Estimating Neutron Spectral Intensities from Cold Source Moderators: Methods and Comparisons to Experiment

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We should always keep in mind that …

All models are wrong. Some models are useful.

George Box, *Statistics for Experiments*

Why Are Accurate Neutronic Simulations Important for Pulsed Spallation Neutron Sources?

- Predict and understand the neutronic performance of target/reflector/moderator systems
- Guide design of instruments
- Predict results of experiments

Moderator Performance Measures

- Neutron Spectral Intensity

$$i(E) = \frac{L^2}{I} \cdot \phi(E)\Big|_L$$

  - metric independent of flight path distance
  - units of $i(E)$ are n/eV/sr/μC
  - calculate with point detector or surface current tallies
- Neutron Emission Time Distribution (pulse shape)

$$i(E) = \int_0^\infty i(E,t)\, dt$$

  - calculate with surface current tally
- Full Width at Half-Maximum (FWHM) of Pulse Shapes

Experimental and Calculational Methods

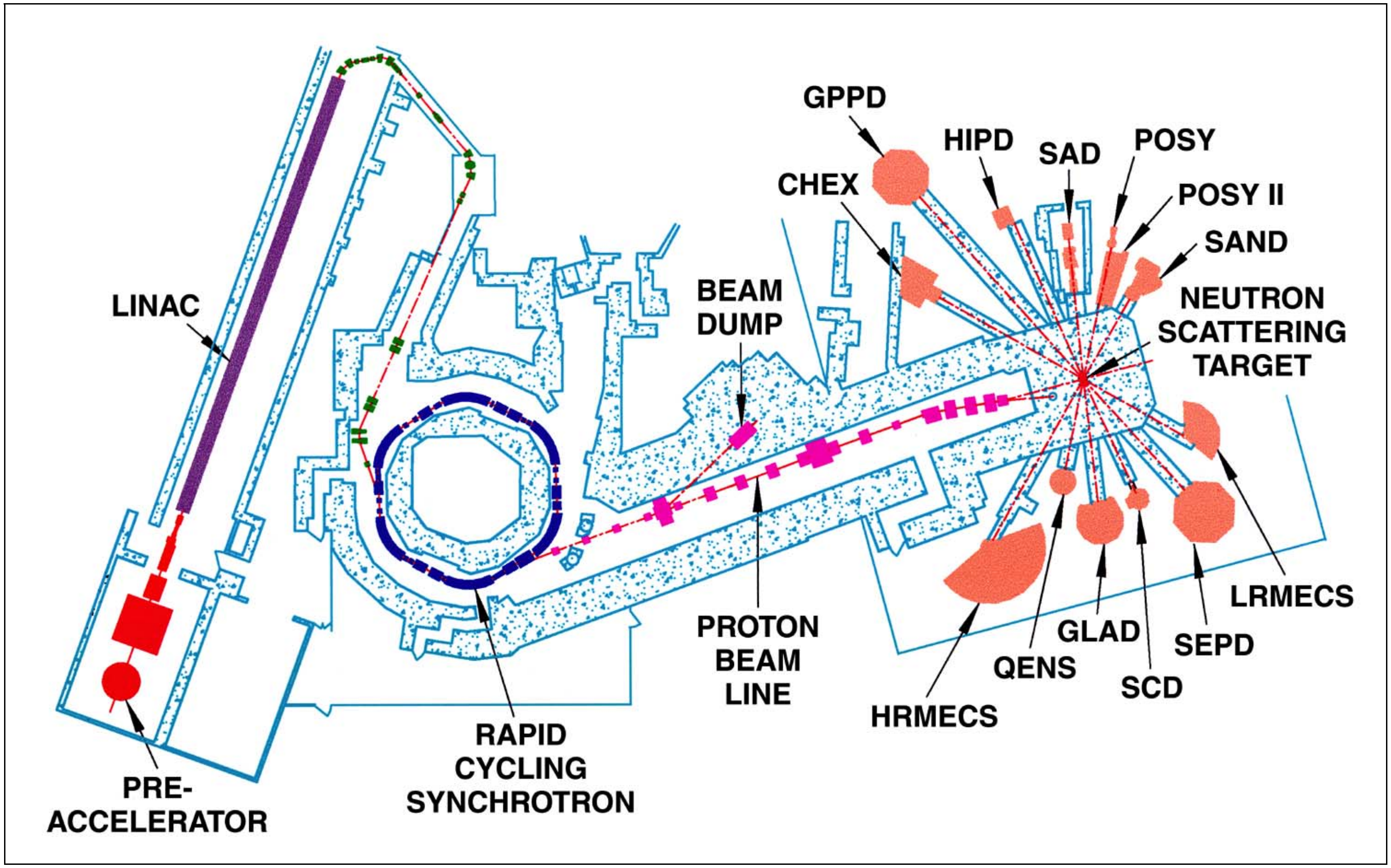
- Neutron Spectral Intensity
  - Neutron energy spectrum recorded by time-of-flight in a low-efficiency 1/*v* detector
  - Gold foil activation measurement provided absolute normalization

$$C(t) = A\eta(E)\,\phi_D(E)\,\frac{2E}{t} + B$$

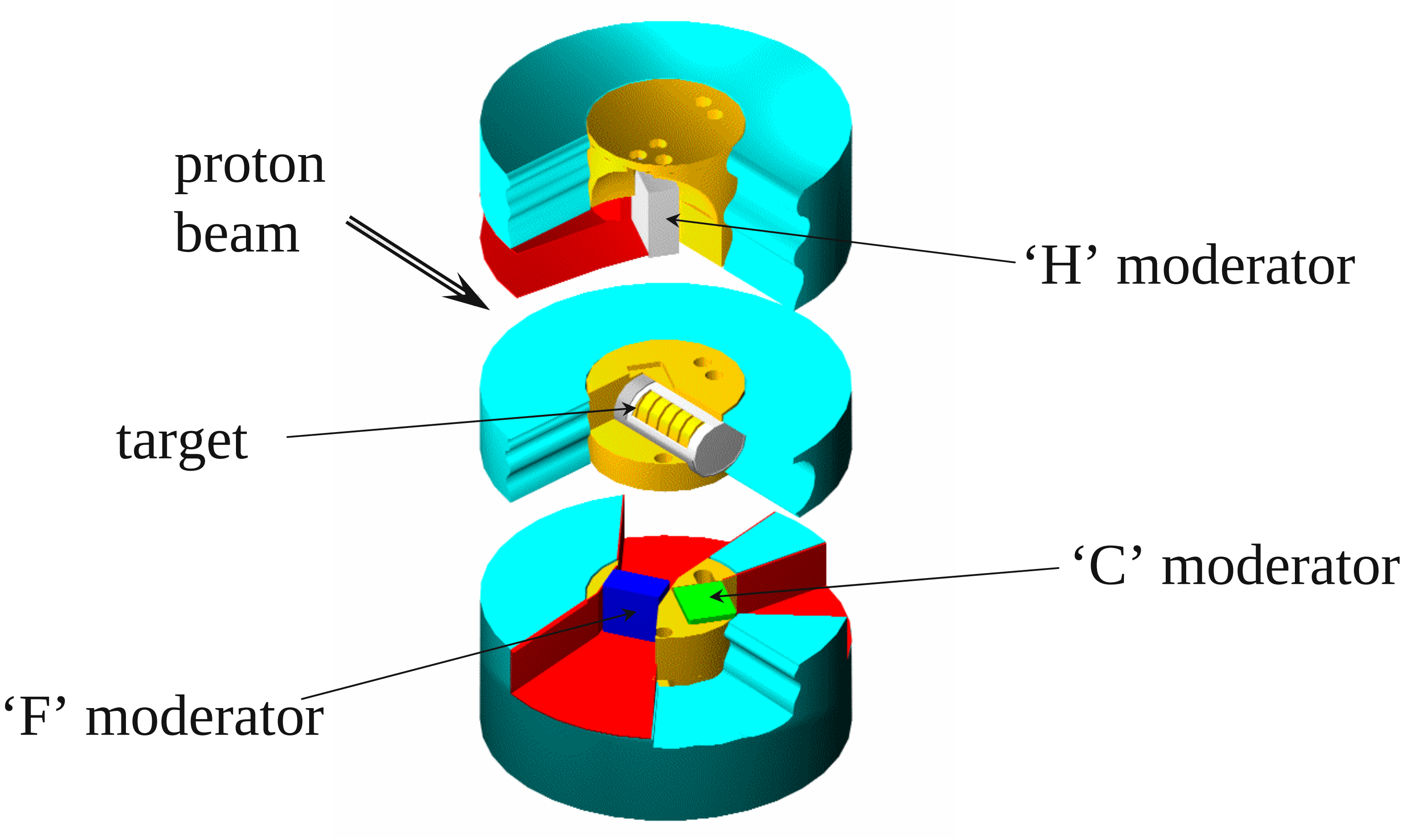
$$E \cdot \phi(E) = \frac{C(t) - B}{K}$$

- Neutron Emission Time Distribution (pulse shape)
  - Neutrons counted as function of time by time-focused crystal analyzer
  - Neutron energies are those obtained by Bragg reflection from (*nnn*) planes in cooled germanium crystal
- Calculations used various versions of MCNPX

Schematic Drawing of the IPNS



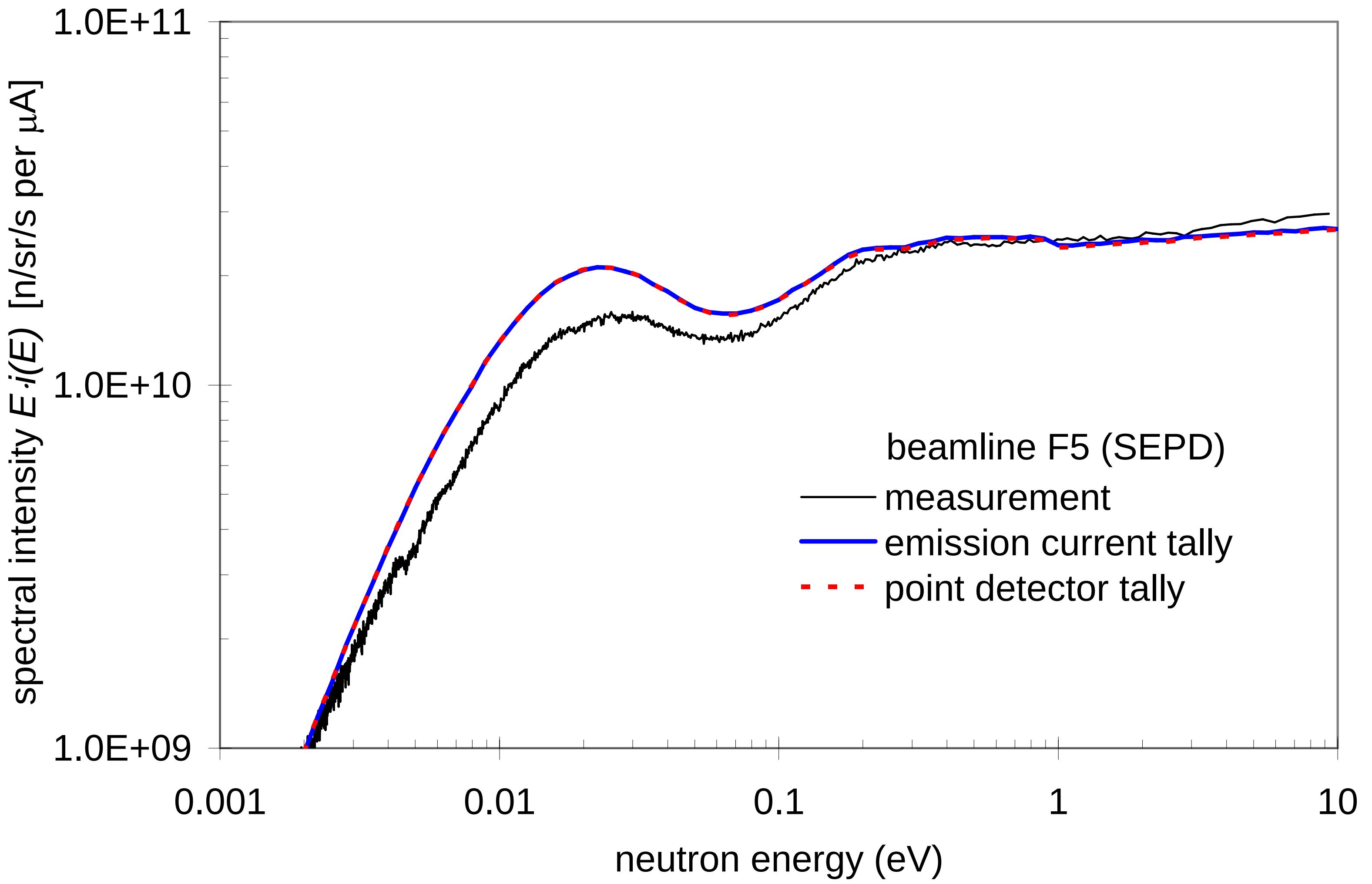
Schematic Drawing of the IPNS Target/Moderator Block



