QinetiQ

User Requirements Document

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Abstract

The user requirements are described for a computer code to be used to simulate microdosimetry in geometries representing features of a semiconductor device. The tool is intended to be based on the Geant4 radiation transport simulation toolkit, which can or will simulate proton nuclear and electromagnetic, and electron interactions in the energy range applicable to microdosimetry effects induced by the space radiation environment. The Geant4-based Microdosimetry Analysis Tool (GEMAT) will be integrated into the ESA SPENVIS web-based space environment simulation tool-set. The output of the code will be text files, including comma-separated variable data files of the calculated energy deposition spectra.

Record of changes

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Issue	Date	Detail of changes
0.a	10 July 2001	First issue to reviewers in draft form
0.b	12 July 2001	Second draft following comments from Sira and QinetiQ reviewers.
0.c	2 August 2001	Third draft following initial input from ESA.
0.d	8 October 2001	Fourth draft following further comments from ESA.

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1 Introduction

1.1 Contractual

This document has been issued by QinetiQ Space Department and Sira Electro-Optics Ltd for ESA/ESTEC under contract 14968/00/NL/EC (ESA Technology Research Programme, Space Environment and Effects Major Axis), in part fulfilment of milestone 2 “development of user requirements for radiation effects shielding tools”.

1.2 Purpose of the Document

This document describes the user requirements for a Geant4-based Microdosimetry Analysis Tool (GEMAT) to allow assessment of single event effects in semiconductor devices, including the assessment of simultaneous energy deposition in several sensitive regions (potentially leading to multiple bit upsets).

1.3 Scope of the Software

GEMAT will utilise the Geant4 radiation transport toolkit as the basis of the simulation to treat the run-management, geometry tracking, physical interaction processes and user interface. Specifically, GEMAT shall use Geant4 4.0, and will interact with and be accessible via the ESA SPENVIS system.

1.4 Definitions, acronyms and abbreviations

ASCII	American Standard Code for Information Interchange
BIRA	Belgisch Instituut voor Ruimte-Aëronomie
CERN	Conseil Europeen pour la Recherche Nuclaire
CRÈME	Cosmic Radiation Effects on Micro-Electronics
CSV	comma-separated value
ESA	European Space Agency
ESTEC	European Space Technology Centre
Geant4	C++ toolkit for Monte Carlo simulation of high-energy, fundamental particle transport, developed by an international collaboration led by CERN.
GEMAT	Geant4 Microdosimetry Analysis Tool
GUI	graphical user interface
HETC	High-Energy Transport Code
OO	object-oriented
PDF	probability distribution function
SPENVIS	SPace ENvironment Information System

UR user requirement

URD User Requirements Document

UrQMD Ultra-relativisitic Quantum Molecular Dynamics

1.5 References

[1] The CERN Geant4 Collaboration provides a significant amount of references information: http://wwwinfo.cern.ch/asd/geant4/geant4.html
From this Web page, access can be obtained to User Documentation:

[2] User Guide for Application Developers: http://wwwinfo.cern.ch/asd/geant4/geant4_public/G4UsersDocuments/UsersGuides/ForApplicationDeveloper/html/index.html

[3] User Guide for Toolkit Developers: http://wwwinfo.cern.ch/asd/geant4/geant4_public/G4UsersDocuments/UsersGuides/ForToolkitDeveloper/html/index.html

[4] The Physics Reference manual: http://wwwinfo.cern.ch/asd/geant4/geant4_public/G4UsersDocuments/UsersGuides/PhysicsReferenceManual/html/index.html

[5] The Software Reference manual provides information on the public methods to the Geant4 classes: http://geant4.kek.jp/cgi-bin/G4GenDoc.csh?flag=1

[6] The parent project reference is the proposed 'ESA Radiation Effects Analysis Tools', QINETIQ/KI/SPACE/7/36/8/2. This parent project is itself defined in Work Order contract 14968/00/NL/EC, file reference QINETIQ/KI/SPACE/7/36/8/1/1 as modified by the minutes of meetings (QINETIQ/KI/SPACE/7/36/8/1/3).

