Infinite 3D medium, Isotropic Point Source, Isotropic Scattering

Exponential Random Flight

This is code to accompany the book:

A Hitchhiker's Guide to Multiple Scattering

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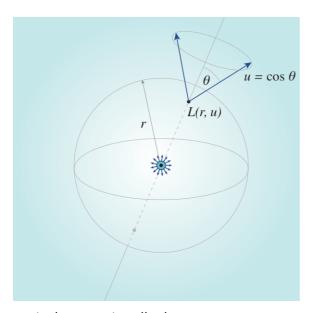
www.eugenedeon.com/hitchhikers

Path Setup

Put a file at ~/.hitchhikerpath with the path to your hitchhiker repo so that these worksheets can find the MC data from the C++ simulations for verification

In[725]:= SetDirectory[Import["~/.hitchhikerpath"]]

Notation



c - single-scattering albedo

 Σt - extinction coefficient

r - radial position coordinate in medium (distance from point source at origin)

 $u = \cos \theta$ - direction cosine

Namespace

In[6706]:= Begin["inf3Disopointisoscatter`"]

Out[6706]= inf3Disopointisoscatter`

Util

In[6770]:= SA[d_, r_] := d
$$\frac{P_{1}^{d/2}}{Gamma\left[\frac{d}{2} + 1\right]} r^{d-1}$$

Diffusion modes

In[6771]:= diffusionMode[v_, d_, r_] :=
$$(2\pi)^{-d/2} r^{1-\frac{d}{2}} v^{-1-\frac{d}{2}}$$
 BesselK[$\frac{1}{2}(-2+d), \frac{r}{v}$]

Analytic solutions

Caseology quantities

In[6739]:= CaseN0[c_, v0_] :=
$$\frac{1}{2}$$
 c v0³ $\left(\frac{c}{v0^2 - 1} - \frac{1}{v0^2}\right)$

In[6740]:= Casev0[c_?NumericQ] := FindRoot[c v ArcTanh[
$$\frac{1}{v}$$
] - 1 == 0, {v, 1.00000000001, 10^{10} }, Method \rightarrow "Brent"][[1]][[2]]

$$ln[6741] := Casev0approx[c_] := 1 / \sqrt{1 - c^{2.4429445001914587^{\circ} + \frac{0.5786368322364553^{\circ}}{c}} - 0.021581332427913873^{\circ} c}$$

$$ln[6742] = CaseN[c_, v_] := v \left(Case\lambda[v, c]^2 + \left(\frac{\pi c v}{2} \right)^2 \right)$$

$$ln[6743] = Case \lambda[v_, c_] := 1 - c v ArcTanh[v]$$

Fluence: exact solution (1)

[Bothe 1942]

[Case et al. 1953]

$$\begin{aligned} &\text{In}[6745] \coloneqq \phi \text{exact1b}[r_, \Sigma t_, c_] \coloneqq \frac{\text{Exp}[-\Sigma t \, r]}{4 \, \text{Pi} \, r^2} + c \, \frac{\Sigma t}{2 \, \text{Pi}^2 \, r} \\ &\text{NIntegrate} \Big[\frac{\text{ArcTan}[z]^2}{z - c \, \text{ArcTan}[z]} \, \text{Sin}[r \, \Sigma t \, z] \,, \, \{z, \, 0, \, \text{Infinity}\} \,, \, \text{Method} \rightarrow \text{"LevinRule"} \Big] \end{aligned}$$

Rigorous diffusion approximation

$$ln[6746]:= \phi rigourousDiffusion[r_, \Sigmat_, c_] := \frac{\Sigma t}{4 Pir} \frac{E^{-r \Sigma t/\#}}{\# CaseN0[c_, \#]} \& [Casev0[c]]$$

$$In[6747]:= \phi transient[r_, \Sigma t_, c_] := \frac{\Sigma t}{4 \, Pi \, r} \, NIntegrate \left[\frac{e^{-\Sigma t \, r \, / v}}{v \, CaseN[c, v]}, \, \{v, \, 0, \, 1\} \right]$$

Expansion of transient term [Case et al. 1953]

$$\begin{aligned} &\text{In}[6748] \coloneqq \phi \text{transient2}[r_, \, \Sigma t_, \, c_, \, M_] \ \coloneqq \frac{\text{Exp}[-r \, \Sigma t]}{4 \, \text{Pi} \, r^2} + \frac{1}{4 \, \text{Pi} \, r} \, \text{Sum} \big[\text{ExpIntegralE}[2 \, n, \, r \, \Sigma t] \\ &\text{SeriesCoefficient} \big[v \big/ \text{CaseN}[c, v], \, \{v, \, 0, \, 2 \, n\} \big], \, \{n, \, 1, \, M\} \big] \end{aligned}$$

Fluence: exact solution (2)

