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

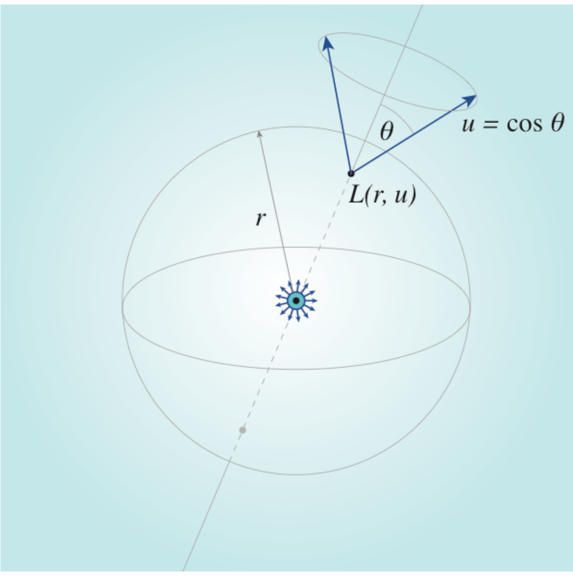
www.eugenedeon.com

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[215]:= SetDirectory[Import["~/.hitchhikerpath"]]

Out[215]= /Users/eug/Documents/research/hitchhikersscatter
```

Notation



α - single-scattering albedo
Σt - extinction coefficient
r - radial position coordinate in medium (distance from point source at origin)
u = cos θ - direction cosine

Util

In[156]:= $$\mathtt{SurfaceArea[d\_,\ r\_]\ :=\ d}\ \frac{\mathtt{Pi}^{d/2}}{\mathtt{Gamma}\left[\frac{d}{2}+1\right]}\ \mathtt{r}^{d-1}$$

Diffusion modes

In[157]:= $$\mathtt{diffusionMode[v\_,\ d\_,\ r\_]\ :=}\ (2\,\pi)^{-d/2}\ \mathtt{r}^{1-\frac{d}{2}}\ \mathtt{v}^{-1-\frac{d}{2}}\ \mathtt{BesselK}\left[\frac{1}{2}\ (-2+d),\ \frac{r}{v}\right]$$

Analytic solutions

Caseology quantities

In[216]:= $$\mathtt{CaseN0[c\_,\ v0\_]\ :=}\ \frac{1}{2}\ c\ \mathtt{v0}^3\left(\frac{c}{\mathtt{v0}^2-1}-\frac{1}{\mathtt{v0}^2}\right)$$

In[217]:= $$\mathtt{Casev0[c\_?NumericQ]\ :=}$$
$$\mathtt{FindRoot}\left[c\ v\ \mathtt{ArcTanh}\left[\frac{1}{v}\right]-1==0,\ \left\{v,\ 1.00000000001,\ 10^{10}\right\},\ \mathtt{Method}\to\text{"Brent"}\right]\mathtt{[[1]][[2]]}$$

In[218]:= $$\mathtt{CaseN[c\_,\ v\_]\ :=}\ v\left(\mathtt{Case\lambda[v,\ c]}^2+\left(\frac{\pi\ c\ v}{2}\right)^2\right)$$

In[219]:= $$\mathtt{Case\lambda[v\_,\ c\_]\ :=}\ 1-c\ v\ \mathtt{ArcTanh[v]}$$

Fluence: exact solution (1)

[Bothe 1942]

In[220]:= $$\mathtt{inf3Disopointisoscatter`\phi exact1a[r\_,\ \Sigma t\_,\ \alpha\_]\ :=}$$
$$\frac{1}{2\ \mathtt{Pi}^2\ r}\ \mathtt{NIntegrate}\left[\frac{z\ \mathtt{ArcTan}[z/\Sigma t]}{z-\alpha\ \Sigma t\ \mathtt{ArcTan}[z/\Sigma t]}\ \mathtt{Sin}[r\ z],\ \{z,\ 0,\ \mathtt{Infinity}\},\ \mathtt{Method}\to\text{"ExtrapolatingOscillatory"}\right]$$

[Case et al. 1953]

In[221]:= $$\mathtt{inf3Disopointisoscatter`\phi exact1b[r\_,\ \Sigma t\_,\ \alpha\_]\ :=}\ \frac{\mathtt{Exp}[-\Sigma t\ r]}{4\ \mathtt{Pi}\ r^2}+\alpha\ \frac{\Sigma t}{2\ \mathtt{Pi}^2\ r}$$
$$\mathtt{NIntegrate}\left[\frac{\mathtt{ArcTan}[z]^2}{z-\alpha\ \mathtt{ArcTan}[z]}\ \mathtt{Sin}[r\ \Sigma t\ z],\ \{z,\ 0,\ \mathtt{Infinity}\},\ \mathtt{Method}\to\text{"LevinRule"}\right]$$

Rigorous diffusion approximation

In[222]:= $$\mathtt{inf3Disopointisoscatter`\phi rigourousDiffusion[r\_,\ \Sigma t\_,\ \alpha\_]\ :=}$$
$$\frac{\Sigma t}{4\ \mathtt{Pi}\ r}\ \frac{\mathtt{E}^{-r\ \Sigma t/\#}}{\#\ \mathtt{CaseN0}[\alpha,\ \#]}\ \&[\mathtt{Casev0}[\alpha]]$$

Fluence: exact solution (2)

[Davison 1947]

In[223]:=

$$\text{inf3Disopointisoscatter`}\phi\text{exact2a}[\text{r\_},\ \Sigma\text{t\_},\ \alpha\text{\_}] := \text{inf3Disopointisoscatter`}\phi\text{rigourousDiffusion}[\text{r},\ \Sigma\text{t},\ \alpha] + \frac{\Sigma\text{t}}{4\ \text{Pi r}}\ \text{NIntegrate}\left[\frac{e^{-\Sigma t\, r\, y}}{\frac{\alpha^2\,\pi^2}{4\,y^2}+\left(1-\frac{\alpha}{2\,y}\ \text{Log}\left[\frac{y+1}{y-1}\right]\right)^2},\ \{\text{y},\ 1,\ \text{Infinity}\}\right]$$

[Case and Zwiefel 1967]

In[224]:=

$$\text{inf3Disopointisoscatter`}\phi\text{exact2b}[\text{r\_},\ \Sigma\text{t\_},\ \alpha\text{\_}] := \text{inf3Disopointisoscatter`}\phi\text{rigourousDiffusion}[\text{r},\ \Sigma\text{t},\ \alpha] + \frac{\Sigma\text{t}}{4\ \text{Pi r}}\ \text{NIntegrate}\left[\frac{e^{-\Sigma t\, r/v}}{\text{v CaseN}[\alpha,\ \text{v}]},\ \{\text{v},\ 0,\ 1\}\right]$$

n-th scattered fluence

In[225]:=

$$\text{inf3Disopointisoscatter`}\phi\text{exact1}[\text{r\_},\ \Sigma\text{t\_},\ \alpha\text{\_},\ \text{n\_}] := \frac{(\alpha\ \Sigma\text{t})^{n}}{2\ \pi^2\ \text{r}}\ \text{NIntegrate}\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]^{1+n}\ \text{Sin}[\text{r z}]}{z^{n}},\ \{\text{z},\ 0,\ \text{Infinity}\},\ \text{Method} \to \text{"ExtrapolatingOscillatory"}\right]$$

In[226]:=

$$\text{inf3Disopointisoscatter`}\phi\text{exact2}[\text{r\_},\ \Sigma\text{t\_},\ \alpha\text{\_},\ \text{n\_}] := \frac{\alpha^{n}\ \Sigma\text{t}}{2^{n+3}\ \text{Pi}^2\ \text{I r}}\ \text{Chop}\left[\text{NIntegrate}\left[\frac{\text{Exp}[-\text{r z}\ \Sigma\text{t}]}{z^{n}}\left(\left(\text{Log}\left[\frac{z+1}{z-1}\right]+\text{I Pi}\right)^{n+1}-\left(\text{Log}\left[\frac{z+1}{z-1}\right]-\text{I Pi}\right)^{n+1}\right),\ \{\text{z},\ 1,\ \text{Infinity}\}\right]\right]$$

In[227]:=

$$\text{inf3Disopointisoscatter`}\phi\text{Gaussian}[\text{r\_},\ \Sigma\text{t\_},\ \alpha\text{\_},\ \text{n\_}] := \frac{3\sqrt{3}\ e^{-\frac{3\,r^2\,\Sigma t^2}{4\,(1+n)}}\ \alpha^{n}\ \Sigma\text{t}^2}{8\sqrt{(1+n)^3}\ \pi^{3/2}}$$

Moments

In[228]:=

$$\text{inf3Disopointisoscatter`}\phi\text{m}[\text{c\_},\ \Sigma\text{t\_},\ \text{m\_?IntegerQ},\ \text{n\_}] := \text{Limit}\left[\text{Simplify}\left[(-1)^{m/2}\left(\frac{2\ \text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]}\ \text{D}\left[\frac{\left(\frac{c\ \Sigma t\ \text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z}\right)^{1+n}}{c\ \Sigma t},\ \{\text{z},\ \text{m}\}\right]\right)\right],\ \text{z} \to 0\right]$$

In[229]:=

