

6 McStas various utils

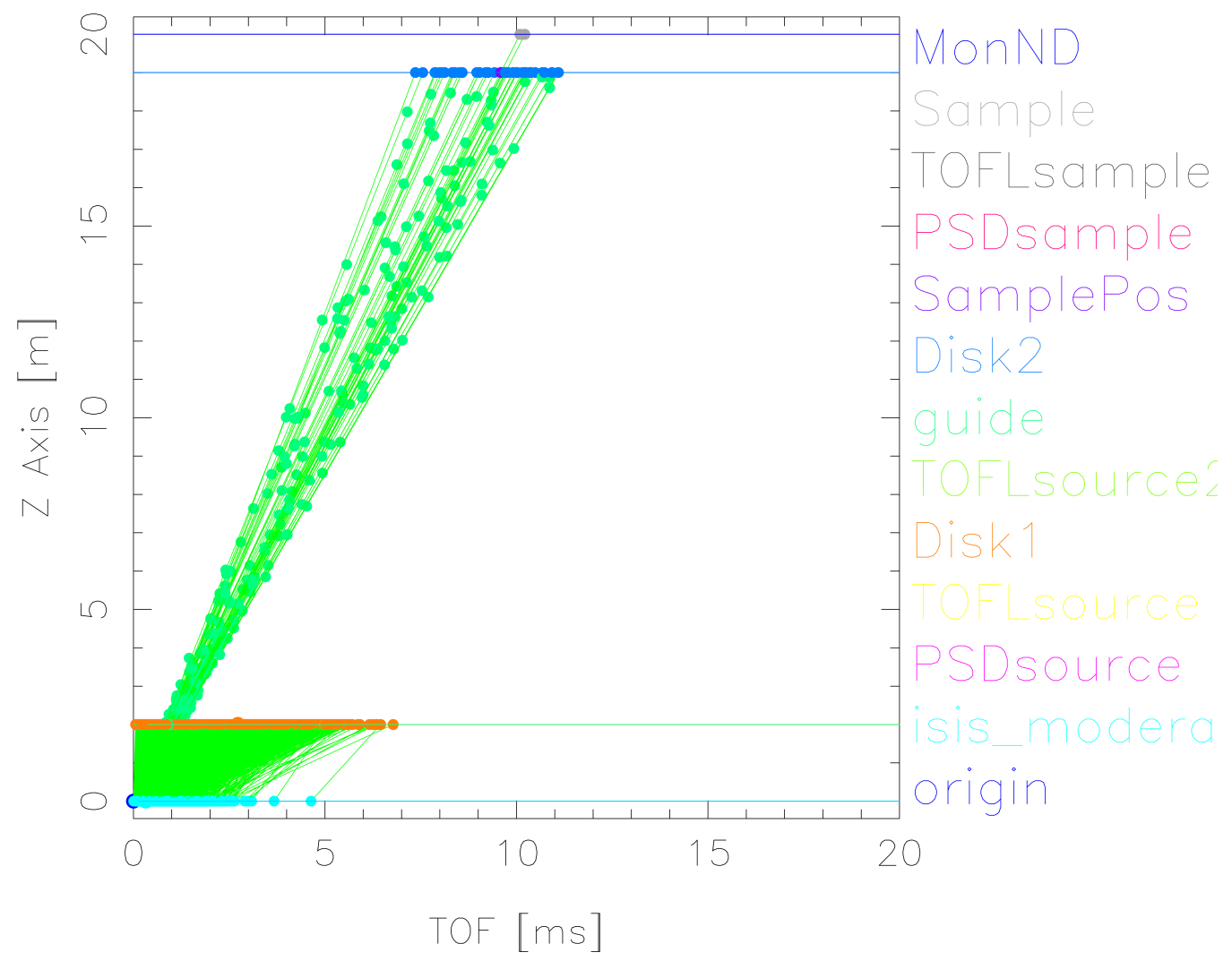
- Hidden gems and useful little things...
- + Disclaimers and tips for the next couple of days...