[Davison 1947]

$$\begin{split} & \underset{\text{In}[6749]:=}{\text{Depart2a}[\texttt{r}_, \texttt{\Sigmat}_, \texttt{c}_] := \phi rigourousDiffusion}[\texttt{r}, \texttt{\Sigmat}, \texttt{c}] + \\ & \frac{\texttt{\Sigmat}}{4\,\text{Pir}}\,\text{NIntegrate}\Big[\frac{e^{-\texttt{\Sigmat}\,\texttt{r}\,\texttt{y}}}{\frac{c^2\,\pi^2}{4\,\texttt{y}^2} + \Big(1 - \frac{c}{2\,\texttt{y}}\,\text{Log}\Big[\frac{\texttt{y}+\texttt{1}}{\texttt{y}-\texttt{1}}\Big]\Big)^2},\,\{\texttt{y},\,\texttt{1},\,\text{Infinity}\}\Big] \end{split}$$

[Case and Zwiefel 1967]

In[6750]:=
$$\phi$$
exact2b[r_, Σ t_, c_] :=
$$\phi$$
rigourousDiffusion[r, Σ t, c] +
$$\frac{\Sigma t}{4 \text{ Pir}} \text{ NIntegrate} \left[\frac{e^{-\Sigma t r/v}}{v \text{ CaseN[c, v]}}, \{v, 0, 1\} \right]$$

n-th scattered fluence

$$\begin{array}{l} & \text{In}[6751] \coloneqq \phi \text{exact1}[r_, \ \Sigma t_, \ c_, \ n_] \ \coloneqq \frac{(\text{c} \ \Sigma t)^n}{2 \ \pi^2 \ r} \ \text{NIntegrate} \Big[\frac{\text{ArcTan} \Big[\frac{z}{\Sigma t}\Big]^{1+n} \ \text{Sin}[r \ z]}{z^n}, \\ & \{z, \ 0, \ \text{Infinity}\}, \ \text{Method} \rightarrow \text{"ExtrapolatingOscillatory"} \Big] \end{array}$$

In[6753]:=
$$\phi$$
Gaussian[r_, Σ t_, c_, n_] := $\frac{3\sqrt{3} e^{-\frac{3r^2 \Sigma t^2}{4(1+n)}} c^n \Sigma t^2}{8\sqrt{(1+n)^3} \pi^{3/2}}$

Moments

$$ln[6754] = \phi m[c_, \Sigma t_, m_?IntegerQ, n_] :=$$

$$\text{Limit} \big[\text{Simplify} \big[\left(-1 \right)^{\text{m/2}} \left(\frac{2 \, \text{Gamma} \left[\frac{3+m}{2} \right]}{\text{Gamma} \left[\frac{1+m}{2} \right]} \, \text{D} \left[\frac{\left(\frac{c \, \text{\Sigmat ArcTan} \left[\frac{z}{\text{St}} \right]}{z} \right)^{1+n}}{c \, \text{\Sigmat}}, \, \{z, \, m\} \big] \right], \, z \rightarrow \emptyset \big]$$

```
In[6755]:= TableForm[Table[\phim[c, \Sigmat, m, n], {m, 0, 6, 2}]]
Out[6755]//TableForm=
             2 c^n (1+n)
             4 c<sup>n</sup> (1+n) (18+5 n)
             \underline{8\ c^n\ (1{+}n)\ \left(810{+}343\ n{+}35\ n^2\right)}
 ln[6756] = \phi m[c_, \Sigma t_, m_?IntegerQ] :=
              \label{eq:limit_simplify} \text{Limit} \big[ \text{Simplify} \big[ \left( -1 \right)^{m/2} \left( \frac{2 \, \text{Gamma} \left[ \frac{3+m}{2} \right]}{\text{Gamma} \left[ \frac{1+m}{2} \right]} \, D \Big[ \frac{\text{ArcTan} \left[ \frac{z}{\Sigma t} \right]}{z - c \, \Sigma t \, \text{ArcTan} \left[ \frac{z}{\Sigma t} \right]}, \, \left\{ z \,, \, m \right\} \Big] \right) \Big] \,, \, z \to 0 \Big]
 ln[6757] = TableForm[Table[\phi m[c, \Sigma t, m], \{m, 0, 6, 2\}]]
             8 (-9+4 c)
             3 (-1+c)^3 \Sigma t^5
             16 (135-144 c+44 c<sup>2</sup>)
                 3 (-1+c)^4 \Sigma t^7
            Recurrence derivation [Case et al. 1953]
In[6758] = CaseB[0, c_] := \frac{1}{1};
            CaseB[m_, c_] := \frac{1}{(1-c)^2} Sum[Caseb[m, s] \left(\frac{c}{1-c}\right)^{s-1}, {s, 1, m}];
            Caseb[m_, 1] := \frac{1}{2 m + 1};
            Caseb[m_, s_] := Sum \left[\frac{Caseb[n, s-1]}{1+2 (m-n)}, \{n, s-1, m-1\}\right]
 ln[6772] = \phi mCase[c_, \Sigma t_, m_?IntegerQ] := \frac{1}{\Sigma + m + 1} CaseB[m/2, c] Factorial[m+1]
 In[6773]:= TableForm[Table[FullSimplify[\phimCase[c, \Sigmat, m]], {m, 0, 6, 2}]]
Out[6773]//TableForm=
             \Sigma t - c \Sigma t
             (-1+c)^2 \Sigma t^3
              8(-9+4c)
             3 (-1+c)^3 \Sigma t^5
             16 (135+4 c (-36+11 c))
                   3 (-1+c)^4 \Sigma t^7
       Classical diffusion approximation
 \label{eq:diffusion} \ln [r\_, \Sigma t\_, c\_] := \frac{1}{\Sigma t \; (1-c)} \; \text{diffusionMode} \left[ \frac{1}{\sqrt{3 \; (1-c)}} \; \Sigma t, \; 3, \; r \right]
 log(6775) = FullSimplify[\phi Diffusion[r, \Sigma t, c], Assumptions <math>\rightarrow 0 < c < 1 \&\& \Sigma t > 0]
```

