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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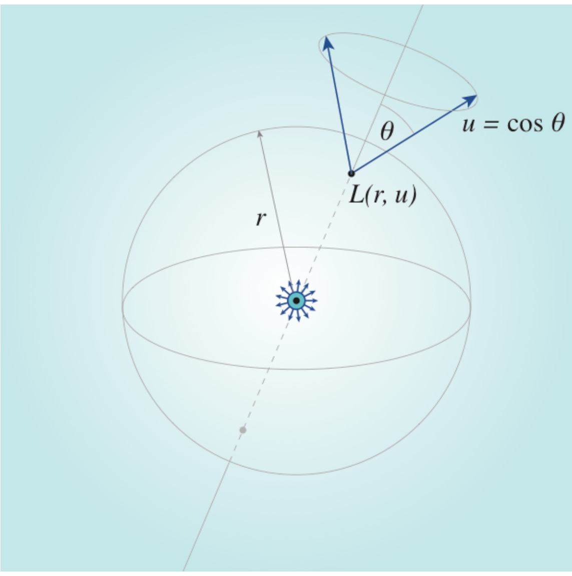
www.eugenedeon.com/hitchhikers

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[2325]:= 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 θ - direction cosine

Namespace

In[2328]:= `Begin["inf3Disopointisoscatter`"]`

Out[2328]= `inf3Disopointisoscatter``

Util

In[2329]:= $$\text{SA}[d\_, r\_] := d \frac{\text{Pi}^{d/2}}{\text{Gamma}\left[\frac{d}{2}+1\right]} r^{d-1}$$

Diffusion modes

In[2330]:= $$\text{diffusionMode}[v\_, d\_, r\_] := (2\pi)^{-d/2} r^{1-\frac{d}{2}} v^{-1-\frac{d}{2}} \text{BesselK}\left[\frac{1}{2}(-2+d), \frac{r}{v}\right]$$

Analytic solutions

Caseology quantities

In[2331]:= $$\text{CaseN0}[c\_, v0\_] := \frac{1}{2} c\, v0^3 \left(\frac{c}{v0^2-1} - \frac{1}{v0^2}\right)$$

In[2332]:= $$\text{Casev0}[c\_?\text{NumericQ}] := \text{FindRoot}\left[c\, v\, \text{ArcTanh}\left[\frac{1}{v}\right] - 1 == 0, \{v, 1.00000000001, 10^{10}\}, \text{Method} \to \text{"Brent"}\right][[1]][[2]]$$

In[2333]:= $$\text{Casev0approx}[c\_] := 1 \Big/ \sqrt{1 - c^{2.4429445001914587` + \frac{0.5786368322364553`}{c} - 0.021581332427913873`\, c}}$$

In[2334]:= $$\text{CaseN}[c\_, v\_] := v\left(\text{Case}\lambda[v, c]^2 + \left(\frac{\pi\, c\, v}{2}\right)^2\right)$$

In[2335]:= $$\text{Case}\lambda[v\_, c\_] := 1 - c\, v\, \text{ArcTanh}[v]$$

Fluence: exact solution (1)

[Bothe 1942]

In[2336]:= $$\phi\text{exact1a}[r\_, \Sigma t\_, c\_] := \frac{1}{2\,\text{Pi}^2 r} \text{NIntegrate}\left[\frac{z\, \text{ArcTan}[z/\Sigma t]}{z - c\,\Sigma t\, \text{ArcTan}[z/\Sigma t]} \text{Sin}[r\, z], \{z, 0, \text{Infinity}\}, \text{Method} \to \text{"ExtrapolatingOscillatory"}\right]$$

[Case et al. 1953]

In[2337]:= $$\phi\text{exact1b}[r\_, \Sigma t\_, c\_] := \frac{\text{Exp}[-\Sigma t\, r]}{4\,\text{Pi}\, r^2} + c \frac{\Sigma t}{2\,\text{Pi}^2 r} \text{NIntegrate}\left[\frac{\text{ArcTan}[z]^2}{z - c\,\text{ArcTan}[z]} \text{Sin}[r\,\Sigma t\, z], \{z, 0, \text{Infinity}\}, \text{Method} \to \text{"LevinRule"}\right]$$

Rigorous diffusion approximation

In[2338]:= ϕrigourousDiffusion[r_, Σt_, c_] := $\frac{\Sigma t}{4\,\text{Pi}\,r}\,\frac{E^{-r\,\Sigma t/\#}}{\#\,\text{CaseN0}[c,\#]}$ &[Casev0[c]]

In[2339]:= ϕtransient[r_, Σt_, c_] := $\frac{\Sigma t}{4\,\text{Pi}\,r}$ NIntegrate$\left[\frac{e^{-\Sigma t\,r/v}}{v\,\text{CaseN}[c,v]}, \{v, 0, 1\}\right]$

Expansion of transient term [Case et al. 1953]

In[2340]:= ϕtransient2[r_, Σt_, c_, M_] := $\frac{\text{Exp}[-r\,\Sigma t]}{4\,\text{Pi}\,r^2} + \frac{1}{4\,\text{Pi}\,r}$ Sum[ExpIntegralE[2 n, r Σt] SeriesCoefficient[v / CaseN[c, v], {v, 0, 2 n}], {n, 1, M}]

Fluence: exact solution (2)

[Davison 1947]

In[2341]:= ϕexact2a[r_, Σt_, c_] := ϕrigourousDiffusion[r, Σt, c] + $\frac{\Sigma t}{4\,\text{Pi}\,r}$ NIntegrate$\left[\frac{e^{-\Sigma t\,r\,y}}{\frac{c^2\pi^2}{4\,y^2} + \left(1 - \frac{c}{2\,y}\,\text{Log}\left[\frac{y+1}{y-1}\right]\right)^2}, \{y, 1, \text{Infinity}\}\right]$

[Case and Zwiefel 1967]

