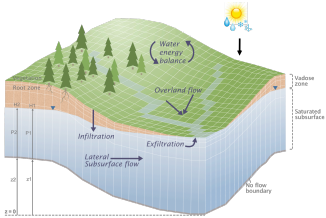
  J. Hokkanen, S. Kollet, et al, EGU General Assembly 2020, 4–8 May 2020, EGU2020-12904, and GPU Seminar Talk

- Model hydrologic processes, hill-slope to continental scale; forecasting, water cycle research, climate change; since 1990s
- Finite-difference scheme with implicit time integration

Team: J. Hokkanen, S. Kollet

→ `parflow.org`

- C, C++, CUDA, MPI
- Fresh GPU port in prepartion for Booster



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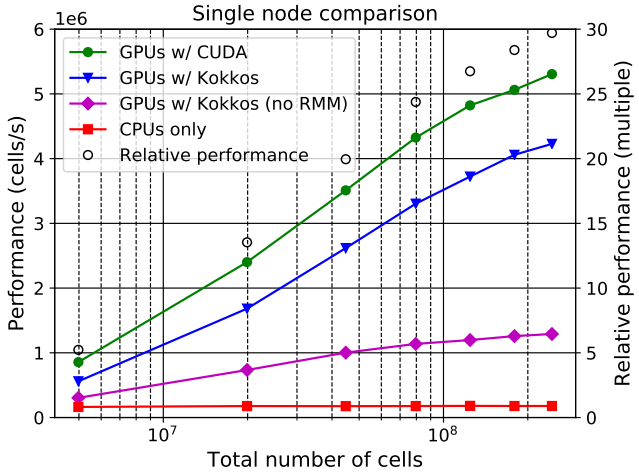
Earth-System Modeling: ParFlow

Single-Node Performance

- Comparing CPU of Booster node with GPUs
- **Good speed-up, max. 29×**
- Memory pool (*RMM*) gives extra boost
- Larger problem sizes solvable per node
- Currently extending to Kokkos

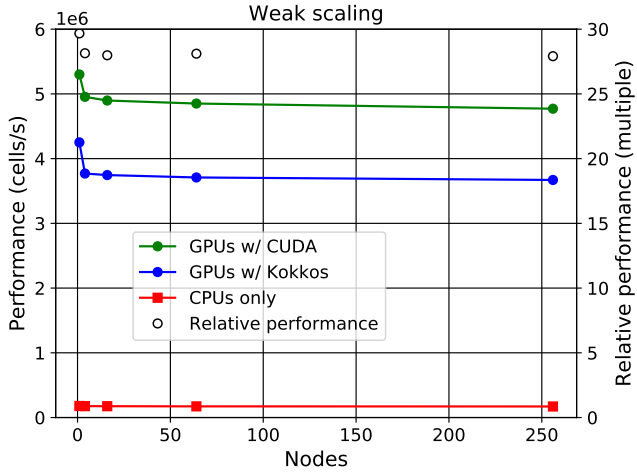


Plot provided by ParFlow / J. Hokkanen

Earth-System Modeling: ParFlow

Weak Scaling

- Fixed problem size per node
- **26× speed-up achieved over $\mathcal{O}(100)$ nodes**

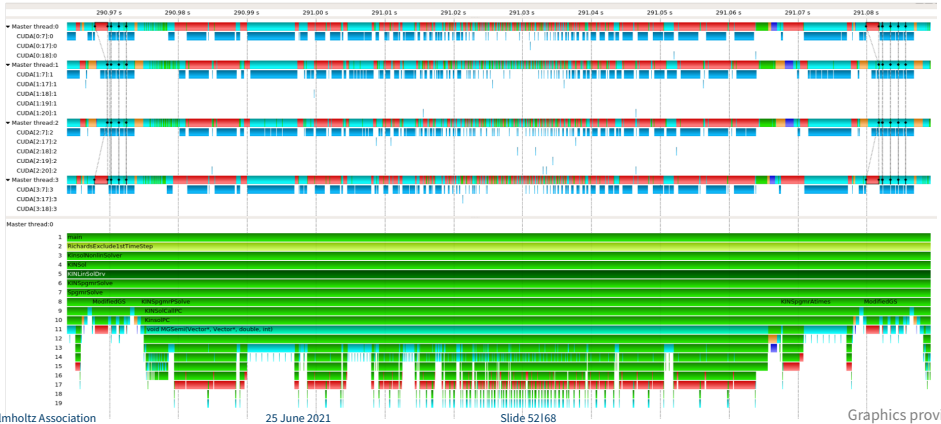


Plot provided by ParFlow / J. Hokkanen

Earth-System Modeling: ParFlow

POP Performance Assessment

- Performance Assessment by I. Zhukov (JSC, POP CoE) at mid of 2020
- 1 node, 4 GPUs
- Instrumentation with Score-P, visualization with Vampir



