Effective behavior for transport of photons and supra-thermal particles in binary mixtures

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Summary

- Physical context
  - numerical simulation of Inertial Confinement Fusion targets
  - hydrodynamical instabilities in imploding capsules
- Physical modeling
  - kinetic equations for photons and supra-thermal particles
  - binary mixtures
- Mathematical tools
  - asymptotic analysis (homogenization theory)
  - renewal theory (random process on the line)
- Numerical computation of effective coefficients

Inertial Confinement Fusion

Lawson's criterium must be fulfilled to achieve nuclear fusion:

(1) $$\text{density} \times \text{Confinment time} \geq C(\text{Temperature}).$$

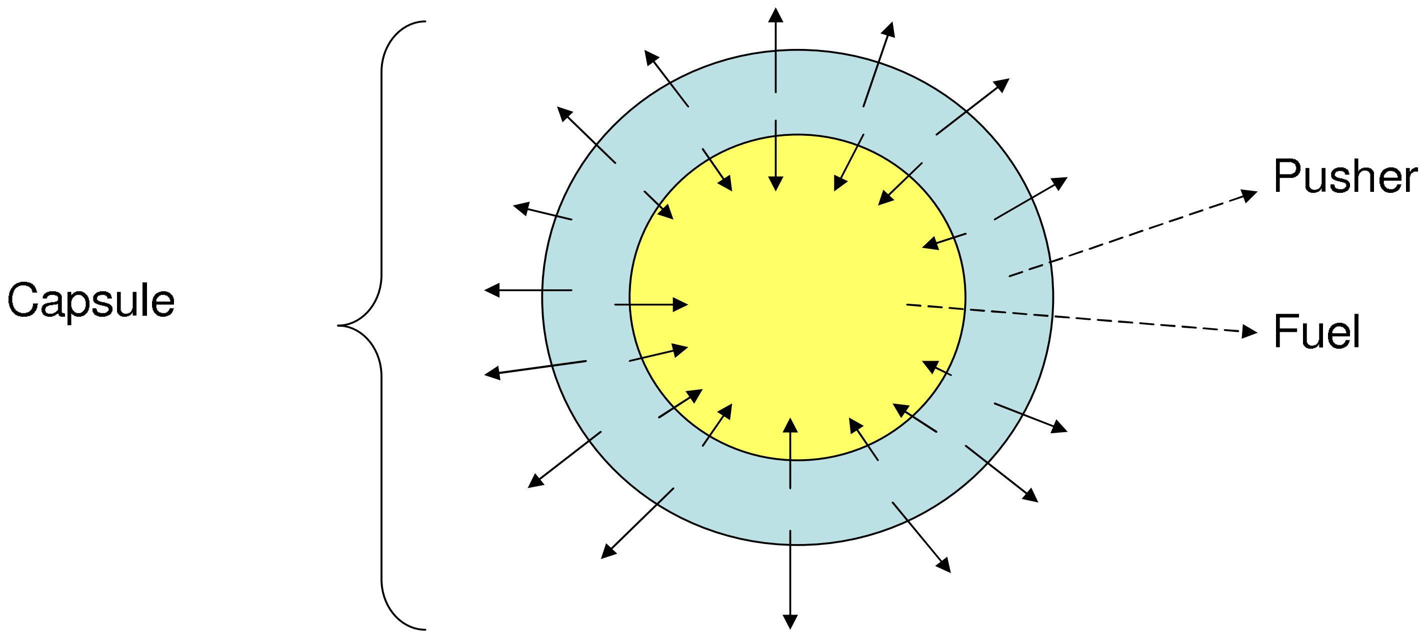
There are three ways to satisfy this constraint:

i/ Long confinement time$\Rightarrow$ Magnetic Confinement fusion

ii/ High density$\Rightarrow$ Inertial Confinement fusion (ICF)

iii/ High density and long time $\Rightarrow$ Gravitational Confinement fusion

In ICF, explosion of the pusher (usually plastic) compress the fuel (isotope of hydrogen) and creates a plasma which eventually ignites

