# Infinite 3D medium, Isotropic Point Source, Rayleigh Scattering

**Exponential Random Flight** 

This is code to accompany the book:

A Hitchhiker's Guide to Multiple Scattering

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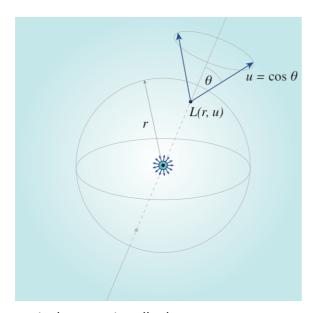
www.eugenedeon.com/hitchhikers

# 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[3200]:= SetDirectory[Import["~/.hitchhikerpath"]]

## **Notation**



c - single-scattering albedo

 $\Sigma t$  - extinction coefficient

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

 $u = \cos \theta$  - direction cosine

#### Namespace

In[3199]:= Begin["inf3DisopointRayleighscatter`"]

Out[3199]= inf3DisopointRayleighscatter`

#### Util

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

#### **Diffusion modes**

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

# **Analytical solutions**

#### Fluence: exact solution

[Grosjean 1963 - A New Approximate One-Velocity Theory for Treating both Isotropic and Anisotropic Multiple Scattering Problems, p. 37]

In[4569]= 
$$\phi exact[r_{-}, \Sigma t_{-}, c_{-}] := \frac{Exp[-r \Sigma t]}{4 \, Pi \, r^2} + \frac{c \, \Sigma t}{2 \, Pi^2 \, r} \, NIntegrate[u \left( \frac{-450 \, ArcTan[u]^2 - \frac{225 \, \left(-3 \, u + \left(3 + u^2\right) \, ArcTan[u]\right) \, \left(-3 \, u + \left(3 - 3 \, c + u^2\right) \, ArcTan[u]\right)}{4 \, u^4} \right) \, Sin[r \, \Sigma t \, u] \, , \, \{u, \, 0, \, Infinity\} \, , \, Method \rightarrow "LevinRule"]$$

In[4570]=  $\phi exact[r_{-}, \, \Sigma t_{-}, \, c_{-}, \, 1] := \frac{c \, \Sigma t}{2 \, Pi^2 \, r} \, NIntegrate[u \left( \frac{9 \, u^2 - 6 \, u \, \left(3 + u^2\right) \, ArcTan[u] + \left(9 + 6 \, u^2 + 9 \, u^4\right) \, ArcTan[u]^2}{8 \, u^6} \right) \, Sin[r \, \Sigma t \, u] \, , \, \{u, \, 0, \, Infinity\} \, , \, Method \rightarrow "LevinRule"]$ 

In[4571]=  $\phi exact[r_{-}, \, \Sigma t_{-}, \, c_{-}, \, 2] := \frac{c \, \Sigma t}{2 \, Pi^2 \, r} \, NIntegrate[u \left( \frac{1}{64 \, u^{11}} \, 3 \, \left(-9 \, u^3 \, \left(3 + u^2\right) + \left(81 \, u^2 + 54 \, u^4 + 57 \, u^6\right) \, ArcTan[u] - u \, \left(81 + 81 \, u^2 + 123 \, u^4 + 35 \, u^6\right) \, ArcTan[u]^2 + 3 \, \left(3 + 2 \, u^2 + 3 \, u^4\right)^2 \, ArcTan[u]^3\right) \, c\right)$ 

Sin[r \( \Sigma t \, u \) , \( \{u, \, 0, \, Infinity\} \) , \( Method \rightarrow "LevinRule" \)

```
ln[4572] = \phi exact[r_, \Sigma t_, c_, 3] := \frac{c \Sigma t}{2 Pi^2 r} NIntegrate[
               u\left(\frac{1}{512\,u^{16}}\,9\,\left(27\,u^4\,\left(3+2\,u^2+3\,u^4\right)-12\,u^3\,\left(27+27\,u^2+45\,u^4+13\,u^6\right)\,\mathrm{ArcTan}[u]\right.+
                          6 u^{2} (81 + 108 u^{2} + 198 u^{4} + 108 u^{6} + 49 u^{8}) ArcTan[u]^{2} - 4 u (81 + 135 u^{2} + 270 u^{4} + 108 u^{6})
                               210 u^6 + 161 u^8 + 39 u^{10}) ArcTan[u]<sup>3</sup> + 3 (3 + 2 u^2 + 3 u^4)<sup>3</sup> ArcTan[u]<sup>4</sup>) c^2
                  Sin[r Σt u], {u, 0, Infinity}, Method → "LevinRule"]
```

