The EGSnrc Monte Carlo system

Iwan Kawrakow

Ionizing Radiation Standards, NRC, Ottawa, Canada





Outline

- History & Overview
- EGSnrc user codes
- Brief review of cross sections
- Brief review of condensed history implementation
- Selected benchmarks
- EGSnrc C++ class library
- Selected recent EGSnrc applications



EGSnrc

- A package for the Monte Carlo simulation of coupled electron-photon transport
- The dynamic range is between 1 keV and several tens of GeV
 - Lower energy limit due to large uncertainties in cross sections and the fact that the track concept increasingly looses validity in the eV range
 - Upper energy limit due to lack of radiative corrections, no production of pp
 -pairs other than e⁺e⁻,
 Landau-Pomeranchuk effect not taken into account
- Elements $Z = 1 \cdots 100$, arbitrary compounds and mixtures using the independent atom approximation
- Uses a class II scheme for the simulation of charged particle transport
- Written in Mortran 3
- Successor of EGS4

Major developments

EGS3 – 1970s

Richard Ford & Ralph Nelson developed the code for high energy particle physics at SLAC

EGS4 – 1980s

Ralph Nelson, Hideo Hirayama (visitor at SLAC) & Dave Rogers (at NRC) released EGS4, focus shifts to lower energy applications

PRESTA – 1986

Alex Bielajew & Dave Rogers (at NRC) improved the condensed history transport at low energies. Released as add-on to EGS4

User codes – late 80s, early 90s Rogers & Bielajew (and numerous students) developed a series of user codes relevant for ion chamber dosimetry



Major developments

Photon cross section improvements – early 1990's Bielajew at NRC and Hirayama, Namito & Ban at KEK improved the treatment of several photon interaction processes

BEAM - 1995

Rogers (and many others at NRC) released BEAM, an EGS4 user code for the simulation of medical linacs. This is currently the most widely used code in the Medical Physics community (300+ citations)

Multiple scattering & transport mechanics – 1997 Kawrakow & Bielajew published a new multiple elastic scattering approach and a new condensed history algorithm that removes most of the EGS4 limitations



Major developments

Work on EGSnrc – 1998 ··· · 2000 Kawrakow at NRC incorporated all previous + many new developments in a new EGS version to become known as EGSnrc

EGS4 not actively maintained – $\sim 1998 \cdots$ present Not actively maintained (except for the KEK version)

Work on EGS5 – $\sim 1998 \cdots$ present Bielajew, Nelson & KEK group announce plans to develop EGS5, only a beta release so far

EGSnrc released – 2000

Kawrakow & Rogers release EGSnrc, now considered by many to be the "golden standard" in the Medical Physics community (200+ citations)



Initial EGSnrc release

- All EGS4 extensions included by default
- Many subroutines rewritten
- Completely new and vastly superior condensed history implementation
- Kawrakow & Bielajew multiple scattering theory extended to elastic scattering with spin effects taken into account
- Compton scattering with binding and Doppler broadening
- Improved photo-absorption
- Atomic relaxations
- Major code clean-up, many bug fixes, algorithm optimizations
- New 300 pages manual

Recent developments

- BEAMnrc 2001 BEAM adapted to work with EGSnrc and renamed BEAMnrc
- Electron Impact Ionization 2002
- EGSnrcMP 2003 A new run-time environment that works on Unix/Linux and Windows
- DBS 2004
 - New variance reduction techniques that dramatically improve the efficiency of linac simulations

egspp – 2005

New C++ class library for EGSnrc that provides a geometry package, several particle source and many useful utility classes. Still under heavy development

 Photon cross section improvements – 2006
 Better treatment of pair production and radiative corrections for Compton scattering

MC papers in Med.Phys. & PMB



 \Rightarrow by 2016 all papers will relate to MC in one way or another

EGSnrc structure



NRC-CNRC

The EGSnrc Monte Carlo system - p.10/71

EGSnrc tutorial user codes

- Tutorial codes tutor1...tutor7
 - Simple hard-coded slab geometry
 - Simple hard-coded particle source
 - Demonstrate basic scoring techniques.
 - See PIRS-701 for more details
- Jutorial codes tutor2pp, tutor7pp
 - Same as corresponding tutorials in Mortran but written in C++
 - Can use arbitrary geometry constructible with egspp
 - Can use any source provided by egspp
 - tutor2pp derives from EGS_SimpleApplication
 - tutor7pp USES EGS_AdvancedApplication

