Mathematica notebook for plotting out particle tracks from an MNCP ptrac file

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After generating a ptrac file from MCNP [1] this is an attempt to plot out some tracks. This notebook is a proof of concept that plotting of particle tracks inside a Mathematica is accomplished at first via hard coding data then developed a methodology for extracting out the necessary data from an ascii ptrac file.

Figure (1): An example MCNP ascii ptrac file.

NOTE: Inside Mathematica this notebook is best viewed after selecting Format → Style Sheet → Report → StandardReport

Assign first two particle tracks to an Array.

In[1]:=
```
PtracArray[1] = {{-5.0000, -0.56379, 0.83193}, {-0.2500, -0.56379, 0.83193},
    {-0.70112 × 10⁻¹, -0.56379, 0.83193}, {0.22250 × 10⁻¹, -0.39029 × 10¹, 0.87590},
    {0.52596 E 10⁻¹, -0.50000 × 10¹, 0.89034}};
PtracArray[2] = {{-5.0000, 1.5413, 2.4723}, {-0.2500, 1.5413, 2.4723},
    {0.90869 × 10⁻¹, 1.5413, 2.4723}, {0.25000, -0.38155 × 10⁻¹, 0.13802},
    {0.28519, -0.50000 × 10¹, -0.37814}};
```

Use ListPointPlot3D() to plot out point and then join points joined with a thin line.

In[3]:=
```mathematica
ListPointPlot3D[{PtracArray[1], PtracArray[2]},
   PlotRange → {{-5, 5}, {-5, 5}, {-5, 5}},
   AxesLabel → {"x", "y", "z"}] /. Point → Line
```

Out[3]=
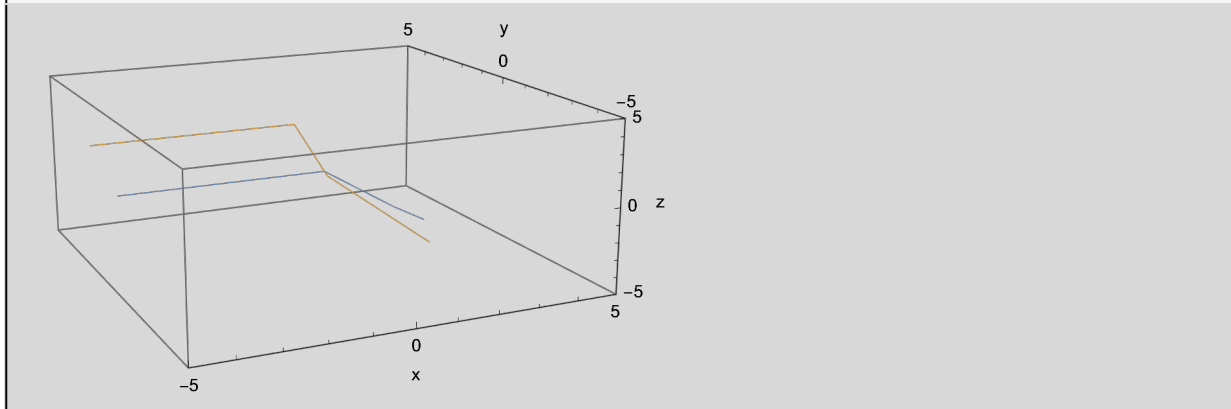
Particles start in Y-Z plane at X = –5. The foil is simulated as a soild disc centered on origin (0,0,0) with a thickness of 0.5 cm in X-direction with a radius of 4 cm.

Hard coding is only for proof of concept. To my knowledge no one else is importing MCNP ptrac files into Mathematica to parse, display, or visualize the data. Simple hard coding will take an excessive amount of time for simply plotting tracks from 10 or 15 particle histories much less plotting several dozens to several hundreds or thousands.

