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Single Crystal Time-of-Flight Neutron Diffraction Data at the IPNS

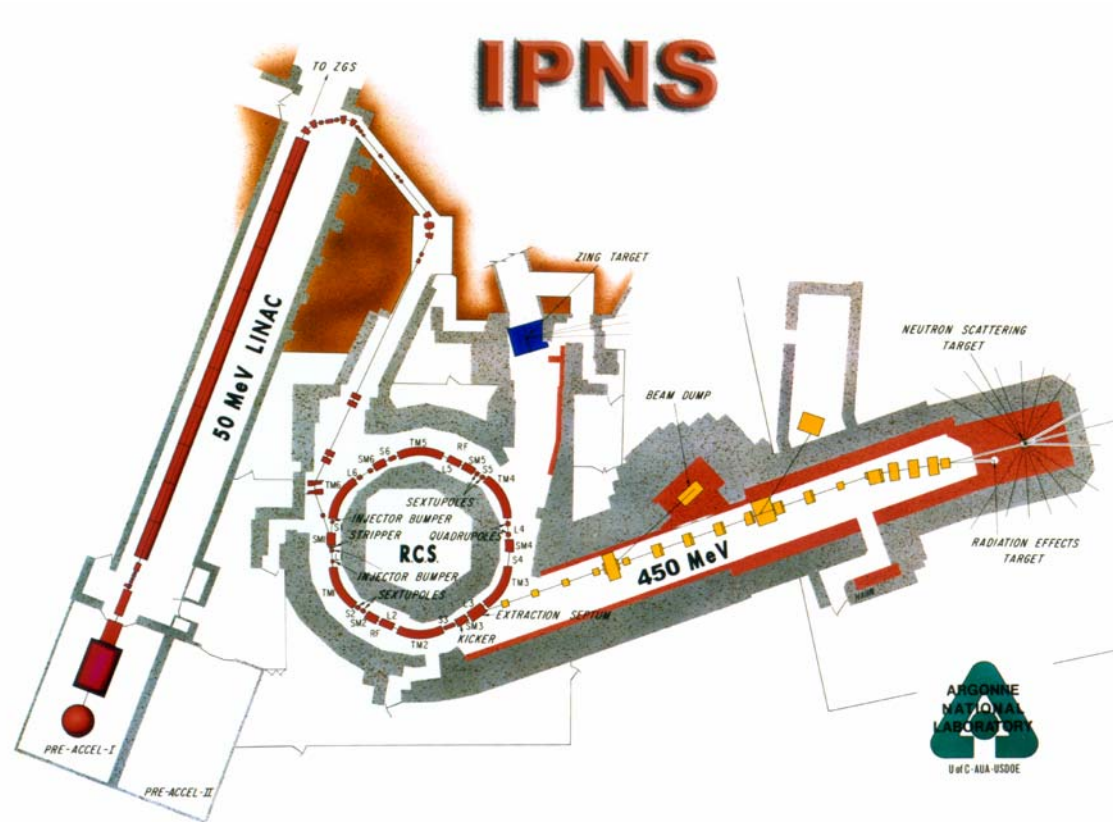
Arthur J. Schultz

Intense Pulsed Neutron Source

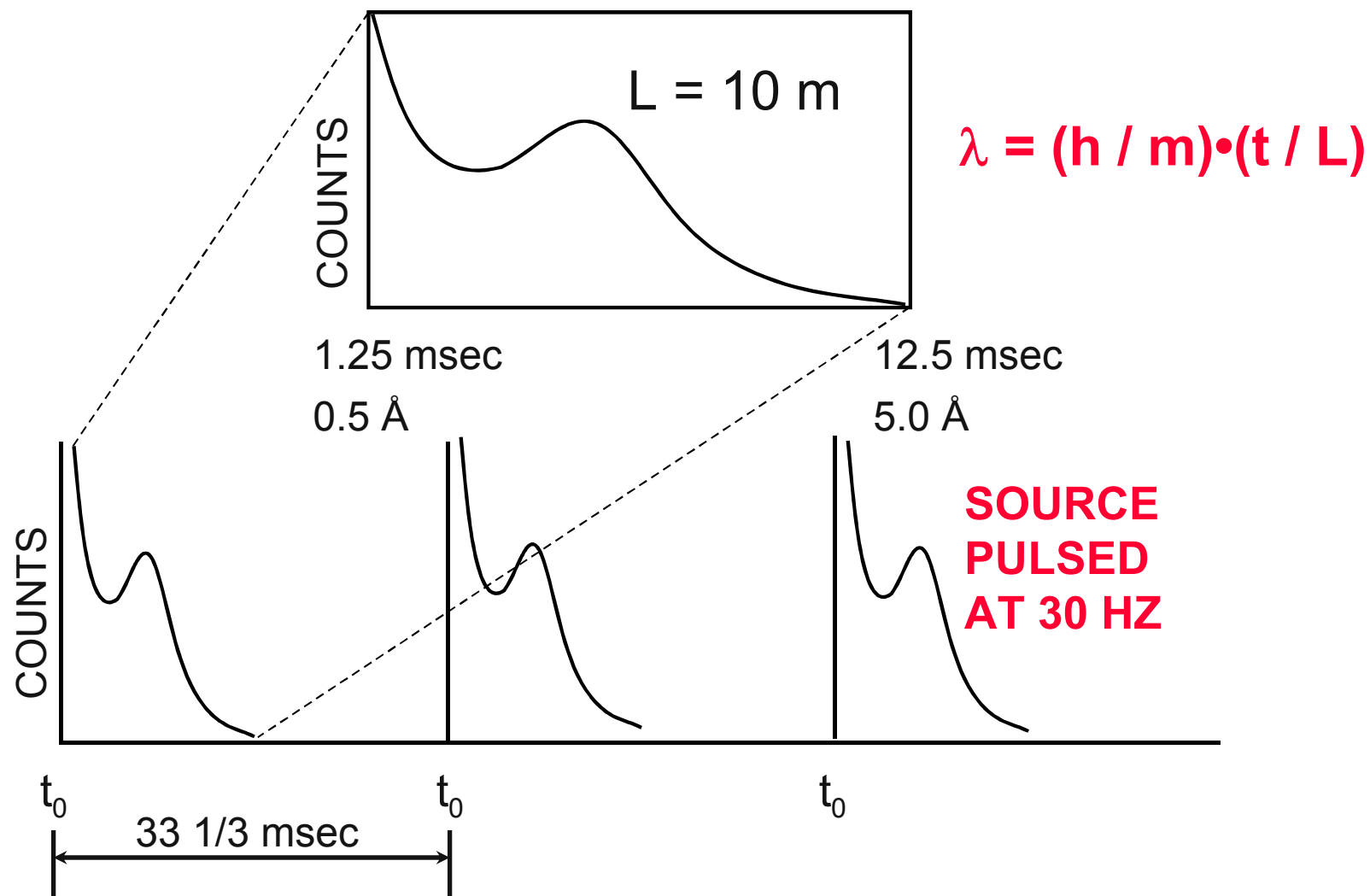
Argonne National Laboratory

Crystallographic Data Management Workshop, April 26-28, 2007, Bloomington, IN

Intense Pulsed Neutron Source

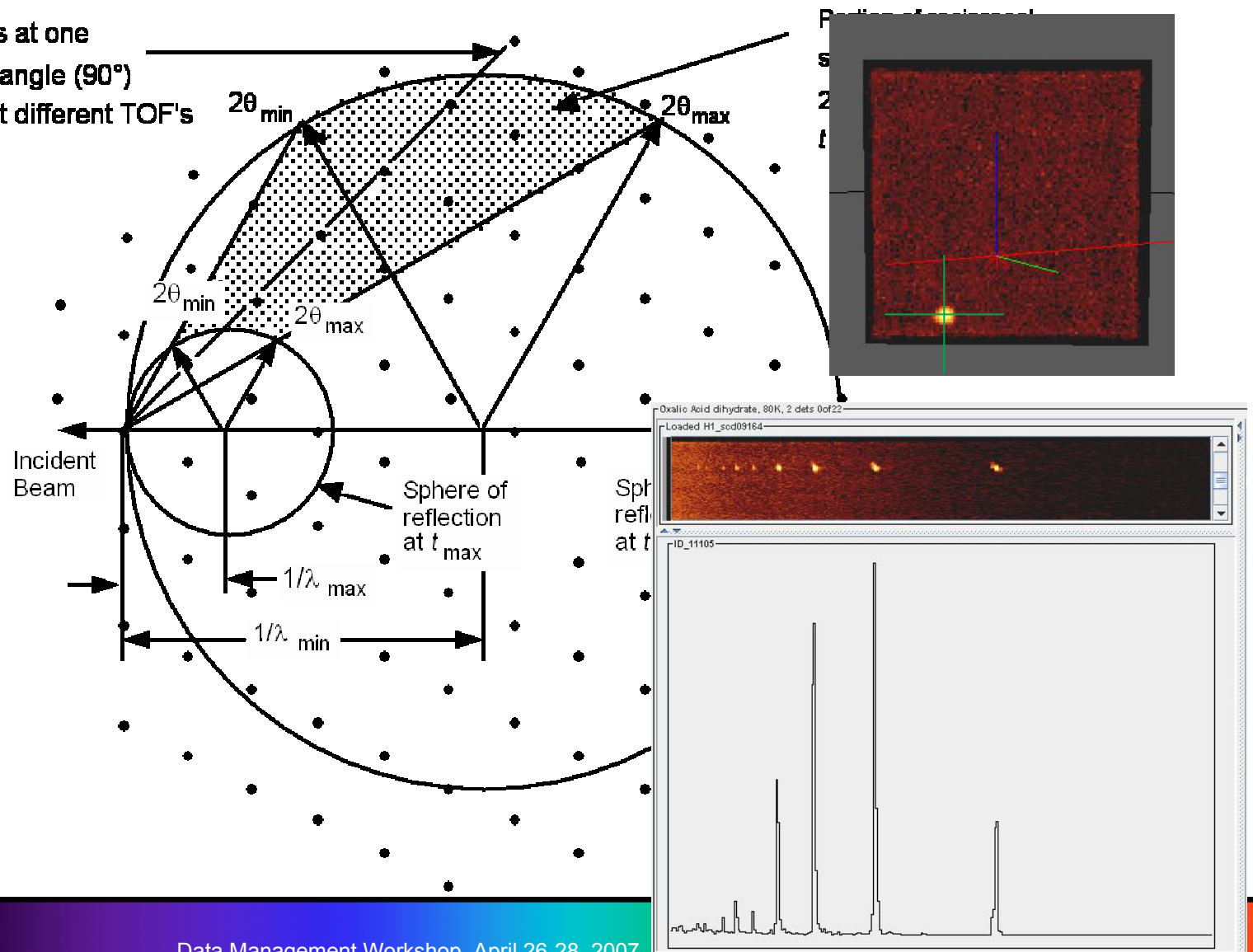


Pulsed Neutron Incident Spectrum



