Infinite 3D medium, Isotropic Point Source, Lambert Sphere Scattering

Exponential Random Flight

This is code to accompany the book:

A Hitchhiker's Guide to Multiple Scattering

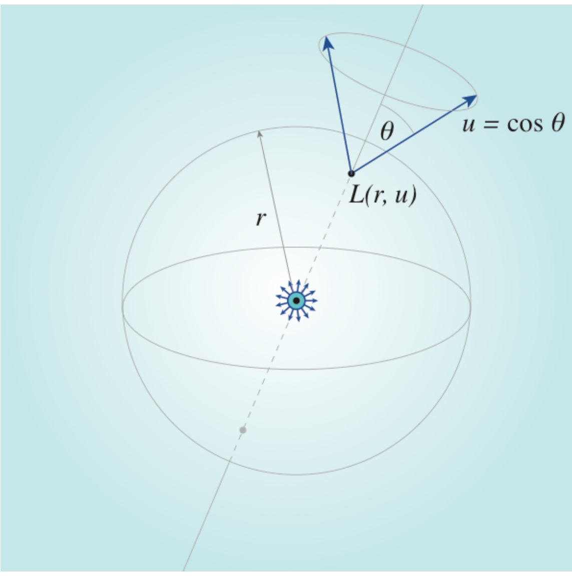
www.eugenedeon.com/hitchhikers

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[•]:= 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[6633]:=
```
Begin["inf3DisopointLambertSpherescatter`"]
```
Out[6633]=
```
inf3DisopointLambertSpherescatter`
```

Util

In[4628]:=
$$\texttt{SA[d\_, r\_] := d}\ \frac{\texttt{Pi}^{d/2}}{\texttt{Gamma}\left[\frac{d}{2}+1\right]}\ r^{d-1}$$

Diffusion modes

In[4629]:=
$$\texttt{diffusionMode[v\_, d\_, r\_] :=}\ (2\,\pi)^{-d/2}\ r^{1-\frac{d}{2}}\ v^{-1-\frac{d}{2}}\ \texttt{BesselK}\left[\frac{1}{2}\,(-2+d),\ \frac{r}{v}\right]$$

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[6634]:=
$$\texttt{\phi exactTruncatedFourierOrder3[r\_, \Sigma t\_, c\_] :=}\ \frac{\texttt{Exp}[-r\,\Sigma t]}{4\,\texttt{Pi}\,r^2}+\frac{c\,\Sigma t}{2\,\texttt{Pi}^2\,r}\ \texttt{NIntegrate}\Big[$$
$$u\,\Big(\big(u^2\,(135+60\,c+256\,u^2)+\texttt{ArcTan}[u]\,\big(15\,(-2+c)\,(9+4\,c)\,u+(-602+236\,c)\,u^3+(-15\,(-1+c)\,(9+4\,c)+(346-c\,(281+20\,c))\,u^2+207\,u^4)\,\texttt{ArcTan}[u]\big)\big)\Big/$$
$$\big(u\,(-15\,(-1+c)\,c\,(9+4\,c)\,u+(301-256\,c)\,c\,u^3+192\,u^5+c\,(15\,(-1+c)\,(9+4\,c)+(-346+c\,(281+20\,c))\,u^2-207\,u^4)\,\texttt{ArcTan}[u])\big)\Big)$$
$$\texttt{Sin}[r\,\Sigma t\,u],\ \{u,\ 0,\ \texttt{Infinity}\},\ \texttt{Method}\rightarrow\texttt{"LevinRule"}\Big]$$

```
In[4980]:= ϕexactTruncatedFourierOrder5[r_, Σt_, c_] := Exp[-r Σt]/(4 Pi r^2) +
  (c Σt)/(2 Pi^2 r) NIntegrate[u ((u^2 (-700 c^2 (21 + 11 u^2) + 35 c (5775 + 4753 u^2 + 16 704 u^4) +
          48 (11 025 + 11 550 u^2 + 28 945 u^4 + 49 152 u^6)) + u (-700 c^3 (21 + 11 u^2) + 35 c^2
           (6615 + 5333 u^2 + 16 740 u^4) - 288 (3675 + 5075 u^2 + 10 605 u^4 + 19 429 u^6) +
          2 c (62 475 + 82 670 u^2 + 94 185 u^4 + 1 084 896 u^6)) ArcTan[u] +
       3 (140 c^3 (35 + 30 u^2 + 3 u^4) - 7 c^2 (10 325 + 11 730 u^2 + 29 685 u^4 + 9024 u^6) -
          c (109 025 + 169 365 u^2 + 304 815 u^4 + 869 739 u^6) +
          48 (3675 + 6300 u^2 + 11 970 u^4 + 22 684 u^6 + 13 275 u^8)) ArcTan[u]^2) /
     (u (u (1 769 472 u^8 + 700 c^4 (21 + 11 u^2) - 35 c^3 (6195 + 4973 u^2 + 16 704 u^4) +
            144 c (3675 + 5075 u^2 + 10 605 u^4 + 19 429 u^6) -
            c^2 (327 075 + 399 070 u^2 + 810 495 u^4 + 2 359 296 u^6)) -
         3 c (140 c^3 (35 + 30 u^2 + 3 u^4) - 7 c^2 (10 325 + 11 730 u^2 + 29 685 u^4 + 9024 u^6) -
            c (109 025 + 169 365 u^2 + 304 815 u^4 + 869 739 u^6) +
            48 (3675 + 6300 u^2 + 11 970 u^4 + 22 684 u^6 + 13 275 u^8)) ArcTan[u]))
    Sin[r Σt u], {u, 0, Infinity}, Method → "LevinRule"]
```

