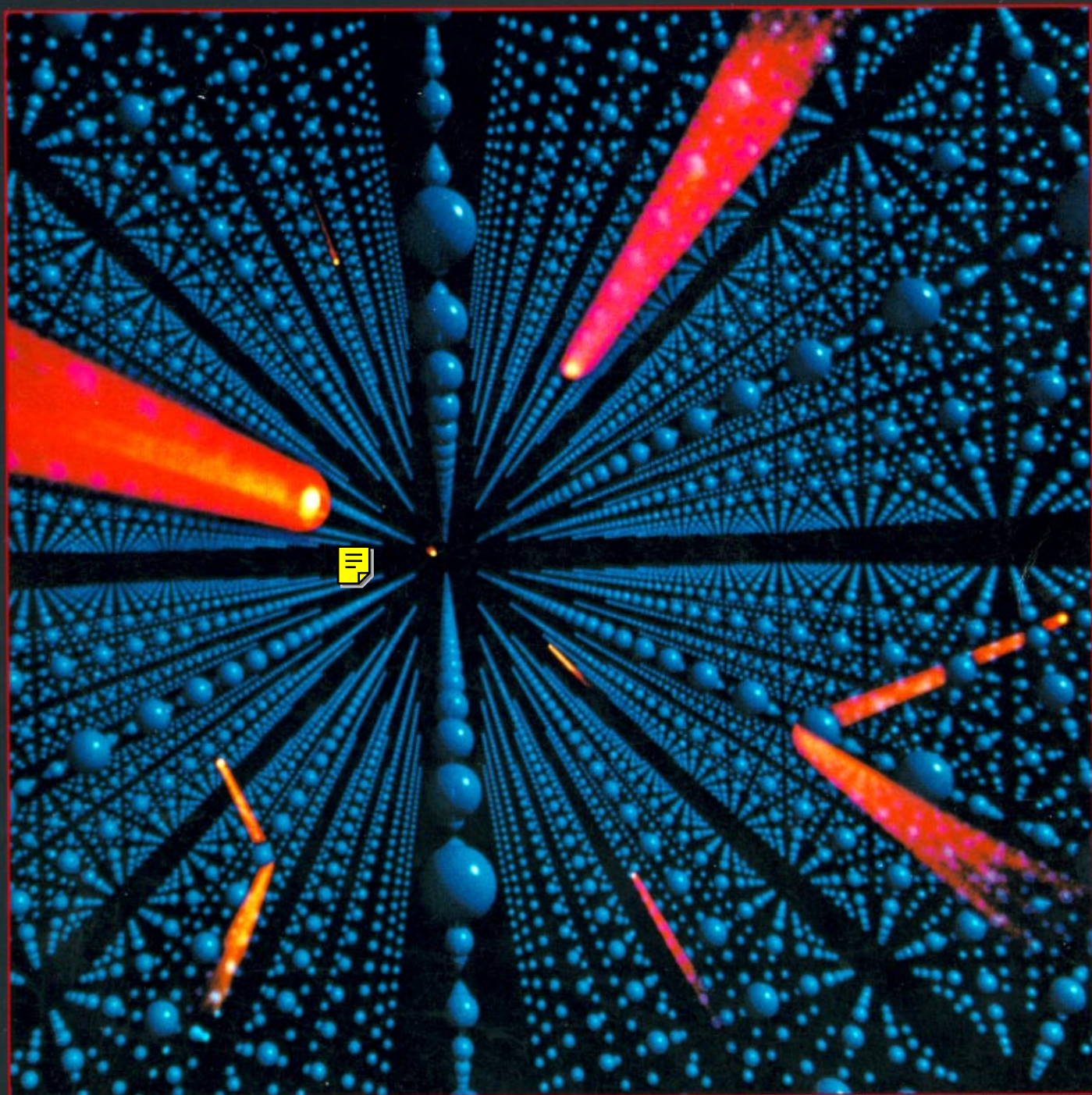
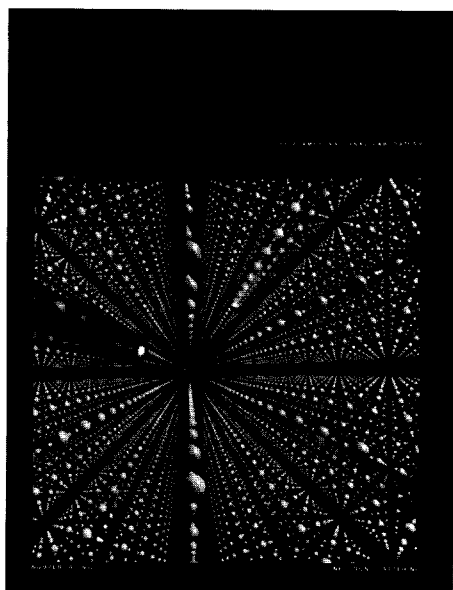