Grosjean-style diffusion approximation

$$\begin{aligned} & & \text{In} [6776] \coloneqq \phi \text{Grosjean} [\text{r}_, \Sigma \text{t}_, \text{c}_] \ \coloneqq \frac{\text{Exp}[-\text{r} \, \Sigma \text{t}]}{4 \, \text{Pi} \, \text{r}^2} + \frac{\text{c}}{\Sigma \text{t} \, (1-\text{c})} \, \text{diffusionMode} \Big[\frac{\sqrt{2-\text{c}}}{\sqrt{3 \, (1-\text{c})} \, \Sigma \text{t}}, \, 3, \, \text{r} \Big] \\ & & \text{In} [6777] \coloneqq \text{FullSimplify} [\phi \text{Grosjean}[\text{r}, \Sigma \text{t}, \text{c}], \, \text{Assumptions} \rightarrow 0 < \text{c} < 1 \, \& \, \Sigma \text{t} > 0] \\ & & & \text{Out} [6777] \coloneqq \frac{\text{e}^{-\text{r} \, \Sigma \text{t}} - \frac{3 \, \text{c} \, \text{e}^{-\sqrt{3 \cdot \frac{3}{2 \cdot \text{c}} \, \text{r} \, \Sigma \text{t}}}}{-2 + \text{c}}}{4 \, \pi \, \text{r}^2} \end{aligned}$$

Angular ϕ Integral

Note: this form leaves out the singular term $\frac{e^{-r\Sigma_t}}{4\pi r^2}\delta(u-1)$, because it doesn't plot:

In[6778]:= Lintegral[r_, u_,
$$\Sigma$$
t_, c_, ϕ _] :=
$$\frac{c \Sigma t}{4 \, \text{Pi}} \, \text{NIntegrate} \left[\phi \left[\sqrt{r^2 + t^2 - 2 \, r \, t \, u} \right], \, \Sigma t, \, c \right] \, \text{Exp[-Σt t], } \{t, \, \theta, \, \text{Infinity}\} \right]$$

Angular Classical diffusion approximation

In[6779]:= Ldiffusion[r_, u_,
$$\Sigma$$
t_, c_] :=
$$\frac{1}{4 \, \text{Pi}} \, \phi \text{Diffusion[r, } \Sigma \text{t, c]} + \frac{1}{4 \, \text{Pi}} \, u \, \frac{3 \, e^{-r \, \sqrt{3-3 \, c}} \, \Sigma \text{t}}{4 \, \pi \, r^2} \left(1 + r \, \sqrt{3-3 \, c} \, \Sigma \text{t}\right)$$

load MC data

```
In[6780]:= ppoints[xs_, dr_, maxx_] :=
         Table[{dr (i) - 0.5 dr, xs[[i]]}, {i, 1, Length[xs]}][[1;; -2]]
In[6781]:= ppointsu[xs_, du_, Σt_] :=
         Table\big[\big\{-1.0 + du \, \big(i\big) - 0.5 \, du, \, xs[[i]] \, \big/ \, \big(2 \, \Sigma t\big)\big\}, \, \{i, 1, \, Length[xs]\}\big][[1 \, ;; \, -1]]
In[6782]:= fs = FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/MCdata/
               inf3D_isotropicpoint_isotropicscatter*"];
ln[6783] = index[x_] := Module[{data, <math>\alpha, \Sigma t},
            data = Import[x, "Table"];
            Σt = data[[1, 13]];
            \alpha = data[[2, 3]];
            \{\alpha, \Sigma t, data\}];
        simulations = index /@fs;
        cs = Union[#[[1]] & /@ simulations]
Out[6785]= \{0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999\}
In[6786]:= mfps = Union[#[[2]] & /@ simulations]
Out[6786]= \{0.3, 1\}
```

```
In[6787]:= numcollorders = simulations[[1]][[3]][[2, 13]];
     maxr = simulations[[1]][[3]][[2, 5]];
     dr = simulations[[1]][[3]][[2, 7]];
      numr = Floor[maxr/dr];
```

