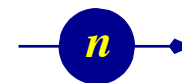# Introducing *iFit*

- a flexible Math framework that plays nicely with McStas

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McStas

n

McStas automation: iFit

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

iFit

McStas

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

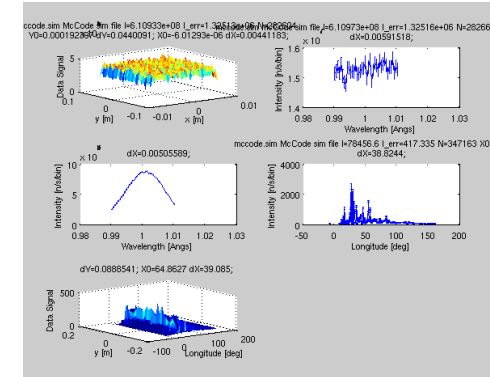 – edit(model)
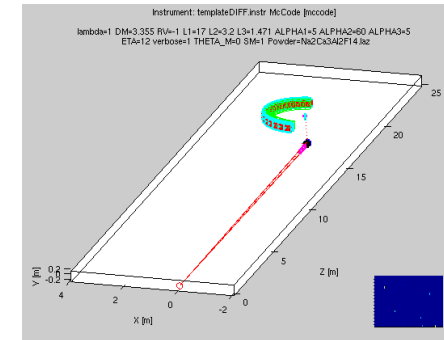
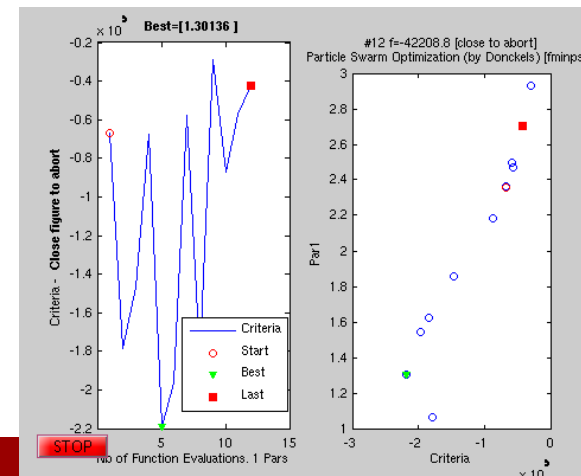# *McStas iFit: eval*

- 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;

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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 and load data from one or more of the TOF monitor outputs of the last scans in the 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

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