

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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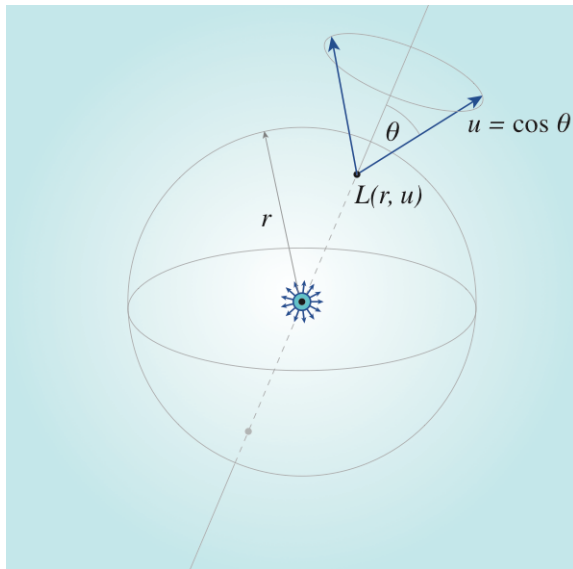
www.eugenedeon.com

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[424]:= SetDirectory[Import["~/hitchhikerpath"]]
```

Notation



α - single-scattering albedo

Σ_t - extinction coefficient

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

$u = \cos \theta$ - direction cosine

Util

In[425]:= **SurfaceArea**[d_, r_] := d $\frac{\text{Pi}^{d/2}}{\text{Gamma}[\frac{d}{2} + 1]}$ r^{d-1}

Diffusion modes

In[426]:= **diffusionMode**[v_, d_, r_] := (2 π)^{-d/2} r^{1-d/2} v^{-1-d/2} **BesselK**[$\frac{1}{2}(-2+d)$, $\frac{r}{v}$]

Analytic solutions

Caseology quantities

In[427]:= **CaseN0**[c_, v0_] := $\frac{1}{2} c v0^3 \left(\frac{c}{v0^2 - 1} - \frac{1}{v0^2} \right)$

In[428]:= **Casev0**[c_?NumericQ] := **FindRoot**[c v **ArcTanh**[$\frac{1}{v}$] - 1 == 0, {v, 1.000000000001, 10¹⁰}, **Method** → "Brent"][[1]][[2]]

In[429]:= **CaseN**[c_, v_] := v $\left(\text{Case}\lambda[v, c]^2 + \left(\frac{\pi c v}{2} \right)^2 \right)$

In[430]:= **Caseλ**[v_, c_] := 1 - c v **ArcTanh**[v]

Fluence: exact solution (1)

[Bothe 1942]

In[431]:= **inf3Disopointisoscatter**ϕexact1a[r_, Σt_, α_] := $\frac{1}{2 \text{Pi}^2 r} \text{NIntegrate} \left[\frac{z \text{ArcTan}[z / \Sigma t]}{z - \alpha \Sigma t \text{ArcTan}[z / \Sigma t]} \text{Sin}[r z], \{z, 0, \text{Infinity}\}, \text{Method} \rightarrow \text{"ExtrapolatingOscillatory"} \right]$

[Case et al. 1953]

In[432]:= **inf3Disopointisoscatter**ϕexact1b[r_, Σt_, α_] := $\frac{\text{Exp}[-\Sigma t r]}{4 \text{Pi} r^2} + \alpha \frac{\Sigma t}{2 \text{Pi}^2 r} \text{NIntegrate} \left[\frac{\text{ArcTan}[z]^2}{z - \alpha \text{ArcTan}[z]} \text{Sin}[r \Sigma t z], \{z, 0, \text{Infinity}\}, \text{Method} \rightarrow \text{"LevinRule"} \right]$

Rigorous diffusion approximation

In[433]:= **inf3Disopointisoscatter**ϕrigorousDiffusion[r_, Σt_, α_] := $\frac{\Sigma t}{4 \text{Pi} r} \frac{\text{E}^{-r \Sigma t / \#}}{\# \text{CaseN0}[\alpha, \#]} \&[\text{Casev0}[\alpha]]$

Fluence: exact solution (2)

[Davison 1947]

```
In[434]:= inf3Disopointisoscatter`phiexact2a[r_, Sigma t_, alpha_] :=
  inf3Disopointisoscatter`phi rigorousDiffusion[r, Sigma t, alpha] +
  
$$\frac{\Sigma t}{4 \pi r} \text{NIntegrate}\left[\frac{e^{-\Sigma t r y}}{\frac{\alpha^2 \pi^2}{4 y^2} + \left(1 - \frac{\alpha}{2 y} \text{Log}\left[\frac{y+1}{y-1}\right]\right)^2}, \{y, 1, \text{Infinity}\}\right]$$

```

[Case and Zwiefel 1967]

```
In[435]:= inf3Disopointisoscatter`phiexact2b[r_, Sigma t_, alpha_] :=
  inf3Disopointisoscatter`phi rigorousDiffusion[r, Sigma t, alpha] +
  
$$\frac{\Sigma t}{4 \pi r} \text{NIntegrate}\left[\frac{e^{-\Sigma t r / v}}{v \text{CaseN}[\alpha, v]}, \{v, 0, 1\}\right]$$

```

n-th scattered fluence

```
In[436]:= inf3Disopointisoscatter`phiexact1[r_, Sigma t_, alpha_, n_] :=
  
$$\frac{(\alpha \Sigma t)^n}{2 \pi^2 r} \text{NIntegrate}\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]^{1+n} \text{Sin}[r z]}{z^n}, \{z, 0, \text{Infinity}\}, \text{Method} \rightarrow \text{"ExtrapolatingOscillatory"}\right]$$

```

```
In[437]:= inf3Disopointisoscatter`phiexact2[r_, Sigma t_, alpha_, n_] := 
$$\frac{\alpha^n \Sigma t}{2^{n+3} \pi^2 r} \text{Chop}\left[\text{NIntegrate}\left[\frac{\text{Exp}[-r z \Sigma t]}{z^n} \left(\left(\text{Log}\left[\frac{z+1}{z-1}\right] + i \pi\right)^{n+1} - \left(\text{Log}\left[\frac{z+1}{z-1}\right] - i \pi\right)^{n+1}\right), \{z, 1, \text{Infinity}\}\right]\right]$$

```

```
In[757]:= inf3Disopointisoscatter`phiGaussian[r_, Sigma t_, alpha_, n_] := 
$$\frac{3 \sqrt{3} e^{-\frac{3 r^2 \Sigma t^2}{4 (1+n)}} \alpha^n \Sigma t^2}{8 \sqrt{(1+n)^3} \pi^{3/2}}$$

```

Moments

```
In[483]:= inf3Disopointisoscatter`phi m[c_, Sigma t_, m_?IntegerQ, n_] :=
  
$$\text{Limit}\left[\text{Simplify}\left[(-1)^{m/2} \left(\frac{2 \text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]} \text{D}\left[\frac{\left(\frac{c \Sigma t \text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z}\right)^{1+n}}{c \Sigma t}, \{z, m\}\right]\right], z \rightarrow 0\right]\right]$$

```