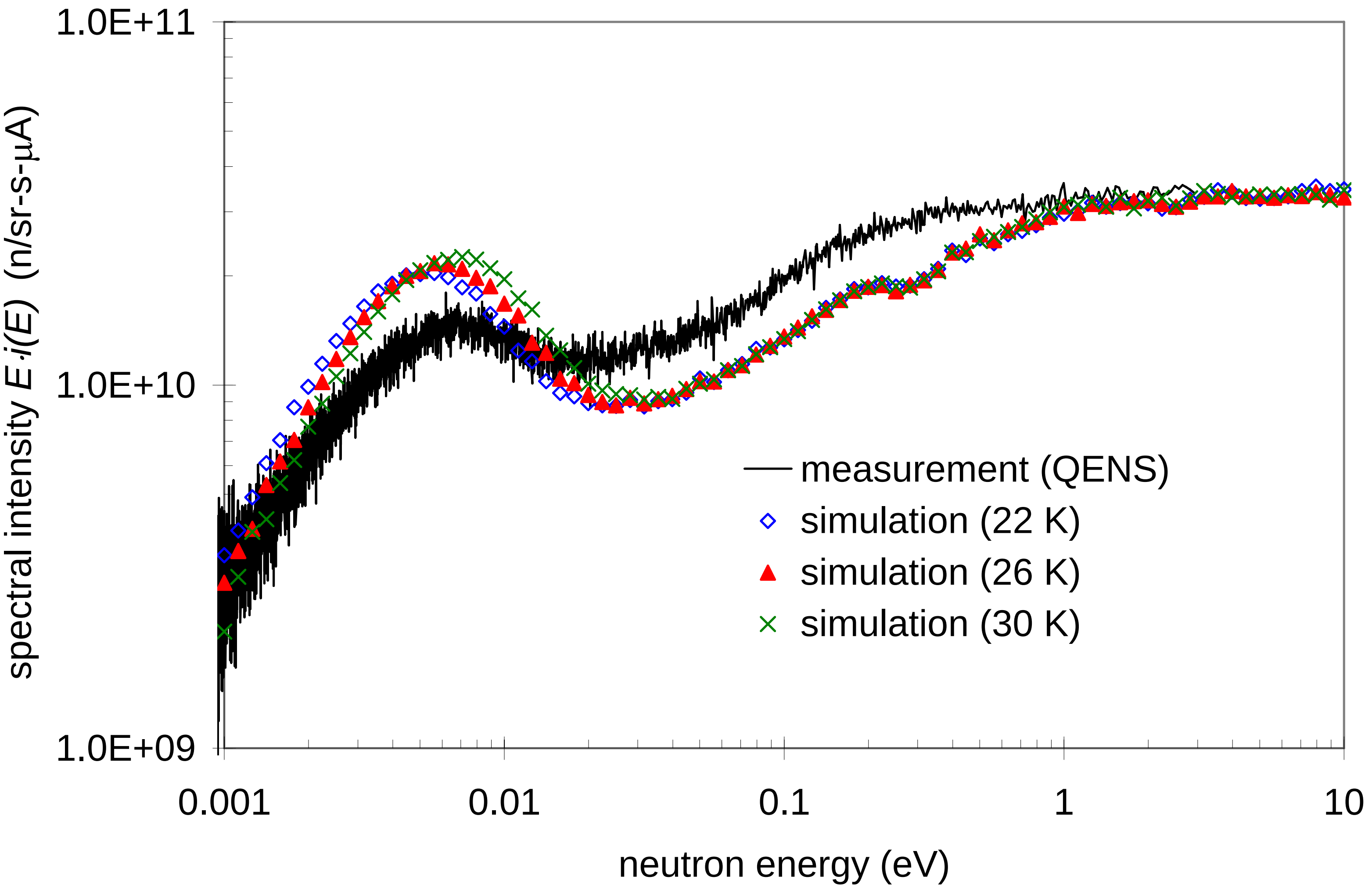
Neutron Spectral Intensities

- Experimental and simulation results are normalized independently
- H moderator is solid methane at 22 K
- F moderator is liquid methane at 100 K

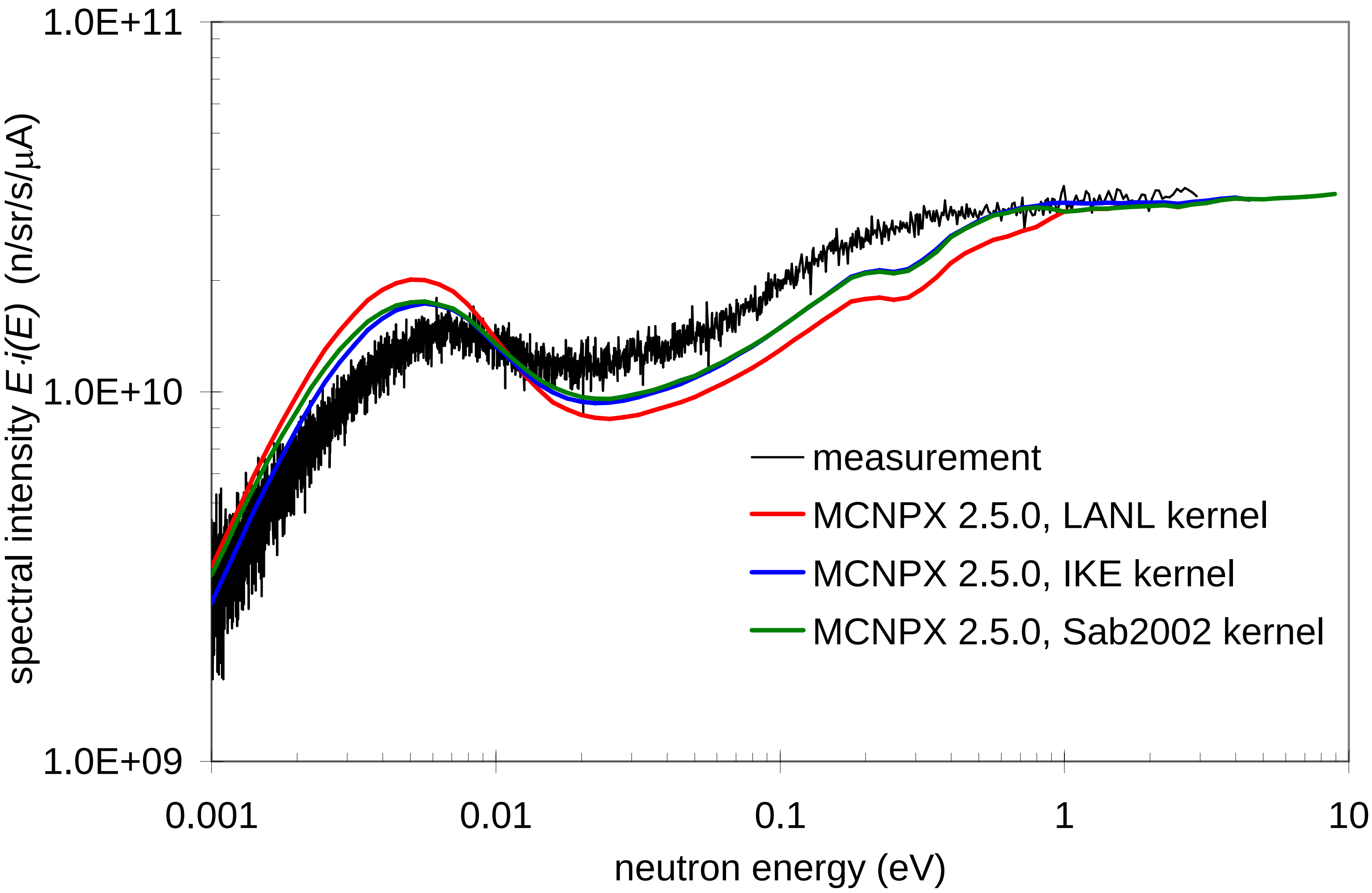
Neutron Spectral Intensity for F Moderator



Neutron Spectral Intensity for H Moderator

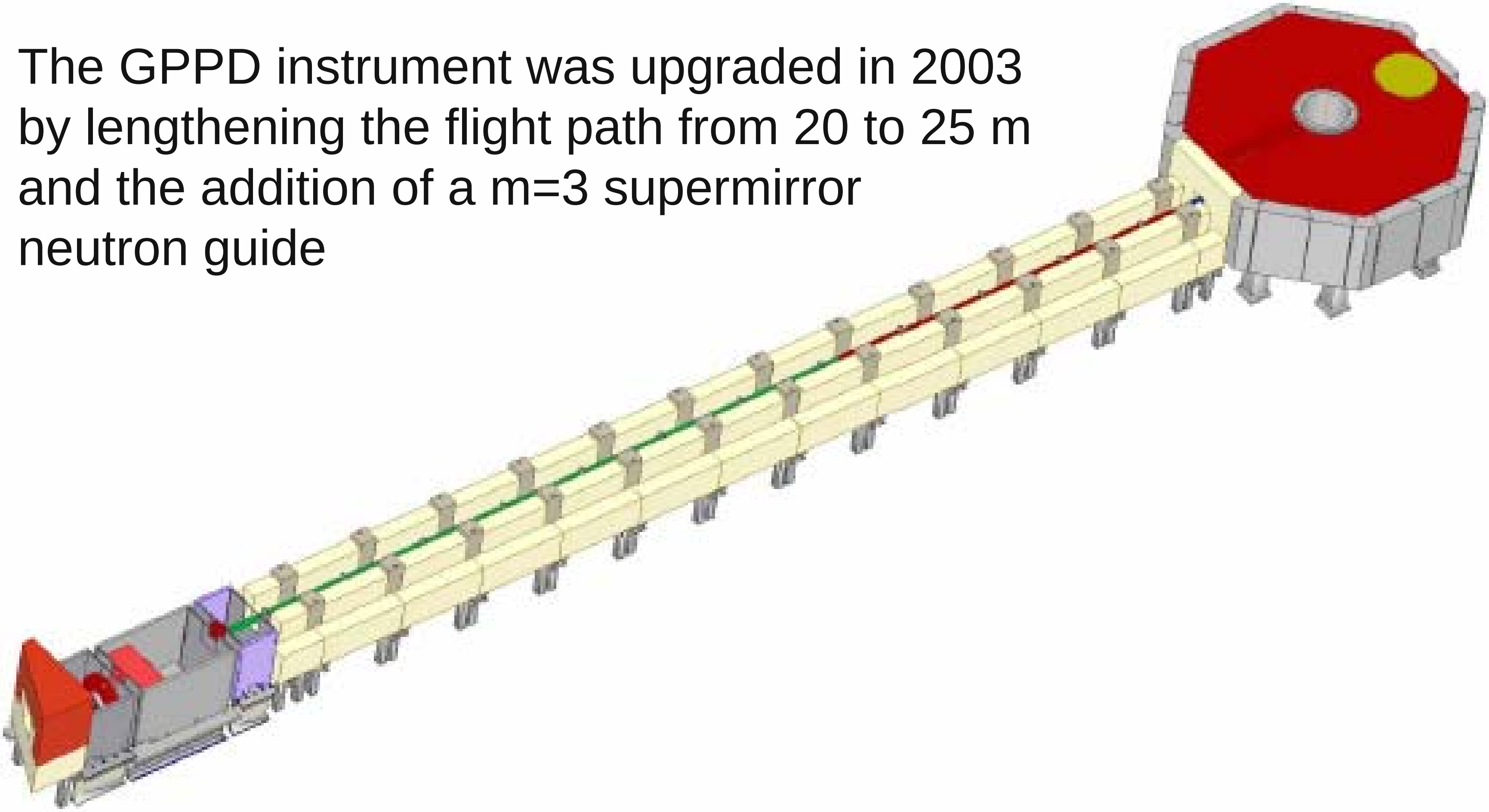


Neutron Spectral Intensity for H Moderator



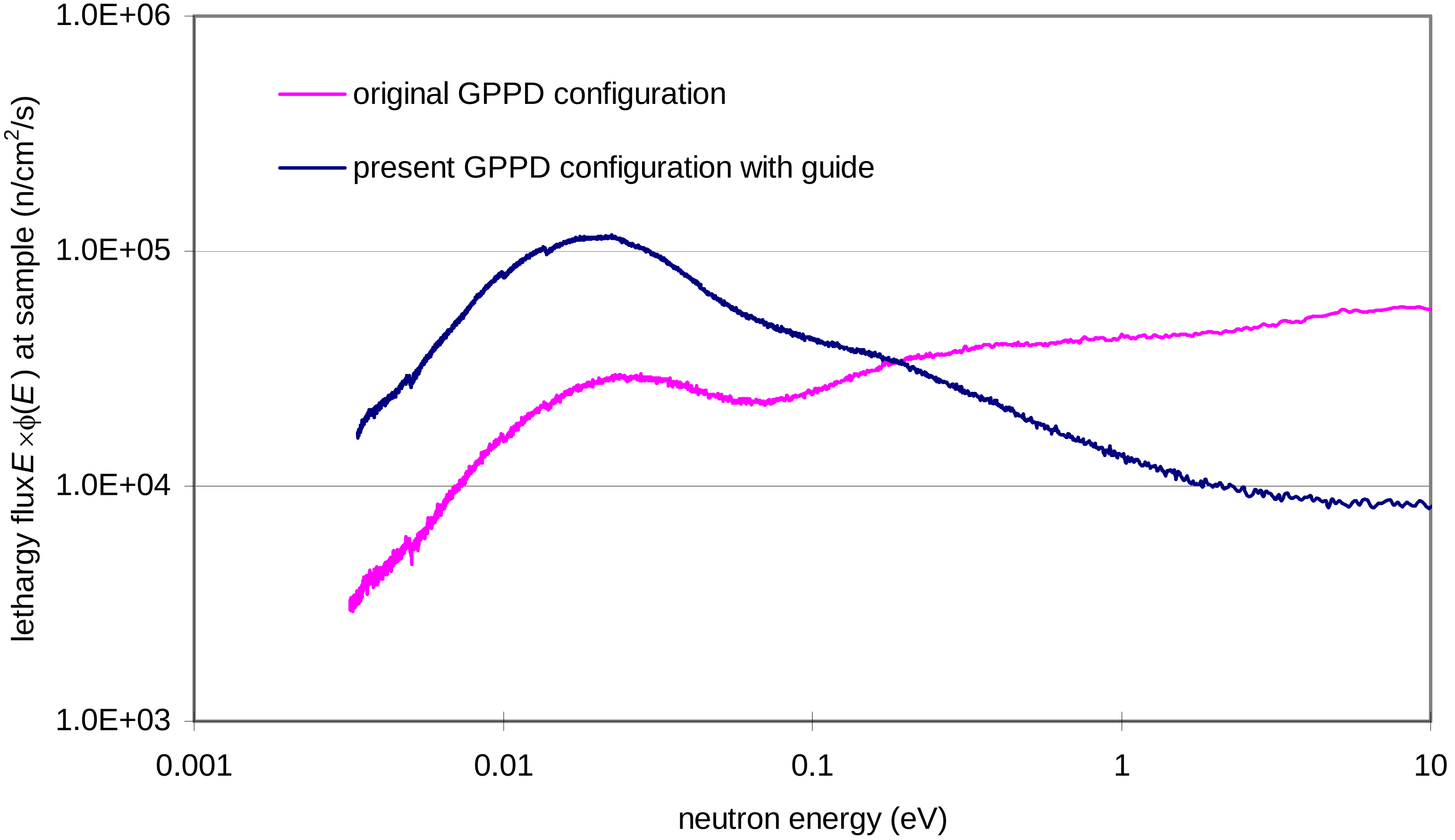
General Purpose Powder Diffractometer

- The GPPD instrument was upgraded in 2003 by lengthening the flight path from 20 to 25 m and the addition of a m=3 supermirror neutron guide