```
TableForm[Table[inf3Disopointisoscatter`ϕm[α, Σt, m, n], {m, 0, 6, 2}]]
```

Out[229]//TableForm=

$$\begin{array}{l} \frac{\alpha^{n}}{\Sigma t} \\ \frac{2\,(1+n)\,\alpha^{n}}{\Sigma t^3} \\ \frac{4\,(1+n)\,(18+5\,n)\,\alpha^{n}}{3\,\Sigma t^5} \\ \frac{8\,(1+n)\,(810+343\,n+35\,n^2)\,\alpha^{n}}{9\,\Sigma t^7} \end{array}$$

In[230]:=

$$\text{inf3Disopointisoscatter`}\phi\text{m}[\text{c\_},\ \Sigma\text{t\_},\ \text{m\_?IntegerQ}] := \text{Limit}\left[\text{Simplify}\left[(-1)^{m/2}\left(\frac{2\ \text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]}\ \text{D}\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z-c\ \Sigma t\ \text{ArcTan}\left[\frac{z}{\Sigma t}\right]},\ \{\text{z},\ \text{m}\}\right]\right)\right],\ \text{z} \to 0\right]$$

In[231]:=
```
TableForm[Table[inf3Disopointisoscatter`ϕm[α, Σt, m], {m, 0, 6, 2}]]
```

Out[231]//TableForm=

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

Recurrence derivation [Case et al. 1953]

In[232]:=
```
inf3Disopointisoscatter`CaseB[0, c_] := 1/(1 - c);
inf3Disopointisoscatter`CaseB[m_, c_] :=
  1/(1 - c)^2 Sum[inf3Disopointisoscatter`Caseb[m, s] (c/(1 - c))^(s-1), {s, 1, m}];
inf3Disopointisoscatter`Caseb[m_, 1] := 1/(2 m + 1);
inf3Disopointisoscatter`Caseb[m_, s_] :=
  Sum[inf3Disopointisoscatter`Caseb[n, s - 1]/(1 + 2 (m - n)), {n, s - 1, m - 1}]
```

In[236]:=
```
inf3Disopointisoscatter`ϕmCase[c_, Σt_, m_?IntegerQ] :=
  1/Σt^(m+1) inf3Disopointisoscatter`CaseB[m / 2, α] Factorial[m + 1]
```

In[237]:=
```
TableForm[
 Table[FullSimplify[inf3Disopointisoscatter`ϕmCase[α, Σt, m]], {m, 0, 6, 2}]]
```

Out[237]//TableForm=

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

Classical diffusion approximation

In[238]:=
```
inf3Disopointisoscatter`ϕDiffusion[r_, Σt_, α_] :=
  1/(Σt (1 - α)) diffusionMode[1/(Sqrt[3 (1 - α)] Σt), 3, r]
```

In[239]:=
```
FullSimplify[inf3Disopointisoscatter`ϕDiffusion[r, Σt, α],
 Assumptions → α > 0 && α < 1 && Σt > 0]
```

Out[239]=

$$\frac{3\,e^{-r\sqrt{3-3\,\alpha}\,\Sigma t}\,\Sigma t}{4\,\pi\,r}$$

Grosjean-style diffusion approximation

In[240]:=
```
inf3Disopointisoscatter`ϕGrosjean[r_, Σt_, α_] :=
  Exp[-r Σt]/(4 Pi r^2) + α/(Σt (1 - α)) diffusionMode[Sqrt[2 - α]/(Sqrt[3 (1 - α)] Σt), 3, r]
```

In[241]:=
```
FullSimplify[inf3Disopointisoscatter`ϕGrosjean[r, Σt, α],
  Assumptions → α > 0 && α < 1 && Σt > 0]
```

Out[241]=

$$\frac{e^{-r\,\Sigma t} - \frac{3\, e^{-r\sqrt{3+\frac{3}{-2+\alpha}}\ \Sigma t}\ r\,\alpha\,\Sigma t}{-2+\alpha}}{4\,\pi\,r^2}$$

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[242]:=

$$\texttt{inf3Disopointisoscatter`Lintegral[r\_, u\_, Σt\_, α\_, ϕ\_] :=}$$
$$\frac{\alpha\,\Sigma\texttt{t}}{\texttt{4 Pi}}\ \texttt{NIntegrate}\left[\phi\left[\sqrt{\texttt{r}^2+\texttt{t}^2-\texttt{2 r t u}}\ ,\ \Sigma\texttt{t},\ \alpha\right]\ \texttt{Exp[-}\Sigma\texttt{t t], \{t, 0, Infinity\}}\right]$$

Angular Classical diffusion approximation

In[243]:=

$$\texttt{inf3Disopointisoscatter`Ldiffusion[r\_, u\_, Σt\_, α\_] :=}$$
$$\frac{1}{\texttt{4 Pi}}\ \texttt{inf3Disopointisoscatter`ϕDiffusion[r, Σt, α]} +$$
$$\frac{1}{\texttt{4 Pi}}\ \texttt{u}\ \frac{3\, e^{-r\sqrt{3-3\,\alpha}\ \Sigma t}\left(1+r\sqrt{3-3\,\alpha}\ \Sigma t\right)}{4\,\pi\,r^2}$$

load MC data

In[256]:=
```
inf3Disopointisoscatter`ppoints[xs_, dr_, maxx_, Σt_] :=
  Table[{dr (i) - 0.5 dr, xs[[i]] / Σt}, {i, 1, Length[xs]}][[1 ;; -2]]
```

In[257]:=
```
inf3Disopointisoscatter`ppointsu[xs_, du_, Σt_] :=
  Table[{-1.0 + du (i) - 0.5 du, xs[[i]] / (2 Σt)}, {i, 1, Length[xs]}][[1 ;; -1]]
```

In[258]:=
```
inf3Disopointisoscatter`fs =
   FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/data/
      inf3D_isotropicpoint_isotropicscatter*"];
```

In[259]:=
```
inf3Disopointisoscatter`index[x_] := Module[{data, α, Σt},
    data = Import[x, "Table"];
    Σt = data[[1, 13]];
    α = data[[2, 3]];
    {α, Σt, data}];
inf3Disopointisoscatter`simulations =
   inf3Disopointisoscatter`index /@ inf3Disopointisoscatter`fs;
inf3Disopointisoscatter`alphas =
  Union[#[[1]] & /@ inf3Disopointisoscatter`simulations]
```

Out[261]=
```
{0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999}
```

In[262]:=
```
inf3Disopointisoscatter`muts =
  Union[#[[2]] & /@ inf3Disopointisoscatter`simulations]
```

Out[262]=
```
{1, 3}
```

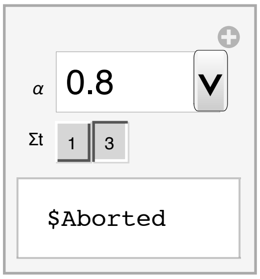
```
In[263]:= inf3Disopointisoscatter`numcollorders =
            inf3Disopointisoscatter`simulations[[1]][[3]][[2, 13]];
          inf3Disopointisoscatter`maxr =
           inf3Disopointisoscatter`simulations[[1]][[3]][[2, 5]];
          inf3Disopointisoscatter`dr =
           inf3Disopointisoscatter`simulations[[1]][[3]][[2, 7]];
          inf3Disopointisoscatter`numr =
            Floor[inf3Disopointisoscatter`maxr / inf3Disopointisoscatter`dr];
```

Compare Deterministic and MC

Fluence - Exact solution (1a) comparison to MC

In[266]:=
```
Clear[alpha, Σt];
Manipulate[
 If[Length[inf3Disopointisoscatter`simulations] > 0,
  Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
   data = SelectFirst[
      inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
   maxr = data[[2, 5]];
   dr = data[[2, 7]];

   pointsϕ = data[[4]];