My intent is to create my own parsing notebook. First import raw data from MCNP ptrac file. Items are by default a string. This is advantageous for further editing and parsing of data (File location is on my own hard drive). Print out first ten items.

```mathematica
MCNPptracRaw = Import[
    "/Users/XXXxxx/Documents/MY_MCNP/TestFoil/ptracFiles/ptracFiveMinTestFoil1"
    , "Data"];
Do[Print[MCNPptracRaw[[n]]], {n, 1, 10}]
```

```
   -1
mcnp    6                         02/20/18 04/01/21 10:27:02
TestFoilInputDeck
  1.4000E+01  1.0000E+00  1.0000E+02  1.0000E+00
  3.0000E+00  0.0000E+00  1.0000E+00  1.0000E+00  0.0000E+00  1.0000E+00

  1.0000E+05  0.0000E+00  0.0000E+00  0.0000E+00
  1.0000E+00 -1.0000E+00  1.0000E+00  1.0000E+00  0.0000E+00  1.0000E+00

  1.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     5    5    3    6    3    6    3
   6    3    6    3    1    4    0    0    0    0    0    0    0
    1    2    3    5    6    7    8    9   17   18   20   21   22
   7    8   10   11   17   18   20   21   22    7    8   12   13   17   18   20   21
   22    7    8   10   11   17   18   20   21   22    7    8   14   15   17   18   20   21   22
      8388      1000         5        34  8.08830E-05
```

Data import is a success. Unfortunately it is not usable and will require several edits

First Edit of Raw Data:

From the raw data use StringReplace() function to take ptrac data that has exponents in form of "...E+01" to a usable form of "...*10^{01}". Hard code to perform this operation from "...E−06" to "...E+06" and evaluate results.

Print out first ten items.

```
MCNPptracFirstEdit = StringReplace[MCNPptracRaw,
    {"E-06" → "*10^-06", "E-05" → "*10^-05", "E-04" → "*10^-04", "E-03" → "*10^-03",
     "E-02" → "*10^-02", "E-01" → "*10^-01", "E+00" → "*10^+00",
     "E+01" → "*10^+01", "E+02" → "*10^+02", "E+03" → "*10^+03",
     "E+04" → "*10^+04", "E+05" → "*10^+05", "E+05" → "*10^+05"}];
Do[Print[MCNPptracFirstEdit[[n]]], {n, 1, 10}]
```

```
     -1
mcnp     6                              02/20/18 04/01/21 10:27:02

TestFoilInputDeck
   1.4000*10^+01   1.0000*10^+00   1.0000*10^+02   1.0000*10^+00   3.0000*10^+00
   0.0000*10^+00   1.0000*10^+00   1.0000*10^+00   0.0000*10^+00   1.0000*10^+00

   1.0000*10^+05   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00   1.0000*10^+00
  -1.0000*10^+00   1.0000*10^+00   1.0000*10^+00   0.0000*10^+00   1.0000*10^+00

   1.0000*10^+00   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00
   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00   0.0000*10^+00

     5    5    3    6    3    6    3
   6    3    6    3    1    4    0    0    0    0    0    0    0
    1    2    3    5    6    7    8    9   17   18   20   21   22
   7    8   10   11   17   18   20   21   22    7    8   12   13   17   18   20   21
   22    7    8   10   11   17   18   20   21   22    7    8   14   15   17   18   20   21   22
        8388       1000         5        34   8.08830*10^-05
```

Second Edit of Raw Data:

After first edit of replacing exponent form of Raw Data, create an list of list of strings by separating out items & removing the whitespace to create a comma separated list utilizing the StringSplit(). Print out first ten items.

In[8]:=
```
MCNPptracSecondEdit = StringSplit[MCNPptracFirstEdit, {Whitespace}];
Do[Print[MCNPptracSecondEdit[[n]]], {n, 1, 10}]
```

{-1}

{mcnp, 6, 02/20/18, 04/01/21, 10:27:02}

{TestFoilInputDeck}

{1.4000*10^+01, 1.0000*10^+00, 1.0000*10^+02, 1.0000*10^+00, 3.0000*10^+00,
 0.0000*10^+00, 1.0000*10^+00, 1.0000*10^+00, 0.0000*10^+00, 1.0000*10^+00}

{1.0000*10^+05, 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00, 1.0000*10^+00,
 -1.0000*10^+00, 1.0000*10^+00, 1.0000*10^+00, 0.0000*10^+00, 1.0000*10^+00}

{1.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00,
 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00, 0.0000*10^+00}

{5, 5, 3, 6, 3, 6, 3, 6, 3, 6, 3, 1, 4, 0, 0, 0, 0, 0, 0, 0}

{1, 2, 3, 5, 6, 7, 8, 9, 17, 18, 20, 21, 22, 7,
 8, 10, 11, 17, 18, 20, 21, 22, 7, 8, 12, 13, 17, 18, 20, 21}

{22, 7, 8, 10, 11, 17, 18, 20, 21, 22, 7, 8, 14, 15, 17, 18, 20, 21, 22}

{8388, 1000, 5, 34, 8.08830*10^-05}

Third Edit of Raw Data:

Remove top 9 items from the ptrac data file since they are simply input parameters and other identifiers used in MCNP. Print out first 15 items.

