LA-UR-07-4595

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Title: A Tutorial on Using MCNP for 1-Group Transport Calculations

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Intended for: MCNP website & classes

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A Tutorial on Using MCNP for 1-group Transport Calculations

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Abstract

A Tutorial on Using MCNP for 1-Group Transport Calculations

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1-group transport calculations are an invaluable R&D tool for developing new algorithms and calculational methods for particle transport applications. They are also important for verifying the correctness of existing transport codes, since many 1-group transport analytical problems exist for which exact solutions are known. MCNP is a general-purpose, 3D, continuous-energy Monte Carlo particle transport code used for a wide variety of applications. In this tutorial, we describe how MCNP can be used to perform 1-group transport calculations. An auxilliary code called ONEGXS is first used to construct 1-group cross-section files in the ACE format required by MCNP. Then, MCNP can be run in a multigroup mode using the 1-group data files. This procedure is illustrated by several examples. It is important for users to understand the limitations on the MCNP Monte Carlo methods: For 1-group problems with isotropic scattering, MCNP results match exact analytical solutions. For linearly anisotropic scattering, MCNP results match exact analytical solutions when $|\bar{\mu}| \leq 1/3$, but will generally not match exact analytical soultions otherwise, due to the non-physical effects of truncating the scattering data representation.

Outline

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  - Importance
  - References
- **Generating 1-Group Cross-section Files**
  - onegxs code
  - Input & output
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- **Running 1-Group Calculations with MCNP**
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  - Referencing 1-group datafiles
  - Examples
- **Discussion**
  - Angular scattering distributions
  - P_0 and P_1 scattering
  - Truncation errors for highly forward- or backward-peaked scatter

1-Group Transport - Background

- **1-group transport calculations are an important R&D tool**
  - Useful for developing new algorithms & computational methods that do not involve energy-dependence

    Examples: geometry tracking, criticality, void streaming

  - Simplifies & speeds up calculations

- **1-group calculations are important for verifying correctness of codes**
  - Many transport problems have known, exact, analytical solutions
  - Typically, these are 1-group with simple geometry

1-Group Transport - Background

- **Criticality benchmarks**
  - A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification", LA-UR-01-3082 (2001)
  - Compilation of 75 criticality problems with exact analytical solutions
    - **30 problems - 1-group, isotropic scatter**
    - **13 problems - 1-group, anisotropic scatter**
    - 26 problems - 2-group, isotropic scatter
    - 4 problems - 2-group, anisotropic scatter
    - 1 problem - 3-group, isotropic scatter
    - 1 problem - 6-group, isotropic scatter
- **Kobiyashi void-streaming benchmark**
  - K. Kobayashi, N. Sugimura, Y. Nagaya, "3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions", OECD/NEA (2000).
- **Many others …..**

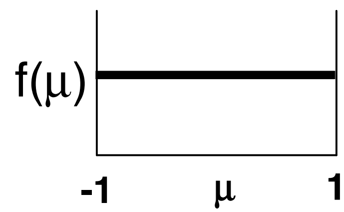
Generating 1-Group Cross-section Files

- **MCNP reads ACE-format cross-section files to obtain cross-section data, scattering distributions, etc., required for performing transport calculations**
  - ACE files - described in MCNP manual, Volume III, Appendix F
  - Very general, to accommodate continuous-energy neutron/photon/electron data & also multigroup data
  - Compact (but complex) data layout
- **onegxs**
  - Auxilliary code to simplify preparing 1-group cross-section datafiles
    - Includes basic cross-section data:
      total, scatter, capture, fission, nu
    - Provides scattering distribution data in the lab system:
      isotropic (P_0) or linearly-anisotropic (P_1) scattering
  - Creates datafile in ACE format