Compare Deterministic and MC

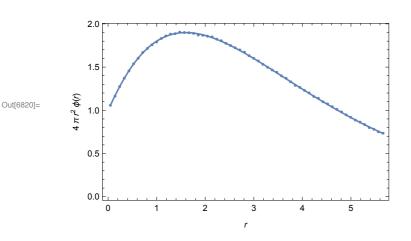
0.3

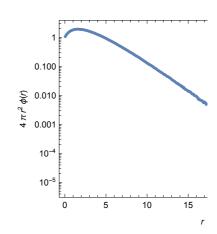
Set mfp

```
Mean Track Length
ln[6872] =  { {ActionMenu["Set c", "c = " <> ToString[#] \Rightarrow (c = #;) & /@ cs], Dynamic[c]},
          {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
           Dynamic[mfp] } // TableForm
Out[6872]//TableForm
                    0.8
        Set c
                    0.3
        Set mfp
In[6791]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
       meanTL = data[[-1]]
Out[6792]= { Mean, track, length:, 1.00046}
Out[6793]= 1.
    Fluence - Exact solution (1a) comparison to MC
ln[6873] =  { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c]},
          {ActionMenu["Set mfp", "mfp = " <> ToString[#] \Rightarrow (mfp = #;) & /@ mfps],
          Dynamic[mfp] } // TableForm
Out[6873]//TableForm=
                    0.8
        Set c
```

```
In[6812]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      MCFluence = ppoints[data[[6]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact1a}[\#[[1]], 1/mfp, c]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact1a}[\#[[1]], 1/\text{mfp, c}]\}] & /@
          MCFluence[[60;;-1;;10]];
      plotφshallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
            ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
            ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
        PlotLabel -> "Exact solution (1a) \nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "\Leftrightarrow
          ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Exact solution (1a) Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.9, Σ_t = 1





Fluence - Exact solution (1b) comparison to MC

```
ln[6874]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
             \left\{ \text{ActionMenu} \left[ \text{"Set mfp", "mfp = "} <> \text{ToString} \right] \right. \Rightarrow \left( \text{mfp = #;} \right) \, \& \, /@ \, \text{mfps} \right],
              Dynamic[mfp] } // TableForm
```

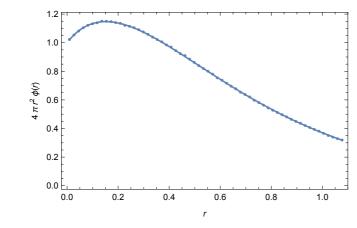
Out[6874]//TableForm=

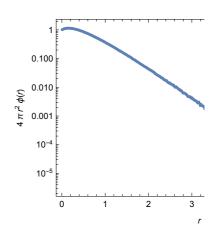


Set mfp

```
In[6830]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      MCFluence = ppoints[data[[6]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact1b}[\#[[1]], 1/mfp, c]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact1b}[\#[[1]], 1/\text{mfp, c}]\}] & /@
          MCFluence[[60;;-1;;10]];
      plotφshallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
            ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
            ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
        PlotLabel -> "Exact solution (1b) \nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "\Leftrightarrow
          ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Exact solution (1b) Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.7, Σ_t = 3.33333





Out[6838]=

Fluence - Exact solution (2a) comparison to MC

```
ln[6875]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c]},
             \left\{ \text{ActionMenu} \left[ \text{"Set mfp", "mfp = "} <> \text{ToString} \right] \right. \Rightarrow \left( \text{mfp = #;} \right) \, \& \, /@ \, \text{mfps} \right],
              Dynamic[mfp] } // TableForm
```

Out[6875]//TableForm=

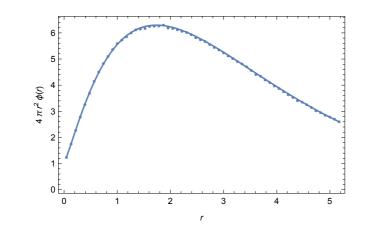


0.8

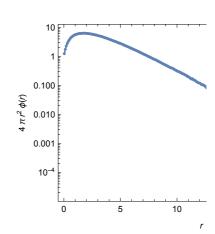
Set mfp

```
In[6839]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      MCFluence = ppoints[data[[6]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact2a} [\#[[1]], 1/mfp, c]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact2a}[\#[[1]], 1/\text{mfp, c}]\}] & /@
          MCFluence[[60;;-1;;10]];
      plot¢shallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
            ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
            ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
        PlotLabel -> "Exact solution (2a) \nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "\Leftrightarrow
          ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Exact solution (2a) Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.99, Σ_t = 3.33333



Out[6847]=



Fluence - Exact solution (2b) comparison to MC

```
ln[6876]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
             \left\{ \text{ActionMenu} \left[ \text{"Set mfp", "mfp = "} <> \text{ToString} \right] \right. \Rightarrow \left( \text{mfp = #;} \right) \, \& \, /@ \, \text{mfps} \right],
              Dynamic[mfp] } // TableForm
```

Out[6876]//TableForm=

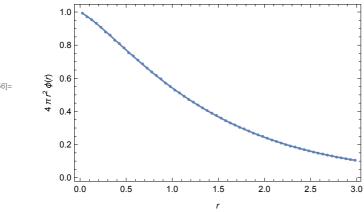


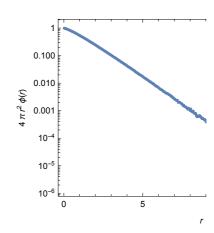
0.8

Set mfp

