Peter Willendrup

Simulation optimisation, brilliance basics, FOM's and tools

Topics

- Optimising your simulation (statistics etc.)
  - Variance reduction / biasing
- Source brilliance and brilliance transfer
- Deciding for a figure of merit
- Tools: scans, iFit and guide_bot

Important points to remember

1. Your simulation will only contain elements you provided / defined

2. … to the precision you defined

3. Answers the questions you posed

4. Background essentially only from “sample”, or sample-near objects

Ensuring efficiency of the simulation is an important start…

- Apply focusing techniques
  - At the source (spatially, temporally, in wavelength…)
  - At the sample, if possible

- (carefully!) Apply SPLIT - but only if immediately followed by Monte Carlo choices, e.g. in sample

- Alternatively use MCPL o/i which allows repetition - beware of biases!

Ensuring efficiency of the simulation is an important start…

- Apply focusing techniques
  - At the source (spatially, temporally, in wavelength…)
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- Alternatively use MCPL o/i which allows repetition - beware of biases!

All of this can be considered "variance reduction"

or biasing

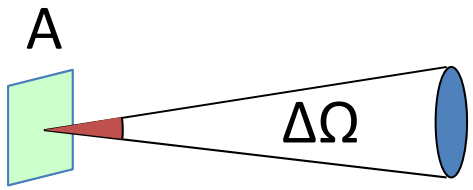
Which hammer?



- Use **MPI** parallelisation - included in macOS install from 2.4, easy to get on Linux… Ready to roll on IDAaaS.
- Choice of compiler and optimisation flags can at times give ~a factor of 2 in speed, clang vs gcc vs Intel C
- Think of moving to McStas 3.0 and GPU's could help you… (see thursday talk)
- - Always consider if you are asking the right question if runtimes reach days/weeks… -> **Pick the right hammer!**

Sledge-hammer / brute force!

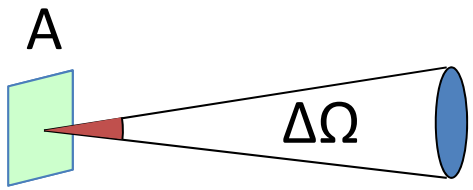
Neutron flux - and brilliance / brightness



B = N per time per A per ΔΩ

units = n/s/cm^2/sr

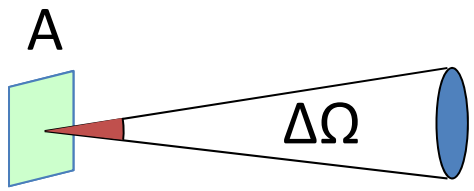
Neutron flux - and brilliance / brightness



