1. Background

In May 1993, Argonne convened a Workshop on Technology and Science at a High-Power Pulsed Spallation Source, attended by more than sixty scientists active in the field. Gabriel Aeppli and Bruce Brown chaired the Workshop. The basis of these considerations was the IPNS Upgrade design, which for the present purposes must be considered as a "worked example" no longer in the running for consideration as a funded construction project. The community's attention and hopes now rest with the National Spallation Neutron Source project, design of which is being funded by the US Department of Energy. Earlier, the Kohn Panel convened by the Basic Energy Sciences Advisory Committee of the Department of Energy, had emphasized the need for new neutron facilities in the U.S. as, more generally, has a symposium sponsored by the Megascience Forum of the Organization for Economic Cooperation and Development.

The Summary of the Workshop Proceedings, quoted below, describes the background for the considerations of the Workshop and for the efforts at pulsed source development:

"Neutrons have played an essential role in engineering and science, first in nuclear physics and more recently in experiments revealing the structure of solids and liquids. For example, neutron results form a large and important part of the empirical basis for solid state science, which underlies much of modern technology. Currently, neutrons are playing a similar role in polymer science and are beginning to make an impact on biology and mechanical engineering. However, even as neutrons are finding vital applications in virtually all fields of science and engineering, U.S. neutron facilities have ceased to lead the world in source strength and instrumentation.

"This [Workshop] report documents the urgency of constructing a pulsed spallation neutron source (PSS) with a beam power of 1 MW or more, describing the many new opportunities such a source presents for science and technology. The authors are 63 scientists from industry, federal laboratories, and academia. Many are young corporate researchers and university faculty whose output will depend strongly on the new source. The authors met at Argonne National Laboratory for four days in May 1993 and divided into groups to write about the following fields:

- Surface and Interfaces
- Engineering
- Materials Science
- Polymers and Complex Fluids
- Chemistry
- Structural Biology
- Nuclear Engineering and Radiation Effects
- Condensed Matter Physics
- Fundamental Physics

"Each group identified the key problems in its field and evaluated the impact that neutrons could have in resolving these problems. The groups confirmed that neutrons are an essential tool in all the areas assessed. Further, they recognized a wide variety of important new capabilities, which do not exist in the U.S. today, that could only be provided at a pulsed source with a 1 MW minimum beam power.

"Most uses of a 1 MW spallation source discussed in this volume involve neutron scattering; however, the working groups identified significant applications of the facility for muon research, for studies of radiation damage, and for neutron nuclear physics. Many of the opportunities described here are unique to the PSS, either because of the neutron energy spectrum that is characteristic of pulsed neutron sources or because of the time structure of the neutron beams.

"Technological applications of neutron scattering loom large in the lists of uses assembled by the discussion groups. Because of their penetrating power, ability to image light elements, and sensitivity to magnetism, we envision that neutrons will become a routine analytical tool for industry. The pulsed nature and wide dynamic range..."
of neutrons at a 1 MW PSS will provide unique analytical capabilities needed to make advances in areas such as:

- Biologically Active Molecules for pharmaceuticals
- High-Temperature Superconductors for electric transmission lines
- Hard Magnets for electric motors
- Fast-ion conductors for battery components
- Amorphous solids for optical and solar devices
- Polymers for adhesive films
- Complex fluids for chemical separations and environmental restoration
- Catalysts for industrial processes
- Engineering Components under stress

"This list demonstrates and the full report extensively documents that a 1 MW pulsed neutron source is essential for progress on a very broad range of important scientific and engineering problems. Until recently, the U. S. led in the production and exploitation of pulsed neutron sources. In view of their great scientific and technical importance of these facilities, it is imperative that we recapture this leadership role. Rapid construction of a 1 MW PSS will recover this leadership and reap its technological and scientific payoff."

In the year following the Workshop, an event took place which further attests to the importance of neutron methods in scientific applications. The Royal Swedish Academy of Sciences awarded the 1994 Nobel Prize in Physics to Clifford Shull and Bertram Brockhouse for their pioneering accomplishments in neutron diffraction and inelastic scattering. Not only does this award honor the achievements of these long-revered scientists, but it recognizes the broad significance of the developments that their works made possible and emphasizes the significance of neutron beam research done since and envisioned for the future.