In[10]:=
```
MCNPptracThirdEdit = Drop[MCNPptracSecondEdit, {1, 9}];
Do[Print[MCNPptracThirdEdit[[n]]], {n, 1, 15}]
```

{8388, 1000, 5, 34, 8.08830*10^-05}

{3000, 1, 40, 4, 0}

{-0.50000*10^+01, -0.56379*10^+00, 0.83193*10^+00}

{4000, 2, 13.3, 179, 3, 1}

{-0.25000*10^+00, -0.56379*10^+00, 0.83193*10^+00}

{3000, 2, 28060, 2, 3, 1}

{-0.70112*10^-01, -0.56379*10^+00, 0.83193*10^+00}

{3000, 3, 13.1, 11, 4, 0}

{0.22250*10^-01, -0.39029*10^+01, 0.87590*10^+00}

{5000, 4, 1.4, 1, 5, 0}

{0.52596*10^-01, -0.50000*10^+01, 0.89034*10^+00}

{9000, 4, 1, 1, 5, 0}

{0.52596*10^-01, -0.50000*10^+01, 0.89034*10^+00}

{25160, 1000, 5, 34, 1.17772*10^-04}

{3000, 1, 40, 4, 0}

Verify That the list works by calling the first item in the first list:

In[12]:=
```
MCNPptracThirdEdit[[1, 1]]
```

Out[12]=
```
8388
```

Extraction works but is it usable numerically? Attempt to add 1 (+1) to the first item in the first list.

In[13]:=
```
MCNPptracThirdEdit[[1, 1]] + 1
```

Out[13]=
```
1 + 8388
```

Fourth Edit of Raw Data:

All of the data is still in a string format. Utilized ToExpression() to convert all data from a string form to a numerical form in order to be useful in calculations. Print out first 15 items.

In[14]:=
```
MCNPptracFourthEdit = ToExpression[MCNPptracThirdEdit];
Do[Print[MCNPptracFourthEdit[[n]]], {n, 1, 15}]
```

```
{8388, 1000, 5, 34, 0.000080883}

{3000, 1, 40, 4, 0}

{-5., -0.56379, 0.83193}

{4000, 2, 13.3, 179, 3, 1}

{-0.25, -0.56379, 0.83193}

{3000, 2, 28060, 2, 3, 1}

{-0.070112, -0.56379, 0.83193}

{3000, 3, 13.1, 11, 4, 0}

{0.02225, -3.9029, 0.8759}

{5000, 4, 1.4, 1, 5, 0}

{0.052596, -5., 0.89034}

{9000, 4, 1, 1, 5, 0}

{0.052596, -5., 0.89034}

{25160, 1000, 5, 34, 0.000117772}

{3000, 1, 40, 4, 0}
```

Separate numerical data:

Data is looking more manageable but there remains excess information in each history. The first number on the first line was "8388" which denotes the Particle ID number 8388 whereas on the 14th line the first number is "25160" for Particle ID number 25160. The event ID number "1000" denotes that this is a beginning of life for the particle. On the next line are the X, Y, & Z coordinates. In this MCNP geometry All particles will start on the Y-Z plane at X = –5.0. Y and Z are random values from –5 to 5. The particles travel perpendicular to the Y-Z plane from the generation point. ID Number "3000" is a surface crossing for example and ID number "9000" is the termination of the problem.

The next steps will be collect X, Y, & Z coordinates following event ID number "1000" and before "9000."

Using an If(), verify ability to extract data on particle starting point.

In[16]:=
```
If[MCNPptracFourthEdit[[1, 2]] == 1000, (*Do*)
  Print[MCNPptracFourthEdit[[1 + 2]]], (*else*)Print["did not work"]]
```

{-5., -0.56379, 0.83193}

X, Y, & Z coordinates extracted successfully. Now attempt to extract all tracks for the first particle and print to screen.

