



10 YEAR ANNIVERSARY WORKSHOP NVIDIA APPLICATION LAB AT JÜLICH

21/22 June 2022 | Andreas Herten | Forschungszentrum Jülich

Workshop Agenda

Tuesday

13:00 Introduction

13:30 JUWELS Booster 

14:00 JUQCS

14:30 JUQMES, et al

15:00 Break

15:30 OpenGPT-X

16:00 PIconGPU 

16:30 Brain Simulation 

17:00 SOMA 

Wednesday

09:00 Hopper

09:40 MPTRAC

10:10 ParFlow 

10:40 Break

11:00 MESSy

11:30 D2Q37 LBM

12:00 M-AIA



EST 2012



Nutshell

- Signed Collaboration Agreement: ISC 2012 (18 June)
- Original team: Dirk Pleiter (JSC), Andrew Adinets (JSC), Jiri Kraus (NVIDIA)
- Changes: -Andrew (2015), +Andreas Herten (JSC, 2015), +Markus Hrywniak (NVIDIA, 2020), -Dirk (2021)
- Hosted by: Application-Oriented Technology Development → Accelerating Devices Lab
- 2014: POWER Acceleration and Design Centre
- 32 Trainings, 11 Conference Trainings, 18 Workshops
- *Many Applications Accelerated*

Systems

- JUDGE (M2050)
- JuHydra (K20X)
- JURECA (K80, K40 on vis nodes)
- JURON (P100)
- JUWELS Cluster (V100)
- JUSUF (V100)
- JUWELS Booster (A100)
- JURECA DC (A100)
- ???

Courses

- Many courses together with *Many-Core Group*
- CUDA Course (Pre-Lab: 2010, 2011, 2012; Lab: 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022)
- OpenACC Course (2015, 2016, 2017, 2018, 2019, 2020, 2021)
- Guest Students (2017, 2018, 2019, 2020, 2021)
- Introduction to Supercomputers at JSC (2018², 2019², 2020², 2021², 2022)
- Dec 2020: JSC GPU Crash Course (*All I want for Christmas is GP-U*) 

Hackathons, Workshops, Trainings

- GPU Hackathons:

- 2016 GPU Hackathon (Dresden)

- 2017 Eurohack (JSC) [↗](#)

- 2018 GPU Hackathon (Dresden)

- 2019 Helmholtz GPU Hackathon (JSC) [↗](#)

- 2020 Helmholtz GPU Hackathon (virtual) [↗](#)

- 2021 Helmholtz GPU Hackathon (virtual)

- 2022 Helmholtz GPU Hackathon (virtual+Berlin) [↗](#)

- Workshops et al

- 2020 JUWELS Booster Early Access Program

- 2020 Tunathon Onlineathon Booster Prep Days

- 2021 JUWELS Booster Early Access Colloquium



- 2021 JUWELS Booster Porting Workshop 2021

- 2022 JUWELS Booster Tuning and Scaling Workshop 2022 [↗](#)

- NVLab/PADC Workshop

- 2012 NVLab Kick-Off Meeting

- 2013 NVLab 1st Annual Workshop

- 2014 NVLab 2nd Annual Workshop

- 2015 PADC Opening Workshop [↗](#)

- 2016 PADC Annual Workshop [↗](#)

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External Trainings

- OpenPOWER Tutorial: SC16, SC17, SC18, SC19
- GTC Tutorial: 2018, 2019
- Multi-GPU Tutorial: SC21, ISC22, SC22
- GridKa Summer School: 2017, 2018, 2019
- MSA GPU Seminar Series (Nov 2019 - Jul 2020)

External Trainings

- OpenPOWER Tutorial: SC16, SC17, SC18, SC19
- GTC Tutorial: 2018, 2019
- Multi-GPU Tutorial: SC21, ISC22, SC22
- GridKa Summer School: 2017, 2018, 2019
- **MSA GPU Seminar Series (Nov 2019 - Jul 2020)**

RECAP GPU SERIES

● Technology ● Applications

- 26 Nov 2019 Introduction to GPU Programming with CUDA C/C++, [Jiri Kraus](#) (NVIDIA) [↗](#)
- 3 Dec 2019 Tools for GPU Computing, [Michael Knobloch](#) (JSC) [↗](#)
- 14 Jan 2020 GPU accelerated Quantum ESPRESSO, [Pietro Bonfà](#) (Uni Parma) [↗](#)
- 21 Jan 2020 Multi-GPU Programming with MPI, [Jiri Kraus](#) (NVIDIA) [↗](#)
- 28 Jan 2020 GPUs at CSCS and Arbor, [Ben Cumming](#) (CSCS) [↗](#)
- 4 Feb 2020 Directive-based GPU programming with OpenACC, [Andreas Herten](#) (JSC) [↗](#)
- 11 Feb 2020 SOMA: Scaling Soft Polymers to many GPUs via OpenACC, [Ludwig Schneider](#) (Uni Göttingen) [↗](#)
- 18 Feb 2020 GPU libraries — Get More for Less, [Jan Meinke](#) (JSC) [↗](#)
- 7 May 2020 Lattice QCD on modern GPU systems, [Mathias Wagner](#) (NVIDIA) [↗](#)
- 7 May 2020 Scaling Lattice QCD on many GPU Nodes of JUWELS, [Eric Gregory](#) (JSC) [↗](#)
- 19 May 2020 PIconGPU: 10 years of living with the HPC hardware zoo, [Michael Bussmann](#) (HZDR) [↗](#)
- 2 Jun 2020 Hydrologic modeling on GPUs with ParFlow, [Jaro Hokkanen](#) (FZJ) [↗](#)
- 9 Jun 2020 Heterogeneous parallelization in GROMACS, [Szilárd Páll](#) (KTH Stockholm) [↗](#)
- 16 Jun 2020 TB-scale Image analysis with HPC-enabled Deep Learning for mapping the human brain, [Christian Schiffer](#) (FZJ) [↗](#)
- 23 Jun 2020 CUDA 11 and A100 - What's new?, [Markus Hrywniak](#) (JSC) [↗](#)
- 30 Jun 2020 More science, fewer bits – Mixed-Precision Comp. with Tensor Cores, [Julien Demouth](#), [Mathias Wagner](#) (NVIDIA) [↗](#)
- 7 Jul 2020 JUWELS Booster – Design of JSC's GPU-Based Flagship System, [Damian Alvarez](#), [Dorian Krause](#) (JSC)

