serco

Serco Assurance

MCFANG – A Monte Carlo Forward Adjoint Neutron Gamma code

Presentation to
MCNEG 2004

by
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The ANSWERS Software Service
Serco Assurance

Overview

- The ANSWERS Software Service of Serco Assurance
- Status of Computational Methods
- Overview of MCFANG
- Multigroup Data
- Variance Reduction
- Graphical User Interface
- MCFANG Example
- Summary

The ANSWERS Software Service

- The main activity of Serco Assurance’s ANSWERS Software Service is supplying :
  - **High Quality Software**
  - **Consultancy Services**
- for customers world-wide in the areas of
  - **Radiation Shielding**
  - **Reactor Physics**
  - **Criticality**
  - **Nuclear Data**

Radiation Shielding Software

- MCBEND
  - A generalised 3D Monte Carlo code for all radiation transport applications.
- RANKERN
  - A 3D point kernel method for design and assessment of gamma-ray shielding.
- MCFANG
  - A simplified 3D multigroup Monte Carlo code.
- *Our products are workstation and PC based and are differentiated from competitor products by a combination of versatility, ease of use and a dedicated delivery and support service.*

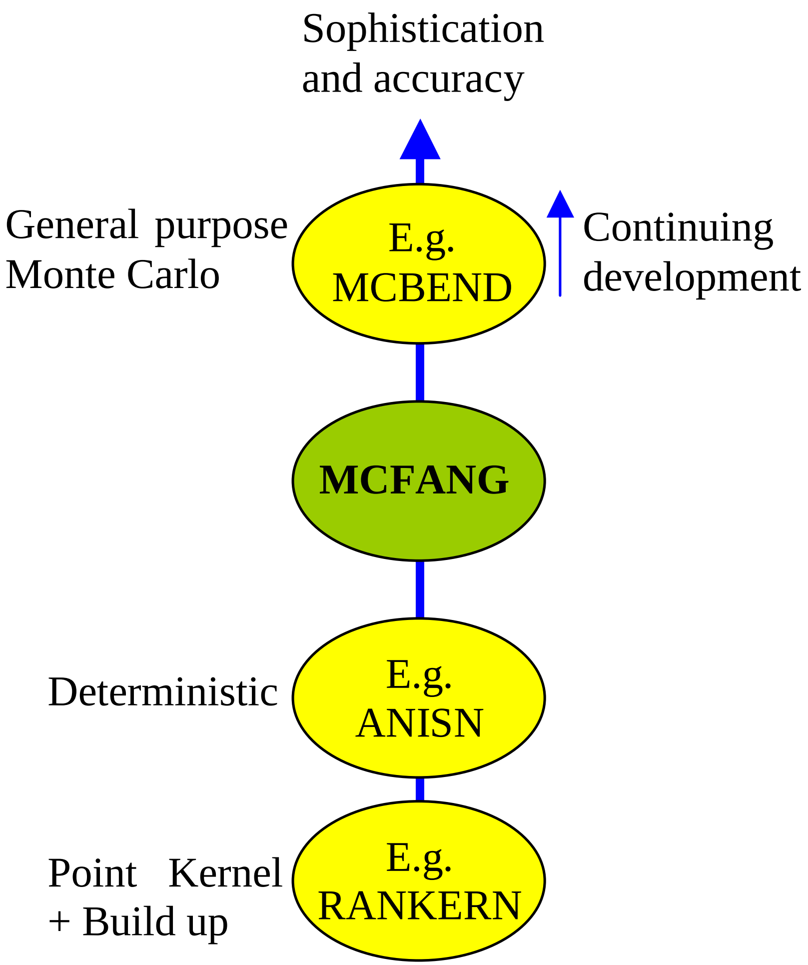
Computational Method Status - 20th Century

- Deterministic Codes
  - Relatively fast (= inexpensive to execute)
  - Very restricted geometry modelling
  - Multigroup nuclear data
  - Results sensitive to modelling simplifications such as mesh spacing, angular quadrature, group scheme.

- Monte Carlo Codes
  - Relatively slow (= expensive to execute)
  - Accurate geometry modelling
  - Detailed nuclear data
  - Results are accurate within reported statistical uncertainty.

Computational Method Status - 21st Century

- Computers are now faster and computing power is cheap and abundant
- Monte Carlo is usually the preferred method but requires expertise.
- Manpower is an expensive commodity
- MCFANG
  - Simplified Monte Carlo
  - Intermediate between deterministic methods and general purpose codes.
- **M**onte **C**arlo **F**orward **A**djoint **N**eutron **G**amma



MCFANG Summary

- Retains the full geometry and source modelling capabilities of MCBEND
- Uses multigroup data for collision processing.
- Handles neutron, gamma or coupled n,γ calculations.
- Executes in forward or adjoint modes – or both
- Includes simple, robust variance reduction methods:
  - Spatial variation relative to defined lines superimposed on the physical geometry
  - MIDWAY variance reduction
- Input is aided by a Graphical User Interface.

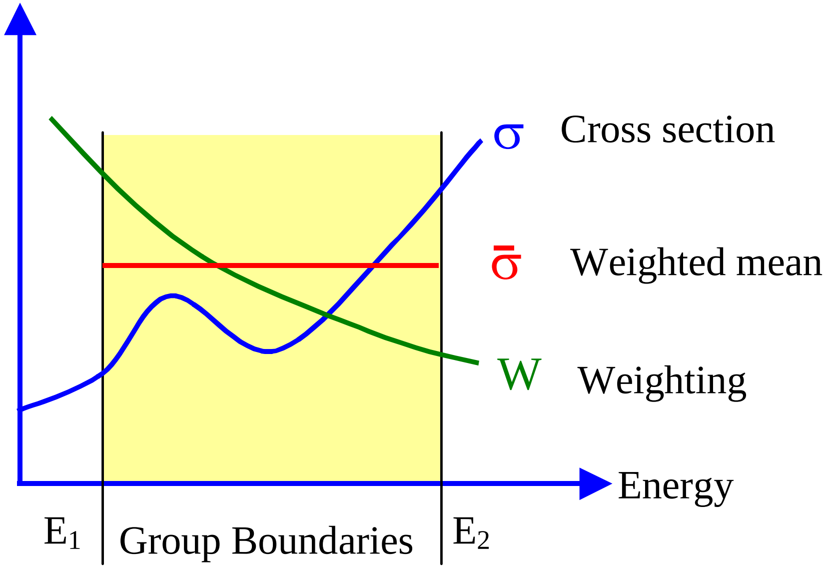
Multigroup Data

- Multigroup data is less accurate than point energy data since fine structure of cross section variation is averaged over each group. However:

  A significant advantage of multigroup data is the ability to execute calculations in forward and/or adjoint mode.