   (* divide by Σt to convert collision density into fluence *)
   plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

   exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
         inf3Disopointisoscatter`ϕexact1a[#[[1]], Σt, α]}] & /@ plotpointsϕ;

   plotϕ = Quiet[Show[
       ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       ListPlot[exact1points, PlotRange → All, Joined → True],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
     ]];
   logplotϕ = Quiet[Show[
       ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       ListLogPlot[exact1points, PlotRange → All, Joined → True],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
     ]];
   Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800],
    PlotLabel -> "Exact solution (1a)\nInfinite 3D, isotropic point
        source, isotropic scattering, fluence ϕ[r], α = " <>
      ToString[α] <> ", Σt = " <> ToString[Σt]]
  ]
  ,
  Text[
   "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
     ensure the data path is setup correctly."]
 ]
 , {{α, 0.8}, inf3Disopointisoscatter`alphas},
 {{Σt, 3}, inf3Disopointisoscatter`muts}]
```

Out[267]=



α 0.8

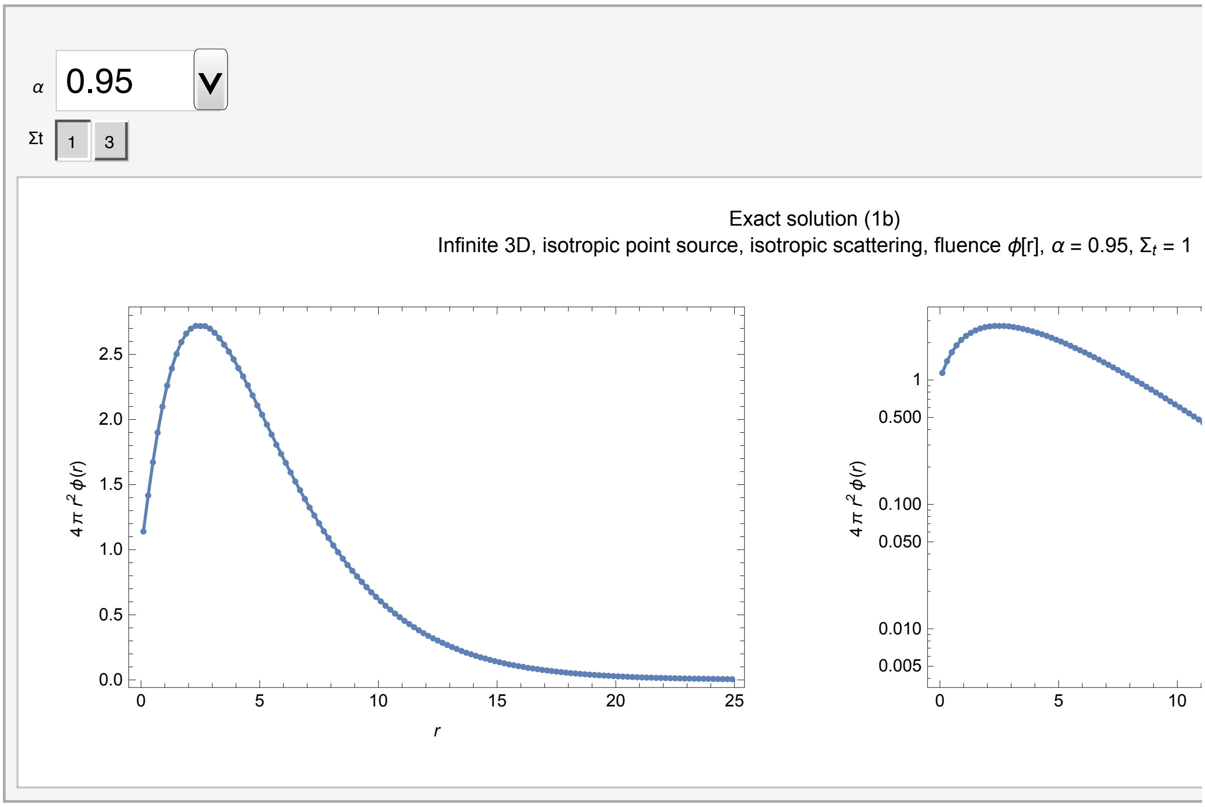
Σt 1 3

```
$Aborted
```

Fluence - Exact solution (1b) comparison to MC

```
In[268]:= Clear[alpha, Σt];
          Manipulate[
            If[Length[inf3Disopointisoscatter`simulations] > 0,
             Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
              data = SelectFirst[
                  inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
              maxr = data[[2, 5]];
              dr = data[[2, 7]];

              pointsϕ = data[[4]];

              (* divide by Σt to convert collision density into fluence *)
              plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

              exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
                    inf3Disopointisoscatter`ϕexact1b[#[[1]], Σt, α]}] & /@ plotpointsϕ;

              plotϕ = Quiet[Show[
                  ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                  ListPlot[exact1points, PlotRange → All, Joined → True],
                  Frame → True,
                  FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
                 ]];
              logplotϕ = Quiet[Show[
                  ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                  ListLogPlot[exact1points, PlotRange → All, Joined → True],
                  Frame → True,
                  FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
                 ]];
              Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800],
               PlotLabel -> "Exact solution (1b)\nInfinite 3D, isotropic point
                   source, isotropic scattering, fluence ϕ[r], α = " <>
                  ToString[α] <> ", Σt = " <> ToString[Σt]]
             ]
             ,
             Text[
              "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
                ensure the data path is setup correctly."]
            ]
            , {{α, 0.95}, inf3Disopointisoscatter`alphas},
            {Σt, inf3Disopointisoscatter`muts}]
```

Out[269]=



α 0.95

Σt 1 3

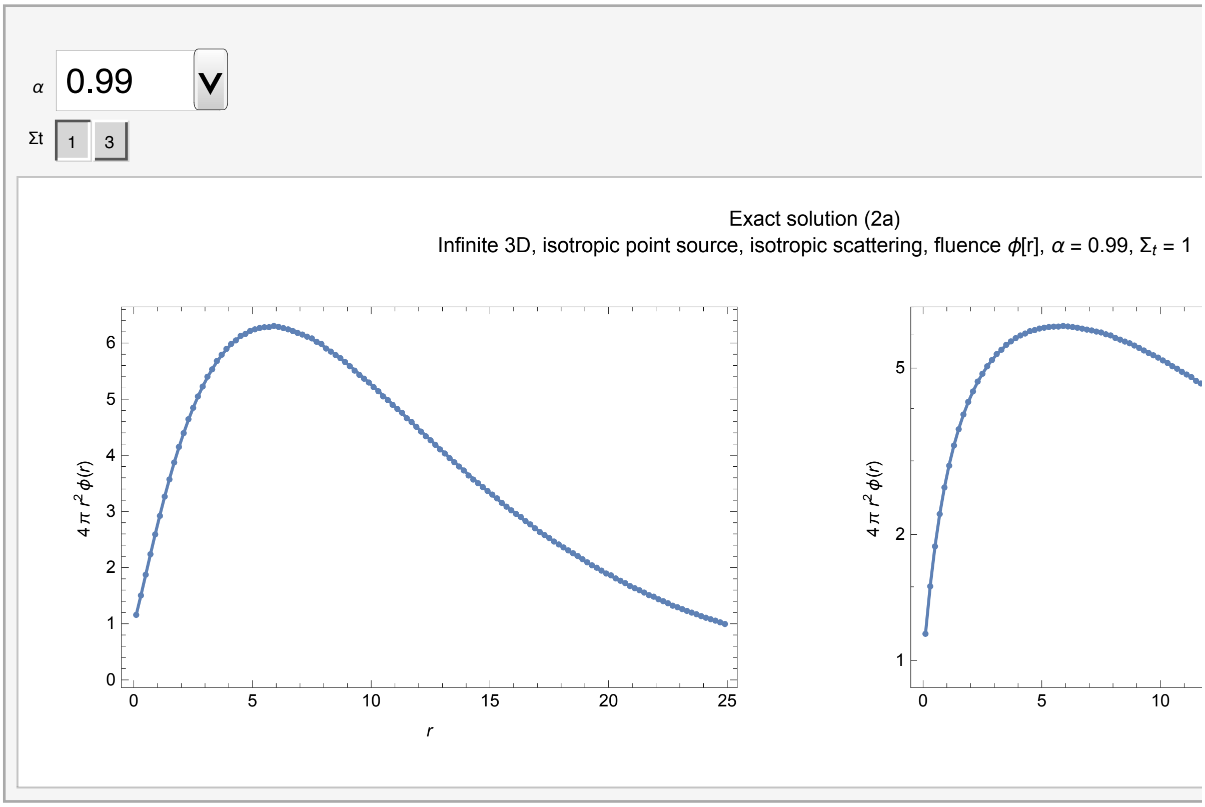
Exact solution (1b)

Infinite 3D, isotropic point source, isotropic scattering, fluence ϕ[r], α = 0.95, Σ_t = 1

Fluence - Exact solution (2a) comparison to MC