```
In[6848]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      MCFluence = ppoints[data[[6]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact2b}[\#[[1]], 1/mfp, c]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{exact2b}[\#[[1]], 1/\text{mfp, c}]\}] & /@
          MCFluence[[60;;-1;;10]];
      plotφshallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
            ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
            ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
        PlotLabel -> "Exact solution (2b) \nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "\Leftrightarrow
          ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Exact solution (2b) Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.3, Σ_t = 1



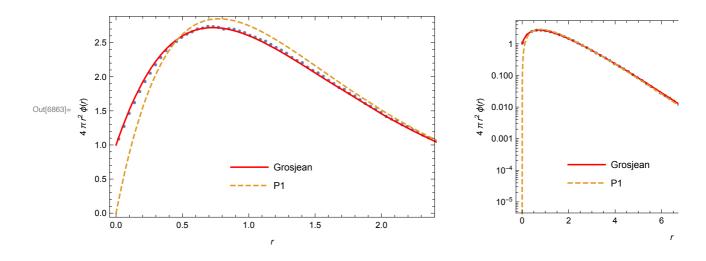


Out[6856]=

Fluence - Diffusion approximations (Classical and Grosjean) comparison to MC

```
ln[6877] = \{ \{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c] \}, \}
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
           Dynamic[mfp] } // TableForm
Out[6877]//TableForm:
                    0.8
        Set c
        Set mfp
                    0.3
In[6857]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
       maxr = data[[2, 5]];
       dr = data[[2, 7]];
       MCFluence = ppoints[data[[6]], dr, maxr];
       plotφshallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            Plot[{
               4 Pi r^2 \phi Grosjean[r, 1/mfp, c],
               4 Pi r<sup>2</sup> φDiffusion[r, 1/mfp, c]
              , {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
             PlotLegends → Placed[{"Grosjean", "P1"}, {0.5, .2}]],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r], \}, \{r,\}\}
           ]];
       logplotφ = Quiet[Show[
            ListLogPlot[MCFluence[[1;; -1;; 5]],
             PlotRange → All, PlotStyle → PointSize[.01]],
            LogPlot[{
               4 Pi r^2 \phi Grosjean[r, 1/mfp, c],
               4 Pi r<sup>2</sup> φDiffusion[r, 1/mfp, c]
              , {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
             PlotLegends → Placed[{"Grosjean", "P1"}, {0.3, .2}]],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
           ||;
       Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
        PlotLabel -> "Diffusion Approximations\nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "<>
           ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Diffusion Approximations Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.95, Σ_t = 3.33333



Fluence - Diffusion approximation (Rigorous) comparison to MC

In[6878]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]}, $\left\{ \texttt{ActionMenu} \left[\texttt{"Set mfp", "mfp = "} <> \texttt{ToString} \texttt{[#]} \Rightarrow \left(\texttt{mfp = #;} \right) \& /@ \, \texttt{mfps} \right], \right.$ Dynamic[mfp]}} // TableForm

Out[6878]//TableForm

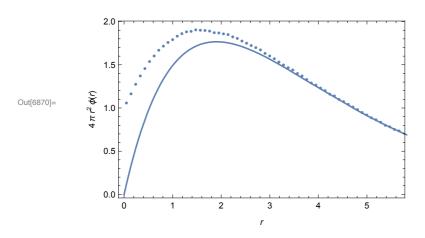
Set c

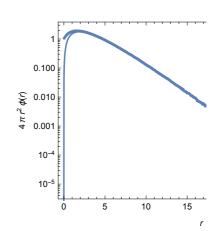
0.8

Set mfp

```
In[6864]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      MCFluence = ppoints[data[[6]], dr, maxr];
      plotφshallow = Quiet[Show[
            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
            Plot[4 Pi r^2 \phi rigourousDiffusion[r, 1/mfp, c], {r, 0, maxr}, PlotRange \rightarrow All],
            Frame → True,
            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
      logplotφ = Quiet[Show[
            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
            LogPlot[
             4 Pi r^2 \phi rigourous Diffusion [r, 1/mfp, c], \{r, 0, maxr\}, PlotRange <math>\rightarrow All],
            Frame → True,
            FrameLabel -> \{\{4 \, \text{Pi} \, r^2 \, \phi[r], \}, \, \{r, \}\}
          11;
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize → 800],
        PlotLabel -> "Rigorous Diffusion Approximation\nInfinite 3D, isotropic
             point source, isotropic scattering, fluence \phi[r], c = "<>
          ToString[c] \leftrightarrow ", \Sigma_t = " \leftrightarrow ToString[1/mfp]]
```

Rigorous Diffusion Approximation Infinite 3D, isotropic point source, isotropic scattering, fluence $\phi[r]$, c = 0.9, Σ_t = 1





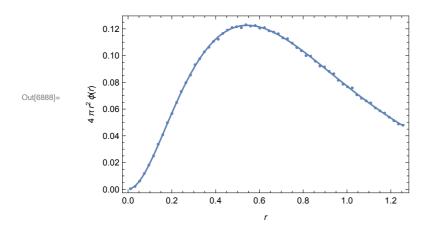
N-th order fluence / scalar flux

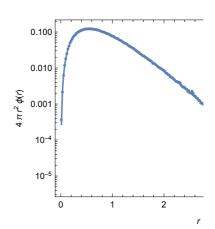
N-th collided Fluence - Exact solution (1) comparison to MC