- The multigroup libraries used by MCFANG are specifically generated for Monte Carlo use.
- The data are derived by sampling from the point energy libraries used by MCBEND.
- New libraries are readily generated for energy group schemes relevant to a given class of problem.

Multigroup Cross Sections



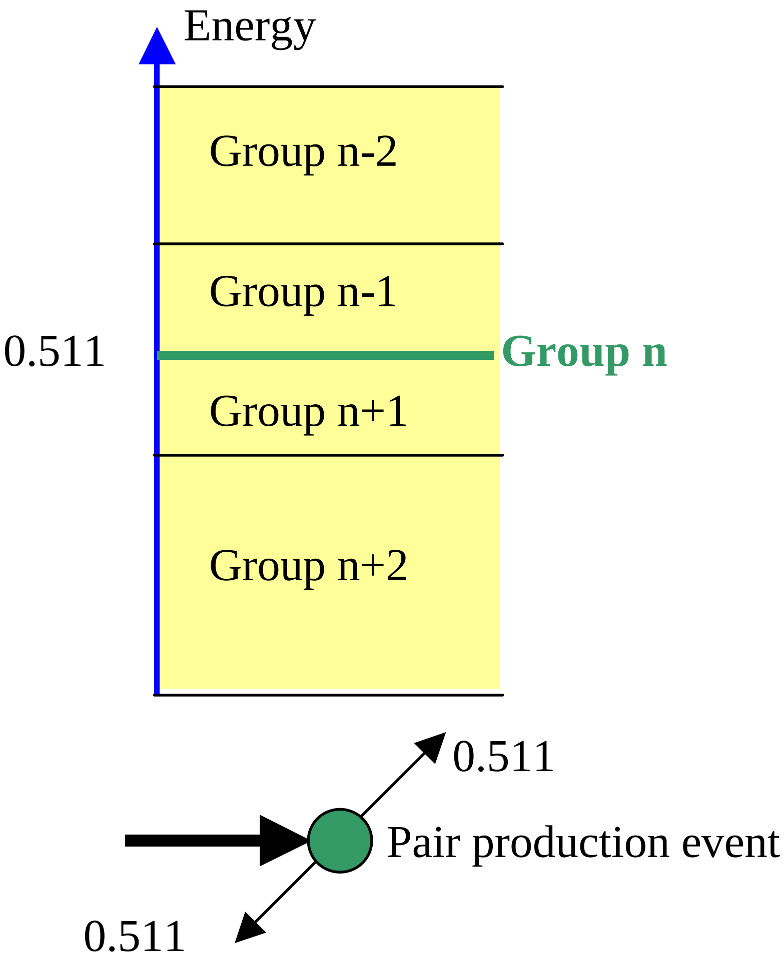
$$\bar{\sigma} = \frac{\int_{E_1}^{E_2} \sigma W dE}{\int_{E_1}^{E_2} W dE}$$

Weighting functions include:

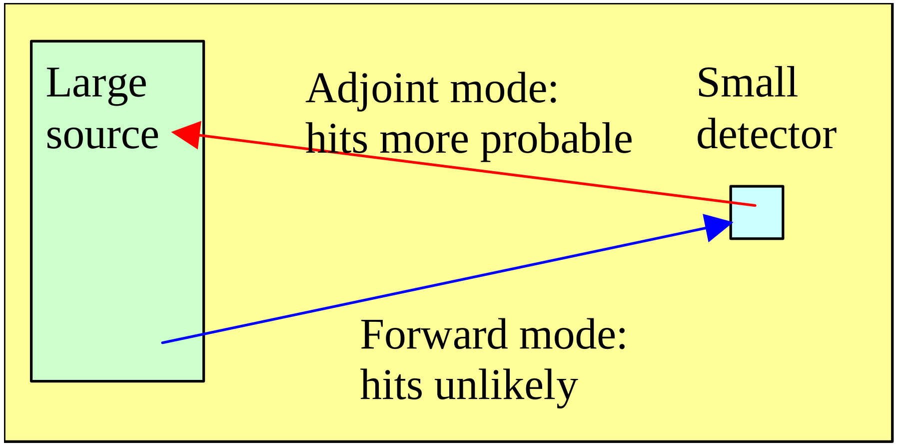
- No weighting
- Fission spectrum
- Inverse energy
- Maxwellian (for thermal neutrons)
- Σ_t (total cross section)

Pair Production

- The multigroup library generation code inserts a line energy at 0.511 MeV into the gamma group scheme
- This allows pair production events to be identified and treated appropriately.
- Two secondary gammas with energy 0.511 MeV are emitted in opposing directions.