B is independent of distance

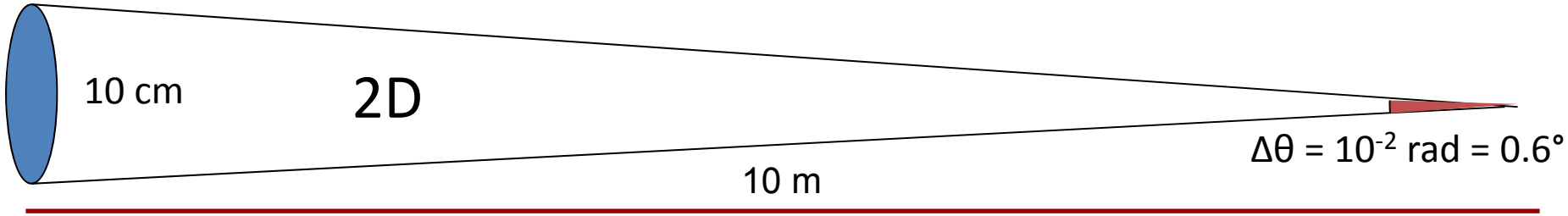
- property of the source

Neutron flux - and brilliance / brightness

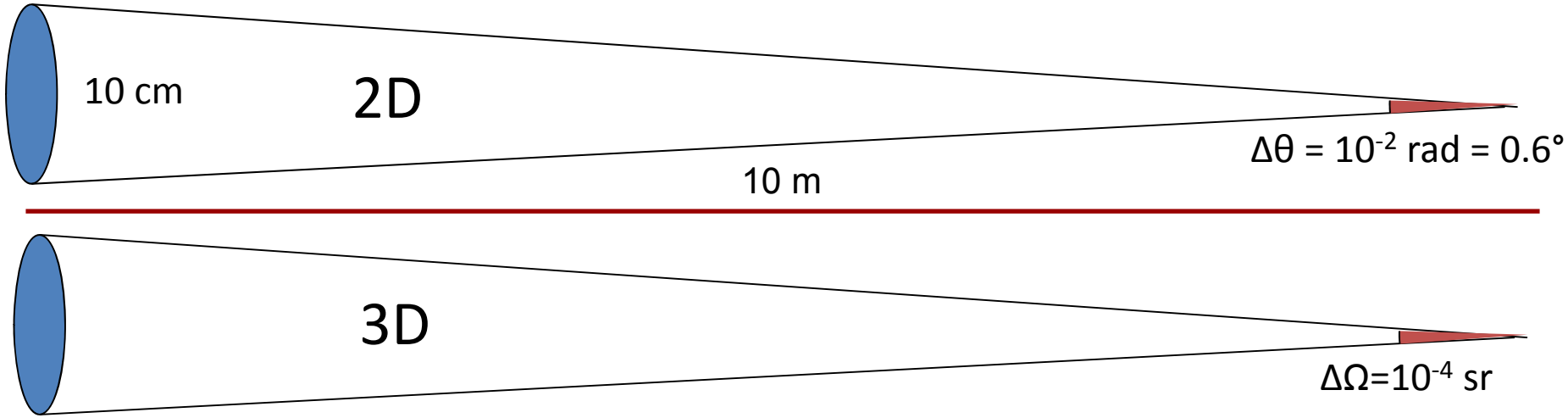


Brilliance/Brightness	B	[n/s/cm^2/sr]
Flux	Ψ	[n/s/cm^2]

Neutron flux - and brilliance / brightness



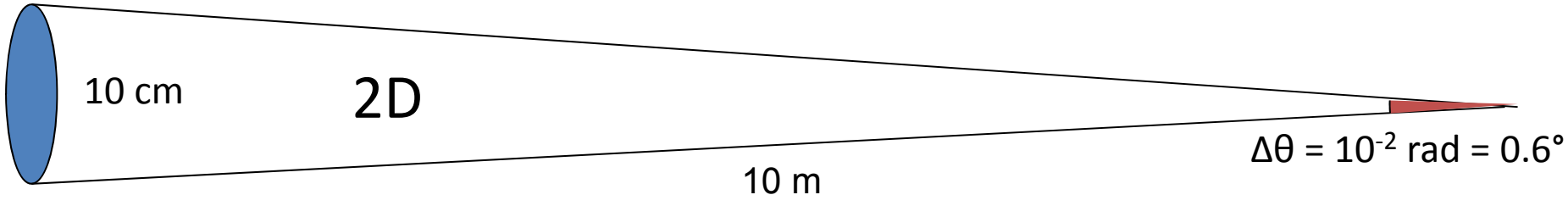
Neutron flux - and brilliance / brightness

