Review of Monte Carlo codes by the Modelling Working Group of the Panel on Gamma and Electron Irradiation

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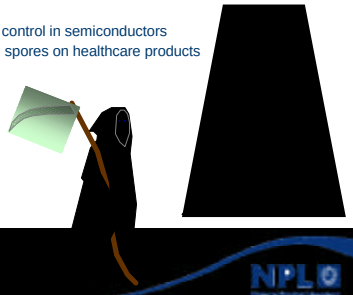
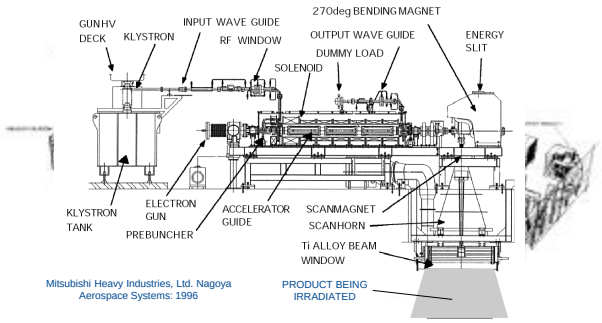
Introduction: Irradiation Industry

- Use irradiation to change the properties of the material being irradiated
  - Crosslinking or chain scission of polymers
  - Colour of gemstones
  - Minority carrier lifetime control in semiconductors
  - Bring death to bacterial spores on healthcare products



Introduction: Irradiation Industry



Mitsubishi Heavy Industries, Ltd. Nagoya Aerospace Systems: 1996

Introduction: Panel on Gamma and Electron Irradiation

- Irradiation Panel: Composed of members from many companies in several countries, promoting best practice in commercial irradiation
  - Regular meetings in UK and Europe with Working Groups in Dosimetry, Modelling, Microbiology, Food Irradiation, Plant Operations (safety, regulations, source transport)
  - Members influence development of national and international standards and regulations through ISO and ASTM committees
  - Runs courses in dosimetry, microbiology
- Modelling Working Group:
  - Currently conducting a review of commonly-used Monte Carlo codes
- Other organisations:
  - iiA
  - RPSMUG

Modelling Working Group Code Review

- Code Review:
  - Looked at several MC codes
  - Identified main features including
    - Usability
    - Physics included
    - Operating system requirements
    - Cost
- Considerations:
  - Trying to provide users with basic information on each code
  - Make an initial choice of the code most suited to their requirements
- Excluded from consideration:
  - Point Kernel methods
    - Unsuited to electron beam
    - Lack of accuracy in dose-rate prediction for more detailed models
  - Thermal modelling

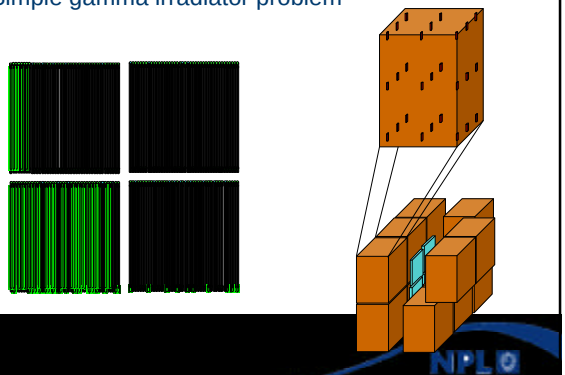
Codes considered

- EGSnrc
  - State-of-the-art electron-photon shower code
  - Very complex geometry input
- Egspp
  - New C++ front end for EGSnrc, macro-based geometry and source inputs
- MCNP
  - Mainly MCNP4C2 in current Code Review but also considering MCNPX (MCNP4 no longer available from NEA Databank)
- MCBEND
  - Serco Assurance commercial code
  - Also MCFANG
- GEANT4
  - “Toolkit” for development of models which can be very complex

Simple gamma irradiator problem

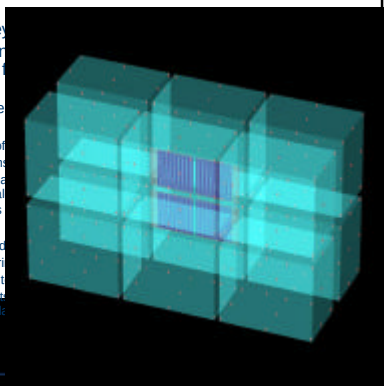
- Object: Create a simplified gamma irradiator with all the main features expected, model this with several different codes, compare results and features
  - Not a code validation in this sense
  - Not a benchmark – simply a comparison exercise
- Vault problem:
  - 12 boxes of low-density water
  - 3 x 3 x 3 array of perspex dosimeters in each box
  - 4 modules of 42 cobalt-60 pencils in source rack
  - Vault surrounded by a concrete shield
- Results
  - Doses and dose rates
  - How easy to code
  - How long to run

Simple gamma irradiator problem



EGSnrc/egspp:

- Set up by Mark Bailey
- Egspp: New C++ fron
  available from NRC, f
  commercial use)
  - Geometry comprehe
  - Pluses
    - Easy generation of
    - Good visualisations
    - Uses state-of-the-a
      spectra directly cal
    - Runs on Windows
  - Minuses
    - Not a 'finished' cod
    - Geometry numberi
    - Care needed in int
    - Repeated element
      used to generate la