[7] Geant4-based Microdosimetry Analysis Tool: Software Project Management Plan QINETIQ/KI/SPACE/SPMP011037.

[8] Guide to applying the ESA software engineering standards to small software projects, ESA BSSC(96)2 Issue 1, May 1996.

The Booch notation will be used for the OO analysis and design diagrams. Good references for this notation are:

[9] 'Object-Oriented Analysis and Design with Applications', Booch G. – 2nd ed., Addison Wesley Publishing Company, 1994

[10] 'Designing Object Oriented Applications using the Booch Method', Robert C. Martin, Prentice Hall, 1995

Good references used for the C and C++ languages are:

[11] 'C++ Nuts and Bolts for Experienced Programmers', Herbert Schildt, Osborne McGraw-Hill, 1995.

[12] C++ How to Program', Deitel and Deitel – 2nd ed., Prentice Hall, 1998.

2 General Description

The general requirement of this software project is to design and implement in the C++ language, and test a set of classes which, when instantiated as objects at run-time, communicate with run-time objects instantiated in the Geant4 toolkit. This software will allow definition of a geometry structure, representing part of a microelectronics device, and an incident particle source. The Geant4 toolkit will provide the user-interface, run-management, geometry tracking, simulation of physics processes, and flagging of ionisation energy loss in different parts of the geometry. The software will then tally these events to generate a summary of the pulse-height energy deposition spectrum (from particle ionisation) in each volume, including information about simultaneous energy deposition in different volumes.

2.1 Product perspective

The Geant4 toolkit is a suite of over 1200 C++ classes which will constitute the vast majority of the simulation code making up the executable GEMAT. GEMAT should include a 'main ()' routine and supporting classes capable of being compiled and linked with the bulk of the Geant4 class libraries. Together, this main routine shall instantiate objects from the selection of classes which then form the dynamic model of the software. The classes should have public interfaces that permit communication, access and control over the Geant4 Monte-Carlo simulation process as a whole.

This project will lie predominantly within the scope of an "Application Developer" as defined in the Geant4 user requirements document, Geant4-URD-v6.4, §2.4.1 (see the CERN Geant4 web pages [1]). However, some of the output of the project may add to the Geant4 toolkit of class libraries and therefore some of the development activity is within the scope of a "Framework Provider". The Geant4 User's Guide for Application Developers is considered highly relevant.

2.2 General capabilities

2.2.1 Geometry definition (UR 1)

The user shall be able to define a geometry representing the features of a semiconductor device using a selection of geometric volumes. The dimensions of these volumes, composition, and material density and relative position shall be variables defined by the user. The user shall also be able to associate one or more threshold energies with each volume, identifying the sensitivity of depleted regions to a change in device state. The user shall be able to associate a funnel length with non-depleted or inactive regions (ionisation in these regions will be considered to contribute to the charge collection to an adjacent depleted region).

2.2.2 Source particle definition (UR 2)

The user shall be able to specify the source particle (species, spectrum and angular distribution). It shall also be possible to define the number of primary particle histories to simulate, and a normalisation factor (the incident particle fluence).

2.2.3 Selection of application scenario (UR 4)

The user shall be able to specify the application scenario and in doing so select the physical interaction processes to be applied to the simulation. The user should also be able to specify variance reduction techniques to apply to the simulation that will improve the efficiency of the calculation.

2.2.4 Section of output (UR 4)

The simulation tool shall be able to provide histogrammed output (in text format) of particle ionisation energy deposition spectra within each volume, and details of the number and type of coincidence events where energy deposition exceeds the threshold levels of more than one active volume. GEMAT should also provide the incident particle fluence as a function of depletion region and particle species. If the source particle is a geantino, the default output shall be a path-length distribution function as a function of volume.

2.2.5 User Interface requirements (UR 5)

GEMAT shall be controlled through ASCII text input, either using a standard terminal (without GUI) or macro-file. Output will be in the form of ASCII text to the terminal screen and, if requested by the user, to one or more CSV (comma-separated value) files.