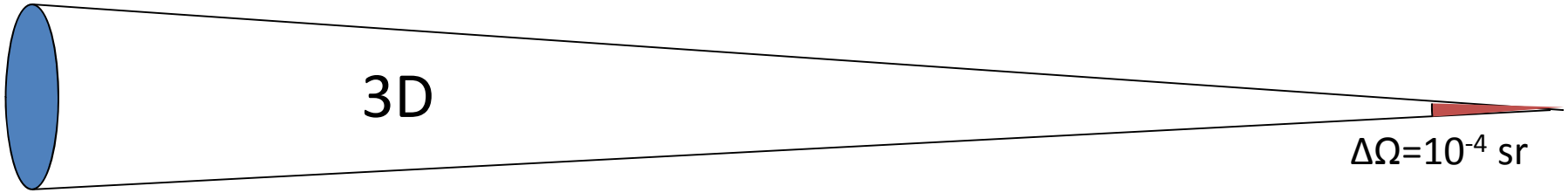


Flux = Source Brightness × Solid Angle

$\Phi = B \times \Delta\Omega$

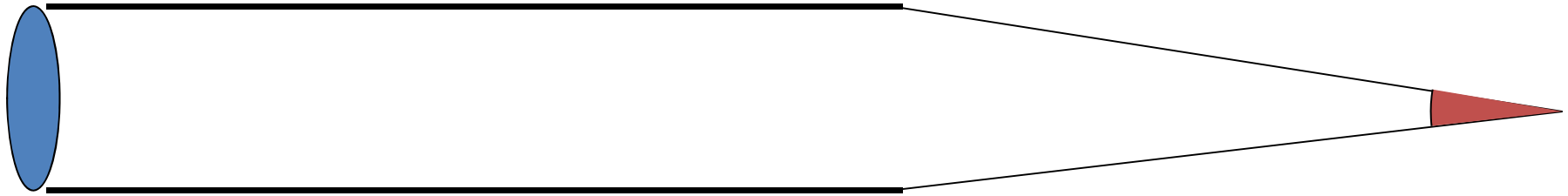
Neutron flux - and brilliance / brightness





Flux = Source Brightness × Solid Angle

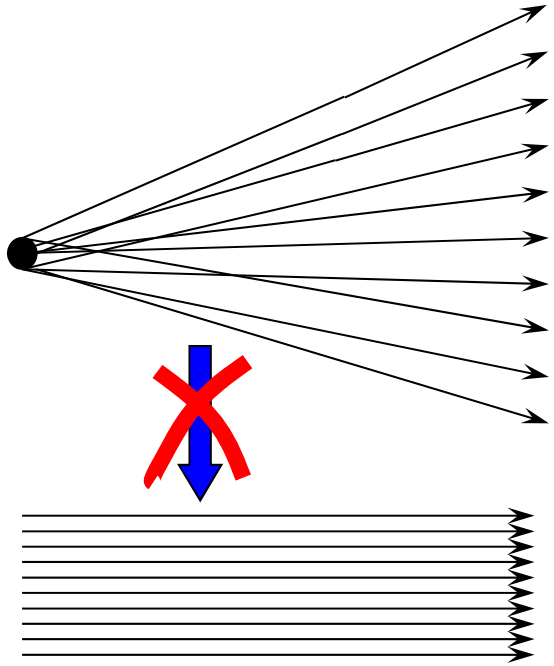
$\Phi = B \times \Delta\Omega$

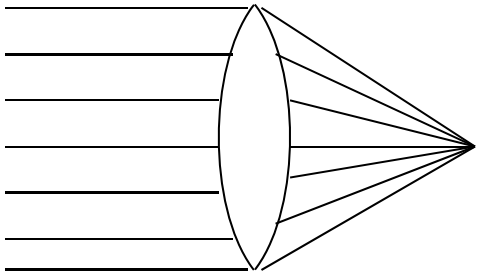


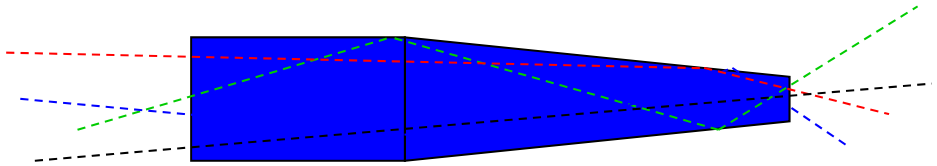
Liouville theorem
→ ΔxΔϕ = const

Liouvilles Theorem

- Conservation laws:
  - neutrons can't be created from thin air
  - neither can "phase space density"
- There is no such thing as a free lunch
  - Beam manipulation transfers distribution between time, area, divergence, energy
- Most common application:
  - Focusing increases divergence
  - improve flux, lose angular resolution