```
In[484]:= TableForm[Table[inf3Disopointisoscatter`phi m[alpha, Sigma t, m, n], {m, 0, 6, 2}]]
```

```
Out[484]//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[485]:= inf3Disopointisoscatter`phi m[c_, Sigma t_, m_?IntegerQ] :=
  
$$\text{Limit}\left[\text{Simplify}\left[(-1)^{m/2} \left(\frac{2 \text{Gamma}\left[\frac{3+m}{2}\right]}{\text{Gamma}\left[\frac{1+m}{2}\right]} \text{D}\left[\frac{\text{ArcTan}\left[\frac{z}{\Sigma t}\right]}{z - c \Sigma t \text{ArcTan}\left[\frac{z}{\Sigma t}\right]}, \{z, m\}\right]\right], z \rightarrow 0\right]\right]$$

```

```
In[486]:= TableForm[Table[inf3Disopointisoscatter`phi[m][alpha, Sigma t, m], {m, 0, 6, 2}]]
```

```
Out[486]//TableForm=
```

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

Classical diffusion approximation

```
In[442]:= inf3Disopointisoscatter`phiDiffusion[r_, Sigma t_, alpha_] :=
```

$$\frac{1}{\Sigma t (1 - \alpha)} \text{diffusionMode}\left[\frac{1}{\sqrt{3} (1 - \alpha) \Sigma t}, 3, r\right]$$

```
In[443]:= FullSimplify[inf3Disopointisoscatter`phiDiffusion[r, Sigma t, alpha],  
Assumptions -> alpha > 0 && alpha < 1 && Sigma t > 0]
```

```
Out[443]=
```

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

Grosjean-style diffusion approximation

```
In[444]:= inf3Disopointisoscatter`phiGrosjean[r_, Sigma t_, alpha_] :=
```

$$\frac{\text{Exp}[-r \Sigma t]}{4 \pi r^2} + \frac{\alpha}{\Sigma t (1 - \alpha)} \text{diffusionMode}\left[\frac{\sqrt{2 - \alpha}}{\sqrt{3} (1 - \alpha) \Sigma t}, 3, r\right]$$

```
In[445]:= FullSimplify[inf3Disopointisoscatter`phiGrosjean[r, Sigma t, alpha],  
Assumptions -> alpha > 0 && alpha < 1 && Sigma t > 0]
```

```
Out[445]=
```

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

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[598]:= inf3Disopointisoscatter`LIntegral[r_, u_, Sigma t_, alpha_, phi_] :=
```

$$\frac{\alpha \Sigma t}{4 \pi} \text{NIntegrate}\left[\phi\left[\sqrt{r^2 + t^2 - 2 r t u}, \Sigma t, \alpha\right] \text{Exp}[-\Sigma t t], \{t, 0, \text{Infinity}\}\right]$$

Angular Classical diffusion approximation

```
In[588]:= inf3Disopointisoscatter`Ldiffusion[r_, u_, Sigma t_, alpha_] :=
```

$$\frac{1}{4 \pi} \text{inf3Disopointisoscatter`phiDiffusion}[r, \Sigma t, \alpha] + \\ \frac{1}{4 \pi} u \frac{3 e^{-r \sqrt{3 - 3 \alpha} \Sigma t} (1 + r \sqrt{3 - 3 \alpha} \Sigma t)}{4 \pi r^2}$$

load MC data

```

In[447]:= inf3Disopointisoscatter`ppoints[xs_, dr_, maxx_, Σt_] :=
  Table[{dr (i) - 0.5 dr, xs[[i]] / Σt}, {i, 1, Length[xs]}][[1 ;; -2]]

In[609]:= inf3Disopointisoscatter`ppointsu[xs_, du_, Σt_] :=
  Table[{-1.0 + du (i) - 0.5 du, xs[[i]] / (2 Σt)}, {i, 1, Length[xs]}][[1 ;; -1]]

In[449]:= inf3Disopointisoscatter`fs =
  FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/data/
    inf3D_isotropicpoint_isotropicscatter*"];

In[450]:= 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[452]= {0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999}

In[453]:= inf3Disopointisoscatter`mutts =
  Union[#[[2]] & /@ inf3Disopointisoscatter`simulations]

Out[453]= {1, 3}

In[454]:= 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[541]:= 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`mutts}]

```

Out[542]=

α 0.8

Σt 1 3

\$Aborted

Fluence - Exact solution (1b) comparison to MC

```

In[534]:= 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]];

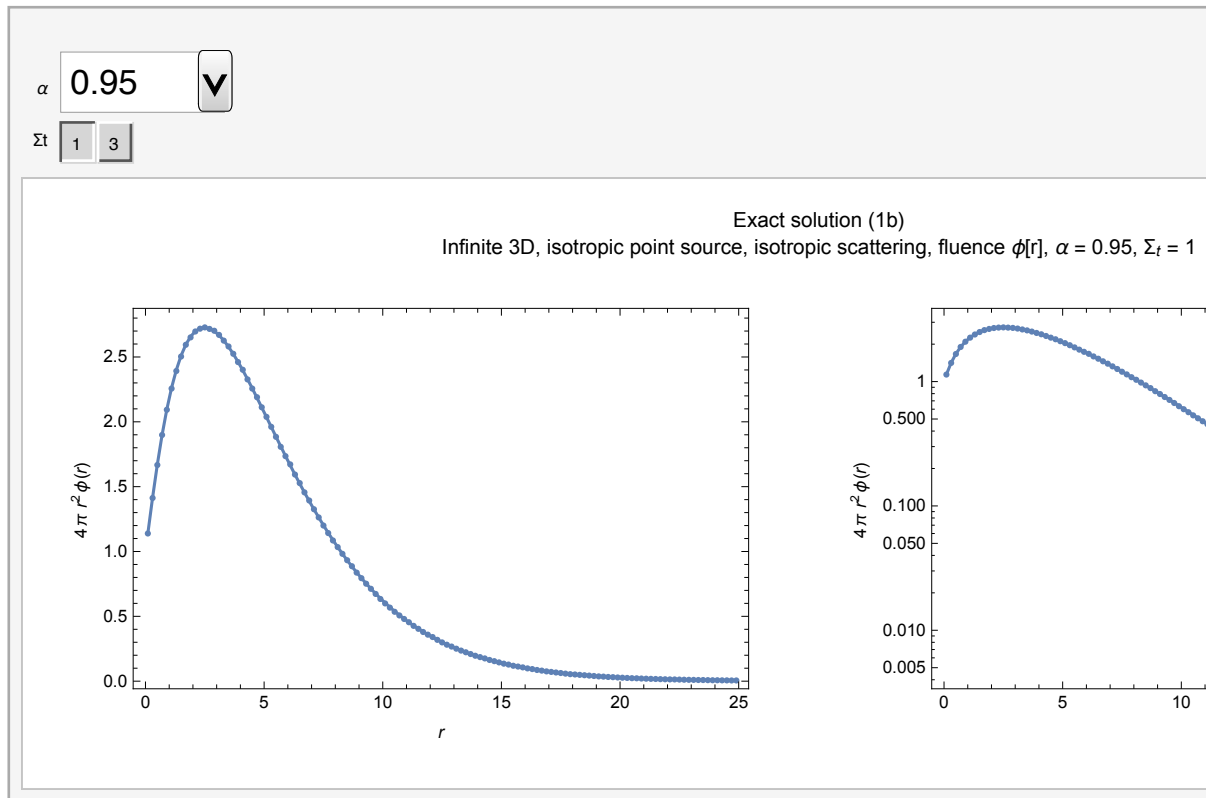
      (* divide by Σt to convert collision density into fluence *)
      plotpointsφ = inf3Disopointisoscatter`ppoints[pointsφ, dr, maxr, Σt];

      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`mutss}]