In[2342]:= ϕexact2b[r_, Σt_, c_] := ϕrigourousDiffusion[r, Σt, c] + $\frac{\Sigma t}{4\,\text{Pi}\,r}$ NIntegrate$\left[\frac{e^{-\Sigma t\,r/v}}{v\,\text{CaseN}[c,v]}, \{v, 0, 1\}\right]$

n-th scattered fluence

In[2343]:= ϕexact1[r_, Σt_, c_, n_] := $\frac{(c\,\Sigma t)^n}{2\,\pi^2\,r}$ NIntegrate$\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]^{1+n}\,\text{Sin}[r\,z]}{z^n},\right.$ {z, 0, Infinity}, Method → "ExtrapolatingOscillatory"]

In[2344]:= ϕexact2[r_, Σt_, c_, n_] := $\frac{c^n\,\Sigma t}{2^{n+3}\,\text{Pi}^2\,I\,r}$ Chop[NIntegrate[$\frac{\text{Exp}[-r\,z\,\Sigma t]}{z^n}\left(\left(\text{Log}\left[\frac{z+1}{z-1}\right] + I\,\text{Pi}\right)^{n+1} - \left(\text{Log}\left[\frac{z+1}{z-1}\right] - I\,\text{Pi}\right)^{n+1}\right)$, {z, 1, Infinity}]]

In[2345]:= ϕGaussian[r_, Σt_, c_, n_] := $\frac{3\sqrt{3}\,e^{-\frac{3\,r^2\,\Sigma t^2}{4\,(1+n)}}\,c^n\,\Sigma t^2}{8\sqrt{(1+n)^3}\,\pi^{3/2}}$

Moments

In[2357]:= ϕm[c_, Σt_, m_?IntegerQ, n_] := Limit$\left[\text{Simplify}\left[(-1)^{m/2}\left(\frac{2\,\text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]}\,\text{D}\left[\frac{\left(\frac{c\,\Sigma t\,\text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z}\right)^{1+n}}{c\,\Sigma t}, \{z, m\}\right]\right)\right], z \to 0\right]$

In[2358]:=
```
TableForm[Table[ϕm[c, Σt, m, n], {m, 0, 6, 2}]]
```

Out[2358]//TableForm=

$$\frac{c^n}{\Sigma t}$$
$$\frac{2\, c^n\, (1+n)}{\Sigma t^3}$$
$$\frac{4\, c^n\, (1+n)\, (18+5\, n)}{3\, \Sigma t^5}$$
$$\frac{8\, c^n\, (1+n)\, \left(810+343\, n+35\, n^2\right)}{9\, \Sigma t^7}$$

In[2359]:=
$$\text{ϕm}[c\_, \Sigma t\_, m\_?\text{IntegerQ}] := \text{Limit}\left[\text{Simplify}\left[(-1)^{m/2} \left(\frac{2\,\text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]} \text{D}\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z - c\, \Sigma t\, \text{ArcTan}\left[\frac{z}{\Sigma t}\right]}, \{z, m\}\right]\right)\right], z \to 0\right]$$

In[2360]:=
```
TableForm[Table[ϕm[c, Σt, m], {m, 0, 6, 2}]]
```

Out[2360]//TableForm=

$$\frac{1}{\Sigma t - c\, \Sigma t}$$
$$\frac{2}{(-1+c)^2\, \Sigma t^3}$$
$$\frac{8\, (-9+4\, c)}{3\, (-1+c)^3\, \Sigma t^5}$$
$$\frac{16\, \left(135-144\, c+44\, c^2\right)}{3\, (-1+c)^4\, \Sigma t^7}$$

Recurrence derivation [Case et al. 1953]

In[2361]:=
$$\text{CaseB}[0, c\_] := \frac{1}{1-c};$$
$$\text{CaseB}[m\_, c\_] := \frac{1}{(1-c)^2} \text{Sum}\left[\text{Caseb}[m, s] \left(\frac{c}{1-c}\right)^{s-1}, \{s, 1, m\}\right];$$
$$\text{Caseb}[m\_, 1] := \frac{1}{2\, m+1};$$
$$\text{Caseb}[m\_, s\_] := \text{Sum}\left[\frac{\text{Caseb}[n, s-1]}{1+2\, (m-n)}, \{n, s-1, m-1\}\right]$$

In[2365]:=
$$\text{ϕmCase}[c\_, \Sigma t\_, m\_?\text{IntegerQ}] := \frac{1}{\Sigma t^{m+1}} \text{CaseB}\left[m/2, c\right] \text{Factorial}[m+1]$$

In[2366]:=
```
TableForm[Table[FullSimplify[ϕmCase[c, Σt, m]], {m, 0, 6, 2}]]
```

Out[2366]//TableForm=

$$\frac{1}{\Sigma t - c\, \Sigma t}$$
$$\frac{2}{(-1+c)^2\, \Sigma t^3}$$
$$\frac{8\, (-9+4\, c)}{3\, (-1+c)^3\, \Sigma t^5}$$
$$\frac{16\, (135+4\, c\, (-36+11\, c))}{3\, (-1+c)^4\, \Sigma t^7}$$

Classical diffusion approximation

In[2367]:=
$$\text{ϕDiffusion}[r\_, \Sigma t\_, c\_] := \frac{1}{\Sigma t\, (1-c)} \text{diffusionMode}\left[\frac{1}{\sqrt{3\, (1-c)}\, \Sigma t}, 3, r\right]$$

In[2368]:=
```
FullSimplify[ϕDiffusion[r, Σt, c], Assumptions → 0 < c < 1 && Σt > 0]
```

Out[2368]=
$$\frac{3\, e^{-\sqrt{3-3\, c}\; r\, \Sigma t}\, \Sigma t}{4\, \pi\, r}$$

Grosjean-style diffusion approximation

In[2369]:=
$$\phi\text{Grosjean}[r\_, \Sigma t\_, c\_] := \frac{\text{Exp}[-r\,\Sigma t]}{4\,\text{Pi}\,r^2} + \frac{c}{\Sigma t\,(1-c)}\,\text{diffusionMode}\left[\frac{\sqrt{2-c}}{\sqrt{3\,(1-c)}\,\Sigma t}, 3, r\right]$$