EGSnrc RZ user codes

- Described in detail in PIRS-702
- All implement an RZ-geometry
- All provide the same set of common particle sources
- Usable via a GUI by Ernesto Mainegra (see PIRS-801)
- CAVRZnrc: Calculates the dose to the cavity of an ionization chamber and correction factors relevant for primary air kerma standards
- DOSRZnrc: Scores the dose deposited in all regions. Can also compute a pulse height distribution
- FLURZnrc: Calculates particle fluence in user defined regions (total and differential in energy)
- SPRRZnrc: Calculates stopping power ratios needed in primary standards and dosimetry protocols

RZ GUI

-•• [dosrznrc_template.eg	sinp] GUI for RZ EGS	urc user codes. Cop	yright 2003 NRC Canada <	2> ? • • •
National Resea Council Canada	rch Conseil national a de recherches Cana	da		-CARC
General I/O control Mo	unte Carlo Geometry (lavity Source Tr	ansport Parameter Transport P.	arameters by Region 1
dosrznrc_template: depth	dosrznrc_template: depth dose in H2O due to Cobalt beam			characters wide
Select EGSnrc user code- C CAVRZnrc C DOSRZnrc C SPRRZnrc C FLURZnrc	Target optimization no optimization debug clean	User code area © EGS_HOME © HEN_HOUSE © Other	Pegs data area	
EGSnrc input file name (*.e	egsinp)			
PEGS4 file name (*.pegs4d	lat)			<u> </u>
Configuration file				
Configuration				view errors
<u>Execute</u> Pre <u>v</u> iewR	Z <u>Print</u> <u>C</u> or	mpile	S <u>a</u> ve&Exit <u>S</u> ave	Exit Help
				The



RZ GUI

eral I/O control Monte	r* dosrznrc template.eg	sinp] GUI for RZ EGSnrc use	er codes. Copy	right 2003 NRC	Canada <2>		? •
tle (80 characters maximum)- osrznrc_template: depth dose	Council Canada	a de recherches Canada	21 - 21			51-1	2
elect EGSnrc user code	General I/O control Mo	onte Carlo Geometry Cavity of front face: 0.	Source Trar	nsport Parameter dia input	Transport Param	eters by Region	1 <u>⊪</u>
DOSRZnrc	C individual		d	lescription by pla	ines 💌		
GSnrc input file name (*.egsir losrznrc_template.egsinp	planes information # slabs thickness 1 10	[cm] 1 cylinder informatio		medium H2O521ICRU	start Z stop Z	start R stop F	₹_▲ 5
EGS4 file name (*.pegs4dat) - i21icru.pegs4dat	2 50 3 4 5	2 2 3 4 5	2 2 5 3 10 4 100 5	AIR521ICRU	11 1		1
onfiguration file gf77.conf	6 7 8	6 7 8	100 6 7 8				
nfiguration	9 10 11 12	9 10 11 12	9 10 11				_
Execute PreviewRZ							

Other EGSnrc user codes

- g: Computes mass energy transfer/absorption coefficients for a given photon spectrum
- CAVSPHnrc: Same as CAVRZnrc but implements a spherical/conical geometry
- EDKnrc: Computes energy deposition kernels needed by convolution/superposition methods
- EXAMIN: Can be used to examine cross section data sets
- 🥭 cavity
 - Full-featured user code in C++
 - Provides same functionality as CAVRZnrc
 - Any geometry or particle source can be used
 - Can compute cavity dose simultaneously in several geometries