Graphics provided by I. Zhukov

Earth-System Modeling: ParFlow

POP Performance Assessment

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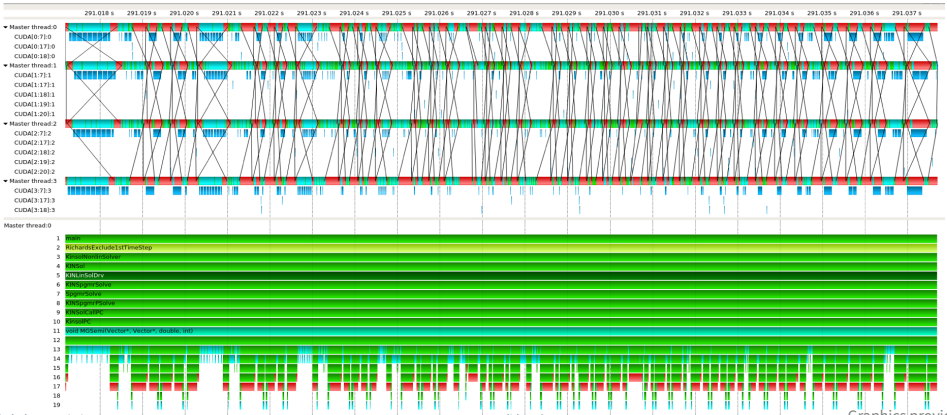
- 1 node, 4 GPUs
- Instrumentation with Score-P, visualization with Vampir
- See MPI connections

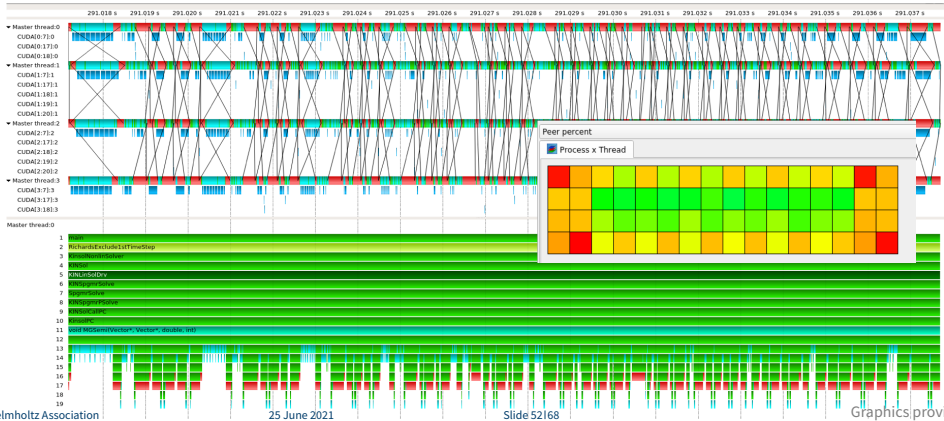


Graphics provided by I. Zhukov

Earth-System Modeling: ParFlow

POP Performance Assessment

- Performance Assessment by I. Zhukov (JSC, POP CoE) at mid of 2020
- 1 node, 4 GPUs
- Instrumentation with Score-P, visualization with Vampir
- See MPI connections, late senders (16 nodes)



Graphics provided by I. Zhukov

Early Experiences

Application-Related: *JUQCS*

Quantum Computing: JUQCS

- **JUQCS**: Jülich Universal Quantum Computer Simulator
  De Raedt et al., Comp. Phys. Comm. 237 47–61 (2019)
- Universal quantum computing on digital computer
- Network-, memory-intensive computations
- Team: Research group Quantum Information Processing

- Fortran, CUDA Fortran
- Frequent JUWELS user

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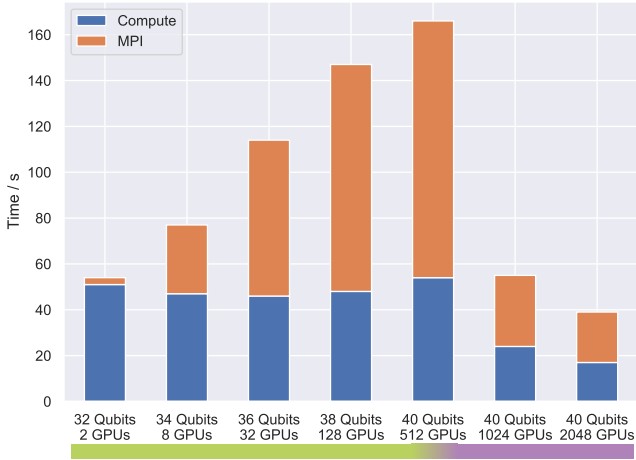
JUQCS

- **40 qubits:**
  - $>$ 16 TiB memory needed
    $\rightarrow$ 512 A100s
  - Each quantum operation: Update states, 8 TB transfer
- Weak scaling: Compute constant, MPI as expected
- Strong scaling: Still investigate DragonFly+ topology

