Backup slides…

DTU

EUROPEAN SPALLATION SOURCE

“Full” list of pragmas and accel-code used

```
#include <accelmath.h>
#pragma acc declare create ( mcgravitation )
#pragma acc declare create ( mcseed )
#pragma acc declare create ( mcgravitation )
#pragma acc declare create ( mcMagnet )
#pragma acc declare create ( mcallowbackprop )
#pragma acc declare create ( mcncount )
#pragma acc routine seq
#pragma acc routine sequential
#pragma acc declare create ( _instrument_var )
#pragma acc declare create ( instrument )
#pragma acc declare create ( _arm_var )
#pragma acc declare create ( _source_var )
#pragma acc declare create ( _coll2_var )
#pragma acc declare create ( _detector_var )
#  include <openacc.h>
acc_attach( (void*)&_arm_var );
acc_attach( (void*)&_source_var );
acc_attach( (void*)&_coll2_var );
acc_attach( (void*)&_detector_var );
#pragma acc update device(_arm_var)
#pragma acc update device(_source_var)
#pragma acc update device(_coll2_var)
#pragma acc update device(_detector_var)
acc_attach( (void*)&_instrument_var );
#pragma acc update device(_instrument_var)
#pragma acc routine seq
#pragma acc atomic
#pragma acc parallel loop
#pragma acc declare device_resident(particles)
_class_particle* particles = acc_malloc(innerloop*sizeof(_class_particle));
#pragma acc enter data create(particles[0:innerloop])
#pragma acc parallel loop present(particles)
acc_free(particles);
#pragma acc update host(_arm_var)
#pragma acc update host(_source_var)
#pragma acc update host(_coll2_var)
#pragma acc update host(_detector_var)
#pragma acc update host(_instrument_var)
```

McXtrace

DTU ESRF

McStas

DTU ESS

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 neutron reworked to be **structures**

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

- **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

- 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 neutron 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/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 neutron 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.