2. IPNS Upgrade: A Worked Example of a High Power Pulsed Spallation Neutron Source

The basis of considerations of scientific applications by the participants in the Workshop was the IPNS Upgrade design and its proposed suite of instruments. Bruce Brown oversaw the overall effort. Yanglai Cho led the accelerator design activities, carried out by a team of Argonne accelerator engineers, and organized the cost summaries. R. Kent Crawford led the instrumentation work within that project with input from Argonne neutron scientists, while J. Carpenter led the target design efforts, done by an Argonne engineering team. The work was carried out under Laboratory sponsorship in response to Kohn Panel recommendations and extended over a period of about four years. The facility was to have fitted into existing Argonne buildings and infrastructure. It represents a documented study of one example of a source configuration; as such, a step in the advancement of the field.

A rapid cycling synchrotron accelerator fed by a medium energy proton linac drives the source. Table 1 summarizes the major parameters of the IPNS Upgrade accelerator system.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection energy (from linac)</td>
<td>400 MeV</td>
</tr>
<tr>
<td>Extraction energy (from synchrotron)</td>
<td>2. GeV</td>
</tr>
<tr>
<td>Time average current</td>
<td>0.5 mA</td>
</tr>
<tr>
<td>Time average beam power</td>
<td>1 MW</td>
</tr>
<tr>
<td>Pulse repetition rate</td>
<td>30 Hz</td>
</tr>
<tr>
<td>Number of extracted bunches per cycle</td>
<td>1</td>
</tr>
<tr>
<td>Extracted pulse length</td>
<td>0.5 μsec</td>
</tr>
</tbody>
</table>

Figure 1 illustrates the layout of the IPNS Upgrade. There are two target stations, one operating at 10 Hz, the other capable of accepting the full 30 Hz beam but normally operating with 2/3 of the pulses. Targets are water-cooled tungsten alloy plates. Each supports six differently optimized moderators chosen appropriately for the scattering instruments. Figure 2 shows a target station (they are basically identical) in more detail. Each provides eighteen beam holes, all provided with gates that enable hands-on work in the sample position of the instrument without requiring interruption of source operation. A servicing cell attached downstream from each target provides for replacement and repair of target and moderator components, which move horizontally together into the cell.
Figure 1. Plan view of the IPNS Upgrade

Figure 2. IPNS Upgrade target station (typical of two).
Table 2 summarizes the spectral parameters of the several types of IPNS moderators, including ambient temperature water, liquid methane, and liquid hydrogen. These are variously poisoned (a sheet of low energy absorber, e.g. cadmium, placed at some depth below the viewed surface) to optimize the pulse characteristics, neutronically coupled to the reflector, or decoupled (by a layer of absorber, for example, cadmium or boron, to prevent long-lived neutrons from the reflector from broadening the pulse). The parameters refer to a time-average spectral function approximately describing the flux in the neutron beams, which is of the form

\[ \phi(E) = \frac{\varphi_{Th} E}{(E_T)^2} \exp\left(\frac{E}{E_T}\right) + \varphi_{epi} \frac{\Delta(E)}{E}, \]

in which \( \phi(E) \) is the flux per unit energy \( E \) and \( E_T \) is the energy corresponding to the spectral temperature. \( \varphi_{Th} \) is the total thermal flux and \( \varphi_{epi} \) is the epithermal flux (constants). \( \Delta(E) \) is a smoothly varying "joining function" which approaches zero for low energies and unity for high energies, for which there are useful representations.

Table 2. Characteristics of IPNS Upgrade moderators

<table>
<thead>
<tr>
<th>Moderator Type</th>
<th>( E_T ), meV</th>
<th>( \varphi_{Th} / \varphi_{epi} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisoned, decoupled, 320 K liquid water</td>
<td>32.</td>
<td>2.3</td>
</tr>
<tr>
<td>Poisoned, decoupled, 95 K liquid methane</td>
<td>11.</td>
<td>2.1</td>
</tr>
<tr>
<td>Decoupled, 18 K liquid hydrogen</td>
<td>3.0</td>
<td>2.4</td>
</tr>
<tr>
<td>Coupled, 320 K liquid water</td>
<td>32.</td>
<td>22.</td>
</tr>
<tr>
<td>Coupled, 18 K liquid hydrogen</td>
<td>2.8</td>
<td>12.</td>
</tr>
</tbody>
</table>

In the absence of neutron guides, which can be incorporated, fluxes vary as the inverse square of the distance from the moderator. Monte Carlo calculations provide absolute values of the fluxes. Wavelength-dependent pulse shapes are known for all these and other moderator choices, based on measurements and calculations.