```
In[270]:= Clear[alpha, Σt];
          Manipulate[
           If[Length[inf3Disopointisoscatter`simulations] > 0,
            Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
             data = SelectFirst[
                inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
             maxr = data[[2, 5]];
             dr = data[[2, 7]];

             pointsϕ = data[[4]];

             (* divide by Σt to convert collision density into fluence *)
             plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

             exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
                   inf3Disopointisoscatter`ϕexact2a[#[[1]], Σt, α]}] & /@ plotpointsϕ;

             plotϕ = Quiet[Show[
                 ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 ListPlot[exact1points, PlotRange → All, Joined → True],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
                ]];
             logplotϕ = Quiet[Show[
                 ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 ListLogPlot[exact1points, PlotRange → All, Joined → True],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
                ]];
             Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800],
              PlotLabel -> "Exact solution (2a)\nInfinite 3D, isotropic point
                 source, isotropic scattering, fluence ϕ[r], α = " <>
                 ToString[α] <> ", Σ_t = " <> ToString[Σt]]
            ]
            ,
            Text[
             "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
               ensure the data path is setup correctly."]
           ]
           , {{α, 0.99}, inf3Disopointisoscatter`alphas},
           {Σt, inf3Disopointisoscatter`muts}]
```

Out[271]=



α 0.99

Σt 1 3

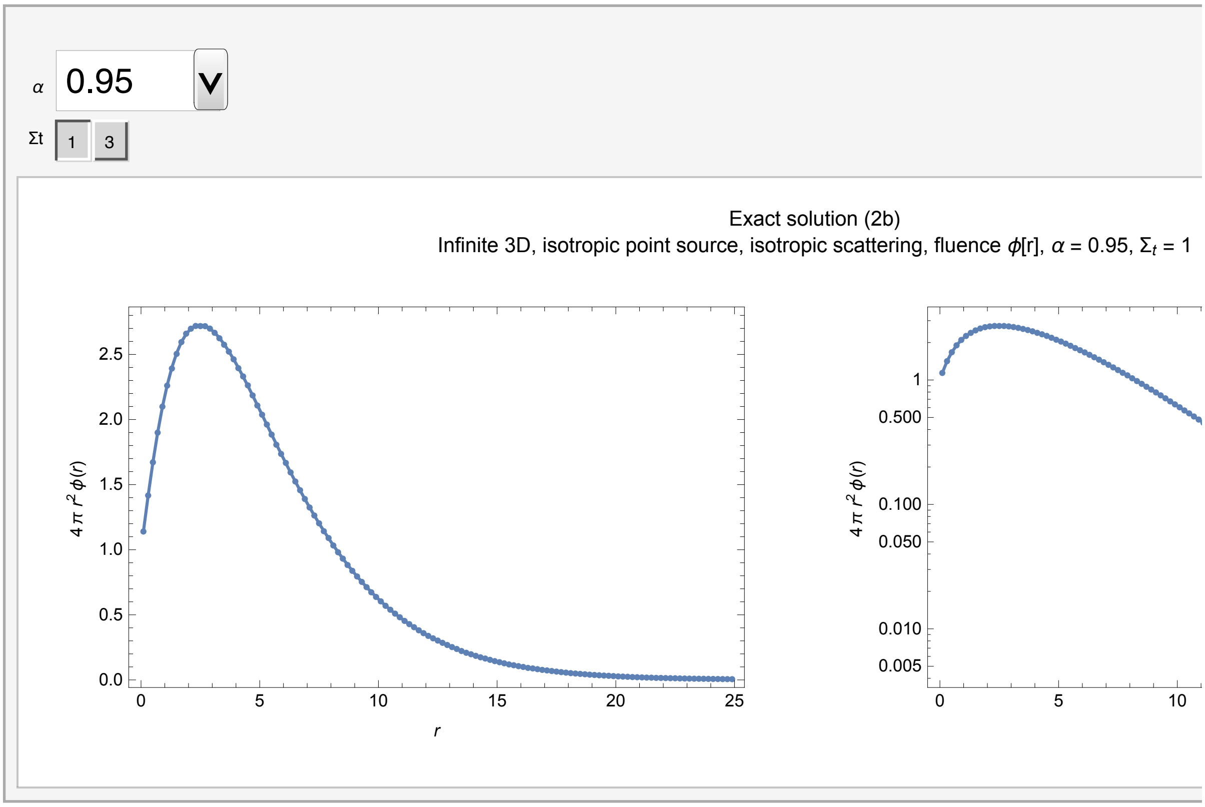
Exact solution (2a)

Infinite 3D, isotropic point source, isotropic scattering, fluence ϕ[r], α = 0.99, Σ_t = 1

Fluence - Exact solution (2b) comparison to MC

In[272]:=
```
Clear[alpha, Σt];
Manipulate[
 If[Length[inf3Disopointisoscatter`simulations] > 0,
  Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
   data = SelectFirst[
      inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
   maxr = data[[2, 5]];
   dr = data[[2, 7]];

   pointsϕ = data[[4]];

   (* divide by Σt to convert collision density into fluence *)
   plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

   exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
         inf3Disopointisoscatter`ϕexact2b[#[[1]], Σt, α]}] & /@plotpointsϕ;

   plotϕ = Quiet[Show[
      ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
      ListPlot[exact1points, PlotRange → All, Joined → True],
      Frame → True,
      FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
     ]];
   logplotϕ = Quiet[Show[
      ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
      ListLogPlot[exact1points, PlotRange → All, Joined → True],
      Frame → True,
      FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
     ]];
   Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800],
    PlotLabel -> "Exact solution (2b)\nInfinite 3D, isotropic point
       source, isotropic scattering, fluence ϕ[r], α = " <>
     ToString[α] <> ", Σt = " <> ToString[Σt]]
  ]
  ,
  Text[
   "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
     ensure the data path is setup correctly."]
 ]
 , {{α, 0.95}, inf3Disopointisoscatter`alphas},
 {Σt, inf3Disopointisoscatter`muts}]
```

Out[273]=



α 0.95

Σt 1 3

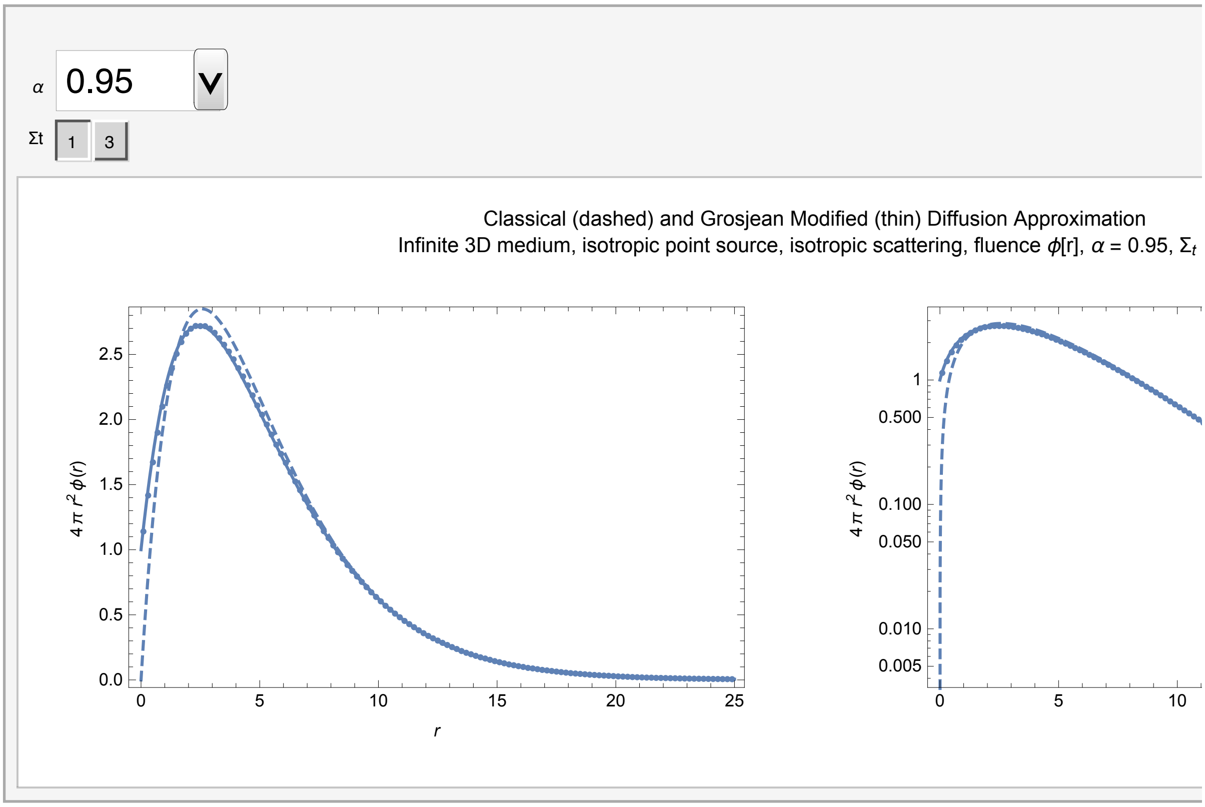
Exact solution (2b)

Infinite 3D, isotropic point source, isotropic scattering, fluence ϕ[r], α = 0.95, Σ_t = 1

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