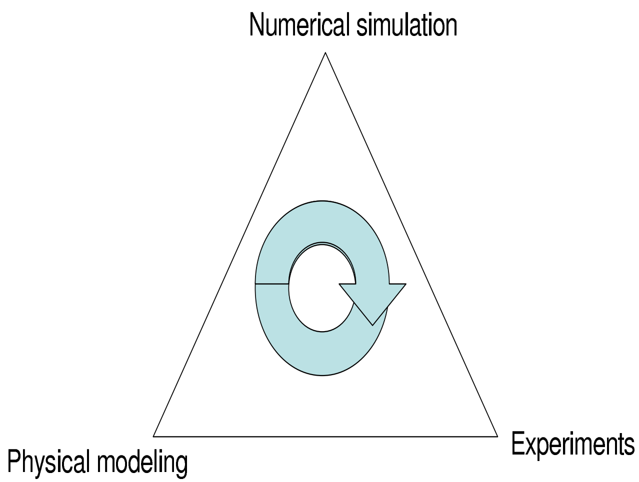


Inertial Confinement Fusion

There are numerous ways to implode the pusher:

- Laser energy irradiating the capsule
- Heavy ions beams
- X-ray

Several laboratories are currently working on the design of such fusion experiments with different energy driver and different capsule design[Lin98]. One challenge is to extrapolate knowledge from today's experiments to specify a target which can perform ignition: use of numerical simulation.



Hydrodynamic Instabilities

One of the major limiting process for ICF is the stability of implosion : hydrodynamic motion is not stable when $\nabla P \cdot \nabla \rho < 0$ (i.e. when a "light" material pushes a "heavy" material).
It means that a given default of wavelength λ at the pusher/fuel interface will grow

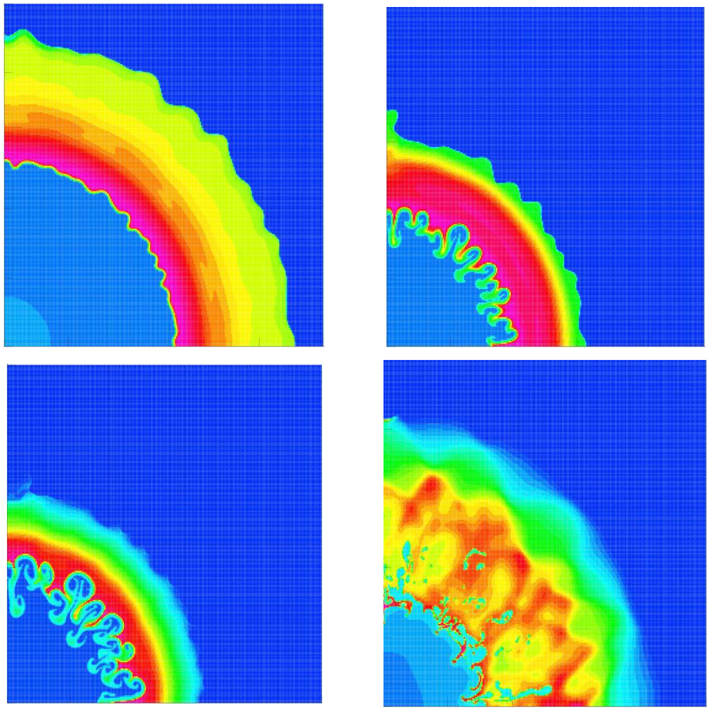
1. linear stage: default grows as $\exp(\gamma(\lambda)t)$
2. non linear stage:
   - saturation of growth
   - coupling between wavelength
3. turbulent stage with fuel/pusher mixing

The importance of each phase depends on the rugosity of the interface and the design of the capsule (convergence ratio, implosion law, ...).