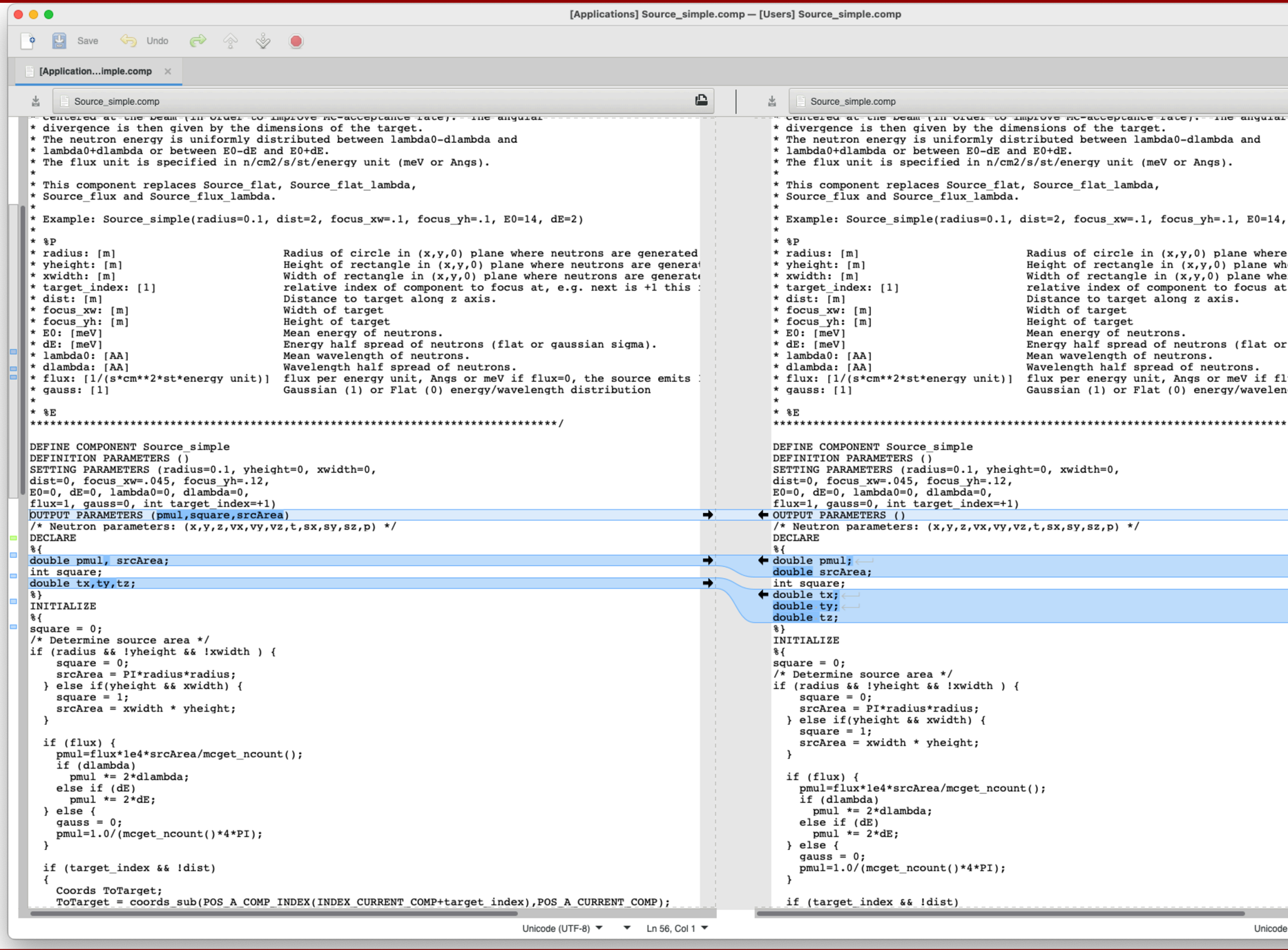
```
struct _struct_particle {
  double x,y,z; /* position [m] */
  double vx,vy,vz; /* velocity [m/s] */
  double sx,sy,sz; /* spin [0-1] */
  unsigned long randstate[7];
  double t, p;    /* time, event weight */
  long long _uid;  /* event ID */
  long _index;     /* component index where to send this 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

Particle state data are not global:
Don't use RESTORE_NEUTRON 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

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.

Various hints

- If you have a candidate-code, apply to join a Hackathon at https://gpuhackathons.org - run by NVIDIA, local compute experts + NVIDIA tech staff - simply great!!

- 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…

- RNG state defined “per particle”, highly parallel setup makes “global” state impossible / impractical / really slow

- Once everything works as expected the GPU run gives exactly the same as corresponding CPU run (± DBL_EPS)

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 McStas 3, if same ncount, same seed, same level of MPI parallelisation, the output should be **identical** on CPU and 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_NEUTRON** in TRACE to do a **local** restore, the macro only raises a flag

What code-parts got #pragma acc

Obviously the **code-generator**…
mcstas/src/cogen.c.in

Examples:

25 **Instruments** that use various global vars in DECLARE that are neither input parameters or USERVARS

These **share/runtime** snippets:
(A good mix of everything)

share/adapt_tree-lib.c
share/interoff-lib.c
share/mccode-r.c
share/mccode-r.h
share/mccode_main.c
share/read_table-lib.c
share/r-interoff-lib.c
share/ESS_butterfly-geometry.c
share/ESS_butterfly-lib.c
share/cov-lib.c
share/monitor_nd-lib.c
share/mcstas-r.c
