Introduction to MCNP

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Overview

- 48000 lines of Fortran and 1000 lines of C code (500 person-years)
- Continuously evolving, by LLNL (now version 5, we will use version 4c)
- Exact transport solution, but takes time
- Successfully parallelized, a factor of 100 speedup is possible
Manual

OAK RIDGE NATIONAL LABORATORY
managed by
UT-BATTELLE, LLC
for the
U.S. DEPARTMENT OF ENERGY

RSICC COMPUTER CODE COLLECTION

MCNP4C

Monte Carlo N-Particle Transport Code System

Contributed by:
Los Alamos National Laboratory
Los Alamos, New Mexico

RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER
Input Deck

Title card
Three blocks (jungles of numbers):

Cell cards [block 1]

Surface cards [block 2]

Data cards (materials, physics) [block3]

Note that each part is separated by a single blank line.
General Card Format

• First line of the input deck is title line
• Input lines can not exceed 80 columns (insensitive to capital/small letters)
• Special characters:
  – C in column 1-5 denotes a comment
  – $ after input data denotes a comment
  – & after input data cont. of prev. line
  – blanks column 1-5 cont. of prev. line
Geometry specification

• Problem treated in terms of regions or volumes (cells) bounded by surfaces
• Cells are defined by intersections, unions and complements of regions

Union \((A \cup B)\)          Intersection \((A \cap B)\)

\(\# (A : B)\) is all space outside union \(A\) and \(B\) (complement)
Basic Cell Card Format – Block 1

\texttt{J M D GEOM PARAMS}

\begin{itemize}
\item J = cell number, starting in columns 1-5
\item M = material number (0 if cell is void)
\item D = cell material density
  \begin{itemize}
  \item * no entry if cell is a void
  \item * positive entry = atom number density (atom/barn-cm)
  \item * negative entry = mass density (gram/cc)
  \end{itemize}
\item GEOM = listed of bounding surfaces
\item PARAMS = optional cell parameters
\end{itemize}
Basic Surface Card Format – Block 2

\[ J \ A \ LIST \]

J=surface number, starting in columns 1-5
A=surface mnemonic
LIST=surface parameters

Example: a cylinder with a radius of 15 cm, extending with a z axis

1 cz 15 $ cylinder of radius 15 cm
# Key Surface Cards

<table>
<thead>
<tr>
<th>Mnemonic</th>
<th>Type</th>
<th>Description</th>
<th>Equation</th>
<th>Card Entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>plane</td>
<td>general</td>
<td>(Ax + By + Cz - D = 0)</td>
<td>A B C D</td>
</tr>
<tr>
<td>PX</td>
<td></td>
<td>normal to (x)-axis</td>
<td>(x - D = 0)</td>
<td></td>
</tr>
<tr>
<td>PY</td>
<td></td>
<td>normal to (y)-axis</td>
<td>(y - D = 0)</td>
<td></td>
</tr>
<tr>
<td>PZ</td>
<td></td>
<td>normal to (z)-axis</td>
<td>(z - D = 0)</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>sphere</td>
<td>centered at origin</td>
<td>(x^2 + y^2 + z^2 - R^2 = 0)</td>
<td>R</td>
</tr>
<tr>
<td>S</td>
<td></td>
<td>general</td>
<td>((x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2 - R^2 = 0)</td>
<td>(x \ y \ z \ R)</td>
</tr>
<tr>
<td>SX</td>
<td></td>
<td>centered on (x)-axis</td>
<td>((x-x_0)^2 + y^2 + z^2 - R^2 = 0)</td>
<td>(x \ R)</td>
</tr>
<tr>
<td>SY</td>
<td></td>
<td>centered on (y)-axis</td>
<td>(x^2 + (y-y_0)^2 + z^2 - R^2 = 0)</td>
<td>(y \ R)</td>
</tr>
<tr>
<td>SZ</td>
<td></td>
<td>centered on (z)-axis</td>
<td>(x^2 + y^2 + (z-z_0)^2 - R^2 = 0)</td>
<td>(z \ R)</td>
</tr>
<tr>
<td>C/X</td>
<td>cylinder</td>
<td>parallel to (x)-axis</td>
<td>((y-y_0)^2 + (z-z_0)^2 - R^2 = 0)</td>
<td>(y \ z \ R)</td>
</tr>
<tr>
<td>C/Y</td>
<td></td>
<td>parallel to (y)-axis</td>
<td>((x-x_0)^2 + (z-z_0)^2 - R^2 = 0)</td>
<td>(x \ z \ R)</td>
</tr>
<tr>
<td>C/Z</td>
<td></td>
<td>parallel to (z)-axis</td>
<td>((x-x_0)^2 + (y-y_0)^2 - R^2 = 0)</td>
<td>(x \ y \ R)</td>
</tr>
<tr>
<td>CX</td>
<td></td>
<td>on (x)-axis</td>
<td>(y^2 + z^2 - R^2 = 0)</td>
<td>R</td>
</tr>
<tr>
<td>CY</td>
<td></td>
<td>on (y)-axis</td>
<td>(x^2 + z^2 - R^2 = 0)</td>
<td>R</td>
</tr>
<tr>
<td>CZ</td>
<td></td>
<td>on (z)-axis</td>
<td>(x^2 + y^2 - R^2 = 0)</td>
<td>R</td>
</tr>
</tbody>
</table>
PWR Lattice