In[2370]:=
```
FullSimplify[ϕGrosjean[r, Σt, c], Assumptions → 0 < c < 1 && Σt > 0]
```

Out[2370]=
$$\frac{e^{-r\,\Sigma t} - \frac{3\,c\,e^{-\sqrt{3+\frac{3}{-2+c}}\,r\,\Sigma t}}{-2+c}}{4\,\pi\,r^2}$$

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[2371]:=
$$\text{Lintegral}[r\_, u\_, \Sigma t\_, c\_, \phi\_] := \frac{c\,\Sigma t}{4\,\text{Pi}}\,\text{NIntegrate}\left[\phi\left[\sqrt{r^2+t^2-2\,r\,t\,u}, \Sigma t, c\right]\,\text{Exp}[-\Sigma t\,t], \{t, 0, \text{Infinity}\}\right]$$

Angular Classical diffusion approximation

In[2372]:=
$$\text{Ldiffusion}[r\_, u\_, \Sigma t\_, c\_] := \frac{1}{4\,\text{Pi}}\,\phi\text{Diffusion}[r, \Sigma t, c] + \frac{1}{4\,\text{Pi}}\,u\,\frac{3\,e^{-r\,\sqrt{3-3\,c}\,\Sigma t}\left(1+r\,\sqrt{3-3\,c}\,\Sigma t\right)}{4\,\pi\,r^2}$$

---

load MC data

In[2373]:=
```
ppoints[xs_, dr_, maxx_] :=
  Table[{dr (i) - 0.5 dr, xs[[i]]}, {i, 1, Length[xs]}][[1 ;; -2]]
```

In[2374]:=
```
ppointsu[xs_, du_, Σt_] :=
  Table[{-1.0 + du (i) - 0.5 du, xs[[i]] / (2 Σt)}, {i, 1, Length[xs]}][[1 ;; -1]]
```

In[2375]:=
```
fs = FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/MCdata/
     inf3D_isotropicpoint_isotropicscatter*"];
```

In[2376]:=
```
index[x_] := Module[{data, α, Σt},
    data = Import[x, "Table"];
    Σt = data[[1, 13]];
    α = data[[2, 3]];
    {α, Σt, data}];
simulations = index /@ fs;
cs = Union[#[[1]] & /@ simulations]
```