Time-of-Flight Laue Technique

Reflections at one scattering angle (90°) resolved at different TOF's



Single Crystal Diffractometers at Pulsed Spallation Neutron Sources

Utilize time-of-flight Laue technique.

Small Molecule Diffractometers

Existing:

- IPNS SCD (ANL)
- ISIS SXD (RAL, UK)

Future:

- SNS Topaz (ORNL)

Macromolecular Diffractometers

Existing:

- LANSCE PCS (LANL)

Future:

- J-PARC BIX-P1 (Japan)
- SNS MaNDi (ORNL)
- ISIS LMX (RAL, UK)

SCD Instrument Parameters

Moderator	liq. methane at 105
Source frequency	30 Hz
Sample-to-moderator dist.	940 cm
Number of detectors	2
Detector active area	155 x 155 mm ²
Scintillator	GS20 ⁶ Li glass
Scintillator thickness	2 mm
Efficiency @ 1 Å	0.86
Typical detector channels	100 x 100
Resolution	1.75 mm
Detector 1:	
angle	75°
sample-to-detector dist.	23 cm
Detector 2:	
angle	120°
sample-to-detector dist.	18 cm
Typical TOF range	1–25 ms
wavelength range	0.4–10 Å
d-spacing range	~0.3–8 Å
TOF resolution, $\Delta t/t$	0.01