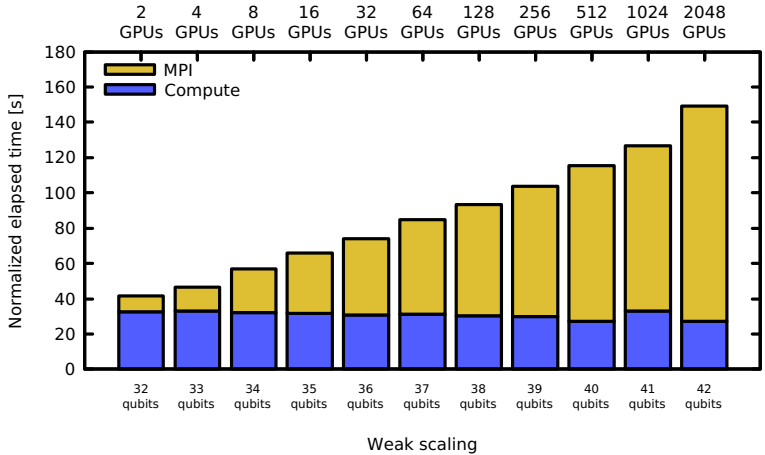


Data provided by JuQCS / H. De Raedt

JUQCS

More Weak Scaling

- Weak scaling to 2048 GPUs / 42 qubits
- Good behavior, but MPI still limiter

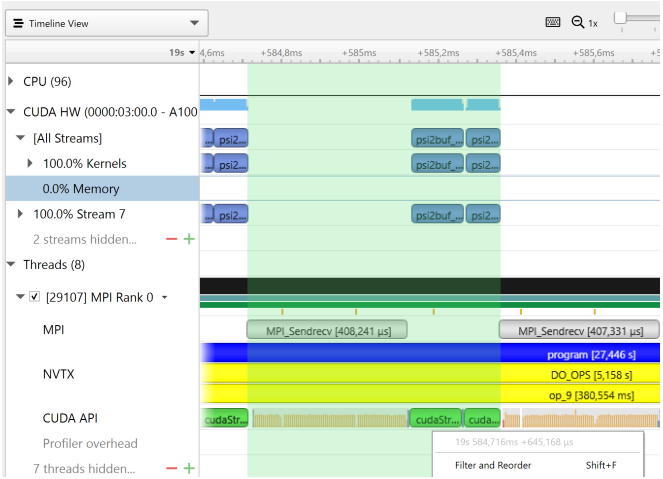


JUQCS

Performance Improvments

- Investigating performance improvements with Nsight Systems
- Focus on gabs between kernels

→ Used by MPI

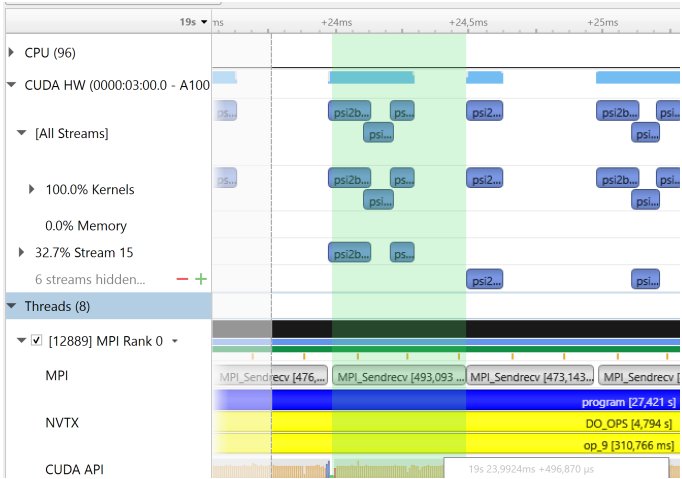


JUQCS

Performance Improvments

- Implement double-buffering
- Overlap GPU kernel and MPI call

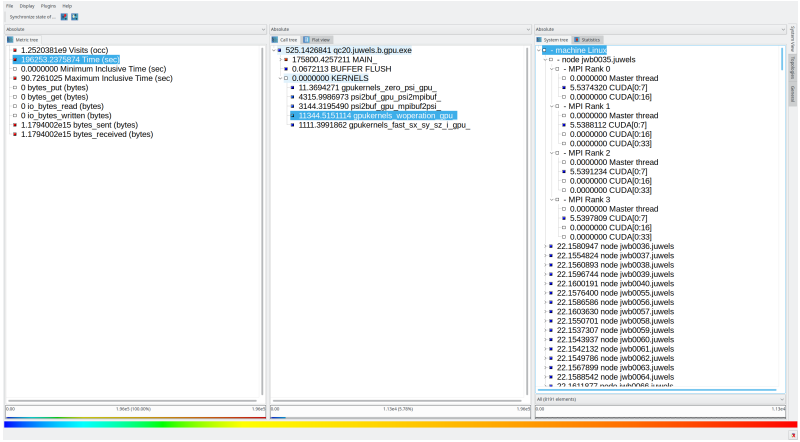
⇒ ≈ 30 % run-time improvement for part of iteration



JUQCS

Performance Analysis

- First analysis with Score-P, Cube, Scalasca, Vampir
- See overview in Cube (2048 GPUs)