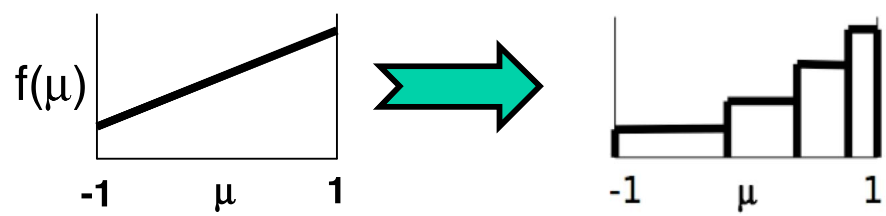
Generating 1-Group Cross-section Files

- **Scattering distributions from onegxs are either isotropic (P_0) or linearly anisotropic (P_1) in the lab system for multigroup MCNP**

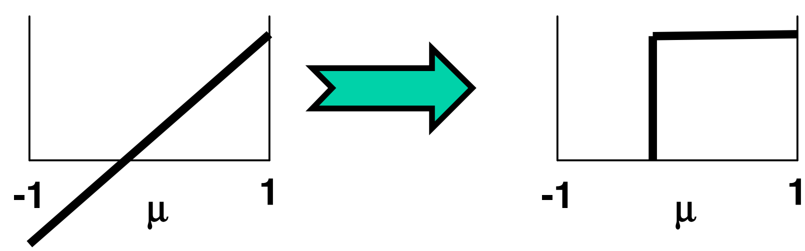
- **Isotropic (P_0)**
  - Flag, no data needed
  - Exact form used in MCNP



- **P_1 scatter, with** $|\bar{\mu}| \leq \frac{1}{3}$
  - 1000 steps, equal-area



- **P_1 scatter, with** $|\bar{\mu}| > \frac{1}{3}$
  - Linear PDF replaced by 1 step
  - Step bounds chosen to preserve $\bar{\mu}$ & remain positive



onegxs Input

- **OneGXS**
  - Takes user-specified, one-group cross sections & writes a cross section file that MCNP can read.
  - The program is driven from the command prompt & has a variety of input options. Use "**`onegxs -h`**" for help.
  - It can handle multiplying or non-multiplying media, and isotropic or linearly anisotropic scattering.
- **Instructions for Use**
  - OneGXS accepts arguments through a flag, followed by data.
  - The one exception is that the first argument is the name of the output file and does not use a flag.
  - General form:

```
onegxs   filename [-z suffix]                         \
                  [-t sigt] [-c sigc] [-s sigs]       \
                  [-n nu  -f sigf]                    \
                  [-s0 sigs] [-s1 sigs1] [-u mubar]
```

onegxs Input

File Name of the output file that MCNP will read & always required. Should be the first item listed.

-c This flag indicates that the next item in the command line is the capture cross section. The capture cross section is defined as the absorption minus the fission, $\Sigma_C=\Sigma_A-\Sigma_F$

-f This flag indicates that the next item in the command line is the fission cross section, Σ_F

-h This flag will print the help page, with a list of all options available for running the program. After displaying the help page, the program will immediately exit. Note: the help page will also be displayed if no arguments are given.

-n This flag indicates that the next item in the command line is ν (nu-bar), the average number of neutrons produced in each fission event.

-s This flag indicates that the next item in the command line is the scattering cross section, Σ_S. This is the isotropic, or P_0, scattering cross section.

-s0 This flag indicates that the next item in the command line is the P_0, or isotropic, scattering cross section, Σ_S. This is the same value as the previous option.

-s1 This flag indicates that the next item in the command line is the P_1 scattering cross section, Σ_{S1}. This provides the next term in the Legendre expansion, causing the scattering to be anisotropic.

-t This flag indicates that the next item in the command line is the total cross section. The total cross section is defined as the sum of the capture, fission, and P_0 scattering cross sections,

$$\Sigma_T = \Sigma_A + \Sigma_S = \Sigma_C + \Sigma_F + \Sigma_S$$

-u This flag indicates that the next item in the command line is μ (mu-bar), the average cosine of the scattering angle, $\mu = \Sigma_{S1} / \Sigma_{S0} = \Sigma_{S1} / \Sigma_S$. If mu-bar is zero, scattering is isotropic. Note: special caution should be taken with mu-bar, since problems with |mu-bar| > 1/3 can give wrong answers. Please read the section on mu-bar.