1100 11 -10.4  (-1100 100 -200) $fuel pin definition

1000 10 7.06685e-2 (1300 500 -600 300 -400 100 -200) $coolant

Blue – surface #
Red – cell #
Data specifications – Block 3

Defines:

- Type of particles
- Problem materials
- Radiation sources
- How results scored (tallies)
- The level of details for physics of particle interactions
- Cross section libraries
- …. and much more
Materials specification

Defines:

- Material unique number
- The elemental (isotopic) composition
- Cross section compilation to be used

ZAID number = ZZZAAA (ZZZ=atomic #Z, AAA=mass #A)

---

c WATER for neutron transport (by mass fraction)
(ignore H-2, H-3, O-17, and O-18)

M1  1001.60c  -0.11190  $ H-1 $ and mass fraction
    8016.60c  -0.88810  $ O-16 $ and mass fraction
Cross section specification

- Cross section data tables
  - Section III of Chapter 2 of MCNP manual
- Comprehensive list of cross sections – Appendix G, Table G2
- Sometimes available for elements
  - 24000.60c – natural chromium
- Sometimes natural elements need to be put together from isotopes
- Watch out for temperatures
  - Xsections available mostly for 300K
  - Doppler broadening important – if library at given temperature not available, needs to be generated using NJOY
Tally specifications

• Surface current tally $F_1$
  
  
  $$F_1 = \int_A dA \int_E dE \int_{4\pi} d\Omega \mathbf{n} \cdot \mathbf{J}(r_s, E, \Omega)$$
  
  *$F_1 = \int_A dA \int_E dE \int_{4\pi} d\Omega E \mathbf{n} \cdot \mathbf{J}(r_s, E, \Omega)$

  – Each time particle crosses a surface, it is added to tally

• Average surface flux tally, $F_2$

  
  $$F_2 = \frac{1}{A} \int_A dA \int_E dE \int_{4\pi} d\Omega \Phi(r_s, E, \Omega)$$
  
  *$F_2 = \frac{1}{A} \int_A dA \int_E dE \int_{4\pi} d\Omega E \Phi(r_s, E, \Omega)$
Tally specifications

• Average cell flux tally, F4

\[ F_4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \Phi(r, E, \Omega) \]

\[ \star F_4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega E \Phi(r, E, \Omega) \]
F4 Tally example

F4:N  CELL#
FC4:N YOUR COMMENTS HERE
E4:N 0.5E-6 20  $ ENERGY STRUCTURE
FM4:N  MULTIPLIERS
MCNP output tables

• Input listing
• Summary of particle loss/creation
• Summary of kcode (neutron criticality)
• Tallies and tally fluctuation charts
• Output controlled by print command
  – Print $ produce everything
  – Print 110 $ print basic + table 110
  – Print -110 $ All tables except 110
Output tables available