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Liouvilles Theorem

- Conservation laws:
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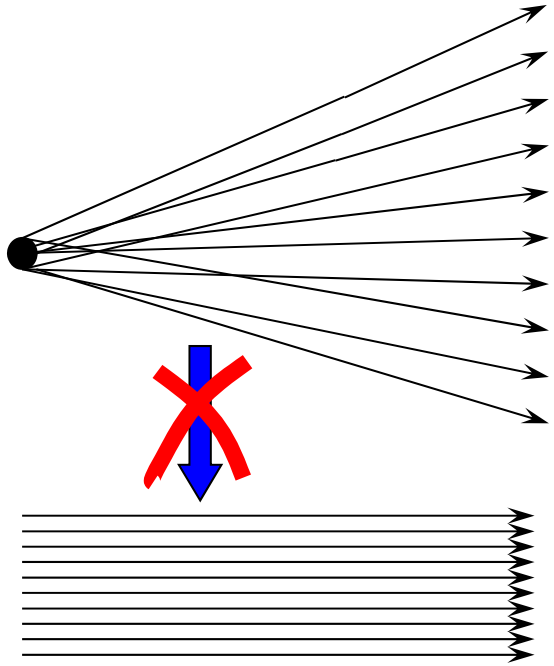
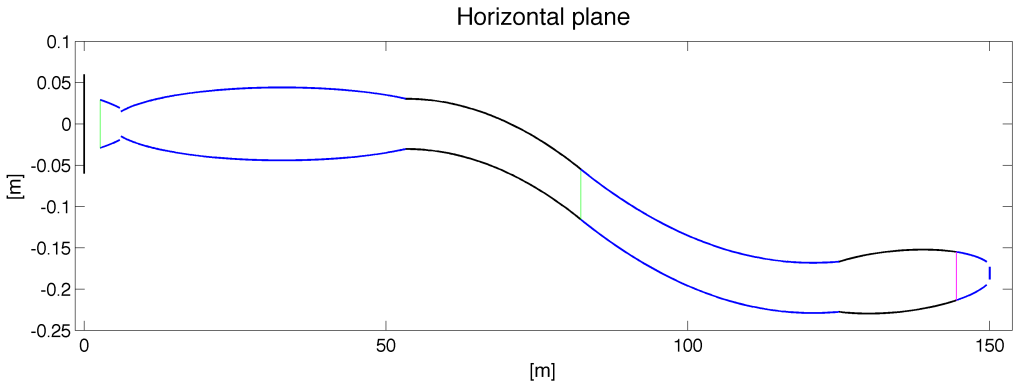
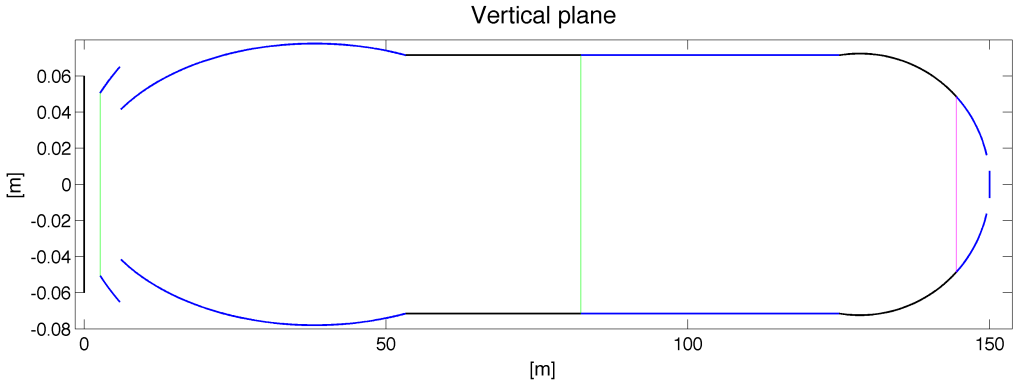


