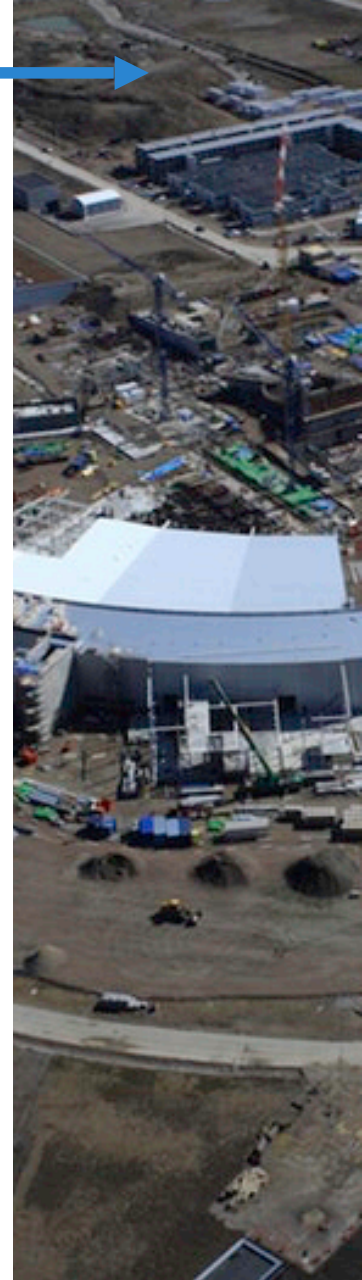


# 6 *McStas various utils*

