Peter Willendrup and Erik Knudsen DTU Physics

mcxtrace-1.x vs. mcxtrace-3.0, status and elements of the GPU port

Agenda

- McXtrace on GPU via OpenACC
  (a “high-level” #pragma driven access to CUDA see https://www.openacc.org and https://developer.nvidia.com/hpc-sdk)
- How well (fast) does it work?
- Simulation flow
- What did we change?
- What needs doing on an instrument / component?
- What does not work

Warning:
1. Assumes some previous experience with McXtrace
2. Does not introduce OpenACC

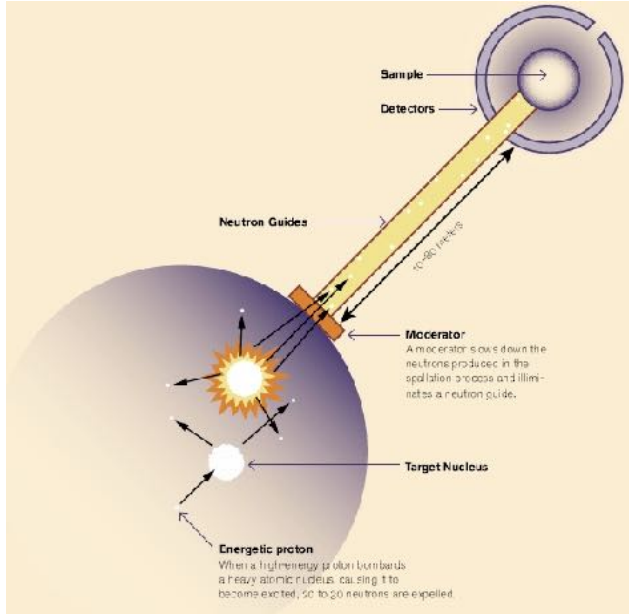
McStas and McXtrace overview

- Portable code (Unix/Linux/Mac/Windoze)
- Ran on everything from iPhone to 1000+ node cluster!

CPU's

+ NVIDIA GPU's

- 'Component' files (~200) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps
- DSL + ISO-C code gen.

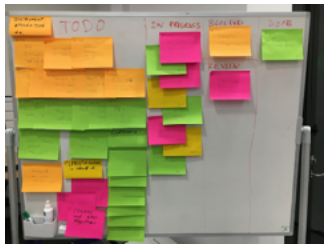


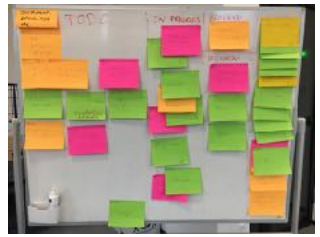
Main events on timeline of road toward GPU

December 15th 2020
McStas 3.0 release!

November 24th 2021
McStas 3.1 release!

February 8th 2022
McXtrace 3.0 release!





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.

January 2020:
One-week local hackathon **@ DTU**

with McCode & RAMP teams

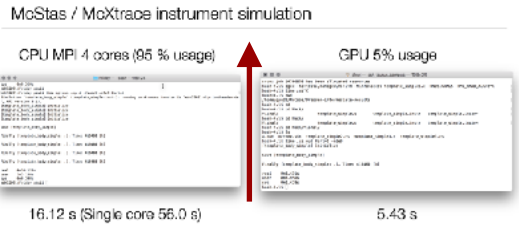
November 2020
Virtual Hackathon, setting release scope

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.

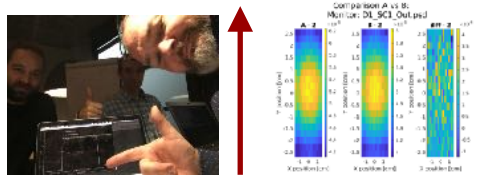
November-December 2019:
First good look at benchmarks and overview of what needs doing for first release with limited GPU support.

2020 1st **Corona** lockdown
P. Willendrup & E. Knudsen continue work on comp and cogen