Hydrodynamic Instabilities

These instabilities alter the efficiency of implosion

- Large instabilities can lead to pusher break-up $\Rightarrow$ no fusion reaction
- Moderate instabilities can significatively reduce the number of reactions

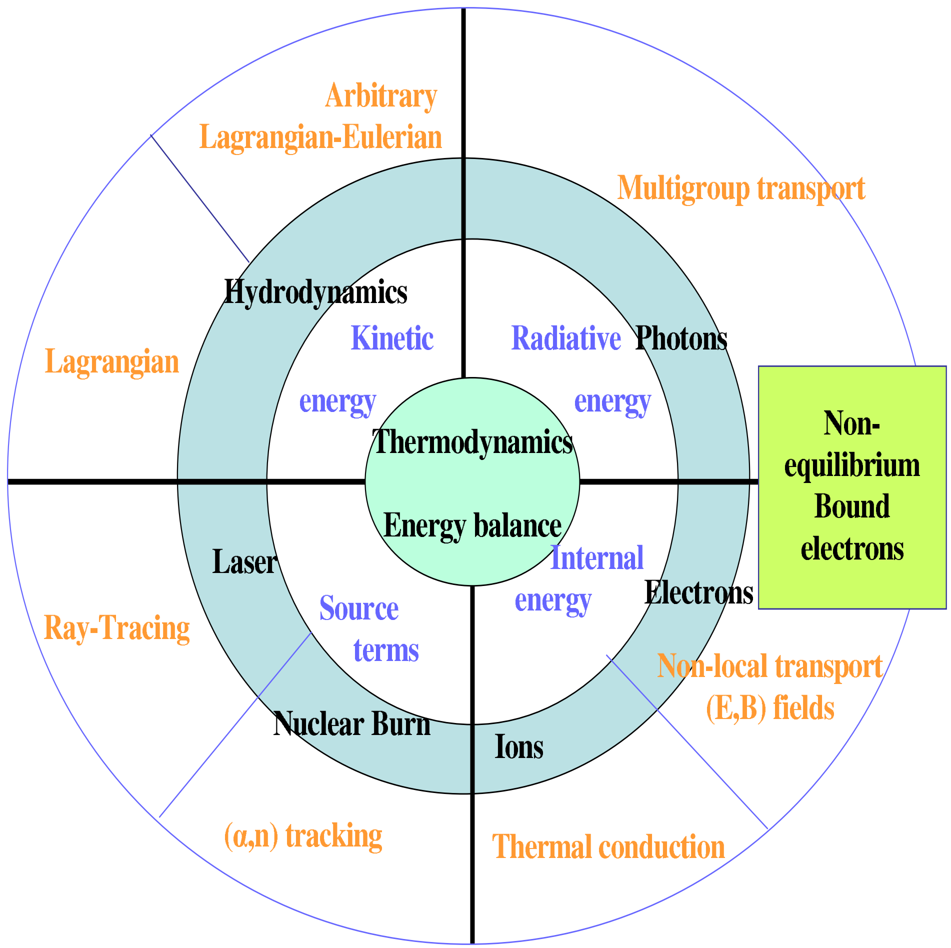


Density map during implosion and nuclear burn

The problem we want to address is the modeling of particle transport in this kind of simulation.

Physical modeling in ICF hydrocode

Hydrocodes are the basic tool for studying the implosion phase[DW93]. They include all necessary physical packages with simplifications due to simulation constraints:



Physical modeling in ICF hydrocode

Concerning particle transport, they distinguish

- thermal particles at equilibrium (maxwellian) distribution $\Rightarrow$ Fluid equations
  - thermal ions $\longrightarrow$ ionic temperature T_i
  - thermal (free) electrons $\longrightarrow$ electronic temperature T_e
- non thermal particles $\Rightarrow$ kinetic equations
  - non-thermal ions coming from nuclear reactions
  - photons coming from laser$\longmapsto$X-ray conversion
  - bound electrons in coronal plasma
  - hot-electrons generated by laser-plasma instabilities
  - neutrons

Modeling for photons

Radiative transfer equations are to be solved.