```
In[274]:= Clear[alpha, Σt];
          Manipulate[
           If[Length[inf3Disopointisoscatter`simulations] > 0,
            Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
             data = SelectFirst[
                inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
             maxr = data[[2, 5]];
             dr = data[[2, 7]];

             pointsϕ = data[[4]];

             (* divide by Σt to convert collision density into fluence *)
             plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

             plotϕ = Quiet[Show[
                 ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 Plot[4 Pi r^2 inf3Disopointisoscatter`ϕGrosjean[r, Σt, α],
                  {r, 0, maxr}, PlotRange → All],
                 Plot[4 Pi r^2 inf3Disopointisoscatter`ϕDiffusion[r, Σt, α],
                  {r, 0, maxr}, PlotRange → All, PlotStyle → Dashed],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
               ]];
             logplotϕ = Quiet[Show[
                 ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 LogPlot[4 Pi r^2 inf3Disopointisoscatter`ϕGrosjean[r, Σt, α],
                  {r, 0, maxr}, PlotRange → All],
                 LogPlot[4 Pi r^2 inf3Disopointisoscatter`ϕDiffusion[r, Σt, α],
                  {r, 0, maxr}, PlotRange → All, PlotStyle → Dashed],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
               ]];
             pp = Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800],
               PlotLabel -> "Classical (dashed) and Grosjean Modified (thin) Diffusion
                   Approximation\nInfinite 3D medium, isotropic point
                   source, isotropic scattering, fluence ϕ[r], α = " <>
                 ToString[α] <> ", Σ_t = " <> ToString[Σt]]
            ]
            ,
            Text[
             "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
               ensure the data path is setup correctly."]
           ]
           , {{α, 0.95}, inf3Disopointisoscatter`alphas},
           {Σt, inf3Disopointisoscatter`muts}]
```

Out[275]=



α 0.95

Σt 1 3

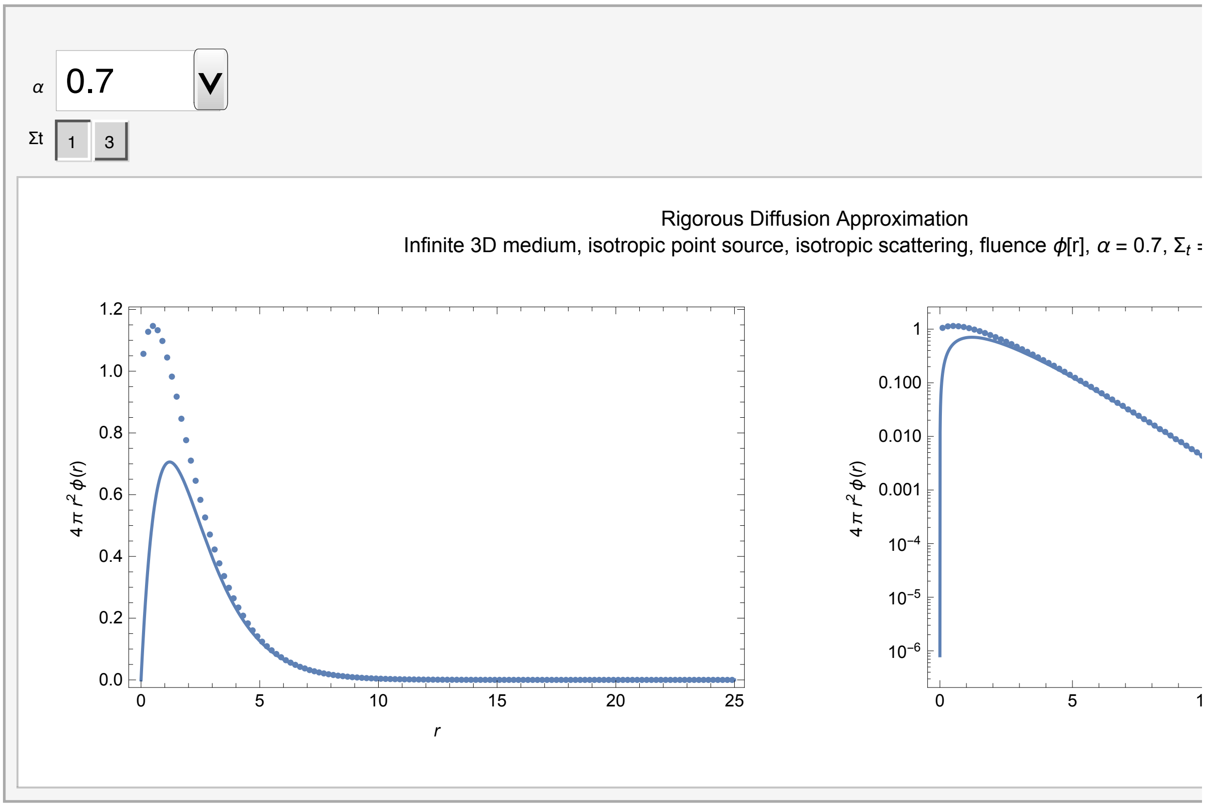
Classical (dashed) and Grosjean Modified (thin) Diffusion Approximation

Infinite 3D medium, isotropic point source, isotropic scattering, fluence ϕ[r], α = 0.95, Σ_t

Fluence - Diffusion approximation (Rigorous) comparison to MC

```
In[276]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
   Module[{data, maxr, dr, pointsϕ, plotpointsϕ, logplotϕ, plotϕ, exact1points},
    data = SelectFirst[
       inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
    maxr = data[[2, 5]];
    dr = data[[2, 7]];

    pointsϕ = data[[4]];

    (* divide by Σt to convert collision density into fluence *)
    plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

    plotϕ = Quiet[Show[
        ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
        Plot[4 Pi r^2 inf3Disopointisoscatter`ϕrigourousDiffusion[r, Σt, α],
         {r, 0, maxr}, PlotRange → All],
        Frame → True,
        FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
       ]];
    logplotϕ = Quiet[Show[
        ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
        LogPlot[4 Pi r^2 inf3Disopointisoscatter`ϕrigourousDiffusion[r, Σt, α],
         {r, 0, maxr}, PlotRange → All],
        Frame → True,
        FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
       ]];
    Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 800], PlotLabel ->
      "Rigorous Diffusion Approximation\nInfinite 3D medium, isotropic
        point source, isotropic scattering, fluence ϕ[r], α = " <>
       ToString[α] <> ", Σt = " <> ToString[Σt]]
   ]
   ,
   Text[
    "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
      ensure the data path is setup correctly."]
  ]
  , {{α, 0.7}, inf3Disopointisoscatter`alphas},
  {Σt, inf3Disopointisoscatter`muts}]
```

Out[276]=



α 0.7

Σt 1 3

Rigorous Diffusion Approximation

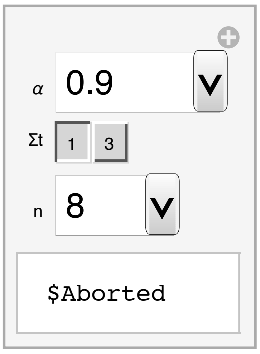
Infinite 3D medium, isotropic point source, isotropic scattering, fluence ϕ[r], α = 0.7, Σ_t =

N-th order fluence / scalar flux

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

```
In[278]:= Clear[alpha, Σt];
          Manipulate[
           If[Length[inf3Disopointisoscatter`simulations] > 0,
            Module[{data, maxr, dr, pointsϕ,
               plotpointsϕ, logplotϕ, plotϕ, exact1points, numorders},
             data = SelectFirst[inf3Disopointisoscatter`simulations,
                 #[[1]] == α && #[[2]] == Σt &][[3]];
             maxr = data[[2, 5]];
             dr = data[[2, 7]];
             numorders = data[[2, 13]];

             pointsϕ  = data[[9 + numorders + n + 1]];

