ICANS-XIII
13th Meeting of the International Collaboration on
Advanced Neutron Sources
October 11-14, 1995
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

# COMPUTATIONAL METHODS

Philip Seeger, Loma del Escolar, Los Alamos 87545 NM, USA

The work reported in the session on "Computational Methods" ran the gamut from accelerator pulses through target calculations and instrument design to data acquisition and reduction. Such diversity, which is typical of ICANS, made the session very interesting. And with one paper being delayed for two days, this was certainly one of the longest sessions. This summary works backwards from the user toward the source.

W. Schmidt *et al.* reminded us that it not always appropriate - or even correct - to treat the resolution of an experiment just by combining standard deviations of the contributing terms and then applying the central-limit theorem. For one example, there may be very significant asymmetric terms such as moderator pulse response which must be treated in more detail. Another situation which is too often ignored is that there are correlations between the terms, *e.g.* angular divergence of the incident neutron beam is correlated with position of interaction in the sample, and the correlations may either increase *or decrease* the width of the resolution function. The solution is to convert all variables to a common coordinate system (the authors use sample coordinates) to unmask the correlations, and then to integrate the convolution of the terms. To make analytic integration easier, they expand all functions as sums of Gaussians or error functions in one or two dimensions. This level of approximation should be quite adequate for resolution calculations, but should be tested using Monte-Carlo integration of the actual distributions.

The paper of Yu. A. Astakhov *et al.*, presented by V. I. Prikhodko, discussed specifications of hardware and software for an upgrade of the Measurement and computational complex at the Frank Laboratory of Nuclear Physics. The present electronics are old and have little standardization. making maintenance difficult. They also anticipate a large increase in data rates as new instruments and new detectors come on-line. Their new generation of electronics involve the VME system and workstations integrated into their local computer network. Control and management of the apparatus will generally be through simple input/output registers from the VME processor. Individual detector systems will not be standardized to the same extent, but encoding and histogramming modules will be standard. To minimize dead time and to leave the VME bus free for other tasks, the accumulation of spectra occur directly in the memory module. Data formats and archiving, graphical user interfaces, and mathematical processing packages will also become standardized for all experiments at FNLP.

Two papers were concerned with the MCLIB library of Monte Carlo subroutines for instrument design. P. A. Seeger described the structures used in the library to define the geometry and various types of beam elements; types include moderator source functions, uniform materials, single-crystal filters, multilayer reflectors, monochromators, choppers, various scattering samples, detectors, *etc.* The written report includes complete subroutine descriptions, a sample problem, and a description of the process by which either experimental flux measurements or detailed moderator source calculations are included in the code. The library is now available to the public. In its present form the user is required to write a specific program to set up the geometry for each class of instrument. The second paper, by T. Thelliez *et al.* (presented by R. P. Hjelm), concerned the development of a graphical user interface (GUI) to overcome this difficulty. Early prototypes of the GUI can already reduce the time to implement certain instrument classes from days of programming to minutes of selecting options. It was noted that the GUI itself is appropriately written in an object-oriented language, but that the Monte Carlo code would remain in Fortran for speed of execution.

N. U. Sobolevsky presented the paper by A. V. Dementyev *et al.* on the universal Monte Carlo hadron transport SHIELD, which has evolved from HETC (High-Energy Transport Code), in particular extending it to energies up to (at least) 100 GeV. At such high energies the code depends on hadron-nucleus interaction models developed in Russia, and it gives an excellent fit to experimental data on neutron production from a Pb target (20-cm diameter, 60-cm length) between 0.5 GeV and 70 GeV. Computed heat deposition in Pb and U for 1-GeV protons is also in excellent agreement with calorimetric measurements. Radiation damage and isotope production may also be inferred from the code. The author concludes that although the specific neutron production (n/MW) falls off at proton energies above about 1.2 GeV (due to increasing pion production), engineering aspects of the energy deposition might favor the use of such energies.

J. N. Carpenter wanted to consider in detail the effect of the shape of the proton pulse on the final result, with the aim of extracting the maximum possible information in the range of higher neutron energies where the moderated pulse is intrinsically narrow. He first considered the ISIS "double-pulse" problem (i.e., accelerator operating at harmonic number 2), and showed that the intuitive result can also be found using Laplace transforms. Since the individual extracted pulses are not delta functions, general pulse-shape broadening must also be considered. The experimental data C(t) may in principal be "deconvoluted" by convoluting with the inverse Laplace transform of the reciprocal of the forward Laplace transform of the broadening function; note that this is done using a model function which is mathematically precise. The example shown was a truncated parabolic function, which generated an embarrassing cubic in the inverse Laplace transform, which can be avoided by taking the third derivative of the data. Since the data are histograms, derivatives are estimated by difference operators, and the integrations of the convolution become matrix multiplications. Thus the effects of different model functions on the recovery of data from counts for different classes of experiments can be estimated on a case by case basis to evaluate accelerator options.