share/mcstas-r.h
share/pol-lib.c
share/ref-lib.c

Sources: (TRACE-functions in SHARE)

sources/Source_Maxwell_3.comp
sources/Source_gen.comp

Samples: (TRACE-functions in SHARE)

samples/Isotropic_Sqw.comp
samples/Magnon_bcc.comp
samples/Phonon_simple.comp
samples/PowderN.comp
samples/SANS_spheres2.comp
samples/Single_crystal.comp

Optics: (TRACE-functions in SHARE + declare create for Gauss structures)

optics/Elliptic_guide_gravity.comp
optics/FermiChopper.comp
optics/Guide_gravity.comp
optics/Monochromator_curved.comp
optics/Monochromator_flat.comp

All **monitors**:

#pragma acc atomic sections for arrays

Misc:
atomic capture for insertion in array of particle events

misc/MCPL_output.comp

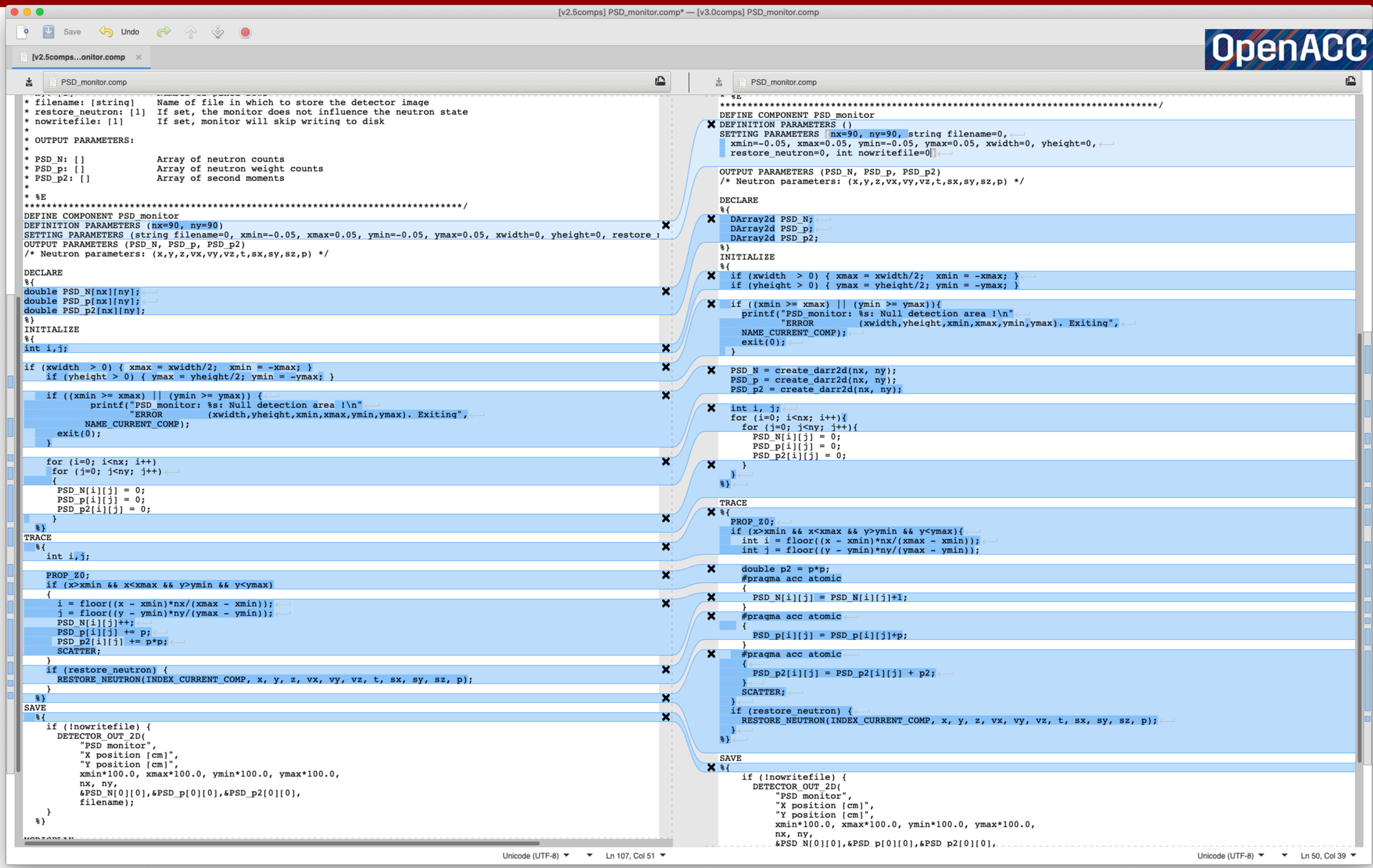
Contrib comps: (atomics in mon's, #pragma acc routine for TRACE-funcs)

contrib/FermiChopper_ILL.comp
contrib/Guide_honeycomb.comp
contrib/ISIS_moderator.comp
contrib/Lens.comp
contrib/Mirror_Elliptic.comp
contrib/Mirror_Parabolic.comp
contrib/PSD_Detector.comp
contrib/PSD_monitor_rad.comp
contrib/SNS_source.comp
contrib/SNS_source_analytic.comp
contrib/ViewModISIS.comp

New RNG ‘KISS’

- We couldn’t easily port Mersenne Twister
- Experimenting with curand showed huge overhead for our relative small number of random numbers
- An RNG ‘state’ carried with each particle - bonus: same seed gives same numbers even when comparing between CPU and GPU
- Required patching prototype of ALL functions making use of e.g. rand01()
- New RNG is simple, fast and “good enough”: Reproduces results of 2.7 over all of the example suite, see http://new-nightly.mcstas.org
-

PSD lots of changes



Same seed and same # mpi nodes -> same output

- Good for debugging
- If they don’t give the same CPU vs GPU, some comp(s) are not fully ported
- Use Event_monitor_simple to follow calculation pr. neutron

Declare section

