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Particularities/difficulties of simulating a unconventional guide instrument

The HRPD case @ ISIS

Jordi Jacas-Biendicho
Aziz Daoud-aladine,
K. Knight, S. Hull

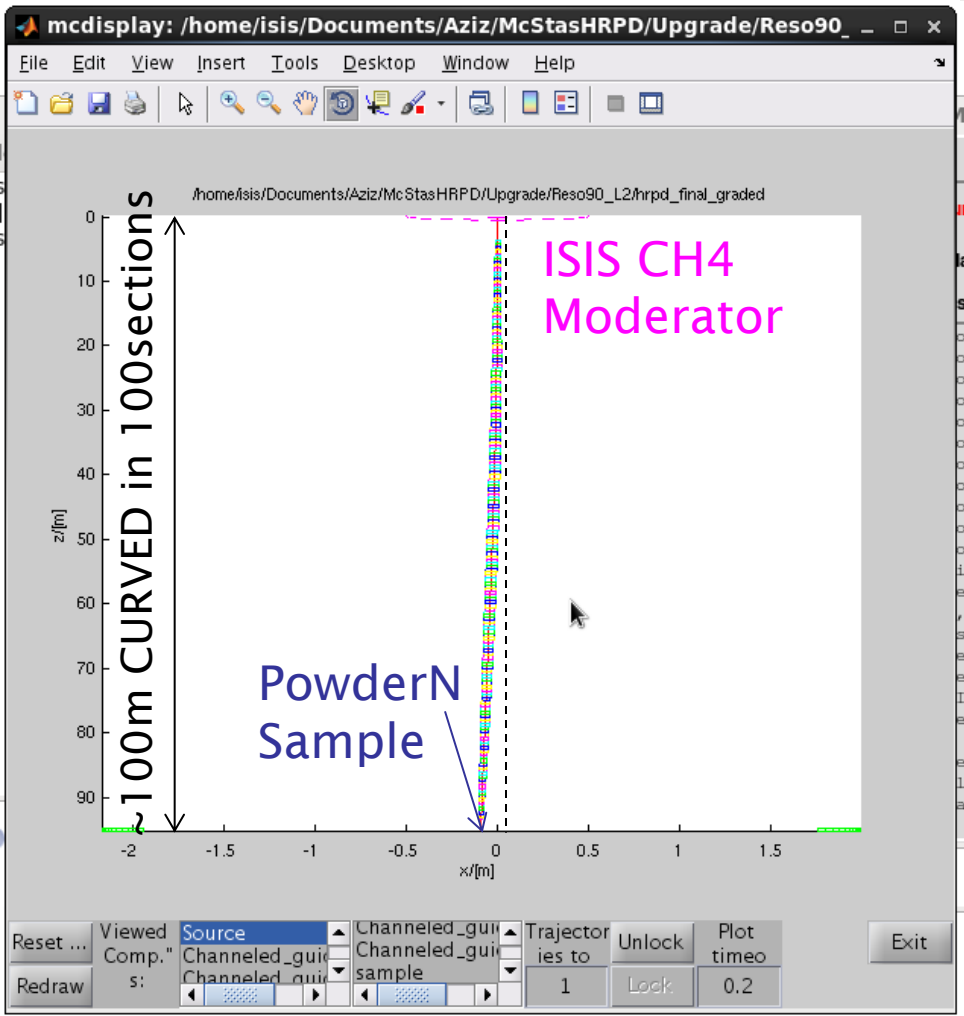
HRPD Upgrade –I (2008) Tapered elliptic-curved guide

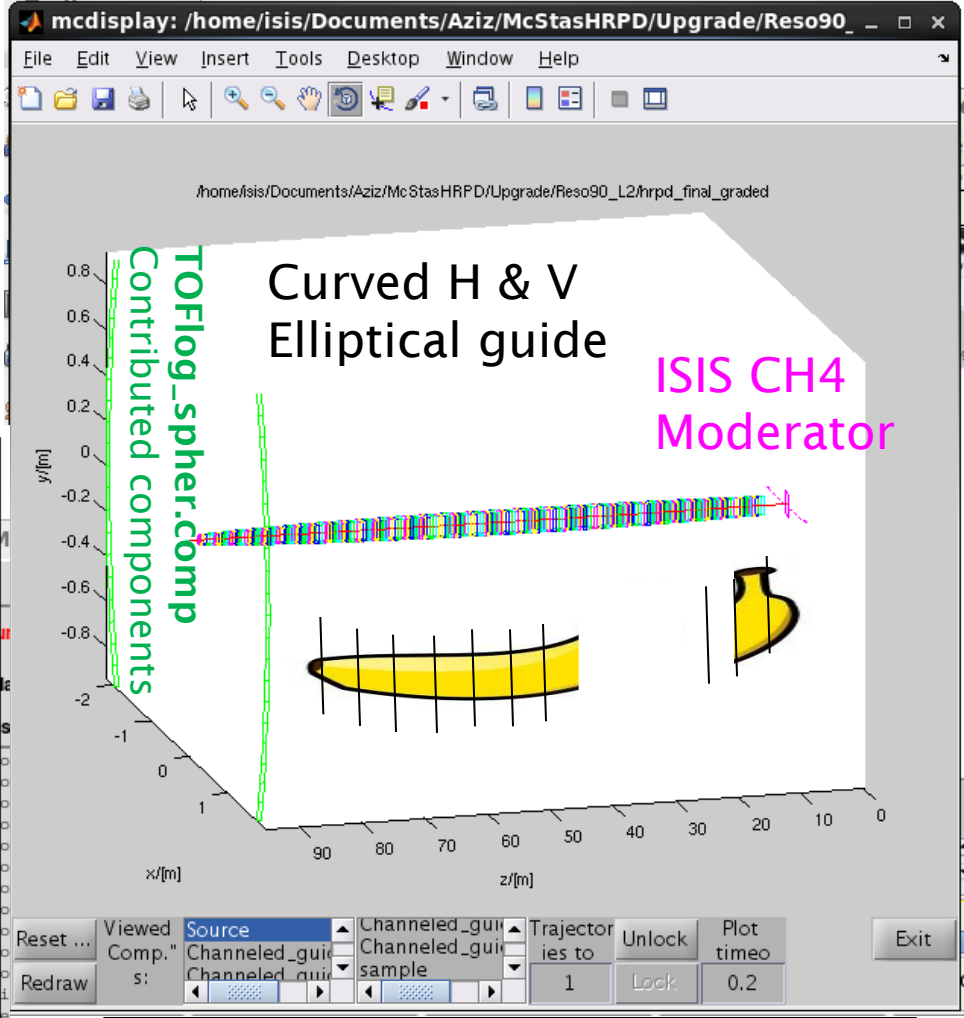
Laurent CHAPON (ILL)

Essential Contributions :

Benchmark against analytic guides

Debugged PowderN, devt of new components





100 (Guide) + few components beam line!!!!