mentor: Vishal Metha

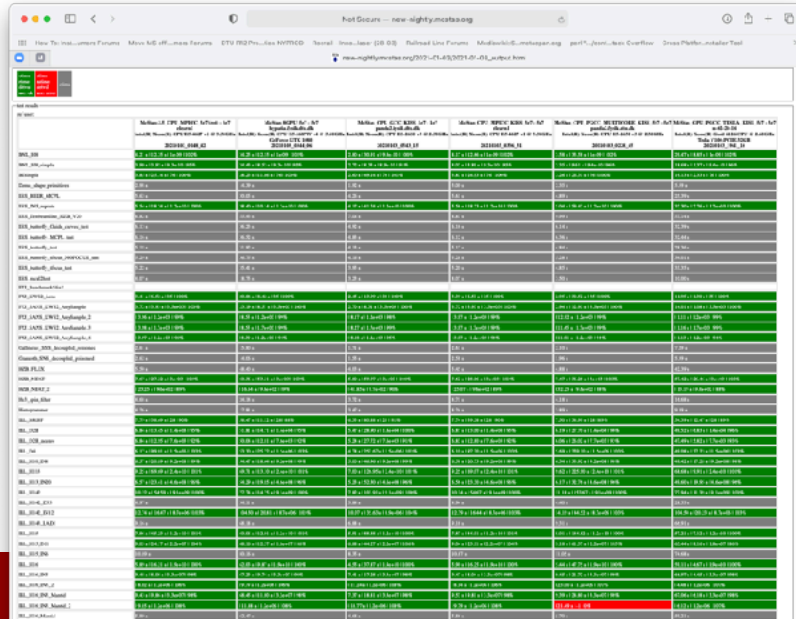
hackathon org.:
Guido Juckeland



mentor: Christian Hundt

hackathon org.:
Sebastian Von Alfthan

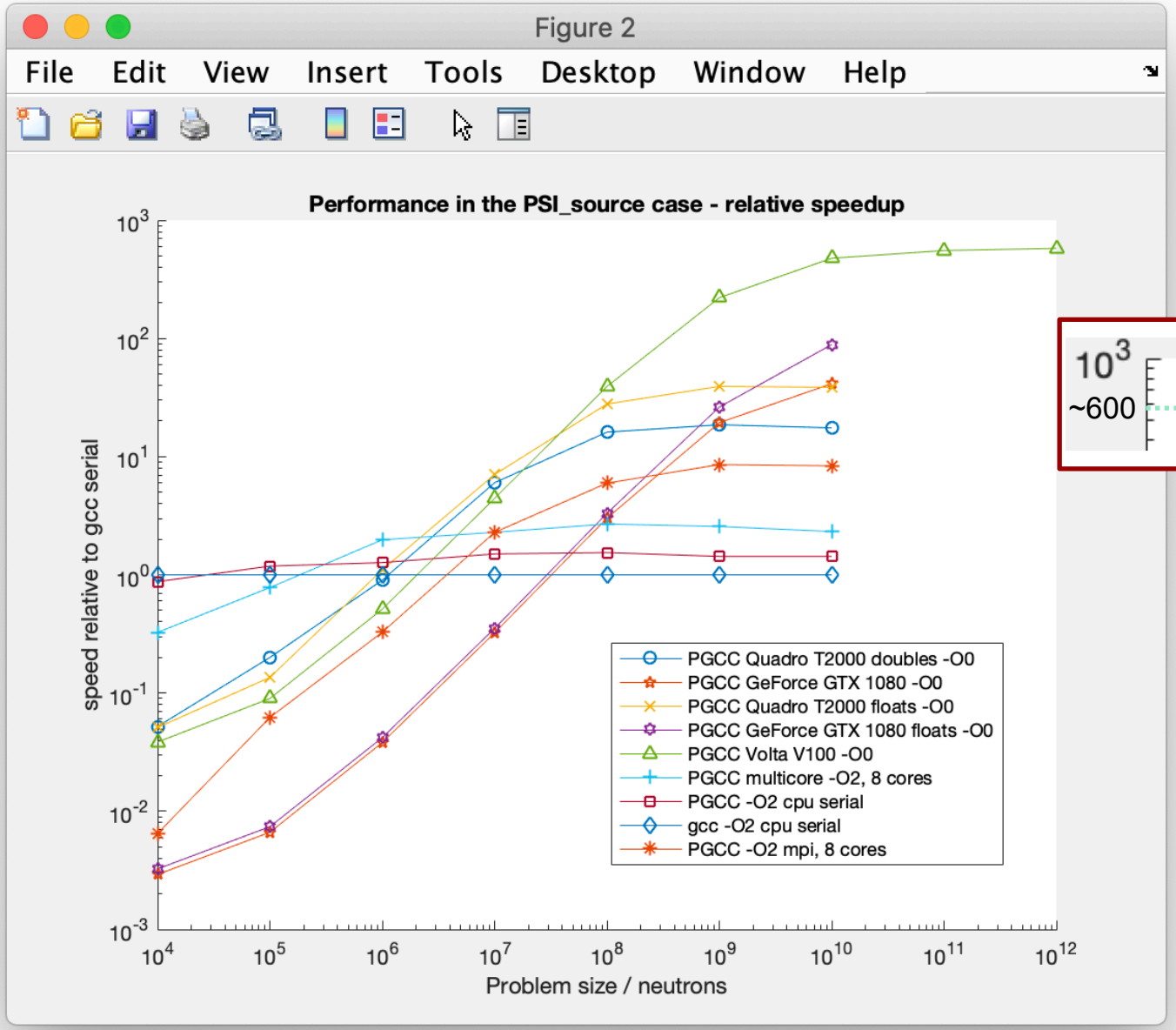
February 2020:
First release McStas **3.0beta** with GPU support was **released** to the public



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

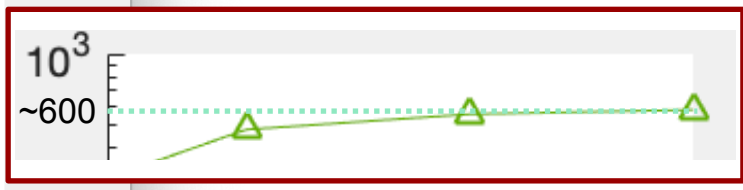
Idealised instrument with source and monitor only - i.e. without any use of the ABSORB macro.

(Likely a good indication of maximal speedup achievable.)



Speedup

Looks like a factor of ~600



V100 execution speedups renormalised to wall-clock of single-core gcc standard simulation,

V100 run is 600 times faster than a single-core CPU run

McStas heading for the GPU… first benchmarking numbers from November 2019

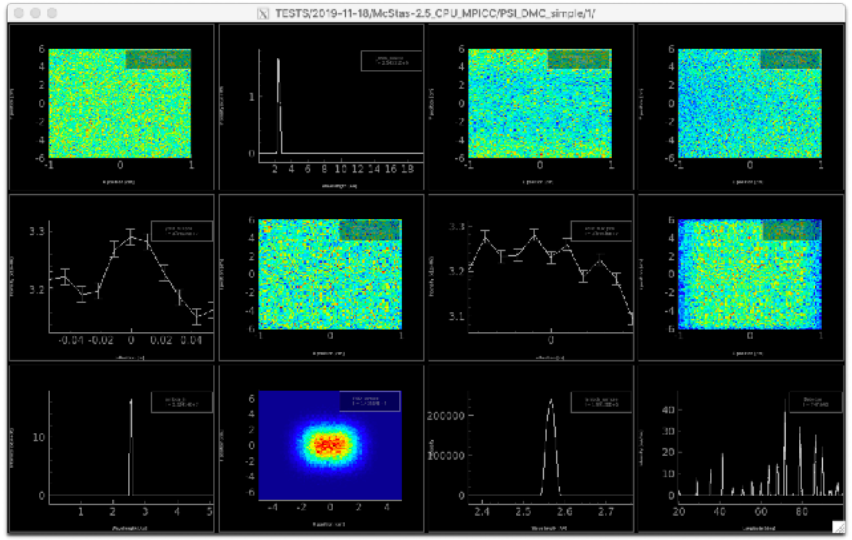
9 instruments fully ported, also realistic ones like PSI_DMC

(Aug 2020: 99 instrs)