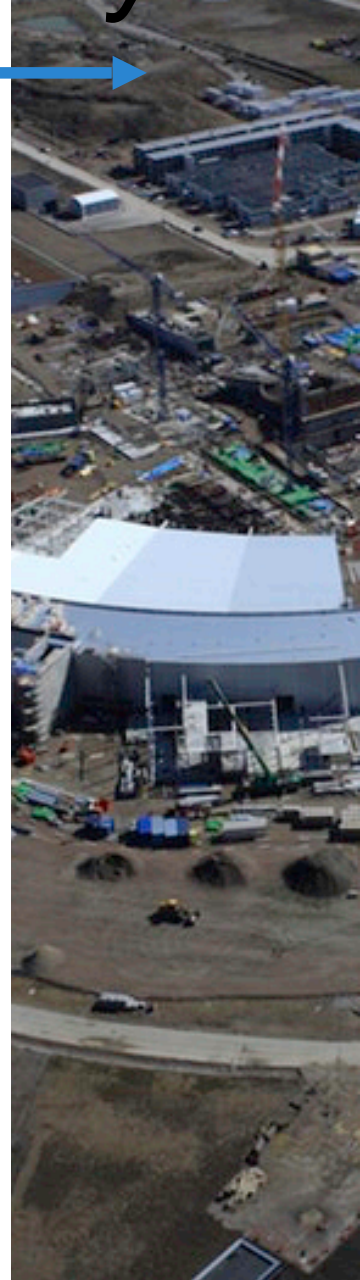
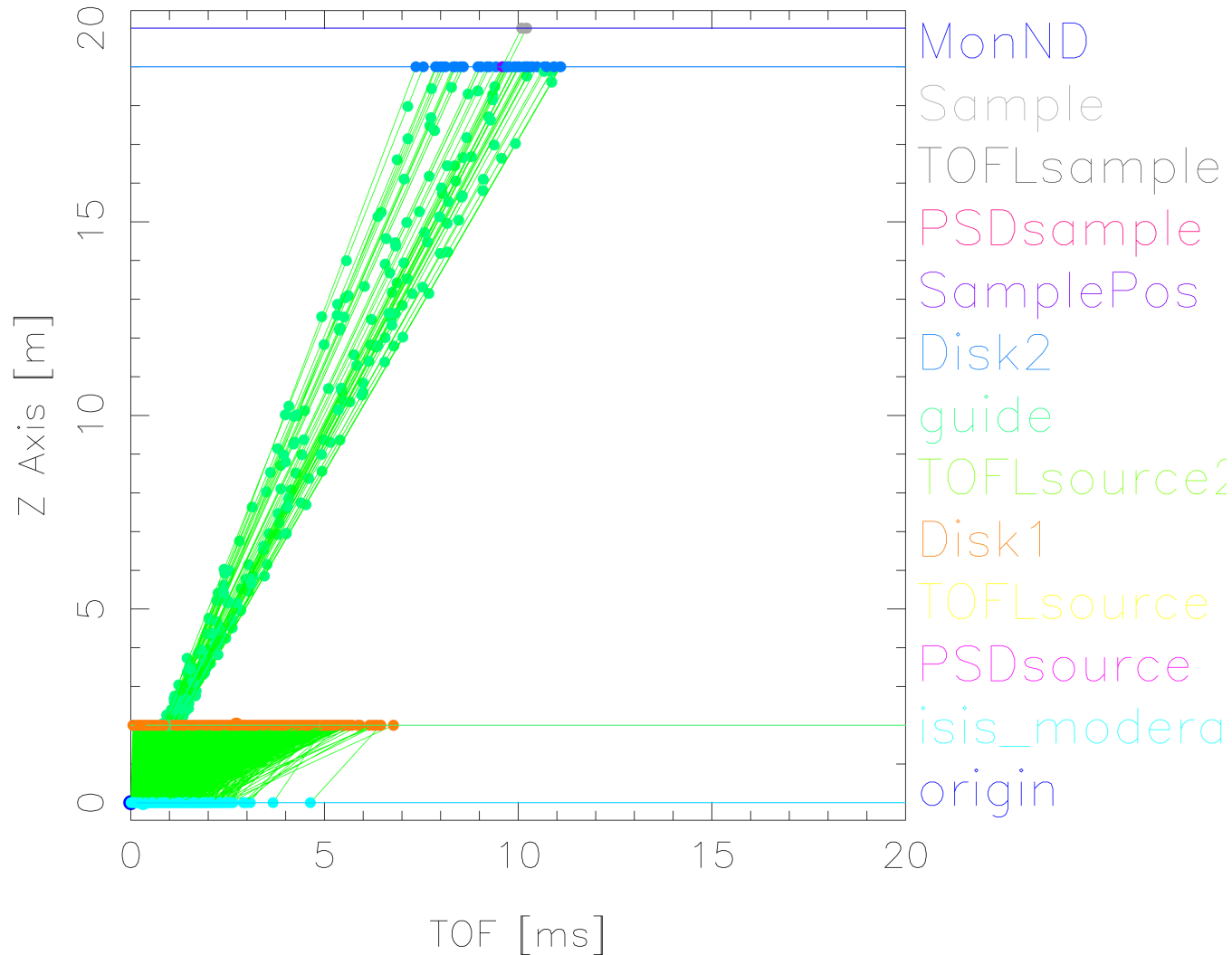
---

