CALOR ON THE WAY FROM A CODE PACKAGE TO AN INTEGRATED CODE

F. X. Gallmeier, P. D. Ferguson

Oak Ridge National Laboratory, P.O. Box 2008, MS6475, Oak Ridge, TN 37831, USA
gallmeierfz@ornl.gov

T. A. Gabriel,

Scientific Investigation and Development, Knoxville, TN 37966, USA

T. Handler

Physics Department, University of Tennessee, Knoxville, TN 37966, USA

The code package CALOR, used for prediction of calorimeter performance, has for decades been a loosely coupled system of the three stand-alone particle transport codes HETC; for high-energy meson and hadron particles, MORSE; for neutrons below 20 MeV, and EGS4; for electron, positron, muon and photon transport. These codes are being forged to a unified code, with the backbone of a single secondary particle bank. Internal scoring routines are being integrated. Furthermore, interfaces are being implemented for plugging in other event generator modules and for plugging in CALOR as a particle transport engine into other code systems. This paper will report on the progress of the effort.

I. INTRODUCTION

ORNL has been involved for many years with the development of high energy radiation transport codes, both Monte Carlo and deterministically based, that can be used for a variety of applications including accelerator shielding, detector analysis and development, and experimental planning and analysis. The current code system that is used at ORNL generally for shielding studies and detector development is the Monte Carlo based CALOR [1] system. Included in the system are the HETC [2] code for hadron transport, the EGS4 [3] code for electromagnetic transport, and the MORSE [4] code for low energy neutron transport. Associated with these codes are a variety of support codes and data sets like PEGS, which generates cross-section data for EGS4, SPECT which calculates energy deposition from the data generated during the running of the HETC code, a score of data sets which deal with low energy neutron cross sections, and gamma ray production data and cross sections. These data sets, which are generated from ENDF evaluated data, are used with the MORSE code. Particle event data were passed between the different codes through history files.

The CALOR system is the father of many of the other transport code systems around the world, including HERMES [5] at Juelich, Germany; PHITS [6] in Japan, LAHET [7] at LANL (which has been merged with MCNP to MCNPX [8]), and GCALOR [9] at University Mainz/Germany.

While in the last decades computational capabilities have grown significantly in speed, memory, storage and connectivity, the CALOR code system has maintained its original structure and is as such no longer well suited to make use of new and changed computing resources. It is evident that one of the major bottlenecks of the code is the need for passing information through history files from sub-code to sub-code. Generating and feeding huge history files from sub-code to sub-code has found to be unpractical and tedious. It was decided that for the code to grow, urgent upgrades are necessary which include merging the different sub-codes to a master code making use of the large memory capabilities of the current computers. Upgrade efforts were launched several years ago but stopped short due to the loss of the lead developer to health problems. These upgrade efforts have been rejuvenated recently. The subsequent sections report on the process and progress of the CALOR code on the transformation from a package of independent sub-codes to an integrated multi-particle transport code.

II. CALOR PHYSICS

The HETC code is the core component of the CALOR package, combining high-energy neutral and charged particle transport including charged particle energy loss, multiple coulomb scattering, charged pion decay in flight and capture at rest, muon decay, and elastic and inelastic nuclear interactions. The Bertini model is used for the internuclear cascade for hadrons and pions up to energies of 3.5 and 2.5 GeV, respectively, and is extended by a scaling model to energies of up to 10-15 GeV. Above 10-15 GeV, the nucleon-nucleus interactions are described by a modified FLUKA87 [9] particle nucleus model, from an early version of the FLUKA code. The fragments resulting from the cascade process are handed over to the DRESNER evaporation model, which includes a fission model for actinides. Neutrons below 20 MeV energy are passed to the MORSE code for further transport using evaluated coupled multigroup neutron/gamma cross sections. Gamma rays resulting from the high-energy interactions and from neutron interactions are further transported by the EGS4 code. Neither HETC nor EGS4 have timing schemes implemented; particles handed to MORSE start with zero time, particles handed to EGS4 keep the time they had at transfer.