- during compression phase for X-ray driven implosion
- during combustion: radiative losses determine the beginning of nuclear reactions

Photons are described by radiative intensity $I(x, \overrightarrow{\Omega}, \nu, t)$ solution of

$$\begin{cases} \frac{1}{c}\partial_t I + \overrightarrow{\Omega} \cdot \nabla I + \sigma_\nu(T) I = \sigma_\nu c \frac{B_\nu(T)}{4\pi} & \text{transport of radiation} \\ \partial_t E(T) + \int d\nu d\overrightarrow{\Omega} \sigma_\nu(T)(c\frac{B_\nu(T)}{4\pi} - I) = 0 & \text{energy balance equation} \end{cases}$$

B_ν is the Planck distribution (equilibrium distribution function for photons) and σ_ν is the opacity.

The relevant quantity for the transport of radiative energy is the Rosseland mean free path [LPB83].

$$\lambda = \frac{\int \frac{\partial_T B_\nu}{\sigma_\nu(T)} d\nu}{\int \partial_T B_\nu d\nu}$$

We would like to define an effective mean free path in the mixing zone.
First step is to simplify the problem:

- we consider a linear problem with one single equation
- neglect the dependency of $\sigma_\nu(T)$ with respect to ν and T (grey assumption).

We are reduced to an integro-differential equation

$$\frac{1}{c}\partial_t\phi + \overrightarrow{\Omega}\cdot\nabla\phi + \sigma(x)(\phi - \int\phi\frac{d\overrightarrow{\Omega}}{4\pi}) = 0$$

where $\sigma(x) = \sigma_f$ in fuel and $\sigma(x) = \sigma_p$ in pusher.
Results concerning the effective mean free path will then be extended without justification to the non-linear and non-grey case.
There are also some effects of the averaging procedure on the equilibrium temperature [Cl97]: we will not consider them here.

Modeling for non-thermal ions

We consider Deuterium targets. Relevant nuclear reactions are

Primary reactions

$$\left\{ \begin{array}{l} D + D \rightarrow T + H \\ D + D \rightarrow He^3 + n \end{array} \right.$$

secondary reactions

$$\left\{ D + T \rightarrow He^4 + H \right.$$

One question is to know if T will stop in the fuel (and can react with D) or in the pusher.

Particles created by nuclear reactions are not at equilibrium and satisfy Fokker-Planck equation for their distribution function f:

$$\partial_t f + v \cdot \nabla f + \partial_v (af + D\partial_v f) + q(E + v \times B) = S.$$

Effects of electromagnetic fields are usually neglected and trajectory of particles are approximated by straight lines (angular deflection becomes dominant near thermalization):

$$\partial_t f + v \cdot \nabla f + \partial_v (af) = S.$$

It describes the slowing down of particles until they go back to the background of thermal particles.

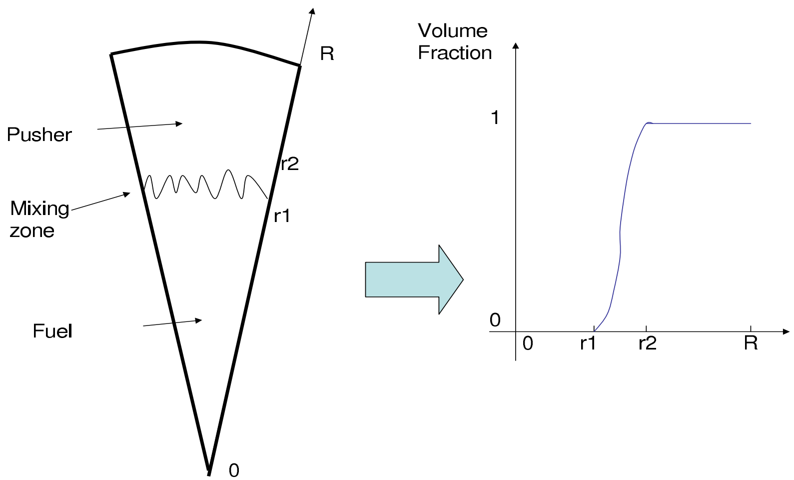
Binary mixtures

The basic method for solving these problems is direct numerical simulation of hydrodynamic and particle transport. The drawbacks are:

- Excessive computational cost (necessity of fine mesh)
- complexity of numerical methods (kinetic equations with mixed cells and interface tracking)

Alternative approach is the following

- use a semi-statistical model for instability growth in the non-linear and pre-turbulent stage[RS04].
- us a subgrid model for particle transport.