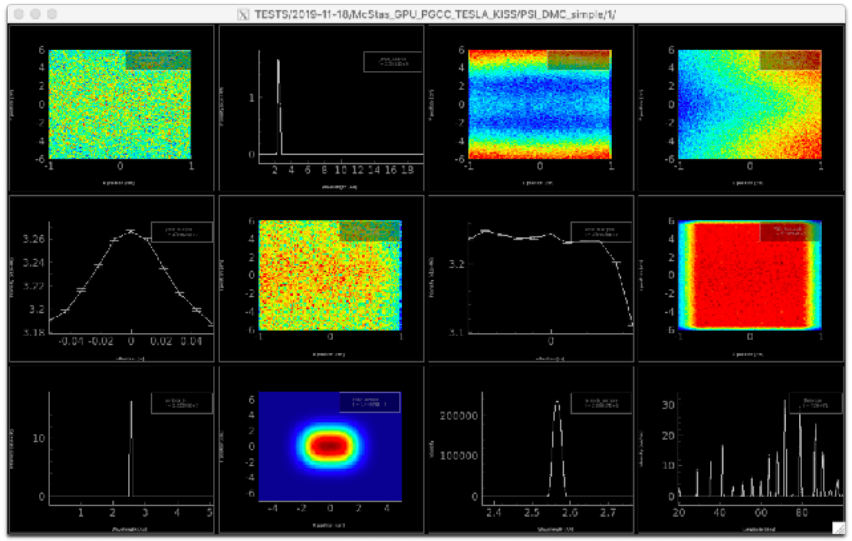
10-core MPI run, **1e9** in 200 secs

(1-core run, **1e9** would be 2000 secs)

VS.



Tesla V100 run, **1e9** in 22 secs



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

- If problem has the right size / complexity, GPU via OpenACC is great!

McXtrace

McStas

McStas 2.x -> McStas 3.0 main differences

- **Rewritten** / streamlined simplified **code-generator** with
  - Much **less generated code**
  - **improved compile time and compiler optimizations**, esp. for large instrs
  - **Much less invasive use of #define**
  - **Component sections -> functions** rather than #define / #undef
  - Much **less global variables,** instrument, component and particle reworked to be **structures**

Advantage of 3.0 also on CPU

- Use of **#pragma** acc … in lots of places (**put in place by cogen** where possible)

OpenACC

- **New random number generator** implemented
  - We couldn't easily port our legacy Mersenne Twister
  - Experimenting with curand showed huge overhead for our relative small number of random numbers
    (we have hundreds or thousands of randnom numbers, not billions)

- Complete change to **dynamic** monitor-arrays

McXtrace

McStas

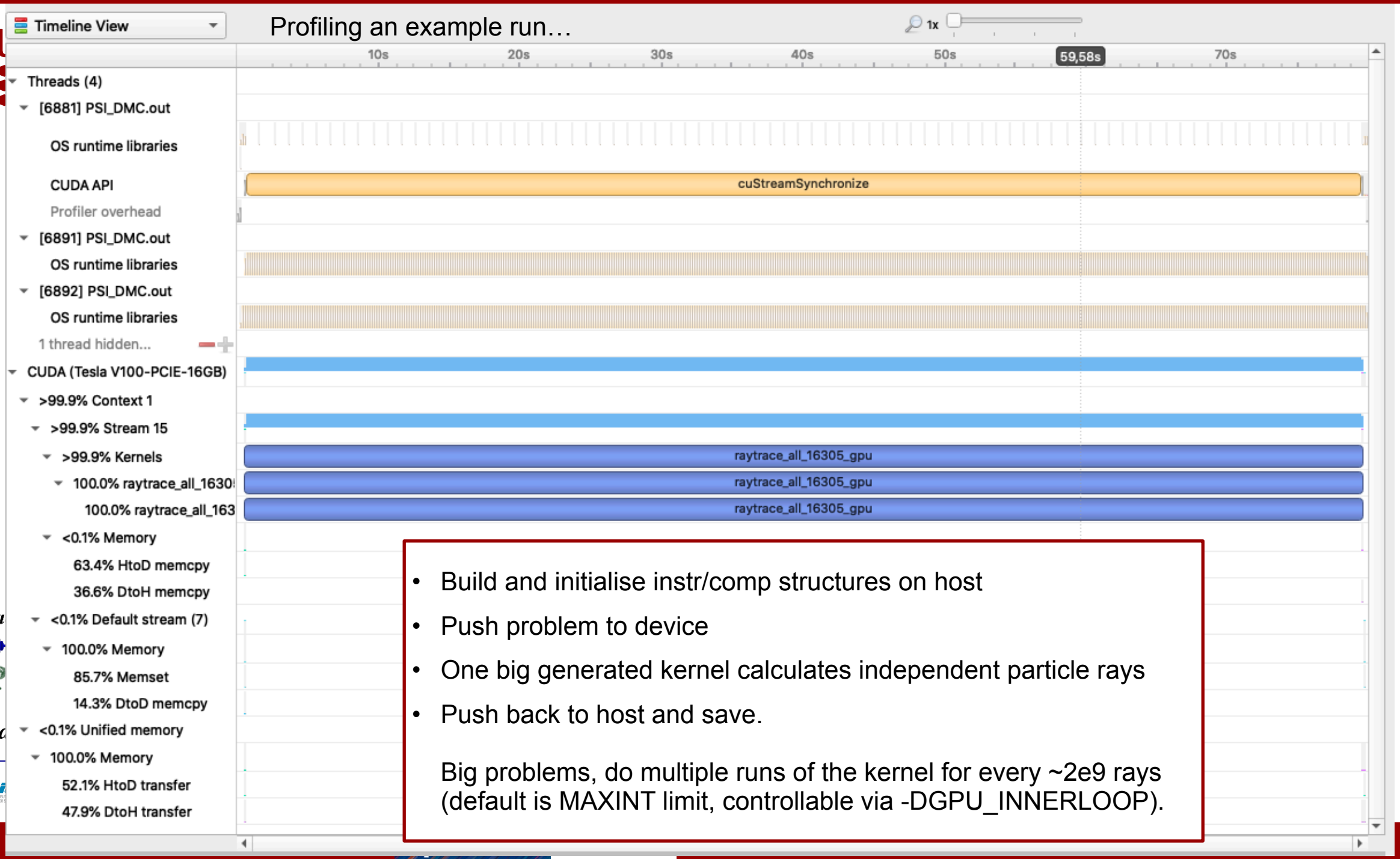
Anatomy of a McStas GPU run (*)