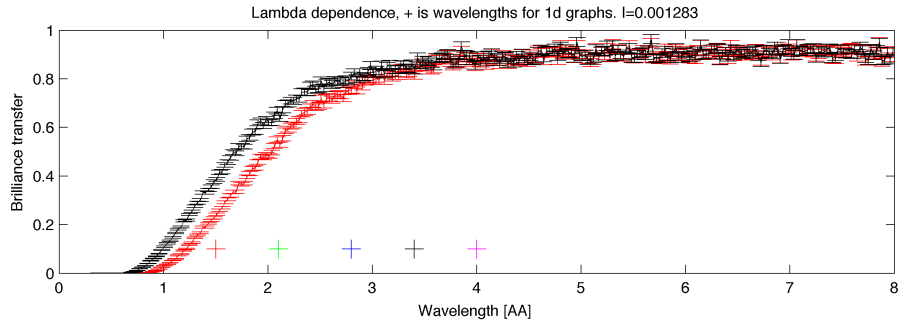
Integrated flux $\int \Psi \, dA \, d\Omega$ can never increase

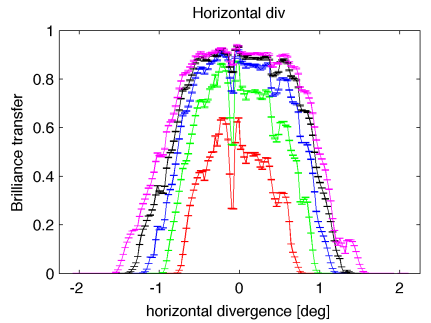
A good optic maximises *transfer* of brilliance

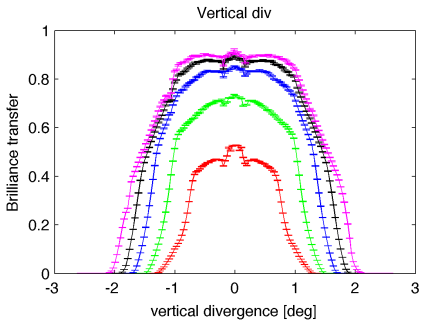
- Example, elliptic guide designed by guide_bot
  → See Thursday talk by Mads Bertelsen

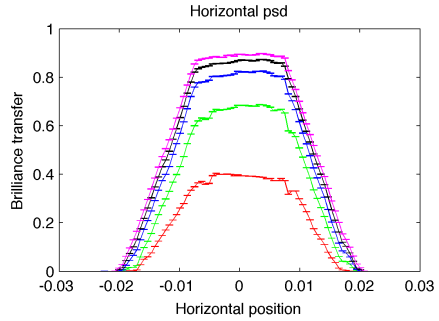


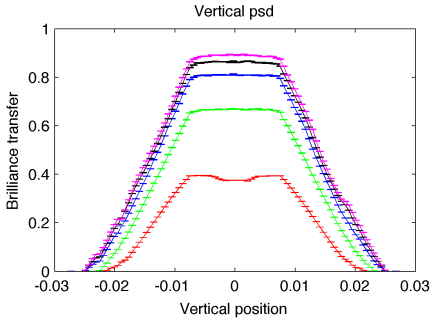












How to implement this in McStas-code? See example folder…

- **BTsimple**, measures phase space before optic…

1.
```
/* Measure incoming phase-space */
COMPONENT BT_in = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_in.dat",
                  Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutron=1)
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0) RELATIVE  origin
```

How to implement this in McStas-code? See example folder…

- **BTsimple**, measures phase space **before** optic…

1.
```
/* Measure incoming phase-space */
COMPONENT BT_in = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_in.dat",
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WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0) RELATIVE  origin
```

Spatial ranges

Spectral range

Directional range

How to implement this in McStas-code? See example folder…

- **BTsimple**, measures phase space **before** and **after** optic…

1.
```
/* Measure incoming phase-space */
COMPONENT BT_in = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_in.dat",
                  Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutron=1)
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0) RELATIVE  origin
```

2.
```
/* Measure outgoing phase-space @ sample position */
COMPONENT BT_out = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_out.dat",
                   Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutron=1)
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0+gL) RELATIVE  guide
```

