

**VECTORIZED MONTE CARLO METHODS FOR  
REACTOR LATTICE ANALYSIS**

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## VECTORIZED MONTE CARLO METHODS FOR REACTOR LATTICE ANALYSIS

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This report details some of the new computational methods and equivalent mathematical representations of physics models used in the MCV code, a vectorized continuous-energy Monte Carlo code for use on the CYBER-205 computer. While the principal application of MCV is the neutronics analysis of repeating reactor lattices, the new methods used in MCV should be generally useful for vectorizing Monte Carlo for other applications. For background, a brief overview of the vector processing features of the CYBER-205 is included, followed by a discussion of the fundamentals of Monte Carlo vectorization. The physics models used in the MCV vectorized Monte Carlo code are then summarized. The new methods used in scattering analysis are presented along with details of several key, highly specialized computational routines. Finally, speedups relative to CDC-7600 scalar Monte Carlo are discussed.

### Introduction

Monte Carlo calculations fill a special and important need in reactor physics analysis -- they represent "truth" against which approximate calculational methods may be calibrated. The Monte Carlo method permits the exact modeling of problem geometry, a highly accurate mathematical model for neutron interactions with matter, and a cross section representation that is as accurate as theory and measurement permit. The precision of Monte Carlo results is primarily limited by the computing time required to reduce statistical uncertainties.

Conventional (scalar) Monte Carlo codes simulate the complete history of a single neutron by repeated tracking through problem geometry and by random sampling from probability distributions that represent the collision physics. The accumulation of data for 1,000,000 neutron histories will typically require three to seven hours of CDC-7600 CPU time. On newer computers such as the CYBER-205, scalar Monte Carlo codes may run one and one-half to two times faster (with some tailoring of the coding) because of the reduced cycle time and improved architecture of the scalar processors. Much larger gains are possible when the vector processing hardware of the CYBER-205 is utilized.

The random nature of the Monte Carlo method seems to be at odds with the demands of vector processing, where identical operations must be performed on streams of contiguous data (vectors). Early known efforts to vectorize Monte Carlo calculations for other vector computers were either unsuccessful or, at best, achieved speedups on the order of seven to ten times for highly simplified problems. Recent results for Monte Carlo in multigroup shielding applications and in continuous-energy reactor lattice analysis have demonstrated that Monte Carlo can be successfully vectorized for the CYBER-205 computer. Speedups of twenty to fifty times faster than CDC-7600 scalar calculations have been achieved without sacrificing the accuracy of standard Monte Carlo methods. Speedups of this magnitude permit the analysis of 1,000,000 neutron histories in only five to ten minutes of CPU time and thus make the Monte Carlo method more accessible to reactor analysts.

## General Considerations for Vectorized Monte Carlo

Conventional scalar Monte Carlo codes may be characterized as a collection of random decision points separated by short and simple arithmetic. Individual neutron histories are simulated, one at a time. The basic idea of vectorized Monte Carlo is to follow many neutrons simultaneously through their random walks, using vector instructions to speed up the computation rates. The many conditional branches (IF...GOTO), few DO-loops, and largely random data retrieval embodied in conventional Monte Carlo codes preclude vectorization through the use of automatic vectorizing software or by a syntactic vectorization of coding. Instead, experience has shown that a comprehensive, highly integrated approach is required. The major elements of such an approach are as follows:

1. The entire cross section and geometry database must be restructured to provide a unified data layout.
2. The entire Monte Carlo code must be restructured (rewritten).
3. Deliberate and careful code development is essential.

Clever programming and machine "tricks" alone will not ensure successful vectorization of a Monte Carlo code. The key to successful vectorization of Monte Carlo is that a well-defined structure must be imposed on both the database and Monte Carlo algorithm before coding is attempted. This structure may arise simply from the reorganization of existing data/algorithms or may entail the development of special mathematics or physics. Careful and systematic development helps to preserve the structure as the vectorized code becomes more complex.

## Vectorization Techniques

The principal obstacle to vectorizing a conventional scalar Monte Carlo code is the large number of IF-statements contained in the coding. Examination of sections of coding shows that, typically, one-third of all essential FORTRAN statements may be IF-tests. Careful consideration of the Monte Carlo program logic and underlying physics permits categorizing these IF-statements and associating them with three general algorithmic features of Monte Carlo codes -- implicit loops, conditional coding, and optional coding. Implicit loops are vectorized using shuffling, and conditional coding is vectorized using selective operations. This approach to vectorizing Monte Carlo is effective on the CYBER-205 and other vector computers having hardware capabilities for vectorized data handling. In successful attempts to vectorize Monte Carlo methods, 40 to 60% of all vector instructions used in actual coding were vector data handling instructions (gather, compress, bit-controlled operations, etc.).

The data-handling operations associated with shuffling and selective operations in the vectorized code constitute extra work that is not necessary in a scalar code. This extra work offsets some of the gain in speed achieved from vectorization. For vectorization to be successful, overhead from shuffling and selective operations should comprise only a small fraction of total computing time. It is thus essential that all data handling operations be performed with vector instructions. Vector computers that must rely on scalar

data handling operations are severely limited in vectorized Monte Carlo performance.

### Conclusions

Continuous-energy Monte Carlo methods have been vectorized for the CYBER-205 and the speedups are large. Due to the drastic restructuring of the Monte Carlo coding and data base, the MCV code has been limited to the treatment of repeating reactor lattice geometry. This restriction has been deliberate, however, to permit an orderly and careful program of development. There are no a priori limitations on the methods used in vectorization that would preclude extension to more general applications. Profound changes in the methods used for reactor physics analysis are anticipated now that 1,000,000 neutron histories may be run in only five to ten minutes with the CYBER-205 vectorized Monte Carlo vs. the three to seven hours that are typical for CDC-7600 scalar Monte Carlo.

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