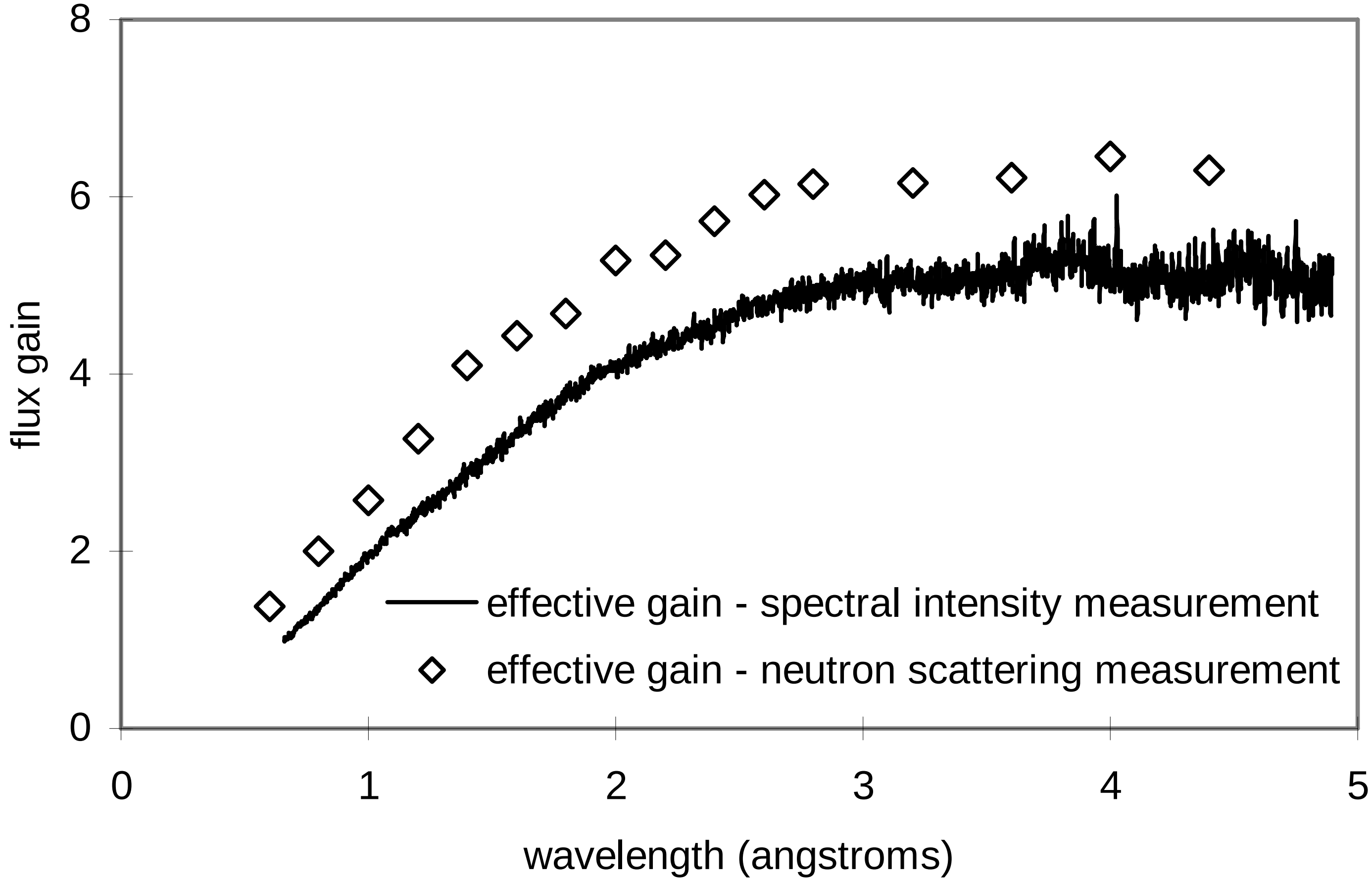
“F” Moderator Results

- Measurements taken on GPPD reported in terms of flux at sample position

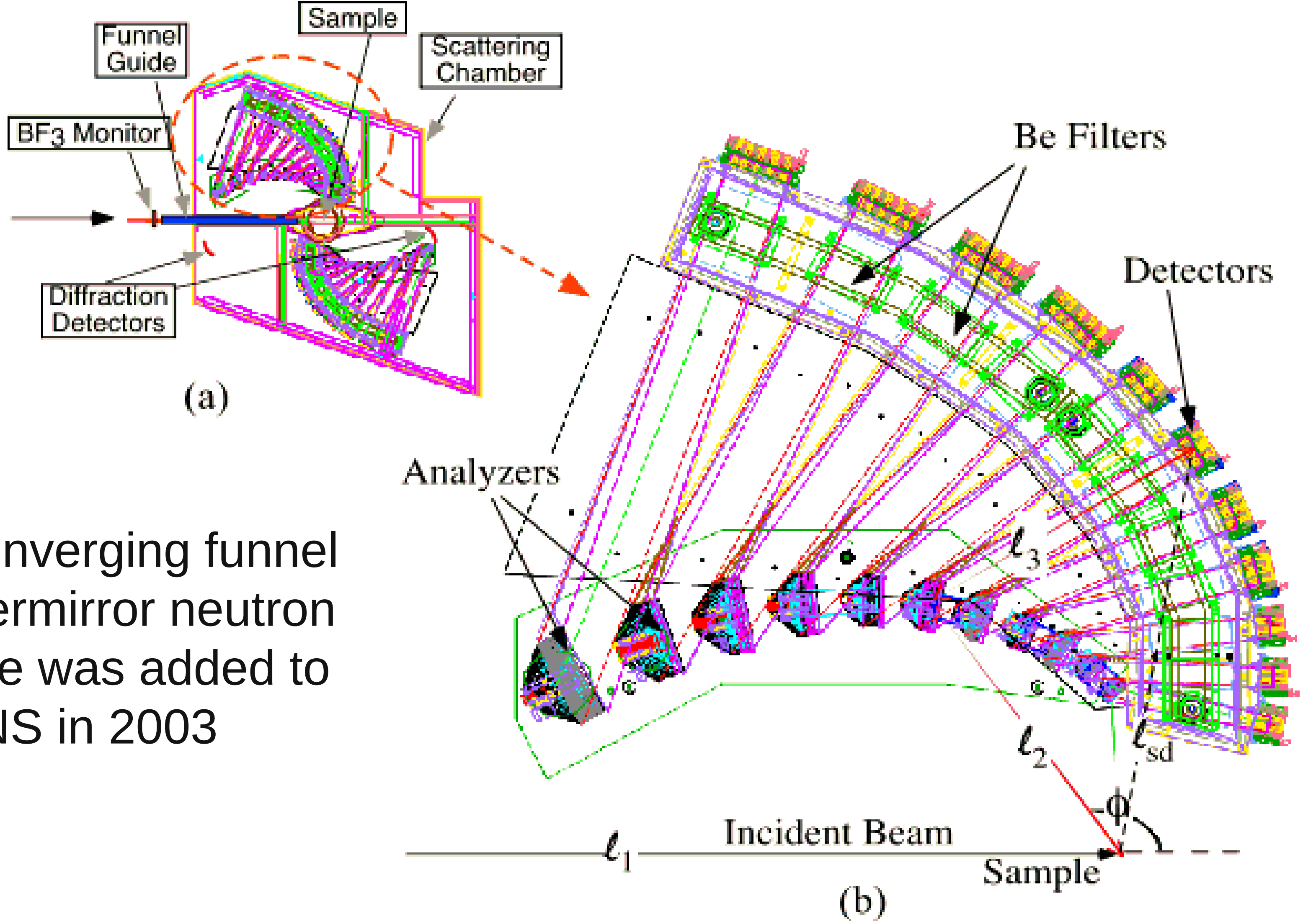


GPPD wavelength-dependent flux gain

- Flux gain defined as ratio of flux at current position with guide to flux at previous position without guide



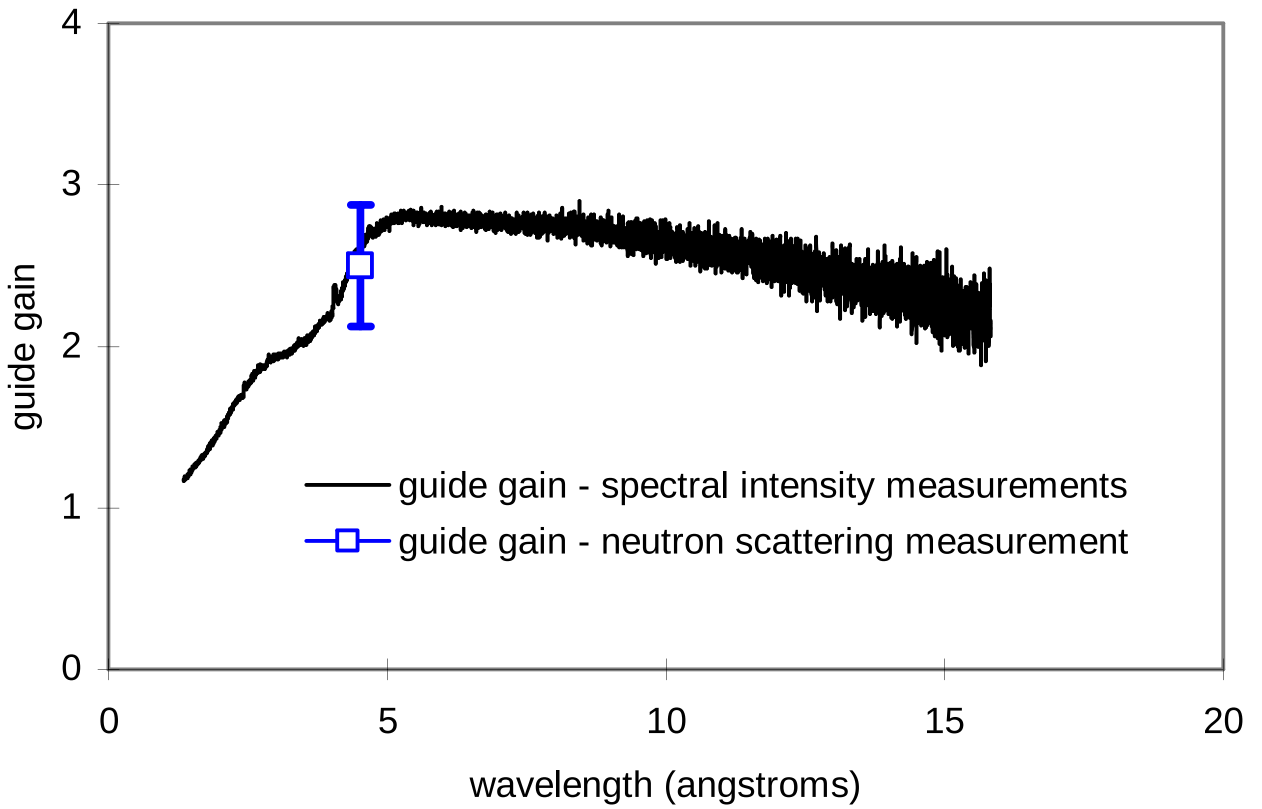
Quasi-Elastic Neutron Spectrometer



- A converging funnel supermirror neutron guide was added to QENS in 2003

QENS wavelength-dependent guide gain

- QENS guide gain determined by comparing results of portable (after guide) and in-situ (before guide) monitors