Binary mixtures

Exact structure of the mixing layer is not known: a random medium assumption is natural. We introduce random variables $\chi_f(x,\omega)$ and $\chi_p(x,\omega) = 1 - \chi_f(x,\omega)$ such that

$$\chi_f(x,\omega) = 1,\ \text{if } x \text{ is in fuel and 0 otherwise}$$

To obtain a subgrid model, it is necessary to suppose that statistical properties of χ vary slowly with respect to radius, i.e. χ is an homogeneous random field. Available knowledge on χ is

- volume fraction $c_f = \int \chi_f(x,\omega) P(d\omega)$
- characteristic length scale: this notion is not well defined.
  - correlation length

$$d(\overrightarrow{\Omega}) = \int_0^\infty \left(\int (\chi_f(x,\omega) - c_f)(\chi_f(x + \overrightarrow{\Omega} h,\omega) - c_f) P(d\omega) \right) dh$$

  - mean chord length $l_f(\overrightarrow{\Omega}) (\neq l_p(\overrightarrow{\Omega}))$

If medium is isotropic $d(\overrightarrow{\Omega})$ and $l_f(\overrightarrow{\Omega})$ do not depend on $\overrightarrow{\Omega}$.

Binary mixtures

If ergodicity is assumed, we can replace statistical means by spatial averages.

$$
\begin{aligned}
c_f &= \lim_{V \to R^3} \frac{1}{|V|} \int_V \chi_f(x,\omega) dx \\
d &= \lim_{V \to R^3} \frac{1}{|V|} \int_0^\infty \left(\int_V (\chi_f(x,\omega) - c_f)(\chi_f(x + \overrightarrow{\Omega} h, \omega) - c_f) dx \right) dh
\end{aligned}
$$

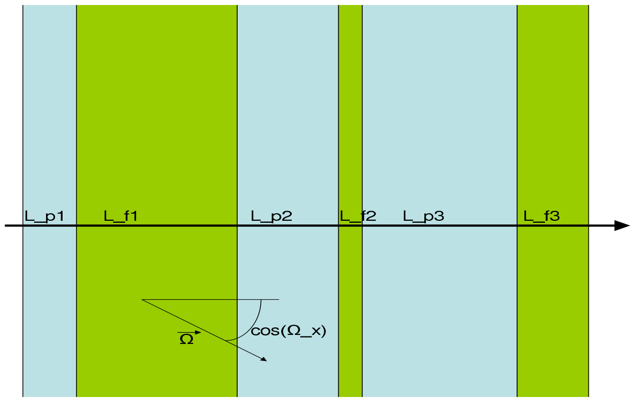
Higher moments can be considered for characterizing the distribution but it is difficult to obtain them from hydrodynamical statistical models: a good model for d is already a challenge.
An important relation is:

$$
c_f = \frac{l_f}{l_f + l_p}, \quad c_p = \frac{l_p}{l_f + l_p}.
$$

As I am interested in computation of effective coefficients, I will give some examples that can be used for simulations.

