McStas McXtrace

Team

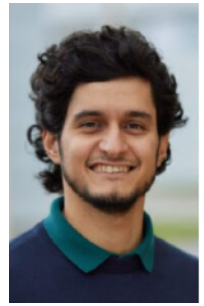
Peter Willendrup
DTU / ESS DMSC

Mads Bertelsen
ESS DMSC

Gregory S Tucker
ESS DMSC

Emmanuel Farhi
Synchrotron SOLEIL

Tobias Weber
Institut Laue-Langevin



José Robledo
FZ Jülich / IAS / JSC

Team Mentors

Jan-Oliver Mirus
FZ Jülich / IAS / JSC

Ilya Zhukov
FZ Jülich / IAS / JSC

OpenACC More Science, Less Programming

OPEN HACKATHONS

- Problem the team is trying to solve.

  Speed up our MC ray-tracing code on GPU, understand bottlenecks

- Scientific driver for the chosen algorithm.

  Used to understand instrumentation at large scale facilities (x-ray / neutron)

- What's the algorithmic motif?

  Monte Carlo ray-tracing framework

- What parts are you focused on?

  Memory transfers, access patterns and structure

Evolution and Strategy

- What was your goal for coming here?

  Our GPU performance had plateaued, needed new knowledge to progress

- What was your initial strategy?

  Hope our mentors would inspire us!

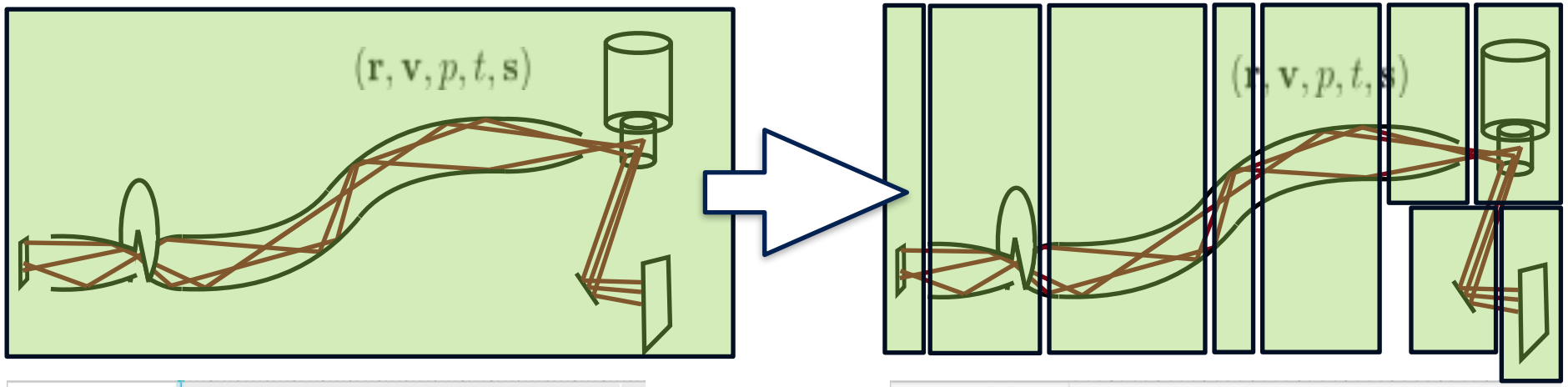
- How did this strategy change?

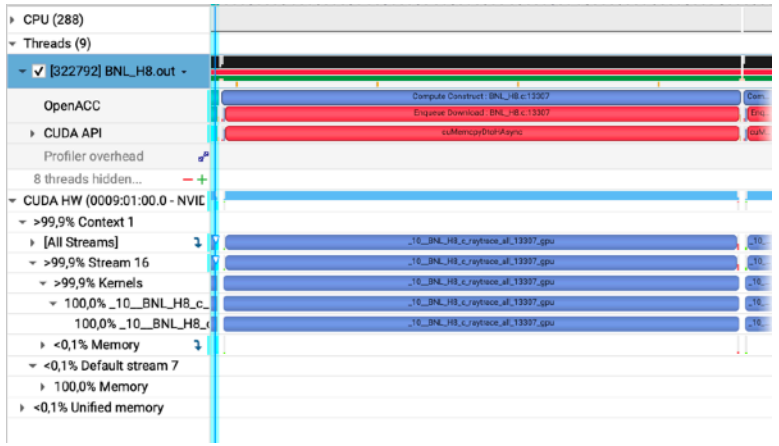
  We almost lost faith as we initially didn't see speedup, but did progress