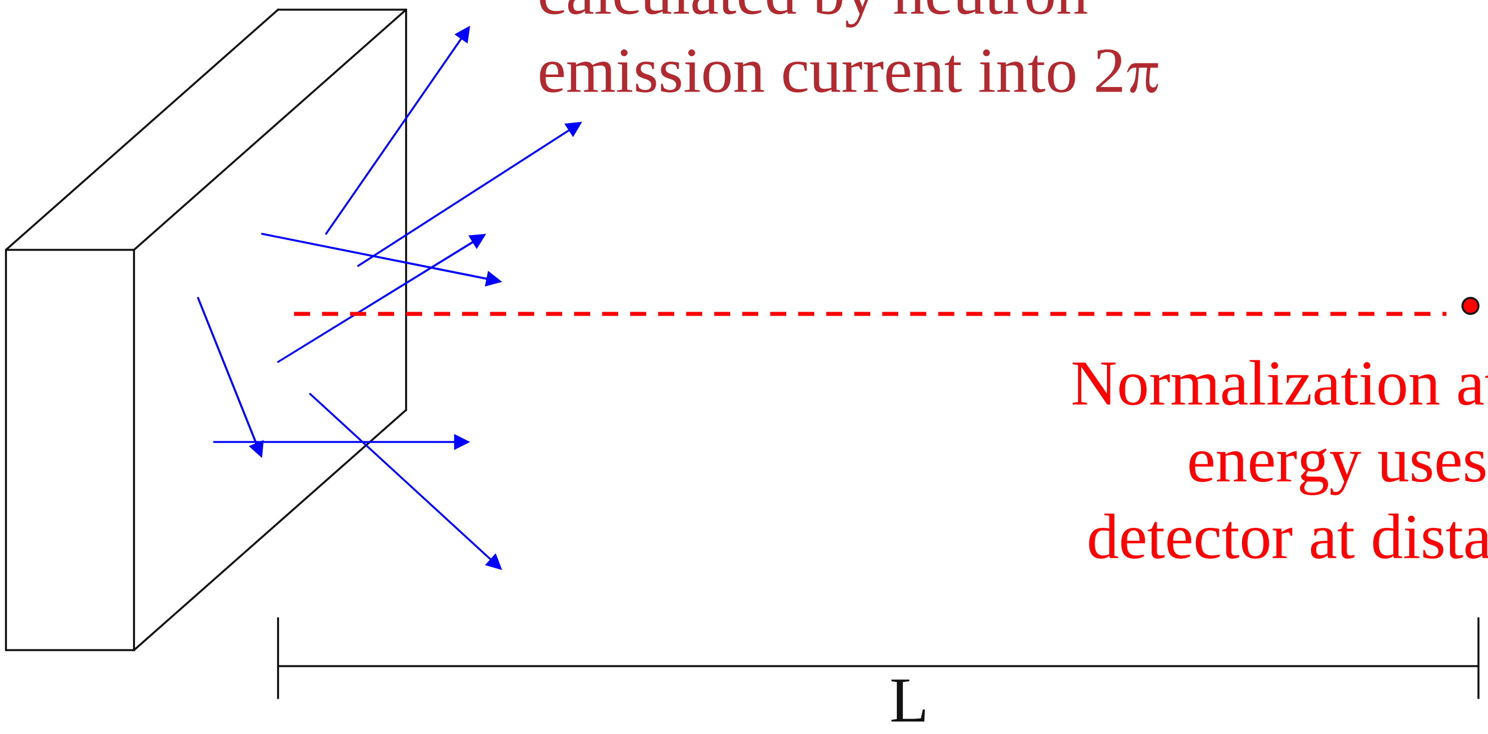
Neutron Spectral Intensities

- Point detector and emission current tallies agree
- Good agreement at 1 eV - details of transport good down to this point
  - discontinuity in spectral intensity curve at 1 eV has been resolved
- Details of spectral intensity not well reproduced below 1 eV
  - features in simulation that are not seen in measured data
  - simulation does not reproduce the same neutron temperature for scattering kernel at the same physical temperature as moderator
- Guide gains predicted to 20% or better

Neutron Pulse Shapes

- F and H moderators are liquid methane at 100 K; C moderator is solid methane at 26 K
- Background subtracted from measured results using linear approximation
- Simulation results normalized to the total counts above background for each neutron energy (i.e., curves will have same area)
- Leading edge of measured pulses broader than simulation results
- Broadening causes peak heights to be reduced

“Traditional” Pulse Shape Calculation Method (basically true for flat moderators)

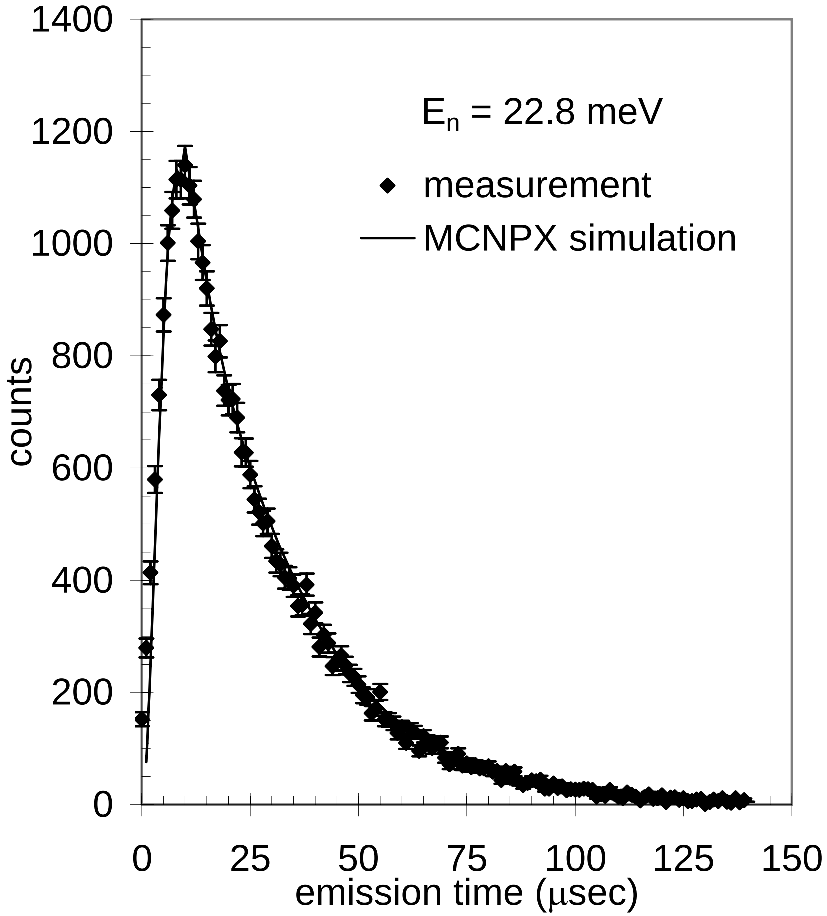


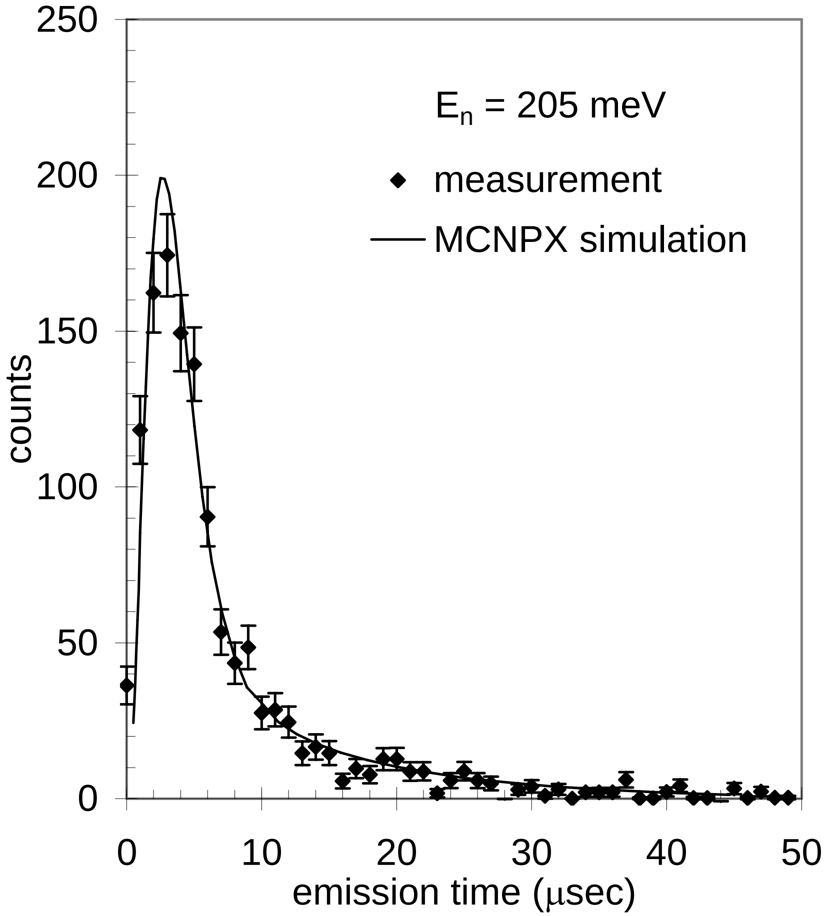
Pulse shapes at each energy calculated by neutron emission current into 2π

Normalization at each energy uses point detector at distance L

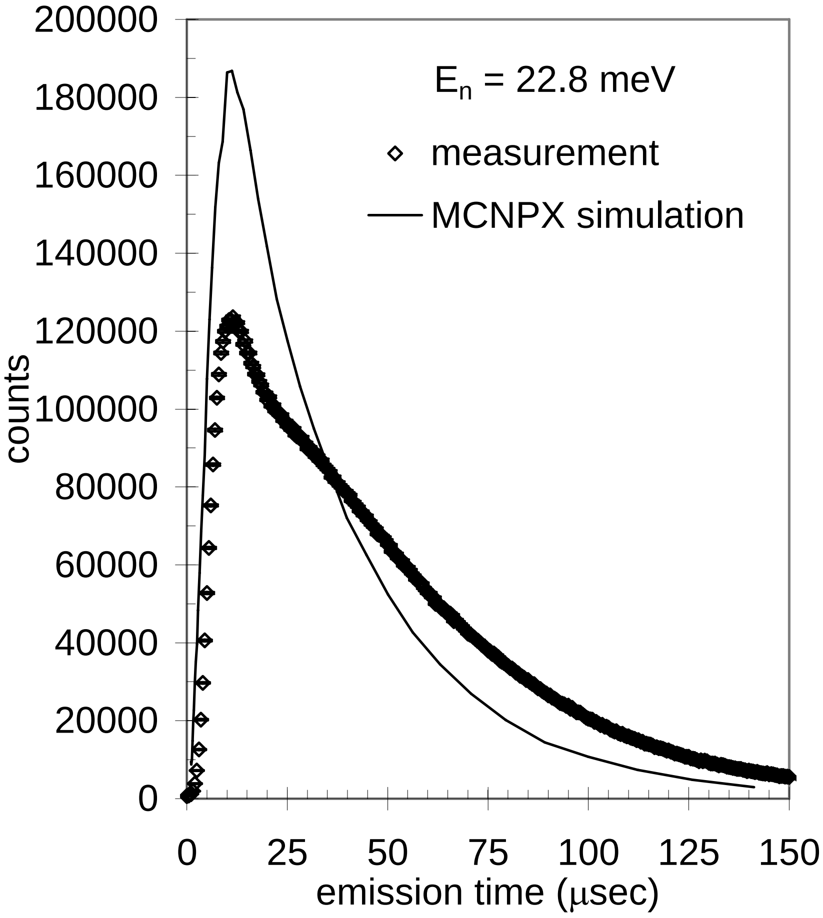
Assumes that time distribution is the same for all directions, but magnitude/energy distribution are different

