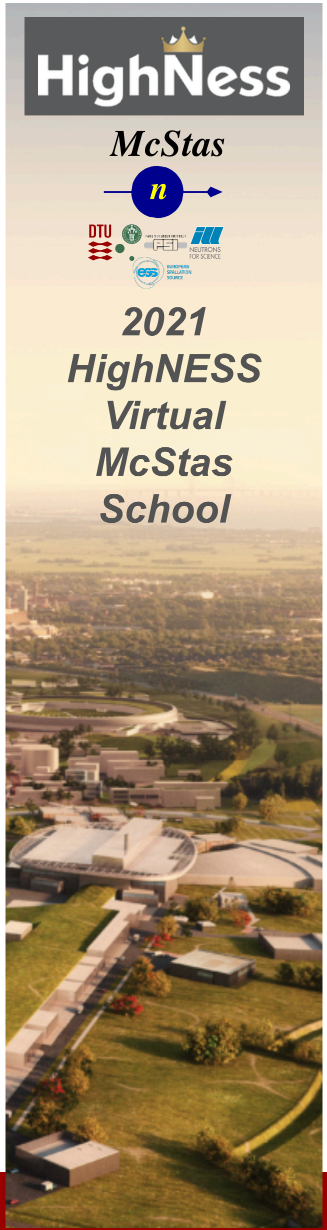
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

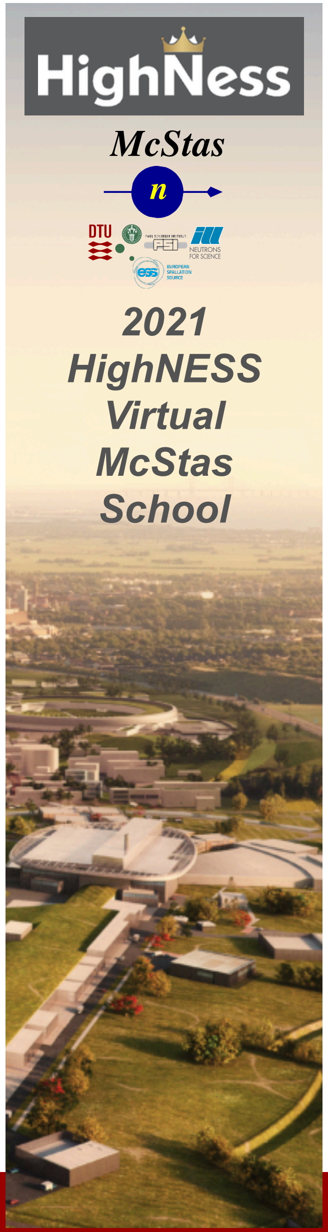
Peter Willendrup

Simulation optimisation, variance reduciton, brilliance basics, FOM’s and tools

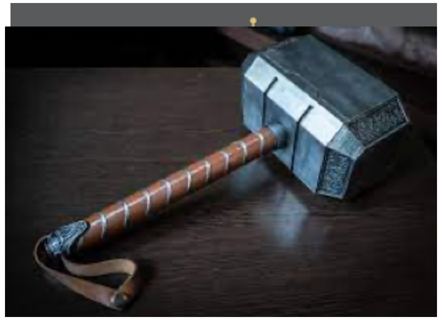


Topics

- 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



Parallelisation for better stats, brute-force… Which hammer?



✦Use **MPI** parallelisation - included in macOS install from 2.4, easy to get on Linux…

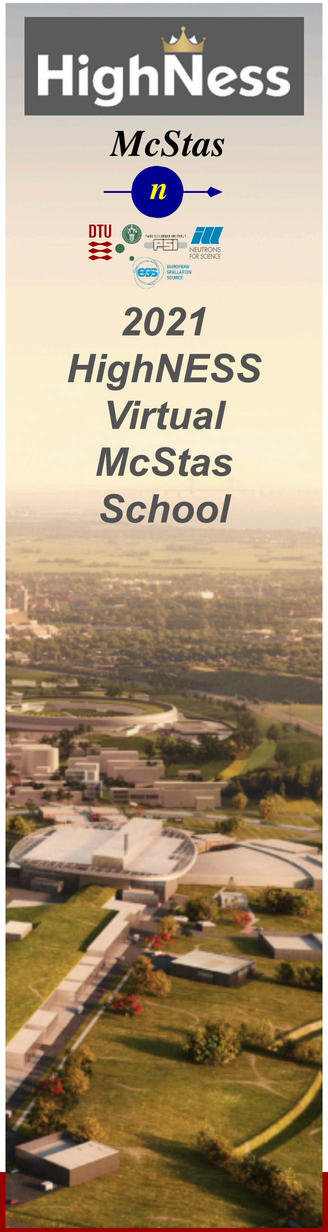
✦Choice of compiler and optimisation flags can at times give ~a factor of 2 in speed, cf. clang vs. Intel C

✦Consider if McStas 3.0 and GPU's could help you… (see Friday talk / demo)

✦- **BUT: Always** consider if you are asking the right question if runtimes reach days/weeks… **Pick the right hammer!**

+

Sledge-hammer / brute force!