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Inaugural Workshop at JSC

NVIDIA Application Lab Kick-off Workshop

Status: 11.09.2012

Wednesday, 19.9.2012

9:00	10:30	Peter Messmer (NVIDIA)	Kepler and CUDA 5 – Overview and first experiences
10:30	11:00	<i>Coffee</i>	
11:00	11:45	Markus Axer/ Marcel Huysegoms (FZJ, INM-1)	How to build a 3D human brain model from thousands of histological sections
11:45	12:30	Frank Winter (U Edinburgh)	Migration of a Data-Parallel, Expression Template based Vector Library to GPU-enabled Multi-Node Systems
12:30	14:00	<i>Lunch</i>	
14:00	14:45	John Romein (ASTRON)	Signal Processing on GPUs for Radio Telescopes
14:45	15:30	Richard Leys (U Heidelberg)	EXTOLL – A feature rich interconnect for HPC
15:30	16:00	<i>Coffee</i>	
16:00	17:30	Jiri Kraus (NVIDIA)	Cuda-aware MPI (incl. Hands-on)

19:30	...	<i>Dinner (Kaiserhof)</i>	
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Thursday, 20.9.2012

9:00	9:45	Rainer Spurzem (NAOC/CAS Beijing and ARI/ZAH U Heidelberg)	GPU Supercomputing in China and Germany and Application to super-massive black holes and gravitational waves from galactic nuclei
9:45	10:30	Fabio Schifano (U Ferrara)	Implementation and optimization of a thermal Lattice Boltzmann Algorithm on a multi-GPU cluster
10:30	11:00	<i>Coffee</i>	
11:00	11:45	Jan Meinke (FZJ, JSC)	Modelling Molecules with Python and GPUs
11:45	13:00	Peter Philippen (FZJ, JSC)	Score-P - Scalable performance analysis on accelerated architectures (incl. Hands-on)

1st Workshop at JSC

NVIDIA Application Lab / 1st Annual Workshop

Status: 03.07.2013

Monday, 8 July 2013		
9:00 – 9:15	D. Pleiter	Welcome
9:15 – 10:00	A. Adinetz / J. Meinke	GPUMAFIA: Subspace Clustering with MAFIA on GPU
10:00 – 10:30	D. Champion	Pulsar Searching with GPUs
10:30 – 11:00		Coffee
11:00 – 11:30	R. Speck	On parallel-in-time integration
11:30 – 12:00	A. Herten	GPUs at High Energy Physics and PANDA
12:00 – 12:30	S. Köhnen	Update on the Jubrain project (TBC)
12:30 – 14:00		Lunch
14:00 – 15:00	T. Bradley	Future Directions for CUDA
15:00 – 15:30	F. Schifano	Benchmarking GPU architectures with Lattice Boltzmann simulations
15:30 – 16:00		Coffee
16:00 – 17:00	J. Kraus	Introduction to OpenACC

20:00 - ...	Dinner
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Tuesday, 9 July 2013		
9:00 – 9:45	L. Oden	GPI2 for GPUs: A PGAS-API for efficient communication in Hybrid Clusters
9:45 – 10:30	M. Bussmann	Playing with Petaflops - Interactive, large-scale Plasma Simulations with GPUs
10:30 – 11:00		Coffee
11:00 – 11:30	P. Wahl	B-CALM: An multi-node multi GPU 3D FDTD simulator
11:30 – 12:00	A. Lintermann	ZFS - Flow Solver AIA
12:00 – 12:30	J. Kraus	OpenACC 2.0 Highlights

Inaugural Announcement at GCS

In InSIDE Spring 2013, Part I

For many applications, using a single GPU is not sufficient, either because more computing power is required, or because the problem size is too large to fit into the memory of a single device. This forces application developers to not only consider parallelization at device level, but also to manage an additional level of parallelism.

Depending on the application this may be challenging since on most architectures device- to-device communication through the network is implemented as split transactions via the host processor. Software solutions like CUDA-aware MPI implementations can help mitigate this problem, but ultimately better hardware support is needed to interconnect GPU and network devices.

Inaugural Announcement at GCS

In InSIDE Spring 2013, Part II

The lab is jointly operated by Jülich Supercomputing Centre (JSC) and NVIDIA since July 2012. For JSC it is yet another step to further strengthen links to vendors that are actively pursuing an exascale strategy.

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To the next years!!
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