TOF diagram util based on mcdisplay

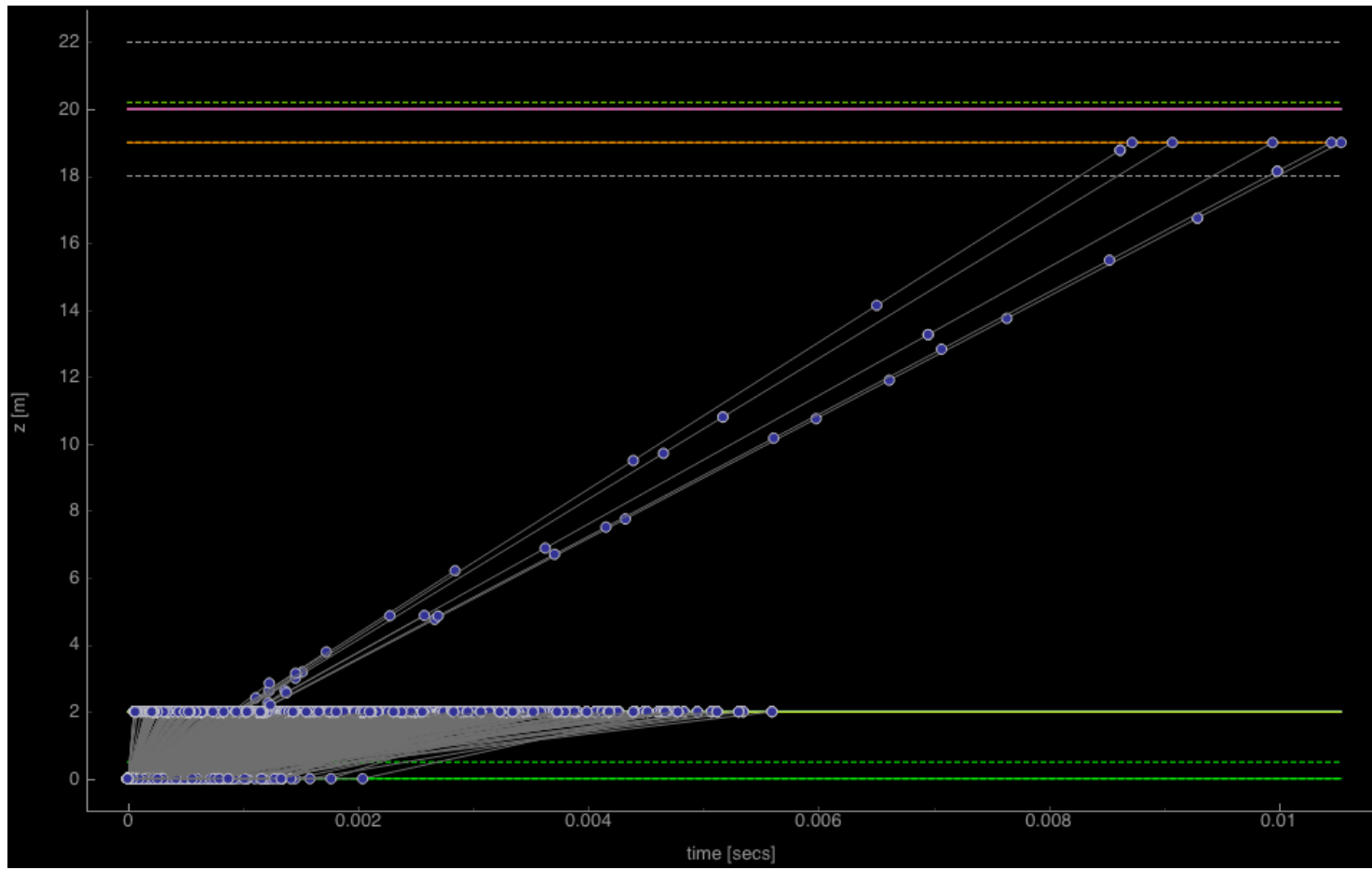
• `mcdisplay.pl --TOF --tmax=20 instrument...`

TOF diagram: STEP3.out



TOF diagram util based on mcdisplay

- `mcdisplay-pyqtgraph --TOF instr`



cif2hkl

- Util for generating McStas style “laz/lau” reflection lists from CIF file
- Based on CrysFML from the ILL (FullProf)
- Compile for your system from <https://github.com/McStasMcXtrace/McCode/tree/master/tools/other/cif2hkl>
- (May also get included in McStas 2.4)



iFit optimiser (<http://ifit.mccode.org>)