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



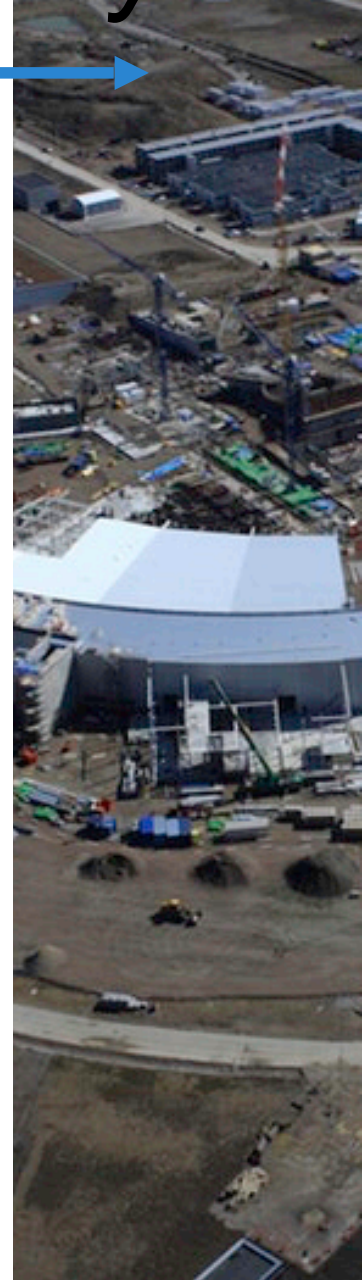
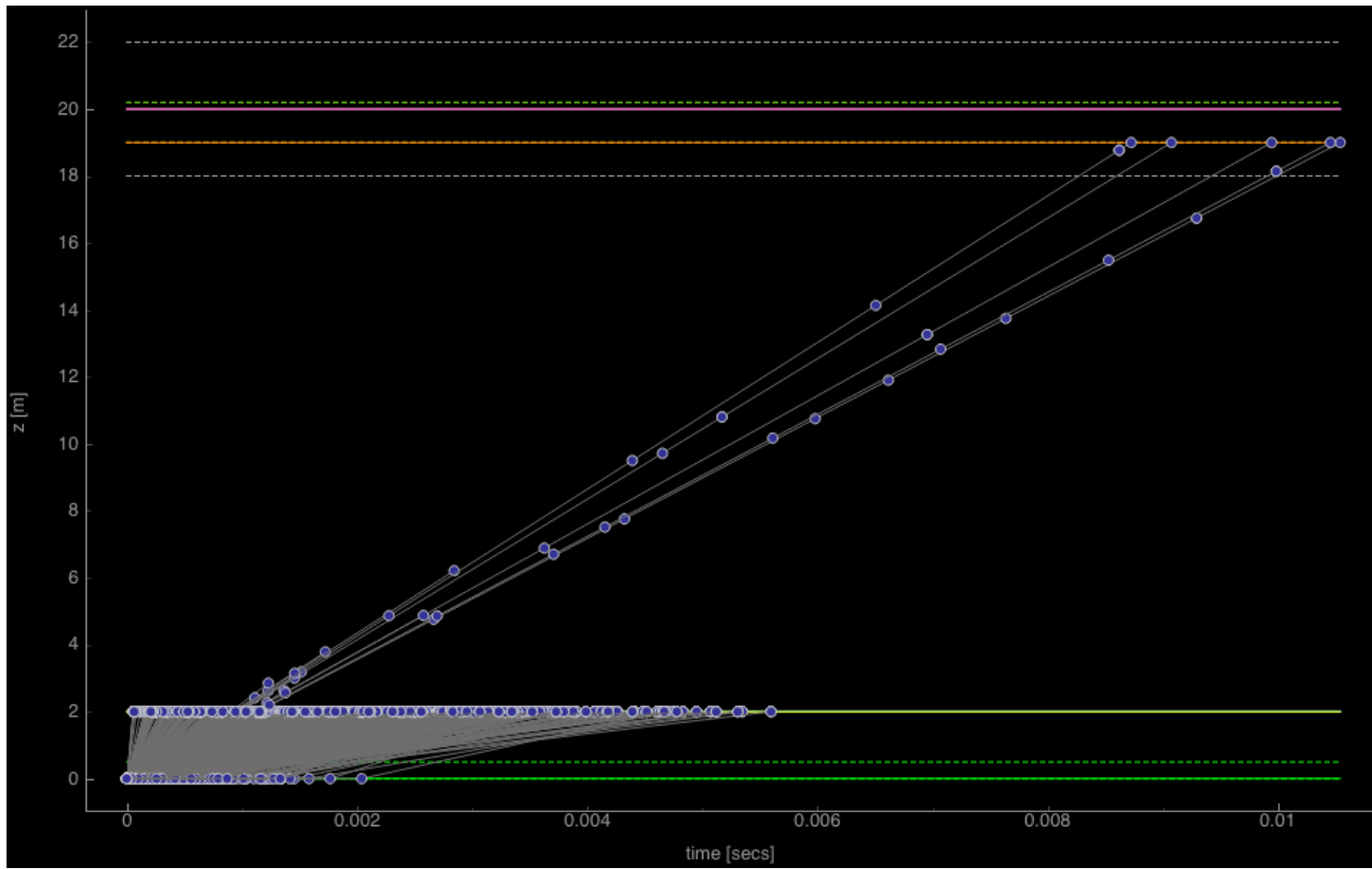
# TOF diagram util based on mcdisplay