INCREDIBLE FLUX GAINS

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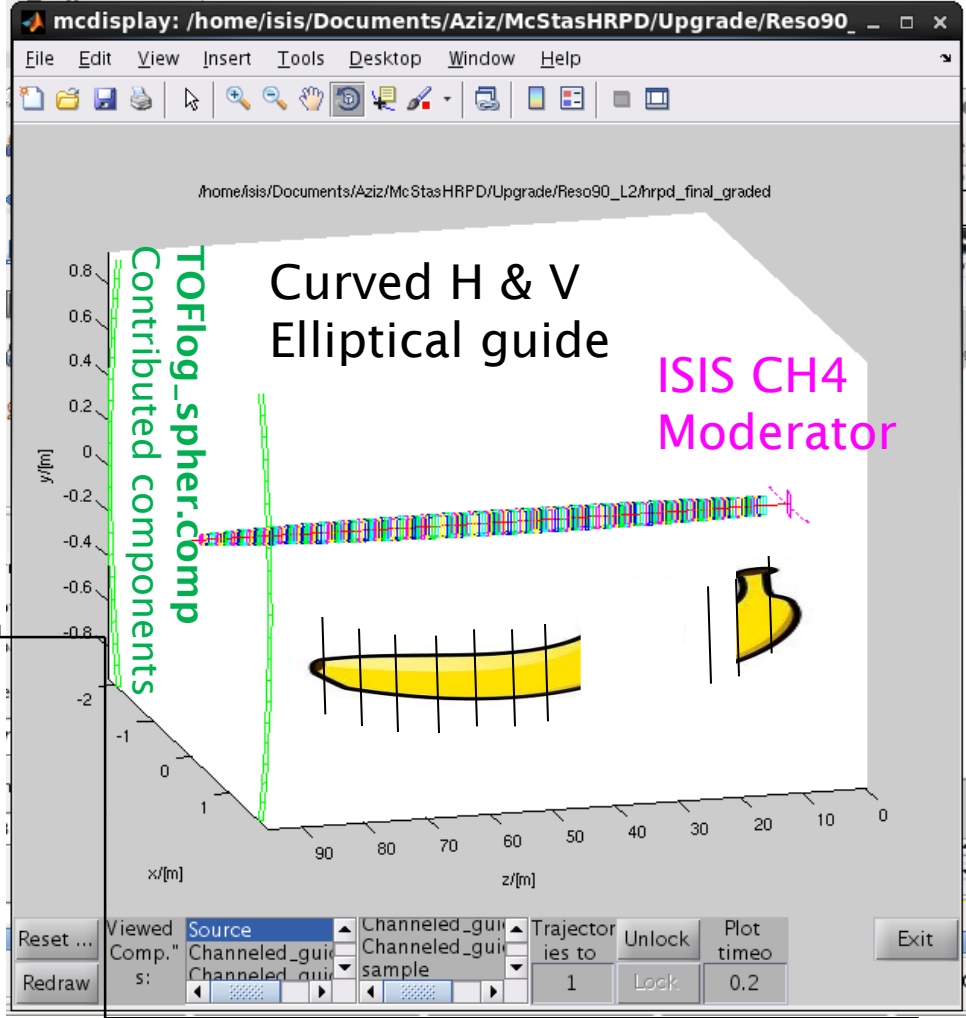
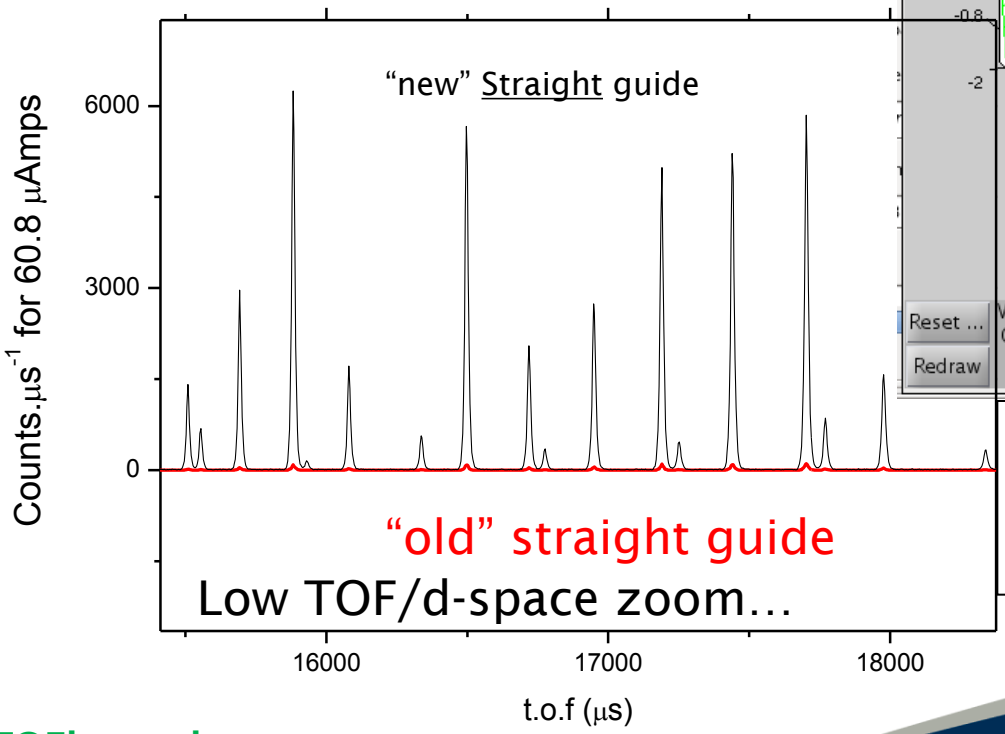


Factor 60 at short wavelengths



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TOFlog_spher.comp

Outputs focused data in log(TOF)

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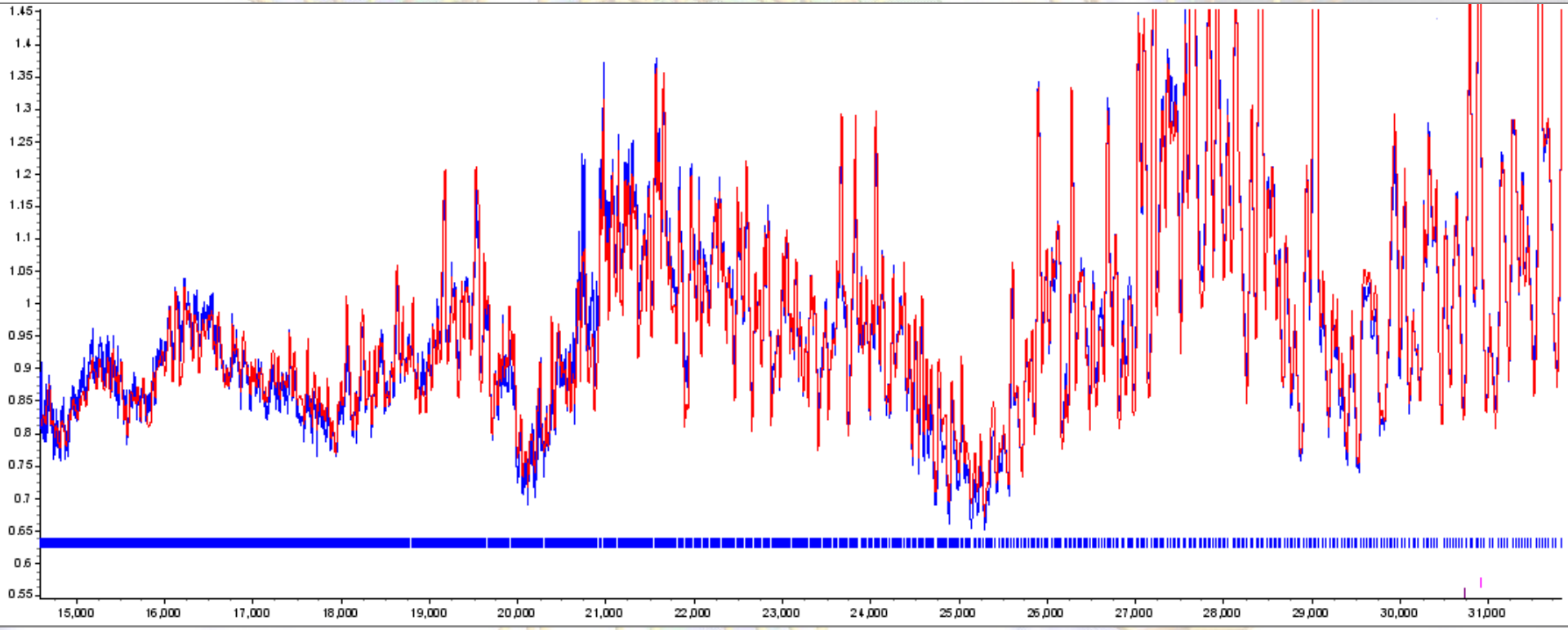
C_{60} revisited on HRPD