```
ln[6871]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
        {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
         Dynamic[mfp] },
        {ActionMenu["Set collision order",
           "collisionOrder = " <> ToString[#] ⇒ (collisionOrder = #;) & /@
            Range[0, numcollorders - 1]], Dynamic[collisionOrder]}} // TableForm
                          0.8
       Set c
                          0.3
       Set mfp
                          2
       Set collision order
```

```
In[6879]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      fluencei = 3 numcollorders + 15 + collisionOrder;
      MCFluence = ppoints[data[[fluencei]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4Pi\#[[1]]^2 \phi exact1[\#[[1]], 1/mfp, c, collision0rder]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[{\#[[1]], 4 \text{ Pi } \#[[1]]}^2 \phi \text{exact1}[\#[[1]], 1/\text{mfp},
                c, collisionOrder]}] & /@MCFluence[[61;; -1;; 10]];
      plotφshallow = Quiet[Show[
           ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
           ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
           ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
           ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
           ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \, \text{Pi} \, r^2 \, \phi[r], \}, \, \{r, \}\}
          ]];
      Show[GraphicsGrid[\{\{plot\phishallow, logplot\phi\}\}, ImageSize \rightarrow 800],
       PlotLabel -> "Exact solution (1) \nInfinite 3D medium, isotropic point source,
             isotropic scattering, n-th scattered fluence \phi[r]" <>
          ToString[collisionOrder] <> "], c =" <> ToString[c] <>
          ", \Sigma_t = " \Leftrightarrow ToString[1/mfp]]
```

Exact solution (1) Infinite 3D medium, isotropic point source, isotropic scattering, n-th scattered fluence $\phi[r|4]$, c =0.8, Σ_t =



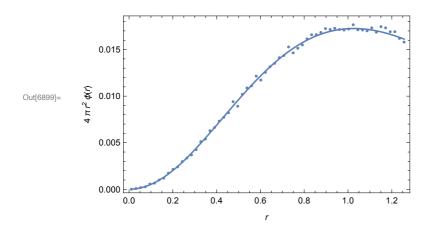


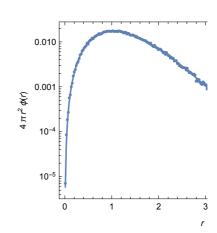
N-th collided Fluence - Exact solution (2) comparison to MC

```
ln[6889]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
          Dynamic[mfp] },
         {ActionMenu["Set collision order",
            "collisionOrder = " <> ToString[#] → (collisionOrder = #;) & /@
             Range[0, numcollorders - 1]], Dynamic[collisionOrder]}} // TableForm
Out[6889]//TableForm=
                            0.8
       Set c
                            0.3
        Set mfp
        Set collision order
                            2
```

```
In[6890]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      fluencei = 3 numcollorders + 15 + collisionOrder;
      MCFluence = ppoints[data[[fluencei]], dr, maxr];
      exact1FluenceShallow =
         Quiet[\{\#[[1]], 4 \text{ Pi} \#[[1]]^2 \phi \text{ exact2}[\#[[1]], 1/mfp, c, collision0rder]\}] & /@
          MCFluence[[1;; 60]];
      exact1Fluence = Quiet[{\#[[1]], 4 \text{ Pi } \#[[1]]}^2 \phi \text{exact2}[\#[[1]], 1/\text{mfp},
                c, collisionOrder]}] & /@MCFluence[[61;; -1;; 10]];
      plotφshallow = Quiet[Show[
           ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
           ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
           ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
           ListLogPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
           ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \, \text{Pi} \, r^2 \, \phi[r], \}, \, \{r, \}\}
          ]];
      Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize → 800],
       PlotLabel -> "Exact solution (2)\nInfinite 3D medium, isotropic point source,
             isotropic scattering, n-th scattered fluence \phi[r]" <>
          ToString[collisionOrder] <> "], c =" <> ToString[c] <>
          ", \Sigma_t = " \Leftrightarrow ToString[1/mfp]]
```

Exact solution (2) Infinite 3D medium, isotropic point source, isotropic scattering, n-th scattered fluence $\phi[r]11$], c =0.8, Σ_t :





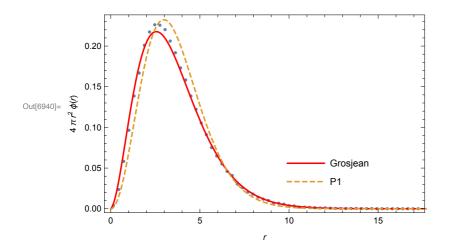
N-th collided Fluence - Approximations

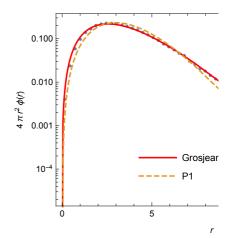
```
In[6900]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
          Dynamic[mfp] },
         {ActionMenu["Set collision order",
            "collisionOrder = " <> ToString[#] → (collisionOrder = #;) & /@
             Range[0, numcollorders - 1]], Dynamic[collisionOrder]}} // TableForm
Out[6900]//TableForm=
                            0.8
       Set c
                            0.3
        Set mfp
        Set collision order
                            2
```