-z This flag indicates that the next item in the command line is the two digit material identifier that accompanies the ZAID number in MCNP. The ZAID will always be 92250. (e.g. 92250.32m)

onegxs Output

- **Using onegxs**
  - Not all of the options are needed to run the program.
  - If the program can not calculate what it needs from the given data, then it will exit.
  - Redundant data is checked against the overlapping data for differences.

- **Onegxs screen output, example**

```
Created MCNP cross section file:

    xsec02

The following cross sections were used:

  sigT= 0.3264, sigF= 0.0816, sigC= 0.019584, sigSO= 0.225216, nu= 3.24, uBar= 0

Please use the following line in your MCNP deck on the xsn card:

    92250.02m 1.0 xsec02 0 1 1 11 0 0 0.0
```

Running 1-Group Calculations with MCNP

- **Run MCNP in multigroup mode**

  – Don't use the MODE card (assume neutron multigroup)

  – Importances should all be given in the form: **imp:n**

  – Use default energy for any SDEF source cards

  – Supply the MGOPT card as one of the data cards

```
mgopt   f   1
```

  – Supply XSn cards in the MCNP input to describe the xsec files

```
xs1  92250.12m  1.0  xsfile1  0  1  1    13  0  0  0.0
xs2  92250.27m  1.0  xsfile2  0  1  1  1013  0  0  0.0
xs3  92250.01m  1.0  xsfile3  0  1  1    11  0  0  0.0
```

Values in red must match the output information from **onegxs**

Example - MCNP Input

PUa-1-1-SL Criticality Benchmark Problem

```
PUa-1-1-SL
10   1     1.0     -1   2    $SEMI-INFINITE SLAB
20   0              1:-2    $OUTSIDE WORLD

1   px  0.77032
2   px -0.77032

kcode    20000  1.0  50  550
ksrc     0.0    0.0  0.0
hsrc   1 -1e20 1e20  1 -1e20 1e20  1 -1e20 1e20
xs1   92250.32m  1.0 xsec32  0  1  1  1013  0  0  0.0
m1    92250.32m  1.0
imp:n    1  0
mgopt f 1
```

Problem PUa-1-0-SL
from
Analytic Criticality
Benchmark Set

Example 1

- **Problem 2 from the analytic criticality benchmark set**
  - Identifier: **PUa-1-0-SL**
  - 1-group slab, with **isotropic scatter (in lab)**
  - From Table 2 in reference:

    $\Sigma_T = .326400$, $\Sigma_S = .225216$, $\Sigma_C = .019584$,

    $\Sigma_F = .081600$, $\nu = 3.24$

  - From Table 3 in reference:

    critical half-thickness = 1.853722

  - Exact eigenvalue: Keff = 1.000000

Example 1

- onegxs input for problem PUa-1-0-SL

```
onegxs xsec02 -z 02     -t .326400   -s .225216  \
                        -c .019584   -f .081600  -n 3.24
```

- onegxs screen output for problem PUa-1-0-SL

```
Created MCNP cross section file:

    xsec02

The following cross sections were used:

     sigT= 0.3264, sigF= 0.0816, sigC= 0.019584, sigS0= 0.225216, nu= 3.24, uBar= 0

Please use the following line in your MCNP deck on the xsn card:

      92250.02m 1.0 xsec02 0 1 1 11 0 0 0.0
```

Example 1

- onegxs file created for problem PUa-1-0-SL (xsec02)

```
92250.02m          250             0    20070629
sigT= 0.3264, sigF= 0.0816, sigC= 0.019584, sigS0= 0.225216, nu= 3.24, uBar= 0



      11     92250         0         0         1         0         0         0
       0         1         0         1         0         0         0         0
       1         3         4         5         6         7         0         0
       0         0         0         0         8         0         0        10
      11         0         0         0         0         0         0         0
       0         0         0         0         0         0         0         0
 5.000000000000e+01  1.000000000000e+02  3.264000000000e-01  8.160000000000e-02
 3.240000000000e+00  1.000000000000e+00  1.958400000000e-02  9.000000000000e+00
 2.252160000000e-01  0.000000000000e+00  0.000000000000e+00
```