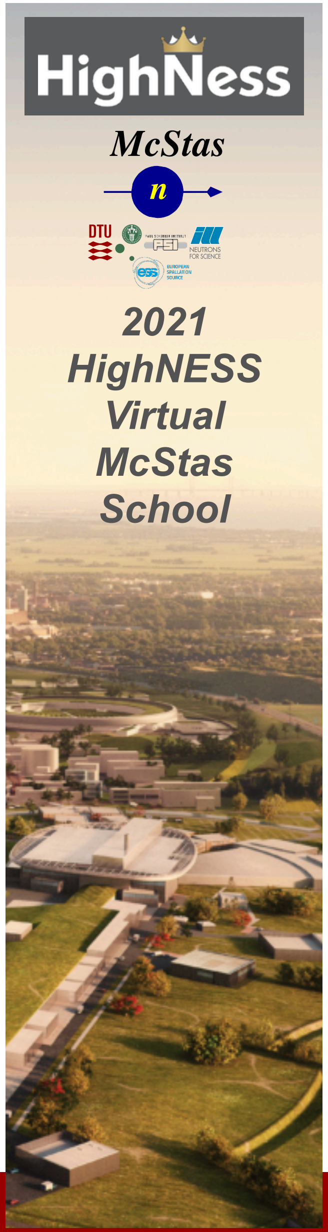


Ensuring efficiency of the simulation is an important start…

- ✦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! Same rule of thumb in order here.



Ensuring efficiency of the simulation is an important start…

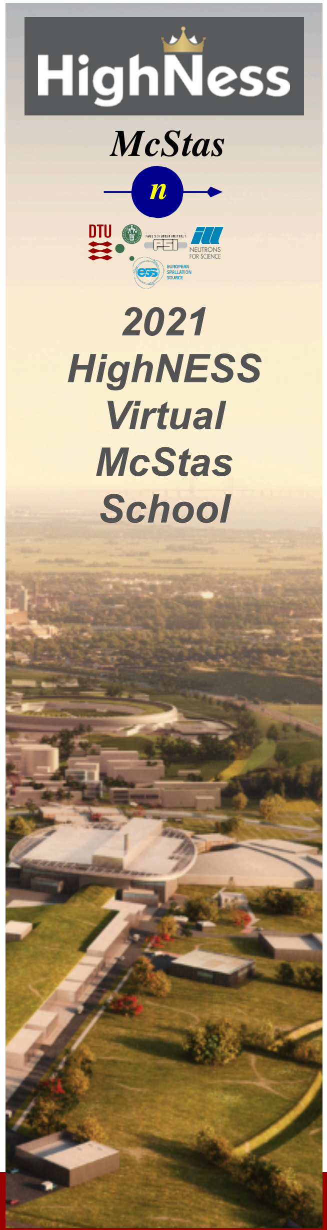
- ✦Apply focusing techniques
  - ✦At the source (spatially, temporally, in wavelength…)
  - ✦At the sample, if possible
- ✦(carefully!) Apply **SPLIT** - but only
  followed by Monte Carlo choices, e

“Repeat the good neutrons that made it here…” - More on Thursday.

- ✦Alternatively use **MCPL** o/i which
  beware of biases! Same rule of thu

I/O mechanism for event files, package independent - More at the end of this section

All of this can be considered “variance reduction” or biasing



Important points to remember

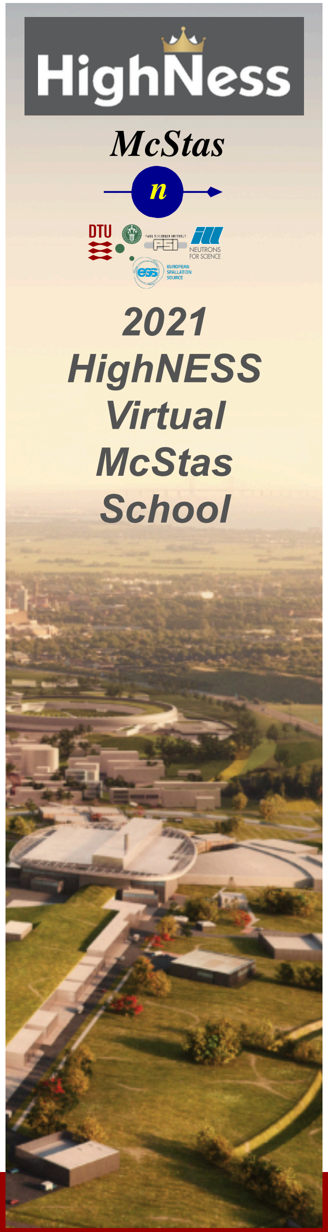
1. Your simulation will only contain elements you provided / defined