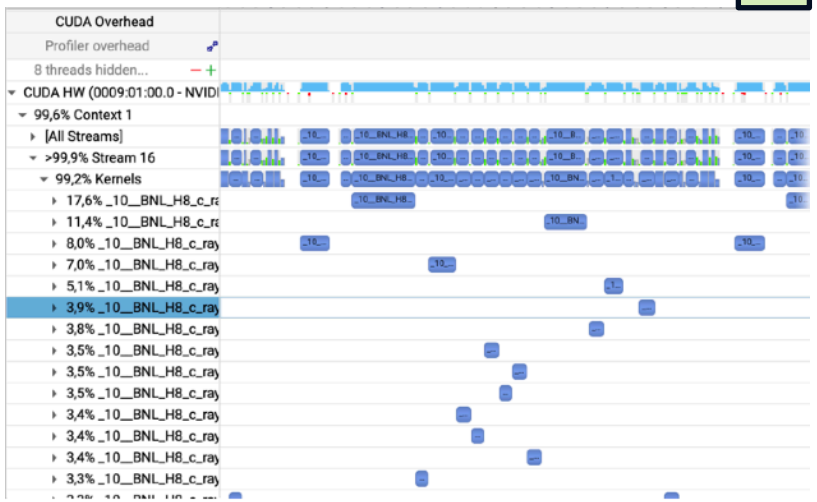
Results and Final Profile

- What were you able to accomplish?
  - Did you achieve a speed up? **Yes! Speed 116% (comparison on GH200)**
  - Show multi-core vs. GPU numbers: **GH200 ~ 112 CPU cores**
- What did you learn?
  Learnt more about registers and profiling tools
  - Did you create a new algorithm?
    We changed memory structure / number of kernels
  - Did you achieve new scientific goals?
    Yes, this speed up is significant for our work!

Results and Final Profile







Energy Efficiency

INPUTS		
Baseline	GPU	*Select the baseline as GPU or CPU*
Baseline GPU Type	4x GH200 (Helios)	*Select the CPU/GPU Type or GPU Node configuration*
Baseline GPU # GPUs	1	*Select the number of CPU cores or GPUs (within one node)*
Final GPU Node	4x GH200 (Helios)	*Select the final GPU Type or GPU Node configuration*
Final # GPUs	1	*Select the number of GPUs (within one node)*
Application Speedup	2.2x	*Enter the amount of achieved speedup*

Node Replacement	2.2x

GPU NODE POWER SAVINGS			
	Baseline	**Comparison**	
	4x GH200 (Helios)	4x GH200 (Helios)	**Power Savings**
Compute Power (W)	6,350	2,940	3,410
Networking Power (W)	216	100	116
Total Power (W)	**6,566**	**3,040**	3,526

Node Power efficiency	**2.2x**

ANNUAL ENERGY SAVINGS PER GPU NODE			
	4x GH200 (Helios)	4x GH200 (Helios)	**Power Savings**
Compute Power (kWh/year)	55,630	25,754	29,875
Networking Power (kWh/year)	1,892	876	1,016
Total Power (kWh/year)	**57,522**	**26,630**	**30,891**

$/kWh	$	0.18
Annual Cost Savings	$	5,560.43
3-year Cost Savings	$	16,681.28

Metric Tons of CO2	22
Gasoline Cars Driven for 1 year	5
Seedlings Trees grown for 10 years	362

(source: Link)

According to calculator:

Saving 31MWh per year if we ran continuously for a year

6.5kW -> 3.0 kW when running

What problems have you encountered?

- Problems with legacy app structure.
  We had array of structures, went to structure of arrays
- Issues with algorithms.
  Single particle at a time didn't leave options for controlling parallelisation
  Working in bunches was the main improvement
- Tool bugs. **None**
- Tool lacking features.
  Would have loved profiling within kernels as our old kernel was huge
- System setup. **No issues!**

Wishlist

What do you wish existed to make your life easier?

