Activities of the computational medical physics working group

Bernadette L. Kirk,[a,*] Glenn Sjoden[b] and Alireza Haghighat[b]

[a]*Nuclear Science and Technology Division*
Oak Ridge National Laboratory
P.O. Box 2008, Oak Ridge, TN 37831-6171 USA

[b]*University of Florida*
Nuclear & Radiological Engineering Department
202 Nuclear Sciences Building
Gainesville, FL 32611 USA

Abstract

Decades of research in reactor physics and software development in the area have benefited various applications, particularly medical and health physics. This paper presents the historical development and activities of the Computational Medical Physics Working Group (CMPWG) as well as an overview of the computational tools widely used for analysis.

1. Historical Development

The development of software tools in the twentieth century was prompted largely by nuclear reactor analysis, nuclear weapons studies, accelerators, fusion reactors, and health physics concerns. As the fields of medical and health physics continue to grow, the implementation of these software codes in cancer research studies (particularly, radiation oncology) and dosimetry becomes more pronounced.

The use of software tools in the analysis of radiation dose and its health effects has been increasing. Such tools include MCNP/MCNPX (X-5, 2003; Pelowitz, 2005; Hendricks *et al.*, 2005), ITS (Halbleib *et al.*, 1992), TORT (Rhoades and Simpson, 1997), ANISN (Engle 1967), EGS4 (Nelson *et al.*, 1985; Bielajew *et al.*, 1994), PENTRAN (Sjoden and Haghighat, 1997), GEANT4 (RD44 Collaboration, 1998), ATTILA (Transpire), PARTISN (Alcouffe *et al.,* 2005), and A^{3}MCNP (Haghighat and Wagner, 2003), FLUKA (Fasso *et al.*, 2005), to name a few.

CMPWG promotes the union of research encompassing nuclear engineering and medical and health physics. CMPWG was established in 2005 within the American Nuclear Society (ANS) and is sponsored by three divisions of the ANS—Mathematics and Computation Division (MCD), Biology and Medicine Division (BMD), Radiation Protection and Shielding (RPSD). The website is http://cmpwg.ans.org.

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[*] Corresponding author, kirkbl@ornl.gov, Tel: 865-574-6176

CMPWG promotes the advancement of computational tools, experimental data, and enabling technologies which are applicable to clinical problems involving computational dosimetry. The group concentrates on a multidisciplinary approach (nuclear engineering, medical physics and health physics) for use by the medical practitioners in the studies of radiation imaging, treatment and effects on human and animal life.

2. Benchmarks

Benchmarking is an important endeavor of CMPWG. Where experimental results exist, efforts are made to use computational models to verify the experimental and computational tools. This is to ensure that the measured dose is computed correctly by the software tools. Computational benchmarks will involve comparisons between software that can model analogous events. A mathematical formulation of a benchmark problem is another case.

The following format will be required for the benchmarks:

1. Detailed description of the experimental benchmark
    a. Overview of the experiment, including objectives
    b. Experimental configuration (materials and methods), including physical dimensions
    c. Description of material data
2. Experimental data
    a. Numerical data and file formats
    b. Experimental uncertainties
3. Benchmark problem definition
    a. Description of the model and the physical problem
    b. Dimensions and geometries
    c. Material composition data
    d. Environmental data
4. Results of sample calculations
5. Computer code inputs

Note that for numerical benchmarks, items 1 and 2 (pertaining to the experiments) will be omitted.

The benchmarks will be classified in accordance to their medical physics applications; some benchmarks will be applicable to more than one group:

1. Radiation therapy (RT)
2. Imaging (IM)
3. Nuclear medicine (NM)
4. Health physics (HP)

A few benchmark examples are as follows: dose distribution on a heterogeneous phantom (RT), computed tomography (CT) density phantom (IM), internal dosimetry (NM-HP), MIRD phantoms (HP), dose distributions on the phantoms acquired with MVCT (IM-RT), and photo-nuclear production during radiation therapy (RT-HP).

The benchmarks will also be classified in accordance to their nature; some will be applicable to more than one:

1. Testing consistency of the codes, noted as theoretical (THE)
2. Clinical benchmarks (CLI): testing clinical—real world—problems
3. Experimental benchmarks (EXP):

A few examples are: pencil beam voxel calculation (THE), electron beam backscattering (CLI), and thick-target bremsstrahlung production measurements (EXP). Heterogeneous phantom dose calculations are noted as THE and THE-EXP if supported by experiments.