Screenshots provided by M. Knobloch

JUQCS

Performance Analysis

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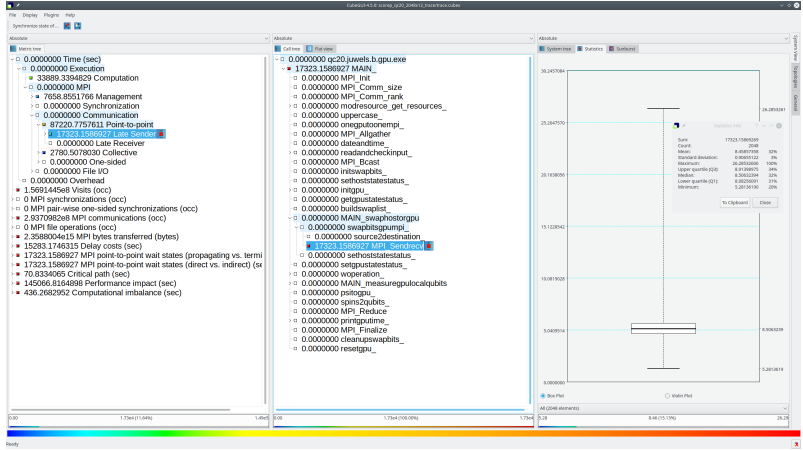
- Study late senders with in Scalasca (2048 GPUs)



Screenshots provided by M. Knobloch

JUQCS

Performance Analysis

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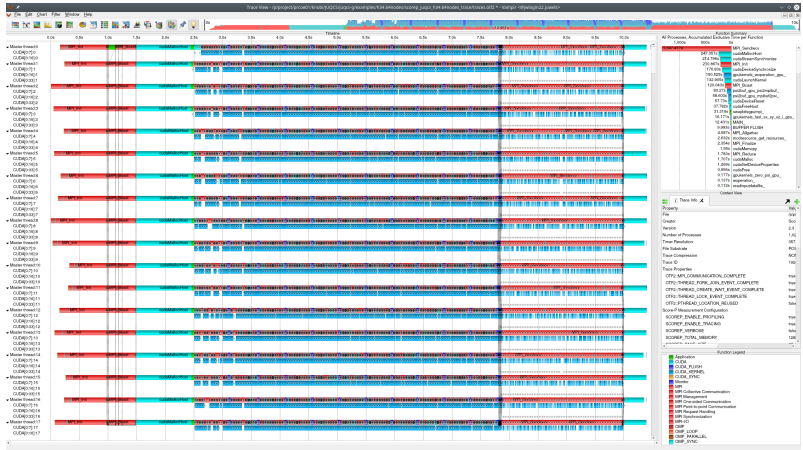

Screenshots provided by M. Knobloch

JUQCS

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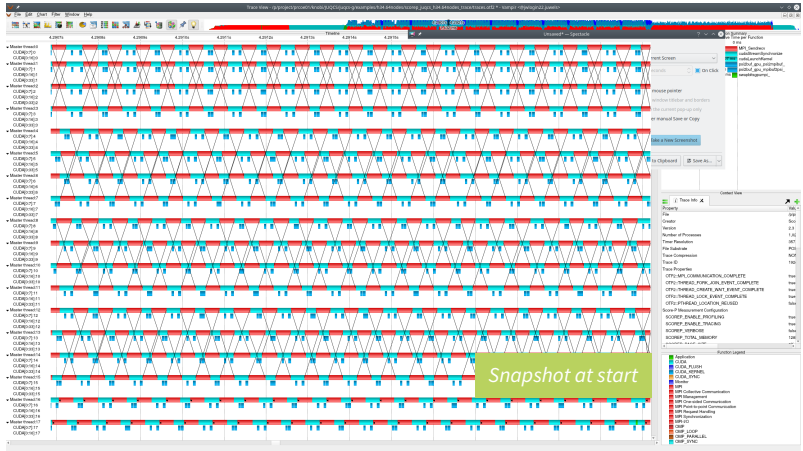

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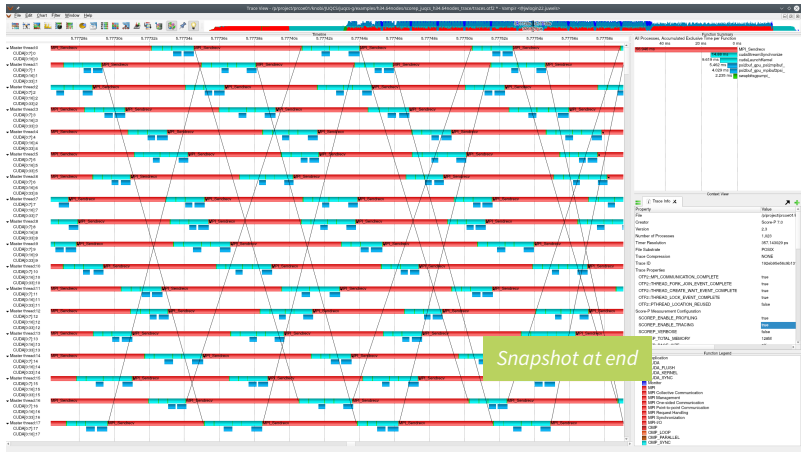

