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Porting McStas to GPU via code-generation and OpenACC pragmas

Main events on timeline of current developments

2017: E. Farhi
initial cogen
modernisation

Fall 2018 onwards: J. Garde
further cogen modernisation and
restructuring

October 2019 onwards:
J. Garde & P. Willendrup:
New RNG, test system, multiple
functional instruments.

March 2018:
Participation at
Dresden Hackathon.
1st “null” instrument
prototype runs.

October 2019:
Participation at Espoo
Hackathon. First meaningful
data extracted. Work on
cogen and realising we need
another RNG.

November-
December 2019:
First good look at
benchmarks and
overview of what
needs doing for first
release with limited
GPU support.



NVIDIA mentor: Vishal Metha



NVIDIA mentor: Christian Hundt

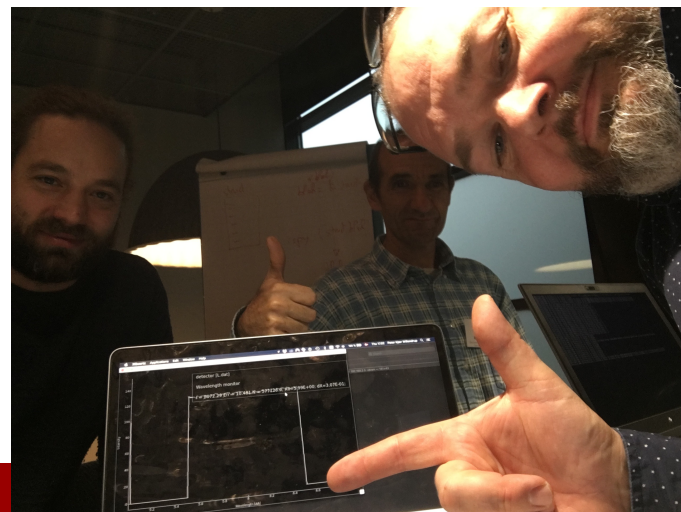
McStas heading for the GPU... October 2019

Rewritten code-
generation with
automated additions of
OpenACC pragmas.

Quite transparent wrt.
CPU vs. GPU

First simulations with
meaningful output

Speed on DELL with
Quadro-card ~ on par
with running on CPU
with MPI



GPU Hackathon

Introduction

CSC is in collaboration with Nvidia and the E-CAM European HPC center of Excellence arranging a 3-day GPU hackathon. The GPU hackathon is a coding event in which teams of developers port their applications or kernels to run on GPUs, or optimize their applications that already run on GPUs. In particular the hackathon focuses on applications that can scale up to multiple GPU nodes.

We are looking for teams of 3-4 developers. Collectively the team should know the application intimately. Please keep in mind that we are looking for teams with plans to develop GPU code – not to just run their code on GPUs. During the hackathon each team is supported by one mentor with in-depth GPU programming expertise.

At CSC the new Puhti-AI partition provides 80 nodes with 4 Nvidia Volta GPUs each. This system provides in total more than 2 petaflops of performance. This system is available during the course and accepted teams will also have access to the system beforehand to do some initial porting of the applications to Puhti.

Date: 16.10.2019 9:00 - 18.10.2019 17:00

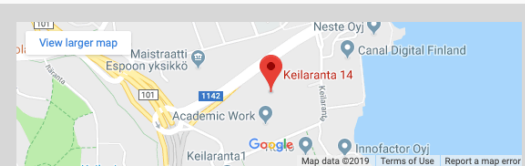
Location details: The event is organised at the CSC Training Facilities located in the premises of CSC at Keilaranta 14, Espoo, Finland. The best way to reach us is by public transportation; more detailed [travel tips](#) are available.