GEMAT will be required to operate as part of the SPENVIS system (§2.6). As such, the user will enter parameters associated with the required simulation through a web-page, and view or download the results (text files or graphs). The requirement is therefore that the text-file input and output be compatible with the SPENVIS system.

It shall be possible to visualise the geometry for confirmation of correct definition.

2.2.6 Performance requirements (UR 6)

The code should be able to provide a rapid microdosimetry analysis for the user-defined geometry. [However, it is difficult to specify the performance as the efficiency will depend upon the type of interactions important for initialising energy deposition (whether direct ionisation by incident particles or from recoiling nuclei), and variance reduction schemes implemented.]

2.3 General constraints

2.3.1 Use of and consistency with Geant4 code (UR 7)

GEMAT will be based on the Geant4 4.0 toolkit. Any new code shall be consistent with existing Geant4 code in terms of modularization and coding approaches.

2.3.2 Quality requirements (UR 8)

The GEMAT code shall be developed to ESA PSS-05 standards for small software projects [8].

2.4 User characteristics

The user will have a basic understanding of the space radiation environment, interaction processes with materials, and single event phenomena arising from direct ionisation and nuclear interactions. The user should be able to use a text editor on the host machine to view and modify the controlling parameters for this software, or in the case of implementation of GEMAT under the SPENVIS system, he/she should be able to input information through a web-page interface. People wishing to extend or modify this code should possess a good understanding of the C++ programming language and at least a basic understanding of a recognised OO analysis and design process and corresponding notation such as Booch or UML. (It is not expected that users undertake this task.)

2.5 Operational environment (UR 9)

GEMAT will be tested using the following platforms:

1. Sun Ultra 1 Workstation
   HD space - sufficient for installation and running Geant4 4.0
   Solaris 2.7 operating system
   Sun Workshop C++ compiler 5.2

2. IBM compatible PC
   Pentium II 500 MHz processor
   128MB memory
   HD space - sufficient for installation and running of Geant4 4.0
   Linux operating system (Redhat 6.2)
   GNU gcc compiler which has g++ 2.95.2

Geant4 guidelines state that it is a necessary and sufficient condition that the software be demonstrated to operate without error on *two* different platforms (under different operating systems).

2.6 Assumptions and dependencies

It is assumed that the physics processes are modelled through existing classes implemented in Geant4, or currently being developed for the toolkit. This software project will **not** involve the development or implementation of any new physical processes. The key physical process missing, which is relevant to the space radiation environment is the treatment of the nuclear interactions of protons or light heavy ions. It is presently understood that the intranuclear cascade code (a re-engineering of HETC) will be available by the end of 2001 in Geant4 4.0 to address proton-nuclear interactions. However, models such as Ultra-relativistic Quantum Molecular Dynamics (UrQMD) model, which will treat nuclear-nuclear interactions, are being developed by the Geant4 collaboration on a longer time-scale.

In addition, the treatment of volume-dependant particle cut-offs is a feature that is a consideration for GEMAT (UR 1.7), and variance reduction for "path-length shrinking" a requirement (UR 3.4) - neither of these are currently treated within Geant4. The inclusion of these facilities in the tool is dependant upon the implementation of such variance reduction features within Geant4 4.0. It is further assumed that Geant4 4.0 is released on 17 December 2001.

GEMAT is intended to be accessible to users of the SPENVIS system, with the code operating on computers at BIRA, Belgium. It is assumed that the developers of the SPENVIS system will be responsible for developing:

- web-page interfaces (GEMAT/web-page);
- utilities to convert text-file data output to graphics files.

It is further assumed that suitably powerful PC/Linux or Sun platforms (see §2.5) are available at BIRA or QinetiQ to operate GEMAT – in the latter case these would be tasked by the SPENVIS system. (Note that contract 14968/00/NL/EC includes provision for the purchase of a computer or computers, potentially for this purpose.)