In[4981]:=
```
ϕexactTruncatedFourierOrder7[r_, Σt_, c_] :=
  Exp[-r Σt]/(4 Pi r^2) + (c Σt)/(2 Pi^2 r) NIntegrate[u ((u^2 (140 140 c^3 (165 + 170 u^2 + 33 u^4) -
            77 c^2 (177 101 925 + 271 313 770 u^2 + 205 154 145 u^4 + 58 729 024 u^6) +
            112 c (1 627 701 075 + 2 990 582 595 u^2 + 2 541 654 225 u^4 + 998 391 449
                u^6 + 2 162 822 400 u^8) + 3072 (156 080 925 + 321 621 300 u^2 +
              298 676 070 u^4 + 138 244 260 u^6 + 191 491 237 u^8 + 314 572 800 u^10)) +
        u (140 140 c^4 (165 + 170 u^2 + 33 u^4) - 77 c^3 (177 702 525 + 272 032 670 u^2 +
              205 350 705 u^4 + 58 735 524 u^6) + 14 c^2 (14 969 729 775 + 27 232 560 355
                u^2 + 22 999 478 535 u^4 + 8 921 729 839 u^6 + 17 350 020 000 u^8) -
            92 160 (10 405 395 + 24 909 885 u^2 + 26 133 954 u^4 + 14 432 110 u^6 +
              14 752 395 u^8 + 24 914 165 u^10) + 32 c (3 589 861 275 + 8 363 415 060 u^2 +
              8 389 598 910 u^4 + 4 353 077 036 u^6 + 2 659 995 975 u^8 + 27 763 977 600 u^10))
         ArcTan[u] - 5 (20 020 c^4 (231 + 315 u^2 + 105 u^4 + 5 u^6) -
            77 c^3 (35 480 445 + 66 151 449 u^2 + 55 997 235 u^4 + 22 249 895 u^6 + 1 725 120 u^8) +
            48 c (1 238 242 005 + 3 176 672 499 u^2 + 3 513 643 210
                u^4 + 2 065 779 870 u^6 + 1 757 994 945 u^8 + 4 460 927 055 u^10) +
            c^2 (39 187 873 725 + 84 226 438 296 u^2 + 80 326 759 590 u^4 +
              38 796 268 280 u^6 + 52 992 099 405 u^8 + 15 584 071 680 u^10) -
            46 080 (2 081 079 + 5 675 670 u^2 + 6 702 465 u^4 + 4 282 740 u^6 +
              3 617 145 u^8 + 5 848 054 u^10 + 3 399 375 u^12)) ArcTan[u]^2) /
      (u (u (724 775 731 200 u^12 - 140 140 c^5 (165 + 170 u^2 + 33 u^4) +
              77 c^4 (177 402 225 + 271 623 170 u^2 + 205 214 205 u^4 + 58 729 024 u^6) -
              7 c^3 (27 991 338 375 + 50 831 295 515 u^2 + 42 920 610 645 u^4 + 16 619 786 953
                  u^6 + 34 605 158 400 u^8) + 46 080 c (10 405 395 + 24 909 885 u^2 +
                26 133 954 u^4 + 14 432 110 u^6 + 14 752 395 u^8 + 24 914 165 u^10) -
              16 c^2 (18 573 630 075 + 41 458 877 460 u^2 + 40 536 011 670 u^4 +
                20 295 123 772 u^6 + 21 838 535 775 u^8 + 60 397 977 600 u^10)) +
          5 c (20 020 c^4 (231 + 315 u^2 + 105 u^4 + 5 u^6) - 77 c^3 (35 480 445 +
                66 151 449 u^2 + 55 997 235 u^4 + 22 249 895 u^6 + 1 725 120 u^8) +
              48 c (1 238 242 005 + 3 176 672 499 u^2 + 3 513 643 210 u^4 +
                2 065 779 870 u^6 + 1 757 994 945 u^8 + 4 460 927 055 u^10) +
              c^2 (39 187 873 725 + 84 226 438 296 u^2 + 80 326 759 590 u^4 +
                38 796 268 280 u^6 + 52 992 099 405 u^8 + 15 584 071 680 u^10) -
              46 080 (2 081 079 + 5 675 670 u^2 + 6 702 465 u^4 + 4 282 740 u^6 +
                3 617 145 u^8 + 5 848 054 u^10 + 3 399 375 u^12)) ArcTan[u])))
    Sin[r Σt u], {u, 0, Infinity}, Method → "LevinRule"]
```