<table>
<thead>
<tr>
<th>Table No.</th>
<th>Table Description</th>
<th>Table No.</th>
<th>Table Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Source information</td>
<td>120</td>
<td>Importance function analysis</td>
</tr>
<tr>
<td>20</td>
<td>Weight windows information</td>
<td>126</td>
<td>Cell particle activity</td>
</tr>
<tr>
<td>30</td>
<td>Tally descriptions</td>
<td>128(b)</td>
<td>Universe map</td>
</tr>
<tr>
<td>35</td>
<td>Coincident detectors</td>
<td>130</td>
<td>Particle weight balances</td>
</tr>
<tr>
<td>40</td>
<td>Material compositions</td>
<td>140</td>
<td>Neutron/photon nuclide activity</td>
</tr>
<tr>
<td>50</td>
<td>Cell vols &amp; masses; surface areas</td>
<td>150</td>
<td>DXTRAN diagnostics</td>
</tr>
<tr>
<td>60(b)</td>
<td>Cell importances</td>
<td>160(d)</td>
<td>TFC bin tally analysis</td>
</tr>
<tr>
<td>62(b)</td>
<td>Forced coll.; expon. transform</td>
<td>161(d)</td>
<td>$p(x)$ tally PDF plot</td>
</tr>
<tr>
<td>70</td>
<td>Surface coefficients</td>
<td>162(d)</td>
<td>Cumulative $p(x)$ plot</td>
</tr>
<tr>
<td>72(b)</td>
<td>Cell temperatures</td>
<td>170</td>
<td>Source frequency; surface source</td>
</tr>
<tr>
<td>85</td>
<td>Electron range &amp; straggling</td>
<td>175</td>
<td>Estimated $k_{eff}$ by cycle</td>
</tr>
<tr>
<td>90</td>
<td>KCODE source data</td>
<td>178</td>
<td>Estimated $k_{eff}$ by batch size</td>
</tr>
<tr>
<td>98</td>
<td>Physics const.&amp; compile options</td>
<td>180</td>
<td>WWG bookkeeping summary</td>
</tr>
<tr>
<td>100(b)</td>
<td>Cross section tables</td>
<td>190(b)</td>
<td>WWG summary</td>
</tr>
<tr>
<td>102</td>
<td>S($\alpha, \beta$) nuclide assignment</td>
<td>198</td>
<td>WW from multigroup fluxes</td>
</tr>
<tr>
<td>110</td>
<td>First 50 starting histories</td>
<td>200(b)</td>
<td>WW generated windows</td>
</tr>
</tbody>
</table>

(d) = default, (b) = basic
MCNP statistics

• 1- relative error

<table>
<thead>
<tr>
<th>Range of $R$</th>
<th>Quality of Tally</th>
</tr>
</thead>
<tbody>
<tr>
<td>$&gt; 0.5$</td>
<td>Meaningless</td>
</tr>
<tr>
<td>0.2 to 0.5</td>
<td>Factor of a few</td>
</tr>
<tr>
<td>$&lt; 0.1$</td>
<td>Reliable (except for point/ring detectors)</td>
</tr>
<tr>
<td>$&lt; 0.05$</td>
<td>Reliable even for point/ring detectors</td>
</tr>
</tbody>
</table>

– Important but not sufficient information

• 2-figure of merit

$$FOM = \frac{1}{R^2 T},$$ T-run time

FOM should remain constant after early cycles
MCNP statistics

- Variance of variance (VOV)
  - R indicates precision of the tally mean
  - VOV indicates how accurate is the estimate of R
  - Hence relative variance of R calculated

\[
VOV = \frac{S^2(S_x^2)}{S_x^2} = \frac{\sum_{i=1}^{N}(x_i - \bar{x})^4}{\left[\sum_{i=1}^{N}(x_i - \bar{x})^2\right]^2} - \frac{1}{N}.
\]

- VOV should be always less than 0.1 for all tallies
### Example of tally fluctuation chart