```
/* User declarations from instrument definition. Can define functions. */
  double constant;
  double two_x_dummy;
```

Initialise section

```
  #define dummy (instrument->_parameters._dummy)
{
  constant=2;
  two_x_dummy=2*dummy;
}
  #undef dummy
  _arm_setpos(); /* type Arm */
  _source_setpos(); /* type Source_simple */
  _coll2_setpos(); /* type Slit */
  _detector_setpos(); /* type PSD_monitor */

  /* call iteratively all components INITIALISE */

  class_Source_simple_init(&_source_var);

  class_Slit_init(&_coll2_var);

  class_PSD_monitor_init(&_detector_var);
```

Functions per component with related component structs

Instrument and component structs built on CPU and transferred to GPU using OpenACC pragmas at the end of

INITIALISE

```
#ifdef USE_PGI
#  include <openacc.h>
acc_attach( (void*)&_arm_var );
acc_attach( (void*)&_source_var );
acc_attach( (void*)&_coll2_var );
acc_attach( (void*)&_detector_var );
#pragma acc update device(_arm_var)
#pragma acc update device(_source_var)
#pragma acc update device(_coll2_var)
#pragma acc update device(_detector_var)
acc_attach( (void*)&_instrument_var );
#pragma acc update device(_instrument_var)
#endif
```

Similar “host” update in FINALLY

“Full” list of pragmas and accel-code used

```
#include <accelmath.h>
#pragma acc declare create ( mcgravitation )
#pragma acc declare create ( mcseed )
#pragma acc declare create ( mcgravitation )
#pragma acc declare create ( mcMagnet )
#pragma acc declare create ( mcallowbackprop )
#pragma acc declare create ( mcncount )
#pragma acc routine seq
#pragma acc routine sequential
#pragma acc declare create ( _instrument_var )
#pragma acc declare create ( instrument )
#pragma acc declare create ( _arm_var )
#pragma acc declare create ( _source_var )
#pragma acc declare create ( _coll2_var )
#pragma acc declare create ( _detector_var )
#  include <openacc.h>
acc_attach( (void*)&_arm_var );
acc_attach( (void*)&_source_var );
acc_attach( (void*)&_coll2_var );
acc_attach( (void*)&_detector_var );
#pragma acc update device(_arm_var)
#pragma acc update device(_source_var)
#pragma acc update device(_coll2_var)
#pragma acc update device(_detector_var)
acc_attach( (void*)&_instrument_var );
#pragma acc update device(_instrument_var)
#pragma acc routine seq
#pragma acc atomic
#pragma acc parallel loop
#pragma acc declare device_resident(particles)
_class_particle* particles = acc_malloc(innerloop*sizeof(_class_particle));
#pragma acc enter data create(particles[0:innerloop])
#pragma acc parallel loop present(particles)
acc_free(particles);
#pragma acc update host(_arm_var)
#pragma acc update host(_source_var)
#pragma acc update host(_coll2_var)
#pragma acc update host(_detector_var)
#pragma acc update host(_instrument_var)
```