For isotropic scattering, no angular distribution data is needed

Example 1

- MCNP input file for problem PUa-1-0-SL,   for 500M histories

```
PUa-1-0-SL
10   1     1.0     -1   2    $SEMI-INFINITE SLAB
20   0               1:-2    $OUTSIDE WORLD

1   px   1.853722
2   px  -1.853722

kcode    20000   1.0   50   2550
hsrc     5 -1.853722 1.853722   1 -1e20 1e20   1 -1e20 1e20
ksrc     0.0   0.0   0.0
xs1      92250.02m 1.0 xsec02  0   1   1   11   0   0   0.0
m1       92250.02m 1.0
imp:n    1   0
mgopt    f   1
```

Example 1

- MCNP output for problem PUa-1-0-SL

```
 cycle    k(col)      ctm   entropy    active     k(col)    std dev       fom
     1   1.11109     0.01  2.20E+00
     2   1.01883     0.03  2.29E+00
     3   1.02007     0.04  2.31E+00
. . . . .
  2544   1.00112    38.41  2.31E+00      2494    1.00004    0.00012   1707942
  2545   0.98849    38.43  2.31E+00      2495    1.00003    0.00012   1706282
  2546   0.99955    38.44  2.31E+00      2496    1.00003    0.00012   1706999
  2547   0.99067    38.46  2.31E+00      2497    1.00003    0.00012   1706142
  2548   0.99723    38.47  2.30E+00      2498    1.00003    0.00012   1706712
  2549   1.00831    38.49  2.31E+00      2499    1.00003    0.00012   1706216
  2550   0.99519    38.50  2.31E+00      2500    1.00003    0.00012   1706499
. . . . .
 final k(col/abs/trk len) = 1.00009     std dev = 0.00010
```

For 1-group problems with isotropic scattering, results using onegxs + MCNP   match the exact analytic solution (within statistics)

Problem Ua-1-1-CY
from
Analytic Criticality
Benchmark Set

Example 2

- **Problem 36 from the analytic criticality benchmark set**
  - Identifier: **Ua-1-1-CY**
  - 1-group infinite cyclinder, with **anisotropic scatter (in lab),** $\bar{\mu} = .171052631$
  - From Table 23 in reference:

    $\Sigma_T = .32640$, $\Sigma_S = .248064$, $\Sigma_{S1} = .042432$

    $\Sigma_C = .013056$, $\Sigma_F = .065280$, $\nu = 2.70$

  - From Table 24 in reference:

    critical radius = 5.514296811

  - Exact eigenvalue: Keff = 1.000000

Example 2

- onegxs input for problem Ua-1-1-CY

```
onegxs xsec36 -z 36     -t .326400   -s .248064  \
                        -c .013056   -f .065280  -n 2.70 \
                        -s1 .042432
```

- onegxs screen output for problem Ua-1-1-CY

```
Created MCNP cross section file:

    xsec36

The following cross sections were used:

   sigT= 0.3264, sigF= 0.06528, sigC= 0.013056, sigS0= 0.248064, nu= 2.7, uBar= 0.171053

Please use the following line in your MCNP deck on the xsn card:

      92250.36m 1.0 xsec36 0 1 1 1013 0 0 0.0
```