Execution times for GEMAT may be significantly longer than other programs in the SPENVIS suite, depending upon the detail of the microdosimetry study. It is assumed that the GEMAT simulation will not be killed, except after a maximum execution time (set by the SPENVIS System Administrator) or cancel signal sent by the user (see URs 5.7, 5.8, and 5.9).

It is recommended that definition of the geometry through the web page should, if possible, be similar to that used to define geometries for shielding analysis in SPENVIS.

3 Specific Requirements

3.1 Geometry definition (UR 1)

UR ID	Description of Requirement
UR 1.1	The user shall be able to define the geometry in terms of a collection of simple bodies (see Appendix A), with covering or underlying layers.
UR 1.2	It shall be possible to define volumes representing depleted regions as having trapezoidal vertical cross-sections (see Appendix A).
UR 1.3	It shall be possible to locate rectangular parallelepiped shapes above the other parts of the geometry to represent contact structures.
UR 1.4	The user shall be able to define the dimensions and positions of the volumes, thicknesses of overlying/underlying layers, and chemical composition and density of the materials.
UR 1.5	The user shall be able to define one or more threshold energies associated with state-change for the volumes representing depleted regions, or a funnel length for non-depleted regions / inactive regions.
UR 1.6	The user shall be able to define the visualisation attributes associated with each volume (see UR 5.5).
UR 1.7	Consideration should be given to allowing the user to apply different cut-off lengths as a function of layer, in order to make the simulation more efficient.
UR 1.8	The maximum number of volumes representing depletion zones shall be restricted to 20.

3.2 Source particle definition (UR 2)

UR ID	Description of Requirement
UR 2.1	The user shall be able to define the incident particle type as geantino, electron, photon, proton, neutron or ion (defined by atomic and nucleon number and excitation state of the nucleus, and charge state of the atom).
UR 2.2	The user shall be able to define the incident particle spectrum as mono-energetic, power-law, exponential, or a piece-wise fit (linear, power-law or exponential) to data.
UR 2.3	The user shall be able to define the source either as a trapped proton or electron spectrum generated by SPENVIS trapped particle models, a solar proton spectrum generated by the SPENVIS solar particle event models, or cosmic ray nuclei defined by CREME, or from a MULASSIS output (input spectrum assumed to be for a single particle species).
UR 2.4	The source particles shall be incident over a rectangle or circle located above (+z) or below (-z) the geometry (see Appendix A). The user shall be able to define the position and dimensions of the rectangle/circle.
UR 2.5	The user shall be able to define the incident particle angular distribution as unidirectional (incident at a specific θ and ϕ to the geometry), isotropic (*i.e.* PDF varies as $\sin\theta$) or cosine-law (*i.e.* PDF varies as $\sin\theta\cos\theta$)
UR 2.6	The user shall be able to specify the normalisation factor in terms of the incident particle fluence, expressed in particles/cm^2 or particles/m^2.
UR 2.7	By default the source particle fluence shall be 1 cm^{-2}.
UR 2.8	The user shall be able to specify the number of primary particle histories to simulate.

UR ID	Description of Requirement
UR 2.9	The default number of primary particle histories shall be 10,000.

3.3 Selection of application scenario (UR 3)

UR ID	Description of Requirement
UR 3.1	The user shall be able to select the application scenario to be applied in the simulation, and based on this the appropriate physical processes within Geant4 should be invoked (see Appendix B).
UR 3.2	If the scenario is not specified, a default set of physical processes shall be applied subject to the source particle and energy (see Appendix B).
UR 3.3	The user shall be able to change the initial random number seed in order to perform several shielding calculations for the same shield and source to increase the statistical accuracy of the results.
UR 3.4	The user should be able to apply variance reduction techniques to the particle transport and interaction processes [TBD].