CMPWG participates in the ANS Joint Benchmark Committee (http://mcd.ans.org/jb/).

3. Computational Tools

The following is a listing of some of the popular software applied to medical and health physics.

A^{3}MCNP (Automated Adjoint Accelerated MCNP) is a revised version of the MCNP code. A^{3}MCNP performs both source and transport biasing for fixed source problems. It automatically prepares weight-window parameters for variance reduction. The weight-window parameters are determined using 3-D, multigroup adjoint function dis-

tributions that are calculated using a discrete ordinates (Sn) code.
http://ufttg.nre.ufl.edu/~haghigha/a3mcnp.html

ATTILA was developed to provide a design based environment for radiation transport simulations. It combines a leading edge solver with intuitive and integrated processes which have evolved over decades in established computer aided engineering (CAE) disciplines. The result is a state-of-the-art tool which will increase productivity, enabling engineers and scientists to spend more time understanding and improving, and less on setting up and running.
http://www.transpireinc.com

COMET is a heterogeneous coarse-mesh transport method for neutron transport to analyze whole-core criticality developed by the Computational Reactor and Medical Physics Group at Georgia Institute of Technology. COMET decomposes a large, heterogeneous global problem into a set of small fixed-source local problems. Response functions, or rather detailed solutions, are obtained for each unique local problem. These response functions are all precomputed and stored in a library. The solution to the global problem is then bounded by a linear superposition of the local problems.
http://smartech.gatech.edu/handle/1853/13960

TORT calculates the flux or fluence of particles due to particles incident upon the system from extraneous sources or generated internally as a result of interaction with the system in two- or three-dimensional geometric systems, and DORT is used in one- or two-dimensional geometric systems. The principal application is the deep-penetration transport of neutrons and photons. Reactor eigenvalue problems can also be solved. TORT and DORT are the main modules in the DOORS 3.2a discrete ordinates code system. http://rsicc.ornl.gov

EGS4 is a Monte Carlo code for simulating the transport of electrons and photons in arbitrary geometries. It was originally developed at the Stanford Linear Accelerator Center (SLAC) for high energy physics applications and has been extended with the help of the Canadian National Research Council (NRC) and Japan's High Energy Accelerator Research Organization (KEK) to apply to lower energy applications.
http://www.irs.inms.nrc.ca/EGS4/get_egs4.html

EVENT (Ziver *et al.*, 2005) is a general purpose deterministic radiation transport code system based on the finite element approximation to the multigroup second-order even-parity neutron transport equation.

FLUKA is a fully integrated particle physics Monte Carlo simulation package that has many applications in high energy experimental physics and engineering, shielding, detector and telescope design, cosmic ray studies, dosimetry, medical physics and radiobiology. http://www.fluka.org/

FOTELP-2K6 is a new compact general purpose version of the previous FOTELP-2K3 code designed to simulate the transport of photons, electrons and positrons through three-dimensional material and sources geometry by Monte Carlo techniques, using subroutine package PENGEOM from PENELOPE 2006. http://rsicc.ornl.gov

GamBet (Version 2.0) is an innovative approach to Monte Carlo simulations of radiation transport in matter. The unitized suite handles the full range of electron/photon/positron interactions with high accuracy. GamBet can be used as a stand-alone tool or as an extension to the Trak or OmniTrak charged-particle-beam codes. Applications include optimization of X-ray targets, electron-beam heating, radiographic imaging, positron physics, radiation therapy research and shielding design. The codes run on personal computers under any version of Windows.
http://www.fieldp.com/gambet.html

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science.
http://geant4.web.cern.ch/geant4/

ITS (Integrated Tiger Series) permits a state-of-the-art Monte Carlo solution of linear time-integrated coupled electron/photon radiation transport problems with or without the presence of macroscopic electric and magnetic fields of arbitrary spatial dependence. http://rsicc.ornl.gov

MCNP (Monte Carlo N-Particle) is a general-purpose code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. http://mcnp-green.lanl.gov/index.html