#### load MC data

```
In[4337]:= ppoints[xs_, dr_, maxx_] :=
        Table [ \{ dr(i) - 0.5 dr, xs[[i]] \}, \{i, 1, Length[xs] \} ] [[1;; -2]] 
In[4338]:= ppointsu[xs_, du_, \Sigmat_] :=
        Table [\{-1.0 + du(i) - 0.5 du, xs[[i]] / (2 \Sigma t)\}, \{i, 1, Length[xs]\}][[1;; -1]]
In[4339]:= fs = FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/MCdata/
              inf3D_isotropicpoint_rayleighscatter*"];
ln[4340] = index[x_] := Module[{data, <math>\alpha, \Sigma t},
           data = Import[x, "Table"];
           Σt = data[[1, 13]];
           \alpha = data[[2, 3]];
           \{\alpha, \Sigma t, data\}\};
       simulations = index /@fs;
       cs = Union[#[[1]] & /@ simulations]
Out[4342]= \{0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999\}
In[4343]:= mfps = Union[#[[2]] & /@ simulations]
Out[4343]= \{0.3, 1\}
In[4344]:= numcollorders = simulations[[1]][[3]][[2, 13]];
       maxr = simulations[[1]][[3]][[2, 5]];
       dr = simulations[[1]][[3]][[2, 7]];
       numr = Floor[maxr/dr];
```

# Compare MC and deterministic

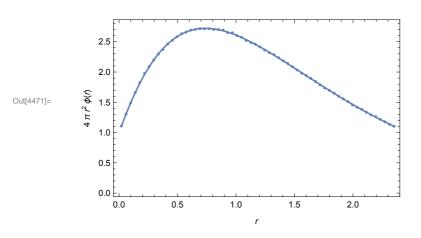
#### Mean Track Length

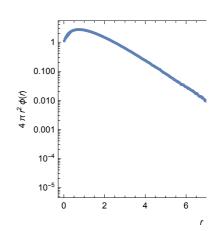
```
ln[4373] =  { {ActionMenu["Set c", "c = "<> ToString[#] \Rightarrow (c = #;) & /@ cs], Dynamic[c]},
         {ActionMenu["Set mfp", "mfp = " <> ToString[#] \Rightarrow (mfp = #;) & /@ mfps],
          Dynamic[mfp] } }
Out[4373]= { { Set c |, 0.95}, { Set mfp |, 0.3}}
```

## Fluence - Exact solution comparison to MC

```
In[4463]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &][[-1]];
      maxr = data[[2, 5]];
      dr = data[[2, 7]];
      pointsFluence = ppoints[data[[6]], dr, maxr];
      exact1FluenceShallow =
         Quiet[{\#[[1]], 4 Pi \#[[1]]^2 \phi exact[\#[[1]], 1/mfp, c]}] & /@
          pointsFluence[[1;;60]];
      exact1Fluence = Quiet[{\#[[1]], 4 Pi \#[[1]]^2 \phi exact[\#[[1]], 1/mfp, c]}] & /@
          pointsFluence[[1;;-1;;10]];
      plotφshallow = Quiet[Show[
           ListPlot[pointsFluence[[1;; 60]],
            PlotRange → All, PlotStyle → PointSize[.01]],
           ListPlot[exact1FluenceShallow, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
          ]];
      logplotφ = Quiet[Show[
           ListLogPlot[pointsFluence, PlotRange → All, PlotStyle → PointSize[.01]],
           ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
           Frame → True,
           FrameLabel -> \{\{4 \operatorname{Pir}^2 \phi[r],\}, \{r,\}\}
      Show[GraphicsGrid[{{plotφshallow, logplotφ}}, ImageSize → 800], PlotLabel ->
         "Exact solution\nInfinite 3D, isotropic point source, Rayleigh scattering,
             fluence \phi[r], c = " \Leftrightarrow ToString[c] \Leftrightarrow ", <math>\Sigma_t = " \Leftrightarrow ToString[1/mfp]
```