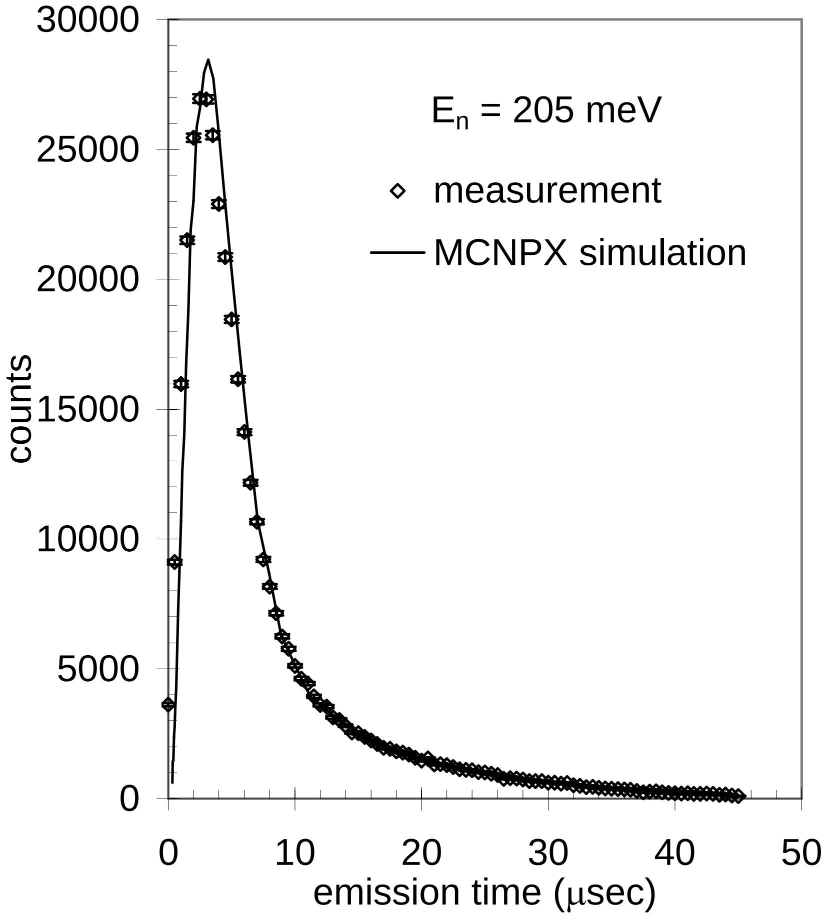
Neutron Pulse Shapes for F Moderator



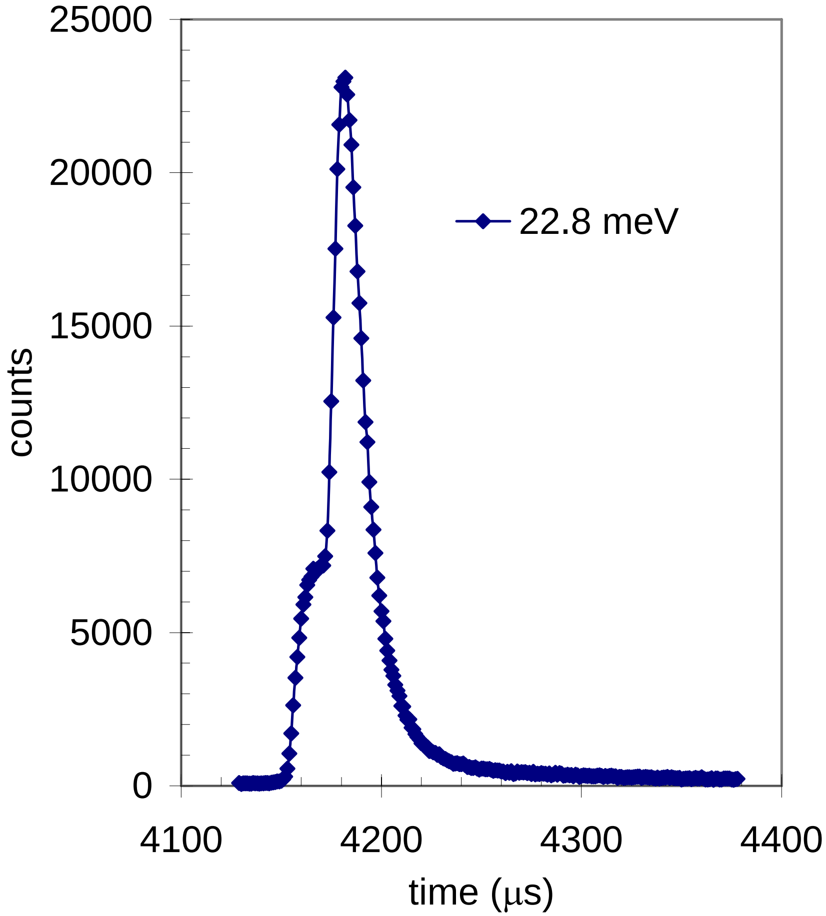


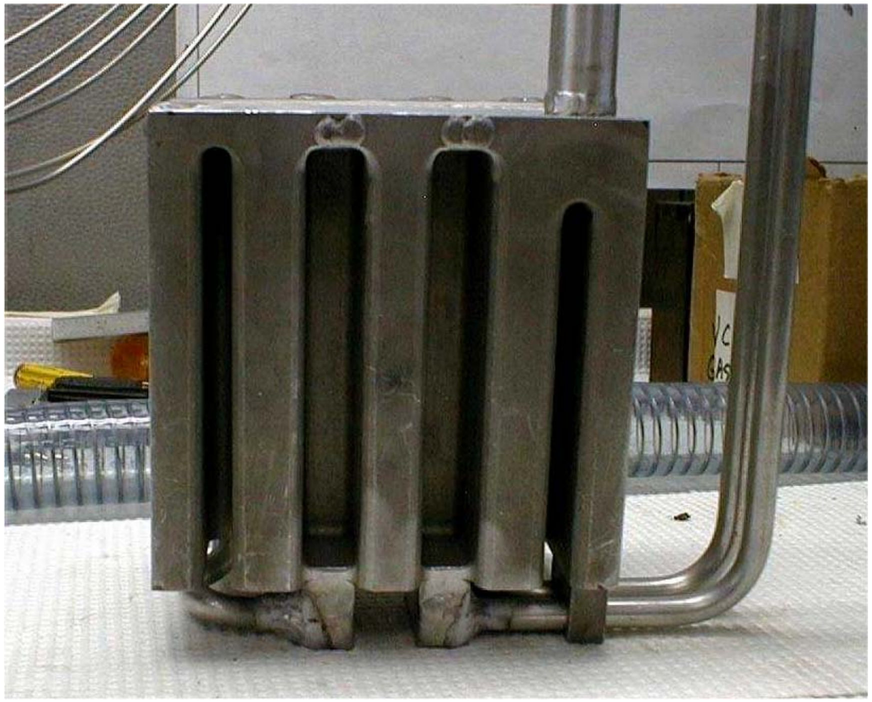
Neutron Pulse Shapes for H Moderator



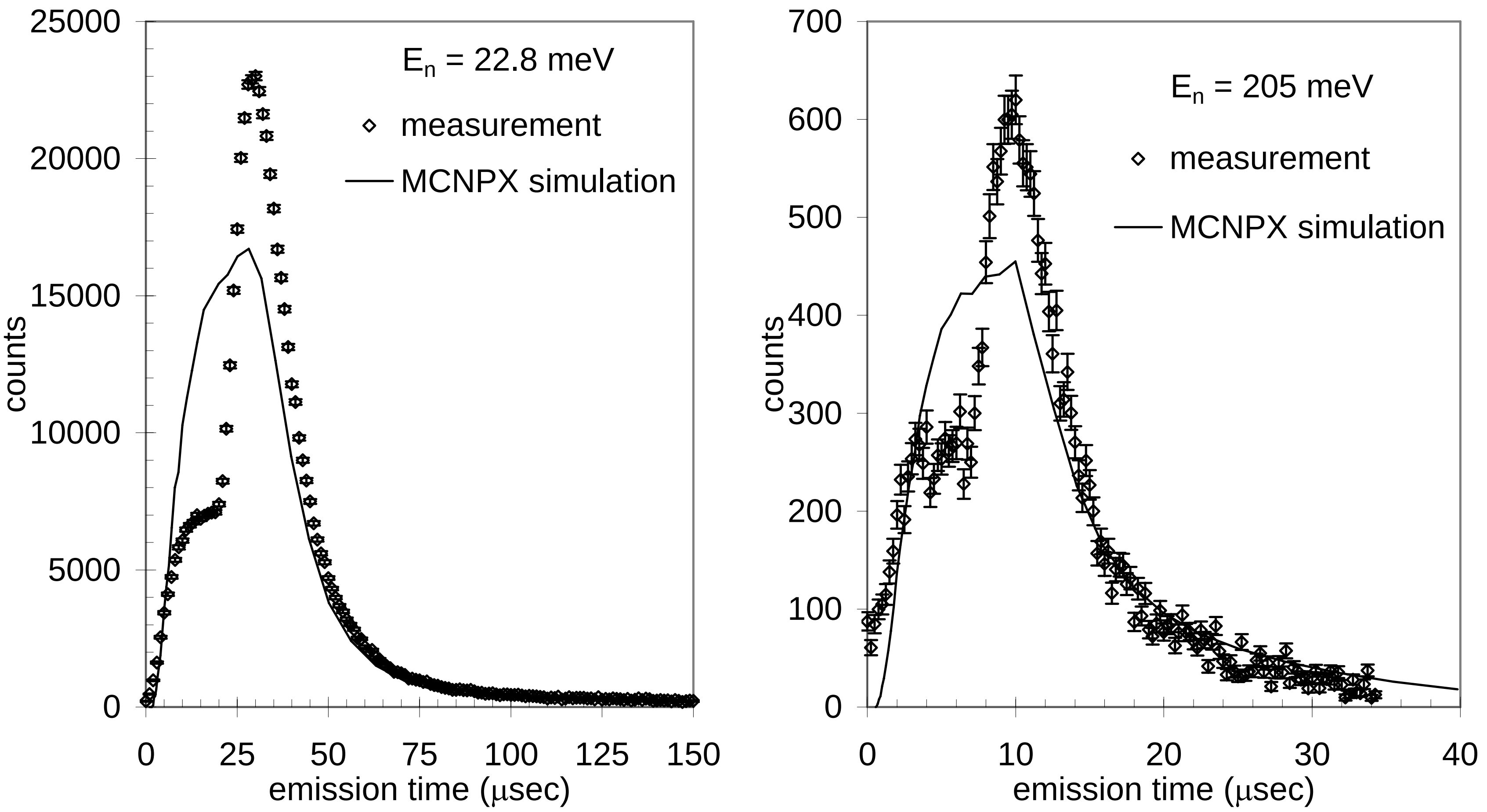


Measured Pulse Shapes for C Moderator

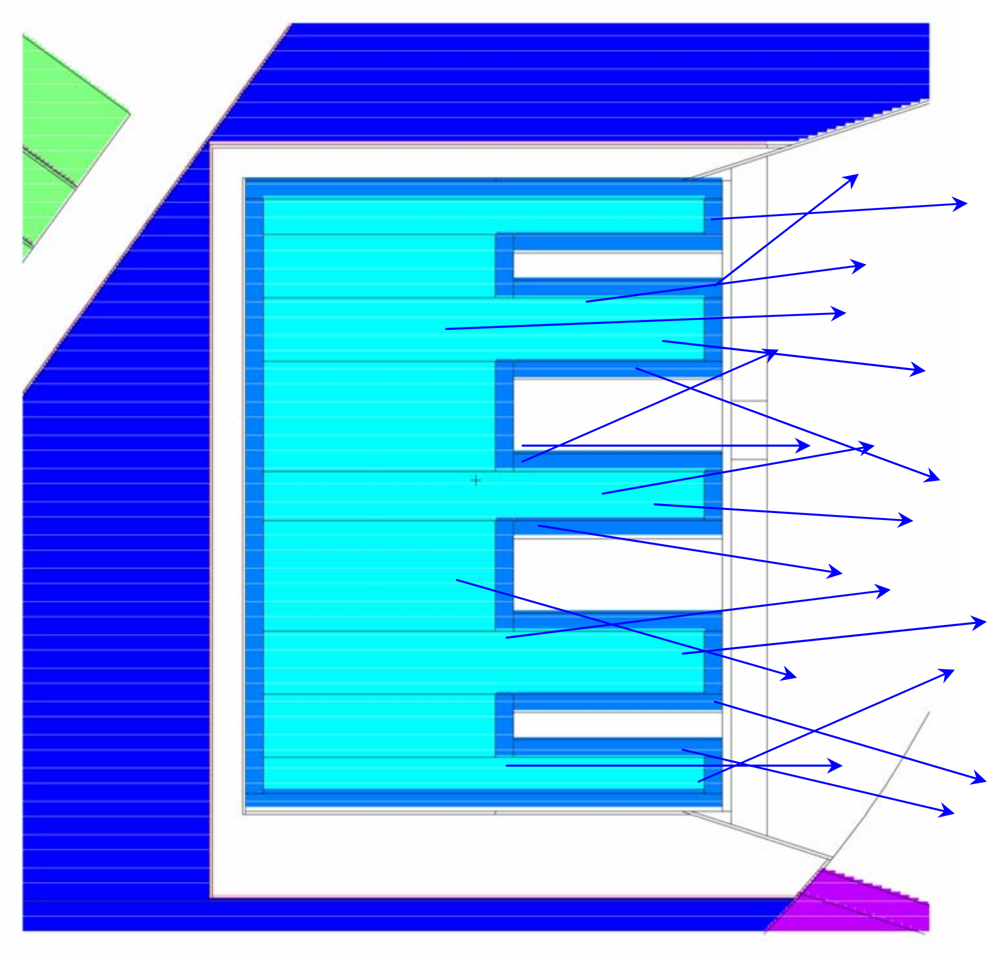




Simple Pulse Shapes for C Moderator



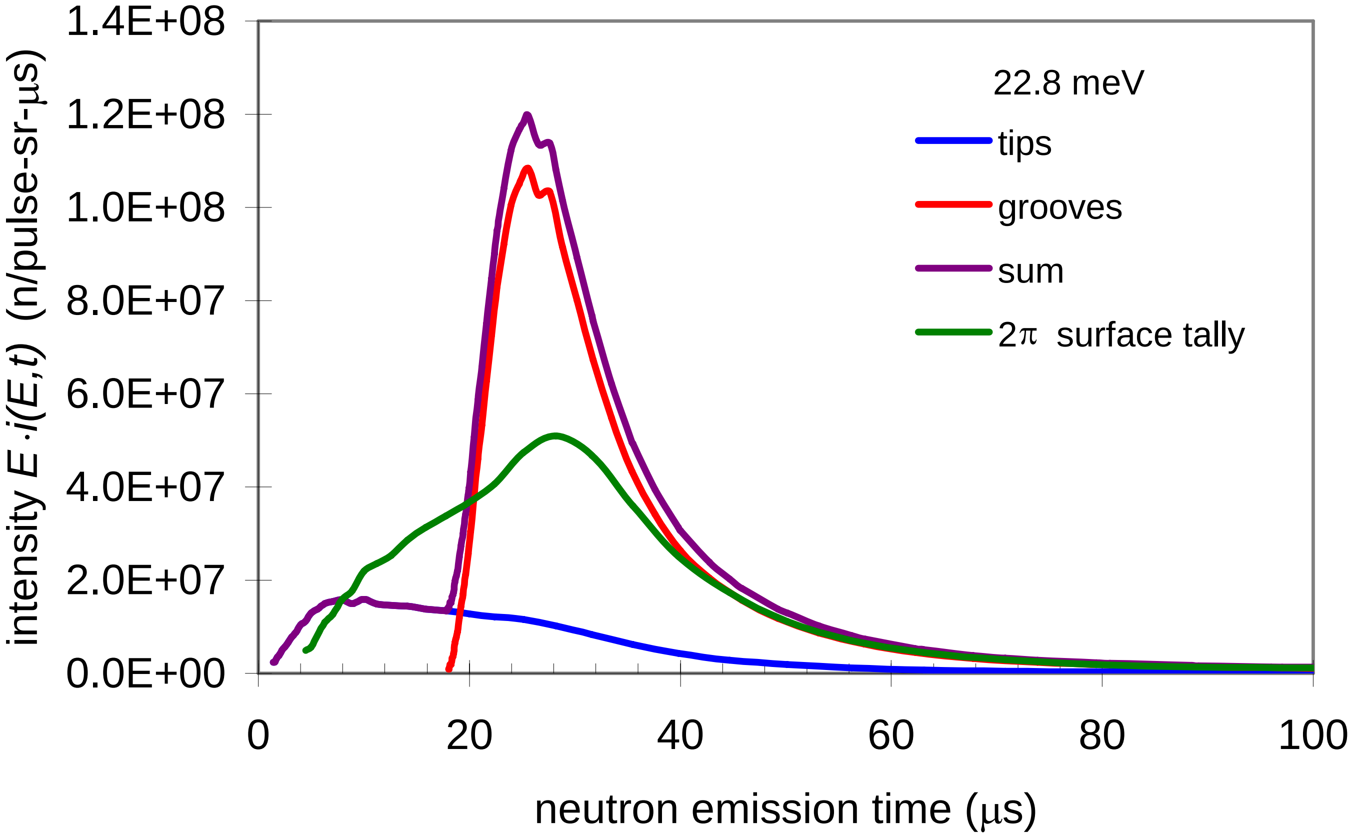
Why The "Traditional" Method Doesn't Work for Reentrant Moderators