0.3Å

0.6Å

These data were not observed in 1992
In 1992, there were 2100 reflections to 0.6Å
In 2007, there are 17820 reflections to 0.3 Å

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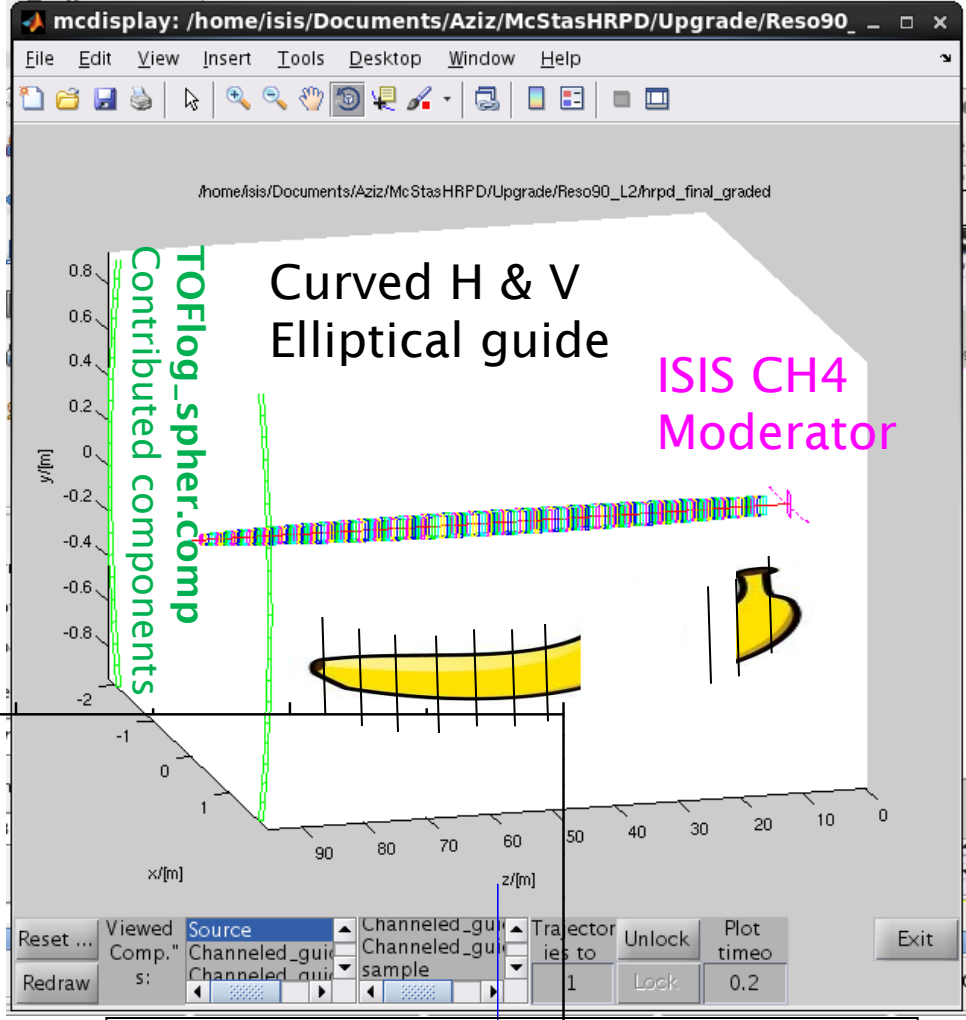