Screenshots provided by M. Knobloch

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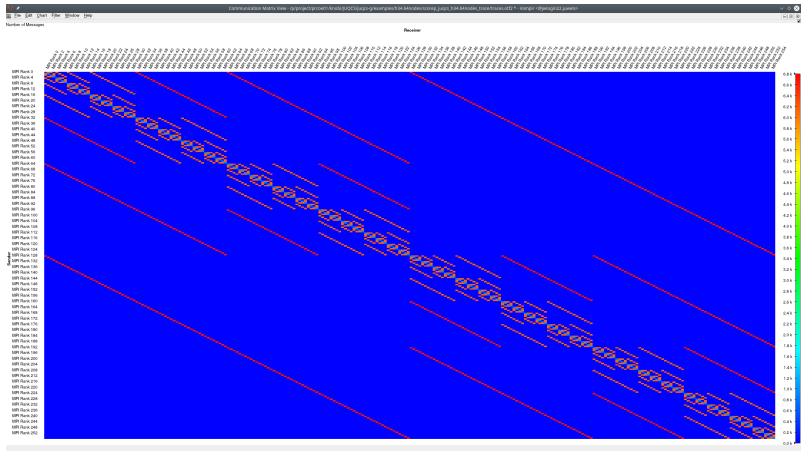


Screenshots provided by M. Knobloch

Early Experiences

Application-Related: *LQCD: Bonn*

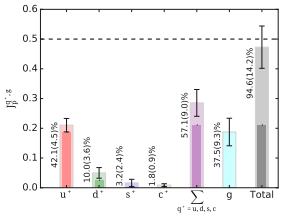
LQCD: Bonn

- **ETMC**: Extended Twisted Mass Collaboration
  C. Alexandrou and S. Bacchio et al, Phys. Rev. D 101 094513 (2020)
- Study of the Flavour Singlet Structure of Hadrons

Team: S. Bacchio, B. Kostrzewa, et al; Uni Bonn, Uni Cyprus, Cyprus Institute, Uni Rome, …

→ `github.com/etmc`, PLEGMA, QUDA, tmLQCD

- C/C++, CUDA, MPI, OpenMP
- Frequent JUWELS user



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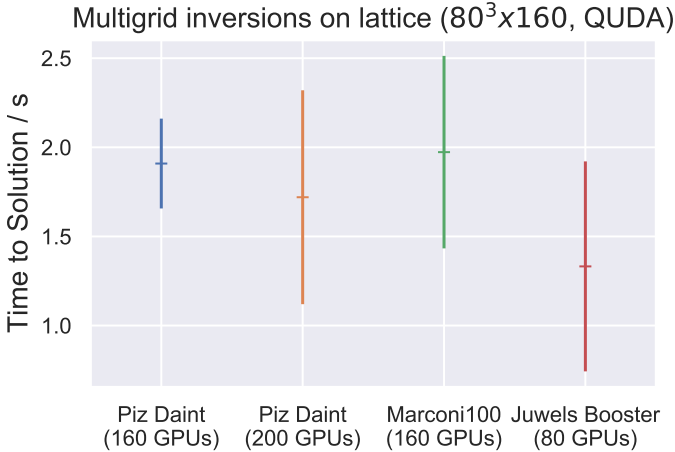
LQCD: Bonn

Comparison of GPU HPC Machines

- Multigrid inversion
- Mean time-to-solution, spread
- Systems

  Piz Daint Haswell, P100; DragonFly

  Marconi100 POWER9, V100; DragonFly+
- JUWELS Booster: Low time to solution; but large spread (being investigated)



Data provided by ETMC / S. Bacchio

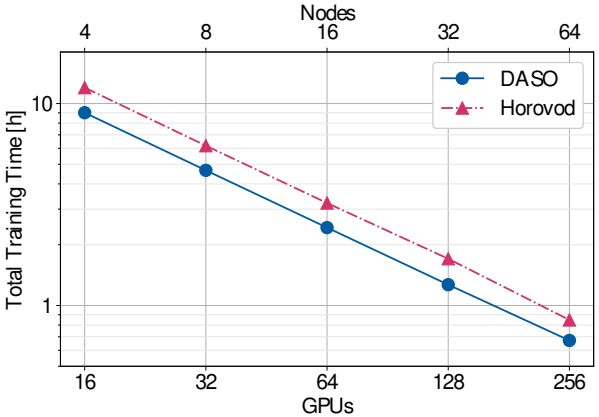
Early Experiences

Application-Related: *Others*

Distributed Training with DASO

Deep-Learning

- **Publication**: Accelerating Neural Network Training with Distributed Asynchronous and Selective Optimization (DASO)
- Authors: D. Coquelin et. al; KIT, DLR
- Unique: 25 % improvement over Horovod
- Status: Preprint arXiv:2104.05588 [cs.LG]

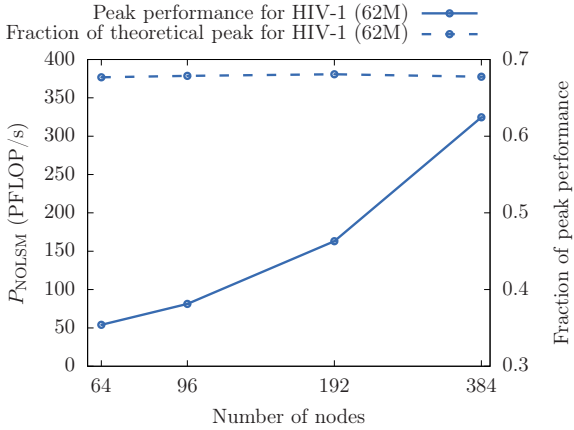


Graph from publication arXiv:2104.05588 [cs.LG]