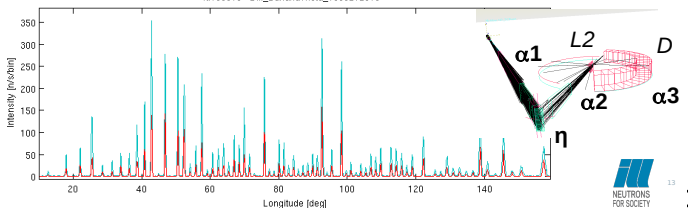
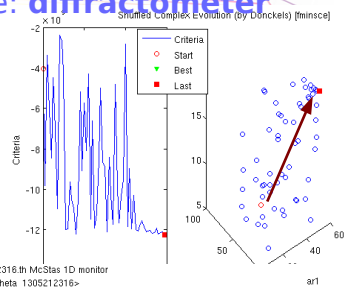
- General data / optimisation framework
- ~ Modern "spec_nd"
- Matlab based, but does not require matlab (binary distribution also)
- Reads and plots McStas
- Can run McStas as a "cost function", varying instrument parameters



iFit/McStas: example: diffractometer

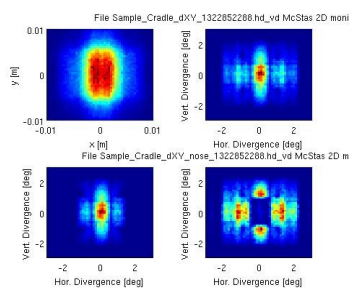
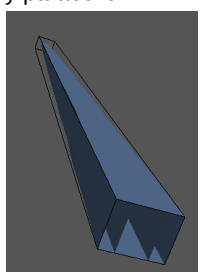
Space: 4 parameters
 Execution: 45 minutes on 2 cores
 Many equivalent solutions.

	start	optimal
$\alpha.1$	10	55
$\alpha.2$	10	50
$\alpha.3$	15	15
η	15	23.5



iFit/McStas: example: IN22 nose

- Gain a factor 3 in flux for 50 k€.**
- No need to use high m coating for top/bottom $\rightarrow m=4$
 - $m=6$ to $m=5$ only reduces flux by 1%.
 - Nose 87 cm long. Profile is not fully parabolic.



Cluster utility scripts

- mcsb cluster scripts

```

./mcsb_slurm.pl
Usage: ./mcsb_slurm.pl [options] [mcrun params]
-h          --help          Show this help
-rN         --runtime=N     Specify maximum runtime (hours) [default 1]
-qQNAME     --queue=QNAME   Specify wanted SLURM queue [default 'express']
-e<mail>    --email=<mail>  Specify address to notify in reg. sim status [default none]
--nodes=NUM Specify wanted number of nodes [default 1]
--name=NAME Specify slurm job name [default
"McSub_<USERNAME>_<TIMESTAMP>"]

After running ./mcsb_slurm.pl NAME.batch is ready for submission using the sbatch command

```

- Takes a “mcrun commandline”
- Writes batch file “template” for use with PBS or slurm cluster queue systems
- <https://github.com/McStasMcXtrace/McCode/tree/master/tools/cluster-scripts>



Vitess - compatibility

- Utility script for converting Vitess reflectivity files for use with McStas
(https://github.com/McStasMcXtrace/McCode/blob/master/tools/other/Refl_Vitess2McStas.sh)
- mcstas2vitess generates Vitess module + tcl snippet from McStas component (poor docs, will improve)



Next: Time for exercises



Forming groups

- | Suggestion for Thursday-Friday exercises:
 - | Often sitting with a colleague is helpful
 - | Form teams of two people for the exercises
 - | Try to gather complementary knowledge by teaming up with someone from a different work area





Next: Exercises

Disclaimers

- You are running a beta - we will likely find new and interesting bugs as we move along... :-)



- Programme is flexible - don't get frustrated if we lag behind, we will either adapt or catch up later!



- Much of the teaching material is new / adapted, so there may be inconsistencies / confusion in some parts... :-)