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



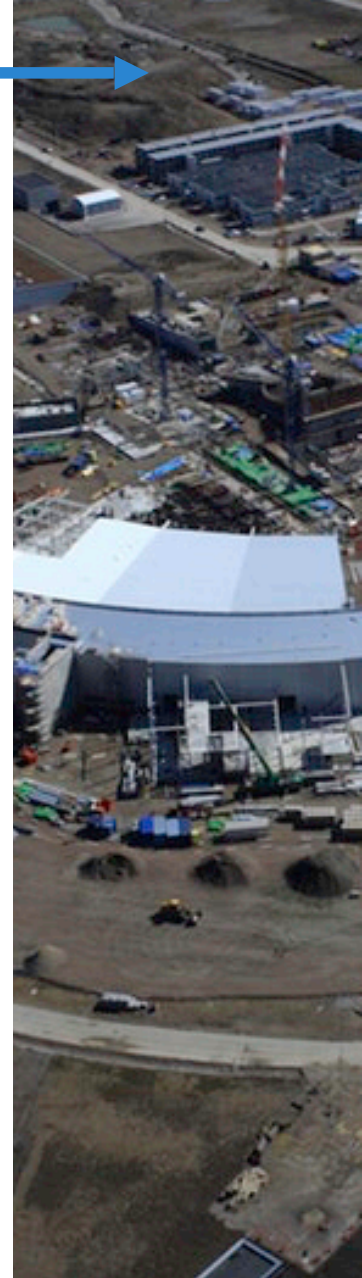
# TOF diagram util based on mcdisplay

- `mcdisplay-pyqtgraph --TOF instr`



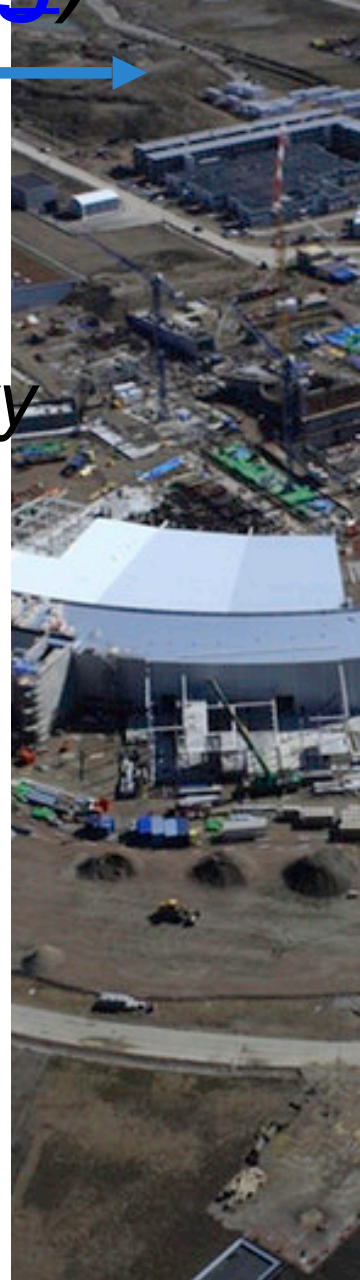
# *cif2hkl*

- *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>)

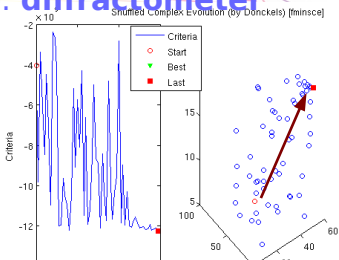
- General data / optimisation framework
- ~ Modern “spec\_nd”
- Matlab based, but does not require matlab (binary distribution also)
- Reads and plots McStas
- Can run McStas as a “cost function”, varying instrument parameters



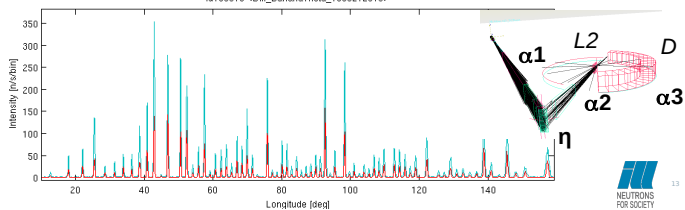
## iFit/McStas: example: diffractometer

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
$\eta$	15	23.5



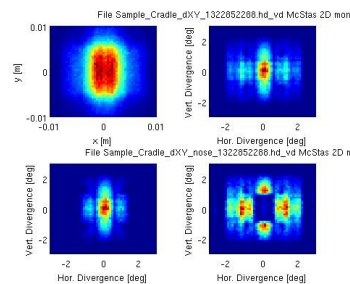
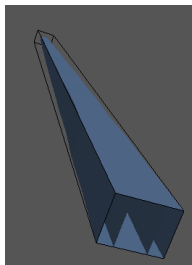
File Diff\_BananaTheta\_1305212316.th McStas 1D monitor  
 id159618 <Diff\_BananaTheta\_1305212316>