<table>
<thead>
<tr>
<th>nps</th>
<th>tally 4 mean</th>
<th>tally 4 error</th>
<th>tally 4 vov</th>
<th>tally 4 slope</th>
<th>fom</th>
<th>tally 14 mean</th>
<th>tally 14 error</th>
<th>tally 14 vov</th>
<th>tally 14 slope</th>
<th>fom</th>
</tr>
</thead>
<tbody>
<tr>
<td>16000</td>
<td>2.5565E-19</td>
<td>0.1546</td>
<td>0.0460</td>
<td>0.0</td>
<td>13</td>
<td>1.6147E-20</td>
<td>0.1550</td>
<td>0.0990</td>
<td>0.0</td>
<td>13</td>
</tr>
<tr>
<td>32000</td>
<td>2.6267E-19</td>
<td>0.1057</td>
<td>0.0219</td>
<td>0.0</td>
<td>14</td>
<td>1.5614E-20</td>
<td>0.1308</td>
<td>0.0400</td>
<td>0.0</td>
<td>13</td>
</tr>
<tr>
<td>48000</td>
<td>2.9321E-19</td>
<td>0.0822</td>
<td>0.0129</td>
<td>10.0</td>
<td>15</td>
<td>1.5964E-20</td>
<td>0.0868</td>
<td>0.0228</td>
<td>0.0</td>
<td>13</td>
</tr>
<tr>
<td>64000</td>
<td>2.9096E-19</td>
<td>0.0725</td>
<td>0.0108</td>
<td>10.0</td>
<td>14</td>
<td>1.6062E-20</td>
<td>0.0760</td>
<td>0.0189</td>
<td>0.0</td>
<td>13</td>
</tr>
<tr>
<td>80000</td>
<td>2.9088E-19</td>
<td>0.0655</td>
<td>0.0086</td>
<td>10.0</td>
<td>14</td>
<td>1.6037E-20</td>
<td>0.0687</td>
<td>0.0161</td>
<td>4.9</td>
<td>13</td>
</tr>
<tr>
<td>96000</td>
<td>2.9487E-19</td>
<td>0.0595</td>
<td>0.0072</td>
<td>10.0</td>
<td>14</td>
<td>1.5578E-20</td>
<td>0.0631</td>
<td>0.0130</td>
<td>2.7</td>
<td>13</td>
</tr>
<tr>
<td>112000</td>
<td>2.9758E-19</td>
<td>0.0545</td>
<td>0.0061</td>
<td>10.0</td>
<td>15</td>
<td>1.5749E-20</td>
<td>0.0571</td>
<td>0.0105</td>
<td>3.0</td>
<td>13</td>
</tr>
<tr>
<td>128000</td>
<td>3.0167E-19</td>
<td>0.0509</td>
<td>0.0052</td>
<td>10.0</td>
<td>15</td>
<td>1.5970E-20</td>
<td>0.0528</td>
<td>0.0086</td>
<td>2.7</td>
<td>14</td>
</tr>
<tr>
<td>144000</td>
<td>3.0142E-19</td>
<td>0.0483</td>
<td>0.0050</td>
<td>10.0</td>
<td>14</td>
<td>1.5824E-20</td>
<td>0.0496</td>
<td>0.0075</td>
<td>2.7</td>
<td>14</td>
</tr>
<tr>
<td>160000</td>
<td>3.0284E-19</td>
<td>0.0461</td>
<td>0.0046</td>
<td>10.0</td>
<td>14</td>
<td>1.6205E-20</td>
<td>0.0465</td>
<td>0.0064</td>
<td>2.8</td>
<td>14</td>
</tr>
<tr>
<td>176000</td>
<td>3.0391E-19</td>
<td>0.0443</td>
<td>0.0042</td>
<td>10.0</td>
<td>14</td>
<td>1.6276E-20</td>
<td>0.0441</td>
<td>0.0056</td>
<td>3.2</td>
<td>14</td>
</tr>
<tr>
<td>192000</td>
<td>3.0143E-19</td>
<td>0.0427</td>
<td>0.0040</td>
<td>10.0</td>
<td>14</td>
<td>1.6351E-20</td>
<td>0.0420</td>
<td>0.0050</td>
<td>3.5</td>
<td>14</td>
</tr>
<tr>
<td>200000</td>
<td>3.0080E-19</td>
<td>0.0420</td>
<td>0.0040</td>
<td>10.0</td>
<td>14</td>
<td>1.6317E-20</td>
<td>0.0410</td>
<td>0.0048</td>
<td>3.9</td>
<td>14</td>
</tr>
</tbody>
</table>
Ten statistical tally tests

Tally Mean, $\bar{x}$:
1. The mean must exhibit, for the last half of the problem, only random fluctuations as $N$ increases. No up or down trends must be exhibited.