BEAMnrc & DOSXYZnrc

- Most widely used codes in the Medical Physics community (300+ citations)
- Developed by Dave Rogers & many others at NRC
- First version (based on EGS4) released in 1995
- Adapted to EGSnrc in 2000
- BEAMnrc: simulation of medical linacs and typical X-ray tubes
- DOSXYZnrc: dose in a rectilinear geometry (possibly defined via CT images)
- Numerous variance reduction techniques
- Maintained and developed by Walters, Kawrakow (NRC) & Rogers (Carleton U)
- Extensive manuals: PIRS–509 & PIRS–794
- Course ~once a year (next course October 2–5 in Ottawa)
- Both codes have own GUI's

Documentation

- PIRS-701: main EGSnrc manual not updated to reflect the recent cross section improvements
- PIRS–702: RZ codes manual
- PIRS–801: RZ-GUI manual
- PIRS–877: EGSnrcMP environment
- PIRS-898: C++ class library (egspp) manual
- PIRS–509: BEAMnrc manual
- PIRS–794: DOSXYZnrc manual
- SLAC–265: original EGS4 manual
- PIRS-436: History, overview and recent improvements of EGS4 (outdated)



Resources

www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html

(search for EGSnrc on Google and follow first link) the EGSnrc distribution site. Includes on-line html and pdf versions of the manuals, list of known bugs/patches, news, etc.

http://rcwww.kek.jp/research/egs/

the EGS home page now maintained at KEK

www.irs.inms.nrc.ca/BEAM/beamhome.html (search for BEAMnrc on Google and follow first link) the BEAMnrc home page and distribution site

EGS list server

low volume, main mode for communication with EGS users (see instructions on EGSnrc or EGS pages how to subscribe)



Courses

- EGSnrc courses every ~18–24 months; next course ~October 2007?
- BEAMnrc courses every ~12–18 months; last course was Oct 2006 in Ottawa
- Courses announced under "News" on the EGSnrc page
- Next (or possibly previous) course brochures at

www.irs.inms.nrc.ca/papers/egsnrc/brochure.html www.irs.inms.nrc.ca/omega/brochure.html



EGSnrc Physics



Photon cross sections

- Incoherent (Compton) scattering
- Coherent (Rayleigh) scattering
- Pair/triplet production
- Photo-absorption



Compton scattering

Theoretical total and differential cross sections: the user has the choice between

- Scattering with free electrons at rest using the Klein-Nishina formula. This is the same as in EGS4 but the sampling algorithm has been optimized
- Binding effects and Doppler broadening in the relativistic impulse approximation (default).
 - The approach used is similar to PENELOPE's
 - The necessary Compton profiles are taken from [Biggs <u>et al</u>, Atomic Data and Nucl. Data Tables 16 (1975) 201.]
 - The relaxation cascade of inner shell vacancies created in Compton scattering events is taken into account
- New: radiative corrections up to $O(\alpha^3)$ can be taken into account



Rayleigh scattering

- Elements: total cross sections from Storm & Israel, XCOM, EPDL–97 or user Bob's cross sections
- Elements: differential cross sections based on atomic form factors from [Hubbell and Øverbø, J. Phys. Chem. Ref. Data (1979) 69.]
- Mixtures: independent atom approximation (known to be not very accurate!)
- TODO list: give the user the option to easily implement and use their own molecular form factors



Pair/triplet production

- Total cross sections from Storm & Israel, XCOM, EPDL–97 or user Bob's cross sections
- Extreme relativistic first Born approximation with screening (Coulomb corrected above 50 MeV) for the cross sections differential in energy.
- Triplet production is not explicitly modeled but taken into account by adding the triplet total cross section to the pair total cross section
- The angular distribution of electrons and positrons is selected from a modified version of Eq. 3D-2003 of [Motz <u>et al</u>, Rev. Mod. Phys. 41 (1969) 581.] or its leading term.
- New: screening corrected exact differential cross sections due to Olsen, Mork & Øverbø up to 85 MeV
- New: explicit simulation of triplet events from the Votruba-Mork cross section (not yet in official release)

New differential pair cross sections





Photo-absorption

- Total cross sections from Storm & Israel, XCOM, EPDL–97 or user Bob's cross sections
- For mixtures the interacting element is explicitly sampled
- The interacting shell is explicitly sampled using photo-absorption branching ratios
- The binding energy of the interacting shell is subtracted from the photo-electron energy
- The relaxation cascade of the shell vacancy is taken into account
- The angular distribution of the photo-electrons is picked from the Sauter distribution