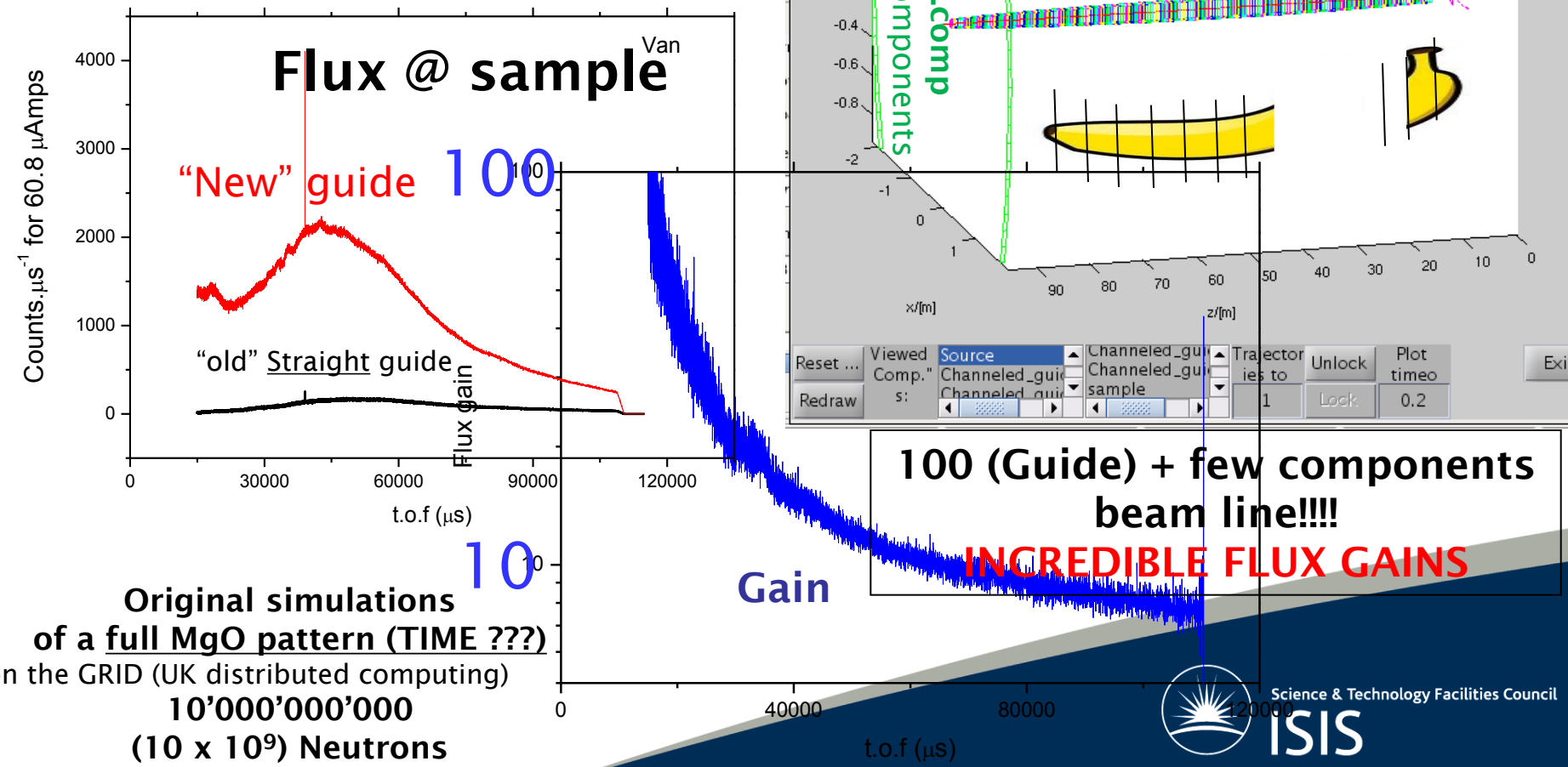

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Original simulations of a full MgO pattern (TIME ???)

on the GRID (UK distributed computing)

10'000'000'000

(10 x 10^9) Neutrons

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HRPD "Upgrade" – II

- Change detector layout to have more space therefore more Sample env. "options", radial collimation, etc..
(pb of trade/improvement flux/resolution)…

Jordi Jacas/myself:
Our initial Problem Different:

First *tests on my PC* (4 cores 2.4GHZ)
~4h20min hours

500'000'000 neutrons

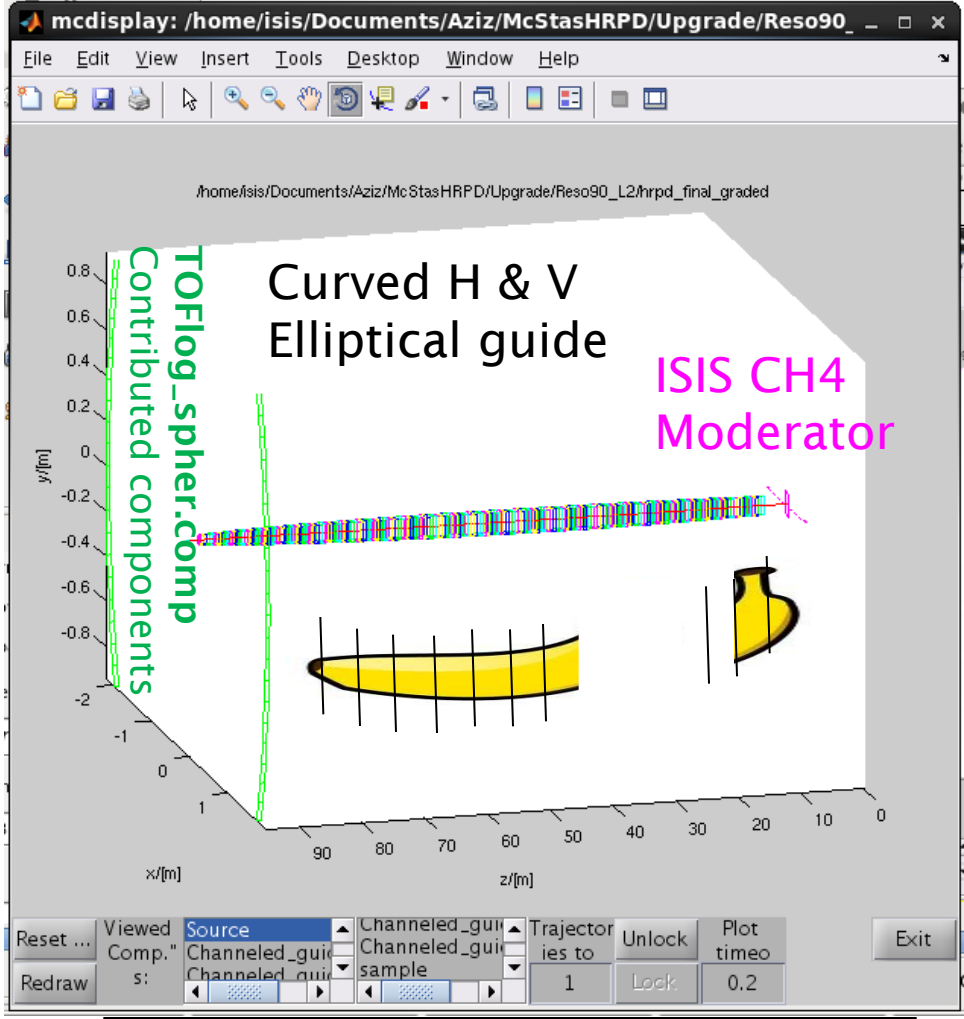
(enough for dealing single peaks, not full pattern)

Would take ~100h

here

↑

Original simulations
of a full MgO pattern (TIME ???)
on the GRID (UK distributed computing)
10'000'000'000
(10 x 10^9) Neutrons



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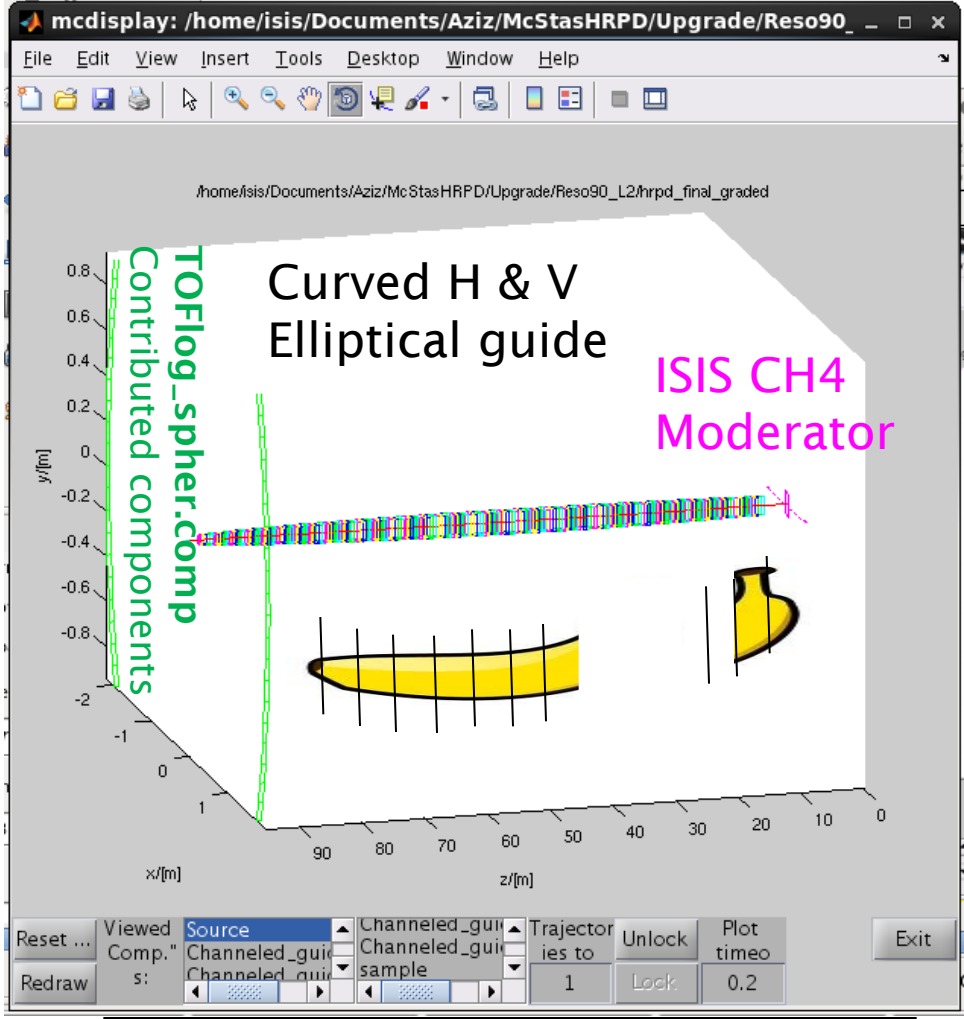
COMPUTATION RESSOURCES
Vs
COMPUTATION TIME

For good Stats?