Out[2378]=
```
{0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999}
```

In[2379]:=
```
mfps = Union[#[[2]] & /@ simulations]
```

Out[2379]=
```
{0.3, 1}
```

In[2380]:=
```
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

Mean Track Length

In[2383]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2383]//TableForm=

Set c	0.7
Set mfp	1

In[2384]:=
```
data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
meanTL = data[[-1]]
```

$$\frac{\text{mfp}}{1 - \text{c}}$$

Out[2385]= {Mean, track, length:, 4.99397}

Out[2386]= 5.

Fluence - Exact solution (1a) comparison to MC

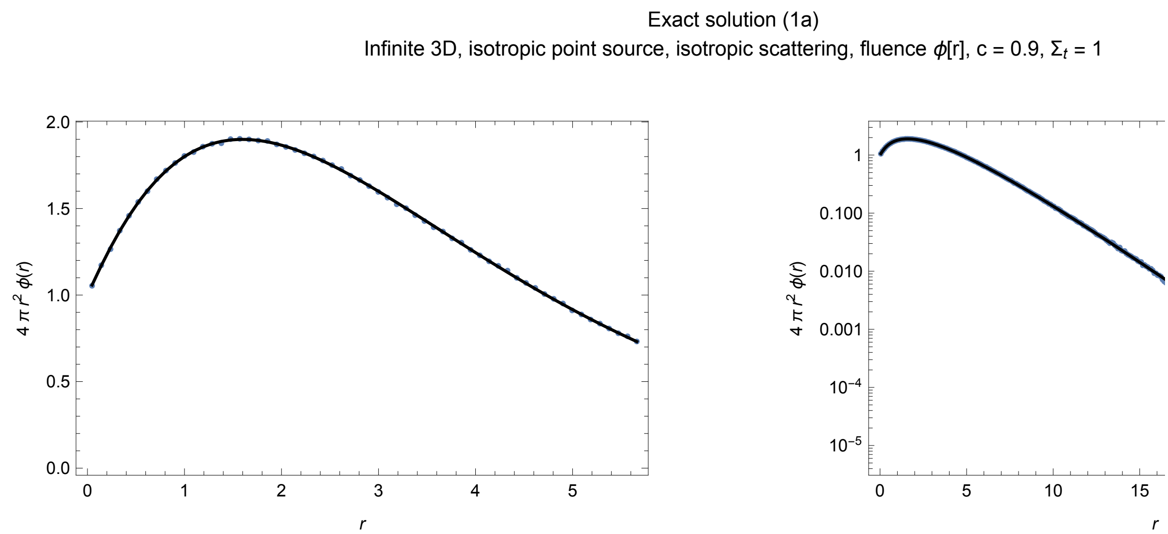
In[2387]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2387]//TableForm=

Set c	0.7
Set mfp	1

In[2397]:=
```
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 Pi #[[1]]^2 ϕexact1a[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact1a[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[60 ;; -1 ;; 10]];
plotϕshallow = Quiet[Show[
    ListPlot[MCFluence[[1 ;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
    ListPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1Fluence,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1FluenceShallow, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (1a)\nInfinite 3D, isotropic
    point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1/mfp]]
```

Out[2405]=



Fluence - Exact solution (1b) comparison to MC

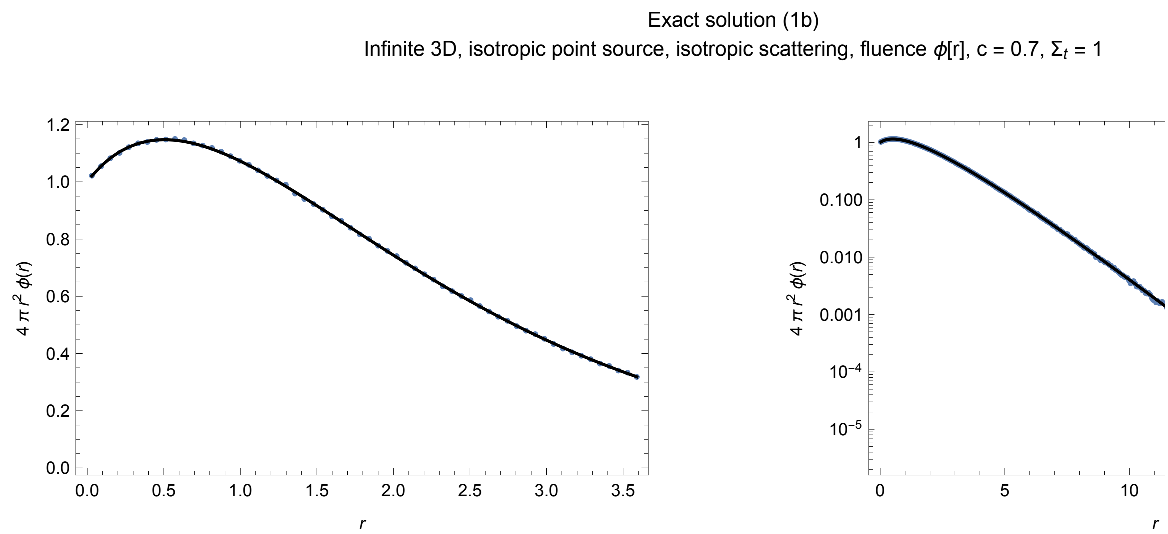
In[ ]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[ ]//TableForm=

Set c	0.7
Set mfp	1

In[2406]:=
```
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 Pi #[[1]]^2 ϕexact1b[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact1b[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[60 ;; -1 ;; 10]];
plotϕshallow = Quiet[Show[
    ListPlot[MCFluence[[1 ;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
    ListPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1Fluence,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1FluenceShallow, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (1b)\nInfinite 3D, isotropic
    point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1/mfp]]
```

Out[2414]=



Fluence - Exact solution (2a) comparison to MC

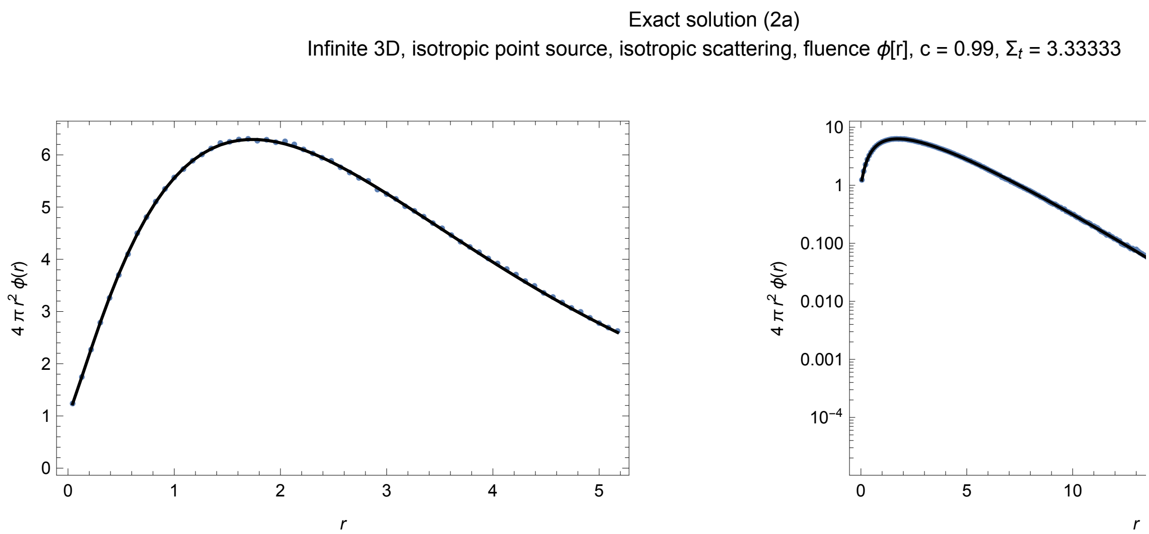
In[2415]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2415]//TableForm=

Set c	0.7
Set mfp	1

In[2416]:=
```
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 Pi #[[1]]^2 ϕexact2a[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact2a[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[60 ;; -1 ;; 10]];
plotϕshallow = Quiet[Show[
    ListPlot[MCFluence[[1 ;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
    ListPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1Fluence,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1FluenceShallow, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (2a)\nInfinite 3D, isotropic
     point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1/mfp]]
```

Out[2424]=



Fluence - Exact solution (2b) comparison to MC

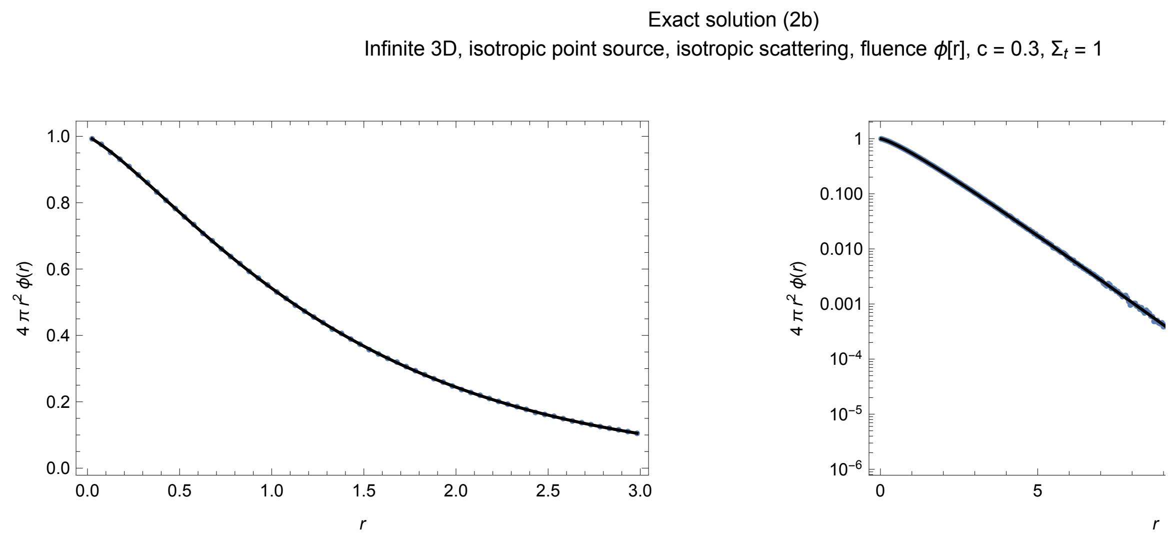
In[2425]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :→ (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :→ (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2425]//TableForm=

Set c	0.7
Set mfp	1

In[2426]:=
```
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 Pi #[[1]]^2 ϕexact2b[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact2b[#[[1]], 1/mfp, c]}] & /@
   MCFluence[[60 ;; -1 ;; 10]];
plotϕshallow = Quiet[Show[
    ListPlot[MCFluence[[1 ;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
    ListPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1Fluence,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1FluenceShallow, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (2b)\nInfinite 3D, isotropic
    point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1/mfp]]
```

Out[2434]=



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

In[2435]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

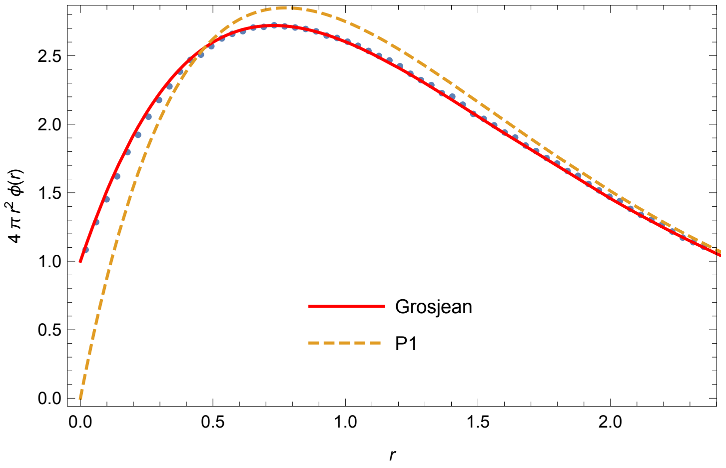
Out[2435]//TableForm=

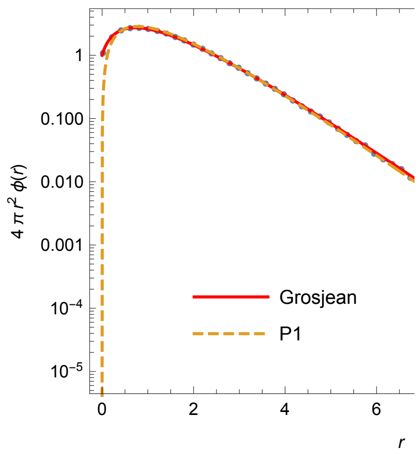
Set c	0.7
Set mfp	1

In[2436]:=
```
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 ϕGrosjean[r, 1 / mfp, c],
      4 Pi r^2 ϕDiffusion[r, 1 / mfp, c]
     }
     , {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
     PlotLegends → Placed[{"Grosjean", "P1"}, {0.5, .2}]],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence[[1 ;; -1 ;; 5]],
     PlotRange → All, PlotStyle → PointSize[.01]],
    LogPlot[{
      4 Pi r^2 ϕGrosjean[r, 1 / mfp, c],
      4 Pi r^2 ϕDiffusion[r, 1 / mfp, c]
     }
     , {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
     PlotLegends → Placed[{"Grosjean", "P1"}, {0.3, .2}]],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Diffusion Approximations\nInfinite 3D, isotropic
     point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1 / mfp]]
```

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

Out[2442]=





Fluence - Diffusion approximation (Rigorous) comparison to MC

In[2443]:=

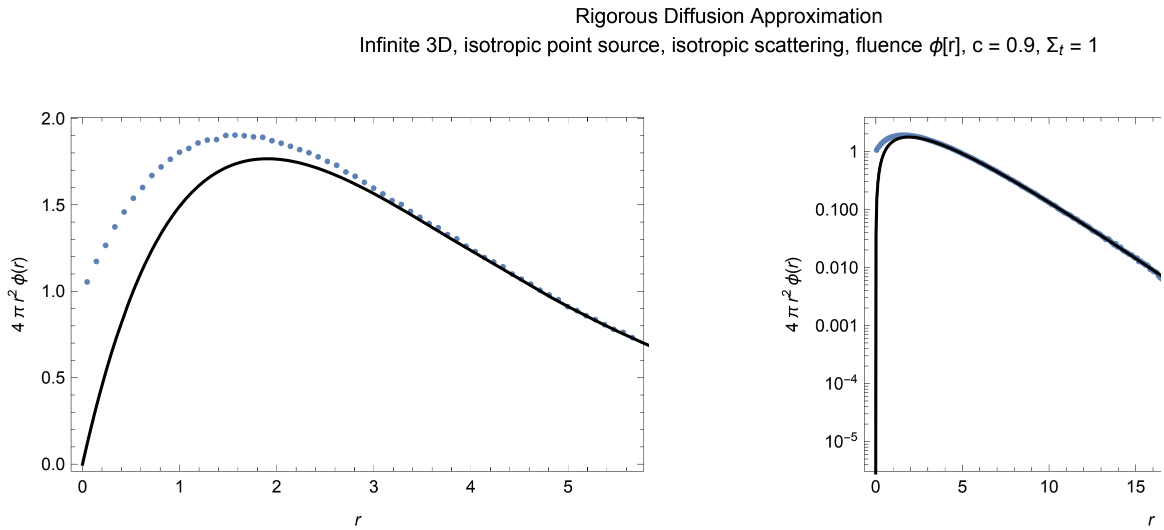
```
{{ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
  {ActionMenu["Set mfp", "mfp = " <> ToString[#] :> (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2443]//TableForm=