```

Out[535]=



Fluence - Exact solution (2a) comparison to MC

```

In[546]:= 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]];

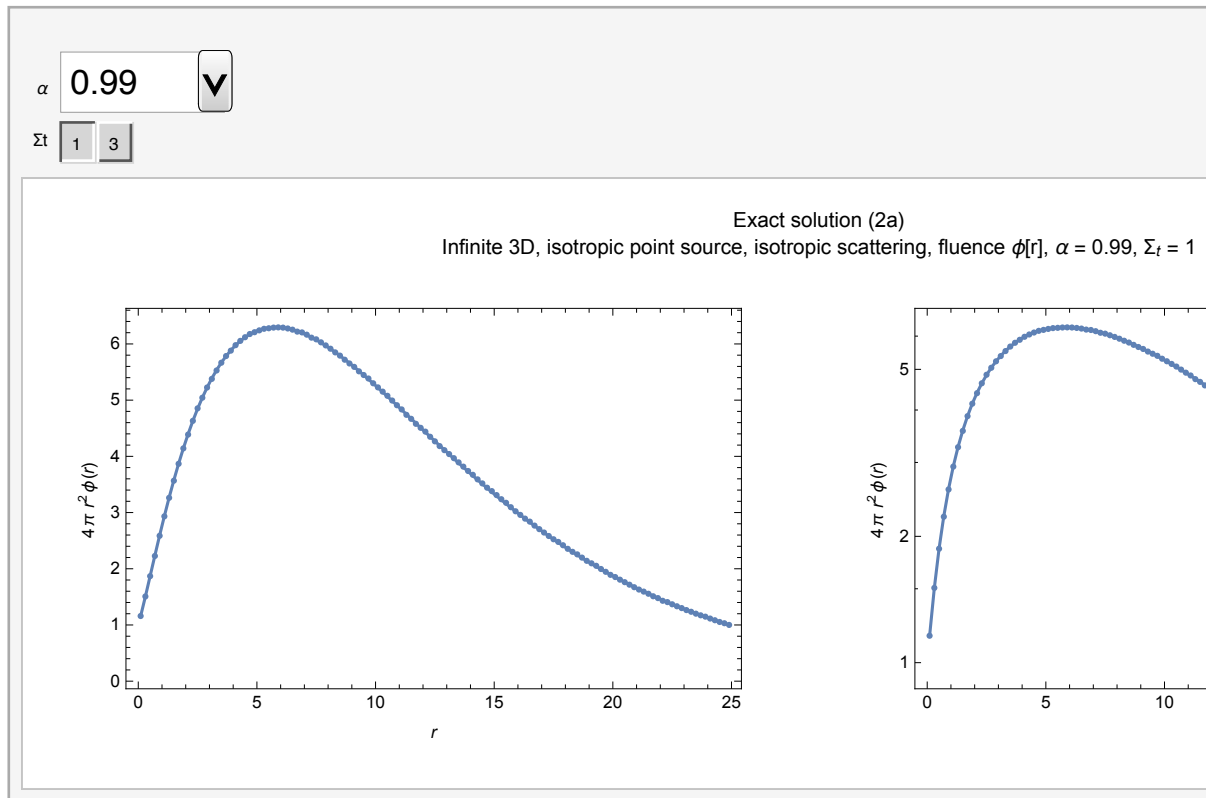
      (* divide by Σt to convert collision density into fluence *)
      plotpointsφ = inf3Disopointisoscatter`ppoints[pointsφ, dr, maxr, Σt];

      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]<> ", 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, 0.99}, inf3Disopointisoscatter`alphas},
{Σt, inf3Disopointisoscatter`mutts}]

```

Out[547]=



Fluence - Exact solution (2b) comparison to MC

```

In[699]:= 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]];

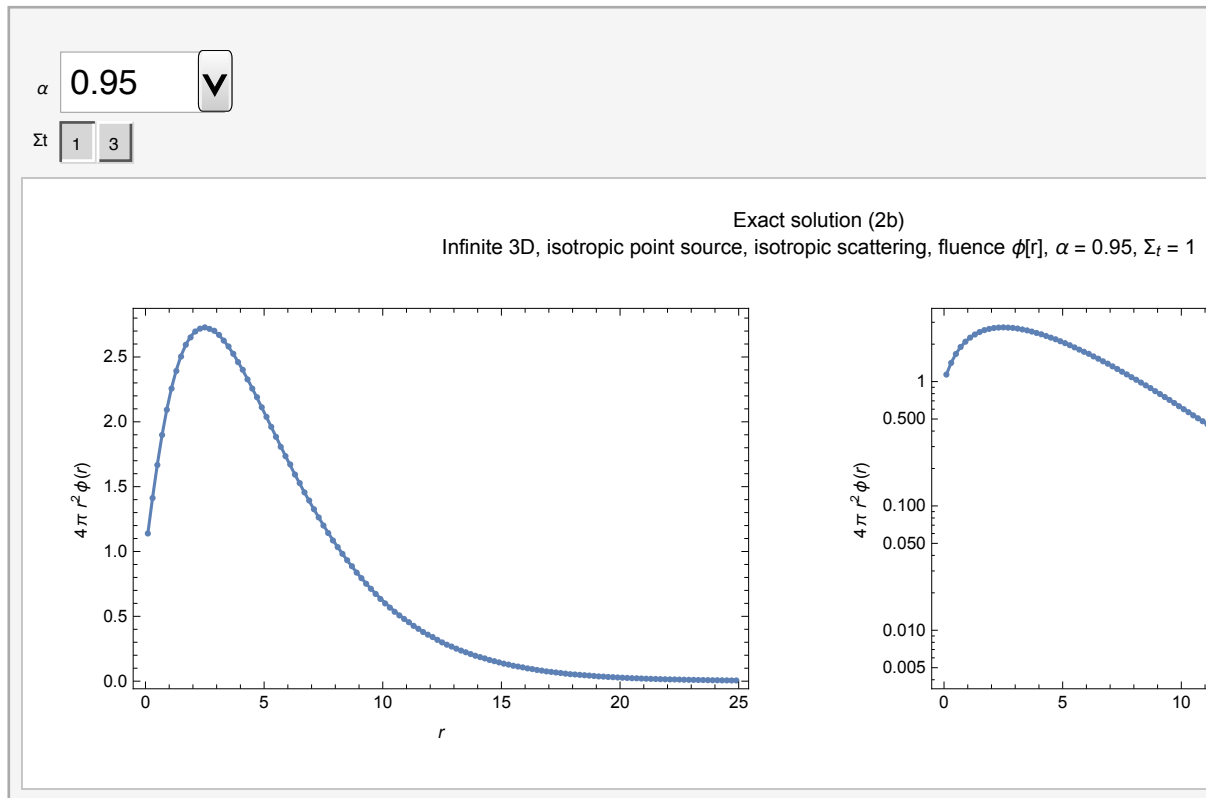
      (* divide by Σt to convert collision density into fluence *)
      plotpointsφ = inf3Disopointisoscatter`ppoints[pointsφ, dr, maxr, Σt];

      exact1points = Quiet[{#[[1]], 4 Pi #[[1]]^2
        inf3Disopointisoscatter`exact2b[#[[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`mutss}]