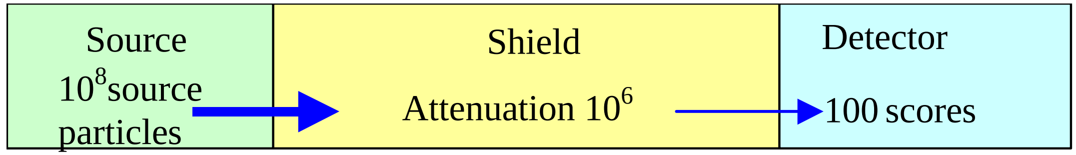


Adjoint Mode

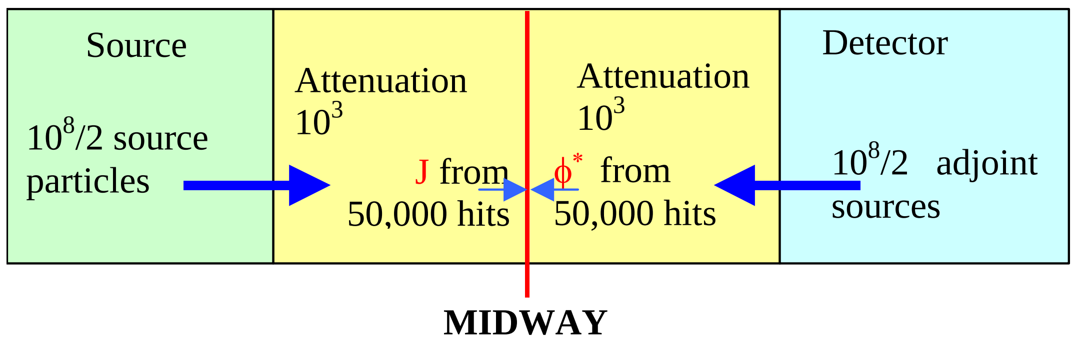


- The source becomes the detector; the source spectrum becomes the response function.
- The detector becomes the source; the response function becomes the source spectrum
- MCFANG performs these transpositions internally and presents response scores as final results.
- Multiple detectors may be defined.

MIDWAY Variance Reduction

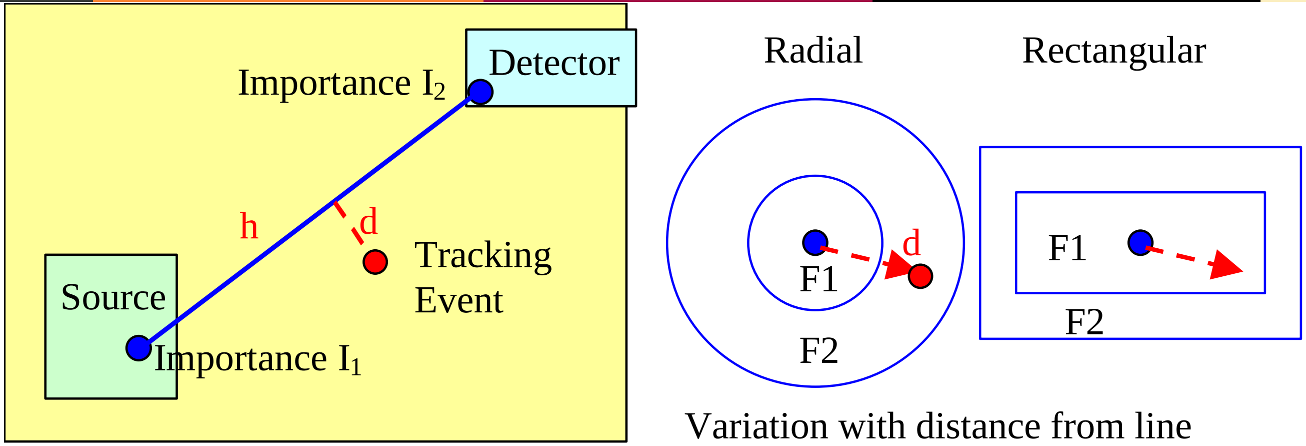


Example analogue scenario



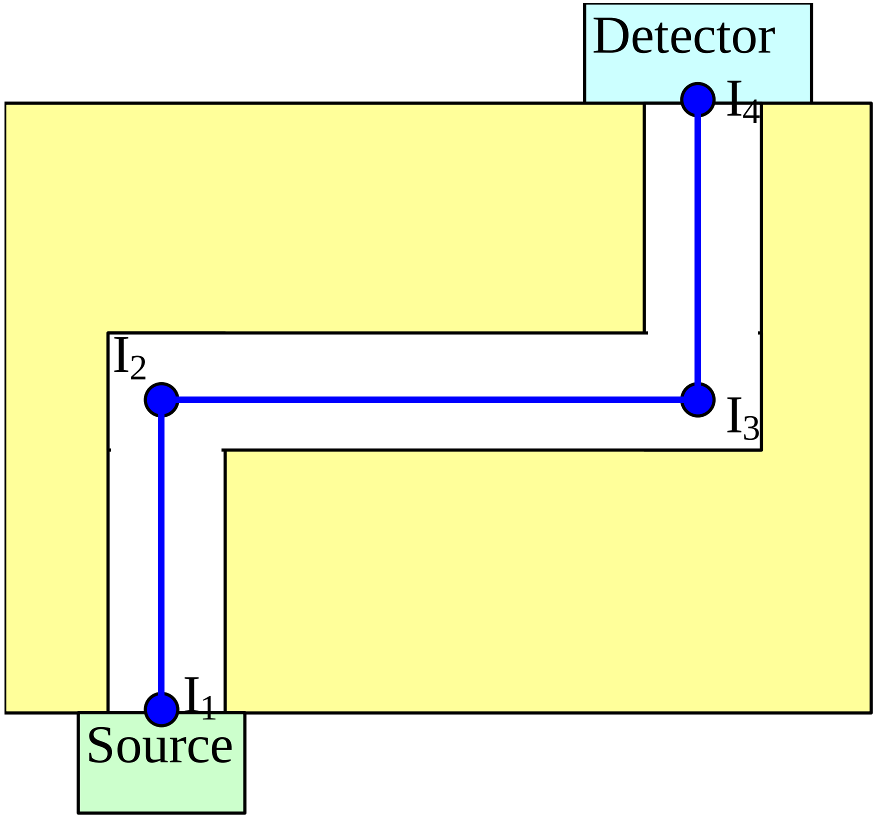
- In the MIDWAY method the detector response is calculated by combining the forward current J and the adjoint flux ϕ^* at an arbitrary surface between source and detector. (J and ϕ^* are scored in subdivisions of the surface in a range of angular bins)
- MCFANG carries out both parts of the calculation and combines the forward/adjoint scores in a single run.

