Neutron Instrument Simulation Package

The Neutron Instrument Simulation Package, *NISP*

http://PASeeger.com

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"Monte Carlo is not a substitute for thinking"
Jack Carpenter

- **Workshop Objectives**
  - Access web site *http://PASeeger.com*
  - Get Manual and install code
  - Tutorial example, *HIPPO*
  - Advanced topics, such as
    - starting a "real" simulation
    - customization (adding new elements)
    - the program "Super_Know"
- **Philosophy & History of NISP**
  - MCLIB, MC_Run, and NISP_Win
- **Examples from Instrument Simulations**
  - *LAPTRON*
  - *VISION*
  - *AMOR*
  - *SPAN*

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http://PASeeger.com **Click here to get Code**

The officially released version of **NISP** is available via http download, NISPforWindows, including *complete* source code and executables for

- a Windows-based GUI interface (NISP_Win), latest update 29 Aug 2006
- the transportable (Fortran) MCLIB library, 11 Sep 2006
- the program to run Monte Carlo simulations (MC_Run, also transportable), 11 Sep 2006
- and a Windows program to view the results (See_MC_Data), 24 Dec 2004

The complete Revision History of MCLIB and MC_Run can be viewed here.

Click here to get Manual

Documentation, including a **Brand New** Manual, conference proceedings with latest updates, and published papers for several innovative algorithms, may be downloaded in a single .zip file from NISP_Documents, **or** as individual documents from Document Menu. In addition to the Manual, I recommend the paper from the 2004 SPIE Proceedings for an overview of NISP.

Other documents as desired

For further information and for assistance in implementing or using NISP, please contact Phil Seeger and Luke Daemen (Los Alamos National Laboratory).

We invite **participation** *in the development of this tool!* Please also send comments and suggestions.

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Code Installation

Download **http://PASeeger.com**/downloads/NISPforWindows.zip

Extract files, including:

`x:\...\NISP\aaaread.me`	installation instructions
`\NISP_Win.exe`	NISP: Construct instrument, write geometry file
`\MC_Run.exe`	MC RUN: Run simulation using geometry file
`\See_MC_Data.exe`	SEE DATA: Plot 1D and 2D detector histograms
`\Super_Know.exe`	Make histograms from "Monitor" file

`\Material.txt`
`\Crystal.txt`
`\Help\NISP.hlp`
`\NISP.cnt`
	REQUIRED by NISP_Win

`\Tables\*.tbl`	moderator energy/time tables
`\Powders\*.pdr`	powder diffraction samples
`\Crystals\*.lau`	single-crystal samples (from McStas)
`\Kernels\*.sab`	inelastic $S(\alpha,\beta)$ data (from MCNP)
`C:\PGPLOT\grfont.dat`	required to get text labels on traces and graphs

Total length of *all* files from the .zip file is 10.3 Mbytes, including *complete* sources.

Note: to view the Virtual Reality, install Octaga Player (http://octaga.com).

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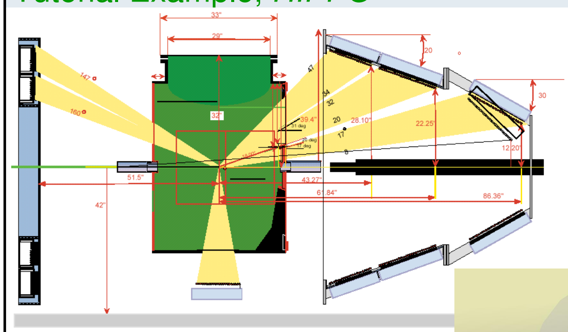
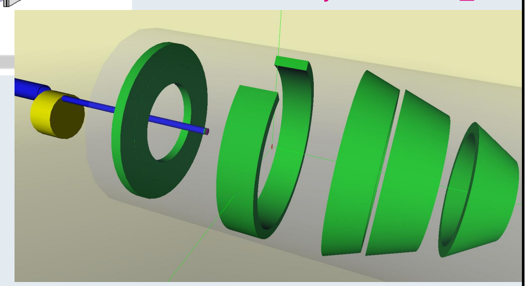
Tutorial Example, *HIPPO*



