Monte Carlo Simulation of ARCS Instrument Using Pyre Framework

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Introduction

In the last year, as part of the DANSE project, two software packages have been developed under pyre framework: "simulation" and "pyre-mcstas". The "simulation" package provides a framework allowing very flexible integration of virtual neutron instruments for simulation. A simulation application can be conveniently constructed as a Python class for a neutron instrument. The package "pyre-mcstas" contains both instruments and generic components that allow for flexible and extensible simulations of samples and detectors.

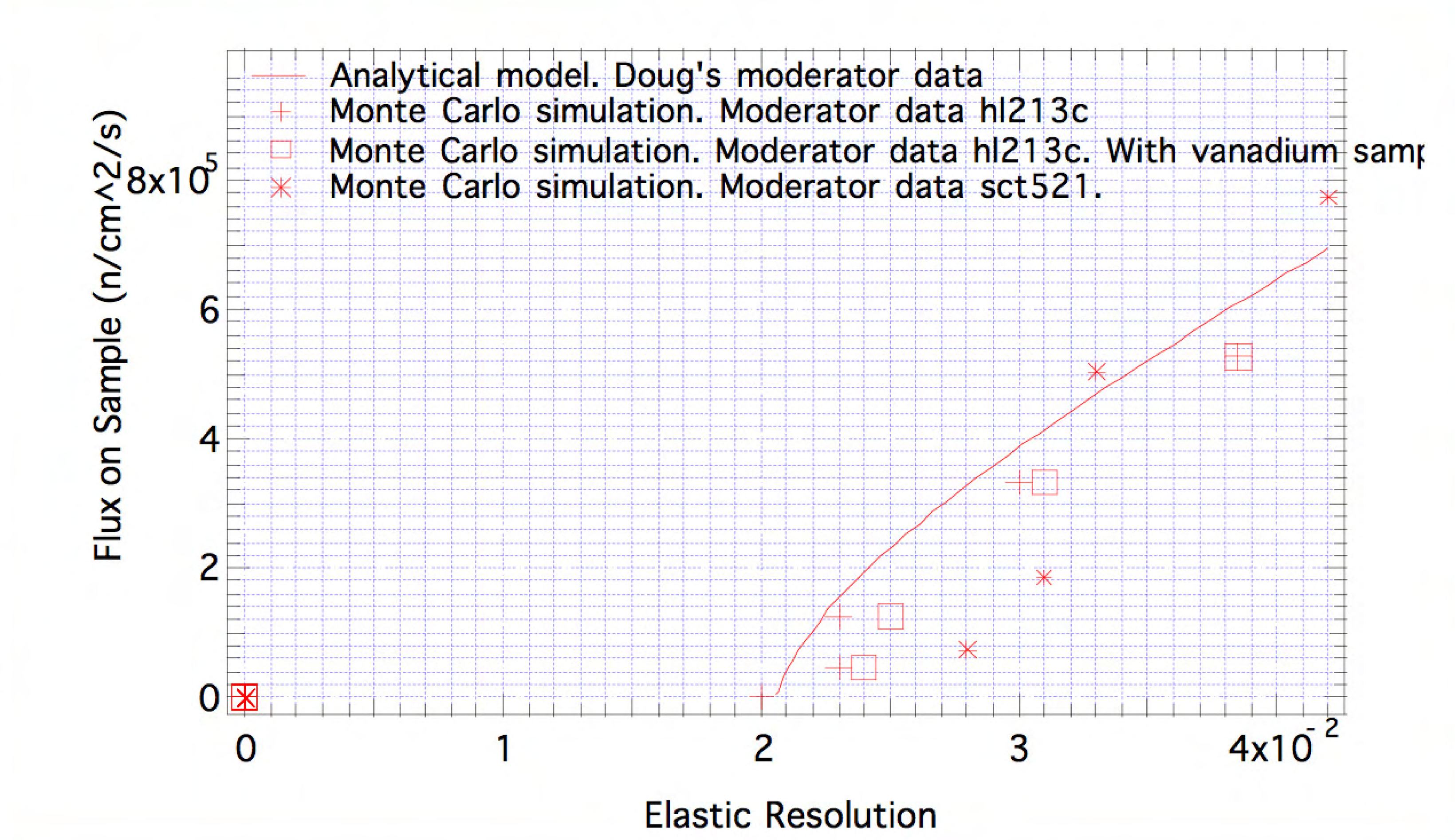
Simulation of ARCS

The simulation pyre application is built from generic sample components and pyre components converted from the McStas package. The moderator component emits neutrons according to the flux distribution function created by Iverson's Monte Carlo simulation. The main guide for the ARCS simulation tapers continuously to produce a 4 cm x 4 cm beam at the sample position, from the shutter to within 1 m of the sample, at 13.5 m. The Fermi chopper is at 11.5 m and is set to 600 Hz. For the purposes of the flux-energy resolution study, the curvature of the chopper blades was optimized for each Ei and ν value. For simulations on polycrystalline tungsten, a package of 32 slits was used, with radius = 0.58 m. A sample component can be constructed with a collection of various kinds of scattering mechanisms. The detector tubes were 3 m from the sample.