Figure 3 shows the target train assembly of the IPNS Upgrade, which carries the target, the moderators, the reflector, and a massive shield block, which all move together, and their method of assembly and disassembly.

Figure 3. The IPNS Upgrade target train, showing target, moderators, reflector, shield block and irradiation tubes.
2. Instruments

Early in the process of facility design, scientists conceived a suite of instruments that would provide a useful and desirable range of capabilities, yet be feasible to construct. The facility design reflects the requirements of these instruments. Of particular importance is the need for a station with pulses at low frequency and for a variety of differently optimized moderators. Tables 3 and 4 list the salient parameters of the instruments. Such a suite of instruments almost certainly would not be built, although they could be. These represent the proof of an existence theorem to the effect that an efficient complement of instruments exists and can be accommodated. And the lists provide the basis for a rational cost estimate. Finally, instruments in such a list would be improved, the list culled and extended in response to scientific needs and technical possibilities.

These lists, with some elaborations, were the basis for considerations of the Workshop on applications of a 1 MW pulsed spallation source in science and technology.

Table 3. Parameters of the instruments for the 30 Hz target of the IPNS Upgrade

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Purpose</th>
<th>Flight Path Lengths L_1 (m)</th>
<th>L_2 (m)</th>
<th>Moderator</th>
</tr>
</thead>
<tbody>
<tr>
<td>SEPD</td>
<td>Powder Diffraction, Low Resolution</td>
<td>12</td>
<td>1.5</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>GPPD</td>
<td>Powder Diffraction, Modest Resolution</td>
<td>25</td>
<td>1.5,4</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>HRDP</td>
<td>Powder Diffraction, High Resolution</td>
<td>50</td>
<td>2</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>RSD</td>
<td>Residual Stress Diffraction</td>
<td>25</td>
<td>1.5,3</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>VSPD</td>
<td>Very Small Sample Diffraction</td>
<td>12</td>
<td>0.75</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>GLAD</td>
<td>Glass and Liquid Diffraction</td>
<td>23.5^b</td>
<td>1.5</td>
<td>CH_4</td>
</tr>
<tr>
<td>SCD</td>
<td>Single Crystal Diffraction</td>
<td>10</td>
<td>0.6</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>HQSCD</td>
<td>High Q, High Resolution Single Crystal Diffraction</td>
<td>30</td>
<td>0.7</td>
<td>CH_4^a</td>
</tr>
<tr>
<td>HRMECS</td>
<td>High Resolution Chopper</td>
<td>18</td>
<td>4</td>
<td>CH_4</td>
</tr>
<tr>
<td>LRMECS</td>
<td>Low Resolution Chopper</td>
<td>12</td>
<td>2.5</td>
<td>CH_4</td>
</tr>
<tr>
<td>SCCS</td>
<td>Single Crystal Excitations</td>
<td>16</td>
<td>4</td>
<td>H_2O</td>
</tr>
<tr>
<td>QENS</td>
<td>Modest Resolution Quasielastic Scattering</td>
<td>9</td>
<td>1</td>
<td>CH_4^c</td>
</tr>
<tr>
<td>TFCA</td>
<td>Chemical Excitation Spectrometry</td>
<td>16</td>
<td>1.5</td>
<td>CH_4</td>
</tr>
<tr>
<td>QSTAXC</td>
<td>Quasi-Steady Cold Neutron Triple Axis Spectrometry</td>
<td>17</td>
<td>2</td>
<td>C-H_2</td>
</tr>
<tr>
<td>MICAS</td>
<td>Multi-Analyzer Coherent Excitations Spectrometry</td>
<td>12</td>
<td>1.5</td>
<td>CH_4</td>
</tr>
</tbody>
</table>

^a Could be H_2O.

^b To low-resolution sample position.

^c Could be poisoned H_2.