Engineering layout

"Virtual Reality" from NISP_Win



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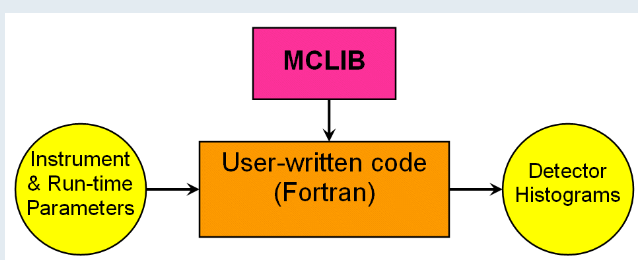
1978:

MCLIB, library of Monte Carlo subroutines for neutron *optics*,
geometry of Surfaces and Regions similar to MCN(P)



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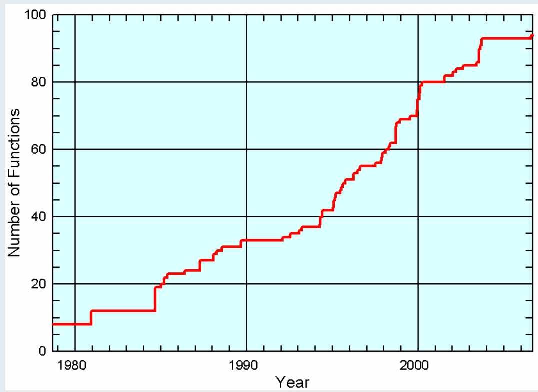
Growth of MCLIB, 1978-2006



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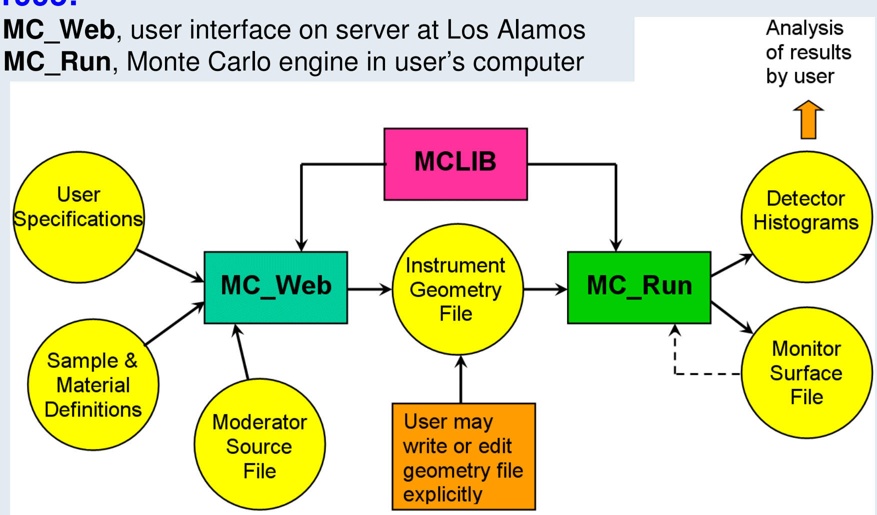
1995:

MC_Web, user interface on server at Los Alamos
MC_Run, Monte Carlo engine in user's computer