Set c	0.7
Set mfp	1

In[2444]:=
```
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 ϕrigourousDiffusion[r, 1 / mfp, c],
     {r, 0, maxr}, PlotRange → All, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    LogPlot[4 Pi r^2 ϕrigourousDiffusion[r, 1 / mfp, c],
     {r, 0, maxr}, PlotRange → All, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Rigorous Diffusion Approximation\nInfinite 3D, isotropic
     point source, isotropic scattering, fluence ϕ[r], c = " <>
   ToString[c] <> ", Σt = " <> ToString[1 / mfp]]
```

Out[2450]=



N-th order fluence / scalar flux

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

In[2451]:=
```
{{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[2451]//TableForm=

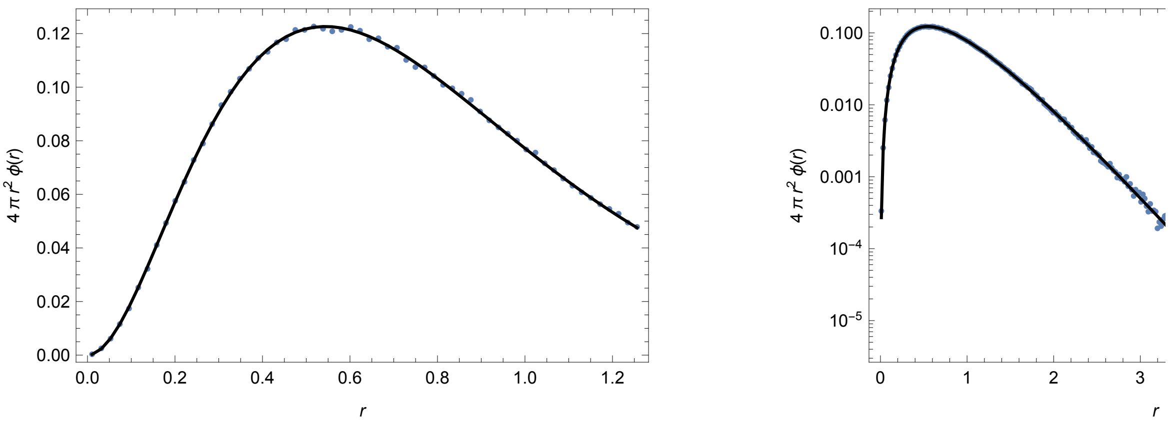
Set c	0.7
Set mfp	1
Set collision order	7

In[2452]:=
```
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 Pi #[[1]]^2 ϕexact1[#[[1]], 1/mfp, c, collisionOrder]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact1[#[[1]], 1/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, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1Fluence, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (1)\nInfinite 3D medium, isotropic point
    source, isotropic scattering, n-th scattered fluence ϕ[r|" <>
   ToString[collisionOrder] <> "], c =" <> ToString[c] <>
   ", Σt = " <> ToString[1/mfp]]
```

Out[2461]=

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



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

In[∘]:=
```
{{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
```

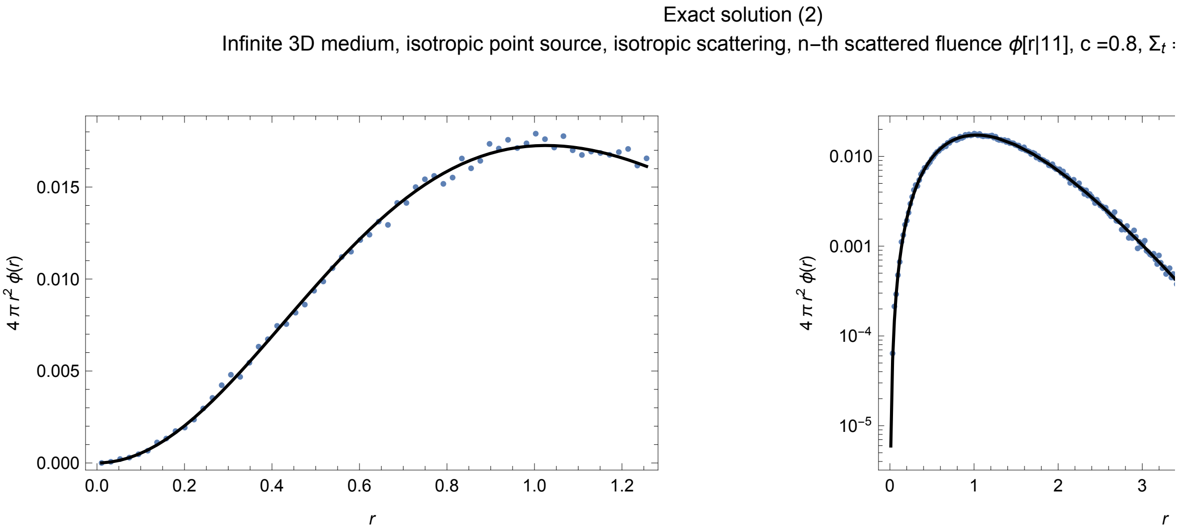
Out[∘]//TableForm=

Set c	0.7
Set mfp	1
Set collision order	7

```
In[2462]:= 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 Pi #[[1]]^2 ϕexact2[#[[1]], 1/mfp, c, collisionOrder]}] & /@
   MCFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexact2[#[[1]], 1/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, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1FluenceShallow,
     PlotRange → All, Joined → True, PlotStyle → Black],
    ListLogPlot[exact1Fluence, PlotRange → All,
     Joined → True, PlotStyle → Black],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution (2)\nInfinite 3D medium, isotropic point
     source, isotropic scattering, n-th scattered fluence ϕ[r|" <>
   ToString[collisionOrder] <> "], c =" <> ToString[c] <>
   ", Σt = " <> ToString[1/mfp]]
```

Out[2471]=



N-th collided Fluence - Approximations

In[∘]:=
```
{{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[∘]//TableForm=