3.4 Selection of output (UR 4)

UR ID	Description of Requirement
UR 4.1	The user shall be able to define the quantities to be histogrammed. Output quantities shall be particle fluence incident upon depleted regions, pulse-height ionising energy-deposition spectra, details of coincidence events and (for geantino particle sources) path-length distributions, all normalised to the incident particle fluence.
UR 4.2	The particle fluence incident on depleted regions shall be calculated as a function of depletion volume.
UR 4.3	The particle fluence incident on depleted regions shall be calculated as a function of particle species.
UR 4.4	The particle fluence incident upon the depletion volumes shall be determined as a function of particle energy, according to an energy binning scheme entered by the user.
UR 4.5	The user shall be able to select the units of particle fluence as either particles/μm^2, particles/cm^2 or particles/m^2.
UR 4.6	The default units of particle fluence shall be particles/cm^2.
UR 4.7	Values of particle fluence shall include associated errors based on Poisson statistics.
UR 4.8	Pulse-height energy deposition shall be calculated as a function of volume.
UR 4.9	Three distinct types of pulse-height energy deposition spectra shall be calculated for: energy associated with charge collection in the depletion region alone; for charge collection from the funnel only; and associated with charge collection from both regions.
UR 4.10	For energy deposition in depleted regions, the energy shall be calculated based on the *total* energy deposited in the volume – even if the volume is complex, and a particle enters, leaves and then re-enters the volume, the energy deposition is determined from the sum of both paths through the volume.

UR ID	Description of Requirement
UR 4.11	The user shall be able to define a binning scheme for the energy deposition spectrum
UR 4.12	The user shall be able to select the units of energy deposition as eV, keV or MeV.
UR 4.13	The default units of energy deposition for energy deposition spectra shall be MeV.
UR 4.14	The energy deposition spectra shall include associated errors based on Poisson statistics.
UR 4.15	Details of coincidence events shall be output as a function of the depletion volume and threshold energy.
UR 4.16	Poisson errors associated with the number of coincidence events shall be provided.
UR 4.17	Path-length distributions shall be output as a function of each depletion volume.
UR 4.18	The user shall be able to define a binning scheme for the path-length.
UR 4.19	The user shall be able to select the units of path-length as actual linear dimensions (*i.e.* μm, mm, cm, m, km) and areal mass (*i.e.* mg/cm^2, g/cm^2, and kg/m^2)
UR 4.20	The default units of path-length shall be mg/cm^2.
UR 4.21	Poisson errors associated with the path-length distributions shall be provided.

3.5 User interface requirements (UR 5)

UR ID	Description of Requirement
UR 5.1	The user shall be able to control the GEMAT through a simple (dumb-) terminal interface.
UR 5.2	It shall be possible for GEMAT to process commands/run-parameters held in an ASCII text file.
UR 5.3	Output (run results and tabulated histograms) shall be to the terminal and/or data file in ASCII text format
UR 5.4	Histogram results to a data file shall be in CSV format.
UR 5.5	It shall be possible to visualise the geometry to confirm its accurate definition, and particle tracks in the geometry.
UR 5.6	If implemented under SPENVIS, the user shall be able to control GEMAT through a web-page interface.
UR 5.7	GEMAT shall provide a prediction of the execution time, based on the time take to process the first few primary particle histories.
UR 5.8	If the expected execution time exceeds the System Administrator – defined maximum execution time, the user shall be informed of this.
UR 5.9	The user should be able to interrupt execution of the simulation in a controlled fashion, so that the results obtained are recorded to the output files before the process is killed.

3.6 Performance requirements (UR 6)

UR ID	Description of Requirement
UR 6.1	TBD

3.7 Use of and consistency with Geant4 code (UR 7)

UR ID	Description of Requirement
UR 7.1	GEMAT shall be based on the Geant4 4.0 toolkit.
UR 7.2	The new software shall be consistent with existing Geant4 code in terms of modularization and coding practice, provided it does not conflict with UR 8.

3.8 Quality requirements (UR 8)

UR ID	Description of Requirement
UR 8.1	GEMAT shall be developed to ESA PSS-05 standards for small software projects.
UR 8.2	The software design will be based on a thorough OO decomposition of the problem.