MCNPX is a general-purpose Monte Carlo radiation transport code for modeling the interaction of radiation with everything. MCNPX stands for Monte Carlo N-Particle eXtended. It extends the capabilities of MCNP4C3 to nearly all particles, nearly all energies, and to nearly all applications without an additional computational time penalty. MCNPX is fully three-dimensional and time dependent. It utilizes the latest nuclear cross section libraries and uses physics models for particle types and energies where tabular data are not available. Applications range from the discovery of water on Mars to the deep underground search for oil. MCNPX is used for nuclear medicine, nuclear safeguards, accelerator applications, nuclear criticality, and much more.
http://mcnpx.lanl.gov/;
http://rsicc.ornl.gov

MCSHAPE is a Monte Carlo code developed to describe the evolution of the polarization state of x-ray photons as a consequence of the multiple scattering collisions during the diffusion into the sample. In order to properly study the transport of photons with an arbitrary state of polarization, the model adopted in this code is derived from the so called ‘vector’ transport equation. Using the Stokes parameters I, Q, U, and V, having the dimension of an intensity and containing all the physical information about the polarization state, MCSHAPE simulates the full state of polarization of the photons at any given position, wavelength and solid angle. http://shape.ing.unibo.it/html/mcshape.html

PARTISN (PARallel, TIme-Dependent SN) is the evolutionary successor to CCC-547/DANTSYS. User input and cross section formats are very similar to that of DANTSYS. The linear Boltzmann transport equation is solved for neutral particles using the deterministic (Sn) method. Both the static (fixed source or eigenvalue) and time-dependent forms of the transport equation are solved in forward or adjoint mode. Vacuum, reflective, periodic, white, or inhomogeneous boundary conditions are solved. General anisotropic scattering and inhomogeneous sources are permitted. PARTISN solves the transport equation on orthogonal (single level or block-structured AMR) grids in 1-D (slab, two-angle slab, cylindrical, or spherical), 2-D (X-Y, R-Z, or R-T) and 3-D (X-Y-Z or R-Z-T) geometries. http://rsicc.ornl.gov

PENELOPE performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials and complex quadric geometries. A mixed procedure is used for the simulation of electron and positron interactions (elastic scattering, inelastic scattering and bremsstrahlung emission), in which ‘hard’ events (i.e. those with deflection angle and/or energy loss larger than pre-selected cutoffs) are simulated in a detailed way, while ‘soft’ interactions are calculated from multiple scattering approaches. Photon interactions (Rayleigh scattering, Compton scattering, photoelectric effect and electron-positron pair production) and positron annihilation are simulated in a detailed way. PENELOPE reads the required physical information about each material (which includes tables of physical properties, interaction cross sections, relaxation data, etc.) from the input material data file. The material data file is created by means of the auxiliary program MATERIAL, which extracts atomic interaction data from the database of 767 ASCII files. http://rsicc.ornl.gov

PENTRAN (Parallel Environment Neutral-particle TRANsport) is a 3-D Cartesian Parallel Sn transport code. The first version was completed in June 1996. PENTRAN is designed for solving large/complex 3-D problems on distributed-memory, distributed computing, and shared memory parallel (SMP) environments. PENTRAN has been operated on all types and configurations of parallel computers and PCs and automatically performs complete and hybrid phase space parallel decomposition among the angular, energy, and spatial variables. PENTRAN performs multigroup, anisotropic, discrete ordinates neutral particle transport calculations in forward and adjoint

modes. PENTRAN is part of the PENTRAN code system, with complete supporting codes for input/3-D mesh preparation preconditioning, and output and data interpretation; tools enable seamless user interface with parallel-memory distributed data.
http://ufttg.nre.ufl.edu/~haghigha/pentran.html

PEREGRINE, a 3-D Monte Carlo dose calculation system, breaks the barriers to accurate dose calculation with the first full-physics model of the radiation treatment process. It uses Monte Carlo calculations, in which statistical sampling techniques are used to obtain a probabilistic approximation of a problem's solution. This enables PEREGRINE to model how trillions of radiation particles interact with the complex tissues and structures in the human body and where they deposit their energy. In the past, Monte Carlo calculations, known to be the best way to model these interactions, would have required days or weeks of supercomputer resources—impractical for radiation treatment planning. The PEREGRINE team has designed and built the Monte Carlo system to plan accurate radiation treatments at a cost and speed practical for widespread medical use. PEREGRINE uses advanced algorithms integrated with off-the-shelf computer hardware configured in sophisticated architectures to bring Monte Carlo-based treatment planning to the desktop.
https://www.llnl.gov/str/Moses.html