Atomic relaxations

- In EGSnrc the relaxation cascade of inner shell vacancies is an independent process that is initiated each time a vacancy is created
 - Currently in photo-absorption, bound Compton scattering, electron impact ionization
 - Future: triplet production, electron-electron bremsstrahlung
- All shells with binding energies above 1 keV
- All radiative and non-radiative transitions to/from K-, LI-, LIIand LIII-shells
- All radiative and non-radiative transitions to/from "average" Mand N-shells.
- TODO list: remove the above limitation

Electron/positron cross sections

- Bremsstrahlung
- Inelastic collisions with atomic electrons
- Elastic collisions with nuclei and atomic electrons
- Positron annihilation



Bremsstrahlung

- For $d\sigma/dk$ the user has the choice between
 - The NIST bremsstrahlung cross section data base (basis for ICRU radiative stopping powers)
 - Extreme relativistic first Born approximation (Coulomb corrected above 50 MeV) with an empirical correction to recover ICRU radiative stopping powers.
- Total bremsstrahlung cross sections for production of photons with energy greater than a user specified threshold are calculated from the selected differential cross section
- Restricted radiative stopping power for sub-threshold bremsstrahlung
- Angular distribution of bremsstrahlung photons from Eq. (2BS) of Koch & Motz, its leading term, or user Bob's approach
- Work in progress: explicit simulation of electron-electron bremsstrahlung

Inelastic collisions

- Møller (e⁻) or Bhabha (e⁺) cross sections for collisions that result in the creation of δ-particles with energies greater than a user specified threshold
- Continuous-slowing-down approximation using the restricted collision stopping power from the Bethe-Bloch theory for sub-threshold processes
- Density effect corrections from ICRU–37 or the empirical Sternheimer formula
- Electron Impact Ionization for K- and L-shells with binding energies above 1 keV. Cross sections from Kawrakow, Casnati, Gryzinski, Kolbenstvedt, or user Bob can be used.
- Work in progress: radiative corrections for e⁺/e⁻ inelastic scattering



Positron annihilation

- Two-photon in-flight annihilation from the first Born approximation neglecting binding
- Two-photon annihilation at rest
- Single- and n-photon ($n \ge 3$) annihilation ignored because cross sections much smaller



Elastic collisions

User has the choice between

- The screened Rutherford cross section with a screening angle from the single scattering theory of Moliére. This is the single elastic scattering cross section effectively used in EGS4 via the multiple scattering theory of Moliére.
- The screened Rutherford cross section times the Mott spin correction factor (which is different for electrons and positrons) with a screening angle selected so that the first elastic scattering moment from PWA cross sections is reproduced.



Ion chamber response

- Early attempts in the '80s with EGS4 revealed ~40% variation of the computed cavity dose with electron step size
- The PRESTA algorithm released in 1987 greatly reduced the problem
- Rogers demonstrated in 1993 that
 - Even with PRESTA, there is still \sim 2.5% variation of cavity dose with step size for graphite wall chambers in 60 Co beams
 - Calculation does not converge to the expected result in the limit of short steps
 - Even larger step-size dependencies in kV beams
- Much larger step-size dependencies for chamber walls other than graphite (e.g. \sim 6% for AI).
- Problem finally solved with release of EGSnrc

Ion chamber response in ⁶⁰Co beams





Condensed history aspects

- Multiple elastic scattering: exact theory valid for arbitrary step sizes, both for the screened Rutherford cross section and the cross sections with spin effects taken into account
- Electron-step algorithm: most accurate algorithm known (truncation error is $O(\Delta s^4)$)
- Evaluation of energy dependent quantities: accurate up to $O(\Delta E^4)$
- Correct implementation of the fictitious cross section method
- Single elastic scattering in the vicinity of interfaces between different materials
- \Rightarrow Step-size independent and artifact free simulation at the sub 0.1% level.