- Emission occurs from many different surfaces
- Need to be added together at some common position

Shift and Add Method

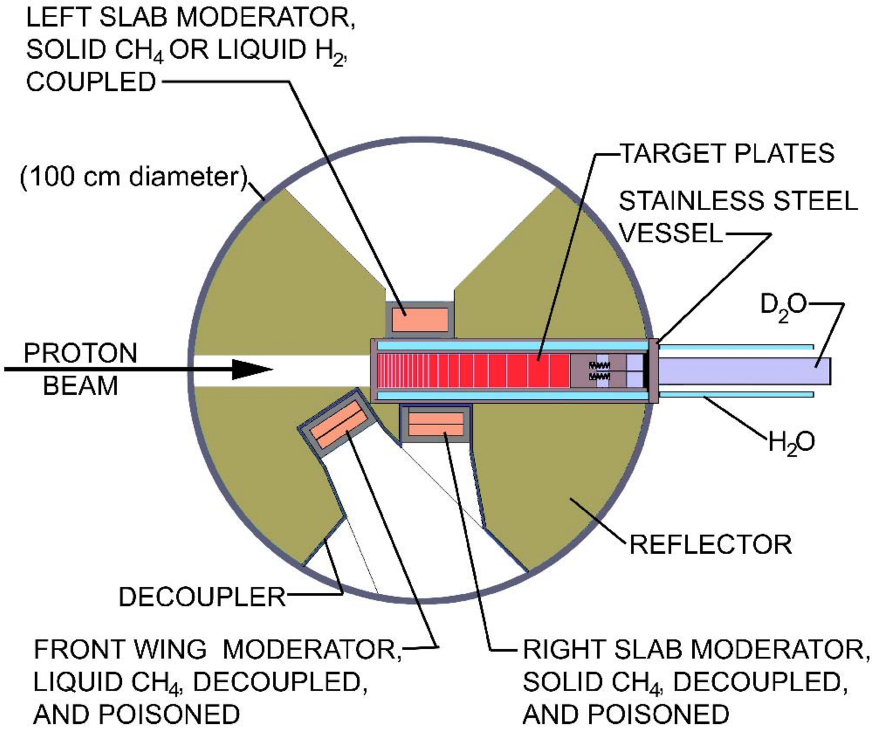
- Add contributions from grooves and tips, time-shifting the emission from the grooves to account for flight time to the moderator face

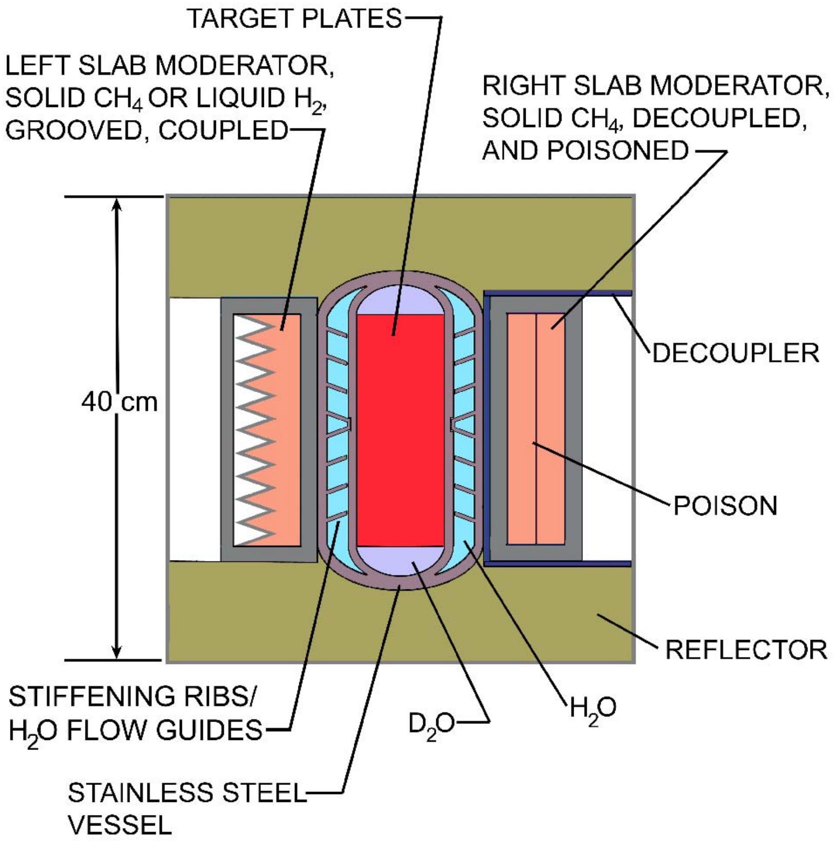


Shift and Add Method

- Advantages
  - rapid computation
- Disadvantages
  - All angles characterized by the same pulse shape
  - Double counting of neutrons
  - Post-processing of MCNPX data required
  - Difficult to generalize to multiple or continuum emission surfaces

LWTS High-Intensity Coupled Moderator



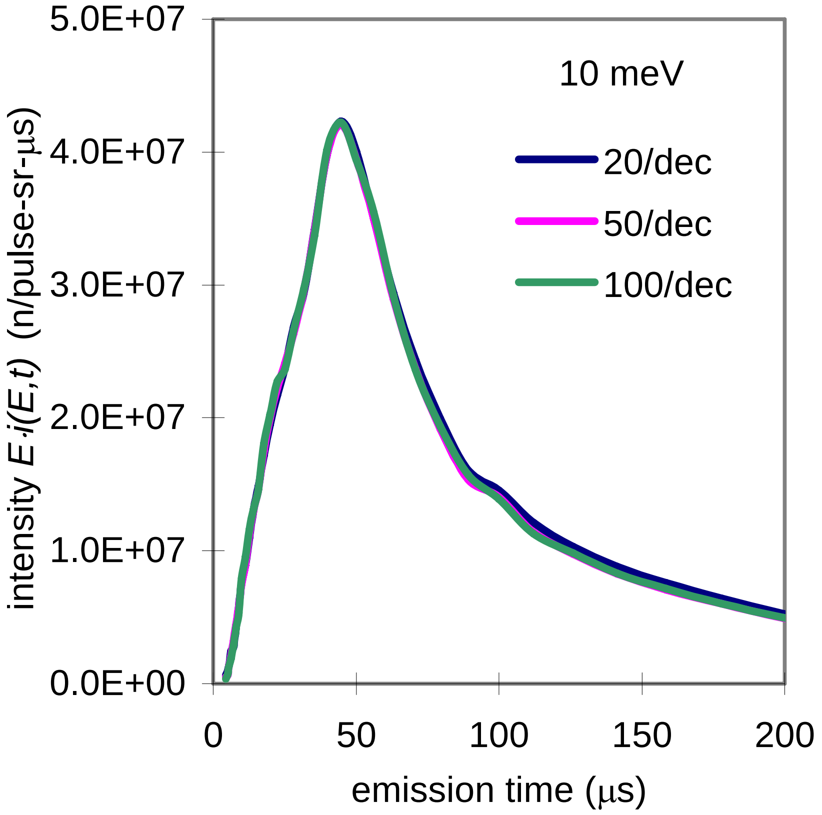


Why Does the 'Traditional' Method Yield a Poor Result?

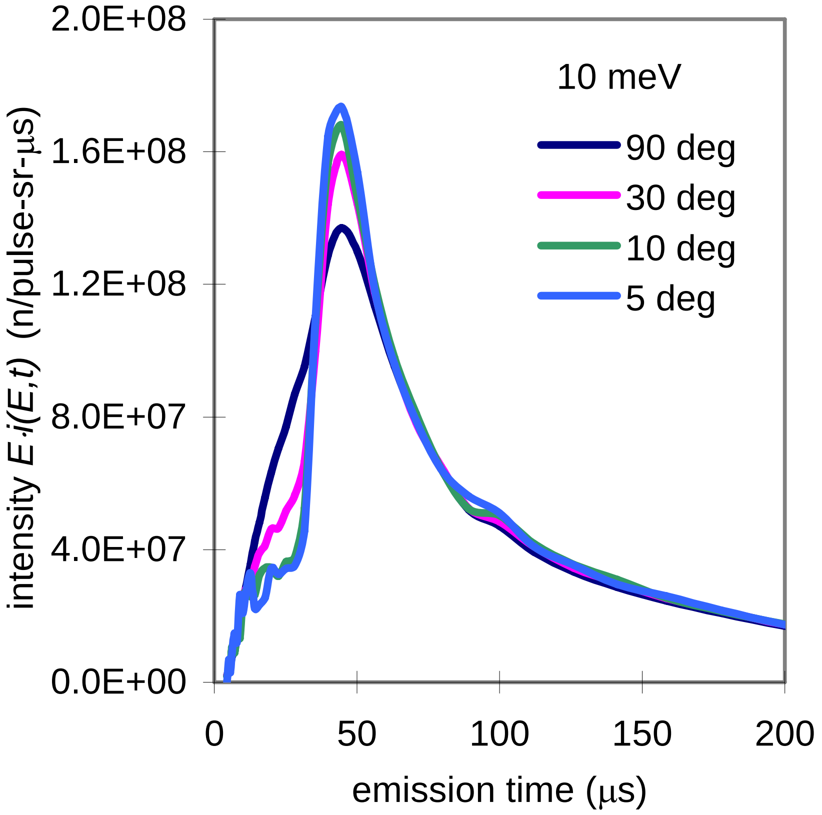
- It had been thought that the smearing of the pulse shapes at the moderator surface was due to velocity dispersion within the MCNPX energy bands
  - But shift-and-add method embodies same assumption
- If this were true, the sharp inflection in the time distribution could be recovered in a single tally at the moderator surface by using narrower energy bins