2. … to the precision you defined

3. Answers the questions you posed

4. Background essentially only from “sample”, or sample-near objects
   - Use *concentric* geometry / Union concept for sample env
   - Source-term backgrounds are usually an MCNP-oriented problem
     (http://coimbra2016.essworkshop.org,
     http://istsi.essworkshop.org,
     https://github.com/McStasMcXtrace/SINE2020WP8)

What to optimise? Figure of merit requires thought…



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

- But brilliance-transfer is probably a good quantity to think of…

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

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

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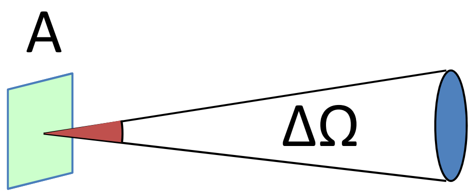
Crawford, R. K., Arai, M., Carlile, C., Chapon, L., Granroth, G., Langridge, S., ... Wiedenmann, A. (2009, Aug 26). Long-Pulse Neutron Instrumentation Workshop, August 26-28, 2009. (Oak Ridge National Laboratory ed.) Oak Ridge, USA.

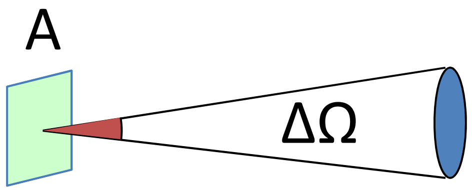
Neutron flux - and brilliance / brightness



B = N per time per A per ΔΩ

units = $n/s/cm^2/sr$

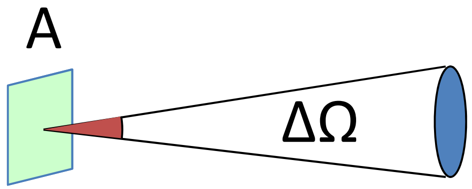
Neutron flux - and brilliance / brightness



B is independent of distance

- property of the source

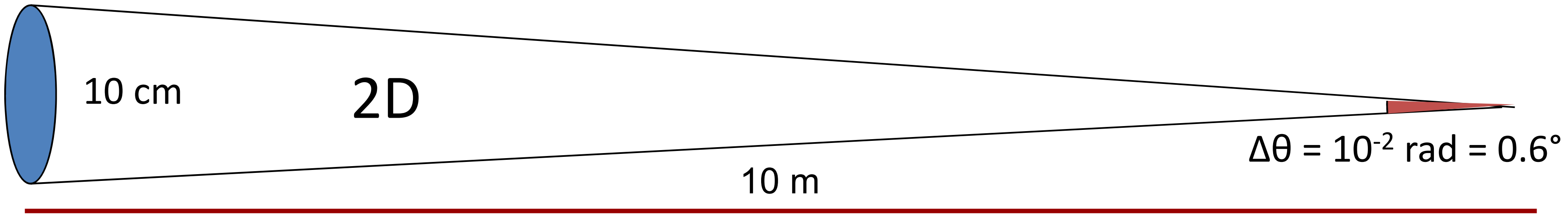
Neutron flux - and brilliance / brightness

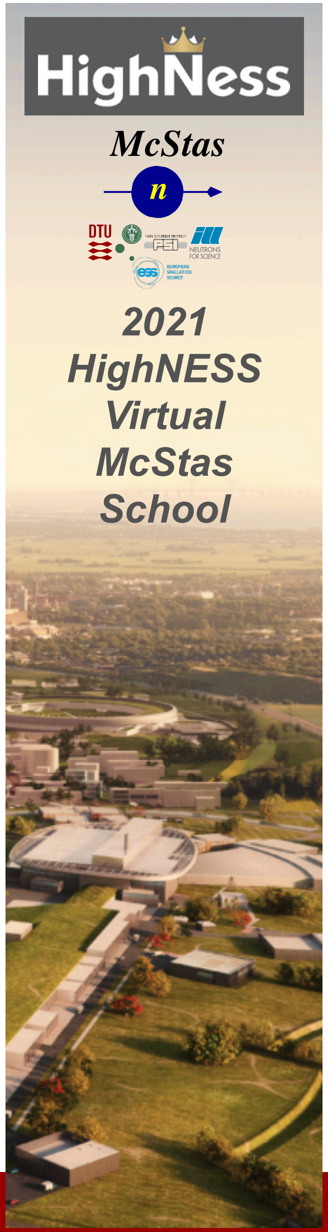


Brilliance/Brightness B [n/s/cm²/sr]