C- → Coupled moderator, otherwise, decoupled.
Table 4. Parameters of the instruments for the 10 Hz target of the IPNS Upgrade

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Purpose</th>
<th>Flight Path Lengths L₁ (m)</th>
<th>L₂ (m)</th>
<th>Moderator</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAND</td>
<td>Small Angle Scattering</td>
<td>12</td>
<td>2</td>
<td>C-H₂</td>
</tr>
<tr>
<td>HRSAND</td>
<td>High Resolution Small Angle Diffraction</td>
<td>20</td>
<td>5</td>
<td>C-H₂</td>
</tr>
<tr>
<td>SPSAND</td>
<td>Special Purpose Small Angle Diffraction</td>
<td>40</td>
<td>-</td>
<td>C-H₂</td>
</tr>
<tr>
<td>POSY-I</td>
<td>Polarized Beam Reflectometry</td>
<td>18</td>
<td>2</td>
<td>H₂</td>
</tr>
<tr>
<td>HIREF</td>
<td>High Intensity Reflectometry</td>
<td>18</td>
<td>2</td>
<td>H₂</td>
</tr>
<tr>
<td>POSY-II</td>
<td>Unpolarized Beam Reflectometry</td>
<td>18</td>
<td>2</td>
<td>H₂</td>
</tr>
<tr>
<td>GREF</td>
<td>Reflectometer for Grazing Incidence</td>
<td>18</td>
<td>5</td>
<td>H₂</td>
</tr>
<tr>
<td>CNCS</td>
<td>Cold Neutron Chopper Spectrometry</td>
<td>20</td>
<td>4</td>
<td>H₂</td>
</tr>
<tr>
<td>HRBS</td>
<td>High Resolution Backscattering</td>
<td>30</td>
<td>3</td>
<td>H₂</td>
</tr>
<tr>
<td>TOFNSE</td>
<td>Time-of-Flight Spin Echo Spectrometry</td>
<td>16</td>
<td>4</td>
<td>C-H₂</td>
</tr>
</tbody>
</table>

3. Some General Observations: Operational requirements of a facility for applications in condensed matter studies

While installations of the scale dealt with here are large and costly, they are

° LARGEST FACILITIES IN SERVICE TO SMALL SCIENCE.

Rather than serving a few, long-standing programs based on expensive instruments, or "detectors," staffed by large groups, facilities must provide for

° > 10³ EXPERIMENTS PER YEAR.

The following represent the results of experience:

° TYPICAL EXPERIMENT INVOLVES A SMALL TEAM, 1-3 SCIENTISTS

RUNS ARE OF MINUTES'-TO-HOURS' DURATION IN-AND-OUT IN ONE DAY OR A FEW DAYS

REQUIRES FACILITY'S SCIENTIFIC AND TECHNICAL SUPPORT

° INSTRUMENTS ARE VERY GENERAL, LIFE = 10 YEARS

° ACCESSIBILITY REQUIRED:

  > 9 MONTHS/YEAR, 24 HOURS/DAY

° RELIABILITY REQUIRED:

  > 90 %

4. Applications of a 1 MW pulsed spallation source in science and technology

Workshop participants produced nine chapters of commentary on applications and required instrumentation. Envisioned future opportunities revolve around the following themes:

° Extensive use of polarized neutrons

° Wide use of isotope substitution

° Small samples

° High resolution

° Real time measurements

Organized in categories according to instruments, some of the general comments and applications discussed are:

REFLECTOMETERS

Surface Characterization 5Å - 5000 Å, 5Å resolution

Magnetization, chemical composition (H/D, general isotope substitution)

APPLICATIONS

Oxidation, corrosion, etching in situ

Multilayer thin films; polymers, giant magnetoresistance, real time growth monitoring

Electrochemical interfaces in situ, H diffusion,

Surface freezing, melting, wetting

Polymer interdiffusion, adsorption

Adhesion, lubrication

Flux line lattices in superconductors
LARGE ANGLE DIFFRACTOMETERS
Excellent Q resolution, $\Delta d/d < 10^{-4}$
Great Q range, angle coverage
Fixed geometry
Polarized beams, polarization analysis
General isotope substitution
APPLICATIONS
Strains: nondestructive, depth studies,
- complete strain tensor determination,
  $1 \text{mm}^2$ fiducial volumes; welds, castings,
  composite materials by constituent;
- New window on engineering materials analysis
Live time, in situ, chemical reactions, annealing
Phases to $< 0.1\%$ at temperatures to $1800 \degree C$
and pressures to $100 \text{kbar}$ in minutes
Simultaneous strain/texture/phase determination
Stroboscopic structure measurements with time resolution $\sim 10 \mu \text{sec}$
Small samples $< 1 \text{mg}$.
Batteries, fuel cells, solid electrolytes, fast ion conductors; H, etc. locations,
charge/discharge in situ
Liquids, glasses; intermediate-range 
(10Å - 30 Å) structure
Ionic configurations in solution [e. g. Ni(H$_2$O)$_6$]
Pressure, field, temperature derivatives: higher-order interatomic correlations