Line Variance Reduction - Outline



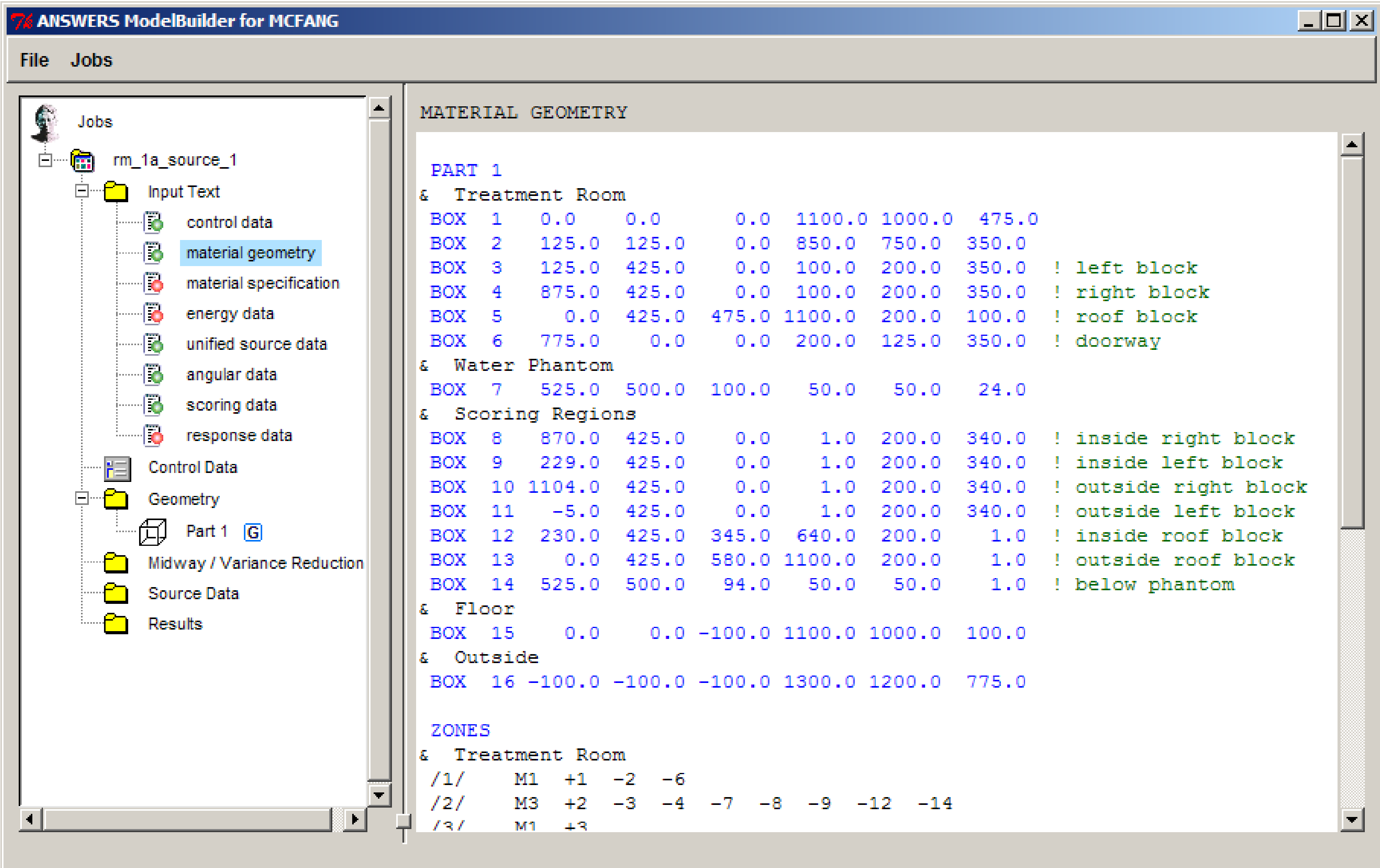
- The importance at a point in the particle history is determined by its projected distance (h) along the line and its normal distance (d) from it.
- An importance is interpolated at h between the values defined at the ends of the line (I_1, I_2). An exponential variation is assumed.
- A factor is applied according to the distance of the point from the line. The factors F_1, F_2 etc. and the off-line boundaries are supplied by the user.