Rigorous asymptotic diffusion

In[6670]:=
```
Clear[c, b, g, x, v];
grosjeanΔ = buildΔ4[3] /. A[0] → 1 /. A[1] → -4/3 /. A[2] → 5/16;
dgrosjeanΔ = D[grosjeanΔ /. u → I v, c];
xpsolve = Solve[D[grosjeanΔ == 0 /. u → I x[c], c], x'[c]][[1, 1, -1]];
grosjeang = buildg4[3] /. A[0] → 1 /. A[1] → -4/3 /. A[2] → 5/16 /. u → I v;
```

In[6646]:=
```
grosjeang (xpsolve x[c] 2 /. x[c] → v) / dgrosjeanΔ /.
  Solve[grosjeanΔ == 0 /. u → I v, ArcTanh[v]] // FullSimplify
```

Out[6646]=
$$\left\{-\left(\left(18432\, v^6 \left(-1+v^2\right)\right) \Big/ \left(c \left(25 (-16+c) (-1+c)^2 (9+4c)^2 + 2 (-1+c) (9+4c) \left(-4568 + c (3283+160c)\right) v^2 - 9 \left(6640 + c (-7417+1152c)\right) v^4 + 9936 v^6\right)\right)\right)\right\}$$

In[6647]:=
```
grosjeanΔ /. u → I V
```

Out[6647]=
$$1+\frac{45 c}{64 V^4}-\frac{25 c^2}{64 V^4}-\frac{5 c^3}{16 V^4}-\frac{301 c}{192 V^2}+\frac{4 c^2}{3 V^2}-\frac{45 c \,\text{ArcTanh}[V]}{64 V^5}+\frac{25 c^2 \,\text{ArcTanh}[V]}{64 V^5}+\frac{5 c^3 \,\text{ArcTanh}[V]}{16 V^5}+\frac{173 c \,\text{ArcTanh}[V]}{96 V^3}-\frac{281 c^2 \,\text{ArcTanh}[V]}{192 V^3}-\frac{5 c^3 \,\text{ArcTanh}[V]}{48 V^3}-\frac{69 c \,\text{ArcTanh}[V]}{64 V}$$