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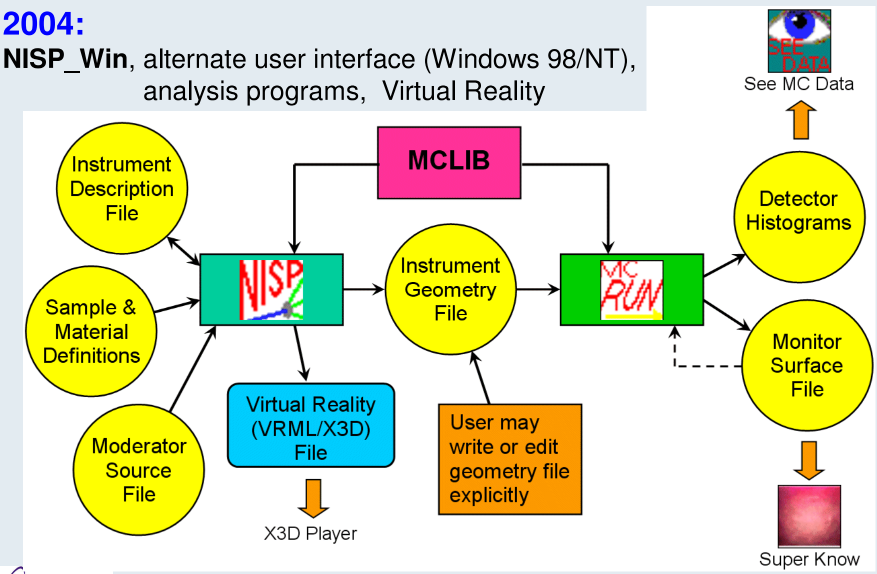
2004:

NISP_Win, alternate user interface (Windows 98/NT), analysis programs, Virtual Reality



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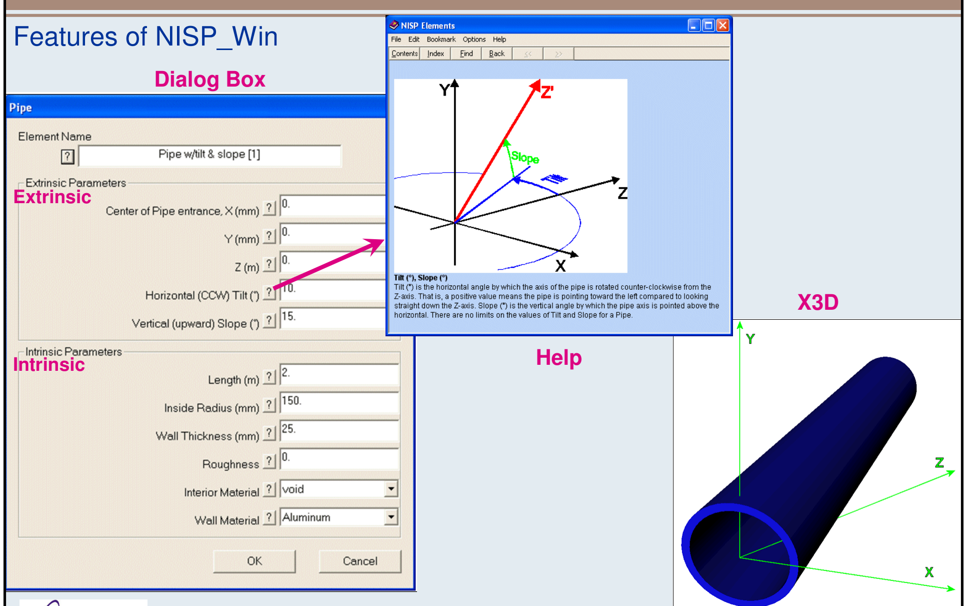
Features of NISP_Win



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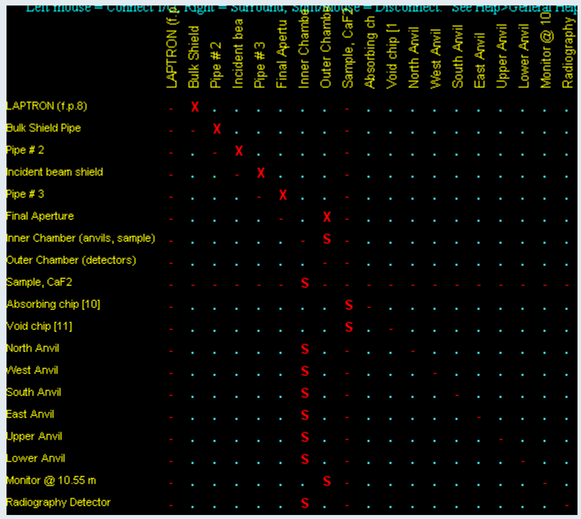
Features of NISP_Win – **Connection Matrix**