Flux Ψ [n/s/cm²]

Neutron flux - and brilliance / brightness





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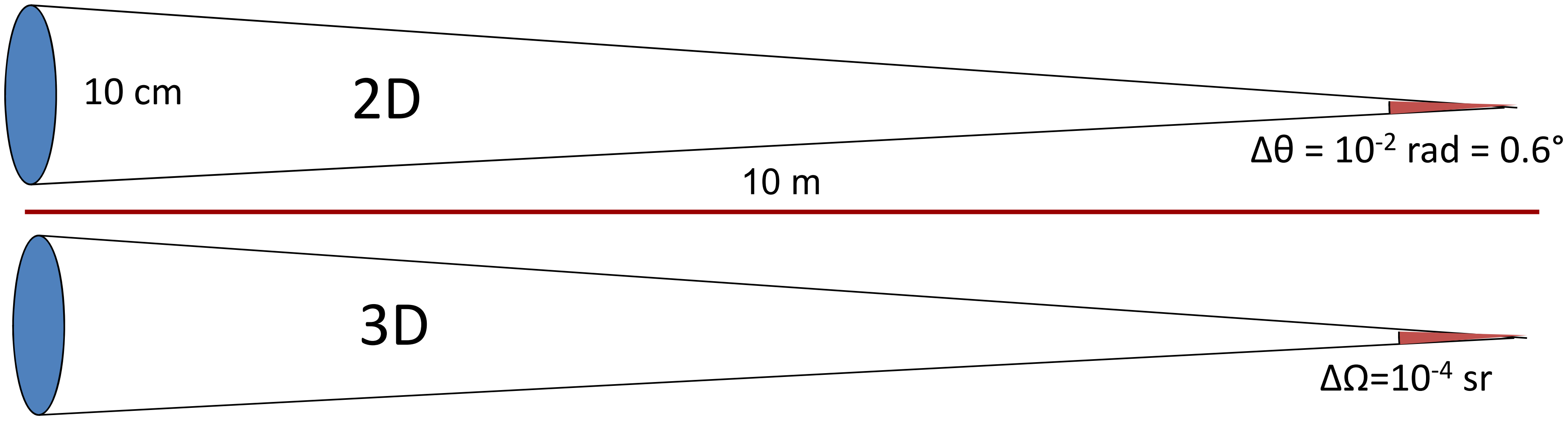
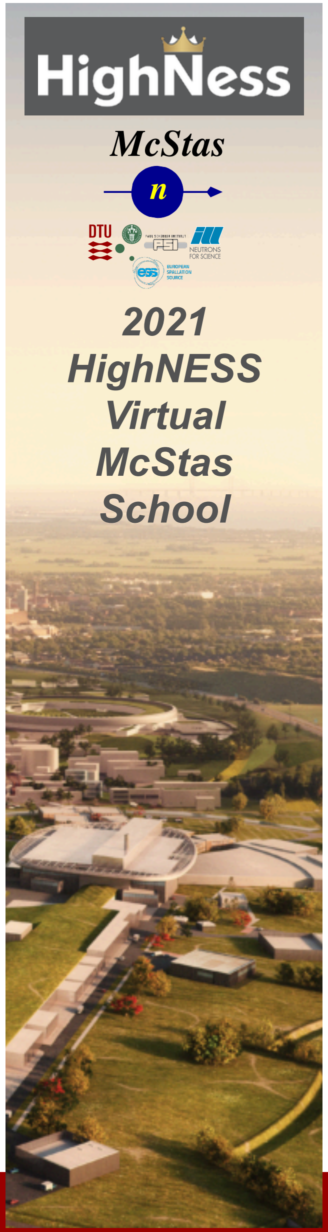
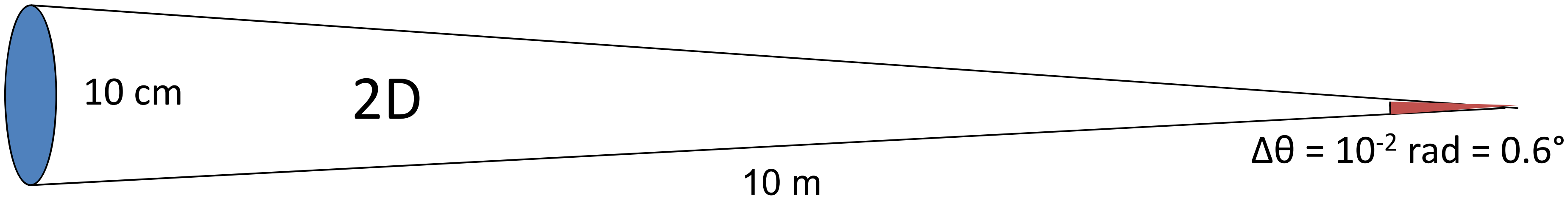