In[6648]:=
```
LSv0inv[c_] := ReplaceAll[Abs[V],
  FindRoot[1 + 45 c/(64 V^4) - 25 c^2/(64 V^4) - 5 c^3/(16 V^4) - 301 c/(192 V^2) + 4 c^2/(3 V^2) - 45 c ArcTanh[V]/(64 V^5) +
    25 c^2 ArcTanh[V]/(64 V^5) + 5 c^3 ArcTanh[V]/(16 V^5) + 173 c ArcTanh[V]/(96 V^3) - 281 c^2 ArcTanh[V]/(192 V^3) -
    5 c^3 ArcTanh[V]/(48 V^3) - 69 c ArcTanh[V]/(64 V), {V, 0.8}]];
```

In[6676]:=
```
ϕrigourousDiffusion[r_, Σt_, c_] :=
  Σt/(4 Pi r) (-((18432 #1^6 (-1 + #1^2)) / (c (25 (-16 + c) (-1 + c)^2 (9 + 4 c)^2 +
        2 (-1 + c) (9 + 4 c) (-4568 + c (3283 + 160 c)) #1^2 -
        9 (6640 + c (-7417 + 1152 c)) #1^4 + 9936 #1^6)))) Exp[-# r Σt] &[LSv0inv[c]]
```

load MC data

In[4982]:=
```
ppoints[xs_, dr_, maxx_] :=
  Table[{dr (i) - 0.5 dr, xs[[i]]}, {i, 1, Length[xs]}][[1 ;; -2]]
```

In[4983]:=
```
ppointsu[xs_, du_, Σt_] :=
  Table[{-1.0 + du (i) - 0.5 du, xs[[i]] / (2 Σt)}, {i, 1, Length[xs]}][[1 ;; -1]]
```

In[4984]:=
```
fs = FileNames["code/3D_medium/infinite3Dmedium/Isotropicpointsource/MCdata/
    inf3D_isotropicpoint_LSscatter*"];
```

In[4985]:=
```
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[4987]=
```
{0.01, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.95, 0.99, 0.999}
```

In[4988]:=
```
mfps = Union[#[[2]] & /@ simulations]
```

Out[4988]=
```
{0.3, 1}
```

In[4989]:=
```
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