Linear connections marked by "**X**"

- LAPTRON (f.p.8)
  - → Bulk Shield Pipe
  - → Pipe # 2 ✱
  - → Incident beam shield
  - → Pipe # 3 ✱
  - → Final Aperture
  - → Outer Chamber ✱

Surrounding regions marked by "**S**"

- ✱Outer Chamber
  - ⊃ Inner Chamber
    - ⊃ Sample, CaF2
      - ⊃ Absorbing chip
      - ⊃ Void chip
    - ⊃ North Anvil
      - · · · total of 6 anvils
    - ⊃ Lower Anvil
    - ⊃ Radiography Detector
  - ⊃ Monitor @ 10.55m
  - ⊃ Top_Left Detector
    - · · · total 14 detector banks
  - ⊃ 144deg_Down Detector
- ✱Pipe # 2
  - ⊃ Guide segment 1
  - ⊃ Guide segment 2
  - ⊃ Guide segment 3
- ✱Pipe # 3
  - ⊃ Final Guide



(partial connection matrix for LAPTRON)

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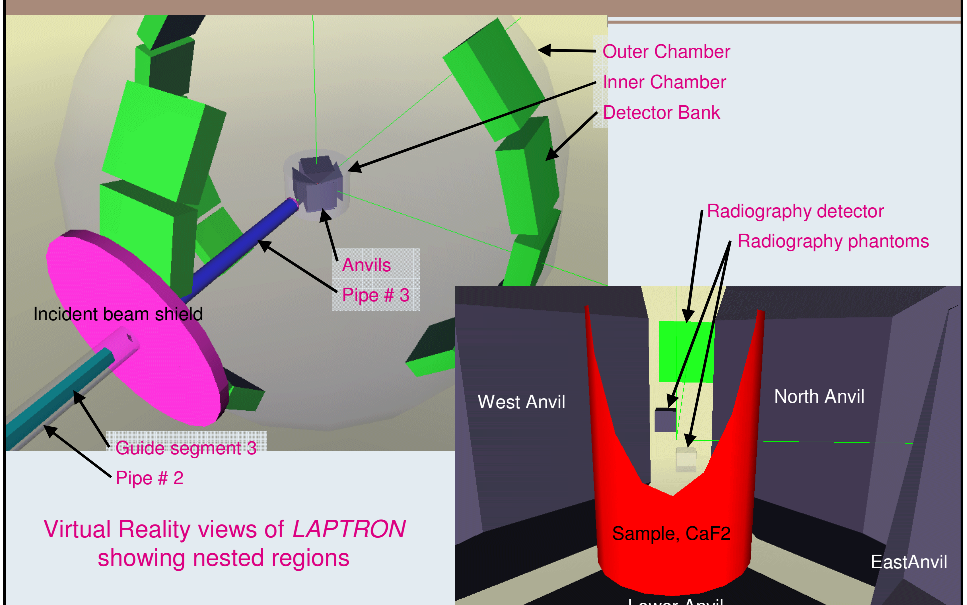