Examples of binary mixtures

The simplest example is the stratified medium



If $(L_p^i)_i$ are independent random variables with identical distribution of mean $\mathbb{E}L_p$(idem for $(L_f^i)_i$ with mean $\mathbb{E}L_f$) then the random field $\chi(x,\omega)$ is ergodic but not isotropic

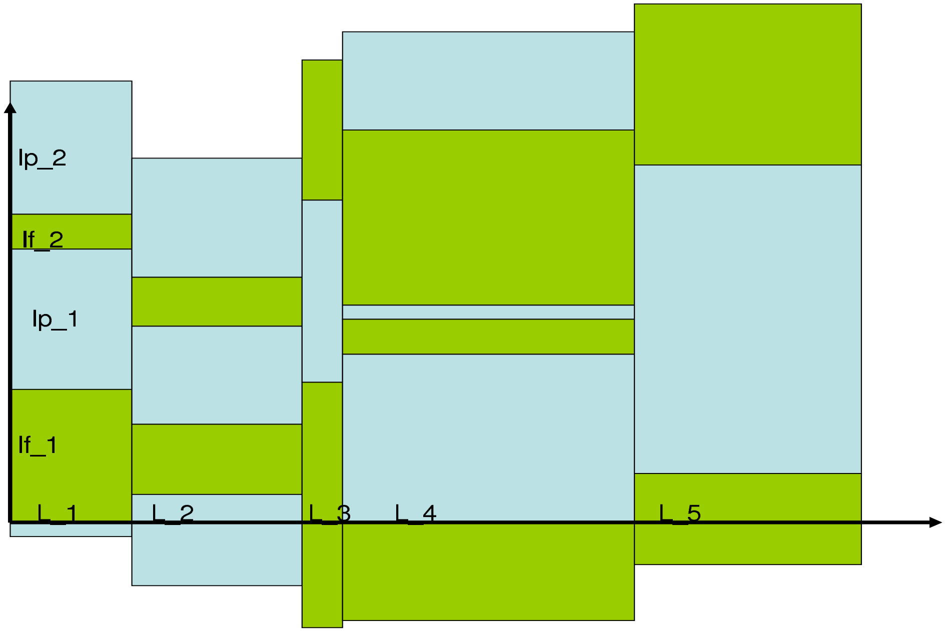
$$c_f = \frac{\mathbb{E}L_f}{\mathbb{E}L_f + \mathbb{E}L_p}, \quad c_p = \frac{\mathbb{E}L_p}{\mathbb{E}L_f + \mathbb{E}L_p}, \quad l_f(\overrightarrow{\Omega}) = \frac{\mathbb{E}L_f}{\cos(\overrightarrow{\Omega}_x)}.$$

This model is the basic model for applying renewal techniques (see below). If random variables have exponential distribution, random medium is markovian and we can compute the correlation length

$$d(\overrightarrow{\Omega}_x) = \frac{(c_p c_f)^2}{\cos(\overrightarrow{\Omega}_x)} \left(\mathbb{E}L_f + \mathbb{E}L_p\right)$$

Example of binary mixture

Construction of multidimensional medium with markovian statistics is not obvious. One possibility is to combine two markovian renewal processes



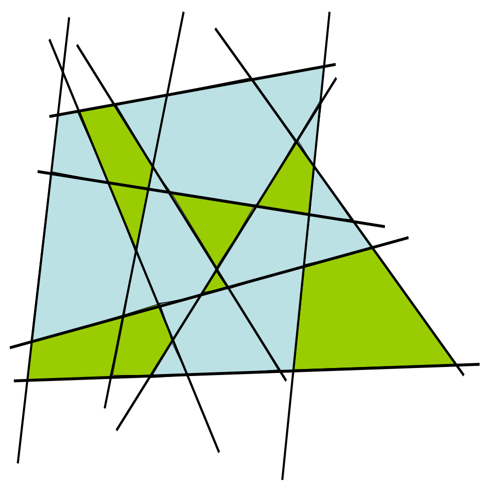
Mean chord length is $l_f = \dfrac{\mathbb{E}L\mathbb{E}l_f}{\cos\overrightarrow{\Omega}_x \dfrac{\mathbb{E}l_f\mathbb{E}l_p}{\mathbb{E}l_f+\mathbb{E}l_p} + \sin\overrightarrow{\Omega}_x\mathbb{E}L\mathbb{E}l_f}$.