Line Variance Reduction – Multiple Lines

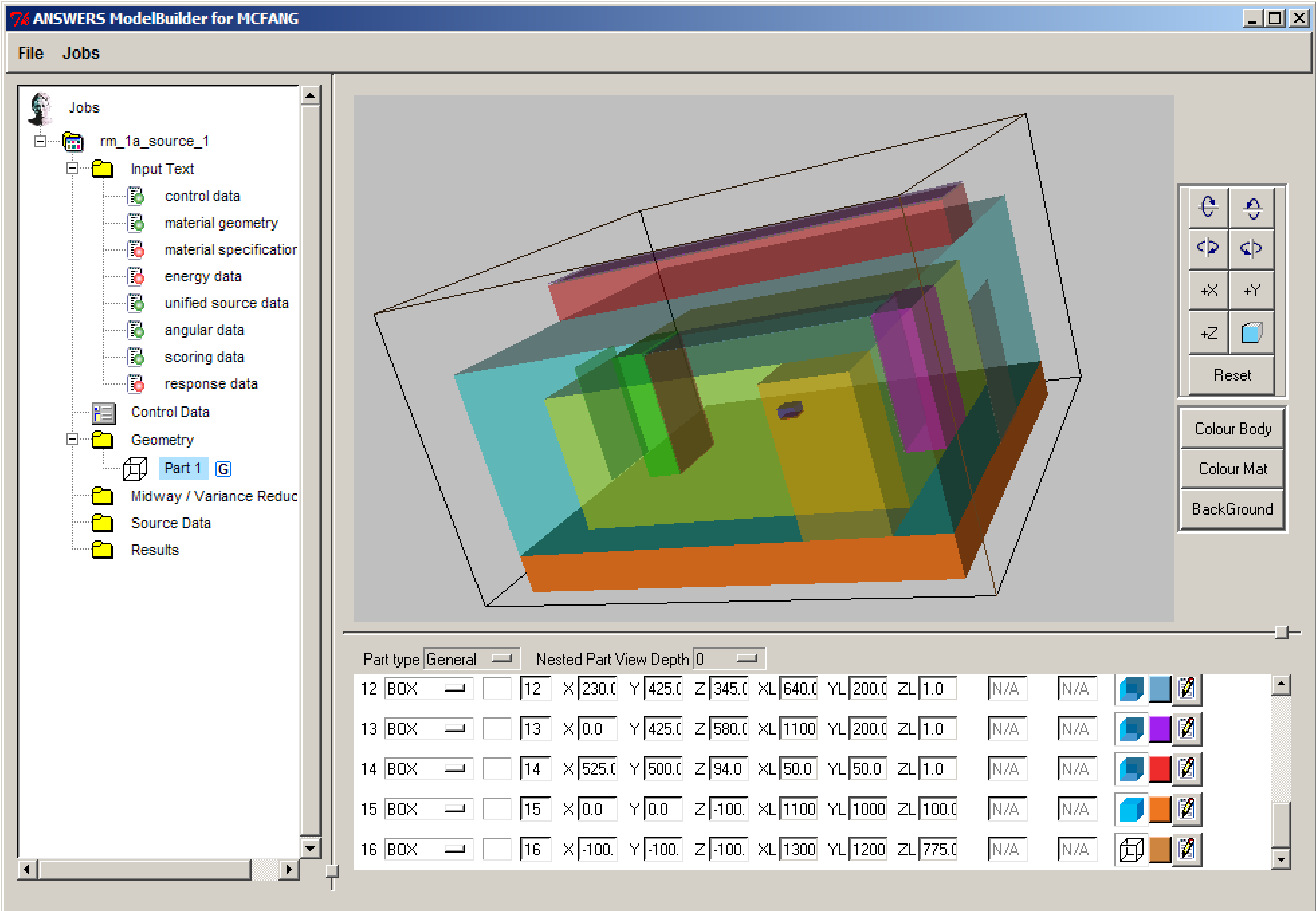


- Multiple lines may be defined.
- The importance at a point is derived from the nearest line

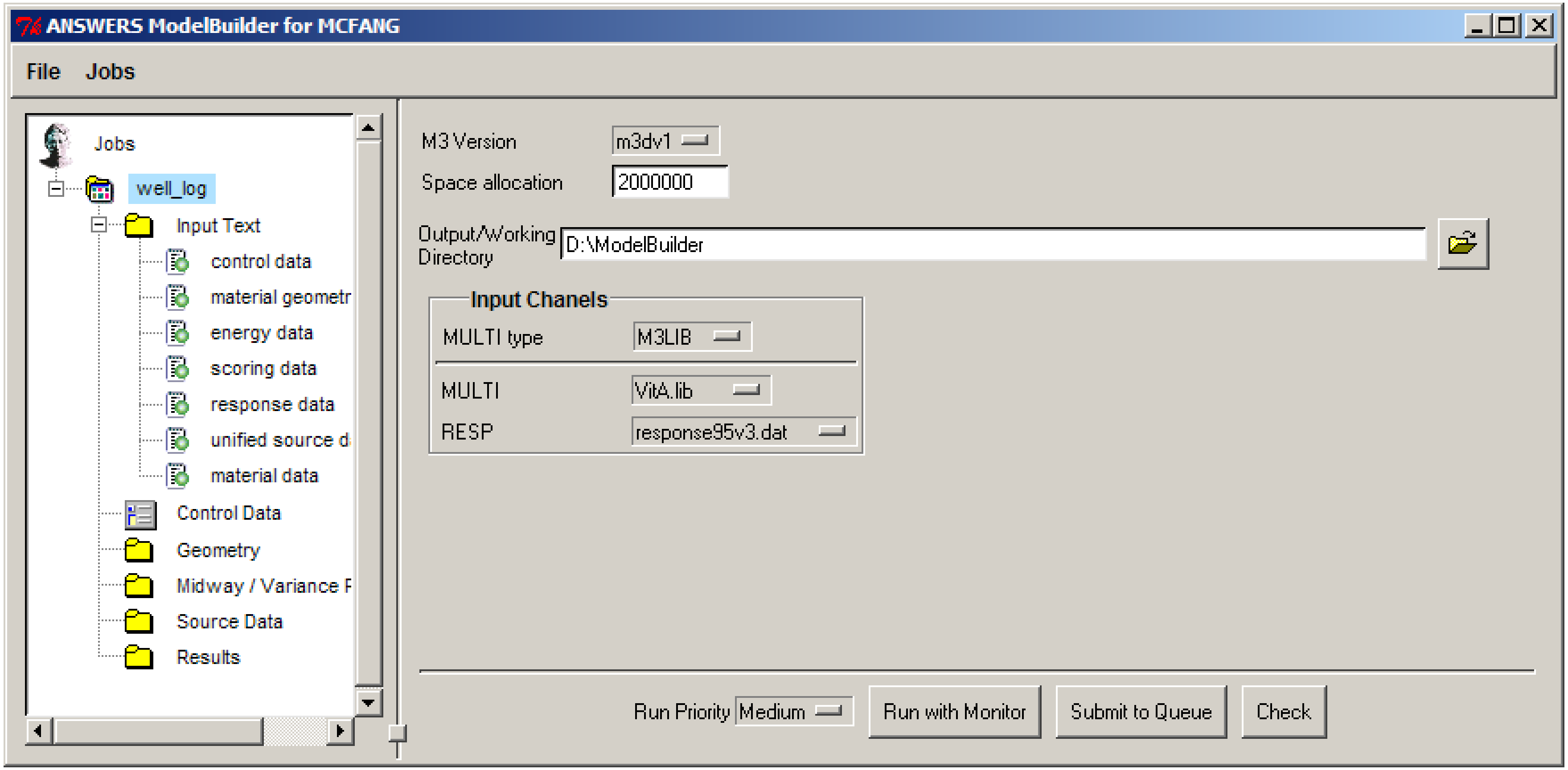
Graphical User Interface – Material Geometry