**Exact solution** Infinite 3D, isotropic point source, Rayleigh scattering, fluence  $\phi[r]$ , c = 0.95,  $\Sigma_t$  = 3.33333



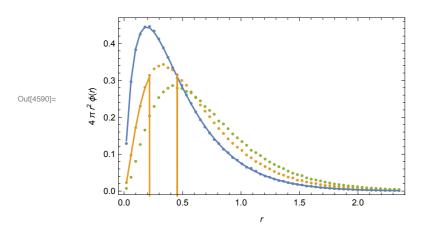


#### N-th collided Fluence - Exact solution comparison to MC

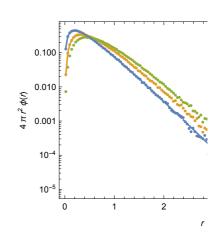
```
ln[4501]:= { {ActionMenu["Set c", "c = "<> ToString[#] :> (c = #;) & /@ cs], Dynamic[c]},
        {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
         Dynamic[mfp] } }
Out[4501] = \{ \{ Set c | , 0.95 \}, \{ Set mfp | , 0.3 \} \}
In[4573]:= data = SelectFirst[simulations, #[[1]] == c && #[[2]] == mfp &] [[3]];
       maxr = data[[2, 5]];
       dr = data[[2, 7]];
       fluencei1 = 3 numcollorders + 15 + 1;
       fluencei2 = 3 numcollorders + 15 + 2;
       fluencei3 = 3 numcollorders + 15 + 3;
       pointsFluence1 = ppoints[data[[fluencei1]], dr, maxr];
       pointsFluence2 = ppoints[data[[fluencei2]], dr, maxr];
       pointsFluence3 = ppoints[data[[fluencei3]], dr, maxr];
       exact1Fluence1Shallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact}[\#[[1]], 1/\text{mfp}, c, 1]\}] & /@
           pointsFluence1[[1;; 60]];
       exact1Fluence1 = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact}[\#[[1]], 1/\text{mfp, c, 1}]\}] & /@
           pointsFluence[[61;; -1;; 10]];
       exact1Fluence2Shallow =
         Quiet[{\#[[1]], 4 Pi \#[[1]]^2 \phiexact[\#[[1]], 1/mfp, c, 2]}] & /@
           pointsFluence1[[1;; 60]];
       exact1Fluence2 = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact}[\#[[1]], 1/\text{mfp}, c, 2]\}] & /@
           pointsFluence[[61;; -1;; 10]];
       exact1Fluence3Shallow =
         Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact}[\#[[1]], 1/mfp, c, 3]\}] & /@
           pointsFluence1[[1;; 60]];
       exact1Fluence3 = Quiet[\{\#[[1]], 4 \text{ Pi } \#[[1]]^2 \phi \text{ exact}[\#[[1]], 1/\text{mfp}, c, 3]\}] & /@
           pointsFluence[[61;; -1;; 10]];
       plotφshallow = Quiet[Show[
            ListPlot[{pointsFluence1[[1;; 60]], pointsFluence2[[1;; 60]],
               pointsFluence3[[1;; 60]]}, PlotRange → All, PlotStyle → PointSize[.01]],
            ListPlot[{exact1Fluence1Shallow, exact1Fluence2Shallow,
               exact1Fluence3Shallow}, PlotRange → All, Joined → True],
            Frame → True,
            FrameLabel -> \{\{4 \, \text{Pi} \, r^2 \, \phi[r], \}, \, \{r, \}\}
           ]];
       logplotφ = Quiet[Show[
            ListLogPlot[{pointsFluence1, pointsFluence2, pointsFluence3},
             PlotRange → All, PlotStyle → PointSize[.01]],
            ListLogPlot[{exact1Fluence1Shallow, exact1Fluence2Shallow,
               exact1Fluence3Shallow}, PlotRange → All, Joined → True],
```

```
ListLogPlot[{exact1Fluence1, exact1Fluence2, exact1Fluence3},
      PlotRange → All, Joined → True],
     Frame → True,
     FrameLabel -> \{\{4 \, \text{Pi} \, r^2 \, \phi[r], \}, \, \{r,\}\}
Show[GraphicsGrid[{{plot\phishallow, logplot\phi}}, ImageSize \rightarrow 800],
 PlotLabel -> "Exact solution (Fourier)\nInfinite 3D medium, isotropic point
      source, Rayleigh scattering, n-th scattered fluence \phi[r]" <>
    ToString[collisionOrder] <> "], c =" <> ToString[c] <>
    ", \Sigma_t = " \Leftrightarrow ToString[1/mfp]]
```