Pulse Shape Dependence on …

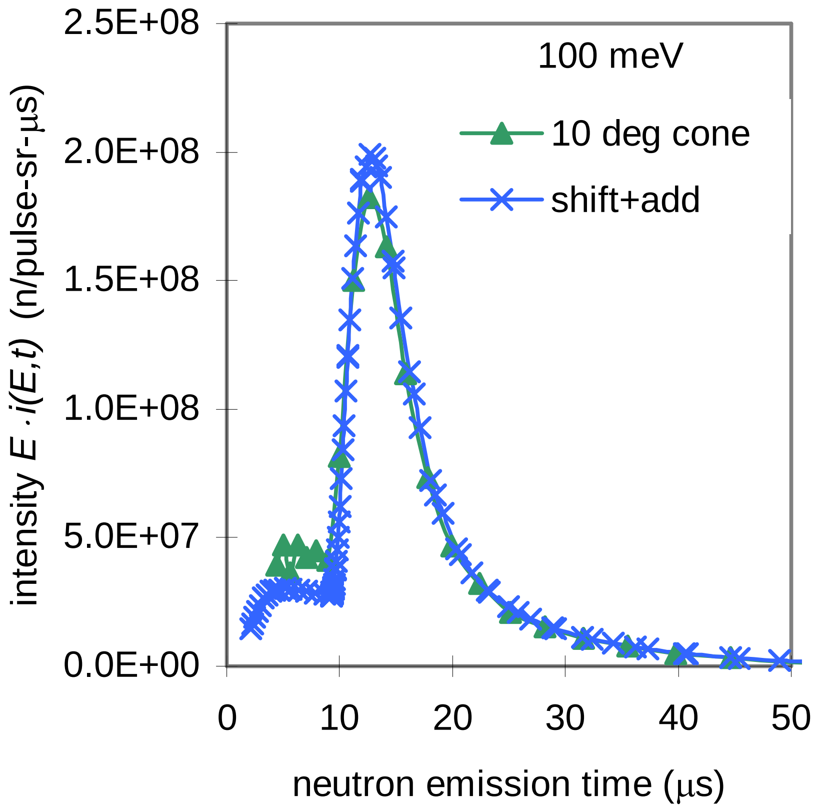
Energy Resolution

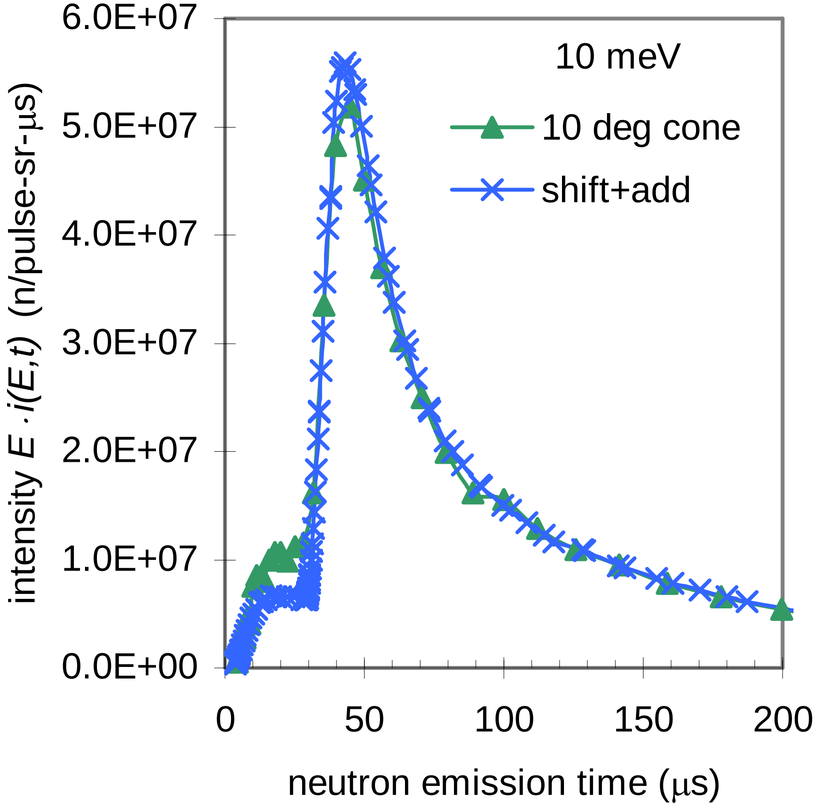


Angular Resolution

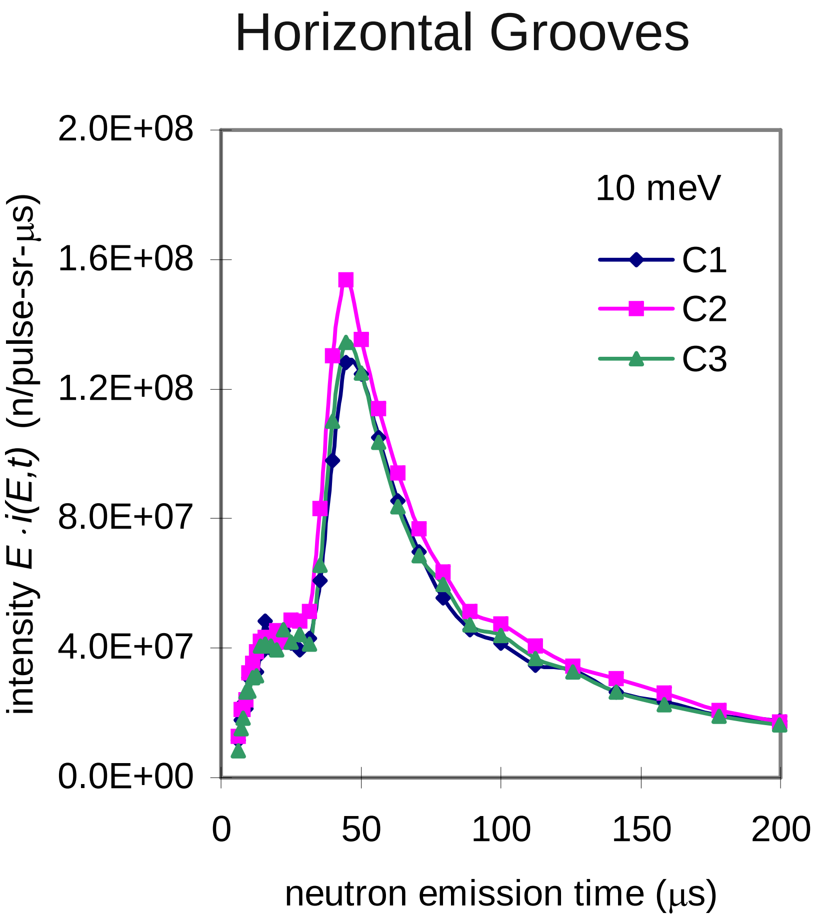


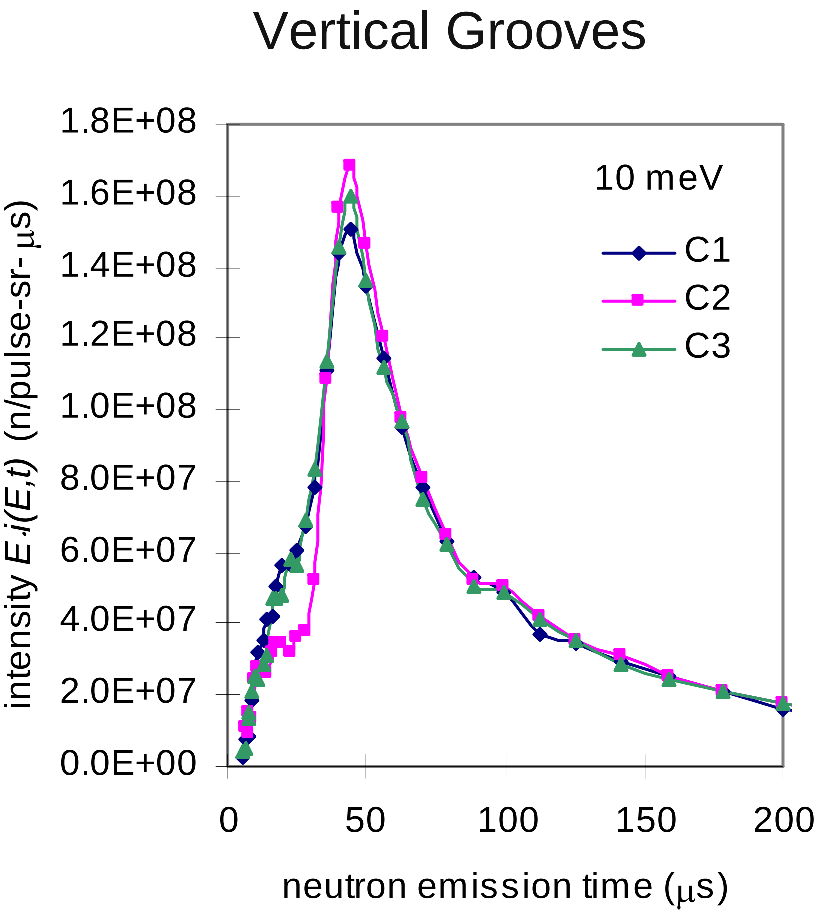
Comparison of Pulse Shape Calculations





Pulse Shapes for IPNS ‘C’ Moderator

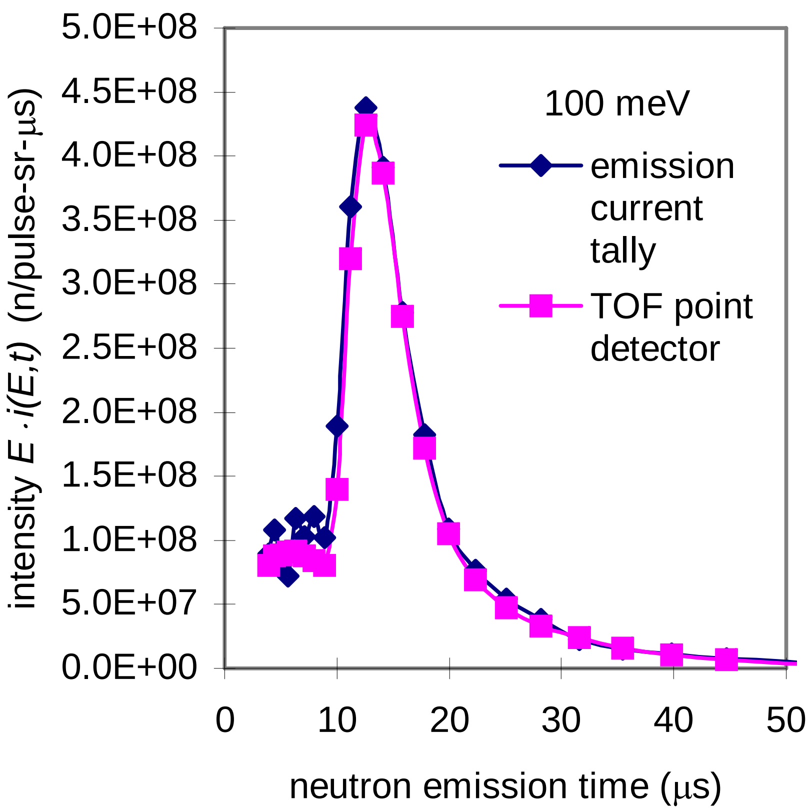


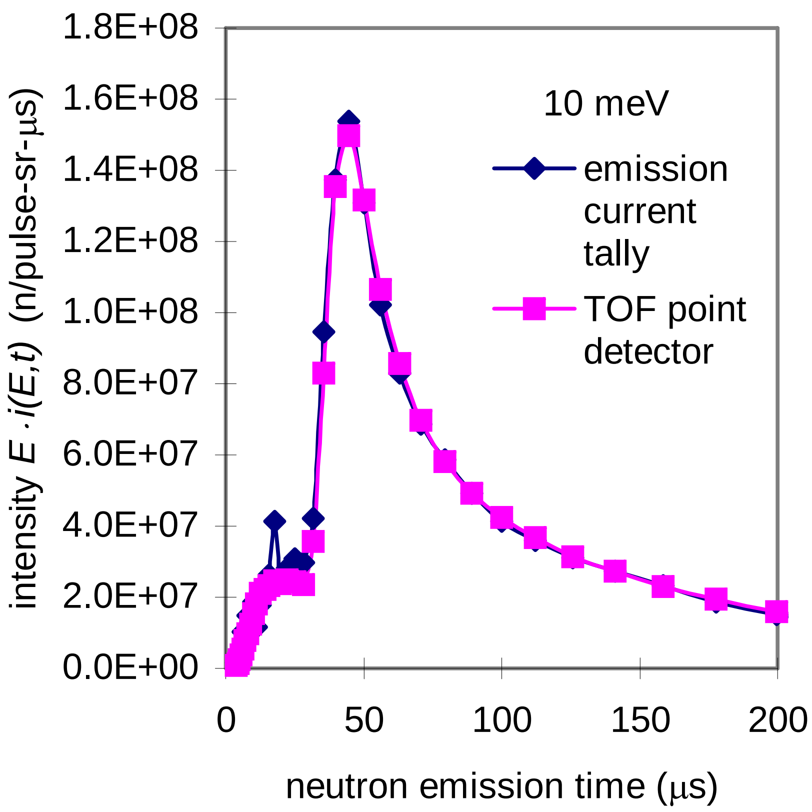


Time-of-Flight Point Detector

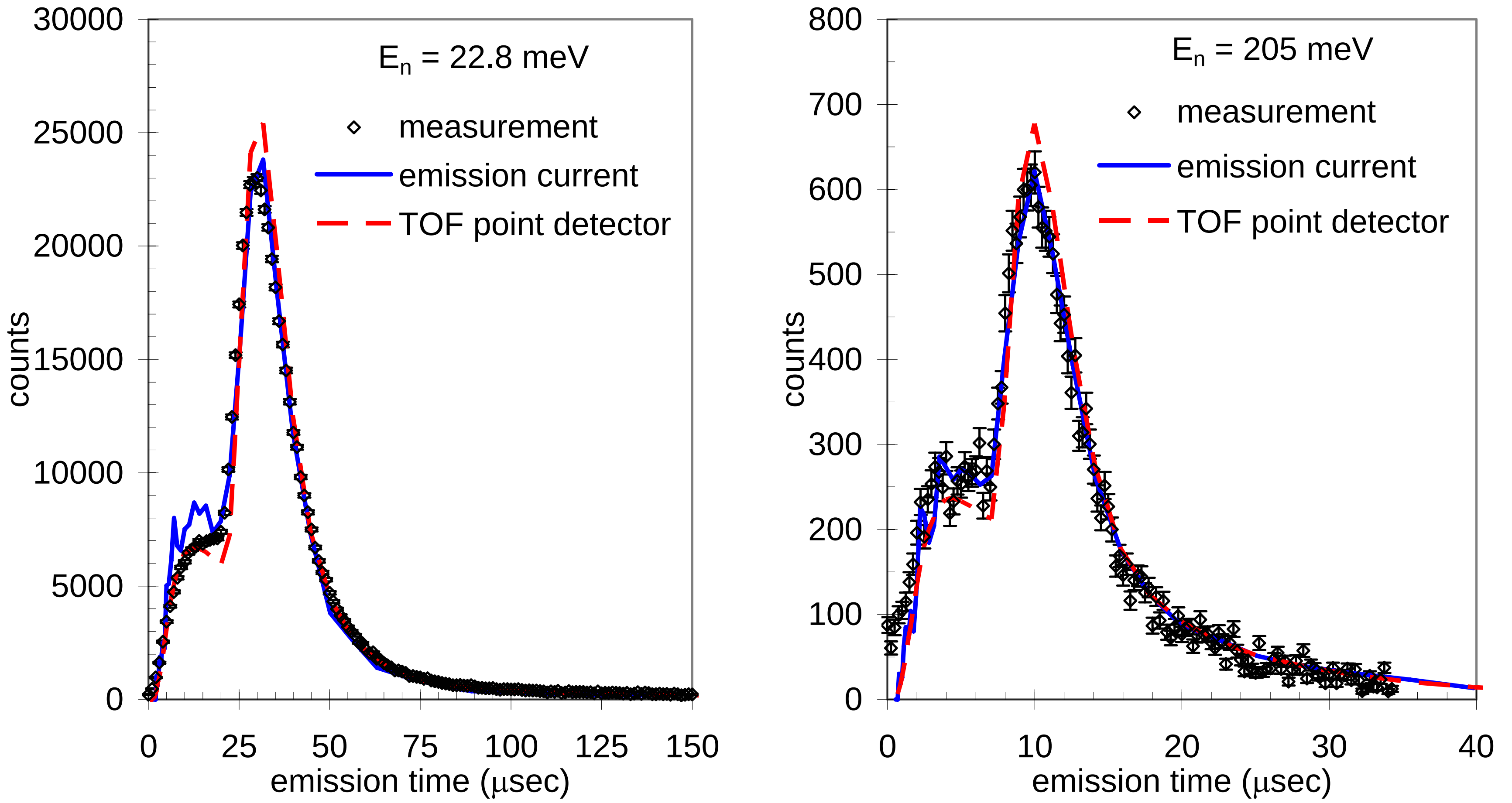
- Obtain detailed time distribution information with the rapid convergence of a point detector tally
- Calculate neutron emission time distribution using remote point detector tally
- Time recorded is the time at which a neutron crosses some specified surface (e.g., the moderator surface) rather than arrival time at detector location