Set c	0.7
Set mfp	1
Set collision order	7

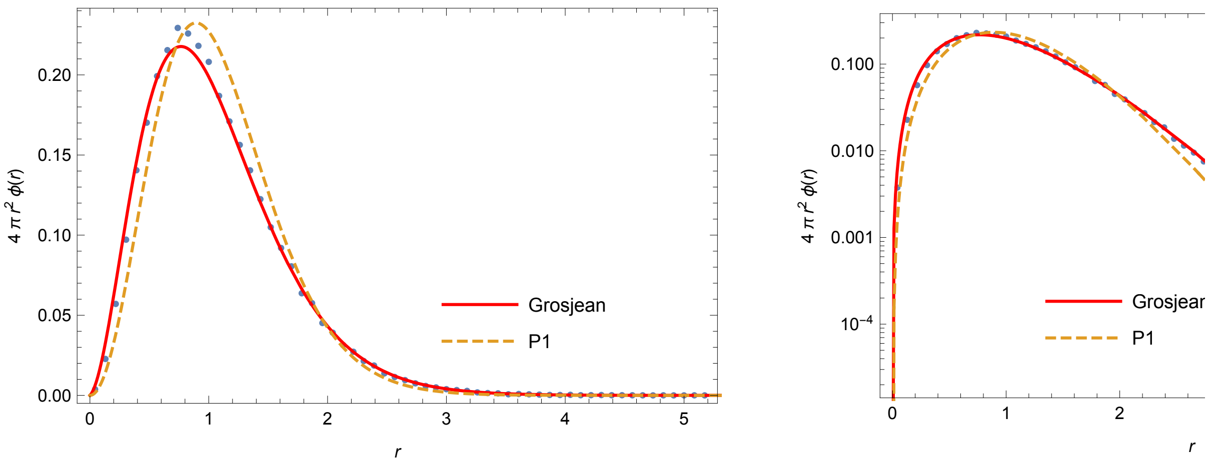
In[2472]:=
```
data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
maxr = data[[2, 5]];
dr = data[[2, 7]];
fluencei = 3 numcollorders + 15 + collisionOrder;

MCFluence = ppoints[data[[fluencei]], dr, maxr];
seriesclassical = c^collisionOrder
   SeriesCoefficient[ϕDiffusion[r, 1/mfp, C], {C, 0, collisionOrder}];
seriesG = c^collisionOrder SeriesCoefficient[
    ϕGrosjean[r, 1/mfp, C], {C, 0, collisionOrder}];
plotϕshallow = Quiet[Show[
    ListPlot[MCFluence[[1 ;; 60]], PlotRange → All, PlotStyle → PointSize[.01]],
    Plot[{4 Pi r^2 seriesG, 4 Pi r^2 seriesclassical},
     {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
     PlotLegends → Placed[{"Grosjean", "P1"}, {0.7, .2}]],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[MCFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    LogPlot[{4 Pi r^2 seriesG, 4 Pi r^2 seriesclassical},
     {r, 0, maxr}, PlotRange → All, PlotStyle → {Red, Dashed},
     PlotLegends → Placed[{"Grosjean", "P1"}, {0.4, .2}]],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Diffusion Approximations\nInfinite 3D medium, isotropic point
     source, isotropic scattering, n-th scattered fluence ϕ[r|" <>
   ToString[collisionOrder] <> "], c =" <> ToString[c] <>
   ", Σt = " <> ToString[1/mfp]]
```

Diffusion Approximations

Infinite 3D medium, isotropic point source, isotropic scattering, n−th scattered fluence ϕ[r|7], c =0.99, Σ_t :

Out[2481]=



Compare moments of ϕ

In[2482]:=

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

Out[2482]//TableForm=

Set c	0.7
Set mfp	1

In[2497]:=
```
data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[3]];
nummoments = data[[2, 15]];
ϕmoments = {data[[10]]};
ks = Table[k, {k, 0, nummoments - 1}];
analytic = Table[ϕm[c, 1 / mfp, k], {k, ks}];
j = Join[{ks}, {analytic}, ϕmoments];
TableForm[
 Join[{{"n", "analytic", "MC"}}, Transpose[j]]
]
```

Out[2503]//TableForm=

n	analytic	MC
0	1.	0.999247
1	0.	0.593242
2	0.6	0.599191
3	0.	0.836826
4	1.488	1.48192
5	0.	3.16635
6	8.02944	7.89526
7	0.	22.4125
8	75.1133	71.0073
9	0.	246.898

In[2504]:=
```
{{ActionMenu["Set mfp", "mfp = " <> ToString[#] :→ (mfp = #;) & /@ mfps],
   Dynamic[mfp]}} // TableForm
```

Out[2504]//TableForm=

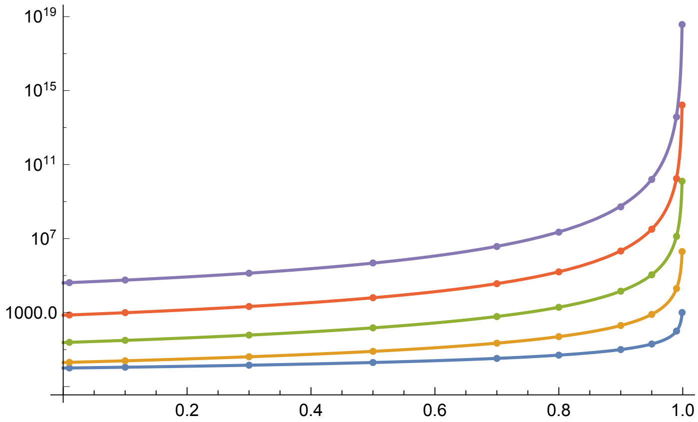
Set mfp   1

In[2507]:=
```
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
  }],
```

$$\text{LogPlot}\left[\left\{-\frac{mfp}{-1+c}, \frac{2\,mfp^3}{(-1+c)^2}, \frac{8\,(-9+4\,c)\,mfp^5}{3\,(-1+c)^3}, \frac{16\,(135-144\,c+44\,c^2)\,mfp^7}{3\,(-1+c)^4}, \frac{128\,(-1575+2808\,c-1836\,c^2+428\,c^3)\,mfp^9}{5\,(-1+c)^5}\right\}, \{c, 0, .999\}, \text{PlotRange} \to \text{All}\right]$$

```
]
```