Large-Scale Ab-Initio Molecular Dynamics

Molecular Dynamics

- **Publication**: Enabling Electronic Structure-Based Ab-Initio Molecular Dynamics Simulations with Hundreds of Millions of Atoms
- Authors: R. Schade et. al; Paderborn University
- Unique: FP16/FP32 mixed precision, 1536 GPUs, 324 PFLOP/s
- Status: Preprint arXiv:2104.08245 [physics.comp-ph]



Graph from publication arXiv:2104.08245 [physics.comp-ph]

Summary and Conclusions

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- JUWELS Booster: European flagship system based on A100 GPUs and HDR200 InfiniBand network
- Highly scalable system design with $> 70\,\mathrm{PFLOP/s_{FP64}}$ compute performance and $749\,\mathrm{Tbit/s}$ acc. injection bandwidth
- In production since end of November, some applications earlier through Early Access Program
- First results incoming; second allocation period started
- Most important tools for performance analysis: Nsight Systems, Nsight Compute, Score-P stack; great overview at in B. Mohr's and M. Knobloch's recent article
- Important models: GPU Utilization, cache hit rate, Roofline (see especially N. Ding's and S. Williams GPU Roofline paper)

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Thank you for your attention!

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Acknowledgements

Acknowledgments

- JSC Application-Oriented Technology Development: Kaveh Haghighi-Mood
- JSC Application Support: Ilya Zhukov, Michael Knobloch, Thomas Breuer, Max Holicki, Filipe Guimaraes
- JSC High Performance Systems: Dorian Krause, Damian Alvarez, Benedikt von St. Vieth
- NVIDIA Collaborators: Markus Hrywniak, Jiri Kraus, Mathias Wagner
- Application owners: Jaro Hokkanen, Dennis Willsch, Hans de Raedt, Ludwig Schneider

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Thank you for your attention!

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Appendix

Tools Wishlist

OSU Micro-Benchmarks: Bandwidth

- Guideline for Tensor Core potential
- Consider node, network affinity / topology

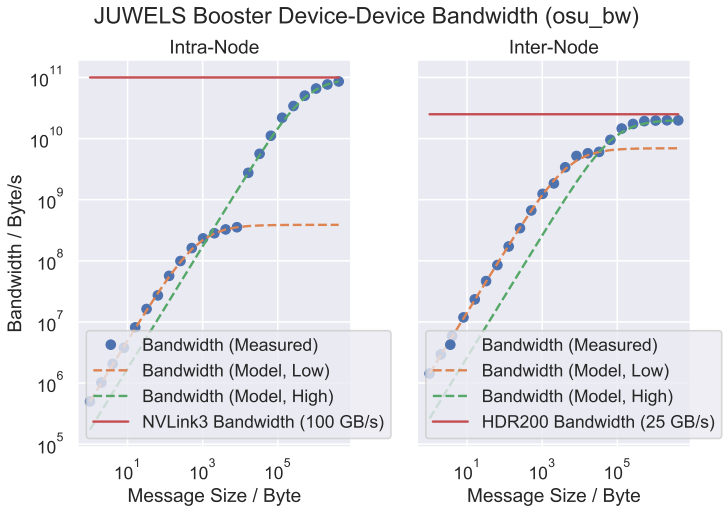
Appendix

Network Performance

Network Performance

OSU Micro-Benchmarks: Bandwidth

- OSU Microbenchmarks: device-device bandwidth (`osu_bw D D`)
- Good results, expected limiters
- Intra-node: NVLink3 bandwidth
- Inter-node: HDR200 bandwidth
- Model fits show 2 regimes (---/ ---)