Exact solution (Fourier) Infinite 3D medium, isotropic point source, Rayleigh scattering, n-th scattered fluence  $\phi[r|1]$ , c =0.95,  $\Sigma_t$ 



sims1 = Select[simulations, #[[2]] == mfp &];



#### Compare moments of $\phi$

```
ln[4361]:= { {ActionMenu["Set c", "c = " <> ToString[#] :> (c = #;) & /@cs], Dynamic[c]},
        {ActionMenu["Set mfp", "mfp = " <> ToString[#] → (mfp = #;) & /@ mfps],
         Dynamic[mfp] }}
Out[4361]= {{ Set c |, 0.95}, { Set mfp |, 0.3}}
       mfp 1
In[4362]:= mfp = 1;
```

```
In[4364]:= 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
                  }],
               \label{eq:logPlot} \text{LogPlot}\big[\big\{\frac{\text{mfp}}{1-c}\,,\,\,\frac{2\,\text{mfp}^3}{\left(-1+c\right)^2}\,,\,-\frac{120\,\left(-2+c\right)\,\text{mfp}^5}{\left(-10+c\right)\,\left(-1+c\right)^3}\,,\,\,\frac{720\,\left(100+c\,\left(-116+37\,c\right)\right)\,\text{mfp}^7}{\left(-10+c\right)^2\,\left(-1+c\right)^4}\,,
                     \frac{5760 \left(49\,000+c \left(-93\,580+c \left(64\,230+c \left(-15\,937+256\,c\right)\right)\right)\right) \, \text{mfp}^9}{7 \, \left(-10+c\right)^3 \, \left(-1+c\right)^5}\right\},
                  \{c, 0, .999\}, PlotRange \rightarrow All
             1
                10<sup>19</sup>
                10<sup>15</sup>
                10<sup>11</sup>
Out[4364]=
                 10<sup>7</sup>
              1000.0
                 0.1
                                                      0.2
                                                                                        0.4
                                                                                                                                                            0.8
                                                                                                                          0.6
```

#### mfp 0.3

```
In[4365]:= mfp = 0.3;
      sims1 = Select[simulations, #[[2]] == mfp &];
```

```
In[4367]:= Show
               ListLogPlot[{
                   {\#[[-1, 2, 3]], \#[[-1, 10, 1]]} \& /@ sims1,
                   {\#[[-1, 2, 3]], \#[[-1, 10, 3]]} \& /@ sims1,
                   {\#[[-1, 2, 3]], \#[[-1, 10, 5]]} \& /@ sims1,
                   {\#[[-1, 2, 3]], \#[[-1, 10, 7]]} \& /@ sims1,
                   {\#[[-1, 2, 3]], \#[[-1, 10, 9]]} \& /@ sims1
                 }],
              LogPlot\left[\left\{\frac{mfp}{1-c},\,\frac{2\,mfp^3}{\left(-1+c\right)^2},\,-\frac{120\,\left(-2+c\right)\,mfp^5}{\left(-10+c\right)\,\left(-1+c\right)^3},\,\frac{720\,\left(100+c\,\left(-116+37\,c\right)\right)\,mfp^7}{\left(-10+c\right)^2\,\left(-1+c\right)^4},\right.
                   \frac{5760 \, \left(49\,000+c \, \left(-\,93\,580+c \, \left(64\,230+c \, \left(-\,15\,937+256 \, c\right)\right)\right)\right) \, \text{mfp}^9}{7 \, \left(-\,10+c\right)^3 \, \left(-\,1+c\right)^5}\right\},
                 \{c, 0, .999\}, PlotRange \rightarrow All
            1
             10<sup>11</sup>
              10<sup>7</sup>
Out[4367]=
             1000
                                                 0.2
                                                                                 0.4
                                                                                                                  0.6
                                                                                                                                                  8.0
```