- Init, geometry, files etc. read on CPU
  - MPI if needed
- Memory-structures
  - Built on CPU
  - Marked for transfer to GPU (#pragma acc declare create etc.)
  - Initialised and synced across
  - Trace-loop is a #pragma acc parallel loop
    - Calculation performed entirely on GPU
  - Component structs (incl. e.g. monitor-arrays) synced across
- Finally and Save runs on CPU
  - MPI merge if needed

No printfs etc. available on GPU, automatically suppressed by #defines

(* Alternative layout via FUNNEL mode, see next 2 slides)

Profiling an example run…

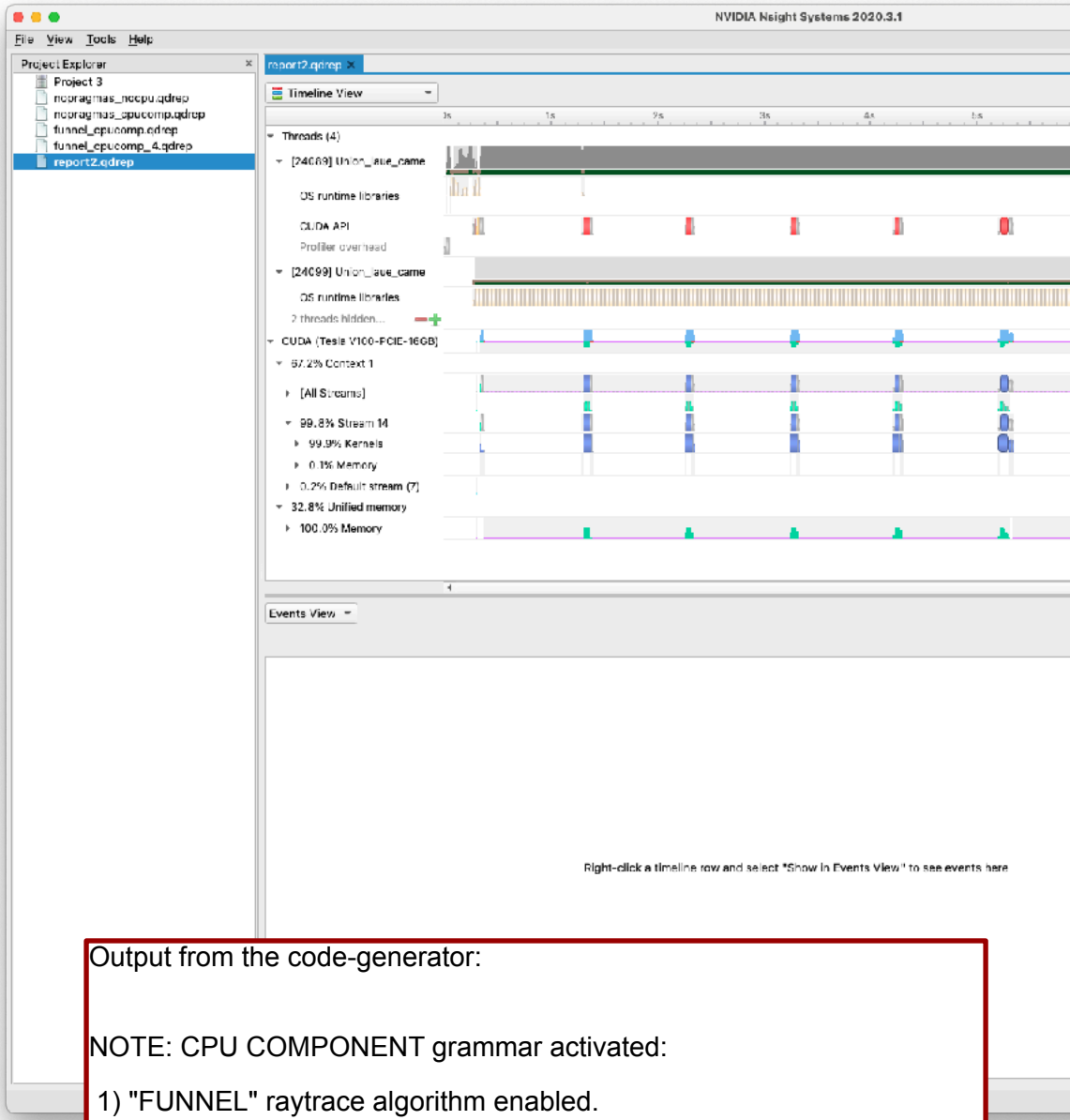


- Build and initialise instr/comp structures on host
- Push problem to device
- One big generated kernel calculates independent particle rays
- Push back to host and save.

Big problems, do multiple runs of the kernel for every ~2e9 rays (default is MAXINT limit, controllable via -DGPU_INNERLOOP).

FUNNEL mode

- Activated **explicitly** using -DFUNNEL or **implicitly** using CPUCOMPONENT in instrument or NOACC in comp header
- Has N kernels / calculation zones instead of one
    1. Separation at SPLIT
    2. Separation if CPUCOMPONENT in instrument file
       (CPUCOMPONENT A=Comp(vars=pars…))
    3. Separation if a component has NOACC in the header
       (See e.g. Multilayer_sample, Union_master)
- Each of these “calculation zones” is finalised before the next one initiated.
- Example:
  Union: Instrument up to Union_master can be GPU, then CPU, then GPU again
    - Can be as slow as single cpu…
    - Copying back and forth to/from GPU is costly…



Output from the code-generator:

NOTE: CPU COMPONENT grammar activated:

1) "FUNNEL" raytrace algorithm enabled.

2) Any SPLIT's are dynamically allocated based on available buffer size.