Language: English

Price:

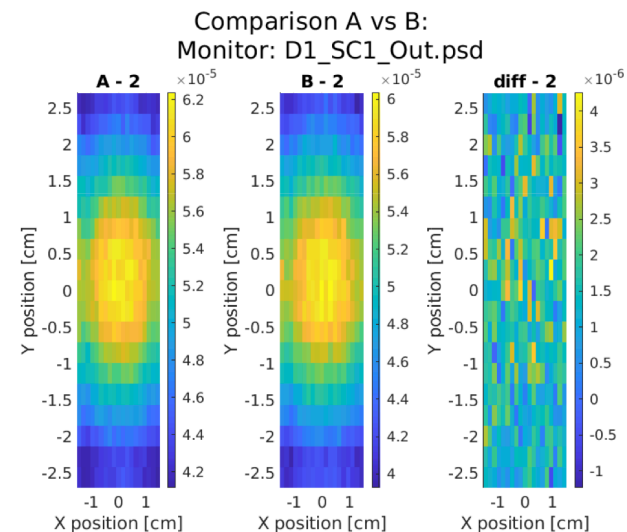
- Free for Finnish universities, universities of applied sciences and governmental research institutes.
- Free for others.

The fee covers all materials, lunches as well as



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McStas heading for the GPU... November 2019

9 instruments fully
ported, also realistic
ones like PSI_DMC*

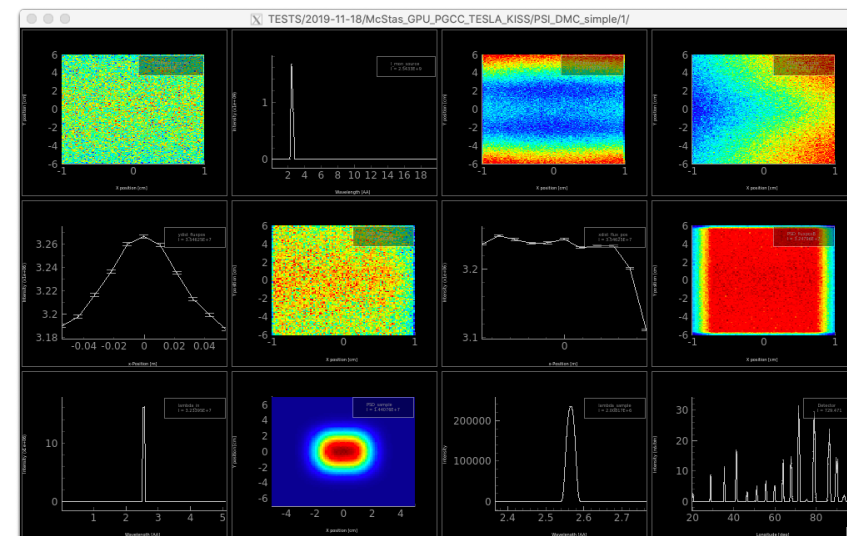
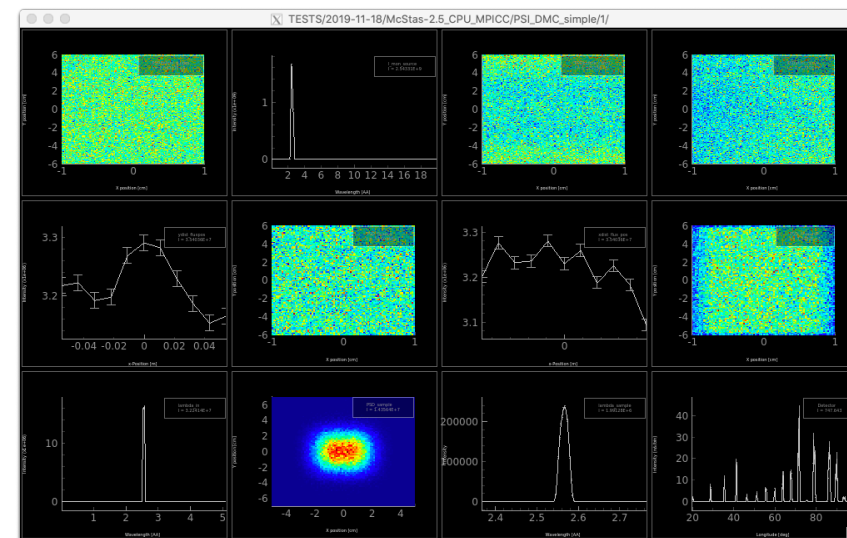
10-core MPI run,
1e7 in 2 secs