Benchmarks



The EGSnrc Monte Carlo system - p.35/71
Benchmark: backscatter coefficients





Benchmark: depth dose curves





Benchmark: Ge detector response



The EGSnrc Monte Carlo system - p.38/71

Benchmark: parallel-plate chamber response





Benchmark: chamber response to ⁹⁰Sr/⁹⁰Y beta



The EGSnrc Monte Carlo system - p.40/71

Benchmark: chamber response to ⁹⁰Sr/⁹⁰Y beta



NRC-CNRC

The EGSnrc Monte Carlo system - p.41/71

Benchmark: Elekta 25 MV beam





Benchmark: Elekta 25 MV beam



difference to chamber dose in water

In both cases full simulation of the detectors

Benchmark: Pancake chamber



EGSnrc C++ class library (egspp)



Motivation

- A Monte Carlo (MC) simulation requires the description of the geometry of interest
- Some general purpose MC codes (<u>e.g.</u> MCNP, Geant4, PENELOPE) provide powerful geometry packages
 - Advantage: simulations can be set up quickly
 - Disadvantage: simulations often run too slow, at least partially because of the generality of the geometry routines
- In EGSnrc the user has to provide the geometry
 - Advantage: optimized geometry routines can be programmed for the problem of interest. EGSnrc is distributed with several user codes that provide geometry implementations for common situations
 - Disadvantage: if no geometry implementation is available, programming it can be very tedious and time consuming

Overview

- Geometry package
- Particle sources
- EGS_SimpleApplication and EGS_AdvancedApplication
- Many other utility classes
- Described in detail in PIRS-898 (html version only)



Abstract geometry objects

Every implementation of a model of geometrical structure must provide several methods to permit the simulation of particle transport:



The EGSnrc Monte Carlo system - p.48/71

Concrete geometry objects

"Elementary" geometries

- Methods implemented directly
- Examples: planes, cylinders, spheres, cones, pyramids, prisms, etc.
- Composite geometries
 - Built from elementary or other composite geometries
 - Use a certain type of logic to put the constituent geometry objects together
 - Examples: envelope geometry, union geometry, transformed geometry, N-dimensional geometry, geometry stack, CD-geometry.



Example: envelope geometry

isWhere(\vec{x}) logic:

- If point \vec{x} is outside the box, then return -1
- If point \vec{x} is inside the box, but outside the sphere, then return 0
- Else return 1



If point \vec{x} is outside the "envelope", then return -1

- If point \vec{x} is inside the "envelope", but outside the inscribed geometry, then return 0
- Else return 1



Example: envelope geometry

- Logic can be generalized to the situation where the "envelope" has many regions, and there is an arbitrary number of inscribed geometries
- Generalization only requires a predetermined region numbering scheme
- howfar and hownear also require a completely generic algorithm that is independent of the envelope and inscribed geometries
- Only requirements are that all inscribed geometries are completely contained within the envelope and don't overlap each other



Example: N-dimensional geometry





howfar logic:

- \bullet Calculate all distances t_i to the "dimensions" of the geometry
- **P** Return $Mint_i$

Examples: XYZ, RZ, spheres & cones, spheres & planes, RZ Φ , etc.

Geometry viewer egs_view

- Geometries are defined in an input file \Rightarrow need for visualization
- Automatic translation of arbitrary complicated geometries in a graphics language (e.g. OpenGL, DirectX) is exceedingly difficult
- Construct the 3D image using the howfar and isWhere methods provided by each geometry
 - Disadvantage: much slower than rendering an OpenGL scene (but still fast enough on modern hardware for real time rotation, transparency, etc.)
 - Advantage: needs the same methods used at run time ⇒ provides additional QA check



Geometry viewer egs_view



Uses simplest OpenGL light model



Geometry examples





Timing benchmarks

Mortran code	C++ code	Calculation	Timing ratio
tutor2	tutor2pp	20 MeV e^- on	0.98
		1 mm Ta	
cavrznrc	cavity	1.25 MeV γ on	1.18 (RZ)
		pancake chamber	0.97 (Envelope)
BEAMnrc	beampp	16 MV photon	0.87 (no VRT)
		linac	0.89 (RR)
			0.36 (DBS + RR)

Simulations use the same physics & VRT's and are run on the same computer

 \Rightarrow Timing differences due to geometry & scoring



Utility classes

- Classes for sampling from a probability distribution
- Classes for handling system-dependent facilities (loading of shared libraries, timing, etc.)
- Classes for run control (including parallel processing)
- Scoring classes
- Random number generator
- Spline and linear interpolations
- Reading an input file
- Transformations
- Etc.