```
In[6931]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
               maxr = data[[2, 5]];
               dr = data[[2, 7]];
               fluencei = 3 numcollorders + 15 + collisionOrder;
               MCFluence = ppoints[data[[fluencei]], dr, maxr];
               seriesclassical = c<sup>collisionOrder</sup>
                         SeriesCoefficient[\phiDiffusion[r, 1/mfp, C], {C, 0, collisionOrder}];
               seriesG = c<sup>collisionOrder</sup> SeriesCoefficient[
                            \phiGrosjean[r, 1/mfp, C], {C, 0, collisionOrder}];
               plotφshallow = Quiet[Show[
                            ListPlot[MCFluence[[1;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
                            Plot[{4 Pi r<sup>2</sup> seriesG, 4 Pi r<sup>2</sup> seriesclassical},
                               \{r, 0, maxr\}, PlotRange \rightarrow All, PlotStyle \rightarrow {Red, Dashed},
                               PlotLegends → Placed[{"Grosjean", "P1"}, {0.7, .2}]],
                            Frame → True,
                            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r], \}, \{r,\}\}
                         ]];
               logplot = Quiet Show
                            ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
                            LogPlot[{4 Pi r<sup>2</sup> seriesG, 4 Pi r<sup>2</sup> seriesclassical},
                               \{r, 0, maxr\}, PlotRange \rightarrow All, PlotStyle \rightarrow \{Red, Dashed\},
                               PlotLegends → Placed[{"Grosjean", "P1"}, {0.4, .2}]],
                            Frame → True,
                            FrameLabel -> \{\{4 \text{ Pi } r^2 \phi[r],\}, \{r,\}\}
               Show[GraphicsGrid[\{\{plot\phishallow, logplot\phi\}\}, ImageSize \rightarrow 800], PlotLabel \rightarrow Robert + Robert
                      "Diffusion Approximations\nInfinite 3D medium, isotropic point source,
                               isotropic scattering, n-th scattered fluence \phi[r]" <>
                         ToString[collisionOrder] <> "], c =" <> ToString[c] <>
                         ", \Sigma_t = " \Leftrightarrow ToString[1/mfp]]
```

Diffusion Approximations

Infinite 3D medium, isotropic point source, isotropic scattering, n-th scattered fluence $\phi[r|7]$, c =0.99,





Compare moments of ϕ

ln[6941]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]}, $\left\{ \texttt{ActionMenu} \left[\texttt{"Set mfp", "mfp = " <> ToString[#] } \right. \right. \\ \left. \left(\texttt{mfp = #;} \right) \, \& \, /@\, \texttt{mfps} \right],$ Dynamic[mfp]}} // TableForm

Out[6941]//TableForm=

Set c

0.8

Set mfp

```
In[6950]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
       nummoments = data[[2, 15]];
       \phimoments = {data[[10]]};
       ks = Table[k, {k, 0, nummoments - 1}];
       analytic = Table [\phi m[c, 1/mfp, k], \{k, ks\}];
       j = Join[{ks}, {analytic}, φmoments];
      TableForm[
        Join[{{"n", "analytic", "MC"}}, Transpose[j]]
       ]
Out[6956]//TableForm=
           analytic
                              MC
      n
       0
           2.
                              2.00096
           0. + 0. i
       1
                              2.98567
                             8.01171
       2
           8.
           0. + 0. i
                              30.4943
       3
       4
           149.333
                             149.478
       5
                             894.305
           0. + 0. i
       6
           6314.67
                              6305.37
       7
           0. + 0. i
                             51051.9
       8
           472269.
                              464 772
            Indeterminate 4.67159 \times 10^6
In[6957]:= \{ \{ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps], \} \}
          Dynamic[mfp] } // TableForm
Out[6957]//TableForm=
                   0.3
        Set mfp
```

```
In[6995]:= sims1 = Select[simulations, #[[2]] == mfp &];
           Show
             ListLogPlot[{
                  {\#[[-1, 2, 3]], \#[[-1, 10, 1]]} \& /@ sims1,
                  {\#[[-1, 2, 3]], \#[[-1, 10, 3]]} \& /@ sims1,
                  {\#[[-1, 2, 3]], \#[[-1, 10, 5]]} \& /@ sims1,
                  {\#[[-1, 2, 3]], \#[[-1, 10, 7]]} \& /@ sims1,
                  {#[[-1, 2, 3]], #[[-1, 10, 9]]} & /@ sims1
               }],
             LogPlot[\left\{-\frac{\text{mfp}}{-1+c}, \frac{2 \text{ mfp}^3}{(-1+c)^2}, \frac{8 \left(-9+4 c\right) \text{ mfp}^5}{3 \left(-1+c\right)^3}, \frac{16 \left(135-144 c+44 c^2\right) \text{ mfp}^7}{3 \left(-1+c\right)^4}, \right\}
                  \frac{128 \left(-1575 + 2808 \text{ c} - 1836 \text{ c}^2 + 428 \text{ c}^3\right) \text{ mfp}^9}{5 \left(-1 + \text{c}\right)^5} \right\}, \text{ {c, 0, .999}}, \text{ PlotRange} \rightarrow \text{All} \right]
           1
              10<sup>19</sup>
              10<sup>15</sup>
              10<sup>11</sup>
Out[6996]=
               107
           1000.0
                                                                  0.6
```

n-th collided moments of ϕ