Graphical User Interface – Geometry Display



Graphical User Interface – Run / Check Window



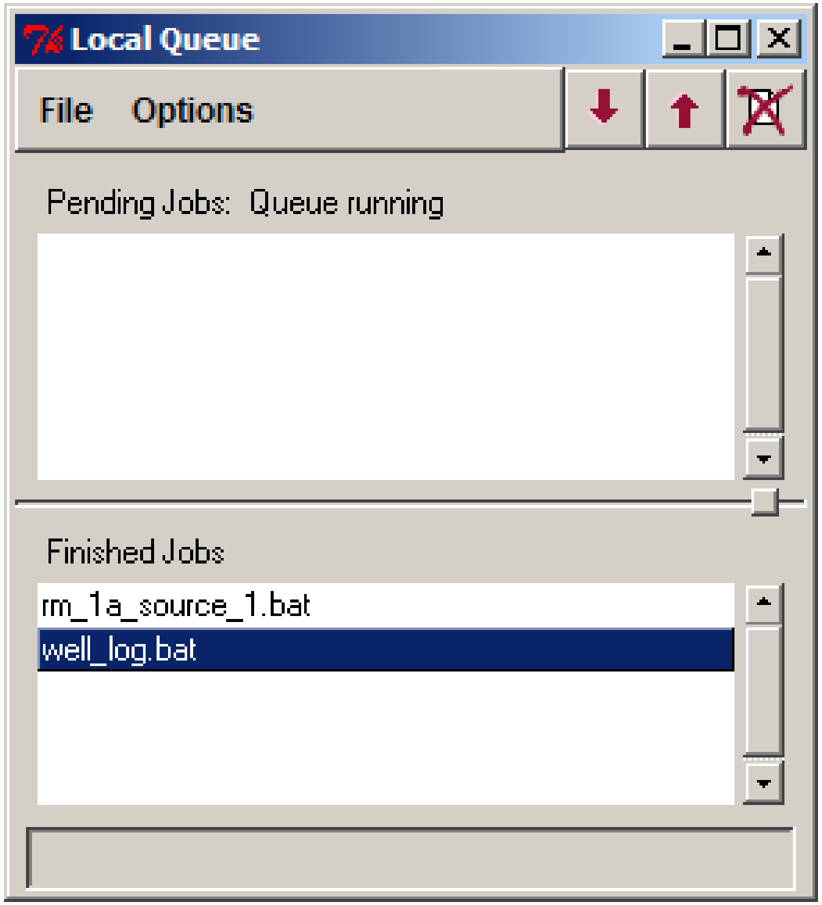
Graphical User Interface – Check Function

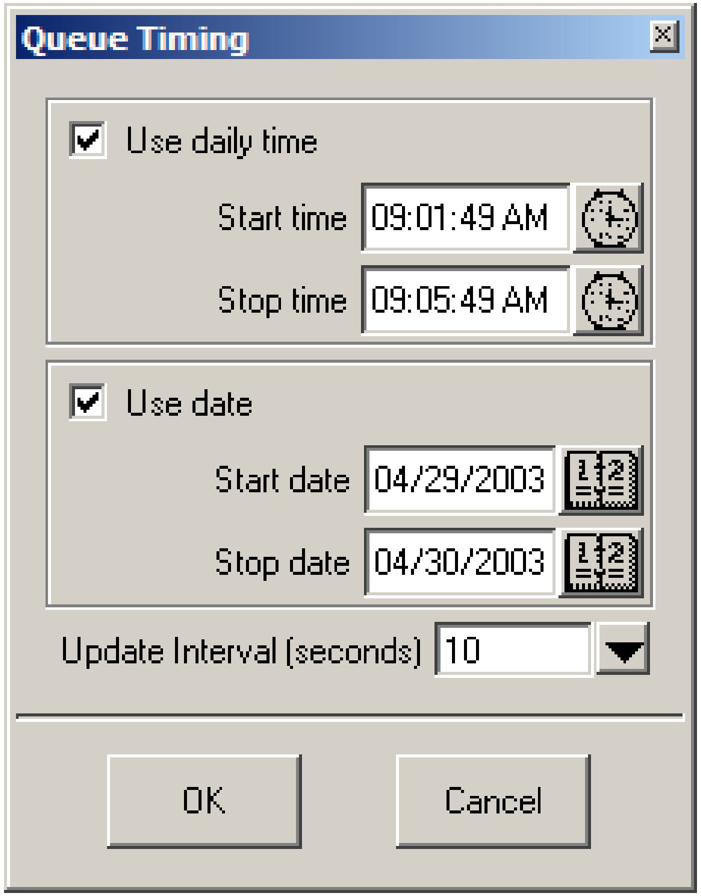
Output file from checking run for rm_1a_source_1

```
FILE C:\DOCUME~1\ADAM_B~1\LOCALS~1\Temp\mb_tmp\rm_1a_source_1.out  Created 09:56 05/03/04
 &
     Free format reading told to echo comment lines only to channel  6

 qb: BEGIN Energy Data
 qx: ERROR of type  1 in RKARD routine RKARDT
 qx  Unrecognised word in field  1 of line 118:
 qx   GAMMA

    The next phrase should be one of the following:
     BEGIN
     END
     MULTIGROUP
     SCORING
     UNIFIED(SOURCE)
     WEIGHTED(COLLISIONS)
     DATA

 qx: Reading error in routine INEDAT    when trying to:
 qx  Read ENERGY DATA control keyword.

     Status of free format reading: Field  1 line number 118 reads:
      GAMMA
     The RKARD processing identified   1 fields.
     Field Type      Start  End  Repeats  Contents
       1   WORD          2      6      0        GAMMA

     Skipped to the end of the input unit after error
```