             (* divide by Σt to convert collision density into fluence *)
             plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

             exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
                   inf3Disopointisoscatter`ϕexact1[#[[1]], Σt, α, n]}] & /@ plotpointsϕ;

             plotϕ = Quiet[Show[
                 ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 ListPlot[exact1points, PlotRange → All, Joined → True],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
                ]];
             logplotϕ = Quiet[Show[
                 ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
                 ListLogPlot[exact1points, PlotRange → All, Joined → True],
                 Frame → True,
                 FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
                ]];
             Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 1000], PlotLabel ->
               "Exact solution (1)\nInfinite 3D medium, isotropic point source,
                  isotropic scattering, n-th scattered fluence ϕ[r|n], α = " <>
                 ToString[α] <> ", Σt = " <> ToString[Σt]]
            ]
            ,
            Text[
             "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
               ensure the data path is setup correctly."]
           ]
           , {{α, 0.9}, inf3Disopointisoscatter`alphas},
           {Σt, inf3Disopointisoscatter`muts},
           {{n, 8}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
               inf3Disopointisoscatter`numcollorders, 1]]}]
```

Out[279]=



α 0.9

Σt 1 3

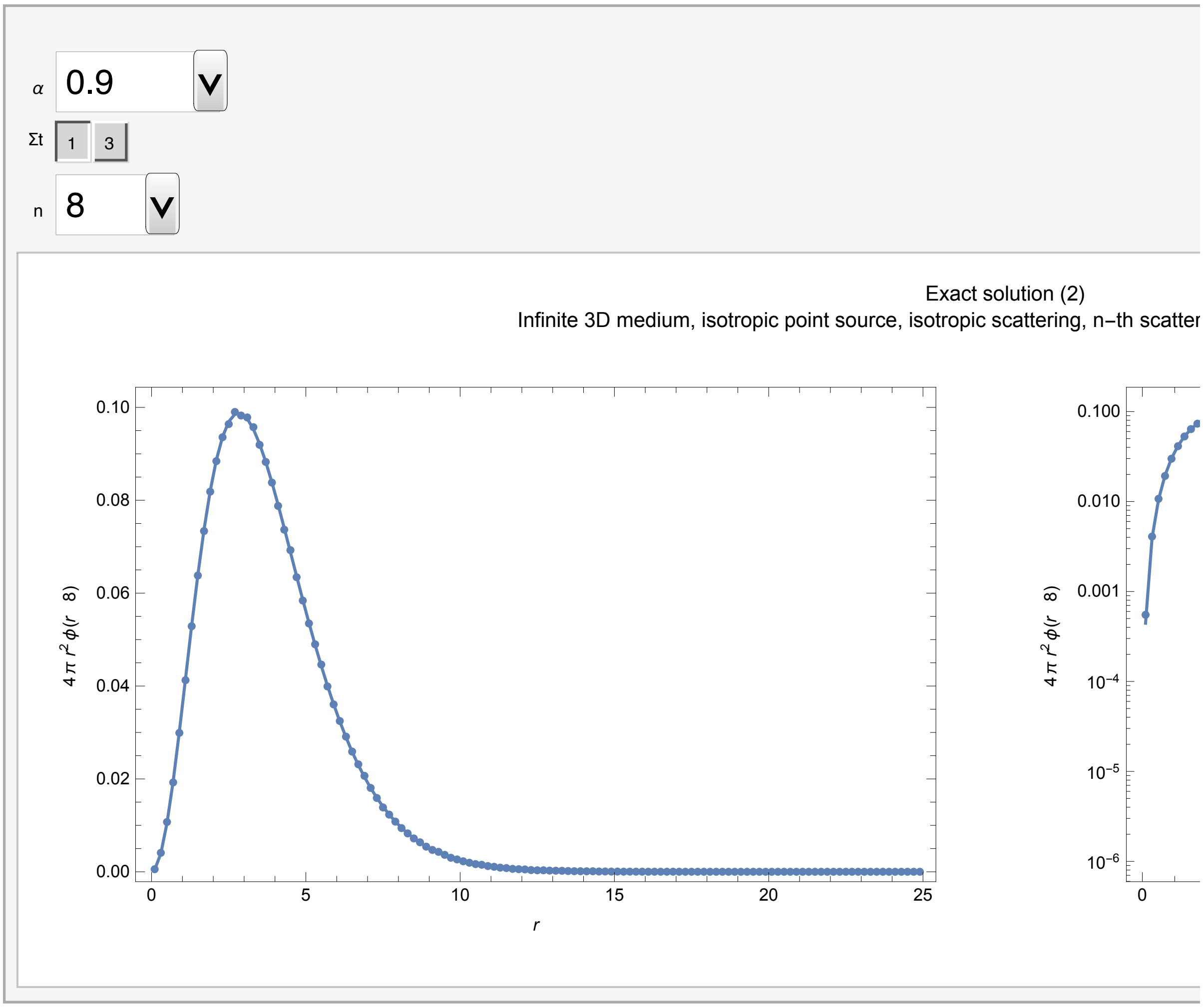
n 8

```
$Aborted
```

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

```
In[280]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
   Module[{data, maxr, dr, pointsϕ,
     plotpointsϕ, logplotϕ, plotϕ, exact1points, numorders},
    data = SelectFirst[inf3Disopointisoscatter`simulations,
       #[[1]] == α && #[[2]] == Σt &][[3]];
    maxr = data[[2, 5]];
    dr = data[[2, 7]];
    numorders = data[[2, 13]];

    pointsϕ  = data[[9 + numorders + n + 1]];

    (* divide by Σt to convert collision density into fluence *)
    plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

    exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
          inf3Disopointisoscatter`ϕexact2[#[[1]], Σt, α, n]}] & /@ plotpointsϕ;

    plotϕ = Quiet[Show[
       ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       ListPlot[exact1points, PlotRange → All, Joined → True],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
      ]];
    logplotϕ = Quiet[Show[
       ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       ListLogPlot[exact1points, PlotRange → All, Joined → True],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
      ]];
    Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 1000], PlotLabel ->
      "Exact solution (2)\nInfinite 3D medium, isotropic point source,
        isotropic scattering, n-th scattered fluence ϕ[r|n], α = " <>
       ToString[α] <> ", Σt = " <> ToString[Σt]]
   ]
   ,
   Text[
    "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
      ensure the data path is setup correctly."]
  ]
  , {{α, 0.9}, inf3Disopointisoscatter`alphas},
  {Σt, inf3Disopointisoscatter`muts},
  {{n, 8}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
     inf3Disopointisoscatter`numcollorders, 1]]}]
```

Out[280]=



α 0.9

Σt 1 3

n 8

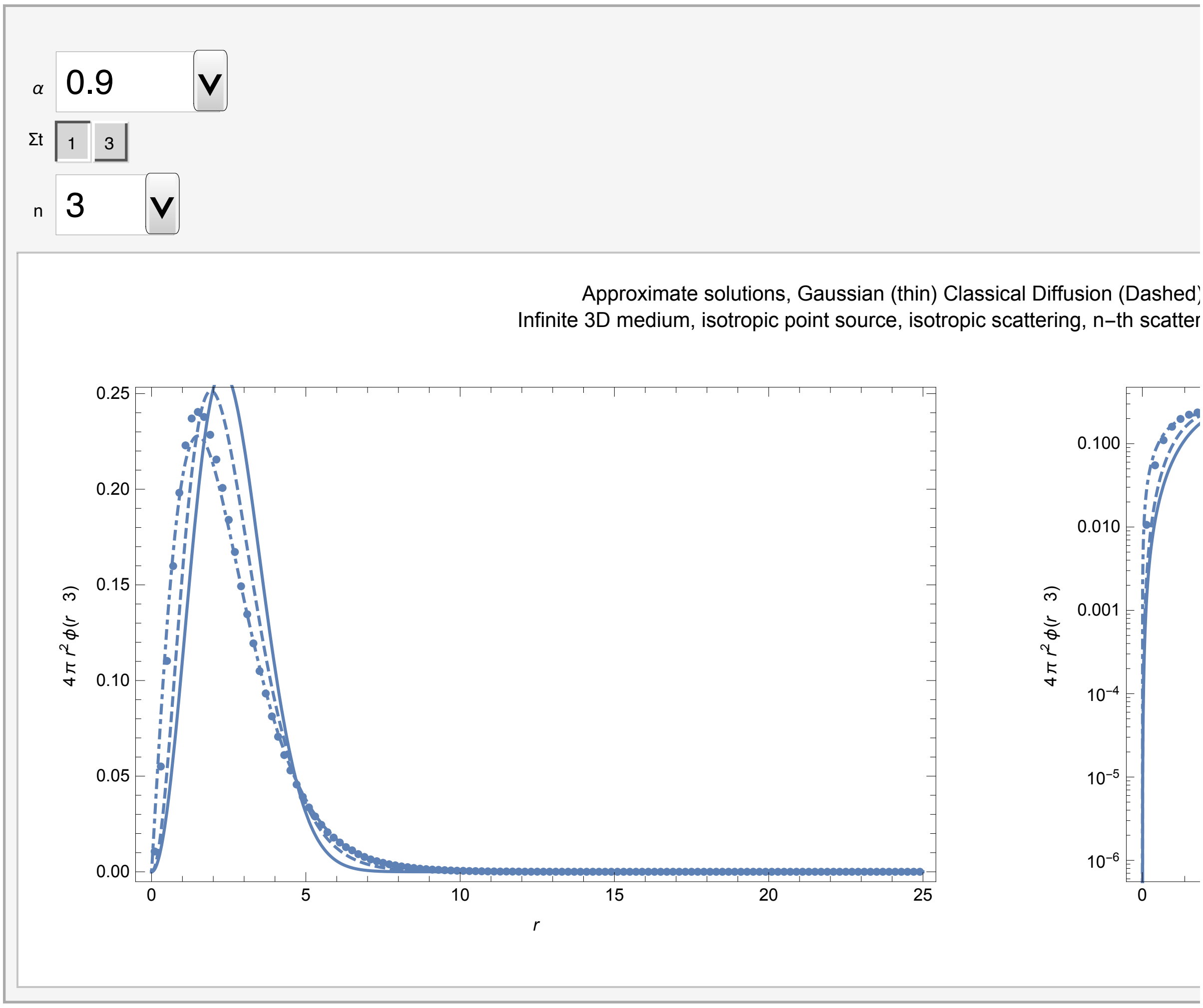
Exact solution (2)

Infinite 3D medium, isotropic point source, isotropic scattering, n–th scatter

N-th collided Fluence - Approximations