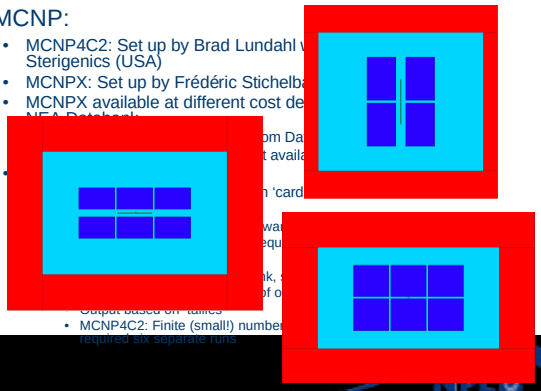


MCBEND:

- Set up by Pat Cowan at Serco
- Serco code, available commercially
  - Developed for nuclear applications
  - Geometry and materials input straightforward with comprehensive checking
  - Pluses
    - Physics built in
    - Very good geometry plotting and debugging, using standard geometric entities, nesting, etc
    - Straightforward coding syntax
  - Minuses
    - Slightly expensive – not really a problem for MCBEND's main target markets
    - MCFANG: Photons only, no electrons

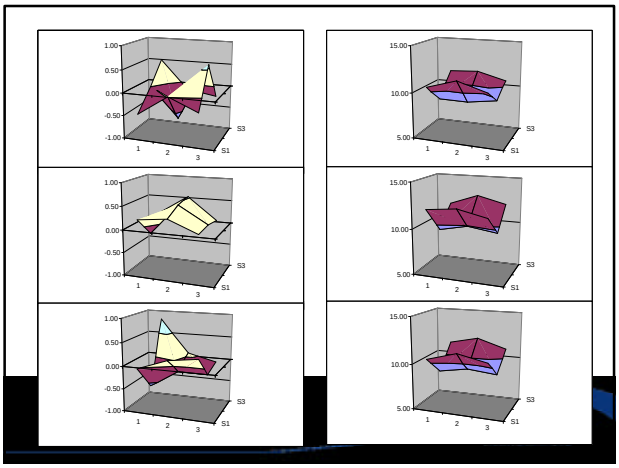
MCNP:

- MCNP4C2: Set up by Brad Lundahl
  Sterigenics (USA)
- MCNPX: Set up by Frédéric Stichelba
- MCNPX available at different cost de
  NEA Databank
- om Da
  t availa
- n 'card
- wa
  equ
- nk,
  of o
  Output based on 'tallies'
- MCNP4C2: Finite (small!) numbe
  required six separate runs



GEANT4:

- Being set up by David Shipley (NPL)
- Available free from Geant4 websites
  - MC toolkit based on C++
  - Not a standalone code: Requires significant programming knowledge
  - Pluses
    - Extremely flexible
    - Can have physics of many particle types and energies included
  - Minuses
    - Need to be familiar with C++ objects
    - Need to be a competent physicist to get the best out of any code, but particularly perhaps with this one!
- Model not yet completed



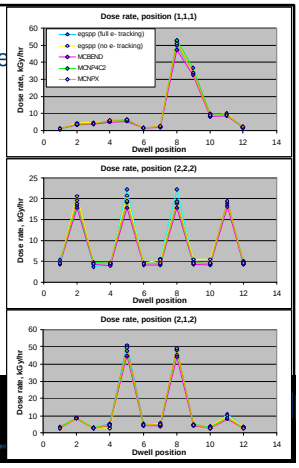
Results from different codes:

- Programming effort:
  - A simple model like this, set up in ~ couple of days for most codes
- Run times:
  - All codes: A few hours (on a modern PC) for a few hundred million histories
  - Longer for the higher accuracy obtained from full tracking of secondary electrons, where this is available
- Overall results:
  - Uncertainties ~ 2%

Average dose rates - kGy/hour	egspp - no electron tracking (effectively kerma)	egspp - with electron tracking	MCBEND - dose based on kerma	MCNPX - dose based on kerma	MCNP4C2 - dosed based on simple electron tracking
Max dose rate average	12.20	12.70	11.17	12.42	12.10
Min dose rate average	8.45	8.52	7.99	8.69	8.70
DUR	1.44	1.49	1.40	1.43	1.39

Results from different code

- Dose rates:
  - Again, very similar between each code (statistical uncertainties ~ 4 – 6%)
  - Need to be careful in geometries with significant symmetry
- General notes:
  - Different ways of scoring dose in different codes: Care required when comparing results between codes
  - Different tallies in MCNP require care in assignment of materials in detector volumes (e.g. f4 and f6 tallies)



Summary:

- The Irradiation Panel Modelling Working Group has produced a Code Review document, describing the main features of several of the more widely-used MC codes
- This document will be reviewed and updated regularly
- Several codes have been used to model a simplified irradiation cell, while retaining all the main features
- Results and techniques from all codes have been compared
  - Has pointed up some interesting differences in how codes are set up, so care is required in interpretation of results from some codes
  - Note this is not a validation or a benchmark
  - Benchmarking different codes for industrial use is a project being followed by RPSMUG (the Radiation Processing Simulation and Modelling Users Group), based in USA
  - A particular validation for a detailed egspp/EGSnrc calculation discribed in next presentation

References:

1. Irradiation Panel Code Review: www.irradiationpanel.org
2. EGSnrc/egspp: I Kawrakow and DWO Rogers: The EGSnrc Code System: Monte Carlo Simulation of Electron and Photon Transport NRCC Report PIRS-701, November 2003
3. MCNP4/5: http://mcnp-green.lanl.gov/index.html
4. MCNPX: http://mcnpx.lanl.gov/
5. MCBEND: http://www.sercoassurance.com/ANSWERS/
6. Geant4: Geant4 Collaboration, “Geant4 – A Simulation Toolkit”, Nuclear Instruments and Methods, A506, pp. 250 – 303