Needs for Automation in the Analysis of simulated data

Fit tools?



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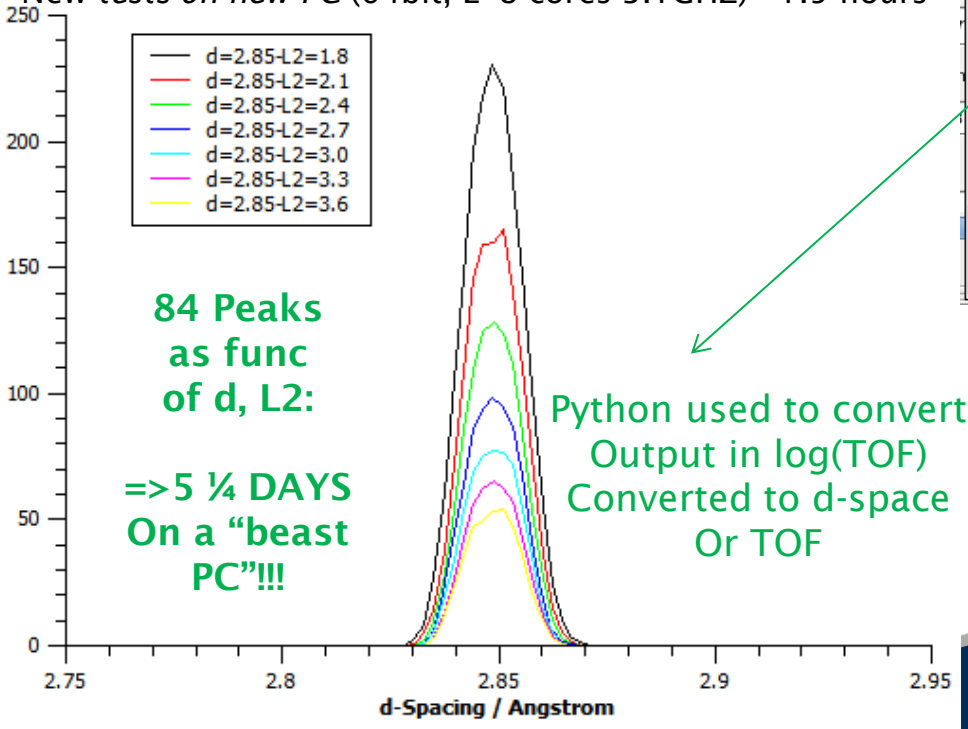
First *tests on my PC* (4 cores 2.4GHZ) ~4h20min hours

500'000'000 neutrons & focused λ-range

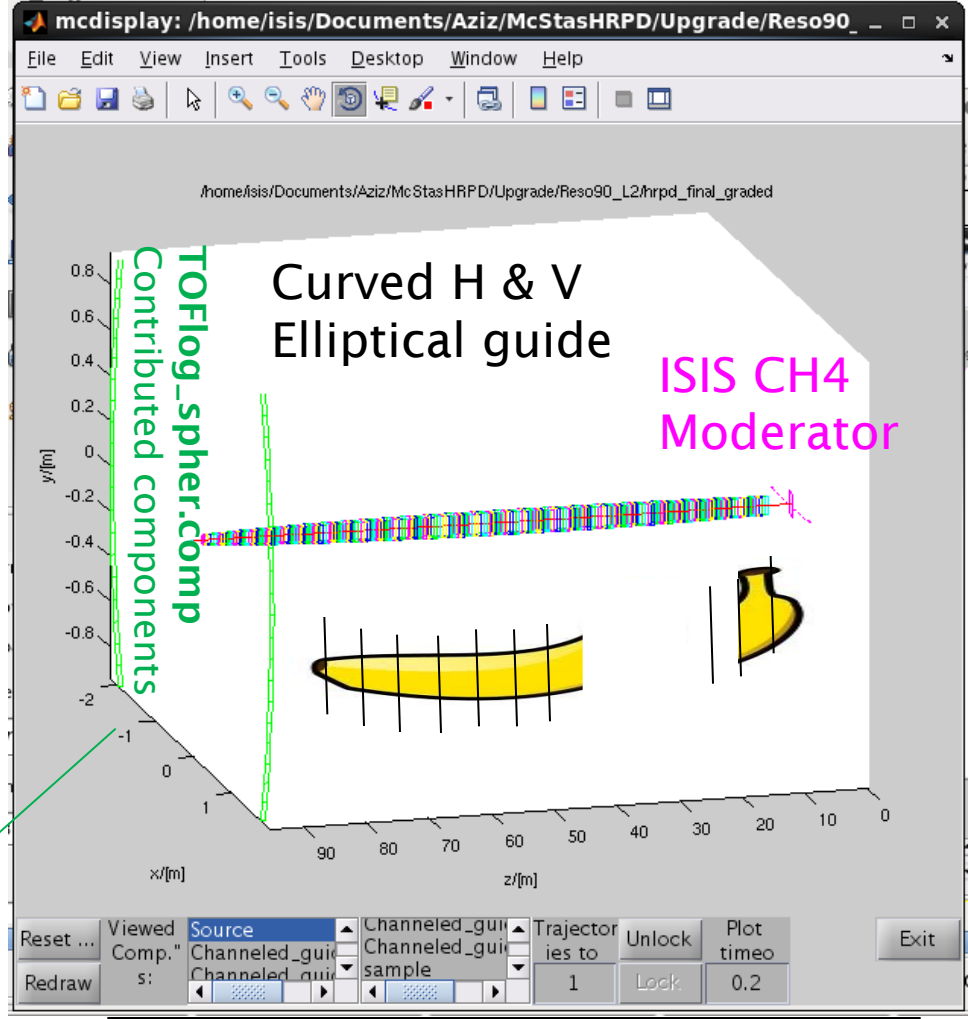
New *tests on new PC* (64bit, 2*8 cores 3.1GHZ) ~1.5 hours



84 Peaks as func of d, L2:

=>5 ¼ DAYS On a "beast PC"!!!