```

Out[700]=



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

```

In[561]:= 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]];

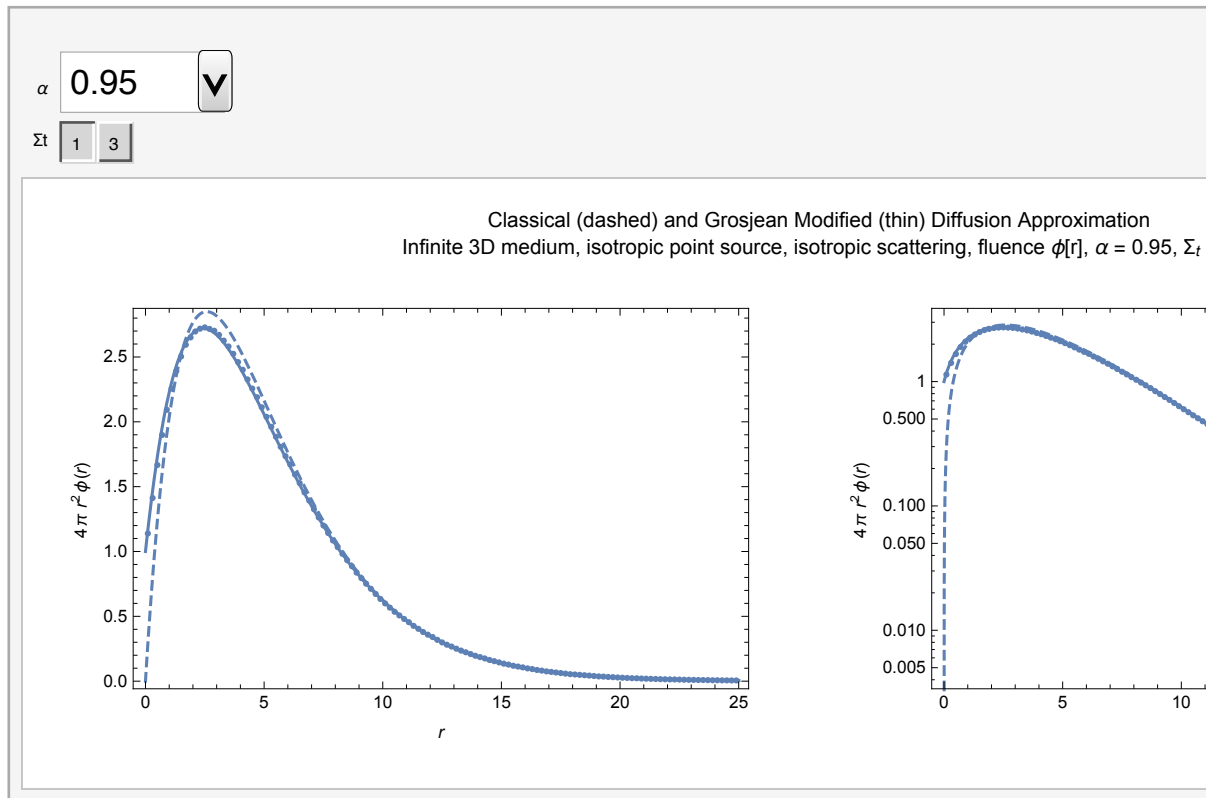
      pointsφ = data[[4]];

      (* 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 r2 inf3Disopointisoscatter`φGrosjean[r, Σt, α],
          {r, 0, maxr}, PlotRange → All],
        Plot[4 Pi r2 inf3Disopointisoscatter`φDiffusion[r, Σt, α],
          {r, 0, maxr}, PlotRange → All, PlotStyle → Dashed],
        Frame → True,
        FrameLabel -> {{4 Pi r2 φ[r]}, {r,}}
      ]];
      logplotφ = Quiet[Show[
        ListLogPlot[plotpointsφ, PlotRange → All, PlotStyle → PointSize[.01]],
        LogPlot[4 Pi r2 inf3Disopointisoscatter`φGrosjean[r, Σt, α],
          {r, 0, maxr}, PlotRange → All],
        LogPlot[4 Pi r2 inf3Disopointisoscatter`φDiffusion[r, Σt, α],
          {r, 0, maxr}, PlotRange → All, PlotStyle → Dashed],
        Frame → True,
        FrameLabel -> {{4 Pi r2 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]<> ", 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`mutss}
]