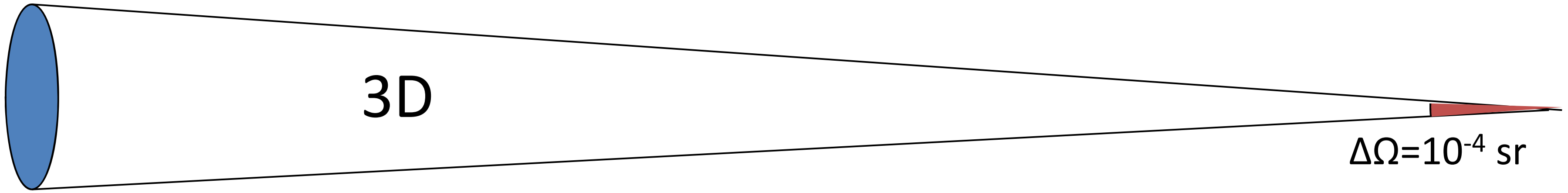
Flux = Source Brightness × Solid Angle

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



Neutron flux - and brilliance / brightness





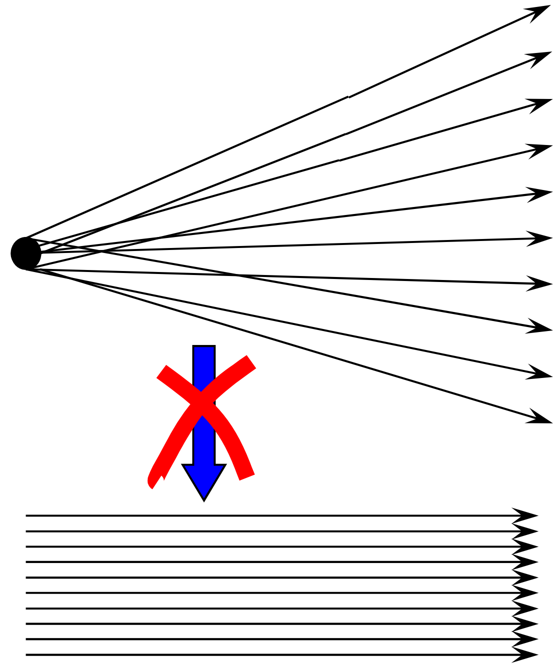
Flux = Source Brightness × Solid Angle

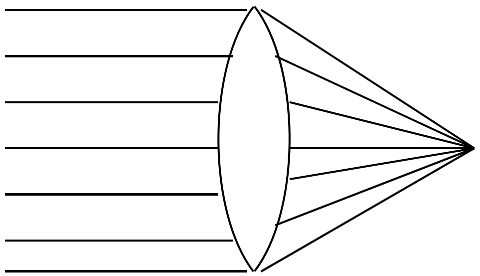
$\Phi = B \times \Delta\Omega$

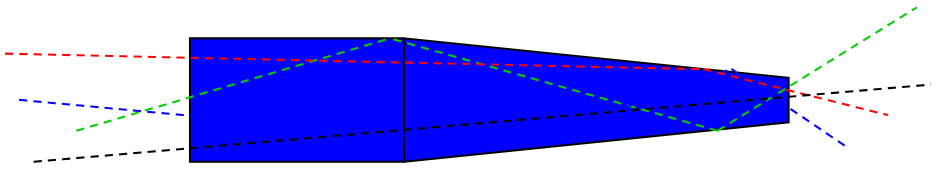
Liouville theorem
→ $\Delta x \Delta \phi$ = const