Sample Environments

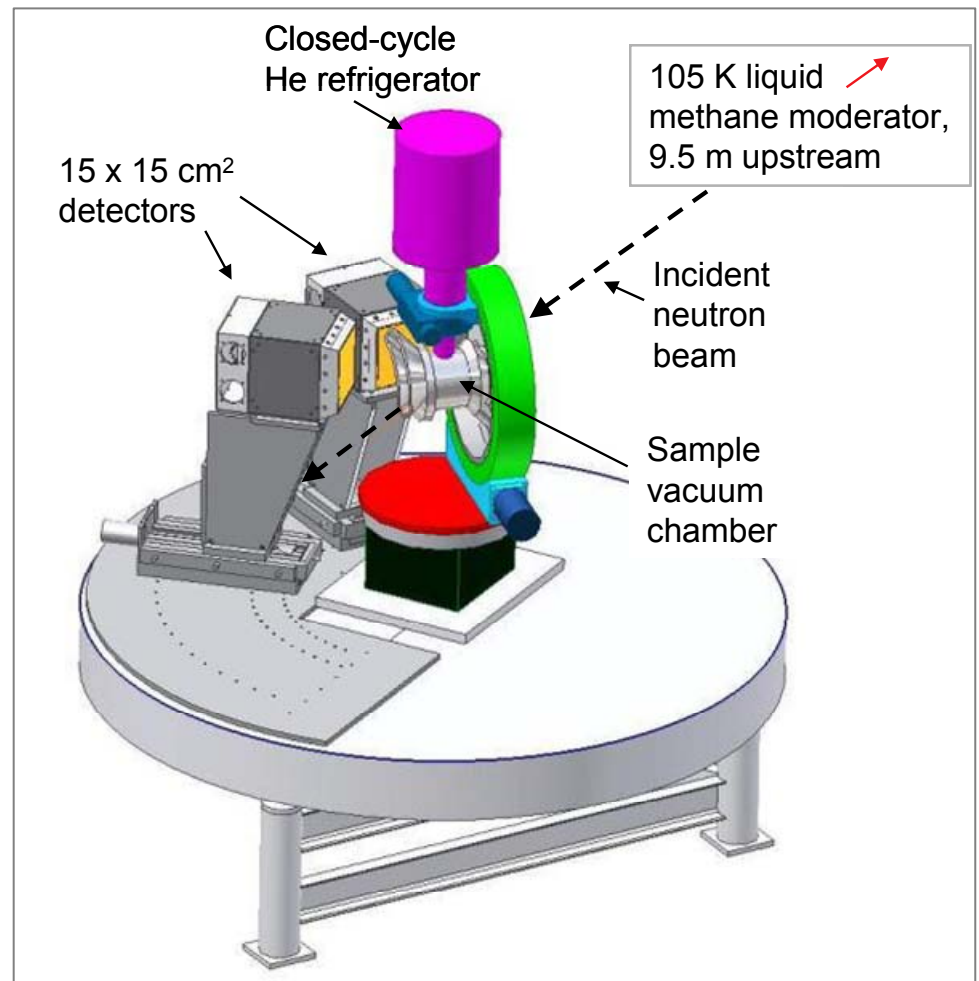
Hot-Stage Displex: 4-900 K

Displex Closed Cycle Helium Refrigerator:
12–473 K

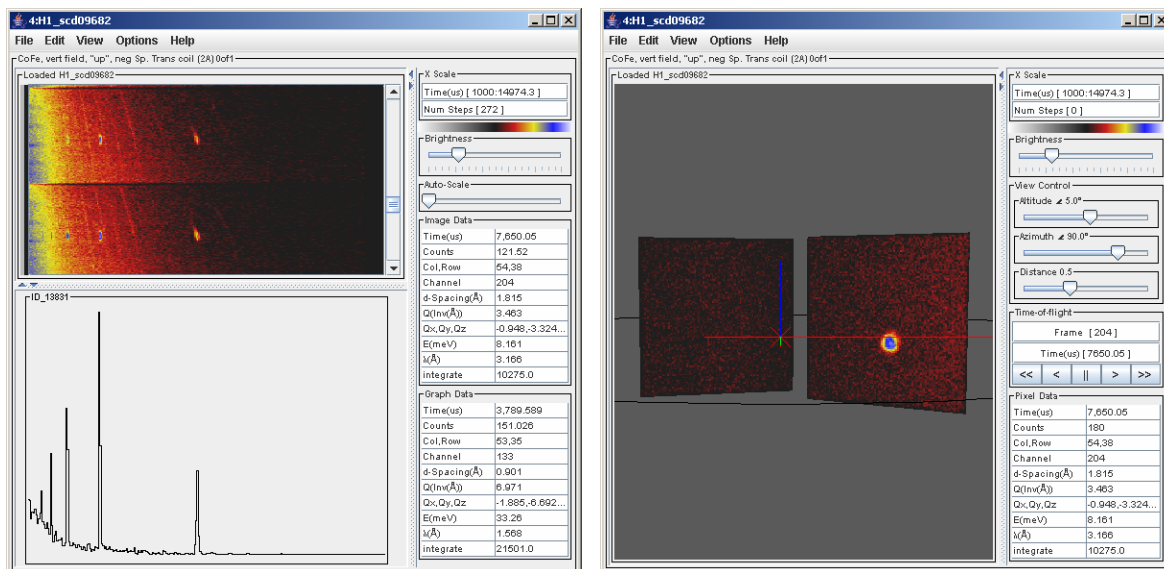
Furnaces: 300–1000 K

Helium Pressure Cell Mounted on Displex:
0–5 kbar @ 4–300 K

Detector distances on locus of constant solid angle in reciprocal space.



Raw Data



Detector size	15 x 15 cm²
Detector channels	100 x 100
Channel width	1.5 mm
Time-of-flight range	1 to 25 ms
Wavelength range	0.4 – 10 Å
TOF channel widths	constant $\Delta t/t = 0.01$

- Number of detector x,y channels = 100 x 100
- Number of tof channels = 322
- Total number of voxels per detector = 3.2M
- Histogram size = 3.2M x 2 detectors x 4 bytes = 26Mb
- Total for hemisphere of data = 22 settings x 26Mb = 572Mb

Data Archival and Retrieval at IPNS

Data Backup:

- At the end of each run, the run file is copied to a server on the Linux cluster.
- A database of information in the header is updated.

Data Retrieval:

- <http://www.pns.anl.gov/>
- Click on Controls and Computing → Get Run File Data → SCD0

Or

- Click on Controls and Computing → ISAW → Database Search

Or

- Click on Instruments → SCD → Software and Procedures → Database Search Tool

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- Tom Worlton
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 - backup and database manager
- Alok Chatterjee
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