Example 2

- **onegxs file created for problem Ua-1-1-CY (xsec36)**

```
92250.36m          250              0    20070702
sigT= 0.3264, sigF= 0.06528, sigC= 0.013056, sigS0= 0.248064, nu= 2.7, uBar= 0.171053




     1013     92250      1001         0         1         0         0         0
        0         1         0         1         0         0         0         0
        1         3         4         5         6         7         0         0
        0         0         0         0         8         0         0        10
       12         0         0         0         0         0         0         0
        0         0         0         0         0         0         0         0
  5.000000000000e+01  1.000000000000e+02  3.264000000000e-01  6.528000000000e-02
  2.700000000000e+00  1.000000000000e+00  1.305600000000e-02  9.000000000000e+00
  2.480640000000e-01  1.100000000000e+01  1.000000000000e+00  1.300000000000e+01
 -1.000000000000e+00 -9.959007501602e-01 -9.918190625466e-01 -9.877547078747e-01
 -9.837074733325e-01 -9.796771402444e-01 -9.756634988818e-01 -9.716663483741e-01
. . . . .
  9.894070569220e-01  9.907332609147e-01  9.920588675273e-01  9.933838764883e-01
  9.947082892934e-01  9.960321076894e-01  9.973553312983e-01  9.986779607410e-01
  1.000000000000e+00
```

For linearly-anisotropic scatter, with |μ-bar| < 1/3,
1000 equiprobable steps are used to represent the angular distribution

Example 2

- MCNP input file for problem Ua-1-1-CY, for 500M histories

```
Ua-1-1-CY
1   1     1.0     -1       $SEMI-INFINITE CYLINDER
2   0              1       $OUTSIDE WORLD

1   rcc 0 0 0   0 0 1e12  5.514296811

imp:n    1   0
kcode    20000  1.0  50   2550
hsrc   1 -1e20 1e20 1 -1e20 1e20 1 -1e20 1e20
ksrc     0.0    0.0  .5e12
xs1   92250.36m 1.0 xsec36 0 1 1 1013 0 0 0.0
m1    92250.36m 1.0
mgopt f 1
```

Example 2

- MCNP output for problem Ua-1-1-CY

```
 cycle    k(col)      ctm   entropy    active     k(col)    std dev        fom
     1   1.23829     0.01  0.00E+00
     2   1.09388     0.02  0.00E+00
     3   1.03832     0.02  0.00E+00
. . . . .
  2544  0.99772     45.99  0.00E+00     2494    0.99995    0.00010    2066295
  2545   1.00139    46.01  0.00E+00     2495    0.99995    0.00010    2067075
  2546   1.01269    46.03  0.00E+00     2496    0.99995    0.00010    2062917
  2547   0.99399    46.05  0.00E+00     2497    0.99995    0.00010    2062640
  2548   0.99587    46.07  0.00E+00     2498    0.99995    0.00010    2062971
  2549   1.00074    46.08  0.00E+00     2499    0.99995    0.00010    2063786
  2550   0.99770    46.10  0.00E+00     2500    0.99995    0.00010    2064459
. . . . .
 final k(col/abs/trk len) = 1.00005     std dev = 0.00008
```

For 1-group problems with linearly-anisotropic scattering, with $|\bar{\mu}| < 1/3$, results using onegxs + MCNP match the exact analytic solution (within statistics)

Problem Ub-1-1-CY
from
Analytic Criticality
Benchmark Set

Example 3

- **Problem 37 from the analytic criticality benchmark set**
  - Identifier: **Ub-1-1-CY**
  - 1-group infinite cyclinder, with **anisotropic scatter (in lab),** $\bar{\mu} = .855263157$
  - From Table 23 in reference:

    $\Sigma_T = .32640$, $\Sigma_S = .248064$, $\Sigma_{S1} = .212160$

    $\Sigma_C = .013056$, $\Sigma_F = .065280$, $\nu = 2.70$

  - From Table 24 in reference:

    critical radius = 6.940205668

  - Exact eigenvalue: Keff = 1.000000

Example 3

- onegxs input for problem Ub-1-1-CY

```
onegxs xsec37 -z 37     -t .326400   -s .248064   \
                        -c .013056   -f .065280   -n 2.70 \
                        -s1 .212160
```

- onegxs screen output for problem Ub-1-1-CY

```
Created MCNP cross section file:

    xsec37

The following cross sections were used:

   sigT= 0.3264, sigF= 0.06528, sigC= 0.013056, sigS0= 0.248064, nu= 2.7, uBar= 0.855263

Please use the following line in your MCNP deck on the xsn card:

      92250.37m 1.0 xsec37 0 1 1 14 0 0 0.0
```