Virtual Reality views of *LAPTRON* showing nested regions

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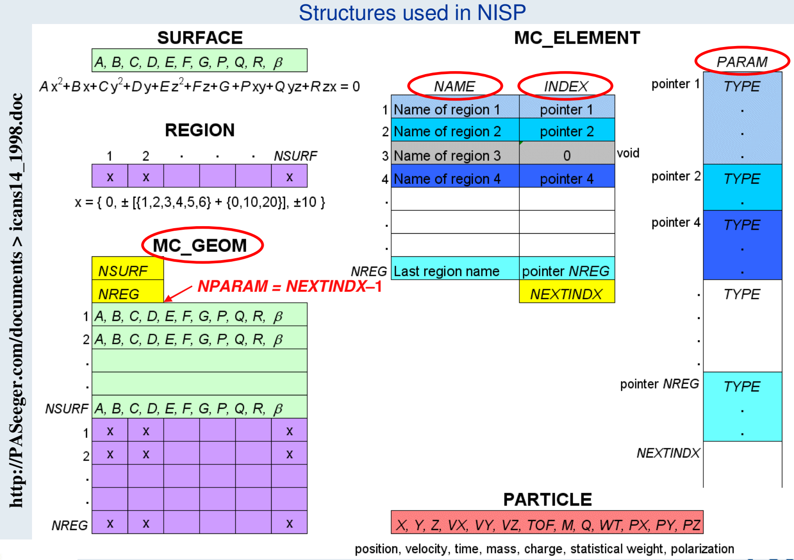
What is in the Geometry file?

Structures used in NISP



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MC_Run: Runtime Parameters

```
$RUN
MON_SURF =  0    Surface number to monitor ("0" for none, negative
                 for corresponding source neutron only)
CORR_SURF =  0   "0" for no correlation, "-1" for preceding surface,
                 "  1" for source, or "nnn" for surface nnn
SCAT = 'N'       Record all detected neutrons in files ('Y' for yes)
BAD = 'N'        Record complete traceback of Bad neutrons ('Y' for yes)
NSPLIT =  1      Neutrons reaching sample may be used more than once
WT_MIN = 1.0E-06 Minimum value of statistical weight to track
WT_FRAC = 1.0E-03 Fraction of histories below WT_MIN to keep
SPEC = 'T'       Spectrum to be 'I'ncident or 'T'ransmitted?
POIS = 'N'       Integer output with Poisson statistics ('Y' for yes)
FIELD = 'N'      Include magnetic induction fields ('Y' for yes)
TRACE = 'N'      Plot trajectories ('Y' for yes).
GRAVITY = 'Y'    Include gravity ('N' for no).
DUMPS = 'N'      Keep ALL intermediate dumps ('Y' for yes).
REUSE =  1       Allowed number of times to reuse input source file
ISEED =   12345678  Random-number seed, 0 to randomize
$
```

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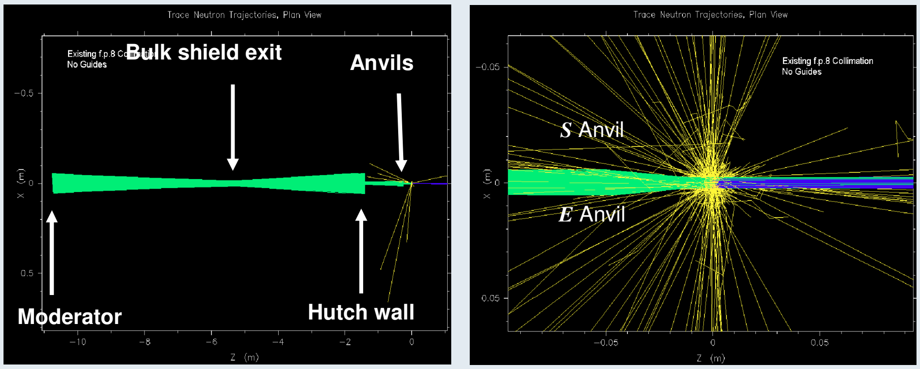
Use of the "Trace" option – *LAPTRON*

Monte Carlo simulation of neutron trajectories:
incident, **transmitted**, **scattered**, and "**bad**"



"Standard Collimation" uses existing f.p. 8 components and a sequence of collimators to define the incident beam (no guides).

