

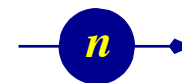
Introducing *iFit*

- a flexible Math framework that plays nicely with McStas

2019 CSNS

McStas
School

McStas



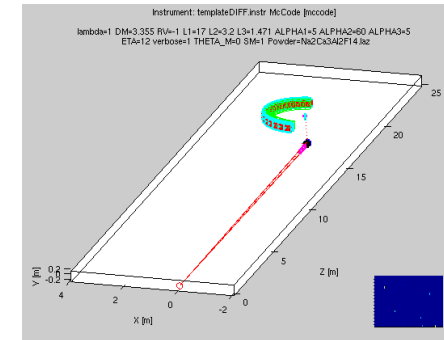
McStas automation: iFit

- iFit is a generic infrastructure which gathers data sets handling, fitting, $S(q,w)$ models, and McStas hooks.

iFit |

McStas iFit: build

- McStas can be controlled from within iFit.
- Open Matlab/iFit
- Create the McStas model with:
 - `model = mccode('instr')`
- Plot the geometry with:
 - `plot(model)` *% has contextual menus*
- Edit the instrument and re-compile
 - `edit(model)`



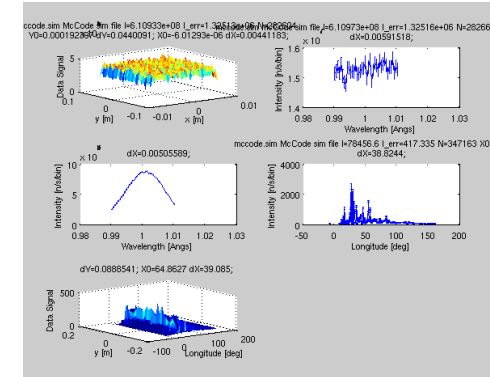
```

Figure 2: TextEdit: /tmp/tp109e7fc7_fd80_
File Edit Help
*****
McStas instrument definition URL=http://www
*****
Instrument: Template monochromator Diffractometer
*****
%Identification
* Written by: E. Farhi
* Date: 13 Apr 2006
* Origin: LLB/ILL
* Release: McStas CVS_080624
* Version: $Revision$
* %INSTRUMENT_SITE: Templates
*
Simple monochromator Diffractometer for powders
*
%Description

```

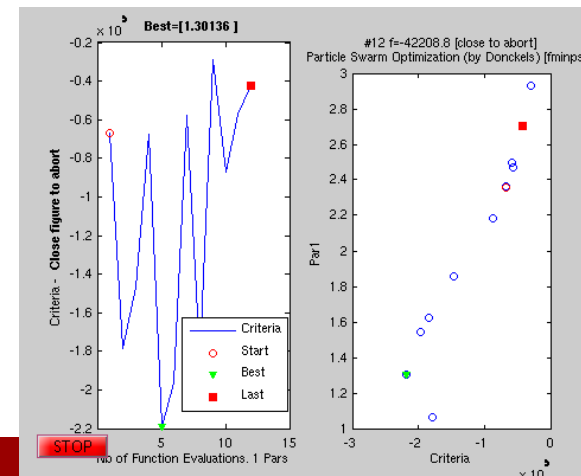
McStas iFit: eval

- Run with (default 1e6 event and pars)
 - `data = iData(model, [], nan);`
 - `subplot(model) % plot monitors, contextual menus`
- Specify parameters
 - `data = iData(model, 'lambda=2.36; coh=Cu.laz')`
- Do a scan:
 - `data = iData(model, 'lambda=[1.2 2.4 3.6]')`
- Change neutron events #
 - `model.UserData.options.ncount = 1e7;`



McStas iFit: optim

- Fix all parameters but *lambda*, Maximize model value:
 - `mlock(model, 'all'); munlock(model, 'lambda')`
 - `xlim(model, 'lambda', [1 3]); % bounds`
 - `fmax(model, 'lambda=2.36', '', nan)`
 - `fmax(model, 'lambda=2.36', 'OutputFcn=fminplot', nan)`



McStas iFit: advanced

- You can add McStas models:
 - `model=mccode('instr1')+mccode('instr2') + ...`
- For instance:
 - Instr1: structure
 - Instr2: spin-wave
 - Instr3: phonons
 - Instr4: incoherent
- The different models can also be assembled as a set of samples chosen at execution in a single McStas instrument.

Exercise:

- Download and install the binary iFit package using the instructions at <http://ifit.mccode.org/Install.html>
- Launch iFit/Matlab and load data from one or more of the TOF monitor outputs of the scan, TOF spectrometer exercise, e.g.
 - `a=iData('folder/5/in5*.t')`
 - `a.error=1`
 - `fits(a,'gauss')`
 - `plot(a)`
- Use the instructions at <http://ifit.mccode.org/McStas.html> to generate some of the example graphics shown in that page