Python used to convert Output in log(TOF) Converted to d-space Or TOF



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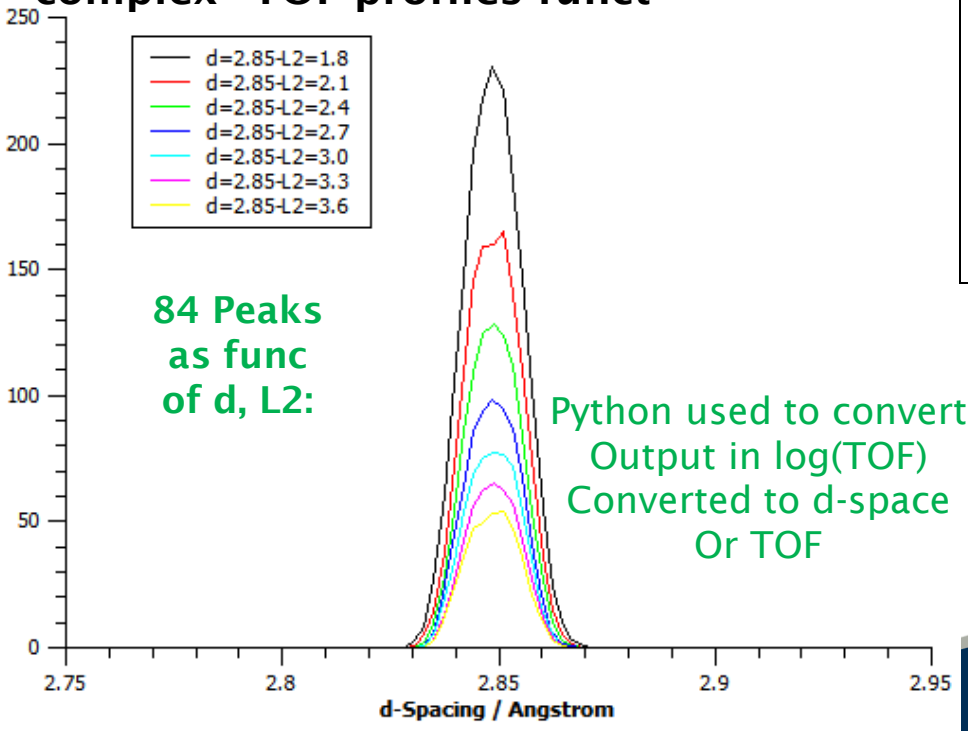
FINAL ANSWERS: Need for Automation

in the **Analysis** of simulated data…

Fit/get and make graph/tables of params in **"complex" TOF profiles funct°**



84 Peaks as func of d, L2:

Python used to convert Output in log(TOF) Converted to d-space Or TOF

This is not only about Monte Carlo…

WHICH TOOL TO USE?

- **Tof-Xrfit in the Rietveld Fullprof Suite** (easiest, but not generic and/or easy to tweak enough)?

- **MANTID (use involves debug, Needed to put constrains ⇒Biased analysis…)**

- **Else?**

So far: more tedious than McStas!!! Requires lots of iterated scripting & fully controlled IO, which do not exist

THIS IS THE HARDEST UNTRUSWORTHY PART
(COMPARED TO the Mc Simulation, Where the main pb is "just" speed)

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Ex: Back to back exp

$$\Omega(x) = pV(x) \otimes E(x) = \int_{-\infty}^{+\infty} pV(x-t)E(t)dt$$

$$pV(x) = \eta L'(x) + (1-\eta)G'(x)$$

Width FWHM $0 \le \eta \le 1$

$$E(t) = 2Ne^{\alpha t} \quad t \le 0$$
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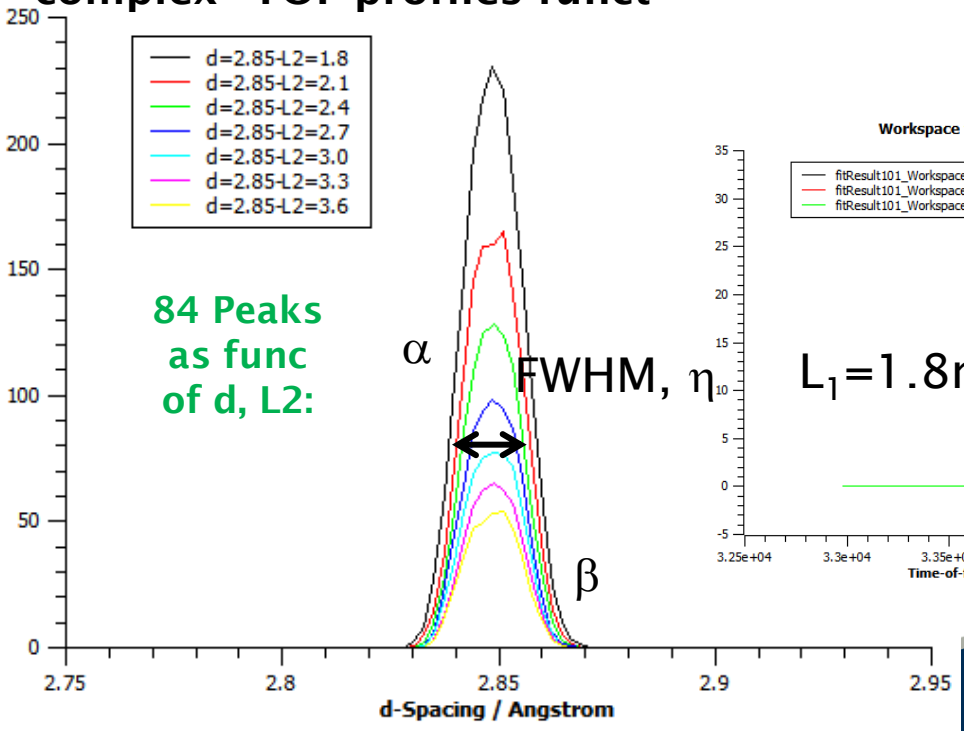
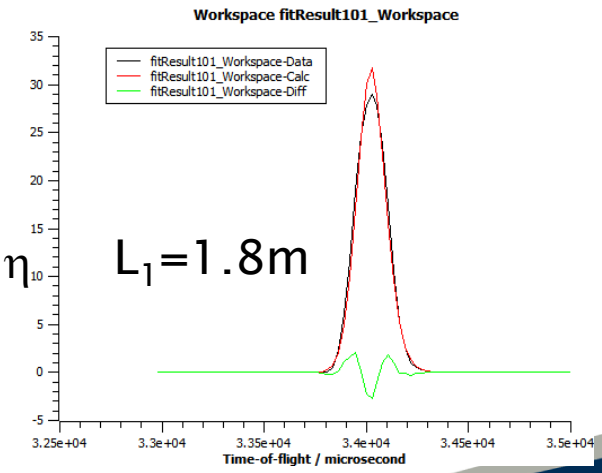
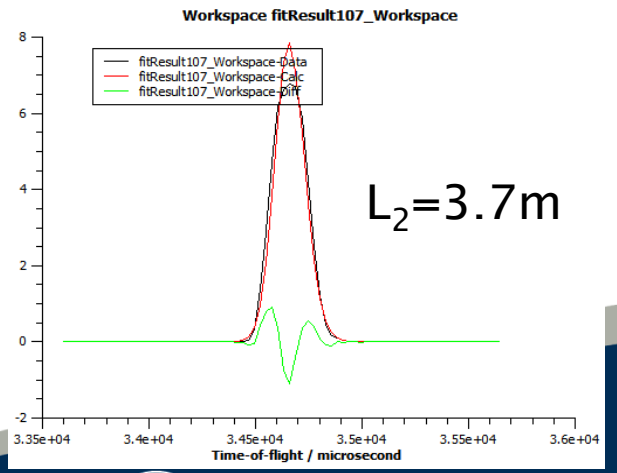
$\Rightarrow$ **Biased analysis…)**