Tesla V100 run,
1e9 in 22 secs



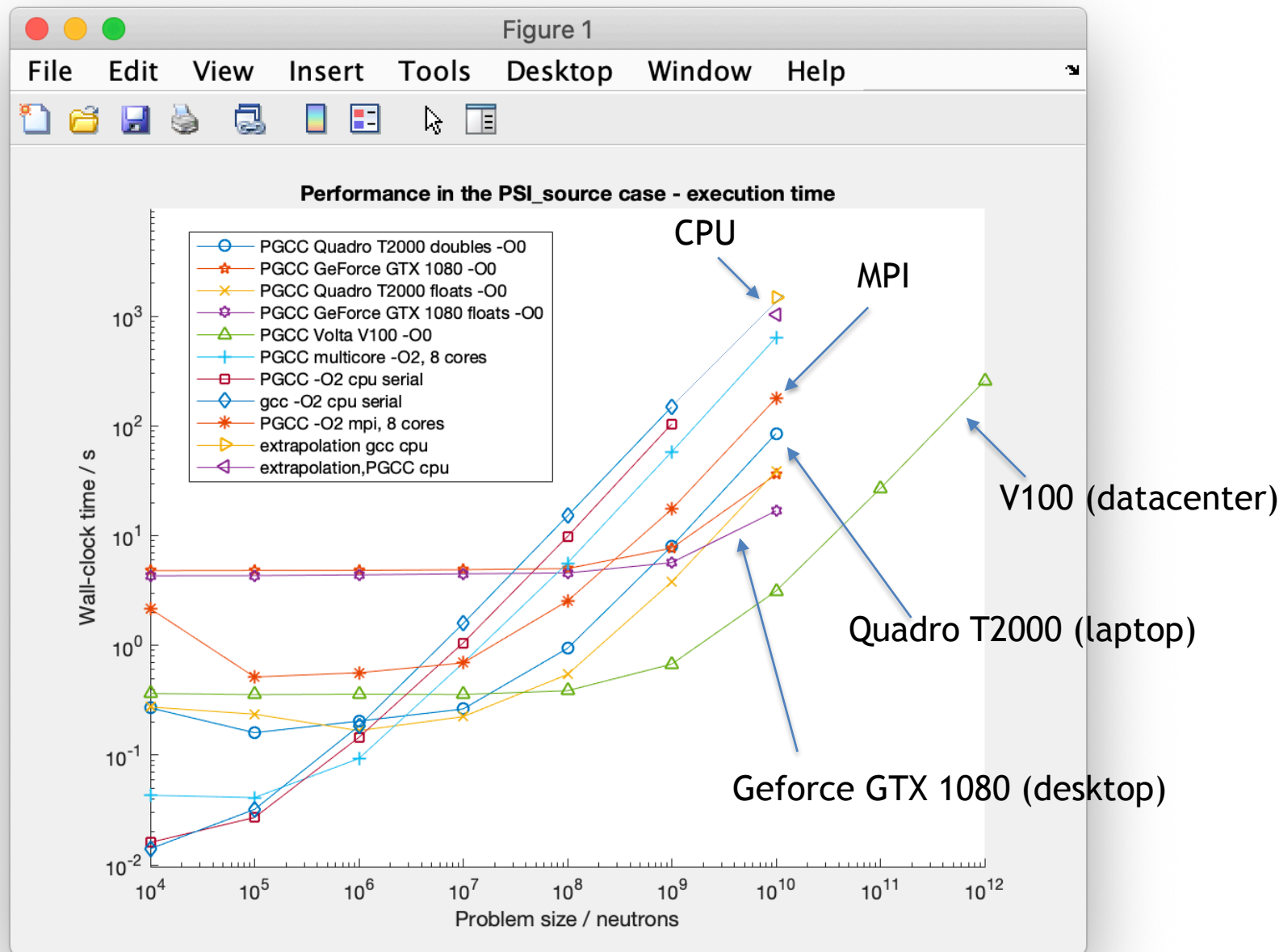
~ i.e. 2 orders of
magnitude wrt. a single,
modern CPU core



*Guide component without reflection-file support, SPLIT disabled, OFF geometry disabled

Idealised instrument
with source and monitor
only - i.e. without any
use of the ABSORB
macro.