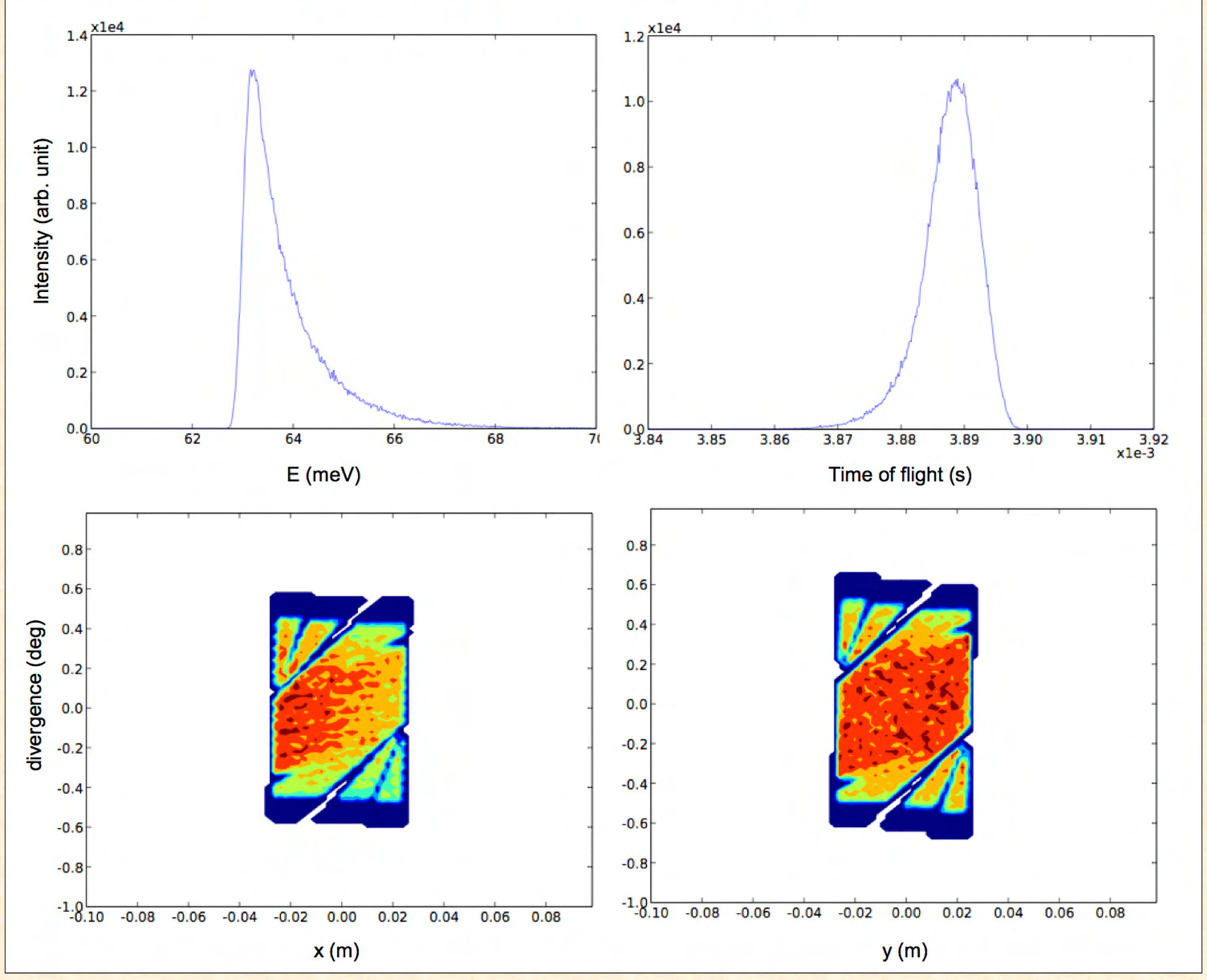
Three sets of simulations were performed. The first one simulates neutrons at the sample position of ARCS instrument. The spectra of these incident neutrons are saved for subsequent simulations. In the second simulation, the saved neutrons are fed to various monitors so energy resolution, flux, divergence, were calculated. In the third simulation the saved neutrons are fed to a sample, and scattered neutrons are collected by various kinds of detectors.