Relative Error, $R$:
2. $R$ must be less than 0.1 (0.05 for point/ring detectors).
3. $R$ must decrease monotonically with $N$ for the last half of the problem.
4. $R$ must decrease as $1/\sqrt{N}$ for the last half of the problem.

Variance of the Variance, VOV:
5. The magnitude of the VOV must be less than 0.1 for all types of tallies.
6. VOV must decrease monotonically for the last half of the problem.
7. VOV must decrease as $1/N$ for the last half of the problem.

Figure of Merit, FOM:
8. FOM must remain statistically constant for the last half of the problem.
9. FOM must exhibit no monotonic up or down trends in the last half of the problem.

Tally PDF, $f(x)$:
10. The SLOPE determined from the 201 largest scoring events must be greater than 3.
Tally Normalization

• Tally results
  – Flux in units of n/cm^2/f-s-n
  – Reaction rates in n-barn/cm^2/f-s-n
• f-s-n (fission source neutron) is directly proportional to power
• Normalization constant will be
  \[(P*\nu)/(Q*keff)\]
  
P=power (Watts)
  \(\nu\) =average number of neutrons per fission
  Q=200Mev*1.602x10^{-13} [J/MeV]
  keff=eigenvalue= \(\nu\) *(f-loss to fission)/f-src
Running MCNP

• Located on MIGHTYALPHA
• Command
  – mcnp4c3 inp=input.in out=outp.out
  – outp.out – output file
  – Other outputs
    • Runtpc – binary restart file
    • Mctal – separate tally file
• File name must be less than 8 characters!
MCNP input file for Lab 04

REPRESENTATIVE PWR UNIT CELL (4.5 w/o UO2 FUEL) - for solution

CELL DEFINITIONS

1000 10 7.06685e-2 (1300 500 -600 300 -400 100 -200) $ Unit Cell Water
   imp:n=1 imp:p=1 tmp=5.0246e-8
1100 11 -10.4 (-1100 100 -200)                   $ fuel pin
   imp:n=1 imp:p=1 tmp=7.7553e-8
1200 12 1.00000e-4 (1100 -1200 100 -200)             $ Gap
   imp:n=1 imp:p=1 tmp=2.53e-8
1300 13 4.34418e-2 (1200 -1300 100 -200)             $ Clad
   imp:n=1 imp:p=1 tmp=5.3512e-8
9999 0 (-100:200:-300:400:-500:600)       $ External Void
   imp:n=0 imp:p=0 tmp=2.53e-8

BLANK LINE MUST FOLLOW
SURFACE DEFINITIONS

*100 pz -2.00  $ bottom of active core
*200 pz 2.00   $ top of active core
*300 px -0.63  $ low-x edge of unit cell
*400 px 0.63   $ high-x edge of unit cell
*500 py -0.63  $ low-y edge of unit cell
*600 py 0.63   $ high-y edge of unit cell
1100 cz 0.4096 $ Fuel Pin
1200 cz 0.4178 $ Gap
1300 cz 0.4750 $ Clad
MCNP input file for lab 04 (Cont.)
c DATA
c H2O
m10 8016.50c 1.0
    1001.50c 2.0
mt10 lwtr.04t
c
4.5 w/o UO2
m11 8016.50c 4.64149E-02
    92234.86c 8.49269E-06
    92235.54c 1.05705E-03
    92238.86c 2.21413E-02
c Helium
m12 2004.50c 1.0
c Zircaloy-4
m13 40000.60c 1.0
c
ksrc 0.0 0.0 -1.0
    0.0 0.0 0.0
    0.0 0.0 1.0
c tally materials
m1000 92235.54c 1.0
m1001 92238.86c 1.0
c
s Reaction Rates
fc4 reaction rates
f4:n 1100
sd4 2.10829
e4 0.625E-6 20.0 T
fm4 (1.0 1000 (-6))
   (1.0 1001 (102))
c
c --------------------------------------------------------------
mode n
kcode 1500 1.01 5 150
prdmp 150 150 150
print