## 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

- *mcs*ub cluster scripts

```

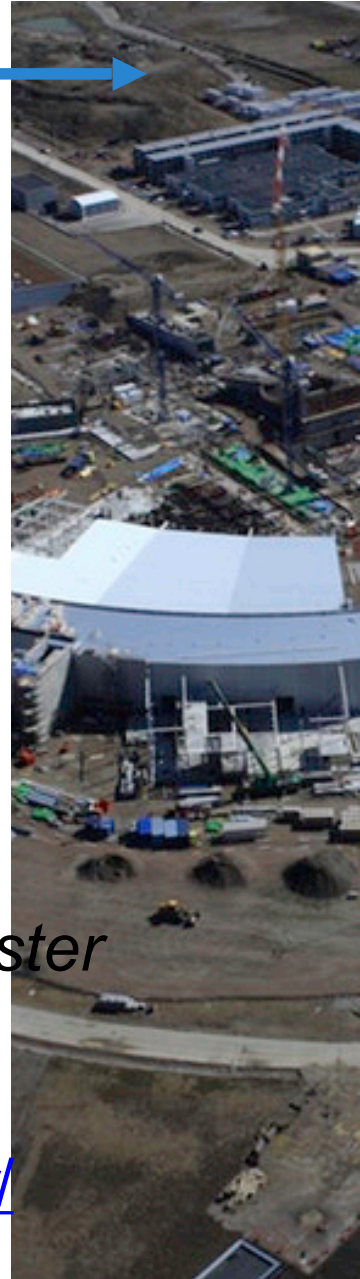
./mcsub_slurm.pl
Usage: ./mcsub_slurm.pl [options] [mcrun params]
-h          --help          Show this help
-rN         --runtime=N     Specify maximum runtime (hours) [default 1]
-qQNAME     --queue=QNAME   Specify wanted SLURM queue [default 'express']
-e<mail>    --email=<mail>  Specify address to 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 ./mcsub_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

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- *Utility script for converting Vitess reflectivity files for use with McStas* ([https://github.com/McStasMcXtrace/McCode/blob/master/tools/other/Refl\\_Vitess2McStas.sh](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)*

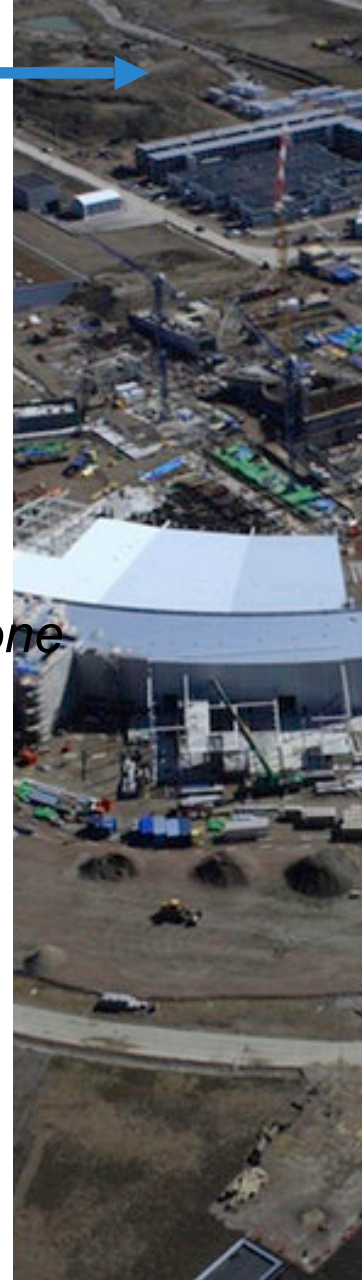


# Next: Time for exercises

## 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... :-)**