Same phase-space element and identical binning…

How to implement this in McStas-code? See example folder…

- **BTsimple**, measures phase space **before** and **after** optic, calculates transferred fraction as fct. of wavelength:

1.
```
/* Measure incoming phase-space */
COMPONENT BT_in = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_in.dat",
                  Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutron
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0) RELATIVE  origin
```

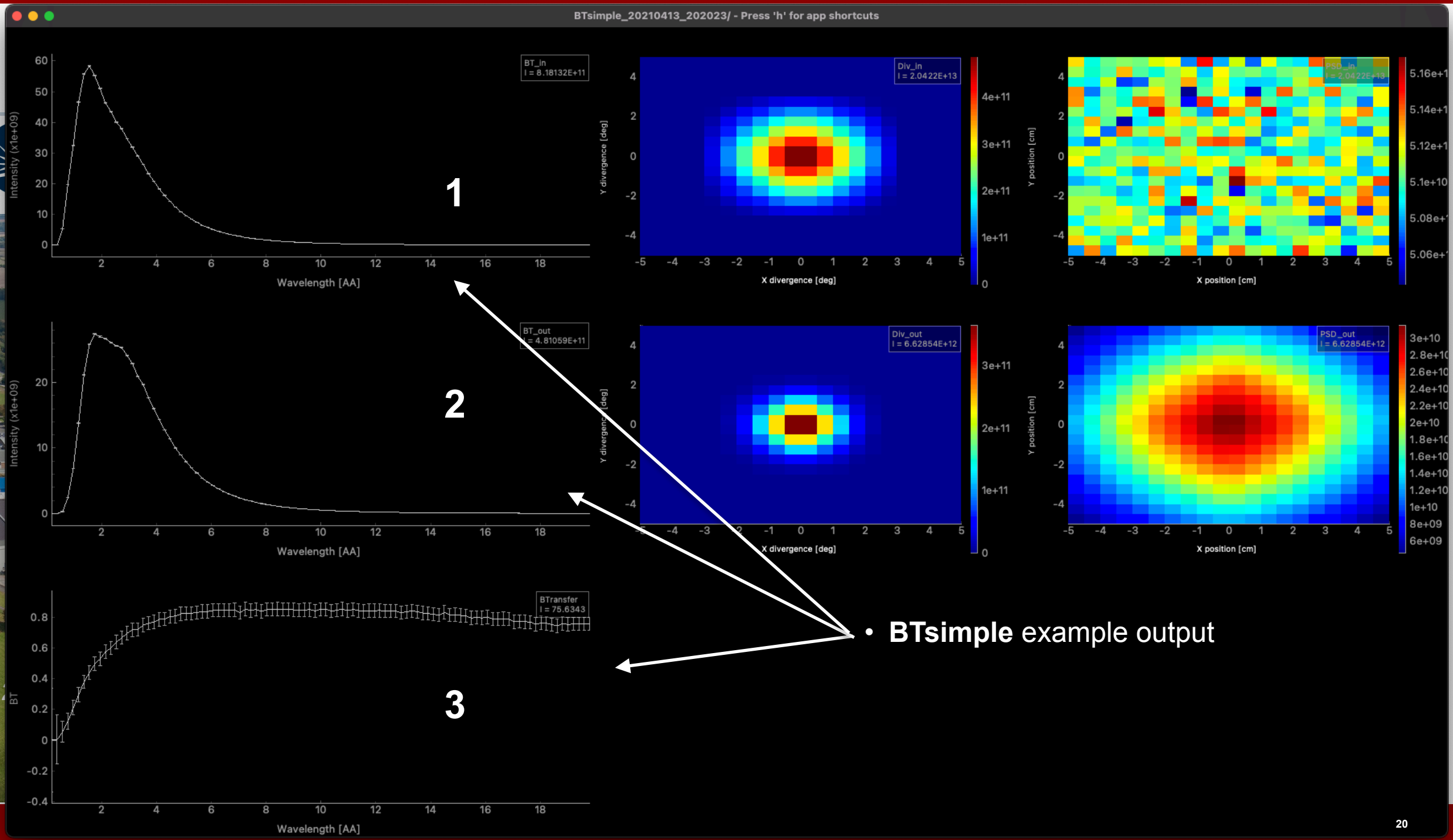
2.
```
/* Measure outgoing phase-space @ sample position */
COMPONENT BT_out = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_out.dat",
                   Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutro
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0+gL) RELATIVE  guide
```