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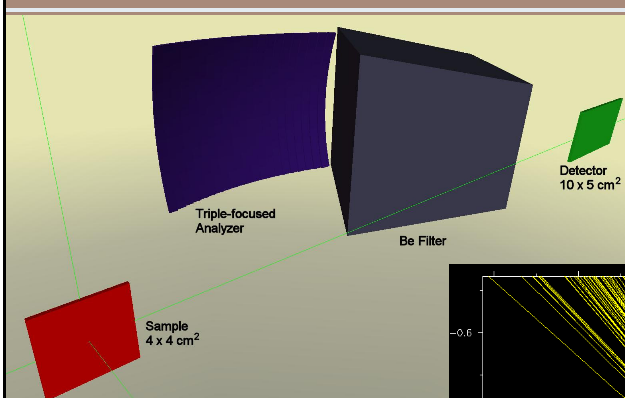
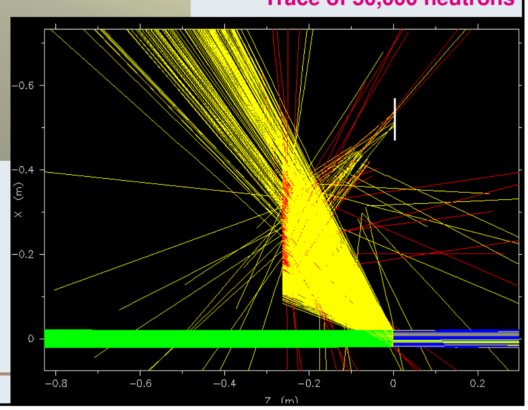
X3D



Trace of 50,000 neutrons



VISION, Chemical Vibration Spectrometer for SNS

The focusing analyzer allows decreased detector size, for improved signal-to-noise ratio.