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Appendix A Geometry definition

The GEMAT geometry shall be defined in terms of one or more active volumes (cylinder, rectangular parallelepiped, 'L' and 'U' shape volumes) corresponding to depleted regions of the semiconductor (see Figure A.1). These shall be embedded in a non-depleted region, and have non-depleted and/or inactive layers above and below (see Figure A.2).

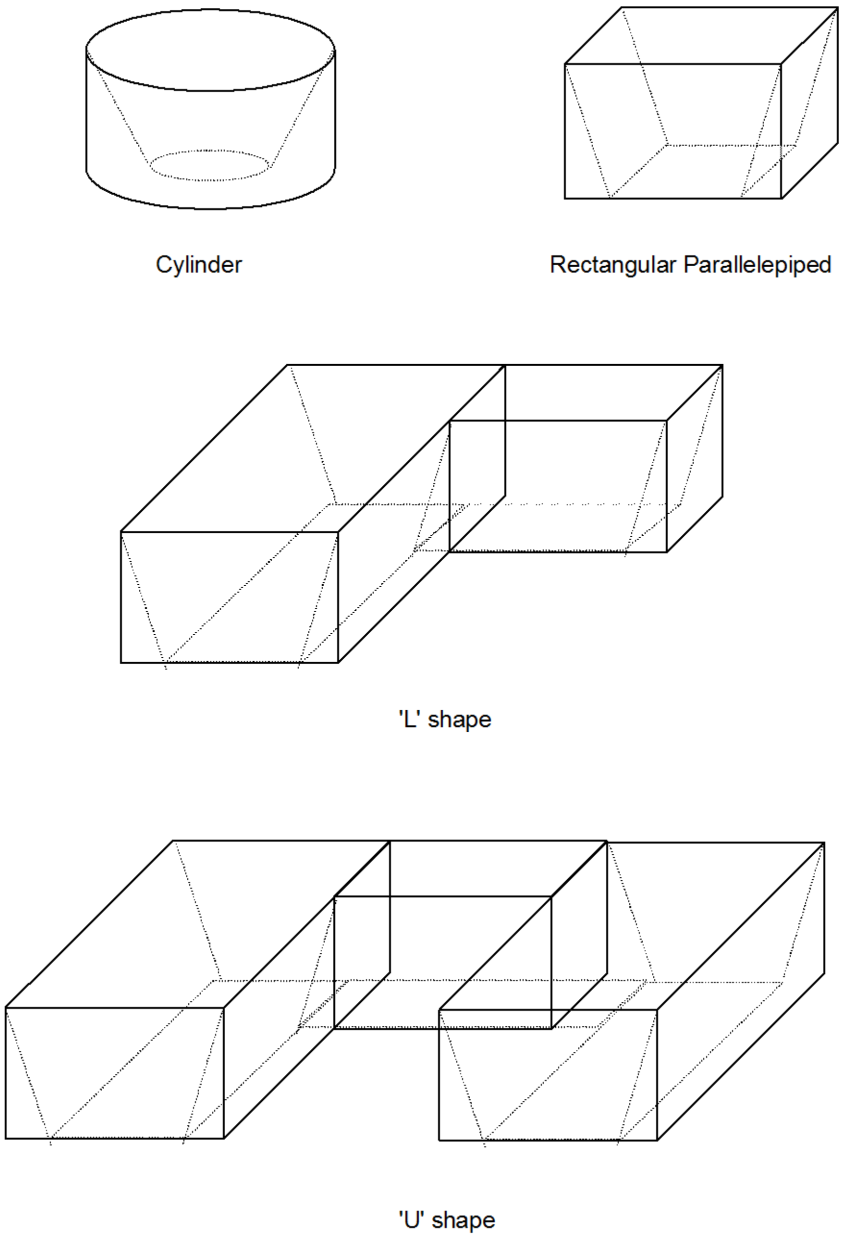

Figure A.1: Possible active volumes.