- Illustration, simple instr with
- Instr vars and “flag”
- Arm
- Source
- Slit
- PSD

example_v25.instr

```
/*
* %Example: example.instr dummy=0 Detector: detector_I=345.995
*/
DEFINE INSTRUMENT Minimal(dummy=0)

DECLARE %{
  double constant=2;
  double two_x_dummy;
  double flag;
%}

INITIALIZE %{
  two_x_dummy=2*dummy;
%}

TRACE

COMPONENT arm = Arm()
AT (0, 0, 0) ABSOLUTE
EXTEND %{
  flag=0;
%}

COMPONENT source = Source_simple(
    radius = 0.02,
    dist = 3,
    focus_xw = 0.01,
    focus_yh = 0.01,
    lambda0 = 6.0,
    dlambda = 0.05,
    flux = 1e8)
AT (0, 0, 0) RELATIVE arm

COMPONENT coll2 = Slit(
    radius = 0.01)
AT (0, 0, 6) RELATIVE arm
EXTEND %{
  flag=SCATTERED;
%}

COMPONENT detector = PSD_monitor(
    nx = 128,
    ny = 128,
    filename = "PSD.dat",
    xmin = -0.1,
    xmax = 0.1,
    ymin = -0.1,
    ymax = 0.1)
AT (0, 0, 9.01) RELATIVE arm

END
```

example_v30.instr

```
/*
* %Example: example.instr dummy=0 Detector: detector_I=345.995
*/
DEFINE INSTRUMENT Minimal(dummy=0)

DECLARE %{
  double constant;
  double two_x_dummy;
%}

USERVARS %{
  double flag;
%}

INITIALIZE %{
  constant=2;
  two_x_dummy=2*dummy;
%}

TRACE

COMPONENT arm = Arm()
AT (0, 0, 0) ABSOLUTE
EXTEND %{
  flag=0;
%}

COMPONENT source = Source_simple(
    radius = 0.02,
    dist = 3,
    focus_xw = 0.01,
    focus_yh = 0.01,
    lambda0 = 6.0,
    dlambda = 0.05,
    flux = 1e8)
AT (0, 0, 0) RELATIVE arm

COMPONENT coll2 = Slit(
    radius = 0.01)
AT (0, 0, 6) RELATIVE arm
EXTEND %{
  flag=SCATTERED;
%}

COMPONENT detector = PSD_monitor(
    nx = 128,
    ny = 128,
    filename = "PSD.dat",
    xmin = -0.1,
    xmax = 0.1,
    ymin = -0.1,
    ymax = 0.1)
AT (0, 0, 9.01) RELATIVE arm

END
```

The particle and USERVARS in the instrument (here shown for McStas)

v2.5: Global variables

```
double x, y, z, vx, vy, vz, t, sx, sy, sz, p;      double flag;
```

v3.0: particle struct, including any USERVARS like flag.

```
struct _struct_particle {
  double x,y,z; /* position [m] */
  double vx,vy,vz; /* velocity [m/s] */
  double sx,sy,sz; /* spin [0-1] */
  unsigned long randstate[7];
  double t, p;    /* time, event weight */
  long long _uid;  /* event ID */
  long _index;     /* component index where to send this event */
  long _absorbed;  /* flag set to TRUE when this event is to be removed/ignored */
  long _scattered; /* flag set to TRUE when this event has interacted with the last component instance */
  long _restore;   /* set to true if neutron event must be restored */
  // user variables:
  double flag;
};
typedef struct _struct_particle _class_particle;
```

Can be probed using e.g. Monitor_nD with user1="flag" which uses the function

double particle_getvar(_class_particle *p, char *name, int *suc)

also works with e.g. "x"

The particle and USERVARS in the instrument

v2.5: Global variables

```
double x, y, z, vx, vy, vz, t, sx, sy, sz, p;      double flag;
```

v3.0: particle struct, including any USERVARS like flag.

```
struct _struct_particle {
  double x,y,z; /* position [m] */
  double vx,vy,vz; /* velocity [m/s] */
  double sx,sy,sz; /* spin [0-1] */
  unsigned long randstate[7];
  double t, p;    /* time, event weight */
  long long _uid;  /* event ID */
  long _index;     /* component index where to send this event */
  long _absorbed;  /* flag set to TRUE when this event is to be removed/
  long _scattered; /* flag set to TRUE when this event has interacted wi
  long _restore;   /* set to true if neutron event must be restored */
  // user variables:
  double flag;
};
typedef struct _struct_particle _class_particle;
```

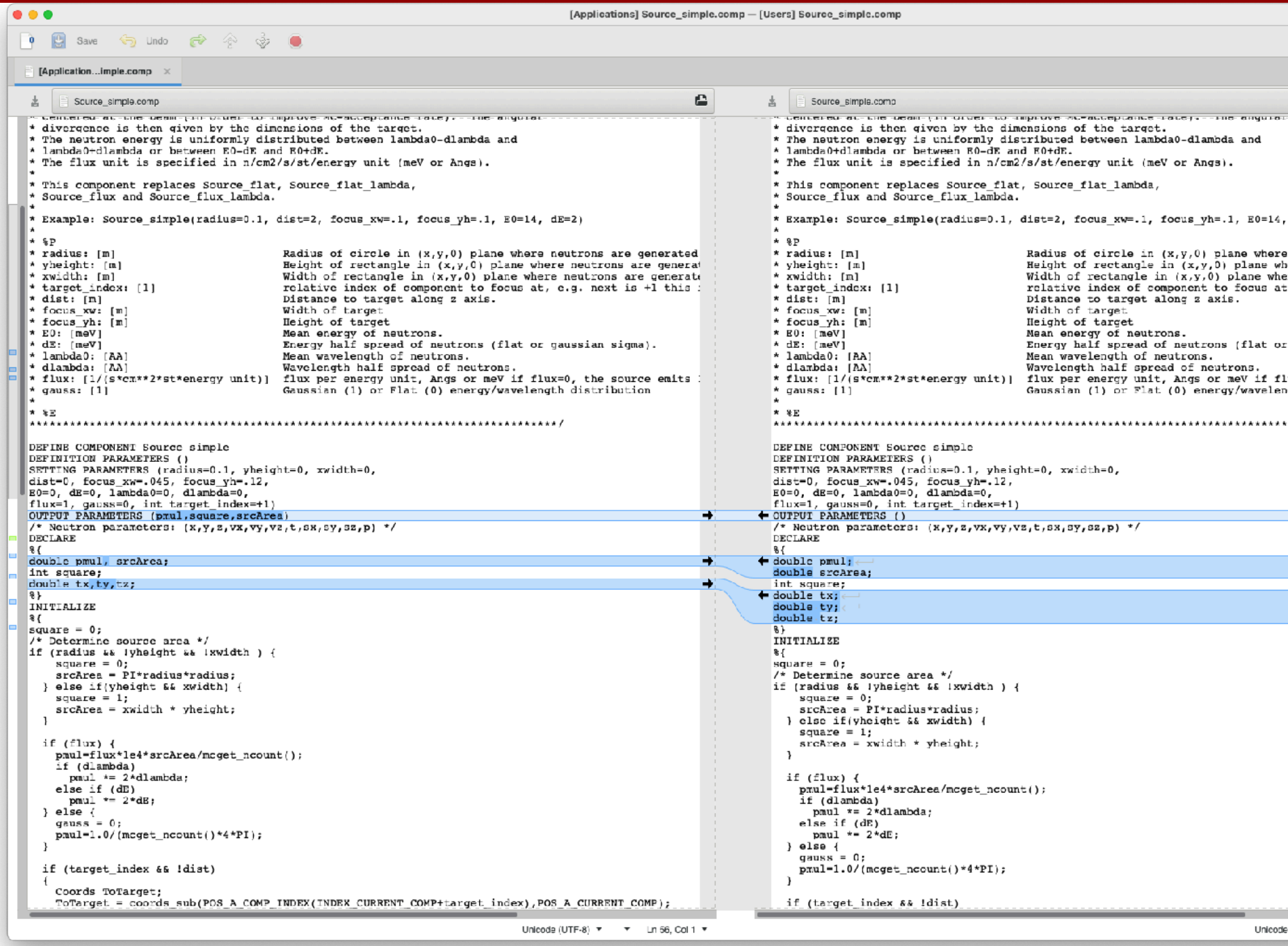
RNG state is a thread-variable contained on the _particle struct. Was earlier a global state in CPU settings