```

Out[562]=



Fluence - Diffusion approximation (Rigorous) comparison to MC

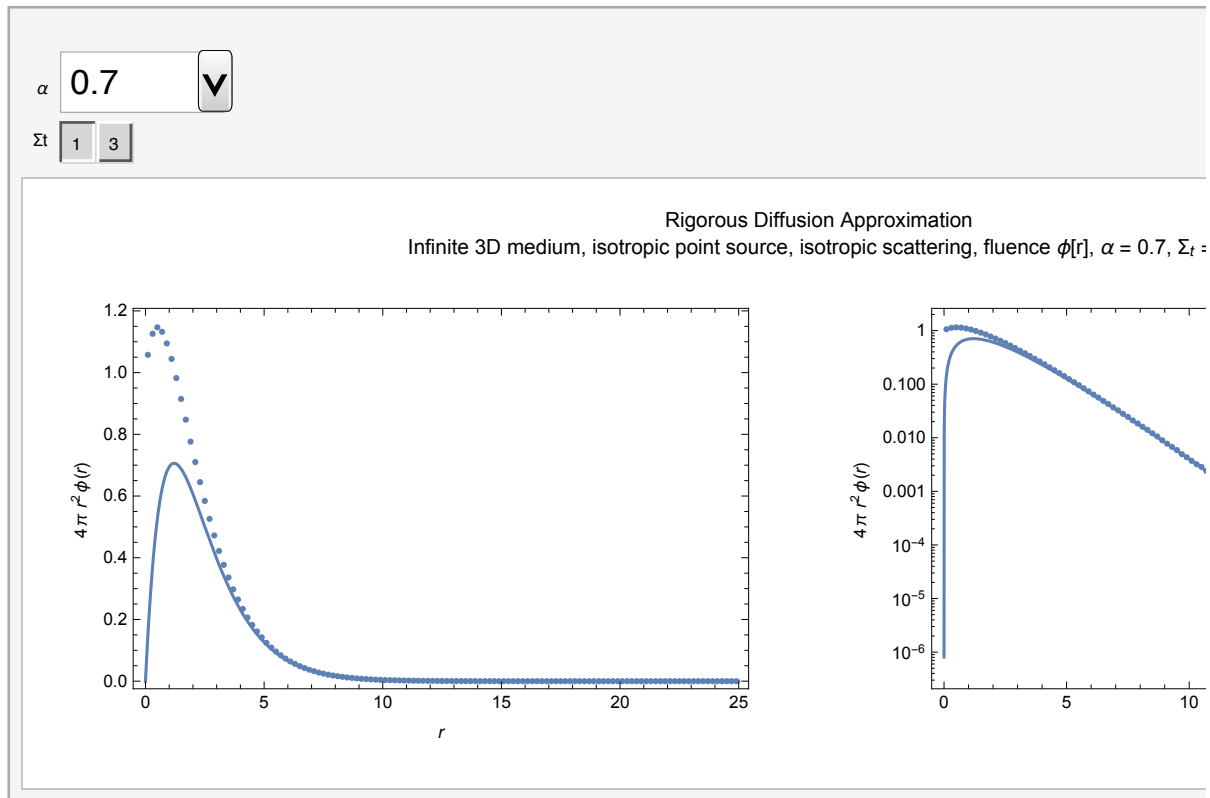
```
In[553]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, maxr, dr, points $\phi$ , plotpoints $\phi$ , logplot $\phi$ , plot $\phi$ , exact1points},
      data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma_t$  &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];

      points $\phi$  = data[[4]];

      (* divide by  $\Sigma_t$  to convert collision density into fluence *)
      plotpoints $\phi$  = inf3Disopointisoscatter`ppoints[points $\phi$ , dr, maxr,  $\Sigma_t$ ];

      plot $\phi$  = Quiet[Show[
        ListPlot[plotpoints $\phi$ , PlotRange → All, PlotStyle → PointSize[.01]],
        Plot[4 Pi r2 inf3Disopointisoscatter` $\phi$ rigorousDiffusion[r,  $\Sigma_t$ ,  $\alpha$ ],
          {r, 0, maxr}, PlotRange → All],
        Frame → True,
        FrameLabel -> {{4 Pi r2  $\phi$ [r]}, {r,}},
      ]];
      logplot $\phi$  = Quiet[Show[
        ListLogPlot[plotpoints $\phi$ , PlotRange → All, PlotStyle → PointSize[.01]],
        LogPlot[4 Pi r2 inf3Disopointisoscatter` $\phi$ rigorousDiffusion[r,  $\Sigma_t$ ,  $\alpha$ ],
          {r, 0, maxr}, PlotRange → All],
        Frame → True,
        FrameLabel -> {{4 Pi r2  $\phi$ [r]}, {r,}},
      ]];
      Show[GraphicsGrid[{{plot $\phi$ , logplot $\phi$ }}, ImageSize → 800], PlotLabel ->
        "Rigorous Diffusion Approximation\nInfinite 3D medium, isotropic
          point source, isotropic scattering, fluence  $\phi$ [r],  $\alpha$  = "<>
          ToString[ $\alpha$ ] <> ",  $\Sigma_t$  = "<> ToString[ $\Sigma_t$ ]]
    ],
    ,
    Text[
      "Uh oh! Couldn't find MC data. Try to evaluate this entire notebook and
        ensure the data path is setup correctly."
    ]
  ],
  {{ $\alpha$ , 0.7}, inf3Disopointisoscatter`alphas},
  { $\Sigma_t$ , inf3Disopointisoscatter`mutss}]
```

Out[553]=



N-th order fluence / scalar flux

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

```

In[557]:= Clear[alpha, Σt];
Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, maxr, dr, pointsφ,
      plotpointsφ, logplotφ, plotφ, exactlpoints, 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]];

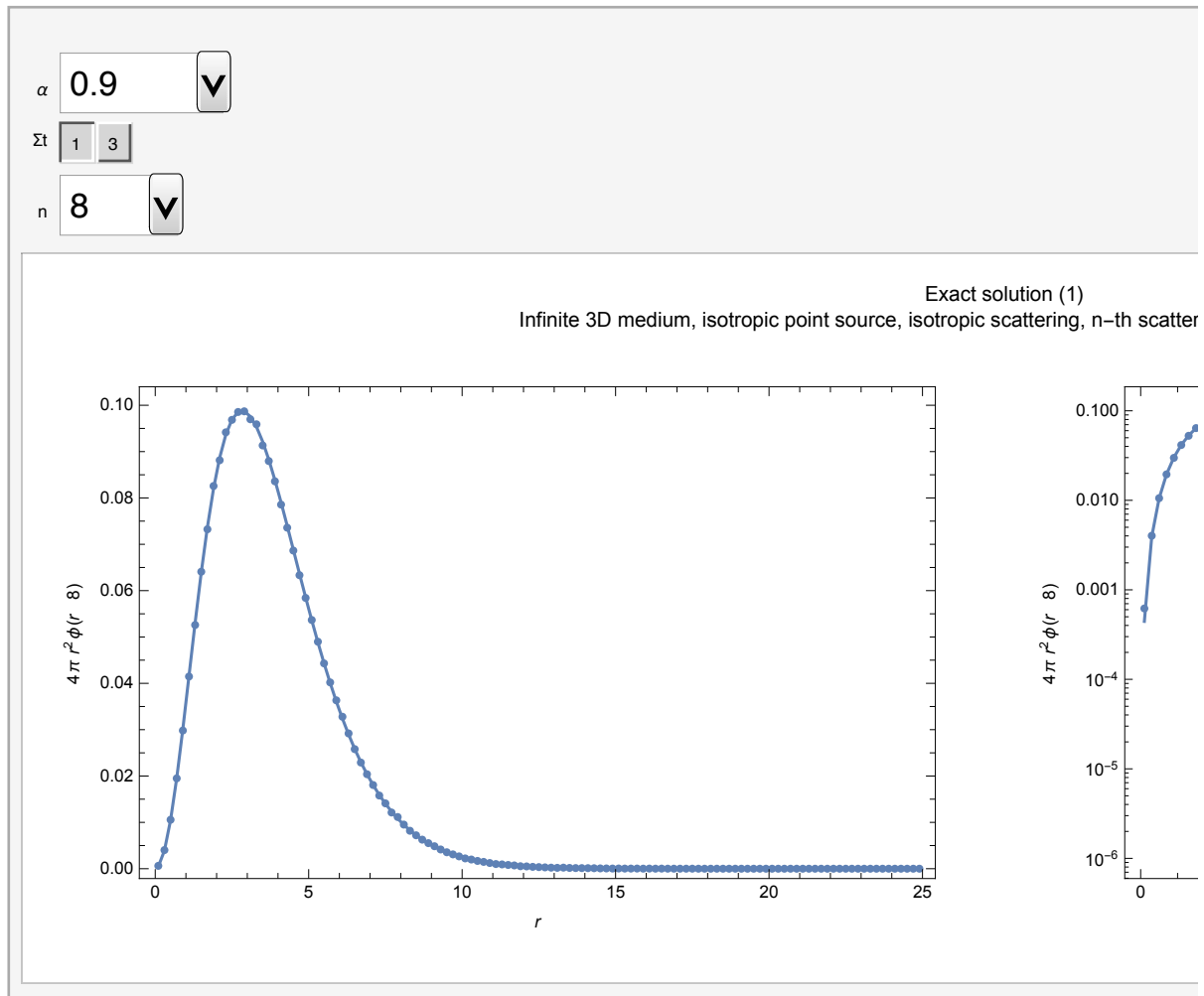
      (* divide by Σt to convert collision density into fluence *)
      plotpointsφ = inf3Disopointisoscatter`ppoints[pointsφ, dr, maxr, Σt];

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

      plotφ = Quiet[Show[
        ListPlot[plotpointsφ, PlotRange → All, PlotStyle → PointSize[.01]],
        ListPlot[exactlpoints, 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[exactlpoints, 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[558]=



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