```
ln[6942] =  {ActionMenu["Set c", "c = "<> ToString[#] \Rightarrow (c = #;) & /@ cs], Dynamic[c]},
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
          Dynamic[mfp] },
         {ActionMenu["Set collision order",
            "collisionOrder = " <> ToString[#] → (collisionOrder = #;) & /@
             Range[0, numcollorders - 1]], Dynamic[collisionOrder]}} // TableForm
Out[6942]//TableForm:
                            0.8
        Set c
```

Set collision order

Set mfp

0.3

2

Out[2437]= 52

```
In[7000]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
       nummoments = data[[2, 15]];

φmoments = N[{data[[numcollorders + 13 + collisionOrder]]}];

       ks = Table[k, {k, 0, nummoments - 1}];
       analytic = Table [\phi m[c, 1/mfp, k, collisionOrder], \{k, ks\}];
       j = Join[{ks}, {analytic}, φmoments];
      TableForm[
        Join[{{"n", "analytic", "MC"}}, Transpose[j]]
       ]
Out[7006]//TableForm=
           analytic
                        MC
      n
       0
           0.192
                        0.192008
       1
           0. + 0. i
                        0.11745
                       0.103751
           0.10368
       2
                        0.120756
       3
           Θ.
           0.174182
       4
                        0.175155
       5
           0.
                        0.305055
       6
           0.610634
                        0.621431
       7
           0.
                        1.45293
       8
           3.68312
                        3.84418
       9
           0.
                         11.3783
    Angular Distributions
ln[7007]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c]},
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
          Dynamic[mfp] } // TableForm
Out[7007]//TableForm=
                   0.8
       Set c
                   0.3
       Set mfp
In[2437]:= depthi = 52
```

```
In[2438]:= Clear[u];
       data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
       du = data[[2, 9]];
       maxr = data[[2, 5]];
       dr = data[[2, 7]];
       fluxi = 17 + 4 numcollorders + Floor[maxr/dr];
       angularFlux = ppointsu[data[[fluxi + depthi]], du, 1];
       r = dr * depthi - 0.5 dr;
       Show
        ListPlot angularFlux, PlotRange → All,
          Frame → True,
          FrameLabel -> {{"4 Pi<sup>2</sup> r<sup>2</sup> L[r,u]",}, {u,}}],
        Plot[4 Pi r^2 Pi Ldiffusion[r, u, 1/mfp, c], \{u, -1, 1\}, PlotRange \rightarrow All]
       ]
          0.7
          0.6
          0.5
          0.4
Out[2446]=
         0.3
          0.1
          0.0
                       -0.5
                                    0.0
                                                0.5
                                                             1.0
```

Angular Distribution: Integral of Grosjean's Diffusion Approximation

```
ln[7008] = \{ \{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c] \}, \}
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
          Dynamic[mfp] } // TableForm
```

Out[7008]//TableForms

Set c

0.8

Set mfp

0.3

In[*]:= depthi = 52

 $Out[\circ] = 52$

```
In[2447]:= Clear[u];
         data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
         du = data[[2, 9]];
         maxr = data[[2, 5]];
         dr = data[[2, 7]];
         fluxi = 17 + 4 numcollorders + Floor[maxr/dr];
         angularFlux = ppointsu[data[[fluxi + depthi]], du, 1];
         r = dr * depthi - 0.5 dr;
         Show
           ListPlot angularFlux, PlotRange → All,
             Frame → True,
             FrameLabel -> \{\{"4 Pi^2 r^2 L[r,u]",\}, \{u,\}\}],
           \mathsf{Plot}\big[4\,\mathsf{Pi}\,\mathsf{r}^2\,\mathsf{Pi}\,\,\mathsf{Lintegral}\big[\mathsf{r},\,\mathsf{u},\,\mathsf{1}\big/\mathsf{mfp},\,\mathsf{c},\,\phi\mathsf{Grosjean}\big],\,\{\mathsf{u},\,\mathsf{-1},\,\mathsf{1}\},\,\mathsf{PlotRange}\to\mathsf{All}\big]
         ]
             0.7
             0.6
             0.5
Out[2455]= 24 0.3
             0.2
             0.1
             0.0
                              -0.5
                                              0.0
                                                              0.5
```

End context

```
In[7009]:= End[]
Out[7009]= inf3Disopointisoscatter`
```