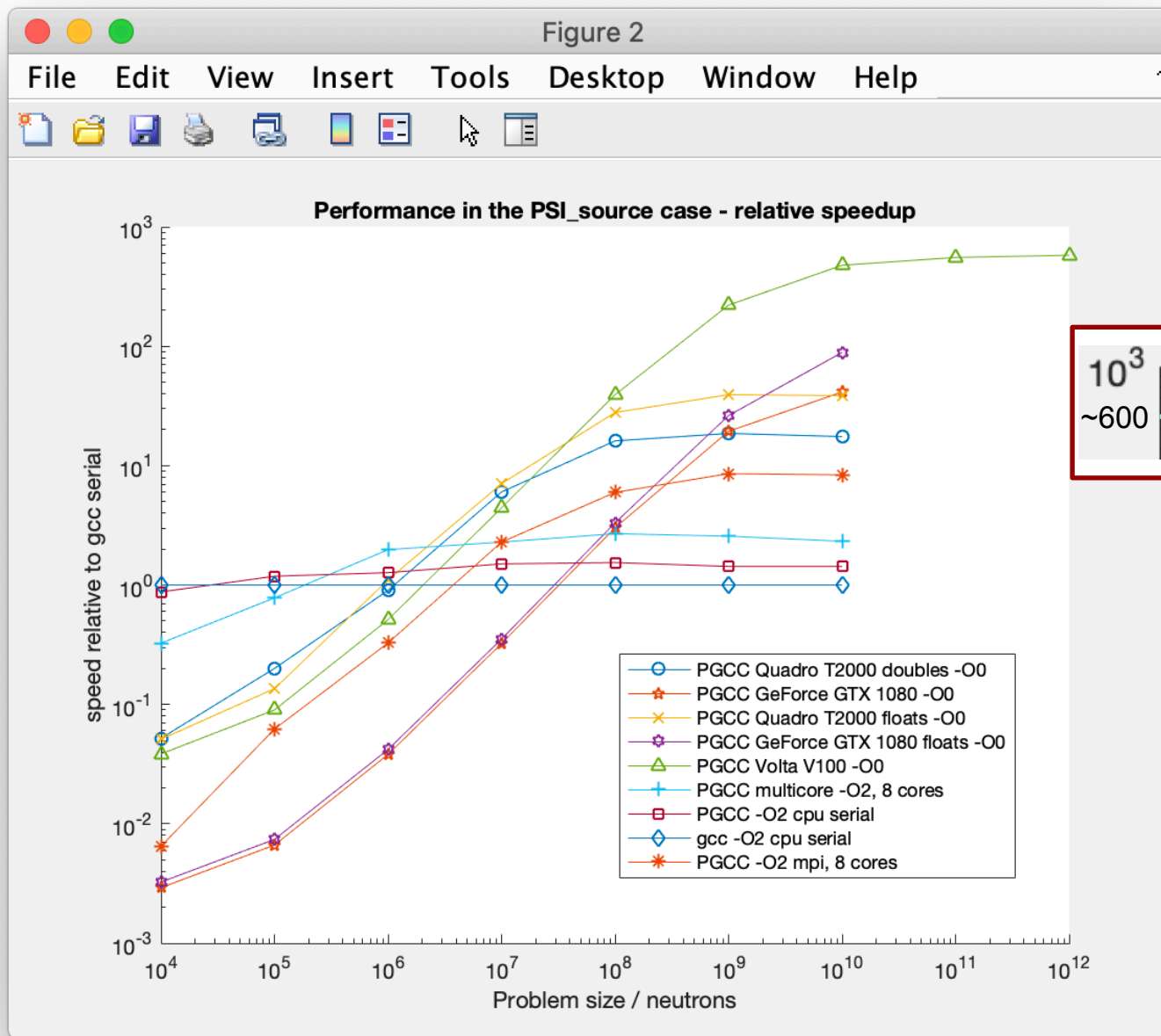
(Likely a good indication
of maximal speedup
achievable.)



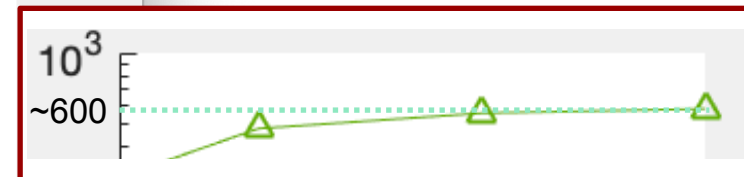
McStas heading for the GPU... November 2019 - first good look at performance. Speedup:

Idealised instrument
with source and monitor
only - i.e. without any
use of the ABSORB
macro.