In[17]:=
```
Do[
 {If[MCNPptracFourthEdit[[n, 2]] == 1000, {}(*this will be a starting point*)],
  If[MCNPptracFourthEdit[[n, 1]] == 3000, Print[MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 4000, Print[MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 5000, Print[MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 9000, Break[]]},
 {n,
  1,
  15}]
```

{-5., -0.56379, 0.83193}

{-0.25, -0.56379, 0.83193}

{-0.070112, -0.56379, 0.83193}

{0.02225, -3.9029, 0.8759}

{0.052596, -5., 0.89034}

First particle X, Y, & Z coordinates with start point on Y-Z plane at X = –5 and ends on X-Z plane with Y=–5. Coordinates extracted & printed successfully.

Show the total number of lines of data elements that need to be parsed and edited.

In[18]:=
```
Length[MCNPptracFourthEdit]
```

Out[18]=
```
75 003
```

NOTE & WARNING:

For best practice to execute this code, the kernel should be stopped, then restarted, each time the following loop is executed.

Now attempt to send information to a create an array with first element with all of the first particle tracks, 2nd element with all of the second particle tracks, and so forth.

In[19]:=
```
m = 1(*start with first history*);
Ptrac[m] = {}(*initialize the first element*);
Do[{If[MCNPptracFourthEdit[[n, 2]] == 1000(*placeholder and starting point*),
    {}], If[MCNPptracFourthEdit[[n, 1]] == 3000(*boundry crossing event*),
   AppendTo[Ptrac[m], MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 4000(*Interaction event*),
   AppendTo[Ptrac[m], MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 5000(*Termination event*),
   AppendTo[Ptrac[m], MCNPptracFourthEdit[[n + 1]]]],
  If[MCNPptracFourthEdit[[n, 1]] == 9000, {m += 1, Ptrac[m] = {}}
   (*particle history terminated, create new history*)]},
 {n, 1, Length[MCNPptracFourthEdit]}]
```

Use Graphics3D() by creating a table of lines from particle tracks in Ptrac array to plot out particle

histories and utilize a cylinder graphic for visualization of the foil. Incorporate the Manipulate() to allow for user to select total number of particle tracks as well as opacity of the target disc.

In[22]:=
```
Manipulate[Graphics3D[{Table[Line@Ptrac[i], {i, 1, max}],

    Opacity[opac/100], Cylinder[{{-0.25, 0, 0}, {0.25, 0, 0}}, 4.0]},
  Axes → True, AxesLabel → {"x (cm)", "y (cm)", "z (cm)"},
  Background → White, PlotRange → {{-5, 5}, {-5, 5}, {-5, 5}},
  PlotLabel → Style[Framed[StringForm["3D Plot of `` neutron collision event
        tracks \nfrom MCNP w/ foil opacity at ``%", max, opac]],
    Black, Background → Yellow], {{max, 5, "number of tracks"},
  1, m - 1, 1}, {{opac, 75, "Opacity %"}, 1, 100, 1},
 FrameLabel → {"", "", "MCNP data visualization", ""}]
```