Appendix

STREAM Benchmark

STREAM

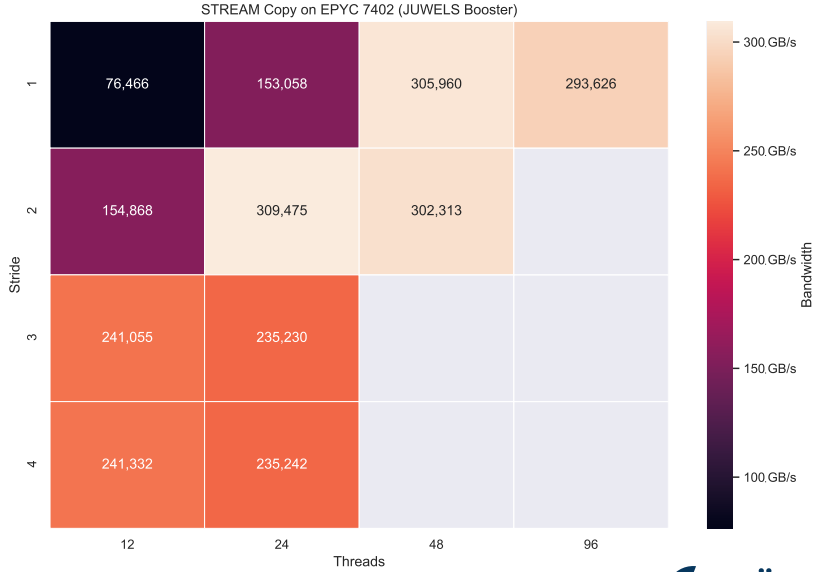
Config

AOCC 3.0.0 on EPYC 7402

```
$ clang -O3 -mcmodel=large -fopenmp -ffp-contract=fast -fnt-store -DSTREAM_ARRAY_SIZE=2500000000
↪  -DNTIMES=200 -DSTREAM_TYPE=double -o stream.exe stream.c
$ srun --cpu-bind=none \
    env \
        OMP_NUM_THREADS=24 \
        OMP_PLACES='{0}:24:2' \
        OMP_PLACES="cores" \
        OMP_PROC_BIND="true" \
        OMP_MAX_ACTIVE_LEVELS=1 \
        OMP_STACKSIZE=256M \
        OMP_SCHEDULE=static \
        OMP_DYNAMIC=false \
        OMP_THREAD_LIMIT=256 \
        OMP_DISPLAY_ENV=true \
    ./stream.exe
```

STREAM

Copy



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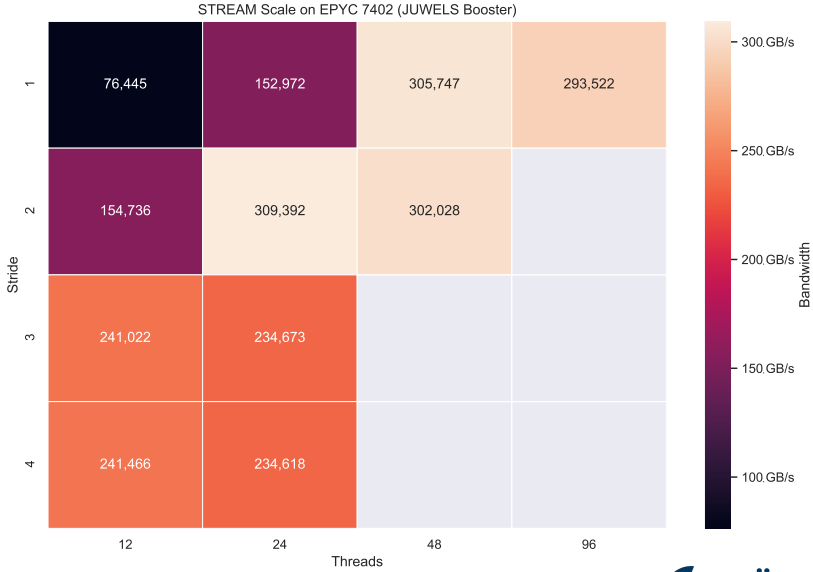
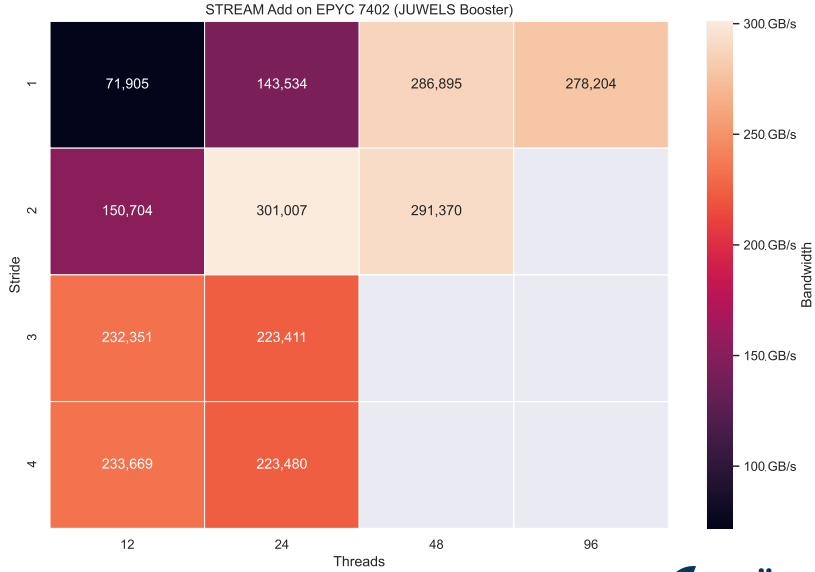
STREAM