Fluence - Exact solution comparison to MC

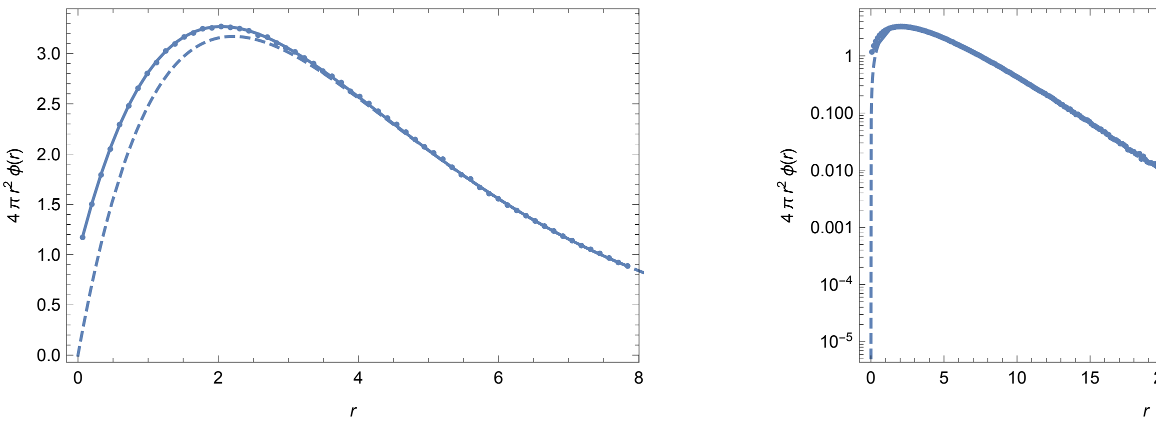
In[4670]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :→ (c = #;) & /@ cs], Dynamic[c]},
 {ActionMenu["Set mfp", "mfp = " <> ToString[#] :→ (mfp = #;) & /@ mfps],
  Dynamic[mfp]}}
```

Out[4670]=
```
{{Set c, 0.95}, {Set mfp, 1}}
```

In[6695]:=
```
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 ϕexactTruncatedFourierOrder3[#[[1]],
       1/mfp, c]}] & /@ pointsFluence[[1 ;; 60]];
exact1Fluence = Quiet[{#[[1]], 4 Pi #[[1]]^2 ϕexactTruncatedFourierOrder3[
       #[[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],
    Plot[4 Pi r^2 ϕrigourousDiffusion[r, 1/mfp, c],
     {r, 0, maxr}, PlotStyle → Dashed, PlotRange → All],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
logplotϕ = Quiet[Show[
    ListLogPlot[pointsFluence, PlotRange → All, PlotStyle → PointSize[.01]],
    ListLogPlot[exact1Fluence, PlotRange → All, Joined → True],
    LogPlot[4 Pi r^2 ϕrigourousDiffusion[r, 1/mfp, c],
     {r, 0, maxr}, PlotStyle → Dashed, PlotRange → All],
    Frame → True,
    FrameLabel -> {{4 Pi r^2 ϕ[r],}, {r,}}
   ]];
Show[GraphicsGrid[{{plotϕshallow, logplotϕ}}, ImageSize → 800],
 PlotLabel -> "Exact solution
     (continuous) and Rigorous Asymptotic Diffusion (dashed)\nInfinite
     3D, isotropic point source, Lambert-Sphere scattering, fluence
     ϕ[r], c = " <> ToString[c] <> ", Σt = " <> ToString[1/mfp]]
```

Out[6703]=