Example 3

- onegxs file created for problem Ub-1-1-CY (xsec37)

```
92250.37m          250             0    20070702
sigT= 0.3264, sigF= 0.06528, sigC= 0.013056, sigS0= 0.248064, nu= 2.7, uBar= 0.855263




      14     92250          2          0          1          0          0          0
       0         1          0          1          0          0          0          0
       1         3          4          5          6          7          0          0
       0         0          0          0          8          0          0         10
      12         0          0          0          0          0          0          0
       0         0          0          0          0          0          0          0
 5.000000000000e+01  1.000000000000e+02  3.264000000000e-01  6.528000000000e-02
 2.700000000000e+00  1.000000000000e+00  1.305600000000e-02  9.000000000000e+00
 2.480640000000e-01  1.100000000000e+01  1.000000000000e+00  1.300000000000e+01
 7.105263157895e-01  1.000000000000e+00
```

For linearly-anisotropic scatter, with |μ-bar| > 1/3, the angular distribution is represented by 1 step is used, with bounds chosen to preserve |μ-bar|

Example 3

- **MCNP input file for problem PUa-1-0-SL, for 500M histories**

```
Ub-1-1-CY
1   1     1.0     -1          $SEMI-INFINITE CYLINDER
2   0              1          $OUTSIDE WORLD

1   rcc 0 0 0    0 0 1e12   6.940205668

imp:n    1   0
kcode    20000  1.0   50   2550
hsrc   1 -1e20 1e20 1 -1e20 1e20 1 -1e20 1e20
ksrc     0.0     0.0   .5e12
xs1   92250.37m 1.0 xsec37 0 1 1 14 0 0 0.0
m1    92250.37m 1.0
mgopt  f 1
```

Example 3

Monte Carlo Codes
X-3-MCC, LANL

- MCNP output for problem Ub-1-1-CY

```
 cycle    k(col)       ctm   entropy     active      k(col)     std dev         fom
     1   1.22206      0.02  0.00E+00
     2   1.09928      0.04  0.00E+00
     3   1.05035      0.06  0.00E+00
. . . . .
  2544   1.01522     45.23  0.00E+00       2494     1.01865     0.00010     2560777
  2545   1.01316     45.25  0.00E+00       2495     1.01865     0.00010     2560448
  2546   1.01781     45.27  0.00E+00       2496     1.01865     0.00010     2561446
  2547   1.01126     45.28  0.00E+00       2497     1.01864     0.00010     2560008
  2548   1.01934     45.30  0.00E+00       2498     1.01864     0.00010     2561015
  2549   1.01609     45.32  0.00E+00       2499     1.01864     0.00010     2561737
  2550   1.01955     45.34  0.00E+00       2500     1.01864     0.00010     2562728
. . . . .
 final k(col/abs/trk len) = 1.01870     std dev = 0.00008
```

For 1-group problems with linearly-anisotropic scattering, with |μ-bar| > 1/3, results using onegxs + MCNP <u>will generally NOT match the exact analytic solution</u>

Angular Scattering Distributions

&

Truncation Errors

Sampling from Truncated Angular PDFs

- **Scattering angle PDFs**
  - Scattering distributions are usually represented by a Legendre polynomial expansion in data libraries (eg, ENDF/B)

$$f(\mu) = \sum_{n=0}^{N} \frac{2n+1}{2} a_n P_n(\mu), \qquad -1 \leq \mu \leq 1$$

  - Typically N=20 Legendre moments a_n are stored
  - The Legendre representation is converted to histogram or piecewise-linear PDFs for use in Monte Carlo codes by NJOY or some other processing program