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







Liouville theorem
$\rightarrow \Delta x \Delta \phi = \text{const}$

Liouvilles Theorem

- Conservation laws:
  - neutrons can’t be created from thin air
  - neither can “phase space density”
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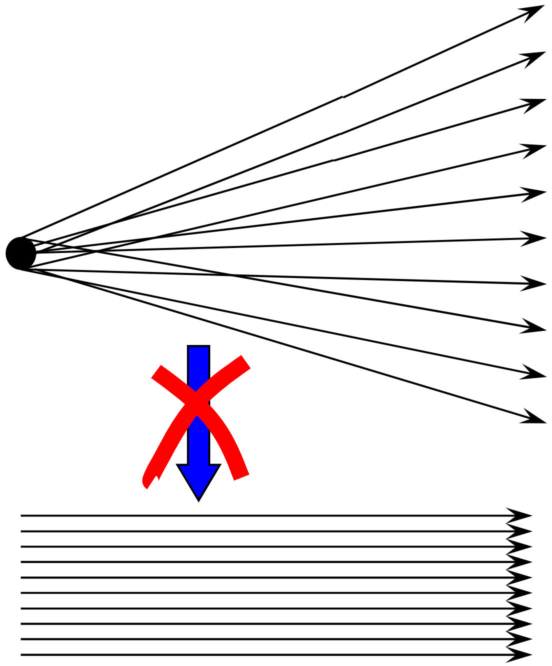
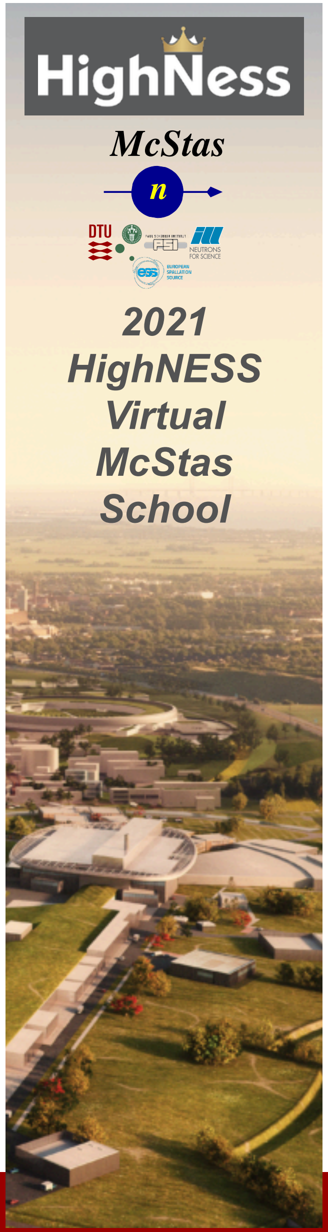
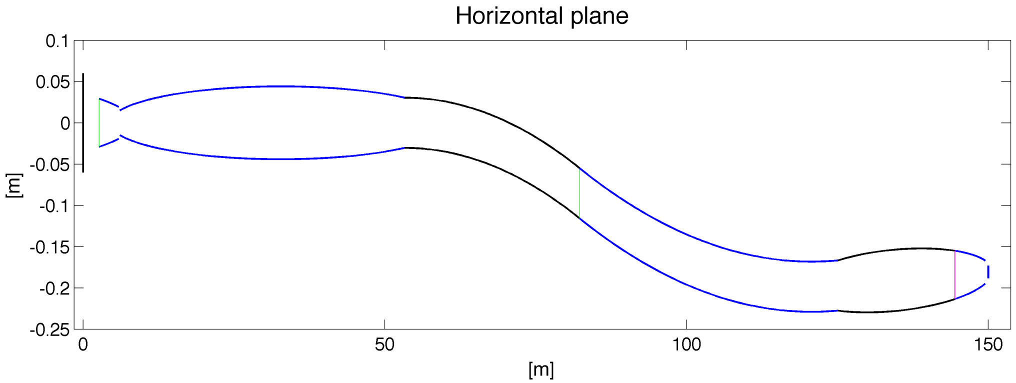


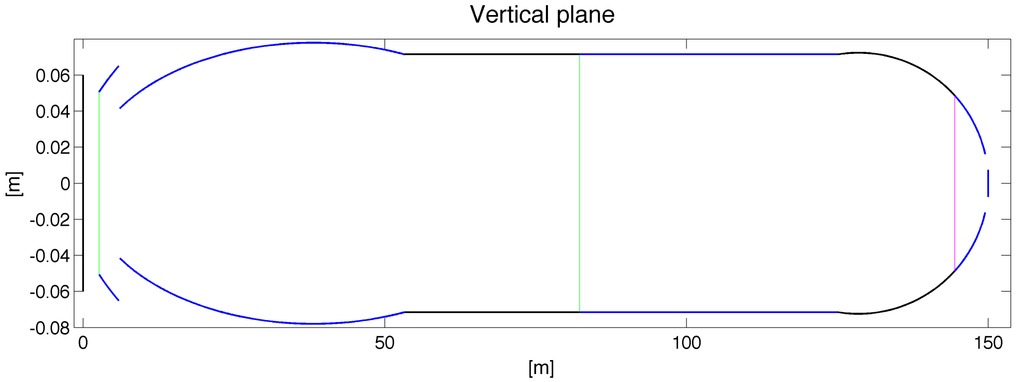
Integrated flux $\int \Psi \, dA \, d\Omega$ can never increase