SMALL ANGLE SCATTERING
Delicate H/D substitutions
Small, dilute samples
Special environments
EXAMPLES
Complex fluids in porous media (e. g. oil in rock)
Surfactants and microemulsions (lubrication,
drug delivery, protein crystallization)
Polymer processing variables (quenching,
  shearing, rapid depressurization)

SINGLE CRYSTAL DIFFRACTOMETERS
Isotope substitution
High pressures, other extreme environments
Polarized beams
Larger unit cells, smaller samples
EXAMPLES
The greatest challenge in neutron single crystal structure studies is to determine the hydrogen locations in large biological molecules, especially proteins. It is not a given that even the highest intensity pulsed neutron sources will open these opportunities widely. Combining high resolution X-ray-determined structures (H information missing) with lower-resolution neutron diffraction results will open them significantly.
Modest sized crystals, modest sized proteins at high spatial resolution
Verification of fundamental interatomic interactions (theoretical chemistry database)

SPECTROSCOPY
Non crystalline materials; glasses, liquids
High frequency magnetic excitations
Coherent excitations in low dimensional materials
High resolution, low frequency ($\mu \text{eV}$) excitations

5. Illustrations of instruments
Below are diagrams of a number of instruments, some of which are in operation, some of which are concepts developed for the IPNS Upgrade design, and some of which are concepts developed by Workshop participants. Names refer to Tables 3 and 4.
5.1 Reflectometers

Figure 4. Posy-I and Posy-II reflectometers which operate at IPNS.

Figure 5. Concept of a multi-beam reflectometer, HIREF in Table 4.

Figure 6. Arrangement for grazing-incidence surface diffraction, GREF in Table 4.
5.2 Wide angle diffractometers

Figure 7. Diffractometer with high resolution 90° arms for stress and special-environment studies, GPPD in Table 3.

Figure 8. Concept for a high resolution diffractometer, HRPD in Table 3.

Figure 9. Concept for a diffractometer for residual stress studies, RSD in Table 3.
5.3 Small Angle Diffractometers

Figure 10. The SAND small angle diffractometer at IPNS, see Table 4.

5.4 Single Crystal Diffractometer

Figure 12. Single Crystal Diffractometer, SCD, at IPNS, represented in Table 3. The number of area detectors could be increased by a factor of five. At some sacrifice in resolution for specific purposes, a funnel could increase the number of neutrons on sample.
5.5 Spectrometers for inelastic scattering studies

Figure 13 The LRMECS chopper spectrometer at IPNS. See Table 3.

Figure 14. The HRMECS chopper spectrometer at IPNS, shown modified by addition of an extended low-angle scattered neutron flight path. See Table 3.

Figure 15. Schematic illustration of the Single Crystal Excitations Chopper Spectrometer, SCCS in Table 3. The concept is similar to that of the Multi Angle Position-Sensitive Spectrometer, MAPS, under construction at the ISIS pulsed spallation source in UK.
Section A–A

Figure 16. Layout of a High Resolution Backscattering Spectrometer, HRBS, similar in concept to the IRIS spectrometer at ISIS.

Figure 17. Concept of the MICAS, Multiple Independent Crystal Analyzer Spectrometer.

Figure 18. Time-Focused Crystal Analyzer Spectrometer, TFCA. Examples of these very simple, high intensity instruments are operating at KENS, ISIS, and IPNS.
This list of instruments and their schematic descriptions is only representative of possibilities. As time goes on, new ideas can be expected to arise, and refinements on these basic ones will be identified. New components are expected to be developed as conceived instruments demand them and new instruments are expected to evolve which exploit independent component developments. Adaptations of steady source instruments may find their place at pulsed sources. In special instances, because the time-average source flux in the more ambitious next-generation pulsed sources may approach what is available in steady sources today, replicas of steady source instruments may be installed in pulsed beams, with similar time-average intensities but capitalizing on pulsed beam characteristics.

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References

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