Scale



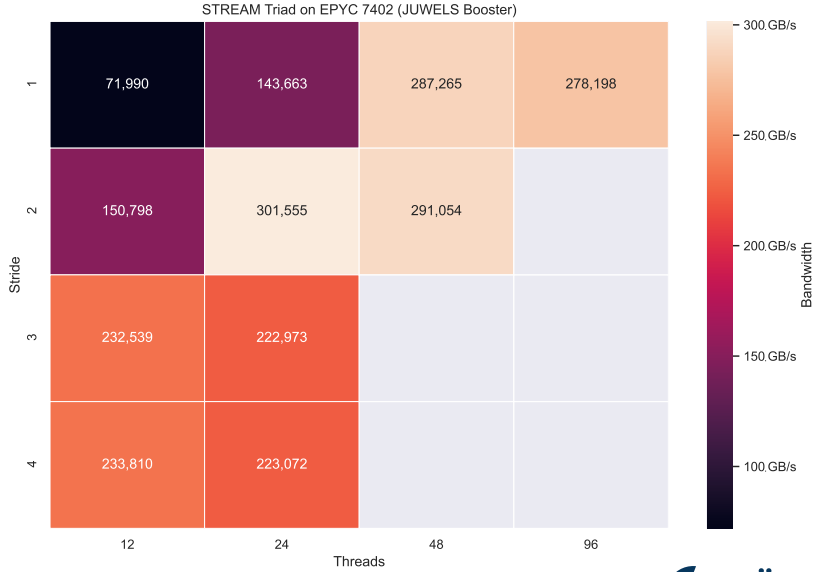
STREAM

Add



STREAM

Triad



Supplement: Application Experiences

PIConGPU

- **PIConGPU**: Plasma simulation

  H. Burau et al, IEEE Transactions on Plasma Science 38 10 (2010)

- Particle-in-cell simulation for Exascale-level GPUs

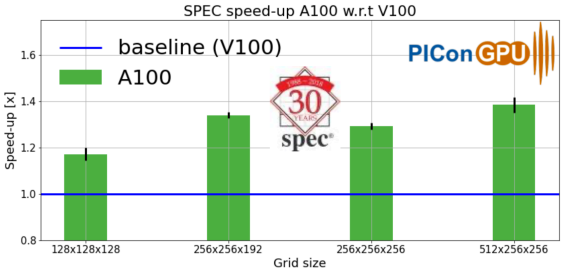
Team: A. Lebedev, A. Debus, M. Bussmann, et. al

→ `github.com/ComputationalRadiationPhysics/picongpu`

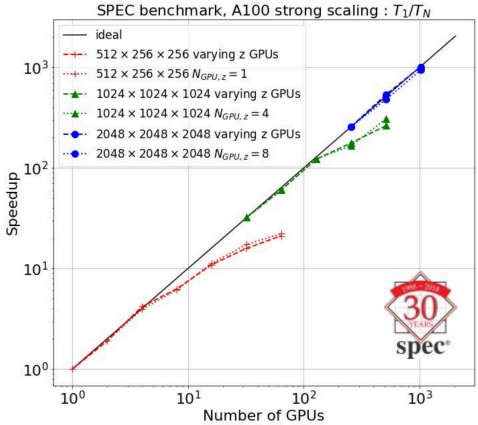
- C/C++, CUDA, MPI, Alpaka

PIConGPU

Results



Comparison A100 vs. V100



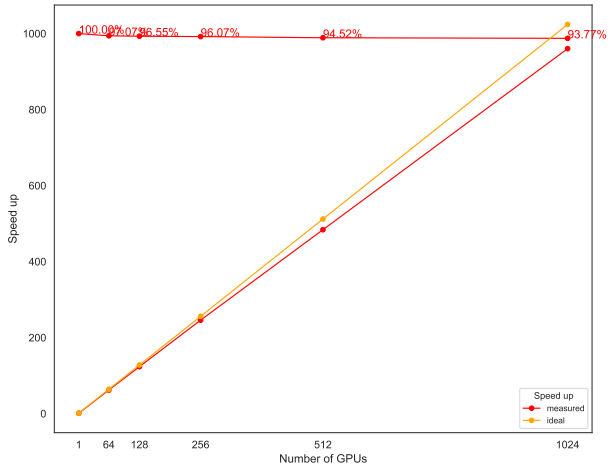
Strong scaling for different grid sizes

Graphs by PIConGPU / M. Bussmann

Large-Scale Pre-Training on Transfer Learning for Images

Deep-Learning

- **Publication**: Effect of large-scale pre-training on full and few-shot transfer learning for natural and medical images
- Authors: Mehdi Cherti, Jenia Jitsev; JSC
- Status: Preprint (under review) arXiv:2106.00116 [cs.LG]



Graph from publication arXiv:2106.00116 [cs.LG]

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References

References I

[5] Hans De Raedt et al. “Massively parallel quantum computer simulator, eleven years later.” In: *Computer Physics Communications* 237 (2019), pp. 47–61. ISSN: 0010-4655 (page 104).

[6] Michael Knobloch and Bernd Mohr. “Tools for GPU Computing – Debugging and Performance Analysis of Heterogenous HPC Applications.” In: *Supercomputing Frontiers and Innovations* 7.1 (2020). ISSN: 2313-8734 (pages 122, 123).

[7] Nan Ding and Samuel Williams. “An Instruction Roofline Model for GPUs.” In: *2019 IEEE/ACM Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS)*. 2019, pp. 7–18 (pages 122, 123).

References: Images, Graphics I

[1] Forschungszentrum Jülich. *Forschungszentrum Bird's Eye*. (Pages 3, 4).

[2] Rob984 via Wikimedia Commons. *Europe orthographic Caucasus Urals boundary (with borders)*. (Pages 3, 4).

[3] Forschungszentrum Jülich GmbH (Ralf-Uwe Limbach). *JUWELS Cluster*.

[4] Forschungszentrum Jülich GmbH (Ralf-Uwe Limbach). *JUWELS Booster*.