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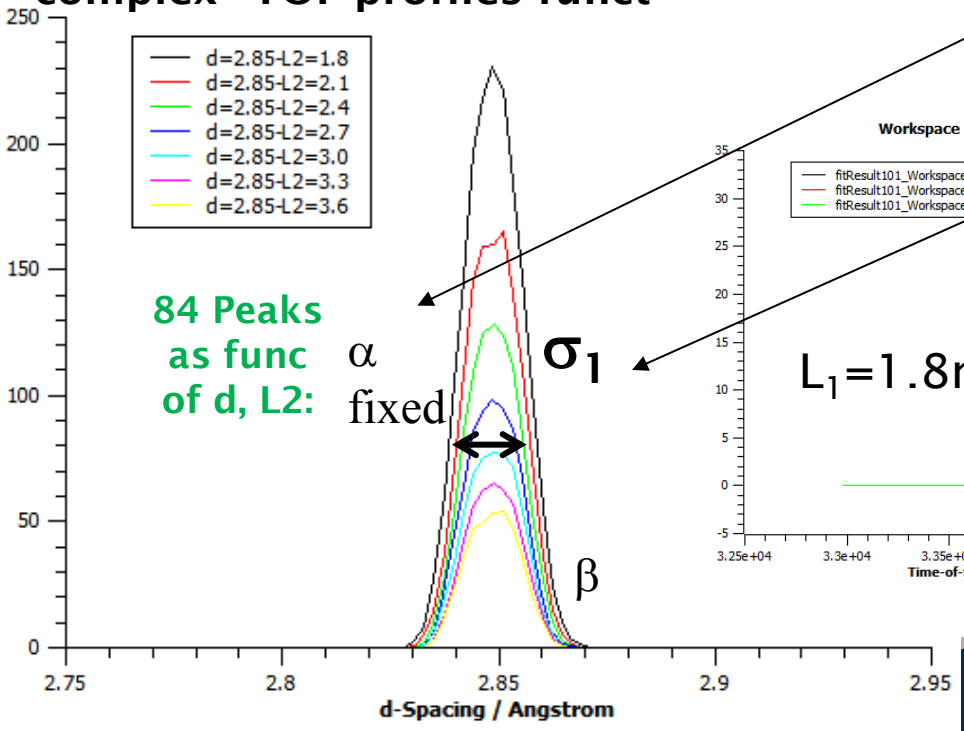

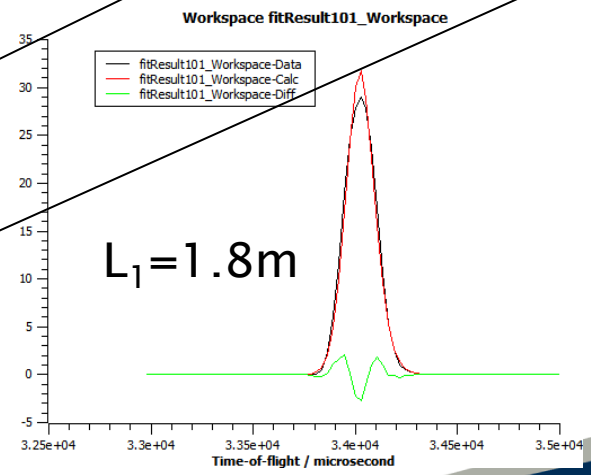

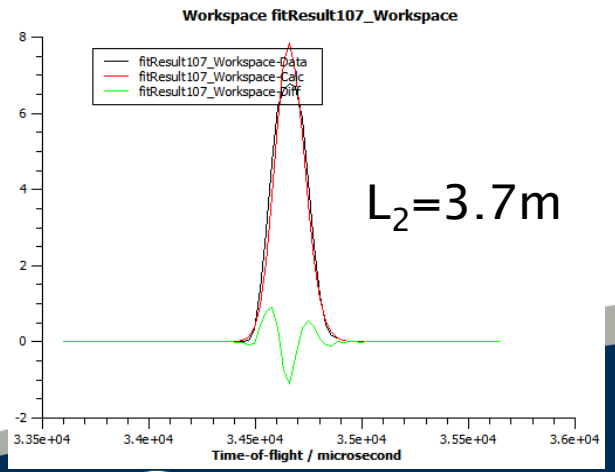

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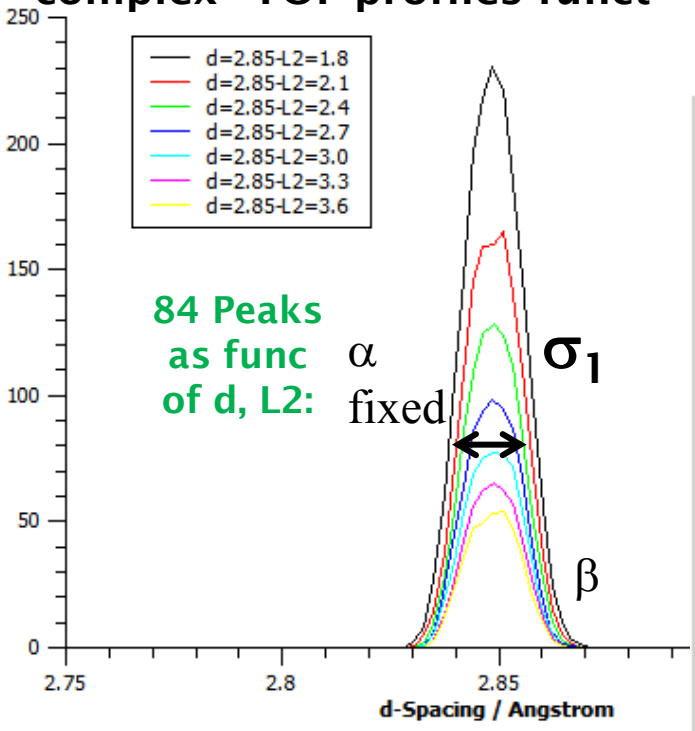

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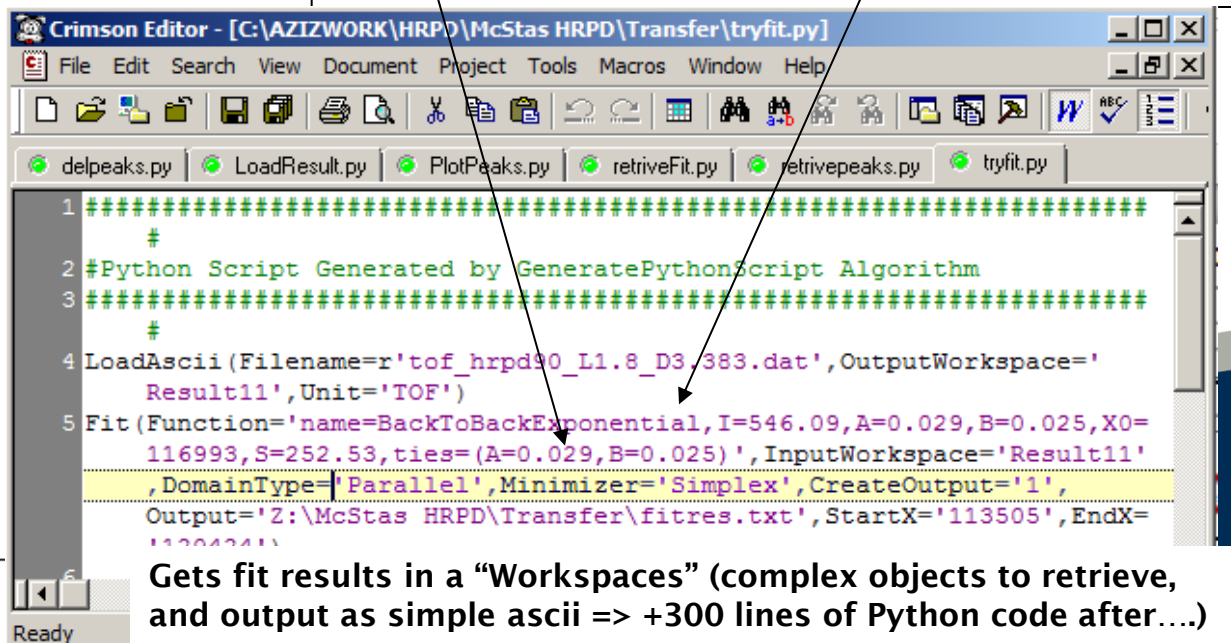