Side-effect:
Every function in TRACE that uses random numbers must have _particle in the footprint

Also:

Particle state data are not global:
Don't use RESTORE_NEUTRON or RESTORE_XRAY in TRACE to do a **local** restore, the macro only raises a flag

Source_simple minor changes



PSD has several changes

No more DEFINITION PARAMETERS

```
* %E
*******************************************************************************/
DEFINE COMPONENT PSD_monitor
DEFINITION PARAMETERS (nx=90, ny=90)
SETTING PARAMETERS (string filename=0, xmin=-0.05, xmax=0.05, ymin=-0.05, ymax=0.05, xwidth=0, yheight=0, restore_
OUTPUT PARAMETERS (PSD_N, PSD_p, PSD_p2)
/* Neutron parameters: (x,y,z,vx,vy,vz,t,sx,sy,sz,p) */

DECLARE
%{
double PSD_N[nx][ny];
double PSD_p[nx][ny];
double PSD_p2[nx][ny];
%}
INITIALIZE
%{
```

```
*******************************************************************************
DEFINE COMPONENT PSD_monitor
DEFINITION PARAMETERS ()
SETTING PARAMETERS (nx=90, ny=90, string filename=0,
  xmin=-0.05, xmax=0.05, ymin=-0.05, ymax=0.05, xwidth=0, yheight=0,
  restore_neutron=0, int nowritefile=0)
OUTPUT PARAMETERS (PSD_N, PSD_p, PSD_p2)
/* Neutron parameters: (x,y,z,vx,vy,vz,t,sx,sy,sz,p) */

DECLARE
%{
  DArray2d PSD_N;
  DArray2d PSD_p;
  DArray2d PSD_p2;
%}
```

Use of new DArray2d for dynamic allocation

```
INITIALIZE
%{
  if (xwidth  > 0) { xmax = xwidth/2;  xmin = -xmax; }
  if (yheight > 0) { ymax = yheight/2; ymin = -ymax; }

  if ((xmin >= xmax) || (ymin >= ymax)){
    printf("PSD_monitor: %s: Null detection area !\n"
           "ERROR        (xwidth,yheight,xmin,xmax,ymin,ymax). Exiting",
    NAME_CURRENT_COMP);
    exit(0);
  }

  PSD_N = create_darr2d(nx, ny);
  PSD_p = create_darr2d(nx, ny);
  PSD_p2 = create_darr2d(nx, ny);

%}
```

PSD lots of changes

```
TRACE
%{
  int i,j;

  PROP_Z0;
  if (x>xmin && x<xmax && y>ymin && y<ymax)
  {
    i = floor((x - xmin)*nx/(xmax - xmin));
    j = floor((y - ymin)*ny/(ymax - ymin));
    PSD_N[i][j]++;
    PSD_p[i][j] += p;
    PSD_p2[i][j] += p*p;
    SCATTER;
  }
  if (restore_neutron) {
    RESTORE_NEUTRON(INDEX_CURRENT_COMP, x, y, z, vx, vy, vz, t, sx, sy, sz, p);
  }
%}
```

```
TRACE
%{
  PROP_Z0;
  if (x>xmin && x<xmax && y>ymin && y<ymax){
    int i = floor((x - xmin)*nx/(xmax - xmin));
    int j = floor((y - ymin)*ny/(ymax - ymin));

    double p2 = p*p;
    #pragma acc atomic
    {
      PSD_N[i][j] = PSD_N[i][j]+1;
    }
    #pragma acc atomic
    {
      PSD_p[i][j] = PSD_p[i][j]+p;
    }
    #pragma acc atomic
    {
      PSD_p2[i][j] = PSD_p2[i][j] + p2;
    }
    SCATTER;
  }
  if (restore_neutron) {
    RESTORE_NEUTRON(INDEX_CURRENT_COMP, x, y, z, vx, vy, vz, t, sx, sy, sz, p);
  }
%}
```

Enabling atomic writes on the detector arrays

```
PROP_Z0;
if (x>xmin && x<xmax && y>ymin && y<ymax){
  int i = floor((x - xmin)*nx/(xmax - xmin));
  int j = floor((y - ymin)*ny/(ymax - ymin));

  double p2 = p*p;
  #pragma acc atomic
  {
    PSD_N[i][j] = PSD_N[i][j]+1;
  }
  #pragma acc atomic
  {
    PSD_p[i][j] = PSD_p[i][j]+p;
  }
  #pragma acc atomic
  {
    PSD_p2[i][j] = PSD_p2[i][j] + p2;
  }
  SCATTER;
```

Samples required a good deal of (detective) work…

Key issue: (mis-) Use of / component DECLARE variables in TRACE for storing particle-dependent information, e.g. reflection list in PowderN etc. must be avoided.