Out[22]=
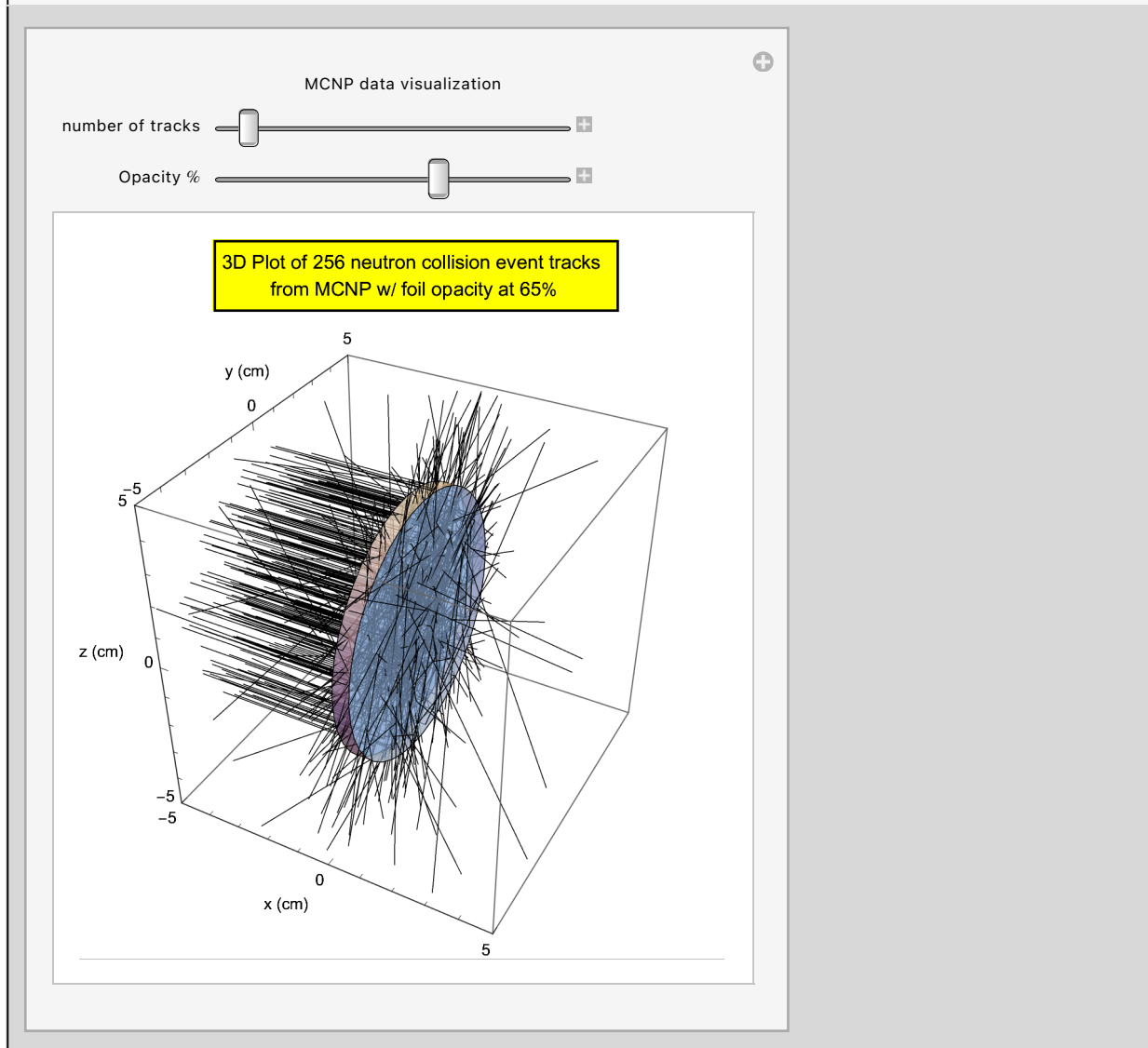
NOTE: After a 5 minute MCNP run with ptrac length of 75003 lines, the data parsed incredibly fast. However, with my laptop, the visualization began to noticeably lag after about 2000 histories or so.

Figure (2): Hardware & OS specifications.

Potential improvements can be made to decrease this lag, however, beyond a few hundred histories this visualization becomes very crowded with data. Although I'm sure this could be better optimized for 10,000 histories or more, the need for this large of a particle tracking plot is not needed at this time.

Total number of histories will be value of: $m - 1$

Print 30 MCNP particle histories (first & last 15) from parsed ptrac file.