```
In[281]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
   Module[{data, maxr, dr, pointsϕ,
     plotpointsϕ, logplotϕ, plotϕ, exact1points, numorders},
    data = SelectFirst[inf3Disopointisoscatter`simulations,
       #[[1]] == α && #[[2]] == Σt &][[3]];
    maxr = data[[2, 5]];
    dr = data[[2, 7]];
    numorders = data[[2, 13]];

    pointsϕ = data[[9 + numorders + n + 1]];

    (* divide by Σt to convert collision density into fluence *)
    plotpointsϕ = inf3Disopointisoscatter`ppoints[pointsϕ, dr, maxr, Σt];

    seriesclassical = α^n SeriesCoefficient[
       inf3Disopointisoscatter`ϕDiffusion[r, Σt, C], {C, 0, n}];
    seriesG = α^n SeriesCoefficient[inf3Disopointisoscatter`ϕGrosjean[r, Σt, C],
       {C, 0, n}];

    plotϕ = Quiet[Show[
       ListPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       Plot[4 Pi r^2 inf3Disopointisoscatter`ϕGaussian[r, Σt, α, n],
        {r, 0, maxr}, PlotRange → All],
       Plot[4 Pi r^2 seriesclassical, {r, 0, maxr},
        PlotRange → All, PlotStyle → Dashed],
       Plot[4 Pi r^2 seriesG, {r, 0, maxr}, PlotRange → All, PlotStyle → DotDashed],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
      ]];
    logplotϕ = Quiet[Show[
       ListLogPlot[plotpointsϕ, PlotRange → All, PlotStyle → PointSize[.01]],
       LogPlot[
        4 Pi r^2 inf3Disopointisoscatter`ϕGaussian[r, Σt, α, n], {r, 0, maxr}],
       LogPlot[4 Pi r^2 seriesclassical, {r, 0, maxr},
        PlotRange → All, PlotStyle → Dashed],
       LogPlot[4 Pi r^2 seriesG, {r, 0, maxr}, PlotRange → All,
        PlotStyle → DotDashed],
       Frame → True,
       FrameLabel -> {{4 Pi r^2 ϕ[r | n],}, {r,}}
      ]];
    Show[GraphicsGrid[{{plotϕ, logplotϕ}}, ImageSize → 1000],
     PlotLabel -> "Approximate solutions, Gaussian (thin) Classical Diffusion
         (Dashed) Grosjean (Dot-Dashed)\nInfinite 3D medium, isotropic
         point source, isotropic scattering, n-th scattered fluence
         ϕ[r|n], α = " <> ToString[α] <> ", Σt = " <> ToString[Σt]]
   ]
   ,
   Text[
    "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
      ensure the data path is setup correctly."]
  ]
  , {{α, 0.9}, inf3Disopointisoscatter`alphas},
  {Σt, inf3Disopointisoscatter`muts},
  {{n, 3}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
     inf3Disopointisoscatter`numcollorders, 1]]}]
```

Out[281]=



α 0.9

Σt 1 3

n 3

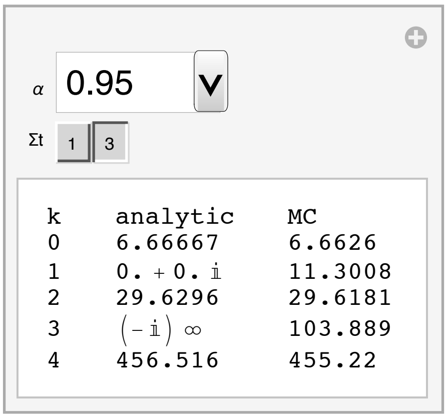
Approximate solutions, Gaussian (thin) Classical Diffusion (Dashed)

Infinite 3D medium, isotropic point source, isotropic scattering, n–th scatter

Compare moments of ϕ

In[282]:=
```
Manipulate[
 If[Length[inf3Disopointisoscatter`simulations] > 0,
  Module[{data, nummoments, ϕmoments, ks, analytic, j},
   data = SelectFirst[
      inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
   nummoments = data[[2, 15]];
                    data[[6]]
   ϕmoments = N[{ ------------ }];
                       Σt
   ks = Table[k, {k, 0, nummoments - 1}];
   analytic = Table[inf3Disopointisoscatter`ϕm[α, Σt, k], {k, ks}];
   j = Join[{ks}, {analytic}, ϕmoments];

   TableForm[
    Join[{{"k", "analytic", "MC"}}, Transpose[j]]
   ]
  ],
  Text[
   "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
     ensure the data path is setup correctly."]
 ]
 , {{α, 0.95}, inf3Disopointisoscatter`alphas},
 {{Σt, 3}, inf3Disopointisoscatter`muts}]
```

Out[282]=

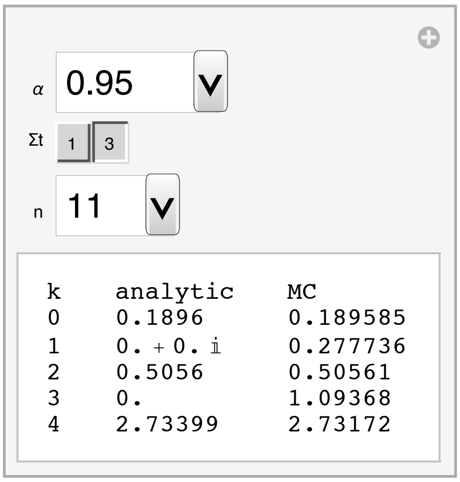


```
k   analytic     MC
0   6.66667      6.6626
1   0. + 0. ⅈ    11.3008
2   29.6296      29.6181
3   (-ⅈ) ∞       103.889
4   456.516      455.22
```

n-th collided moments of ϕ

In[283]:=
```
Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
   Module[{data, nummoments, ϕmoments, ks, analytic, j},
    data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
    nummoments = data[[2, 15]];
    ϕmoments = N[{data[[9 + n]]}/Σt];
    ks = Table[k, {k, 0, nummoments - 1}];
    analytic = Table[inf3Disopointisoscatter`ϕm[α, Σt, k, n], {k, ks}];
    j = Join[{ks}, {analytic}, ϕmoments];