Figure 1 shows a flow diagram of a CALOR analysis in the original code setup including a crude sketch of the data flow. Material, geometry and scoring information were input to five different codes in various formats. Also MORSE and EGS4, the low-energy neutron and electro-magnetic transport engines, respectively, were fed through event files. While the MORSE and EGS4 based scores were directly sampled in user supplied subroutines, the HETC based scores were obtained by the post-processing code SPECT (including user supplied coding), which evaluated the HETC event file. All score contributions were finally merged to the final result.

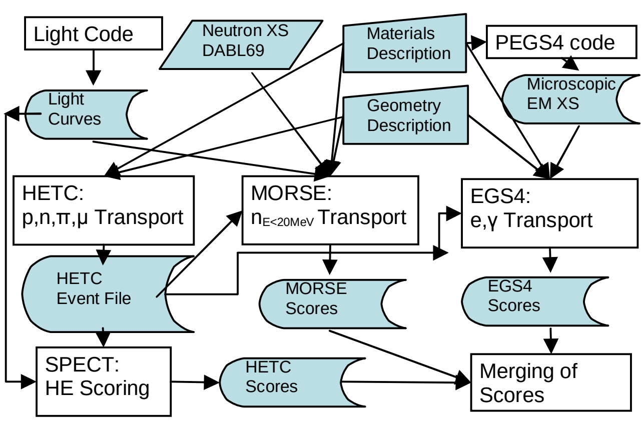

Fig. 1. Flow of an original CALOR transport analysis.

III. CHOICE OF BASELINE CODE

At the start of the effort, we had the choice of picking a reference version as starting point. Besides a standard CALOR version operated and maintained on a LINUX platform at the University of Tennessee, a first cut integrated version prepared by Peter Fu [10] was recovered, which was developed on an IBM-RISC6000 workstation. Also other specialized versions of HETC were identified that were used for early SNS design calculations. Furthermore, a heavy ion transport capability was developed and implemented into an experimental version of HETC at the University of Knoxville.

It felt natural to pick Peter Fu's version as the start of the development and to continue his effort, especially since it had implemented the CEM95 [11] code as optional event generator for hadron and meson reactions below 5 GeV particle energy. The code was ported from IBM to the Linux PC platform and compiled with the Portland Group Fortran compiler PGF77. However, many undocumented code changes were identified, especially in the FLUKA87 part, which caused numerous instabilities, such that we finally decided to replace this part by the cleaner version maintained at the University of Tennessee. At that stage we restructured the more than 300 subroutines of source codes into subdirectories resembling functional units and built compile scripts based on the GNU make utility. Also a modern random number generator was implemented based on Marsaglia & Tang [12] and replaced a compiler provided intrinsic function. After we were confident in running the sample problems provided by Peter Fu, the code was entered into configuration control using CVS.

The integrated baseline code version had, besides simple coding errors, several structural deficits severely limiting its performance:

- The code was run in batch mode accumulating secondary neutrons and photons in a secondary bank. Neutrons were processed after the HETC batch was complete requiring a large secondary bank. The size of secondary bank was hardwired.
- The sizes of scoring arrays were hardwired. Keeping scores on a per source particle basis limited the size of problems that could be processed.
- Scoring routines were problem specific.
- Material input was redundantly read for HETC, MORSE and EGS4.
- Macroscopic neutron cross sections, electro-magnetic cross sections, and light curves still have to be processed before starting the CALOR analysis.

Except for the external processing of cross sections for EGS4 and MORSE, all deficits have been resolved to date.

IV. DEVELOPMENTS

After having established a baseline code, the first effort was dedicated to integrating capabilities of other CALOR versions into the code. The heavy-ion fragment generator

HEDS [13] was integrated first. Besides implementing the event generator, the effort needed an upgrade of the HETC secondary particle bank, significant work in the energy-deposition scoring routines, and in the light conversion routines.