In[23]:=
```
Print["Total number of particle histories:  ", m - 1]
Do[Print["History: ", i, "\n", Ptrac[i]], {i, 1, 15}]
Do[Print["History: ", i, "\n", Ptrac[i]], {i, m - 16, m - 1}]
```

```
Total number of particle histories:  5191

History: 1
{{-5., -0.56379, 0.83193}, {-0.25, -0.56379, 0.83193},
   {-0.070112, -0.56379, 0.83193}, {0.02225, -3.9029, 0.8759}, {0.052596, -5., 0.89034}}

History: 2
{{-5., 1.5413, 2.4723}, {-0.25, 1.5413, 2.4723},
   {0.090869, 1.5413, 2.4723}, {0.25, -3.8155, 0.13802}, {0.28519, -5., -0.37814}}

History: 3
{{-5., 0.8024, -3.6844}, {-0.25, 0.8024, -3.6844}, {0.19748, 0.8024, -3.6844},
   {-0.12012, 1.9908, -1.9128}, {-0.25, 1.7398, 2.595}, {-0.3193, 1.6059, 5.}}

History: 4
{{-5., -1.7488, -0.30272}, {-0.25, -1.7488, -0.30272},
   {-0.14455, -1.7488, -0.30272}, {0.055065, -0.40073, 0.057923},
   {-0.077465, 2.3359, 2.517}, {0.24361, 2.8326, 2.8242}, {1.6446, 5., 4.1647}}

History: 5
{{-5., -0.37332, -1.0908}, {-0.25, -0.37332, -1.0908}, {0.18938, -0.37332, -1.0908},
   {0.21671, -0.33736, -0.99041}, {-0.11659, 0.44199, 3.9755}, {-0.18535, 0.60278, 5.}}

History: 6
{{-5., 1.0861, -3.2176}, {-0.25, 1.0861, -3.2176}, {0.021462, 1.0861, -3.2176},
   {0.19112, -1.6386, -2.4409}, {0.24982, -3.4713, -1.9875}, {0.29879, -5., -1.6093}}
```

```
History: 7
{{-5., -2.3022, 2.334}, {-0.25, -2.3022, 2.334},
  {0.077326, -2.3022, 2.334}, {0.020044, 1.4238, -0.56234},
  {0.062515, 1.7276, -0.96147}, {0.25, 2.0545, -1.1158}, {1.9392, 5., -2.5063}}
History: 8
{{-5., -1.3346, -0.073455}, {-0.25, -1.3346, -0.073455},
  {0.12915, -1.3346, -0.073455}, {0.16578, -0.56458, -3.96}, {0.17558, -0.35853, -5.}}
History: 9
{{-5., -1.3544, 3.1585}, {-0.25, -1.3544, 3.1585},
  {0.023944, -1.3544, 3.1585}, {-0.06972, 0.38912, -3.981}, {-0.083088, 0.63796, -5.}}
History: 10
{{-5., 0.43199, 3.567}, {-0.25, 0.43199, 3.567}, {0.047362, 0.43199, 3.567},
  {-0.092285, 1.0164, 3.0202}, {0.25, 3.1477, 0.71754}, {0.54747, 5., -1.2836}}
History: 11
{{-5., -2.0477, -2.665}, {-0.25, -2.0477, -2.665},
  {0.14596, -2.0477, -2.665}, {0.22133, -0.90986, 3.8951}, {0.23402, -0.71822, 5.}}
History: 12
{{-5., 2.1478, 2.1567}, {-0.25, 2.1478, 2.1567}, {0.072368, 2.1478, 2.1567},
  {-0.11758, 1.887, -0.77558}, {-0.16042, 1.8276, -0.99193},
  {-0.157, 1.5789, -3.3913}, {0.034565, 1.4099, -3.7433}, {0.71851, 0.80689, -5.}}
History: 13
{{-5., 1.217, 1.5682}, {-0.25, 1.217, 1.5682},
  {-0.0003646, 1.217, 1.5682}, {0.11723, 1.3234, -1.6883},
  {0.11447, 1.317, -1.7009}, {-0.25, 1.0151, -2.8928}, {-0.89436, 0.48142, -5.}}
History: 14
{{-5., 0.96812, 3.818}, {-0.25, 0.96812, 3.818},
  {0.065185, 0.96812, 3.818}, {0.042747, 3.8123, 1.211}, {0.033377, 5., 0.12236}}
History: 15
{{-5., 1.768, 2.0813}, {-0.25, 1.768, 2.0813},
  {0.23151, 1.768, 2.0813}, {-0.045243, -3.4922, -1.9506}, {-0.12457, -5., -3.1063}}