```
In[701]:= 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]];

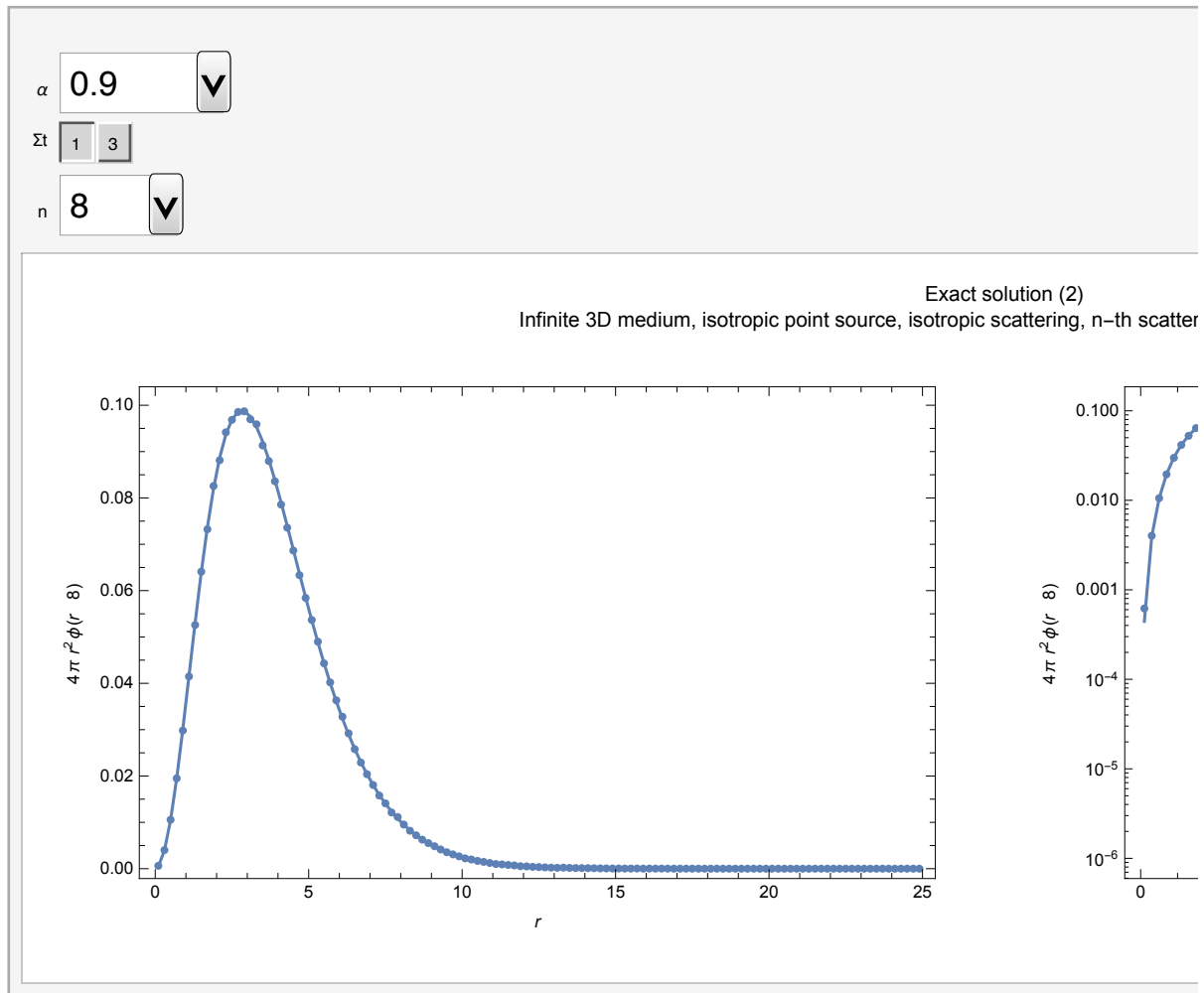
      pointsφ = data[[9 + numorders + n + 1]];