PHITS (Particle and Heavy Ion Transport Code System) is a general purpose Monte Carlo transport code which is used in atom/nuclear physics, shielding design, material science, medical support, environment and space radiation studies and so on, in various countries. The former version of PHITS is NMTC/JAM which is a spin-off of the NMTC code and has been maintained at the Japan Atomic Energy Agency (JAEA). The MCNP code is included in PHITS and calculations are automatically connected between PHITS and MCNP at binding energies which can be set by users for any energy at which cross section data exist.
http://rcwww.kek.jp/research/shield/phits.html

SERA (The Simulation Environment for Radiotherapy Applications) was developed for boron-neutron capture therapy (BNCT) patient treatment planning by researchers at the Idaho National Engineering and Environmental Laboratory (INEEL) and students and faculty at Montana State University (MSU) Computer Science Department. Unique neutron transport geometry provides rapid Monte Carlo solutions. Geometric modeling fidelity is equivalent to image resolution. SERA is a suite of command line or interactively launched software modules, including graphical, geometric reconstruction, and execution interface modules for developing BNCT treatment plans. The program allows the user to develop geometric models of the patient as derived from CT and Magnetic Resonance Imaging (MRI) images, perform dose computation for these geometric models, and display the computed doses on overlays of the original images as three dimensional representations. A three-dimensional Monte Carlo radiation transport model, seraMC, developed at INL, is used to calculate the complex radiation fields present in BNCT treatment.
http://rsicc.ornl.gov

SIMIND is a Monte Carlo simulation code that describes a standard clinical SPECT camera and can easily be modified for almost any type of calculation or measurement encountered in SPECT imaging. The entire code is written in FORTRAN-90 and includes versions that are fully operational on Linux systems (x86), and on Windows (x86). The majority of the main code structure is similar for all of the operating systems; but, in cases where the operating system becomes unique, additional information on the code as it pertains to the specific system is provided. http://www.radfys.lu.se/simind/

TransMED is advanced particle transport software using three-dimensional deterministic methods in arbitrary geometry.
http://www.transware.net/.

4. Workshops

CMPWG has held two workshops to bring the community together. The Nuclear Science and Technology Division (NSTD) of Oak Ridge National Laboratory (ORNL) sponsored CMPWG I on October 26, 2005. The workshop was held to address several key areas:

- Identify the medical physics problems and experiments for computational benchmarks

- Identify the software tools, their applications, strengths and weaknesses
- Identify applications suitable for parallel computing
- Identify the roadmap for benchmarking activities.

Discussions centered on the need for experimental data, the importance of both Monte Carlo and deterministic methods, and the need to evaluate current nuclear data for medical physics. These activities are aimed at improving dose predictions for radiation therapy and other medical activities that utilize ionizing radiation. Proceedings of the workshop are published in the ORNL report "ORNL/TM-2006/7" (Kirk and Rice, 2006) and on the CMPWG website.

The University of Florida at Gainesville sponsored CMPWG II from September 30 to October 3, 2007. The focus of the workshop was on major software tools like PENTRAN, MCNP/MCNPX, GEANT4, ADEIS and A^{3}MCNP and PENELOPE. In addition, emerging need in clinical applications of computation from medical physics practitioners, including radiotherapy, diagnostic applications, and the importance of image guided methodologies were major themes covered in this meeting. A highly-related topic is computational phantom modeling, which was also covered in detail by several presentations. An electron/photon transport bibliographic database consisting of over 4000 citations was presented. Proceedings (Sjoden, 2007) are available on DVD and on the CMPWG website.

CMPWG III is planned for 2009 at the Georgia Institute of Technology, and CMPWG IV is planned in 2011 in Seoul, South Korea.

5. Conclusion

CMPWG is dedicated to advancing the research that merges nuclear engineering with computational dosimetry applications in medical and health physics. The success will greatly depend on the contribution of the scientific community.

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