TOF Point Detector Results - C2 Beamline





Neutron Pulse Shapes for C Moderator

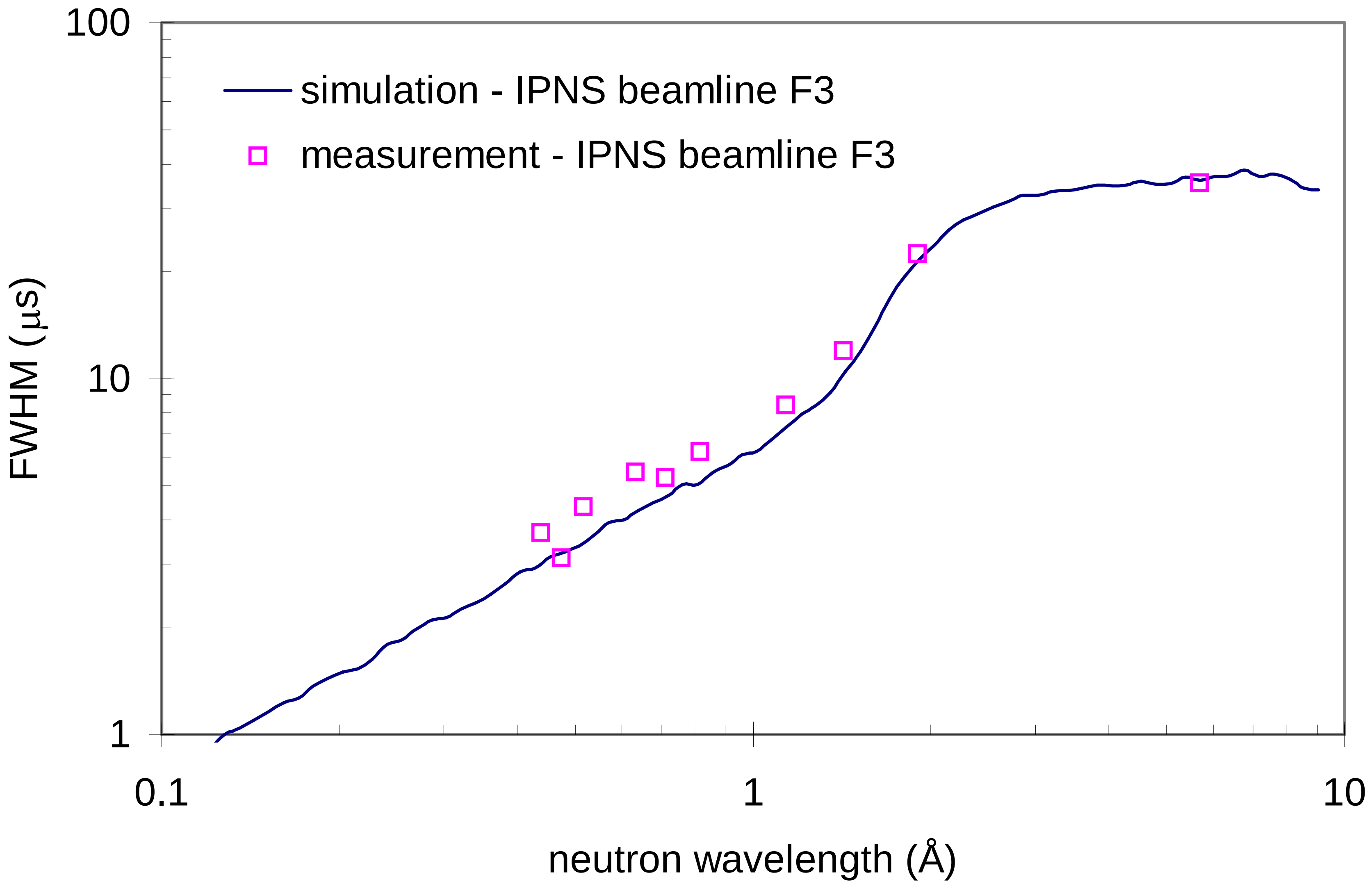


Are We There Yet?

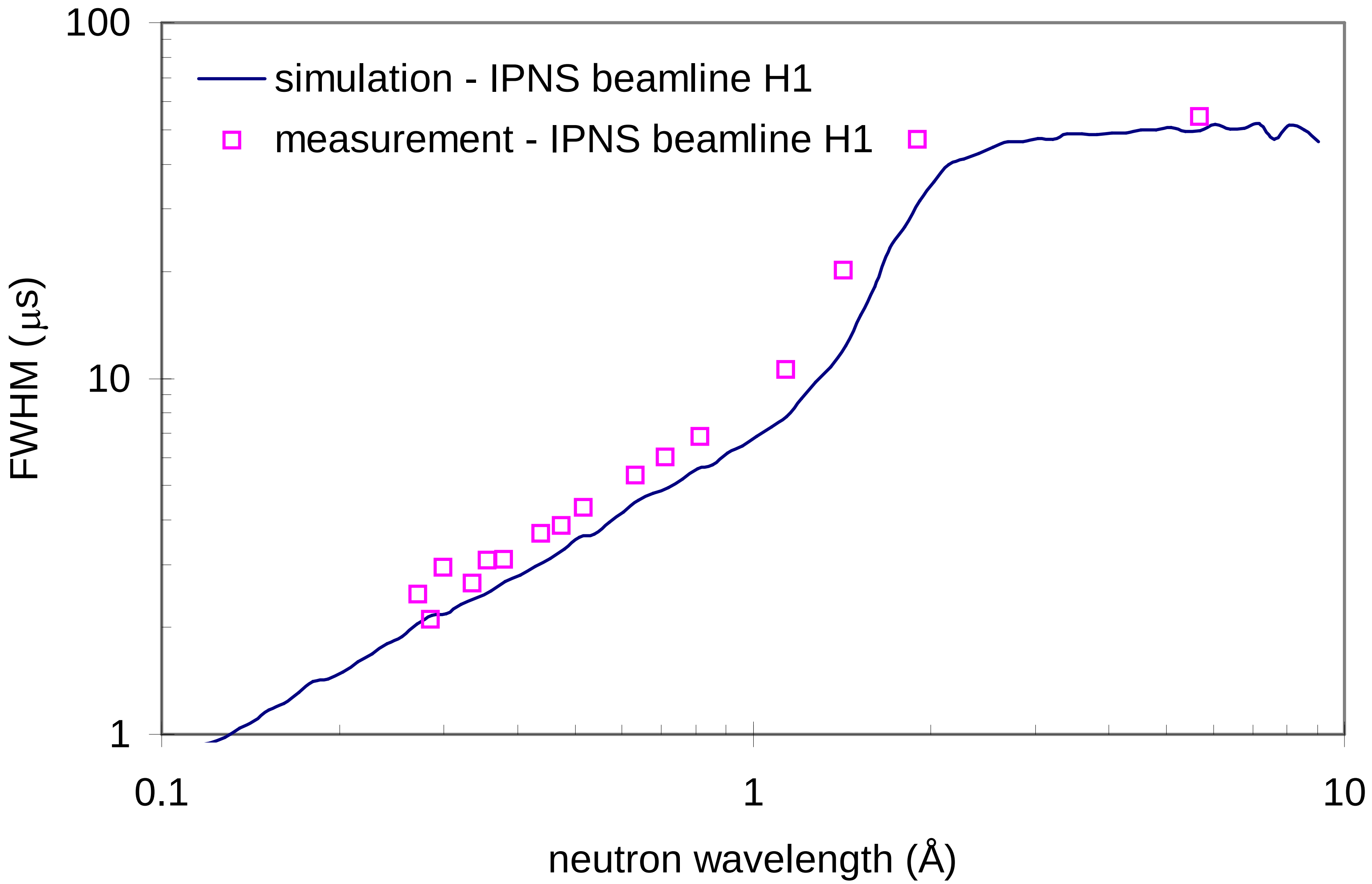
- Metric is time to get 5% fractional standard deviation in the peak emission for 10 meV neutrons
- Time for shift and add = 373 min
- Time for 10 deg cone = 4464 min
- Time for TOF point detector = 22 min !

» Two caveats about the TOF point detector
  - The implementation we used still has some kinks in it
    - *Doesn't apply time bin multipliers correctly*
    - *Doesn't work properly with macrobody surfaces*
  - It has the same limitations as the regular point detector

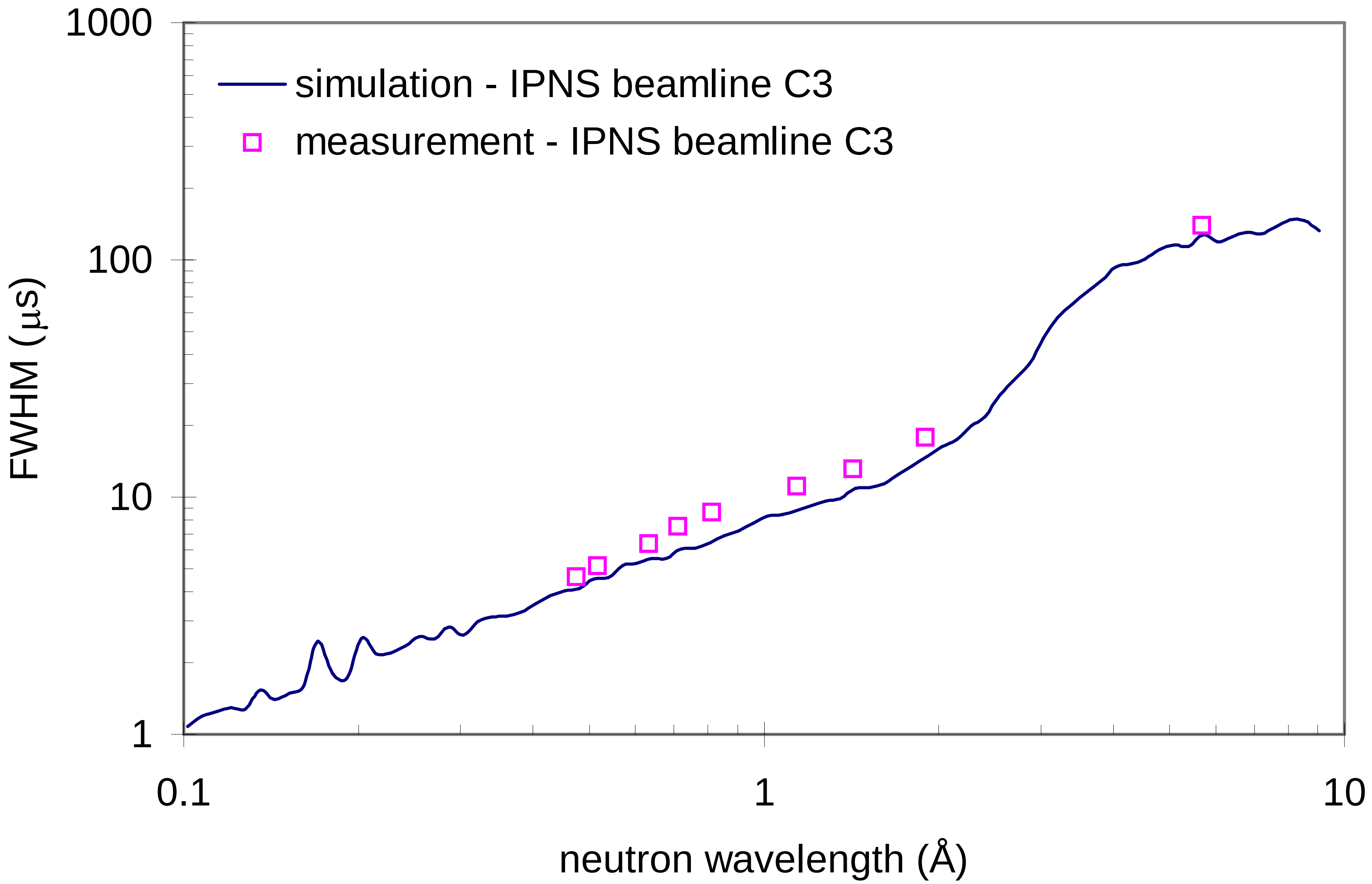
FWHM vs. Neutron Energy – F Moderator



FWHM vs. Neutron Energy – H Moderator



FWHM vs. Neutron Energy – C Moderator



FWHM Curves

- Notice that even though the H moderator pulse shapes have a different appearance, the FWHM values are close to what one might expect
  - Use pulse shapes rather than FWHM in instrument design
- Can deduce a measurement resolution effect from computing $\delta t^2 = \delta t_m^2 - \delta t_s^2$ and noticing that $v \cdot \delta t \approx 2$ cm
- This resolution effect may be responsible for the discrepancies seen on the leading edge of the pulse (symmetric function convoluted with asymmetric function shows largest effect on the rapidly-changing part)

Summary

- Calculational tools (e.g., MCNPX) are good, and improvements continue to be made
- There are some critical data that need refinement (e.g., thermal neutron scattering kernels)
- Comparisons between measured and simulated spectral intensities and pulse shapes show better agreement than previously obtained (1 eV moderator coupling), but significant differences still exist
- Methods used to calculate quantities of interest (spectral intensity, emission time distribution) are adequate but some improvements desired