    TableForm[
     Join[{{"k", "analytic", "MC"}}, Transpose[j]]
    ]
   ],
   Text[
    "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
      ensure the data path is setup correctly."]
  ]
  , {{α, 0.95}, inf3Disopointisoscatter`alphas},
  {{Σt, 3}, inf3Disopointisoscatter`muts},
  {{n, 11}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
      inf3Disopointisoscatter`numcollorders, 1]]}
]
```

Out[283]=



α 0.95

Σt 1 3

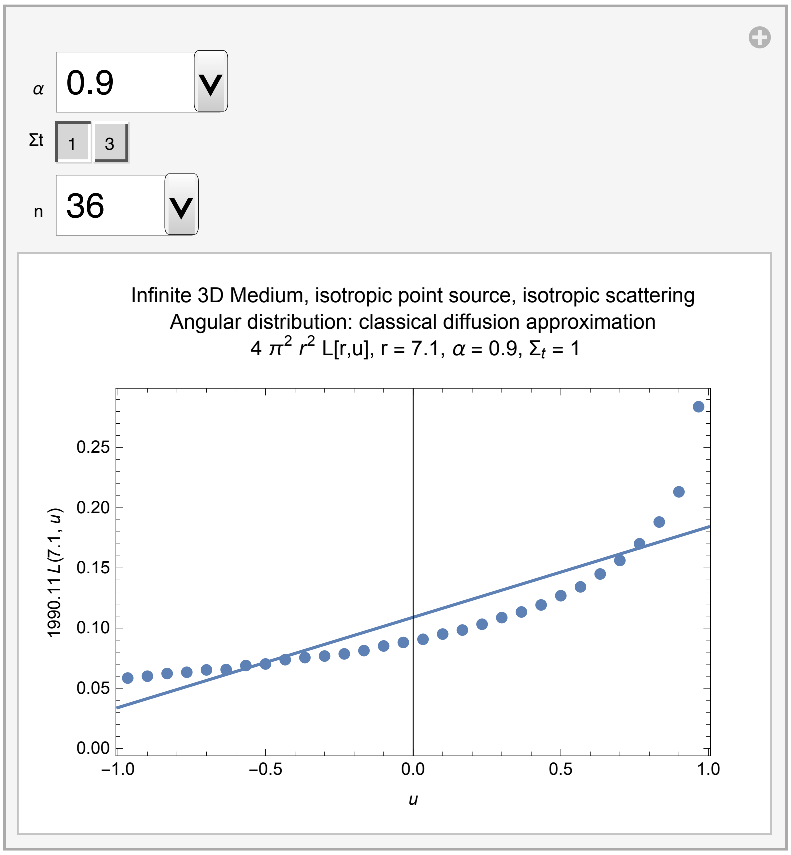
n 11

```
k    analytic     MC
0    0.1896       0.189585
1    0. + 0. ⅈ    0.277736
2    0.5056       0.50561
3    0.           1.09368
4    2.73399      2.73172
```

Angular Distributions

```
In[284]:= Manipulate[
    If[Length[inf3Disopointisoscatter`simulations] > 0,
     Module[{data, numorders, pointsu, plotpointsu, du, r, dr},
      data = SelectFirst[
          inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
      numorders = data[[2, 13]];
      du = data[[2, 9]];
      dr = data[[2, 7]];

      pointsu  = data[[9 + 2 numorders + n]];

      r  =  dr * n - 0.5 dr;

      (* divide by Σt to convert collision density into fluence *)
      plotpointsu = inf3Disopointisoscatter`ppointsu[pointsu, du, Σt];
      Show[
       ListPlot[plotpointsu, PlotRange → All,
        Frame → True,
        FrameLabel -> {{4 Pi^2 r^2 L[r, u],}, {u,}}],
       Plot[4 Pi r^2 Pi inf3Disopointisoscatter`Ldiffusion[r, u, Σt, α],
        {u, -1, 1}, PlotRange → All
       ],
       PlotLabel -> "Infinite 3D Medium, isotropic point source,
           isotropic scattering\nAngular distribution: classical
           diffusion approximation\n 4 π^2  r^2  L[r,u], r  =  " <>
         ToString[r] <> ", α  =  " <> ToString[α] <> ", Σt  =  " <> ToString[Σt]
      ]

     ],
     Text[
      "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
        ensure the data path is setup correctly."]
    ]
    , {{α, 0.9}, inf3Disopointisoscatter`alphas},
    {{Σt, 1}, inf3Disopointisoscatter`muts}, {{n, 36}, Range[If[
       NumberQ[inf3Disopointisoscatter`numr], inf3Disopointisoscatter`numr, 1]]}]
```

Out[284]=



α 0.9

Σt 1 3

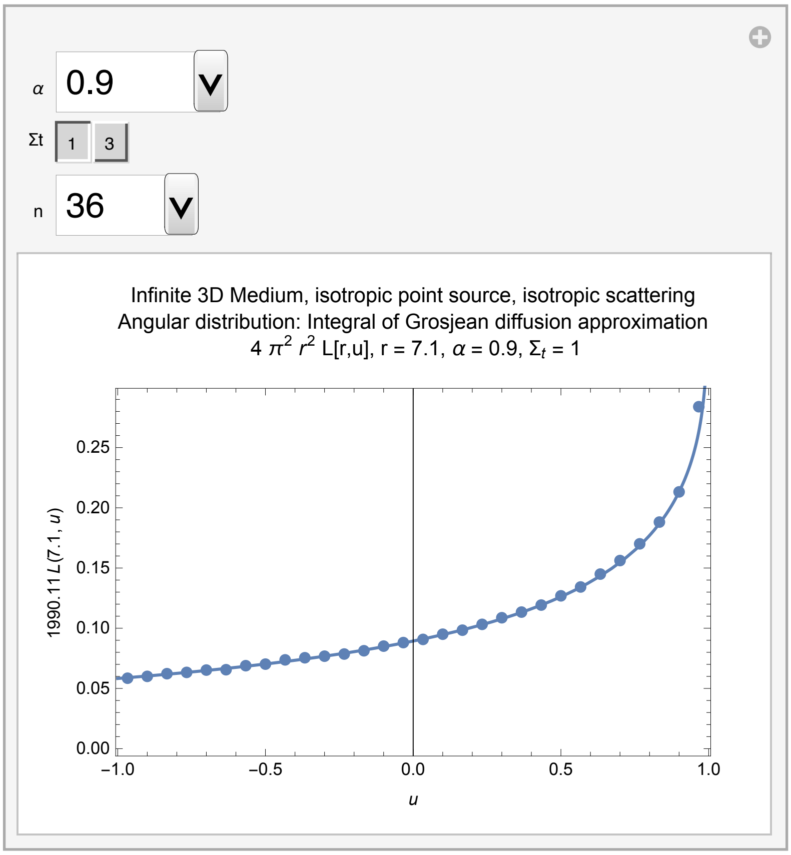
n 36

Infinite 3D Medium, isotropic point source, isotropic scattering
Angular distribution: classical diffusion approximation
$4\,\pi^2\,r^2$ L[r,u], r = 7.1, α = 0.9, Σ_t = 1

Angular Distribution: Integral of Grosjean’s Diffusion Approximation

```
In[285]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
   Module[{data, numorders, pointsu, plotpointsu, du, r, dr},
    data = SelectFirst[
       inf3Disopointisoscatter`simulations, #[[1]] == α && #[[2]] == Σt &][[3]];
    numorders = data[[2, 13]];
    du = data[[2, 9]];
    dr = data[[2, 7]];

    pointsu  = data[[9 + 2 numorders + n]];

    r  =  dr * n - 0.5 dr;

    (* divide by Σt to convert collision density into fluence *)
    plotpointsu = inf3Disopointisoscatter`ppointsu[pointsu, du, Σt];
    pp = Show[
      ListPlot[plotpointsu, PlotRange → All,
       Frame → True,
       FrameLabel -> {{4 Pi^2 r^2 L[r, u],}, {u,}}],
      Plot[4 Pi r^2 Pi inf3Disopointisoscatter`Lintegral[r, u, Σt, α,
         inf3Disopointisoscatter`ϕGrosjean], {u, -1, 1}, PlotRange → All
      ],
      PlotLabel -> "Infinite 3D Medium, isotropic point source, isotropic
          scattering\nAngular distribution: Integral of Grosjean
          diffusion approximation\n 4 π^2  r^2  L[r,u], r  =  " <>
        ToString[r] <> ",  α  =  " <> ToString[α] <> ",  Σt  =  " <> ToString[Σt]
     ]

   ],
   Text[
    "Uh oh!  Couldn't find MC data.  Try to evaluate this entire notebook and
      ensure the data path is setup correctly."]
  ]
  , {{α, 0.9}, inf3Disopointisoscatter`alphas},
  {{Σt, 1}, inf3Disopointisoscatter`muts}, {{n, 36}, Range[If[
     NumberQ[inf3Disopointisoscatter`numr], inf3Disopointisoscatter`numr, 1]]}]
```

Out[285]=



α 0.9

Σt 1 3

n 36

Infinite 3D Medium, isotropic point source, isotropic scattering
Angular distribution: Integral of Grosjean diffusion approximation
$4\,\pi^2\,r^2$ L[r,u], r = 7.1, α = 0.9, Σ_t = 1