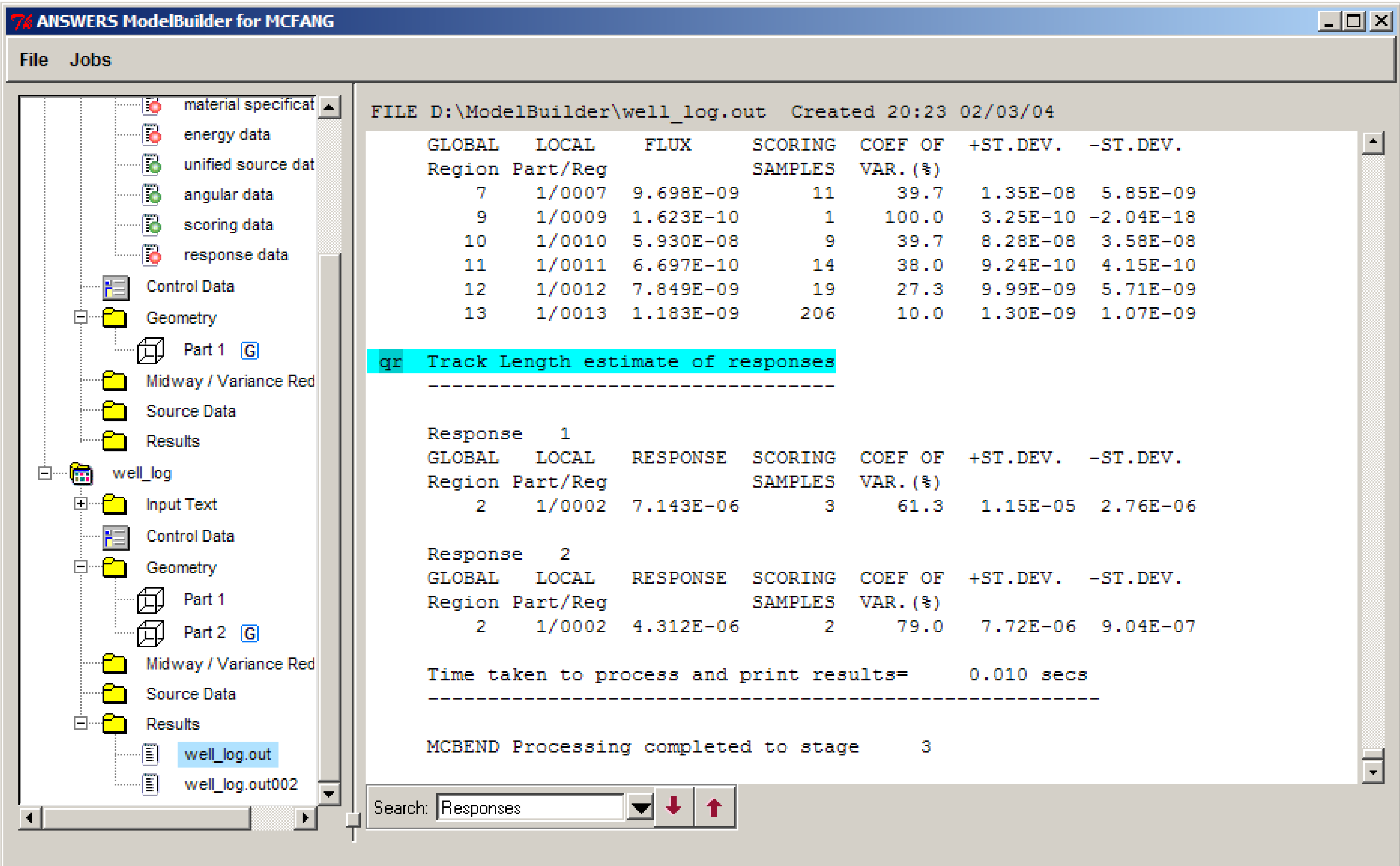
Search: Error Message

Graphical User Interface – Submitting Calculations

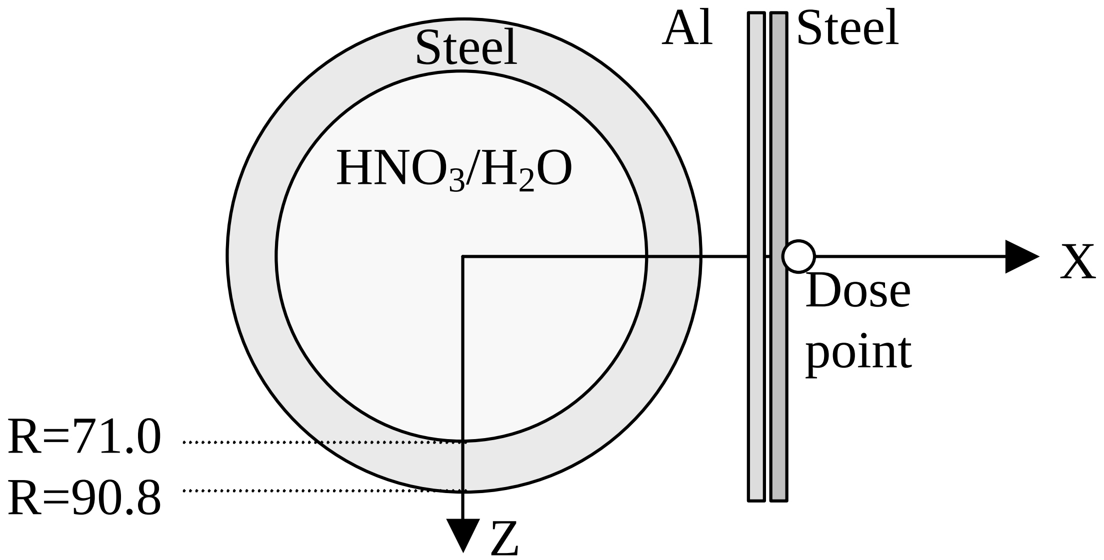




Graphical User Interface – Results



Application Example



- Simple steel vessel containing active liquor
- Dose point off the surface behind some steel and aluminium plates