Out[2508]=



n-th collided moments of ϕ

In[∘]:=
```
{{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[∘]//TableForm=

Set c	0.7
Set mfp	1
Set collision order	7

```
In[•]:= 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[ϕm[c, 1/mfp, k, collisionOrder], {k, ks}];
j = Join[{ks}, {analytic}, ϕmoments];
TableForm[
 Join[{{"n", "analytic", "MC"}}, Transpose[j]]
]
```

Out[•]//TableForm=

n	analytic	MC
0	0.192	0.192008
1	0. + 0. i	0.11745
2	0.10368	0.103751
3	0.	0.120756
4	0.174182	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

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

Out[•]//TableForm=

Set c	0.7
Set mfp	1

```
In[•]:= depthi = 81
Out[•]= 81
```

```
In[•]:= af1integral[r_, c_] :=
  NIntegrate[(-(3 c (u - ArcTan[u]) ArcTan[u] (r u Cos[r u] - Sin[r u]))/(2 π^2 r^2 u^2 (u - c ArcTan[u]))),
   {u, 0, Infinity}, Method → "ExtrapolatingOscillatory"];
```

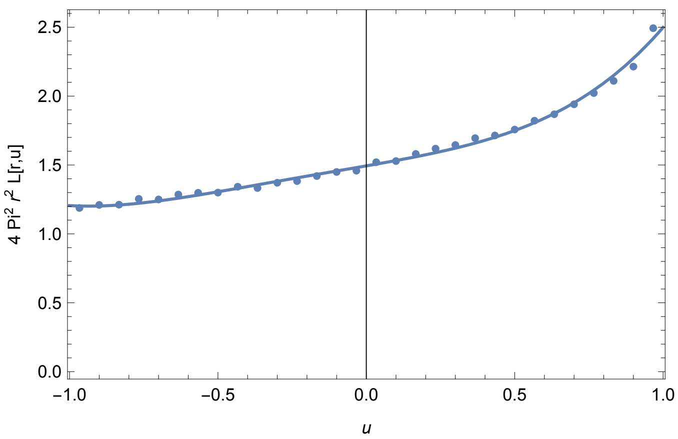
```
In[•]:= af2integral[r_, c_] := NIntegrate[
   (-((5 c ArcTan[u] (-3 u + (3 + u^2) ArcTan[u]) (3 r u Cos[r u] + (-3 + r^2 u^2) Sin[r u])) /
       (4 π^2 r^3 u^4 (u - c ArcTan[u])))),
   {u, 0, Infinity}, Method → "ExtrapolatingOscillatory"];
```

```
In[•]:= af3integral[r_, c_] := NIntegrate[
   (7 c ArcTan[u] (u (15 + 4 u^2) - 3 (5 + 3 u^2) ArcTan[u]) (r u (-15 + r^2 u^2) Cos[r u] +
       3 (5 - 2 r^2 u^2) Sin[r u])) / (12 π^2 r^4 u^6 (u - c ArcTan[u])),
   {u, 0, Infinity}, Method → "ExtrapolatingOscillatory"];
```

In[∘]:=
```
af4integral[r_, c_] :=
  NIntegrate[(3 c ArcTan[u] (-5 u (21 + 11 u^2) + 3 (35 + 30 u^2 + 3 u^4) ArcTan[u])
      (5 r u (-21 + 2 r^2 u^2) Cos[r u] + (105 - 45 r^2 u^2 + r^4 u^4) Sin[r u])) /
    (16 π^2 r^5 u^8 (u - c ArcTan[u])), {u, 0, Infinity},
   Method → "ExtrapolatingOscillatory"];
```

In[∘]:=
```
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;
af0 = ϕexact1b[r, 1 / mfp, c];
af1 = af1integral[r, c];
af2 = af2integral[r, c];
af3 = af3integral[r, c];
af4 = af4integral[r, c];
Show[
 ListPlot[angularFlux, PlotRange → All,
  Frame → True,
  FrameLabel -> {{"4 Pi^2  r^2  L[r,u]",}, {u,}}],
 Plot[ Pi  r^2  (af0 + LegendreP[1, u] af1 + LegendreP[2, u] af2 +
     LegendreP[3, u] af3 + LegendreP[4, u] af4), {u, -1, 1}, PlotRange → All]
]
```

Out[∘]=



Angular Distribution: Integral of Grosjean’s Diffusion Approximation

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

Out[•]//TableForm=

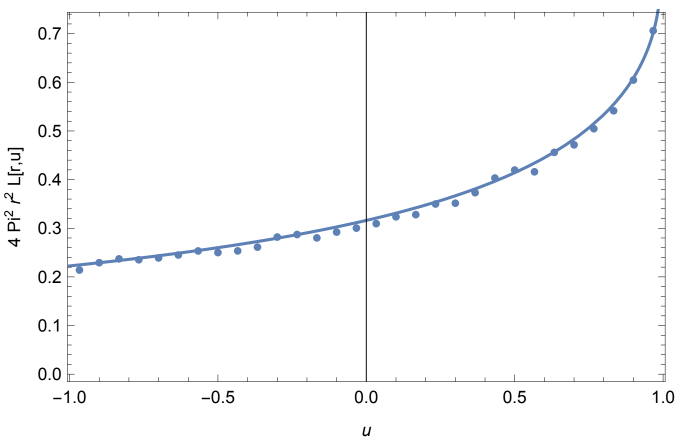
Set c	0.7
Set mfp	1

In[•]:=
```
depthi = 52
```

Out[•]=
```
52
```

In[•]:=
```
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 Pi² r² L[r,u]",}, {u,}}],
 Plot[4 Pi r² Pi Lintegral[r, u, 1 / mfp, c, ϕGrosjean], {u, -1, 1}, PlotRange → All]
]
```

Out[•]=



End context

In[•]:=
```
End[]
```

Out[•]=
```
inf3Disopointisoscatter`
```