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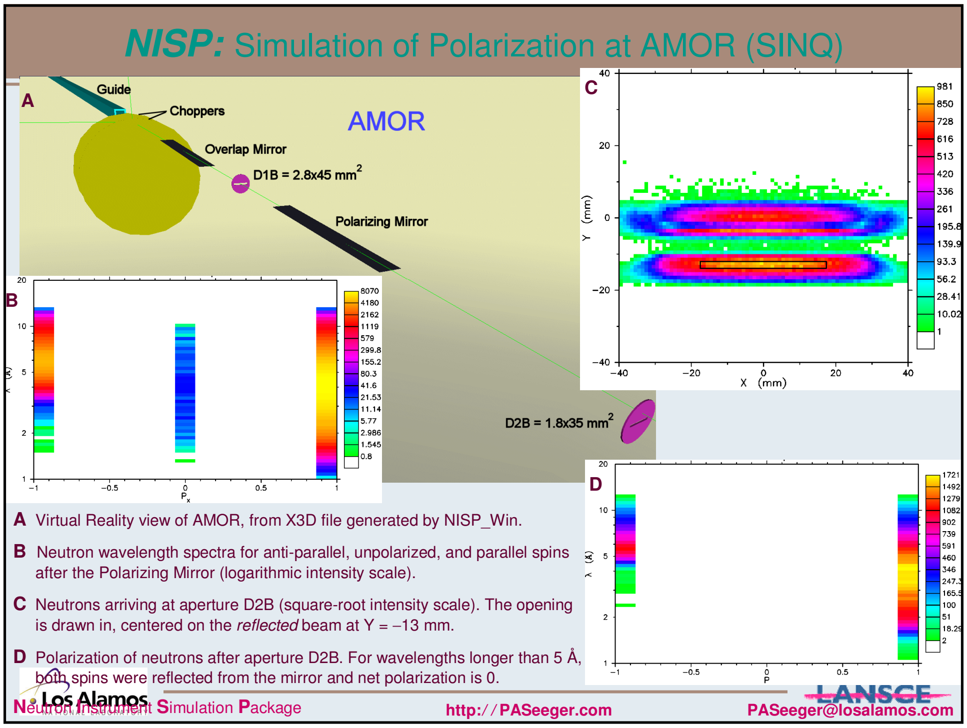
NISP: Simulation of Polarization at AMOR (SINQ)
A
Guide
Choppers
AMOR
Overlap Mirror
D1B = 2.8x45 mm2
Polarizing Mirror
D2B = 1.8x35 mm2
B
C
D
A Virtual Reality view of AMOR, from X3D file generated by NISP_Win.
B Neutron wavelength spectra for anti-parallel, unpolarized, and parallel spins after the Polarizing Mirror (logarithmic intensity scale).
C Neutrons arriving at aperture D2B (square-root intensity scale). The opening is drawn in, centered on the reflected beam at Y = –13 mm.
D Polarization of neutrons after aperture D2B. For wavelengths longer than 5 Å, both spins were reflected from the mirror and net polarization is 0.
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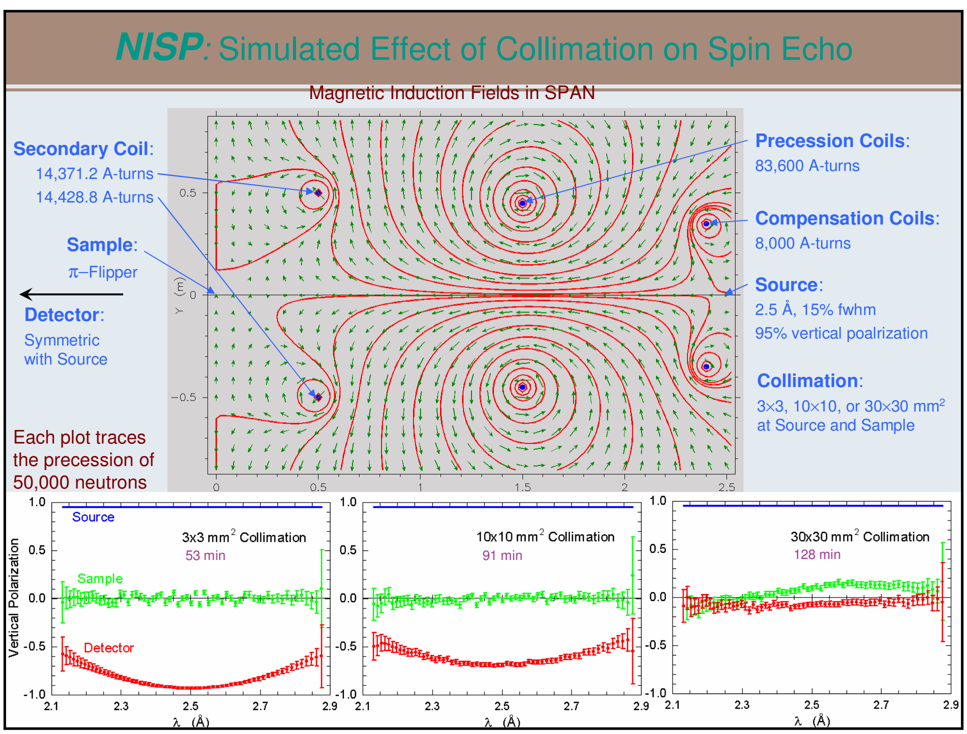
NISP: Simulated Effect of Collimation on Spin Echo
Magnetic Induction Fields in SPAN
Secondary Coil:
14,371.2 A-turns
14,428.8 A-turns
Sample:
π–Flipper
Detector:
Symmetric with Source
Each plot traces the precession of 50,000 neutrons
Precession Coils:
83,600 A-turns
Compensation Coils:
8,000 A-turns
Source:
2.5 Å, 15% fwhm
95% vertical poalrization
Collimation:
3×3, 10×10, or 30×30 mm2 at Source and Sample
Source
Sample
Detector
3x3 mm2 Collimation
53 min
10x10 mm2 Collimation
91 min
30x30 mm2 Collimation
128 min
Vertical Polarization
λ (Å)

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Importing a McSTAS component: Single-Crystal sample