      (* 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[701]=



N-th collided Fluence - Approximations

```

Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, maxr, dr, points $\phi$ ,
      plotpoints $\phi$ , logplot $\phi$ , plot $\phi$ , exactlpoints, numorders},
      data = SelectFirst[inf3Disopointisoscatter`simulations,
        #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma t$  &][[3]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      numorders = data[[2, 13]];

      points $\phi$  = data[[9 + numorders + n + 1]];

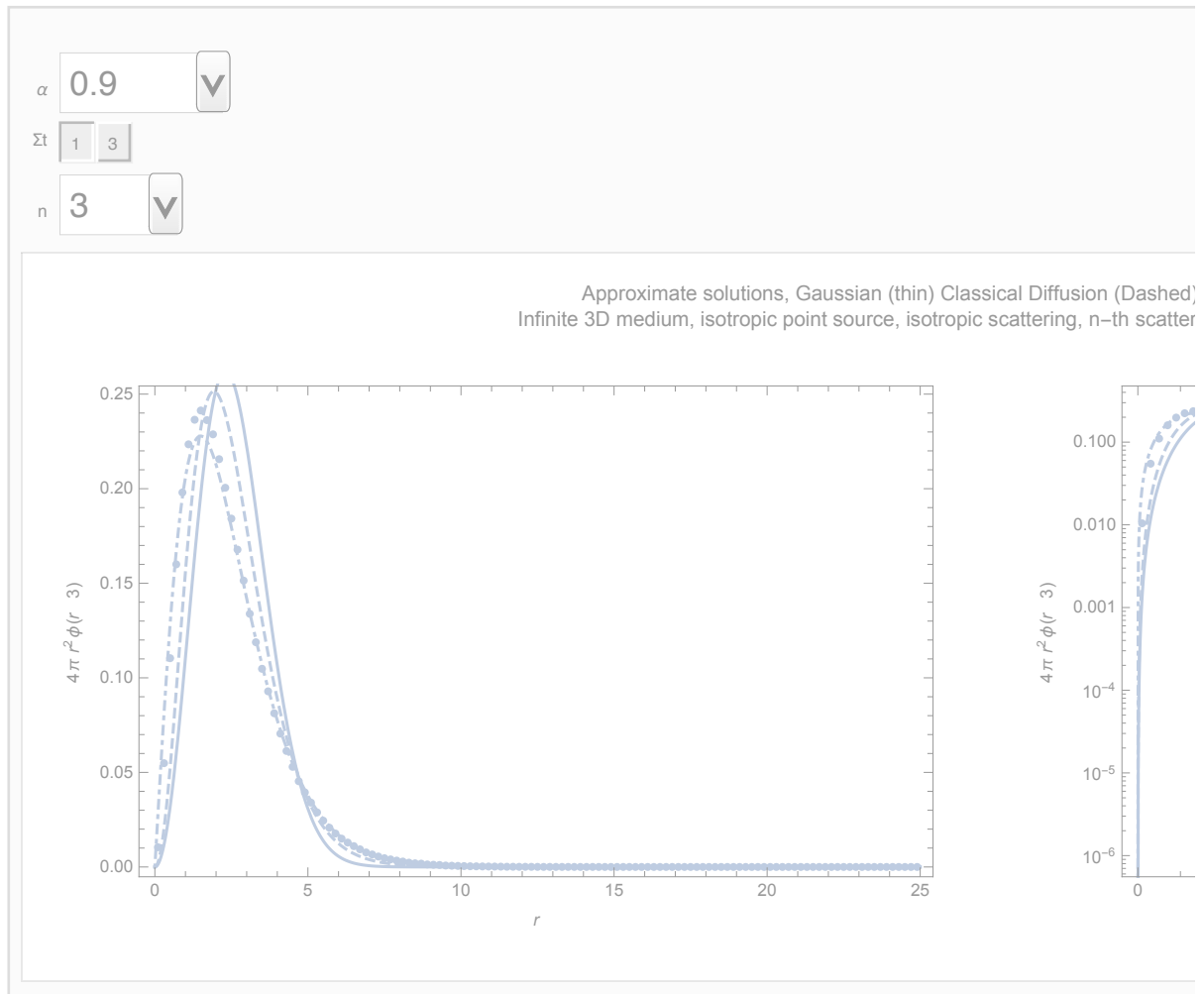
      (* divide by  $\Sigma t$  to convert collision density into fluence *)
      plotpoints $\phi$  = inf3Disopointisoscatter`ppoints[points $\phi$ , dr, maxr,  $\Sigma t$ ];

      seriesclassical =  $\alpha^n$  SeriesCoefficient[
        inf3Disopointisoscatter` $\phi$ Diffusion[r,  $\Sigma t$ , C], {C, 0, n}];
      seriesG =  $\alpha^n$  SeriesCoefficient[inf3Disopointisoscatter` $\phi$ Grosjean[r,  $\Sigma t$ , C],
        {C, 0, n}];

      plot $\phi$  = Quiet[Show[
        ListPlot[plotpoints $\phi$ , PlotRange  $\rightarrow$  All, PlotStyle  $\rightarrow$  PointSize[.01]],
        Plot[4 Pi r2 inf3Disopointisoscatter` $\phi$ Gaussian[r,  $\Sigma t$ ,  $\alpha$ , n],
          {r, 0, maxr}, PlotRange  $\rightarrow$  All],
        Plot[4 Pi r2 seriesclassical, {r, 0, maxr},
          PlotRange  $\rightarrow$  All, PlotStyle  $\rightarrow$  Dashed],
        Plot[4 Pi r2 seriesG, {r, 0, maxr}, PlotRange  $\rightarrow$  All, PlotStyle  $\rightarrow$  DotDashed],
        Frame  $\rightarrow$  True,
        FrameLabel  $\rightarrow$  {{4 Pi r2  $\phi$ [r | n],}, {r,}}
      ]];
      logplot $\phi$  = Quiet[Show[
        ListLogPlot[plotpoints $\phi$ , PlotRange  $\rightarrow$  All, PlotStyle  $\rightarrow$  PointSize[.01]],
        LogPlot[
          4 Pi r2 inf3Disopointisoscatter` $\phi$ Gaussian[r,  $\Sigma t$ ,  $\alpha$ , n], {r, 0, maxr}],
        LogPlot[4 Pi r2 seriesclassical, {r, 0, maxr},
          PlotRange  $\rightarrow$  All, PlotStyle  $\rightarrow$  Dashed],
        LogPlot[4 Pi r2 seriesG, {r, 0, maxr}, PlotRange  $\rightarrow$  All,
          PlotStyle  $\rightarrow$  DotDashed],
        Frame  $\rightarrow$  True,
        FrameLabel  $\rightarrow$  {{4 Pi r2  $\phi$ [r | n],}, {r,}}
      ]];
      Show[GraphicsGrid[{{plot $\phi$ , logplot $\phi$ }}, ImageSize  $\rightarrow$  1000],
        PlotLabel  $\rightarrow$  "Approximate solutions, Gaussian (thin) Classical Diffusion
          (Dashed) Grosjean (Dot-Dashed)\nInfinite 3D medium, isotropic
          point source, isotropic scattering, n-th scattered fluence
           $\phi$ [r|n],  $\alpha$  = "<>ToString[ $\alpha$ ]<>",  $\Sigma t$  = "<>ToString[ $\Sigma t$ ]]
      ]
    ],
    Text[
      "Uh oh! Couldn't find MC data. Try to evaluate this entire notebook and
        ensure the data path is setup correctly."
    ]
  ]
, {{ $\alpha$ , 0.9}, inf3Disopointisoscatter`alphas},
  { $\Sigma t$ , inf3Disopointisoscatter`mutss},
  {{n, 3}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
    inf3Disopointisoscatter`numcollorders, 1]]}]

```

Out[772]=



Compare moments of ϕ

```
In[524]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, nummoments,  $\phi$ moments, ks, analytic, j},
      data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma t$  &][[3]];
      nummoments = data[[2, 15]];
       $\phi$ moments = N[{ $\frac{\text{data}[[6]]}{\Sigma t}$ }];
      ks = Table[k, {k, 0, nummoments - 1}];
      analytic = Table[inf3Disopointisoscatter` $\phi m[\alpha, \Sigma t, k]$ , {k, ks}];
      j = Join[{ks}, {analytic},  $\phi$ moments];

      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`mutts}]

Out[524]=

α	0.7	<input type="button" value="v"/>
Σt	<input type="button" value="1"/>	<input type="button" value="3"/>
k	analytic	MC
0	3.33333	3.33223
1	$0. + 0. i$	6.59823
2	22.2222	22.2373
3	$(-i) \infty$	103.736
4	612.346	614.906

n-th collided moments of ϕ

```

In[526]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, nummoments,  $\phi$ moments, ks, analytic, j},
      data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma t$  &][[3]];
      nummoments = data[[2, 15]];
       $\phi$ moments = N[ $\frac{\{data[[9 + n]]\}}{\Sigma t}$ ];
      ks = Table[k, {k, 0, nummoments - 1}];
      analytic = Table[inf3Disopointisoscatter` $\phi m[\alpha, \Sigma t, k, n]$ , {k, ks}];
      j = Join[{ks}, {analytic},  $\phi$ moments];