Gets fit results in a "Workspaces" (complex objects to retrieve, and output as simple ascii => +300 lines of Python code after….)

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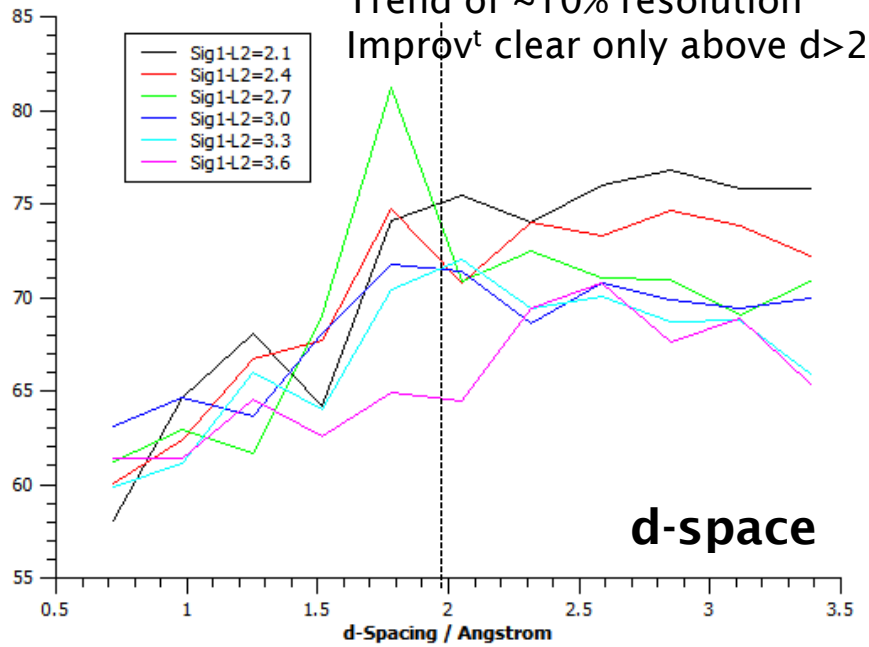
Resolution : For L2<3m
Trend of ~10% resolution
Improvᵗ clear only above d>2A



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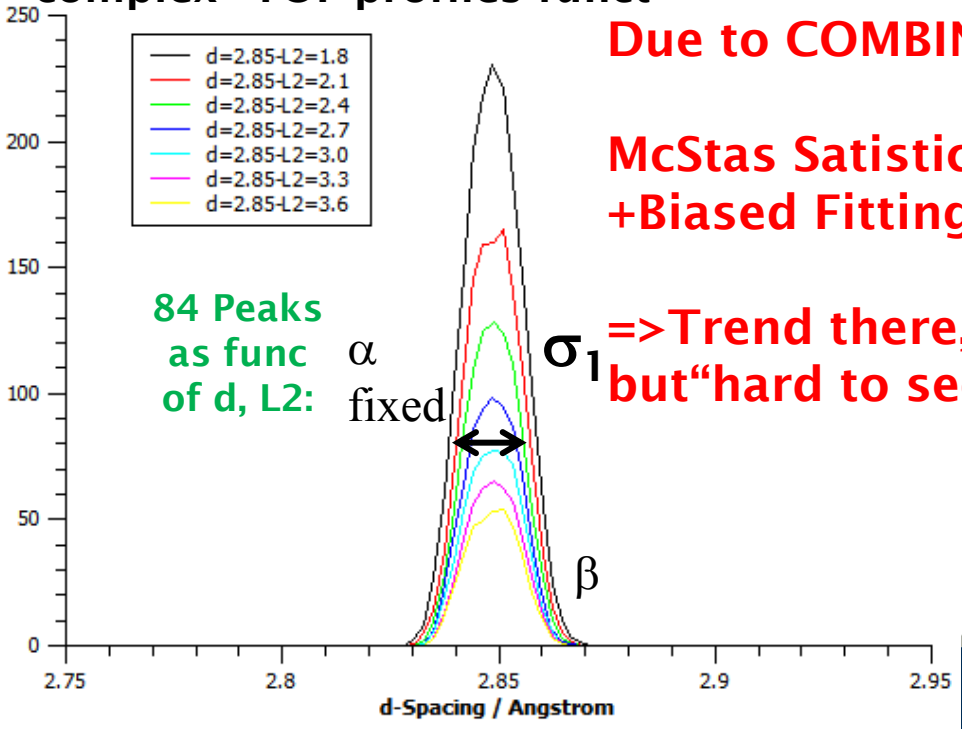
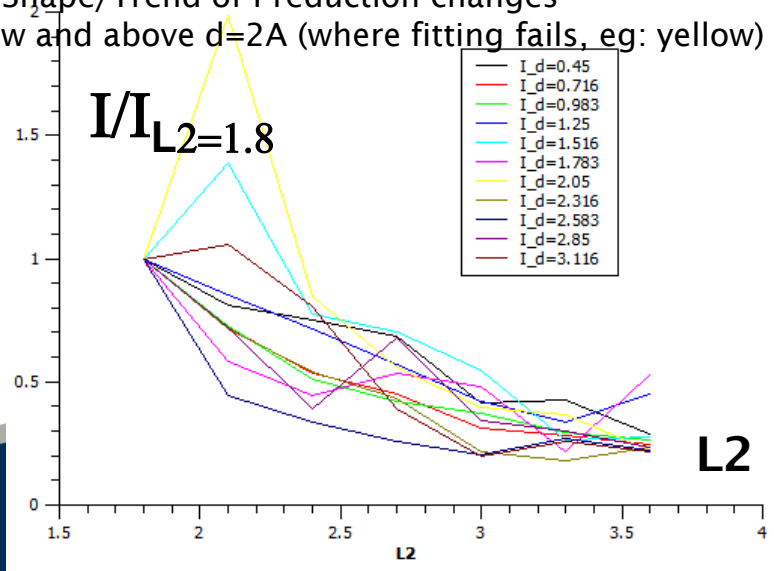


Due to COMBINED

McStas Satistics, +Biased Fitting

=>Trend there, but"hard to see"

Intensity: Peaks not "seem" to all
Follow solid angle change,
The Shape/Trend of I-reduction changes
below and above d=2A (where fitting fails, eg: yellow)



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CONCLUSION

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