Solutions:

1) Make local thread-variables, e.g. →

```
// Variables calculated within thread for thread purpose only
char type = '\0';
int itype = 0;
double d_phi_thread = d_phi;
// These ones are injected back to struct at the end of TRACE in non-OpenACC case
int nb_reuses = line_info.nb_reuses;
int nb_refl = line_info.nb_refl;
int nb_refl_count = line_info.nb_refl_count;
double vcache = line_info.v;
double Nq = line_info.Nq;
double v_min = line_info.v_min;
double v_max = line_info.v_max;
double lfree = line_info.lfree;
double neutron_passed = line_info.neutron_passed;
long   xs_compute = line_info.xs_compute;
long   xs_reuse   = line_info.xs_reuse;
long   xs_calls   = line_info.xs_calls;
int    flag_warning = line_info.flag_warning;
double dq = line_info.dq;

#ifdef OPENACC
#ifdef USE_OFF
off_struct thread_offdata = offdata;
#endif
#else
#define thread_offdata offdata
#endif
```

2) Where meaningful, one could make atomic sections ala the monitors

Side-effect of thread-local vars:

Next neutron(s) in a SPLIT are no longer aware of e.g. available powder lines.

Potential, future solution: Mechanism to inject comp-specific code in the _particle

New monitor-tools for debugging use

- **Event_monitor_simple(nevents=1e6)**
  - basic non-Monitor_nD event monitor. Writes a “log” file, independent from detector_out macros

- **Flex_monitor_1D** , **Flex_monitor_2D**, **Flex_monitor_3D**,
  simple 1/2/3D “uservar” monitors tapping into the instrument USERVARS ala Monitor_nD

- Useful for **debugging** even **component** internals:
  On mccode-3, if same ncount, same seed, same level of MPI parallelisation, the output should be **identical** on CPU and GPU

Each component will correspond to a set of function. Trace is a GPU'ified function…

+ particle-loop and logic around, also running on GPU.

Init and finalisation codes run purely CPU.

```
#pragma acc routine seq
_class_Source_simple *class_Source_simple_trace(_class_Source_simple *_comp
  , _class_particle *_particle) {
  ABSORBED=SCATTERED=RESTORE=0;

  #define radius (_comp->_parameters.radius)
  #define yheight (_comp->_parameters.yheight)
  #define xwidth (_comp->_parameters.xwidth)
  #define dist (_comp->_parameters.dist)
  #define focus_xw (_comp->_parameters.focus_xw)
  #define focus_yh (_comp->_parameters.focus_yh)
  #define E0 (_comp->_parameters.E0)
  #define dE (_comp->_parameters.dE)
  #define lambda0 (_comp->_parameters.lambda0)
  #define dlambda (_comp->_parameters.dlambda)
  #define flux (_comp->_parameters.flux)
  #define gauss (_comp->_parameters.gauss)
  #define target_index (_comp->_parameters.target_index)
  #define pmul (_comp->_parameters.pmul)
  #define square (_comp->_parameters.square)
  #define srcArea (_comp->_parameters.srcArea)
  #define tx (_comp->_parameters.tx)
  #define ty (_comp->_parameters.ty)
  #define tz (_comp->_parameters.tz)
  SIG_MESSAGE("[_source_trace] component source=Source_simple() TRACE [Source_simple.comp:127]");
double chi,E,lambda,v,r, xf, yf, rf, dx, dy, pdir;

t=0;
z=0;

if (square == 1) {
  x = xwidth * (rand01() - 0.5);
  y = yheight * (rand01() - 0.5);
} else {
  chi=2*PI*rand01();                    /* Choose point on source */
  r=sqrt(rand01())*radius;              /* with uniform distribution. */
  x=r*cos(chi);
  y=r*sin(chi);
}
randvec_target_rect_real(&xf, &yf, &rf, &pdir,
                         tx, ty, tz, focus_xw, focus_yh, ROT_A_CURRENT_COMP, x, y, z, 2);
```

…. etc

Contains component trace section

"Scatter-gather" approach not far from what we do in MPI settings, i.e. :

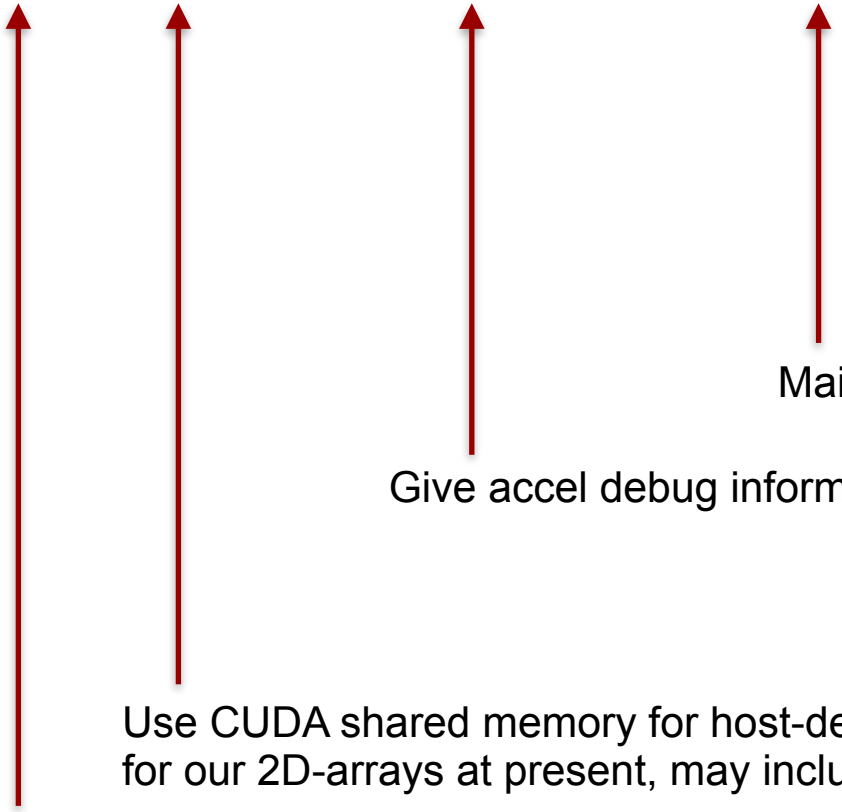
GPU case:
N particles are calculated in parallel in N GPU threads. (Leave to OpenACC/ device how many actually are running at one time)

CPU case:
N particles are calculated in M serial chunks over M processors.