      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."]
],
, {{ $\alpha$ , 0.95}, inf3Disopointisoscatter`alphas},
{{ $\Sigma t$ , 3}, inf3Disopointisoscatter`mut},
{{n, 11}, Range[If[NumberQ[inf3Disopointisoscatter`numcollorders],
  inf3Disopointisoscatter`numcollorders, 1]]}
]

```

Out[526]=

α	<input type="text" value="0.95"/>	<input type="button" value="v"/>
Σt	<input type="text" value="1"/>	<input type="text" value="3"/>
n	<input type="text" value="6"/>	<input type="button" value="v"/>

k	analytic	MC
0	0.245031	0.244959
1	0. + 0. i	0.268885
2	0.381159	0.380743
3	0.	0.66009
4	1.35523	1.35476

Angular Distributions

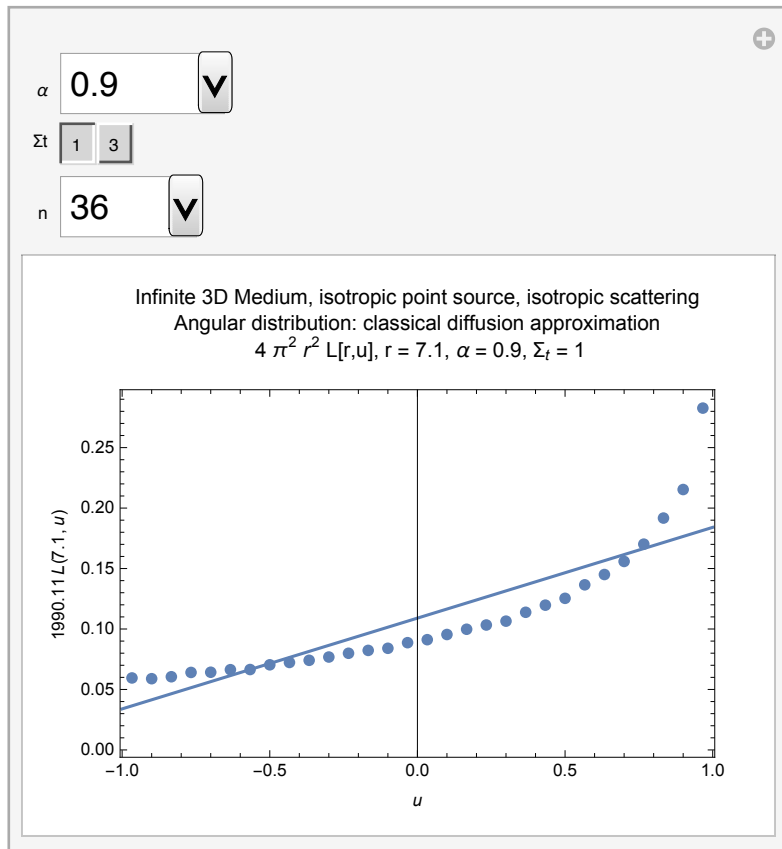
```
In[704]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, numorders, pointsu, plotpointsu, du, r, dr},
      data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma_t$  &][[3]];
      numorders = data[[2, 13]];
      du = data[[2, 9]];
      dr = data[[2, 7]];

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

      r = dr * n - 0.5 dr;

      (* divide by  $\Sigma_t$  to convert collision density into fluence *)
      plotpointsu = inf3Disopointisoscatter`ppointsu[pointsu, du,  $\Sigma_t$ ];
      Show[
        ListPlot[plotpointsu, PlotRange → All,
          Frame → True,
          FrameLabel → {{4  $\pi^2$   $r^2$  L[r, u], }, {u, }},
        Plot[4  $\pi^2$   $\pi$  inf3Disopointisoscatter`Ldiffusion[r, u,  $\Sigma_t$ ,  $\alpha$ ],
          {u, -1, 1}, PlotRange → All
        ],
        PlotLabel → "Infinite 3D Medium, isotropic point source,
          isotropic scattering\nAngular distribution: classical
          diffusion approximation\n4  $\pi^2$   $r^2$  L[r,u], r = "<>
          ToString[r]<>" ,  $\alpha$  = "<>ToString[ $\alpha$ <>" ,  $\Sigma_t$  = "<>ToString[ $\Sigma_t$ 
        ]
      ],
      Text[
        "Uh oh! Couldn't find MC data. Try to evaluate this entire notebook and
          ensure the data path is setup correctly."
      ]
    ],
    {{ $\alpha$ , 0.9}, inf3Disopointisoscatter`alphas},
    {{ $\Sigma_t$ , 1}, inf3Disopointisoscatter`mutss}, {{n, 36}, Range[If[
      NumberQ[inf3Disopointisoscatter`numr], inf3Disopointisoscatter`numr, 1]]}]
  ]
]
```

Out[704]=



Angular Distribution: Integral of Grosjean's Diffusion Approximation

```
In[705]:= Manipulate[
  If[Length[inf3Disopointisoscatter`simulations] > 0,
    Module[{data, numorders, pointsu, plotpointsu, du, r, dr},
      data = SelectFirst[
        inf3Disopointisoscatter`simulations, #[[1]] ==  $\alpha$  && #[[2]] ==  $\Sigma t$  &][[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  $\Sigma t$  to convert collision density into fluence *)
      plotpointsu = inf3Disopointisoscatter`ppointsu[pointsu, du,  $\Sigma t$ ];
      pp = Show[
        ListPlot[plotpointsu, PlotRange -> All,
          Frame -> True,
          FrameLabel -> {{4  $\pi^2 r^2 L[r, u]$ , {u}}, {u, {}}],
        Plot[4  $\pi r^2 \pi$  inf3Disopointisoscatter`Lintegral[r, u,  $\Sigma t$ ,  $\alpha$ ,
          inf3Disopointisoscatter` $\phi$ Grosjean], {u, -1, 1}, PlotRange -> All
        ],
        PlotLabel -> "Infinite 3D Medium, isotropic point source, isotropic
          scattering\nAngular distribution: Integral of Grosjean
          diffusion approximation\n 4  $\pi^2 r^2 L[r, u]$ , r = "<>
          ToString[r]<> ",  $\alpha$  = "<> ToString[ $\alpha$ <> ",  $\Sigma t$  = "<> ToString[ $\Sigma t$ 
        ]
      ],
    Text[
      "Uh oh! Couldn't find MC data. Try to evaluate this entire notebook and
        ensure the data path is setup correctly."
    ]
  ],
  {{ $\alpha$ , 0.9}, inf3Disopointisoscatter`alphas},
  {{ $\Sigma t$ , 1}, inf3Disopointisoscatter`mutst}, {{n, 36}, Range[If[
    NumberQ[inf3Disopointisoscatter`numr], inf3Disopointisoscatter`numr, 1]]}]
]
```

Out[705]=