Recent EGSnrc applications



Topics of MC papers in 2006

Characterization of irradiation devices:

MV linacs, Tomotherapy, X-ray tubes, Gamma- and Cyberknife, Micro beams, Brachytherapy (seeds and miniature X-ray tubes), Protons and Ions, etc.

Imaging

CBCT, digital radiography, PET, SPECT, dose to imaged patient, mammography, new X-ray tube designs, indirect CT, scattered X-rays, etc.

IMRT & Optimization

Direct MC optimization, corrections for and comparisons with traditional optimization methods, new MLC designs, EMRT & MERT, patient motion, etc.

Detector response

EPIDs, phosphor screens, scintillation detectors, CZT detectors, CdWO₄ detectors, etc.



Topics of MC papers in 2006 (cont'd)

Radiation dosimetry

correction factors (P_{wall} , effective point of measurement, etc.), ion chamber design, conversion factors, film dosimetry, etc.

Brachytherapy

shielding, seed self-attenuation, new techniques, combination with external beams, dosimetric properties and constants, dose escalation near Au seeds, etc.

Dose calculation

4D, Comparisons with and improvements of traditional algorithms, fast algorithms, verification of commercial implementations, particle therapy, MC based brachytherapy planning, dose kernels, neutron capture therapies, etc.

New treatment techniques

converging stereotactic delivery of kV X-rays, synchrotron radiation, several of the above

Topics of MC papers in 2006 (cont'd)

Design of new devices

Linacs without flattening filters, Photons and Electron MLC's, X-ray tubes, Detectors, IMRT with ⁶⁰60, new integrated delivery and imaging devices, Laser accelerated protons and electrons, etc.

Miscellaneous

Dose outside of treatment fields, radiation shielding and protection, interaction cross sections, efficiency of MC simulations, dose enhancement due to contrast agents and gold seeds, presence of strong magnetic fields, denoising of MC computed dose distributions, etc.



Fast X-ray tube simulations





Fast X-ray tube simulations



120 kV spectrum from a BEAMnrc/DBS simulation after 2 min. on a single 2.66 GHz CPU.

Free Air Chamber correction factors



Free Air Chamber correction factors





Uncertainty analysis



CBCT scatter calculations



toms. Each particle was used eight times to ensure an uncertainty on the scatter distribution below 15%. In all tests the

The simulations for scatter correction were run on a Pentium 4 Xeon processor 2.8 GHz for 430 h. On a 20-computer cluster, which can now be readily available at acceptable cost, the simulation time can be reduced to 21.5 h. This is

Can the calculation be done faster?

Fast CBCT scatter calculations

- Forced detection for photons towards screen
- Interaction splitting
- Russian Roulette for photons away from screen
- Delta tracking for photons away from screen
- Variable splitting number to guarantee similar weights of detected photons
- Systematic sampling of primary photons
- $\Rightarrow ~\sim \!\! 300$ times faster compared to analog, $\sim 3 \times 10^4$ times compared to full
- ⇒ 0.1 seconds/projection on modern desktop PC for 15% statistics using 5 mm voxels



Fast ⁶⁰**Co simulations**

Motivation:

- Primary air kerma standard
 - Correction factors have never been computed using a realistic ⁶⁰Co source
 - Number of particles required is too large to be stored in a phase space file
- Recent interest in using ⁶⁰Co for IMRT
 - ⁶⁰Co IMRT as a cheaper alternative to IMRT with MV linacs
 - ⁶⁰Co source combined with imaging modality such as MRI
- \Rightarrow Need for fast generation of particles emerging from the 60 Co device

Approach: Combine directional source biasing with DBS in BEAMnrc/beampp



Fast ⁶⁰**Co simulations**





Skeletal dosimetry





See R. Kramer et al, PMB 51 (2006) 6265