Results

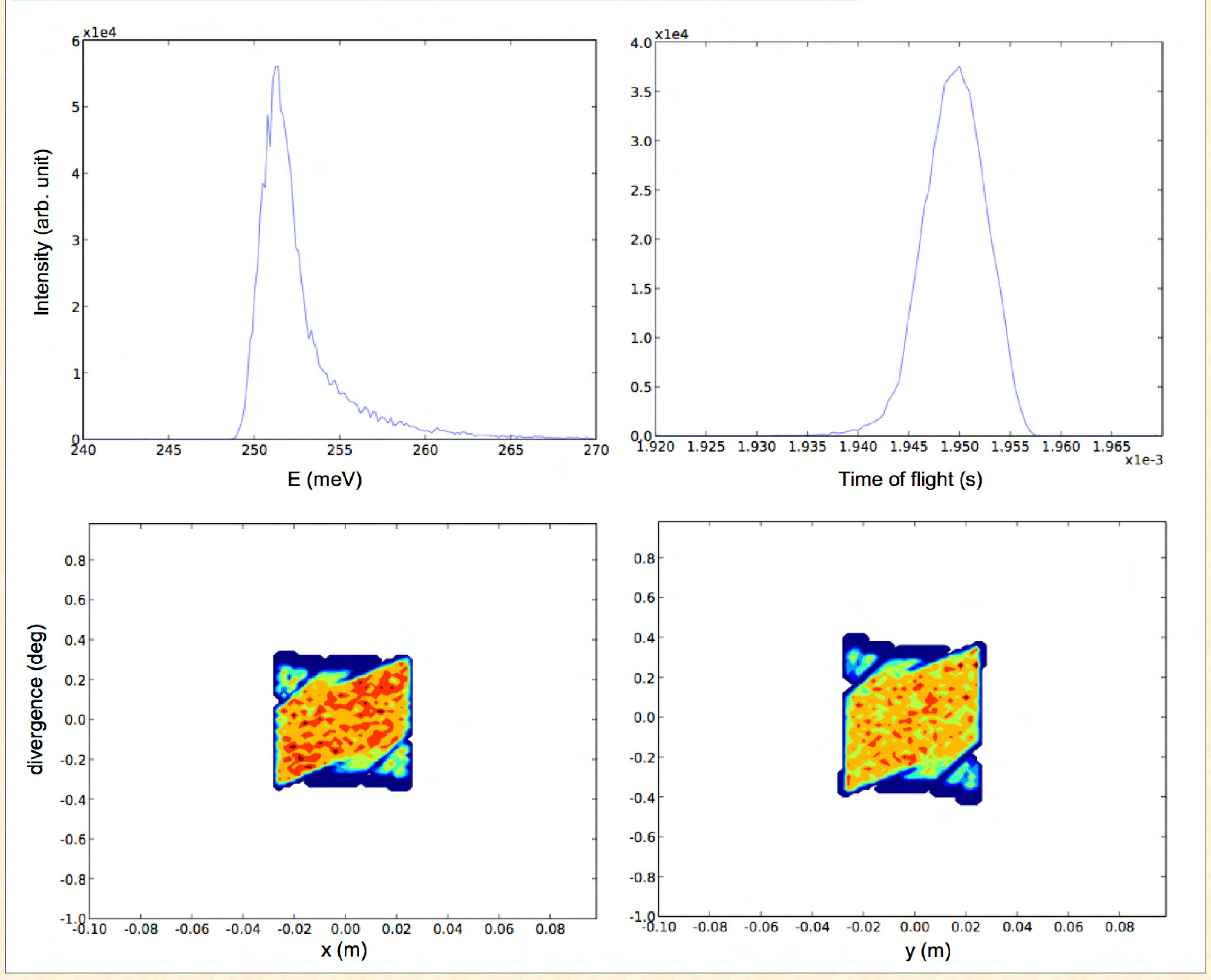
Flux and Energy Resolution



Energy Resolution and Beam Divergence: E = 63meV



Energy Resolution and Beam Divergence: E = 250meV



Coherent Inelastic Phonon Scattering from bcc Tungsten

Tungsten was chosen as a sample for the simulation of coherent inelastic scattering. Tungsten is isotropic elastically, so S(Q,E) remains sharp in Q when dispersions are averaged over all directions of Q, as shown in the lower left figure for a perfect instrument and a perfect incident beam. Sharp dispersions are seen in the first Brillouin zone, and more complex structures in the higher zones. The effect of the spectrum from the incident beam is shown in the middle figure. The third figure shows effects of the sample size and secondary flight path. In the future, this Q information will be utilized in refining experimental results on lattice dynamics.