- Tools: **More detailed information about workload inside each kernel**
- Language standards: **Would be great with function pointers in openACC**
- Event: **All great, thanks!**
- Systems: **Perhaps option of testing on less forgiving GPU**

Final Thoughts

- Was this Open Hackathon worth it?
  Yes, our simulations now take less than half the time

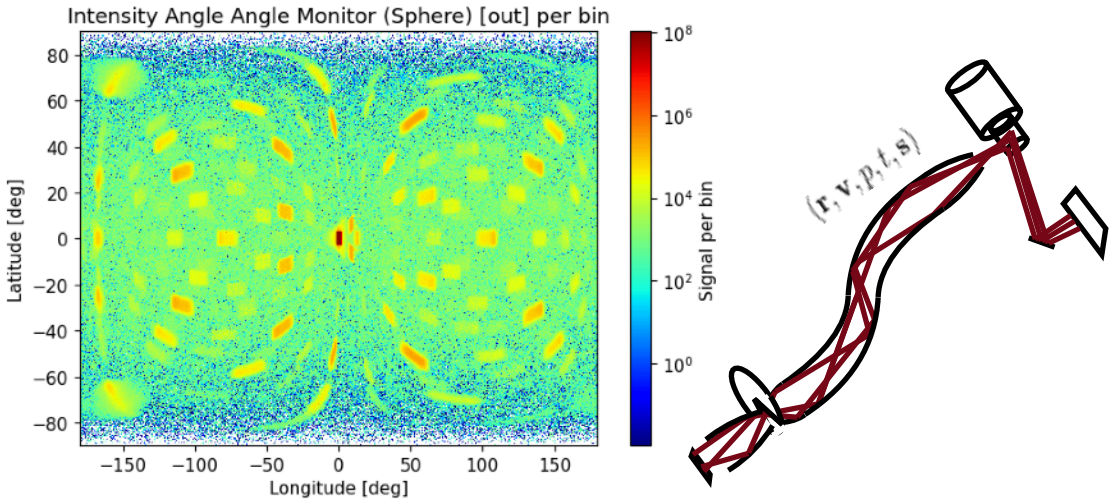
- Will you continue development?
  - **Yes, our faster version is a prototype with disabled features**
  - **Envision further speed / efficiency improvements**

- What sustained resources or support will be critical for your work after the event?

  Occasional conversation with mentors

Application Background

- Simulation tool for x-ray and neutron instrumentation at large scale facilities
- Instruments can be up to 20M€, needs to be carefully studied before construction
- Costs around 1€ per second o use, each usecase should be carefully considered



Single crystal Laue diffraction for large crystal

Hackathon Objectives and Approach

- Improve computation speed on GPU
- Change memory structure
- Change kernel size
- Correctness, removed several race conditions that prevented deterministic results

Technical Accomplishments and Impact

- Improved computation efficiency by simulating particles in batches
- Speedup: 116%
- Faster simulations allow us to imagine more complex instruments and understand how they would work

Project Summary

Please summarize your team's achievements during the Open Hackathon (100 words).

The McStas/McXtrace team arrived with a code that did run reasonably well on GPU, but with with confidence that it could be significantly faster. Our mentors quickly understood our code and memory structure and suggested restructuring from array of structures to structure of arrays. This was accomplished, but did not immediately show a speed up. The new structure allowed the computation to be done in bunches of particles instead of individually, which did lead to a 116% speed up. In addition several race conditions were found and eliminated and we gained experience in using the critical profiling tools.

PROMOTING YOUR WORK: AVAILABLE OPPORTUNITIES

- **Papers and Talks:** Please acknowledge the Open Hackathons program and OpenACC Organization in any planned or upcoming papers, presentations, or talks.
  "This work was completed in part at the Helmholtz GPU Hackathon, part of the Open Hackathons program. The authors would like to acknowledge OpenACC-Standard.org for their support."
- **Social Media Support:** Please feel free to promote your participation across your social media channels. Tag **@OpenACCorg** and **#OpenHackathons** and we are happy to amplify.
- **Blogs and Technical Write-ups**: Create a blog post or technical article that highlights the work being done and results achieved.
- **Quotes and Testimonials:** Highlight your quote or feedback on our channels (i.e. social, website, etc.).

***Please reach out to Izumi Barker (ibarker@nvidia.com) to discuss marketing options and opportunities.**