- **A McSTAS "Component" is like a NISP "Element" because it has both geometric and algorithmic information.**
- **Create a Region type `SnglXtal`**
  - convert C source code to Fortran by global editing, type declarations, DO and IF-THEN-ELSE structures, etc.
  - omit pointer arrays, and allocate data structures directly
  - remove all references to geometry, absorption, transmission, and neutron transport, which are handled in the calling program
  - 2nd entry point for the scatter calculation
  - same data files as McSTAS, *but* include unit-cell parameters
- **Create an Element type "Single Crystal Sample"**
  - orientation requires ***3*** extrinsic parameters: Slope, Tilt, Rotate
  - used same geometry as McSTAS, but *any* shape is allowed
  - Select x'tal data file from list, read unit-cell parameters from file

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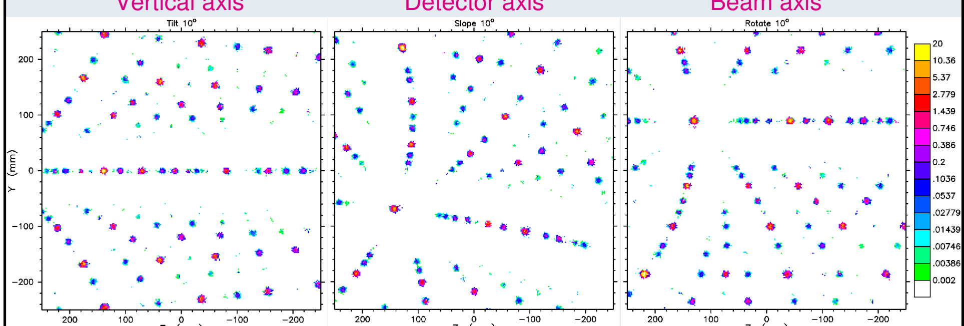
Laue patterns from Adrenaline crystal rotated by 10º about each axis

Vertical axis — Detector axis — Beam axis



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What are the *UNIQUE* features of NISP?

- Separation of *geometry* and *content* of regions
  - use same algorithm in any shape
  - may import algorithms directly from MCNP (*e.g.*, S(α,β))
- Neutrons **not** constrained to specific sequence of elements
  - use connection matrix instead of linear sequence
  - multiple detector banks
  - cradle-to-grave simulation
  - find unexpected pathways
  - see (some) background sources
- Splitting of neutrons in common materials
  - track low-probability events
  - track background scattered neutrons
- Help button for every entry in the user interface
- Virtual Reality file to view instrument geometry
- All programs coded in structured Fortran
  - **fast** execution of simulations
  - may import C routines fairly easily (*e.g.*, Single_crystal.comp)
- Magnetic fields
  - integrates precession
  - hexapole lenses (work in progress)
  - may include 1/ t dependence for pulsed source
- Pulsed spallation sources defined from MCNP output
- Structures support tracking *photons* and other particles

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Shared features between NISP and other codes

- Speed, fast enough to make parameter searches practical
  - simple TAS benchmark: NISP faster than McStas, slower than VITESS
  - exception: integrating precession in a varying field is a little (8000×) slower
- Algorithms of varying complexity, as needed
- Trace mode to visualize neutron trajectories at run time
- Open-source, all codes publicly available
- Portability across platforms
  - NISP user interface is ***not*** portable, but MCLIB and MC_Run are
- Documentation
  - *http://PASeeger.com*, “NISP_Documents” *or* “Document Menu”
- *Some* thinking *required!*

Needed Improvements in NISP

- Portable User Interface
- Benchmarks
- Make it easier to add algorithms and beamline elements
- More algorithms for polarized neutrons and devices
- File outputs in NEXUS format
- Institutional support *and* user support
- *You* tell *us*: PASeeger@losalamos.com, lld@lanl.gov

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Help NISP grow!

All Contributions Gratefully Accepted

PASeeger@losalamos.com (please include “NISP” in subject)

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