History: 5176
{{-5., -2.7931, 2.8213}, {-0.25, -2.7931, 2.8213}, {-0.0332, -2.7931, 2.8213},
  {-0.15576, -0.22947, -0.7173}, {0.25, 0.037311, -0.54137}, {5., 3.1603, 1.5181}}
History: 5177
{{-5., 3.0326, -1.8923}, {-0.25, 3.0326, -1.8923},
  {-0.22506, 3.0326, -1.8923}, {-0.14937, -2.8102, -2.8465}, {-0.121, -5., -3.2041}}
History: 5178
{{-5., -1.4241, -0.34608}, {-0.25, -1.4241, -0.34608}, {-0.03705, -1.4241, -0.34608},
  {0.10616, -0.066754, 1.3303}, {-0.25, 0.67529, 2.2004}, {-1.3958, 3.0626, 5.}}
History: 5179
{{-5., -0.79521, 2.82}, {-0.25, -0.79521, 2.82},
  {-0.098635, -0.79521, 2.82}, {0.16637, 2.5061, 3.1176}, {0.36657, 5., 3.3424}}
```

```
History: 5180
{{-5., 3.3023, 1.6131}, {-0.25, 3.3023, 1.6131},
   {0.14905, 3.3023, 1.6131}, {-0.25, -0.92893, 1.5663}, {-0.63395, -5., 1.5214}}
History: 5181
{{-5., 0.76406, -2.3538}, {-0.25, 0.76406, -2.3538}, {-0.16707, 0.76406, -2.3538},
   {0.059123, 0.73655, -2.3656}, {-0.25, -0.1331, 2.7818}, {-0.38321, -0.50786, 5.}}
History: 5182
{{-5., 0.89887, -2.0249}, {-0.25, 0.89887, -2.0249},
   {-0.15453, 0.89887, -2.0249}, {0.10565, -3.9955, -0.19043}, {0.15905, -5., 0.1861}}
History: 5183
{{-5., 3.9034, -0.14479}, {-0.25, 3.9034, -0.14479},
   {0.0029528, 3.9034, -0.14479}, {0.021919, 3.7974, -0.16775},
   {0.036837, 1.6375, -0.20907}, {0.25, -1.2789, 0.78167}, {0.52199, -5., 2.0458}}
History: 5184
{{-5., 3.6816, -1.3446}, {-0.25, 3.6816, -1.3446},
   {-0.23043, 3.6816, -1.3446}, {-0.19317, -2.6652, -2.9827}, {-0.17946, -5., -3.5853}}
History: 5185
{{-5., -2.9701, 0.66477}, {-0.25, -2.9701, 0.66477},
   {-0.10348, -2.9701, 0.66477}, {-0.16724, -2.7425, 0.58919},
   {0.020339, 0.41375, -0.12594}, {-0.038264, 0.6257, -0.24609},
   {0.020213, 0.97272, -0.34269}, {-0.14401, 3.9279, -0.75605}, {-0.20359, 5., -0.90601}}
History: 5186
{{-5., -1.2971, 1.2165}, {-0.25, -1.2971, 1.2165},
   {0.14577, -1.2971, 1.2165}, {0.033225, 3.682, -1.5629}, {0.0034333, 5., -2.2987}}
History: 5187
{{-5., -1.5305, 0.20334}, {-0.25, -1.5305, 0.20334},
   {0.2286, -1.5305, 0.20334}, {-0.0057493, -0.57778, 3.9581}, {-0.070781, -0.31339, 5.}}
History: 5188
{{-5., 1.6773, 0.94936}, {-0.25, 1.6773, 0.94936},
   {0.026477, 1.6773, 0.94936}, {0.027433, 0.4324, 3.9766}, {0.027757, 0.01152, 5.}}
History: 5189
{{-5., -3.0788, -0.82468}, {-0.25, -3.0788, -0.82468},
   {-0.078818, -3.0788, -0.82468}, {0.2082, 2.5248, -3.1025}, {0.33498, 5., -4.1086}}
History: 5190
{{-5., -2.7757, 1.0445}, {-0.25, -2.7757, 1.0445}, {-0.063987, -2.7757, 1.0445},
   {0.12461, 3.2393, 2.1568}, {0.18266, 3.3553, 2.1777}, {1.0057, 5., 2.4728}}
History: 5191
{{-5., 3.7742, -0.10875}, {-0.25, 3.7742, -0.10875},
   {0.106, 3.7742, -0.10875}, {0.20156, -1.4851, -3.7141}, {0.23565, -3.3609, -5.}}
```

Reference:

A.   1.   MCNP®, Monte Carlo N–Particle Transport Code System, Version 6.2