# Los Alamos Science

LOS ALAMOS NATIONAL LABORATORY





Artist's conception of neutrons flying through matter. Low-energy neutrons (red) scatter to new trajectories by interacting with the atomic nuclei (blue). Since the nuclei are small, the neutrons see mostly empty space and scattering are rare. Cynthia L. Boone created the computer art using Alias software. The 14,000 nuclei were generated by 50 translations of an original lattice plane.

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## Part 1. Introduction to Neutron Scattering

### Neutron Scattering—A Primer . . . . . 1

*by Roger Pynn*

Neutrons are a little-known but remarkably powerful probe of condensed matter on length scales ranging from interatomic distances to a few thousand angstroms. This article explores the physics of various neutron-scattering processes, introduces the experimental techniques and instruments that make neutron scattering so versatile, and discusses the single equation that unifies the interpretation of neutron-scattering data.

Mathematical Foundations of Neutron Scattering

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The director of the Los Alamos neutron-scattering facility discusses the history of the field, its successes around the world, its present problems in the United States, and the plans for opening it to a wide spectrum of users from academia and industry.

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*by Dianne K. Hyer and Roger Pynn*

The accelerator neutron source at the Los Alamos neutron-scattering center is proving at least as effective as traditional reactor sources. This article traces neutrons from their “birth” in the spallation target through beam-tailoring devices and scattering samples to their “death” in neutron detectors. Electronic measurements of times of flight and scattering angles are also discussed, as well as the mechanics of the user program at LANSCE.

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Small-angle neutron-scattering experiments provide evidence that calmodulin, a protein that mediates calcium regulation of biological processes, is flexible in solution. Such experiments also clearly show that calmodulin closes around one of its target enzymes as it stimulates that enzyme’s catalytic function.

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**Neutrons, Sludge Physics, and the Liberty Bell . . . . . 90**

*by Roger Pynn*

The precursors of many advanced materials are disordered systems such as colloidal suspensions and polymeric chains—sludge by another name. Neutron scattering can detect subtle structures beneath the disorder that give advanced materials their extraordinary combinations of strength, elasticity, and low density. By penetrating deep into metal and ceramic components, neutrons also make possible the nondestructive measurement of residual strains.

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Catalyzing chemical reactions with metal atoms remains a mysterious art. But recent neutron-scattering experiments on model systems are revealing the molecular mechanisms of catalytic activity in astonishing detail, including how metal atoms loosen the bonds of hydrogen molecules, an essential first step in hydrogenation reactions.

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*by Richard N. Silver*

Since 1938, theorists have attributed the unusual properties of superfluid helium-4 to the presence of a Bose condensate, an exotic state of matter in which all the condensed helium atoms have exactly zero momentum. Although the Bose condensate cannot be observed directly, an interpretation of neutron-scattering data according to a new first-principles theory of final-state effects has at last confirmed its existence.

How Final-State Effects Were *Really* Calculated

**Bayesian Inductive Inference, Maximum Entropy, and Neutron Scattering 180**

*by Devinderjit Singh Sivia*

With its roots in Bayesian logic, the maximum entropy method of data analysis avoids the “cookbook” approach to statistics. By treating all unknowns in a logically consistent manner, it yields the “best” interpretation of the data at hand. It has been applied successfully to neutron-scattering data and could even influence the design of neutron-scattering instruments.

**W**hat is neutron scattering? Why is it becoming more and more useful in both basic and applied science? And why are materials scientists, in particular, very worried about its future in the United States? At first glance the technique appears forbidding. You shine a large number of neutrons on a sample, but—because neutrons have no electric charge—only a very small fraction are scattered. Therefore generating measurable signals requires a great deal of ingenuity. Also, the neutrons are expensive to produce and are available at only a small number of specialized facilities. It seems like the last technique to choose—except that its results are so valuable. For many questions in condensed-matter physics, in biology, in chemistry, and in the study of modern synthetic materials, neutron scattering is the only technique that provides answers.