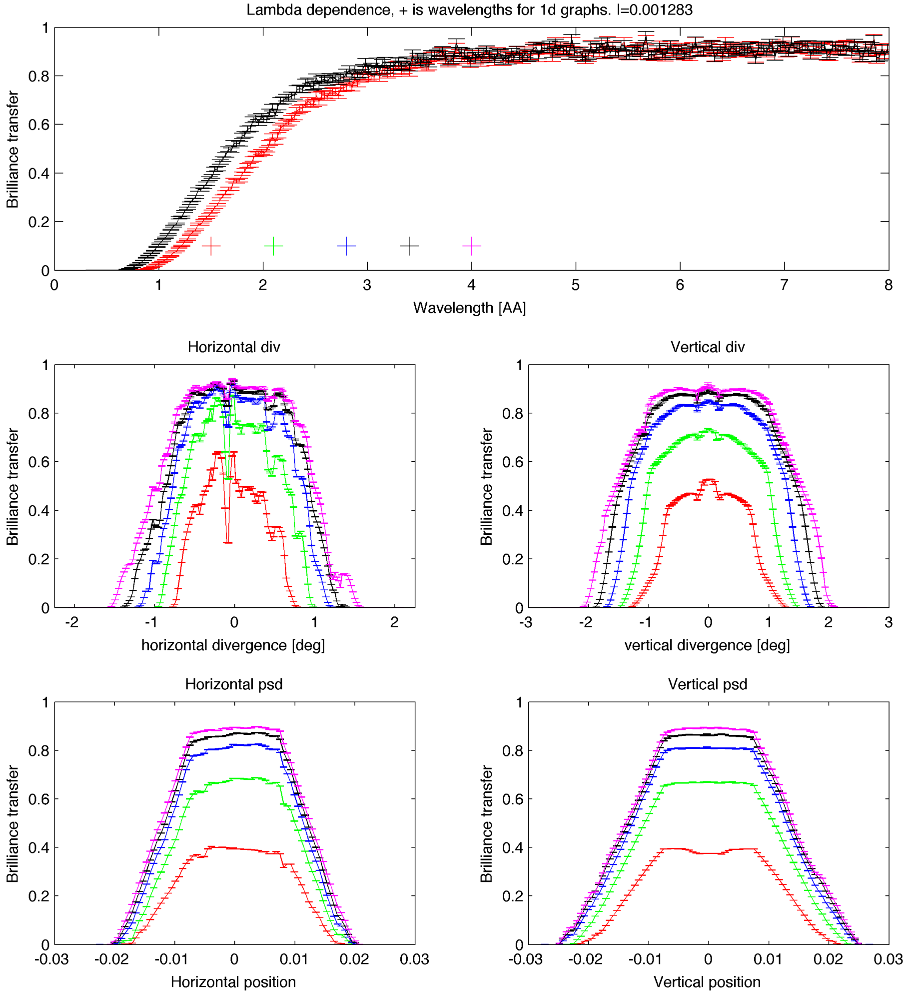


A good optic maximises *transfer* of brilliance

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







Simple BT-means by 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
```

Simple BT-means by McStas-code? See example folder…

McStas

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

Spatial ranges

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
```