Exact solution (continuous) and Rigorous Asymptotic Diffusion (dashed)
Infinite 3D, isotropic point source, Lambert–Sphere scattering, fluence ϕ[r], c = 0.95, Σ_t = 1



Compare moments of ϕ

In[4231]:=
```
{{ActionMenu["Set c", "c = " <> ToString[#] :→ (c = #;) & /@ cs], Dynamic[c]},
 {ActionMenu["Set mfp", "mfp = " <> ToString[#] :→ (mfp = #;) & /@ mfps],
  Dynamic[mfp]}}
```

Out[4231]= {{Set c, 0.95}, {Set mfp, 0.3}}

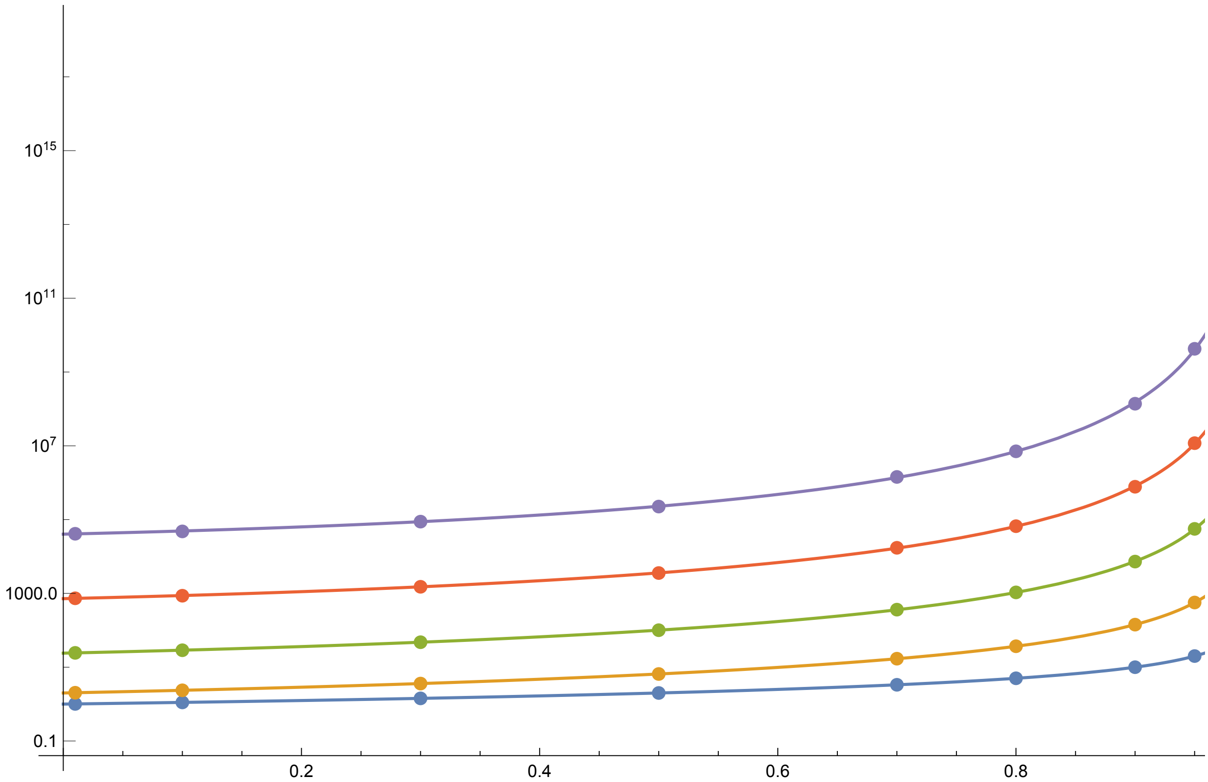
mfp 1

In[4245]:=
```
mfp = 1;
sims1 = Select[simulations, #[[2]] == mfp &];
```

In[4254]:=
```
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[{mfp/(1 - c), -3! mfp mfp^2/((-3 - 4c/3) (-1 + c)^2),
   5! mfp ((9 - 69c/16) mfp^4)/((-3 - 4c/3)^2 (-5 + 5c/16) (-1 + c)^3), mfp 7! ((-675 + 5691c/8 - 36399c^2/256 - 48 c^3) mfp^6)/(7 (-3 - 4c/3)^3 (-5 + 5c/16)^2 (-1 + c)^4),
   mfp 9! ((-496125 + 52729425c/64 - 367391171c^2/1024 - 1099685881c^3/16384 + 11363604819c^4/262144 + 312487c^5/32 - 329 c^6) mfp^8)/
    (49 (-3 - 4c/3)^4 (-9 + c/64) (-5 + 5c/16)^3 (-1 + c)^5)}, {c, 0, .999}, PlotRange → All]
]
```

$$\texttt{LogPlot}\Big[\Big\{\frac{mfp}{1-c},\ -3!\,mfp\,\frac{mfp^2}{\left(-3-\frac{4c}{3}\right)(-1+c)^2},\ 5!\,mfp\,\frac{\left(9-\frac{69c}{16}\right)mfp^4}{\left(-3-\frac{4c}{3}\right)^2\left(-5+\frac{5c}{16}\right)(-1+c)^3},\ mfp\,7!\,\frac{\left(-675+\frac{5691c}{8}-\frac{36399c^2}{256}-48c^3\right)mfp^6}{7\left(-3-\frac{4c}{3}\right)^3\left(-5+\frac{5c}{16}\right)^2(-1+c)^4},$$