Unlike x-rays, neutrons “see” light and heavy elements equally well, interact with the magnetic moments of electrons, and detect atomic vibrations as well as average atomic positions. These properties make neutrons a unique and extremely versatile probe of material structure and dynamics. A look at the table of contents will convince you—measurements of the structure of high-temperature superconductors, of the Bose condensate in liquid helium, of the change in shape of the protein calmodulin as it mediates involuntary muscle contraction, of the catalytic effect of metal atoms on the dissociation of molecular hydrogen, of the fractal structures of precursors to today’s materials, of the layered structures of polymer films, of residual strains in metals and ceramics—and these diverse topics are a sampling of the work at only one facility. High-intensity neutron beams, high-resolution spectrometers, and computerized data acquisition and analysis systems are opening a wide range of phenomena to more precise study, especially in materials technology and other fields tied to economic growth.

Although the promise of neutron scattering is growing, its future in the United States is uncertain. At present, all but two neutron-scattering centers are located at aging nuclear reactors whose budgets are escalating every year to pay, not for research and upgrades, but for enhanced safety. Moreover, access to those facilities has not been easy in the past. Even now, few university scientists use the technique—many fewer than in Europe. But a change is in the works. In the early eighties a user program began at the Intense Pulsed Neutron Source at Argonne National Laboratory, and in 1987 the Los Alamos Neutron Scattering Center (LANSCE) officially opened its doors to users from academia and industry. (Both facilities house accelerator sources, which produce pulsed neutron beams by a nuclear reaction called spallation.) A cold-neutron research center is being built at the National Institute of Standards and Technology, and a spectrometer upgrade at the Brookhaven High-Flux Reactor is planned. The response to these initiatives has been gratifying. For example, more than 140 outside users mounted experiments at LANSCE last year—and this year’s participation is even greater. A technique that was practiced by a small community of professionals is now accessible to “amateurs” from industry and academia.

Experience at the Los Alamos facility is proving that data obtained at pulsed neutron sources can compete with data obtained at reactors. Five years ago when several new spallation sources were just coming on line, conventional wisdom said

that small-angle neutron scattering, which requires intense beams to measure the sizes and shapes of biological macromolecules and colloidal particles, could be done well only at reactors. Today small-angle experiments work as well at LANSCE as at the best reactor sources in the world, except for the very smallest angles. Powder-diffraction experiments here are also highly effective; for example, polycrystalline samples weighing less than 50 milligrams have yielded excellent data. And Los Alamos researchers are leading the way in using spallation sources for reflectometry, one of the newest applications of neutron scattering. These successes reflect the high neutron flux available here as well as the efficient utilization of that flux through innovative spectrometer design. LANSCE and other pulsed sources are demonstrating that they can more than fulfill their original promise.

With all its successes the Los Alamos source is not without problems. Beam availability during 1990 has so far been less than last year because of budget cuts, investment in environmental and safety precautions, and some accelerator problems. Also, though LANSCE generates a higher peak flux than any other spallation source, it has yet to achieve the design value. Nevertheless this year's users report they are getting better data in less time than they could elsewhere.

What of the future? Since neutron scattering is a signal-limited technique, progress depends on building higher-intensity neutron sources. The U.S. neutron-scattering community plans to build a state-of-the-art research reactor, the Advanced Neutron Source, which will deliver five times greater neutron fluxes than today's most powerful research reactors. The new reactor, still in the design stage, should begin operation around the turn of the century. Construction will cost about one billion dollars, and increasingly stringent safety regulations will make it very costly to run. The decision to build the advanced reactor was made several years ago, before spallation sources had proven their worth. We asked Roger Pynn, the director of LANSCE, whether in light of recent progress he thought the next-generation facility ought to be a spallation source. His answer: "If societal concerns should make it impractical to build and operate a research reactor, then an advanced spallation source could meet the needs of the community without raising as many safety and environmental issues. But, for a balanced program, the country needs sources of both types." Whatever happens in the long run, it is clear from the presentations in this issue that neutron scattering is a fertile and expanding field and that LANSCE is providing inspiration for the future in the areas of technical innovation, opportunities for young people, outreach to the larger scientific community, and tangible scientific results.

The editors thank all the authors and the numerous other scientists who contributed their thought and energy to the contents of this volume. It was a pleasure for us to learn about the technically difficult but thoroughly absorbing world of neutron scattering.

A handwritten signature in black ink, reading "Sheila Grant Cooper". The signature is written in a cursive, flowing style with a large initial 'S'.