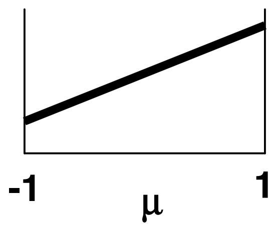
- **Sometimes, truncated angular PDFs must be used**
  - S_N codes typically use P1, P3, P5, …, truncated expansions
  - May want to compare MC & S_N using same cross-section data
  - Truncated Legendre expansions may produce angular PDFs with negative data over part of range

Sampling from Truncated Angular PDFs

- **Simplest case - P1 scattering**

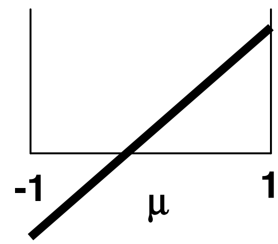
$$f(\mu) = \frac{1 + a\mu}{2}, \qquad -1 \le \mu \le 1, \qquad a = 3\bar{\mu}$$

$|\bar{\mu}| \le \frac{1}{3}$



f(μ) > 0 in [-1,1]

$|\bar{\mu}| > \frac{1}{3}$

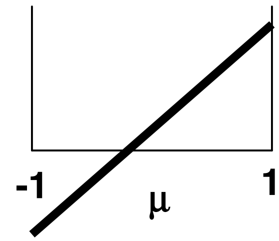


f(μ) < 0 for some μ

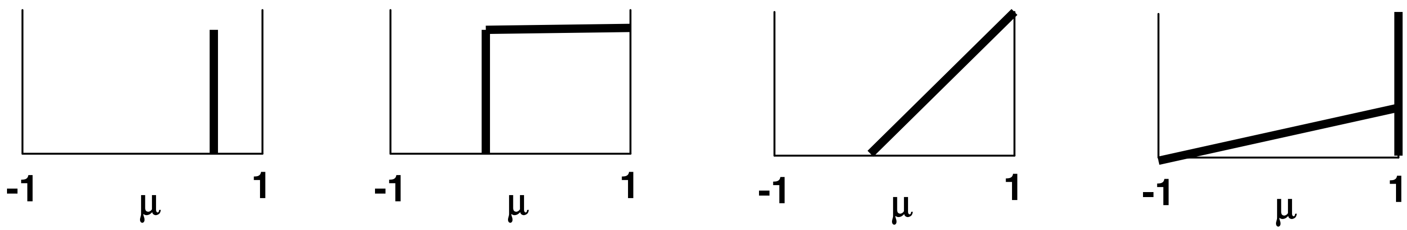
- **If $|\bar{\mu}| > 1/3$, need to replace f(μ) by another PDF g(μ)**
  - Non-negative PDF: $g(\mu) \ge 0$
  - Preserve physical condition: $\int_{-1}^{1} \mu g(\mu) d\mu = \bar{\mu}$

Sampling from Truncated Angular PDFs

- **Non-physical PDF, linear with** $|\bar{\mu}| > \frac{1}{3}$



- **Alternate forms of PDF that can preserve 1st moment**



  – All of these can be chosen to preserve the physical data, $<\mu>$

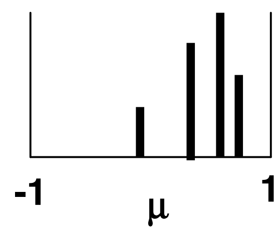
  – The second form, a 1-step histogram, can be accommodated by MCNP using the standard data formats, and does not require code modifications

For $\bar{\mu} > 1/3$, **choose bounds** $[\ 2\bar{\mu}-1,\ \ 1\ ]$

For $\bar{\mu} < -1/3$, **choose bounds** $[\ -1,\ \ 2\bar{\mu}+1\ ]$

Sampling from Truncated Angular PDFs

- **For higher order truncated Legendre expansions, more elaborate schemes must be used to preserve the moments & guarantee non-negative PDFs**
  - For a P_N expansion, can find (N+1)/2 discrete angles which preserve all N moments & have positive weights
    - Use generalized orthogonal polynomials
    - See description in MORSE code manual



  - Can use nonlinear least-squares fitting to find equiprobable histogram distribution that approximately preserves moments