$$mfp\,9!\,\left(\left(-496125+\frac{52729425c}{64}-\frac{367391171c^2}{1024}-\frac{1099685881c^3}{16384}+\frac{11363604819c^4}{262144}+\frac{312487c^5}{32}-329c^6\right)mfp^8\right)\Big/\left(49\left(-3-\frac{4c}{3}\right)^4\left(-9+\frac{c}{64}\right)\left(-5+\frac{5c}{16}\right)^3(-1+c)^5\right)\Big\},\ \{c,0,.999\},\ \texttt{PlotRange}\to\texttt{All}\Big]$$

Out[4254]=



mfp 0.3

In[4255]:=
```
mfp = 0.3;
sims1 = Select[simulations, #[[2]] == mfp &];
```

In[4257]:=
```
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
  }],
```

$$\text{LogPlot}\Big[\Big\{\frac{\text{mfp}}{1-c},\ -3!\,\text{mfp}\,\frac{\text{mfp}^2}{\left(-3-\frac{4c}{3}\right)(-1+c)^2},$$

$$5!\,\text{mfp}\,\frac{\left(9-\frac{69c}{16}\right)\text{mfp}^4}{\left(-3-\frac{4c}{3}\right)^2\left(-5+\frac{5c}{16}\right)(-1+c)^3},\ \text{mfp}\,7!\,\frac{\left(-675+\frac{5691c}{8}-\frac{36399c^2}{256}-48c^3\right)\text{mfp}^6}{7\left(-3-\frac{4c}{3}\right)^3\left(-5+\frac{5c}{16}\right)^2(-1+c)^4},$$

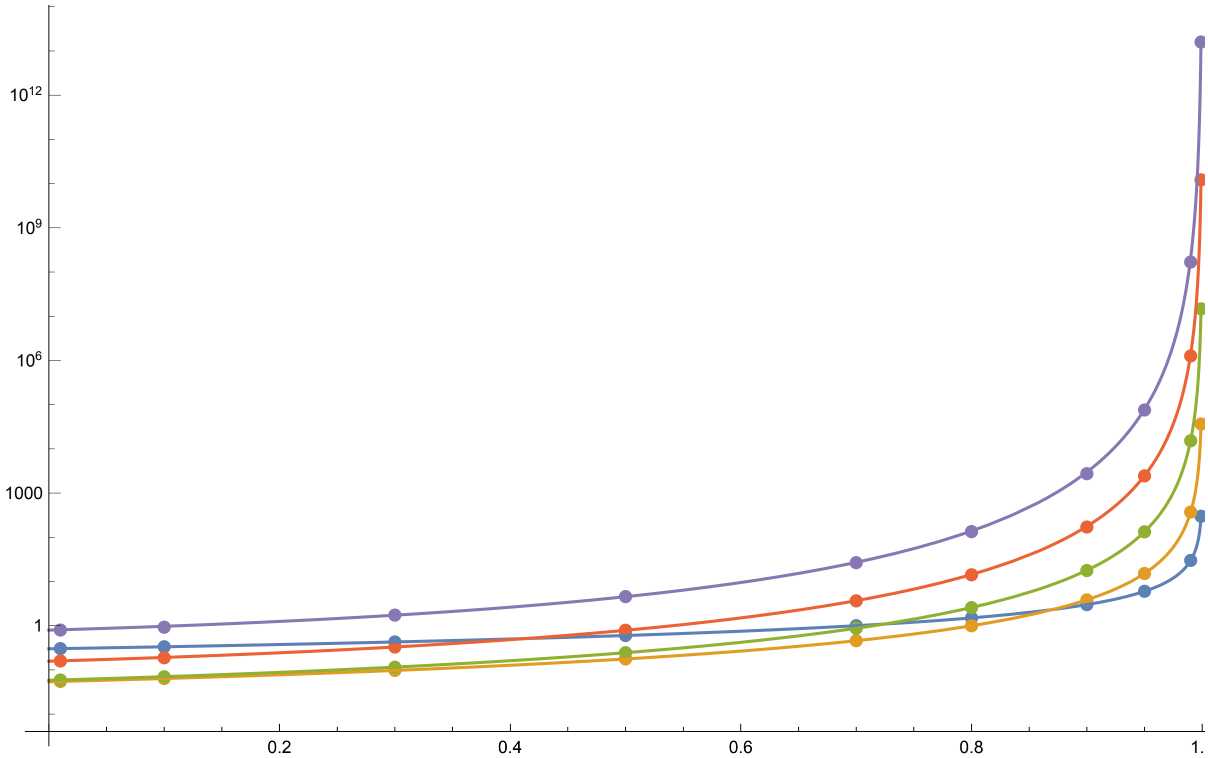
$$\text{mfp}\,9!\,\Big(\Big(-496125+\frac{52729425c}{64}-\frac{367391171c^2}{1024}-$$

$$\frac{1099685881c^3}{16384}+\frac{11363604819c^4}{262144}+\frac{312487c^5}{32}-329c^6\Big)\text{mfp}^8\Big)\Big/$$

$$\left(49\left(-3-\frac{4c}{3}\right)^4\left(-9+\frac{c}{64}\right)\left(-5+\frac{5c}{16}\right)^3(-1+c)^5\right)\Big\},\ \{c,0,.999\},\ \text{PlotRange}\to\text{All}\Big]$$

```
]
```

Out[4257]=



Namespace

```
End[]
```