(Likely a good indication
of maximal speedup
achievable.)



Looks like a factor of ~600



Renormalised to wall-
clock of single-core
gcc standard simulation

McStas heading for the GPU... December 2019 - today's compilation status:

Numerical output with graphics:

http://new-nightly.mccode.org/2019-12-06/2019-12-06_output.html

Statistics:

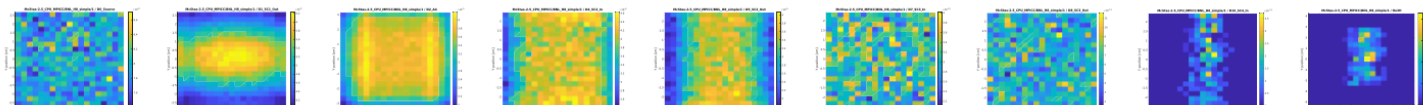
<http://new-nightly.mccode.org/2019-12-06/stats.txt>

(38 of 142 instruments, 62 of 207 components)

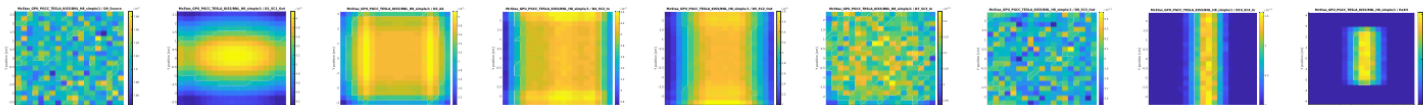
BNL_H8_simple/1 - comparison McStas-2.5_CPU_MPICC vs McStas_GPU_PGCC_TESLA_KISS

(Click to access files)

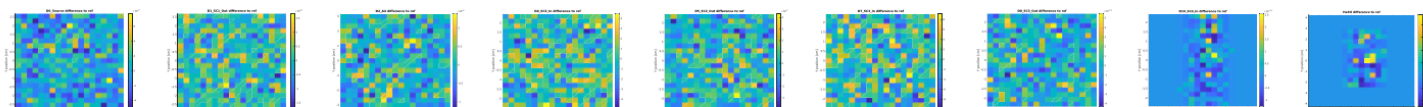
McStas-2.5_CPU_MPICC (reference)



McStas_GPU_PGCC_TESLA_KISS



Difference



test results

ref user: pkwi

	McStas-2.5_CPU_MPICC (ref) - 1e7 n-62-23-6 Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80GHz 20191120_0127_38	McStas_CPU_GCC_KISS - 1e6 n-62-21-99 Intel(R) Xeon(R) CPU E5-2650 v4 @ 2.20GHz 20191205_0058_36	McStas_CPU_GCC_MT - 1e6 n-62-21-99 Intel(R) Xeon(R) CPU E5-2650 v4 @ 2.20GHz 20191205_0122_14	McStas_CPU_MPICC_KISS - 1e7 n-62-23-9 Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80GHz 20191205_0034_53	McStas_GPU_PGCC_TESLA_KISS - 1e9 n-62-20-6 Intel(R) Xeon(R) Gold 6126 CPU @ 2.60GHz Tesla V100-PCIE-16GB 20191205_0012_04
BNL_H8_simple	5.80 s 1.99 s 9.7e-10 99%	4.32 s 1.03 s 1.3e-09 136%	4.35 s 0.99 s 1e-09 106%	4.11 s 1.50 s 1.1e-09 110%	17.59 s 8.16 s 9.7e-10 98%

McStas 3.0 - next generation code generator - release plans

- Limited-functionality “beta” release to be made public soon (jan-mar) after **2.6 (january)**
 - Expect bugs!
 - Only a subset of components / instruments
 - Event interchange with 2.6 possible via MCPL
- Main purpose: **get this working in ‘the wild’**
 - Your instruments will likely **require (limited) rewriting**
 - E.g. the declare section **cannot include assignments**
 - Your own components will **likely require rewriting**
 - E.g. the declare section **cannot include assignments**
 - Arrays must be declared/initialized using a new set of functions (i.e. not double PSD_I[nx][ny] with definition parms)
- Hence some backward compatibility is lost and we need **to increment major release #**