Compiler settings used for GPU:

(McStas 3.0 mcrun is preconfigured on Linux - excluding -Minfo=accel, simply use mcrun --openacc when compiling, can also combine with e.g. --mpi=N)

nvc -ta=tesla,managed -Minfo=accel -DOPENACC



Main “enable GPU”/OpenACC switch

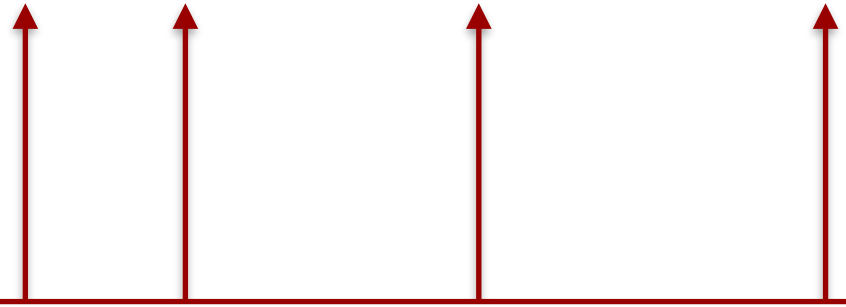
Give accel debug information

Use CUDA shared memory for host-device-host allocation. Needed for our 2D-arrays at present, may include penalty, we could get rid.

Generate Tesla code. “compute capability” e.g. tesla:cc70 may be specified to indicate specific card.

Compiler settings used for GPU:

nvc -ta=tesla,managed -Minfo=accel -DOPENACC



Defaults for “GPU neutron loops”:
1) non-funnelled
   GPU_INNERLOOP=2147483647
2) funnelled
   GPU_FUNNEL_INNERLOOP=1024*1024

For CPU/threading, use below settings, with -DMULTICORE e.g. printfs are not nullified in TRACE

nvc -ta=multicore -Minfo=accel -DOPENACC (-DMULTICORE)

What doesn’t work

- **Function pointers are not available on GPU**
  - Solutions:
    - Code around if possible (integration routine pr. specific function to be integrated…)
    - Mark the component NOACC
- **Variadic functions are not available on GPU**
- **Anonymous structs as comp pars are not available on GPU**
  - Unfold into comp struct
- **User-defined fieldfunctions for polarisation had to be abandoned**
  - No solution yet, may become handled via grammar
- **External libs generally can not be used in TRACE** (“#pragma….” hard to add on 3rd party codes)
  - Handle in INIT / FINALLY (MCPL)
  - NOACC (GSL etc.)
- **Union master is for now NOACC**, will eventually become supported on GPU

CROSS CHECK
Should give the SAME on CPU and GPU!

Porting an instrument to 3.0 and GPU

- **Instrument-level variables** that are to become particle-dependent “**flags**”, e.g. for use in EXTEND WHEN must be put in the new section **USERVARS %{ double flag; %}**
- Use of **instrument input pars** in extend and WHEN must use **INSTRUMENT_GETPAR(varname)**
- **Non-flag instrument vars** to be used during TRACE / EXTEND / WHEN must be injected via **#pragma acc declare create(var)** and **#pragma acc update device(var)**
- **Declare-functions** to be used in **trace** (e.g. in an EXTEND) must have #pragma acc routine

Common error-messages:

- At compile-time, nvc is quite informative if using -Minfo:accel

```
PGC-S-0155-Invalid atomic expression
PGC-S-0000-Internal compiler error. Error: Detected unexpected atomic store opcode.
PGC-S-0155-External variables used in acc routine need to be in #pragma acc create() - flag
…
```

- At runtime, this indicates a GPU segfault

```
Failing in Thread:1
call to cuMemcpyDtoHAsync returned error 700: Illegal address during kernel execution
```

  - Often a symptom of “illegal access”, colliding memory, something isn’t thread-safe…

CROSS CHECK
Should give the SAME on CPU and GPU!

Porting a comp to GPU

- **All pars must be setting parameters.**
  New types: string a="none" and vector b (either ={1,2,3,4} static init or via pointer.)
- **All function-declarations must be moved to SHARE**
- **DECLARE** must ***only*** contain variable **declarations**. All initialization resides in INITIALIZE
- **If the comp uses external libs** either
  - **Avoid use in component TRACE** (e.g. MCPL_input and output, handled in INIT/FINALLY)
  - **Use NOACC keyword** (e.g. Multilayer_sample use of GSL) - implies FUNNEL mode
- **Add #pragma acc routine** to functions to execute in TRACE
- **Functions that call rand01()** and friends **must include _class_particle *_particle in footprint.**
  (rand01() etc. are macros that carry thread-seed on _particle)s
- Generally, **don't store ANY** particle-derived vars on comp struct, **make local TRACE vars** instead.
  - Exception: Monitors, handle arrays in #pragma acc atomic clauses
- **Don't** use **RESTORE_XRAY/NEUTRON** in TRACE to do a **local** restore, the macro only raises a flag

Highlights of comps that work differently

- Monitor_nD
  uservars are strings user1="flag", they use _particle_getvar to access instrument USERVARS

- MCPL_input and MCPL_output
  do most of their work in INIT/FINALLY - buffers transferred for TRACE use

- PowderN + Single_crystal + Isotropic_sqw
  don't check for "same particle as before"
  - in SPLIT cases, no particle state info is kept
  (we could potentially use _particle and "USERVARS" injected from the comps…)

Conclusions

- **It really does work nicely!**
- **Code changes** much **less invasive** than envisioned!
- It often gives a speedup of **1-2 orders** of magnitude over 1 cpu
- **Most things work**
  (we have workarounds or solutions in the pipe for the rest)
- **Documentation** comes in the form of the released code + this set of slides…
- McXtrace 3.0 and McStas 3.1 fully support GPU but **not fully "optimised" performance-wise**, we will try to go to another Hackathon
- **Union** needs a dedicated **Hackathon**
- **Compilation** with GCC 10 offloading support achieved May 2021 - but produces 0 on detectors…
  - hope for better GCC support and non-NVIDIA cards in 1-2 years

The team, Nvidia mentors and Hackathon hosts :-)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Sebastian von Alfthan