MCBEND Run

- MCBEND scoring region - 1cm thick normal to the X axis, its lateral extent in the Y and Z directions is between co-ordinate limits ±10cm.
- This still represents a fairly small target so a splitting mesh was required to accelerate the problem. An XYZ mesh with dimensions 30 x 13 x 30 was overlaid on the problem. A diffusion adjoint (‘MAGIC’) calculation was carried out to obtain an importance map.
- Result (gamma dose rate) = 0.313 ± 4.78%.
  Execution time 42 minutes (50M samples)
  Estimated time for σ = 5% = 38min
- In this example source points were sampled uniformly over the entire volume of the active liquor. A more efficient calculation would have been to use automatic weighting to concentrate on that part of the source closest to the detector.

MCFANG Run - Adjoint

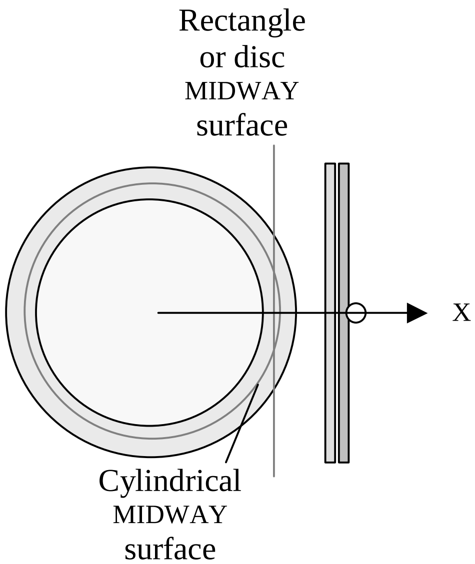
- A number of options are available for solving this case with MCFANG. Given that the source is large and the detector small, an adjoint calculation is favoured.
- A scoring region was specified corresponding to that in the MCBEND calculation. The keywords **ADJOINT AUTO** were included to invoke an adjoint calculation.
- Result (gamma dose rate) = 0.360 $\pm$ 5.1%.
  Execution time 7.6 minutes (50M samples)
  Estimated time for σ = 5% = 7.9min
- In principle, this adjoint calculation could have been carried out using MCBEND. However, it would require significant user effort to interchange the source and detector definitions. MCFANG takes care of this process internally.

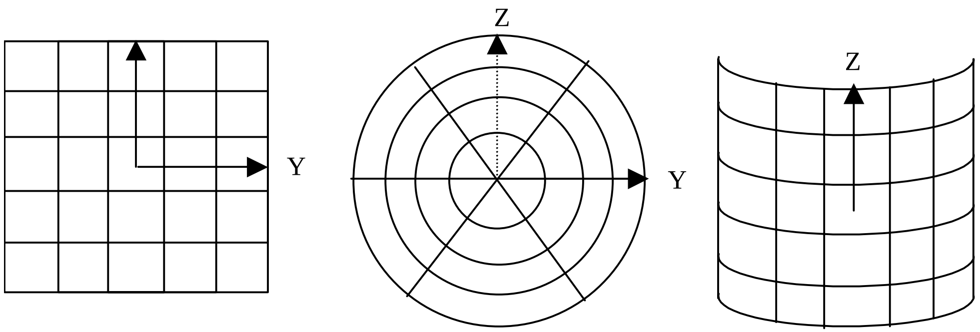
MCFANG Run – Midway Method

- The midway method scores the adjoint flux from the detector and the forward current from the source at a surface placed between the two.
- The surface is divided spatially and the fluxes/currents are scored as a function of polar angle about the surface normal and azimuthal angle within the surface. The forward and adjoint results are combined to give the net score at the detector.
- Three forms of surface are available in MCFANG
  - A rectangular plane surface normal to one of the co-ordinate axes. The surface may be subdivided by an orthogonal mesh.
  - A disc normal to one of the co-ordinate axes. The surface may be subdivided radially and azimuthally
  - A cylindrical shell with axis parallel to the Z axis. The surface may be divided azimuthally and axially.

MCFANG Run – Midway Method

- All three variations were tried:





Rectangle at X=78 Disc at X=78 Cylinder R=80

- Nine azimuthal intervals and eight polar intervals were used for scoring the angular distribution of the fluxes and currents in each spatial subdivision.

MCFANG Run – Midway Method

- The three alternatives gave equivalent results in similar execution times.

- <u>Rectangle</u>

Result (gamma dose rate) =	0.3381 $\pm$ 2.1%
Execution time (50M samples)	18 min
Estimated time for σ = 5% =	3.2 min

- <u>Disc</u>

Result (gamma dose rate) =	0.3360 $\pm$ 2.1%
Execution time (50M samples)	19 min
Estimated time for σ = 5% =	3.3 min

- <u>Cylinder</u>

Result (gamma dose rate) =	0.3587 $\pm$ 2.3%
Execution time (50M samples)	19 min
Estimated time for σ = 5% =	4.0 min

Current Status of MCFANG

- The MCFANG code has been fully developed.

- In the next few months MCFANG will be applied to a variety of applications.
  - Applications where general purpose Monte Carlo codes may encounter difficulties (e.g. labyrinths with large voids)
  - Applications which are traditionally run by non Monte Carlo specialists including medical applications

- The Graphical User Interface is presently designed as a general purpose tool.
  - Full functionality will be developed over the coming months
  - The GUI can be tailored to specific applications

- Field trials of MCFANG would be encouraged.

Summary

- The ANSWERS Software Service of Serco Assurance
- Status of Computational Methods
- Overview of MCFANG
- Multigroup Data
- Variance Reduction
- Graphical User Interface
- MCFANG Example
- Current Status of MCFANG