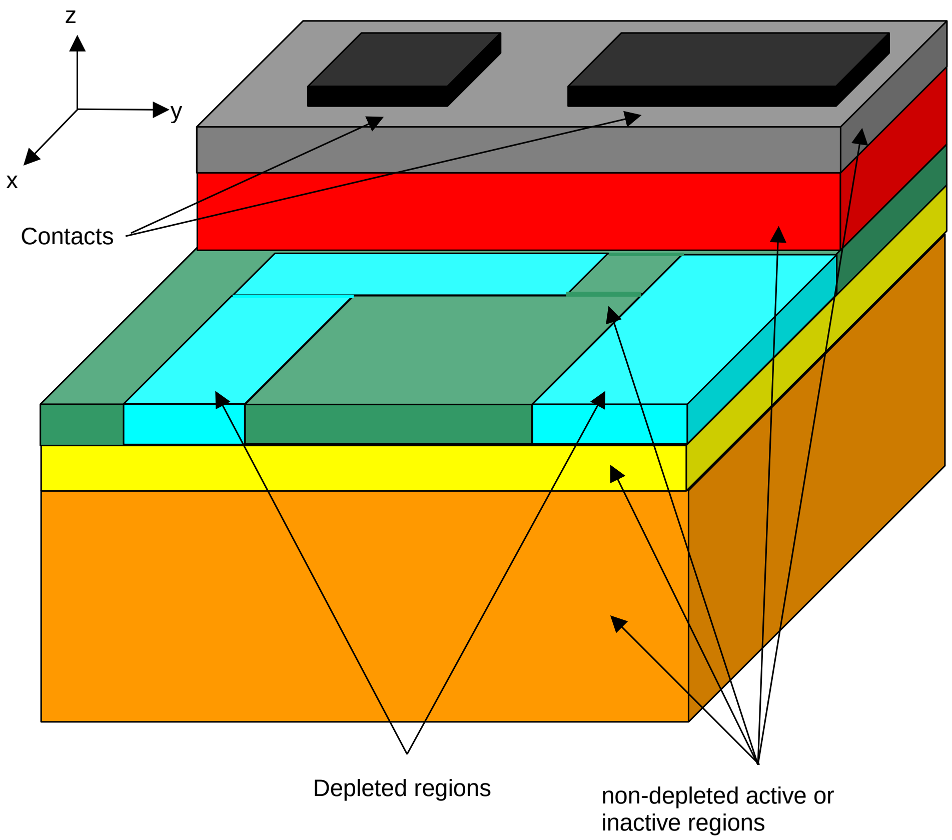

Figure A.2: Example geometry showing depleted and non-depleted or inactive layers.

It shall be possible to define the volumes representing depleted regions as having "tapered" edges so that the vertical cross-section is trapezoidal (indicated by dotted lines in figure A.1).

Appendix B Application scenarios

Particle	Energy Range of source	Physics Processes	Application Scenario
Geantino	all	G4Transportation	Path length analysis (PATH)
proton	20 – 600 MeV	low-energy EM neutron_hp precompound low-energy hadron or INC[1] or kinetic[2]	Mono, trapped and solar Protons (LE proton)
	20 MeV – 100 GeV	Above + high-energy hadron	Mono and cosmic ray protons (HE Proton)
alpha	all	As above + UrQMD[3] instead of INC or kinetic	Mono, solar and cosmic ray alphas (Alpha)
neutron	thermal -20MeV	neutron_hp	Reactor, fission, D-T, D-D sources (LE neutron)
	up to ~1 GeV	As above + precompound INC[1] or kinetic[2]	Spallation neutrons (HE neutron)
electron	10 keV – 30 MeV	Std EM or low-energy EM	Mono, trapped and planetary electrons (Electron)

[1]Intra-nuclear cascade mode (based on HETC), due for release with Geant4 4.0 (December 2001)
[2]Kinetic model – release date is not known.
[3]Ultra-relativisitic Quantum Molecular Dynamics model – release date is not known.

Table B.1: Cross-reference of applications to Geant4 physics models employed.