

Fast Monte Carlo Simulations of SEQUOIA

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Outline

- SNS status and overview
- SEQUOIA overview
- Specialized Monte Carlo Components
- Method of Parallelization
- Results
- Comments on Data Analysis
- Resolution tests
- Summary





SNS site - Spring 2006







SNS first neutrons on April 28







CD4 Beam Line 7 Intensity Measurement



SNS Instrument Suite







Overview







Parameters

- Decouple poisoned ambient H₂O moderator
- Moderator to Fermi chopper distance 18 m
- Fermi chopper to sample distance 2m
- Sample to detector distance in horizontal 5.5m
- Narrow bandwidth vertical axis T₀ chopper at 10 m from moderator operates at multiples of 30 Hz up to 180 Hz
- Elliptical shaped guide with focal point after sample
- 5 cm x 5 cm sample
- Fermi chopper, $E_i = 100 \text{ meV}$, v = 420 Hz, 2 mm slits, $r_{curve} = 1.0048 \text{ m}$
- Detector y = 500, 12mm x φ = 360, 0.25° x t=2000, 5μs 360 x 500 x 2000 = 3.6 x 10⁸ pixels!!





Specialized components

- SNS Source In current McStas release
- T₀ chopper
 Fermi chopper

Slit package can be changed with only a few lines of code

- 1-D Dispersion sample
- Cylindrical Event based detector





1-D dispersion component







Event Detector Component

- 10⁸ pixels is too many for standard cylindrical detectors
- Records Time, phi_bin, y_bin, and probability.
- Histogramming performed after simulation complete
 - Facilitates parallelization

```
tunits: (mus)
    imits: -3.000000e+01 6.000000e+01
 hibins: 360
 hins: 500
         -3.00000e+00 3.000000e+00
  imits:
  .me phi_bin y_bin prob
          266
               [5]
          273
       446
           282
                    .083
          276
       28
               265.99
          275
               0.000450935
     5
       85
```





Processing diagram



- 1x10¹⁰ n distributed over 21 processors
- ~ 3 hour calculation time
- useable on the Teragrid in the near future.
- Requires no knowledge of MPI, PVM, grid access, etc.



Results



Used for Developing Data Analysis Algorithms

- Results too large for mslice
 - 1/5 of detector bank OK on high end linux machine (2003)
- Algorithms tested
 - 1. Event data read and histogrammed into t and ϕ bins
 - Pixels stored as vertices and connections (computer graphics standard)
 - Only pixels with events are kept
 - 2. Vertices converted to Q and ω
 - Note volume of pixel is discrete Jac post
 - 3. Data projected into 2-D plane
 - 3-D projection algorithms and viewing routines in progress
 - Plan to capitalize on computer graphics algorithms from this point
 - 4. Data gridded onto regular array
 - 5. Cuts made
 - Cuts from step 2 in progress





Views in t and $\boldsymbol{\omega}$









200 μs

18.1

18

() 17.9 3

17.8

17.7 2.15







18.1

18

17.8

17.7 2.15











2.2

Q_z(Å⁻¹)

2.25









5μ**S**

18.1

18

(Nem) 17.9 3

17.8

17.7 2.15









18.1

18

17.8

17.7 -2.15







2.2 Q_z(Å⁻¹) 2.25



2.26



2.2

Q_z(Å⁻¹)

2.25







Summary

- 1-D dispersions have been measured using Mcstas
- Cluster simulations were performed in ~ 3 hr
 - All ~10⁸ pixels included in simulation
- These results are useful for testing data analysis software





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