- **Performs piece-wise division of the bins w. error propagation**

3.
```
FINALLY
%{
  /* This adds another "monitor" that measures BT_out / BT_in */
  int j;
  double* tmpN;
  double* tmpp1;
  double* tmpp2;
  double* tmpd1;
  double* tmpd2;
  tmpN=MC_GETPAR(BT_out,L_N);
  tmpp1=MC_GETPAR(BT_in,L_p);
  tmpp2=MC_GETPAR(BT_out,L_p);
  tmpd1=MC_GETPAR(BT_in,L_p2);
  tmpd2=MC_GETPAR(BT_out,L_p2);
  for (j=0;j<101;j++) {

    BT_N[j]=tmpN[j];
    if (tmpp1[j] != 0) {
      BT_p[j]=tmpp2[j]/tmpp1[j];
    } else {
      BT_p[j]=0;
    }
    if ((tmpp1[j] != 0) && (tmpp2[j] != 0)) {
      BT_p2[j]=sqrt((tmpd1[j]/tmpp1[j])*(tmpd1[j]/tmpp1[j])
                + (tmpd2[j]/tmpp2[j])*(tmpd2[j]/tmpp2[j]));
    } else
      BT_p2[j]=0;
  }
// This set of defines is to avoid getting a '.' in the component na
#ifdef NAME_CURRENT_COMP
#undef NAME_CURRENT_COMP
#define NAME_CURRENT_COMP "BTransfer"
#endif
  DETECTOR_OUT_1D(
                  "Brilliance transfer",
                  "Wavelength [AA]",
                  "BT",
                  "L", lambda-dlambda, lambda+dlambda, 101,
                  &BT_N[0],&BT_p[0],&BT_p2[0],
                  "Brilliance_transfer.dat");

%}
```


BTsimple_20210413_202023/ - Press 'h' for app shortcuts
BT_in
I = 8.18132E+11
Intensity (x1e+09)
Wavelength [AA]
1
Div_in
I = 2.0422E+13
Y divergence [deg]
X divergence [deg]
PSD_in
I = 2.0422E+13
Y position [cm]
X position [cm]
BT_out
I = 4.81059E+11
2
Div_out
I = 6.62854E+12
PSD_out
I = 6.62854E+12
BTransfer
I = 75.6343
BT
3
• BTsimple example output

What to optimise? Figure of merit requires thought…

- Brilliance-transfer is probably a good quantity to think of, yet…

- Otherwise a case-specific FOM should be chosen
  - Usually not a matter of simply maximising flux…
  - Depends strongly on the science to be done
  - Wavelength-band, dynamical range of instrument
  - Typical sample size, q and E resolution needed etc.
  - Price (e.g. in the form of shielding requirements and guide coatings)

- See parallel sessions!