Spectral range

Directional range

Simple BT-means by 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…

Simple BT-means by McStas-code?
See example folder…

HighNess McStas

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

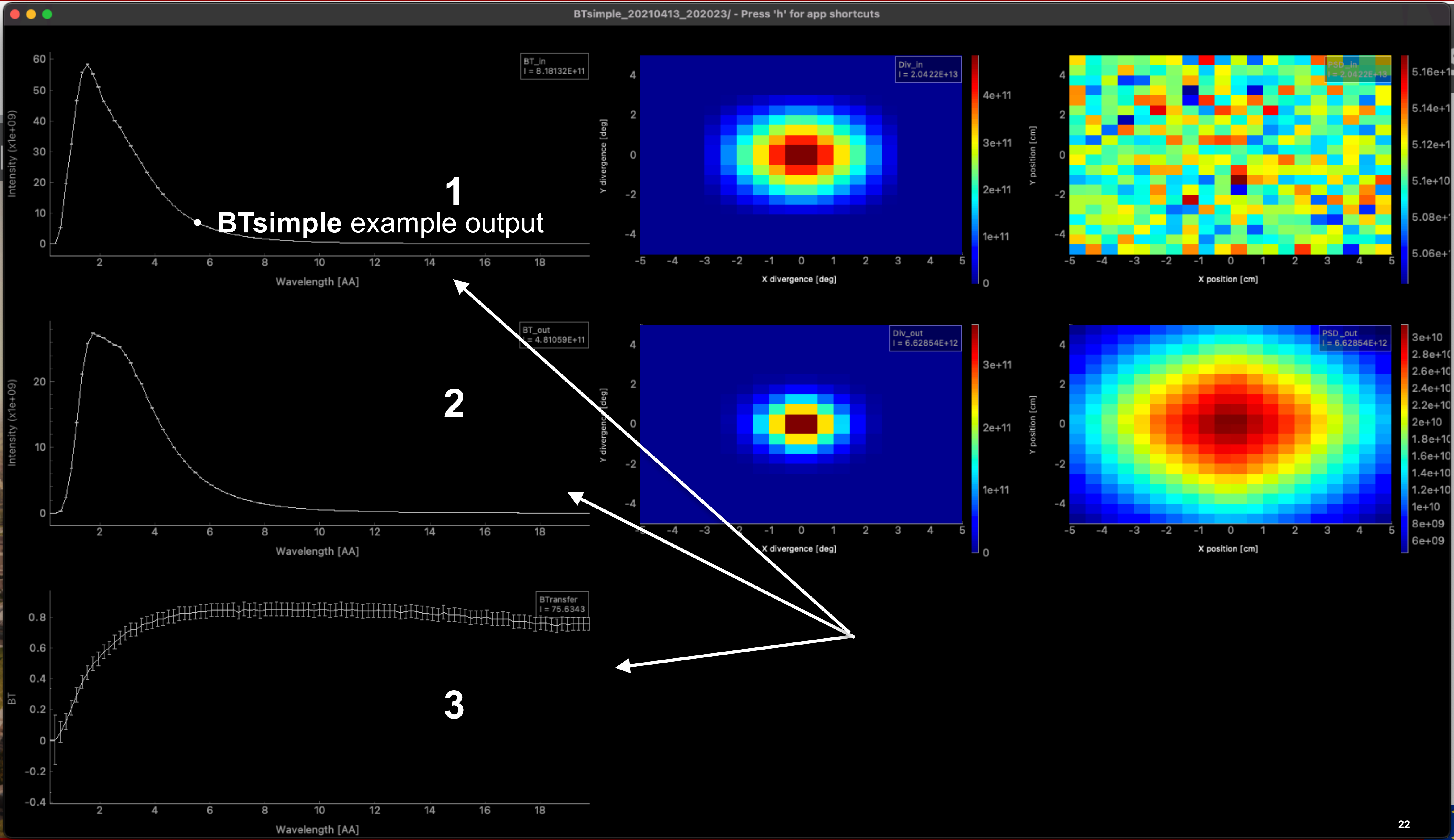
1.
```
/* Measure incoming phase-space */
COMPONENT BT_in = L_monitor(xwidth=0.02, yheight=0.02, filename="BT_in.dat",
                  Lmin=lambda-dlambda, Lmax=lambda+dlambda, nL=101, restore_neutron
WHEN ((VertDiv <= maxvd) && (HorDiv <=  maxhd)) AT (0,0,2.0) RELATIVE  origin
```

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
```

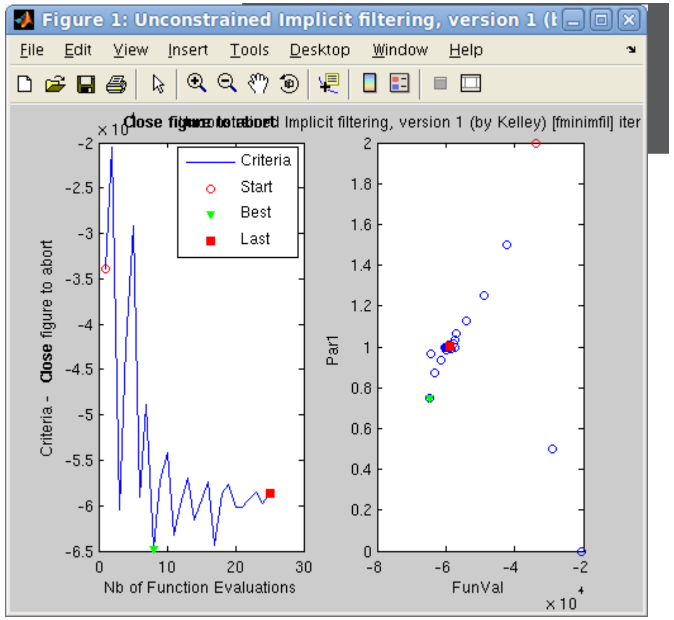
- **Performs piece-wise division of the bins w. error propagation**

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** example output



Optimisation tools…



- 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. Mads recommends Matlab 2012 and iFit 1.3…

2021 HighNESS Virtual McStas School

Connectivity with other codes… Esben?