In the traditional scheme, saturation effect corrected light curves for each possible secondary particle were stored and utilized. This scheme is impractical because with heavy ions as interaction particles, many more types of secondaries can contribute to the light production in a detector assembly. According to Birk's law, saturated light production rates depend on the energy loss of charged particles, meaning that they are dependent on the mass and charge number of the projectile. Fig. 2 shows light production for carbon isotopes on scintillator material relative to C-12. Instead of storing light curves for each isotope, we changed the scheme to store energy-dependent light production *L(A,Z)* for a stable isotope of an element (*Z*,*A*) and the difference of light production

$$R(Z) = \frac{L(Z, A+1)}{L(Z, A)} \qquad (1)$$

for an isotope with an atomic number increased by one. A corrected light output is calculated for a particular isotope applying corrections for a particular isotope with atomic number *A* with different in atomic number *A'*:

$$L(Z, A') = L(Z, A) \times R(Z)^{(A'-A)}. \qquad (2)$$

Figs. 3 show light curves retrieved by our new algorithm. These correction effects are much more pronounced for light element ions as for carbon than for medium and heavy mass ions. While small differences between the original and correction algorithm exist, the correction algorithm quite successfully duplicates the light production with significantly reduced memory requirements.

In this process, we also revised the treatment of neutron-initiated recoil in scintillator material in the energy range from 1-20 MeV. Originally, all neutron energy loss due to scattering was attributed to interaction with hydrogen. This seemed to overestimate the low-energy neutron induced light production as comparisons of light output with SCINFUL [14] calculations showed. While no microscopic cross sections are available in MORSE that would allow identifying the collision partner, we decided to sample a collision partner from the material composition assuming the microscopic cross sections for all collision partners are equal.

V. PLANS FOR THE FUTURE

After resolving the outstanding deficits outlined in above section III, we intend to generalize the scoring routines and an interface easy accessible to user provided routines.

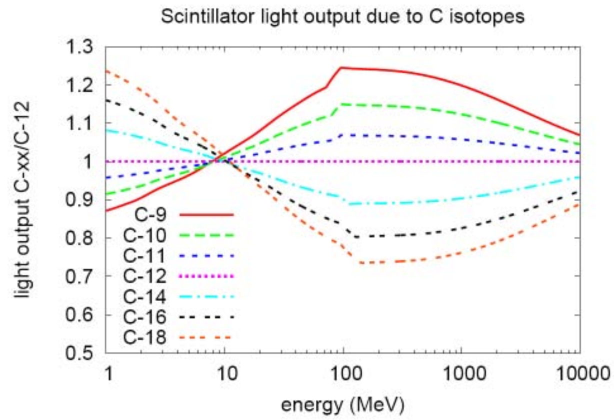

Fig. 2. Ratio of saturation light output of a carbon isotope with respect to C-12 in plastic scintillator as obtained by Birk's law.

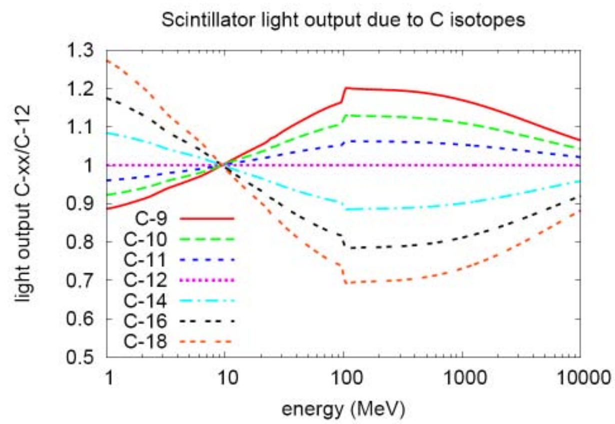

Fig. 3. Ratio of saturation light output of a carbon isotope with respect to C-12 in plastic scintillator as obtained by Birk's law involving the correction formalism.

Before packaging the revived code to a new release, the user interface will obtain a brush-up possibly converting to a keyword-based system more intuitive to the user.

Beyond a first release, ideas come up interfacing the code into a dynamic data analysis system like ROOT developed at CERN. On the geometry side, users would like to see options of geometry packages like the possibility of using MCNP type models, GEANT4 [15] type geometry and even the possibility of importing CAD type geometry.

We are also considering modernizing the physics offered in CALOR by replacing EGS4 with EGS5 [16], and CEM95 with CEM03[17] . Also the high-energy range presently covered by FLUKA87 needs alternatives. MICAP [18] as alternative for the MORSE code as low-energy neutron engine may be revived since it operates on continuous-energy cross section data libraries. Naturally for a Monte Carlo transport code, distributed computing capabilities must be included in future versions to be able to utilize today's computing resources. More extended particle-biasing schemes are desired, especially for shielding applications, but a full analog transport mode must be established and conserved for detector analysis applications.