FOM examples for different types of instruments

STS04-41-TR0002, R00

Table 7.2 – Metrics proposed by the individual working groups

Instrument group	Flux metric	Shape metric
Small angle neutron scattering	$\max\left(\int_{1.5A}^{20A} IF(\lambda)\lambda^{2-3}d\lambda\right)$	N/A
Reflectometry	$\max\left(\int_{3A}^{15(20)A} IF(\lambda)\lambda^{4}d\lambda\right)$	N/A
Spin-Echo	$\max\left(\int_{4A}^{20A} IF(\lambda)\lambda^{2-3}d\lambda\right)$	N/A
Spectroscopy	$\max\left(\int_{1A}^{10A} PF(\lambda)\lambda^{0}d\lambda\right)$	$\min\left(\int_{1A}^{10A}\left\lvert\frac{dPF(\lambda)}{d\lambda}\right\rvert d\lambda\right)$
Nuclear (classical) diffraction	$\max\left(\int_{0.5(0.2)A}^{4A} PF(\lambda)\lambda^{0}d\lambda\right)$	$\min\left(\int_{0.5(0.2)A}^{4A}\left\lvert\frac{dPF(\lambda)}{d\lambda}\right\rvert d\lambda\right)$
Magnetic diffraction	$\max\left(\int_{1A}^{10A} PF(\lambda)\lambda^{0}d\lambda\right)$	$\min\left(\int_{1A}^{10A}\left\lvert\frac{dPF(\lambda)}{d\lambda}\right\rvert d\lambda\right)$

Here $IF(\lambda)$ is defined as the pulse-integrated flux and $PF(\lambda)$ is the pulse-peak flux for a particular wavelength λ.

STS04-41-TR0002, R00

Long-Pulse Neutron Instrumentation Workshop, August 26-28, 2009

Report

R. K. Crawford (editor), M. Arai, C. Carlile, L. Chapon, G. Granroth, S. Langridge, K. Lefmann, F. Mezei, M. Monkenbusch, G. Muhrer, A. Wiedenmann

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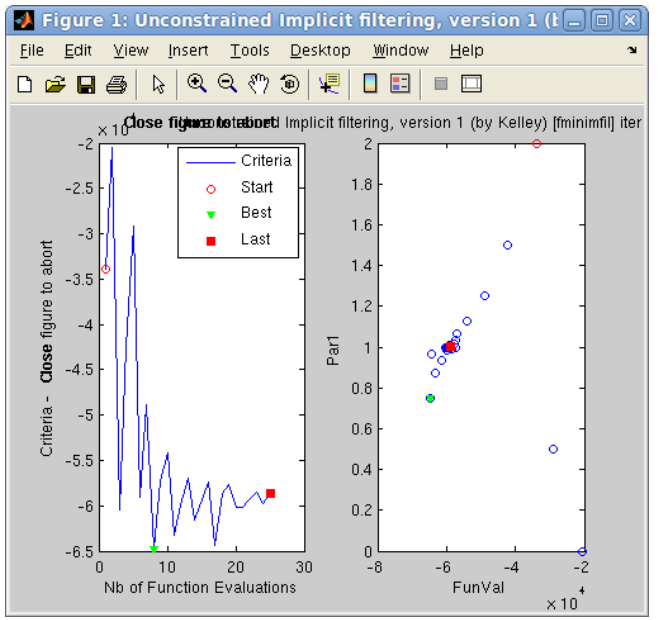
Crawford, R. K., Arai, M., Carlile, C., Chapon, L., Granroth, G., Langridge, S., ... Wiedenmann, A. (2009, Aug 26). Long-Pulse Neutron Instrumentation Workshop, August 26-28, 2009. (Oak Ridge National Laboratory ed.) Oak Ridge, USA.



Parameter-variation

- mcrun and mcgui provide
  - Simple equidistant line-scans or colinear scans
    par=a,b -N k. / par1=a,b par2=c,d -Nk

- mcrun further provides
  - -L list mode (can be non-equidistant, user chooses order, still a form of scan)
    par1=a,b,c,d,e,f par2=g,h,i,j,k,l

- Run your simulations via iFit http://ifit.mccode.org - see http://ifit.mccode.org/McStas.html
  - McStas simulation becomes an **object function**, monitor(s) an **optimisation criterion**
  - Includes a host of different optimisers, e.g. particle swarms in parameter-space
  - Matlab-based, perform calculations based on monitor outputs (!! use Matlab <= 2017b !!)
  - Can work as a recompiled binary, but not as stable as a pure Matlab
  - Use official distribution package from http://ifit.mccode.org/Downloads/iFit.zip, GitHub code is too 'bleeding edge'

iFit

→ guide_bot tool is built on iFit, see Thursday talk. Relies on iFit v. x.y.