VI. CONCLUSIONS

Efforts are underway to modernize the high-energy Monte Carlo transport code CALOR, which has been a tool for scientists for more than four decades. While the initial efforts are focused on merging the six stand-alone codes in the original CALOR analysis to a single executable, we have laid the groundwork for future planed extensions of the code. CALOR was formed as a code system for high-energy detector calorimetry and strives to continue to play a role in this field, where other more general-purpose particle transport codes show weaknesses.

ACKNOWLEDGMENTS

This work has been supported by the U.S. Department of Energy (DOE) through Oak Ridge National Laboratory managed by UT-Battelle under contract no DE-AC-5-00OR22725.

REFERENCES

1. CALOR95, RSIC Computer Code Collection C00610, Oak Ridge National laboratory, Oak Ridge, December 1993.
2. Chandler, K. C. and Armstrong, T. W., "Operating instructions for the high-energy nucleon–meson transport code, HETC," Report No. ORNL-4744 (Oak Ridge National Laboratory, Oak Ridge, TN) (1972).
3. Bielajew, A. F., Hirayama, H., Nelson, W. R. and Rogers, D. W. O., "History, overview and recent improvements of EGS4," SLAC-PUB-6499 (NRC-PIRS-0436, KEK Internal 94-4) (Revised June 1) (1994).
4. Emmett, M. B., "MORSE-CGA, a Monte Carlo radiation transport code with array geometry capability," Report No. ORNL-6174 (Oak Ridge National Laboratory, Oak Ridge, TN) (April 1985).
5. P. Cloth et al, HERMES A Monte Carlo Program System for Beam-Material Interaction Studies, Report JUEL 2203, May 1988.
6. K. Niita, PHITS Ver 2.08 User's Manual, Research Organization for Information Science and Technology (RIST), Tokai, Japan, January 2006.
7. R. E. Prael and H. Lichtenstein, User Guide to LCS: The LAHET Code System, LA-UR-89-3014, September 1989.
8. J. S. Hendricks, MCNPX, VERSION 26C, LA-UR-06-7991, Los Alamos National Laboratory, Los Alamos, December 2006.
9. C. Zeitnitz and T. Gabriel, The GEANT-CALOR Interface User Guide, GCALOR Version 1.05/03, University Mainz, September 2001.
10. P. Fu and T. A. Gabriel, CALOR as a single code including a modular version of HETC, in Proceedings of the Fourth Workshop on Simulating Accelerator Radiation Environments (SARE4), Knoxville, Tennessee, September 14-16, 1998.
11. S. G. Mashnik, User manual for the code CEM95, OECD NEA Data Bank, Paris, France (1995), http://www.nea.fr/abs/html/iaea1247.html.
12. G. Marsaglia and W. W. Tsang, The 64-bit universal RNG, Statistics and Probability Letters, 66 no. 2, pp 183-187 (2004).
13. T. M. Miller et al, Heavy Ion Collision Event Generator for the 3D Monte Carlo Transport Code HETC, 11th International Conference on Nuclear Reaction Mechanisms, Varena, Italy, June 12-16, 2006.
14. J. K. Dickens, SCINFUL - A Monte Carlo Based Computer Program to Determine a Scintillator Full Energy Response to Neutron Detection for Energies between 0.1 and 80 MeV: User's Manual and FORTRAN Program Listing, ORNL-6462, Oak Ridge national Laboratory, March 1988.
15. J. Allison et al, Geant4 developments and applications, IEEE Transactions in Nuclear Science, 53 vol 1, pp 270-278, (2006).
16. H. Hirayama, The EGS5 Code System, SLAC-R-730, Stanford University, December 2005.
17. S. Mashnik et al, CEM03.01 User Manual, Los Alamos National Laboratory, Report LA-UR-05-7321 (2005).
18. J. O. Johnson and T. A. Gabriel, "A User's Guide to MICAP: A Monte Carlo Ionization Chamber Analysis Package," ORNL/TM-10340, Oak Ridge National Laboratory (January 1988).