Medium is markovian and ergodic but not isotropic.

Examples of binary mixtures

One algorithm for constructing isotropic binary mixture with markovian statistics is described in [Swi65]:

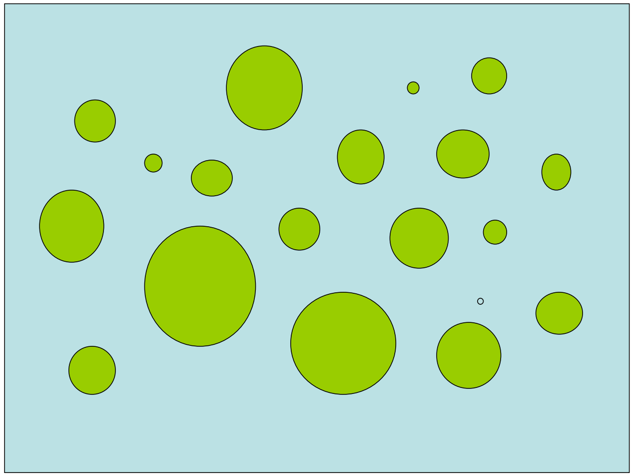
1. For given radius R, choose randomly $n = \dfrac{\pi R}{\lambda}$ couples (θ_i, ρ_i) in $(0, \pi) \times (-R, R)$.
2. The n lines $x \cos(\theta_i) + y \sin(\theta_i) = \rho_i$ define polygonal cells with mean chord length λ.
3. Fill each cell with material p or f according to the volume fraction
4. The resulting mean chord length is $l_f = \dfrac{\lambda}{c_p}$



Examples of binary mixtures

Frequent modeling use inclusion of spheres (or disk in 2D).

- Center of spheres obeys Poisson statistic
- radius are random variables with given PDF $F(r)$ of mean $\mathbb{E}r$ (constant radius is a particular case).



For overlapping spheres[TL93], chord length PDF for the background medium is exponential.
For non overlapping spheres[OMLM05] chord length PDF for the background medium is approximately exponential and chord length PDF for spheres is

$$d(r) = \frac{r}{4\langle r\rangle}\int_{r/2}^{\infty}\frac{F(s)}{\sqrt{s^2-(r/2)^2}}$$

mathematical tools: homogenization

Homogenization theory is a popular tool for computing effective coefficients: it relies on separation of scales

$$\varepsilon = \frac{d}{\delta} = \frac{\text{correlation length}}{\text{size of the mixing zone}} \ll 1.$$

First, it has been applied to elliptic problems in periodic medium [BLP78].

- Extension to more general medium has been extensively studied [Koz80][Tar79][All92]. Application to random medium requires strong assumptions on the random field: existence of measure preserving transformation τ_x such that $\chi(x,\omega) = \tilde{\chi}(\tau_x \omega)$. It can be difficult to prove this property for a given random medium (for example non overlapping spheres).
- Extension to kinetic equations has been made in [BLP79][Sen80] [Gol91][Cl98][DG00].
- Computation of effective coefficients for elliptic equations in random medium is based on periodization of a finite sample of the medium[BP04][BDW04].

mathematical tools: renewal theory

Renewal theory is a well known probabilistic tool[Fel66] aimed at studying random events on a line. Basic tools are

- The renewal measure U defined by $U = \sum_0^\infty F^{*n}$ where F is the PDF for chord length of the medium $(p + f)$.
- The renewal theorem which states that

$$\lim_{x \to \infty} U((x, x + dy)) = \frac{dy}{\int zF(z)dz}$$

- The renewal equation obtained by conditional expectation on the length of the first chord. This equation can be explicitly solved only for markovian statistics.

Comparison of the methods

- Homogenization theory
  - rigorous derivation of the limit: deterministic behavior of the limiting PDE.
  - Need for numerical simulations to compute effective coefficients
- Renewal theory
  - Need to approximate the random geometry
  - Neglect scattering
  - Analytic computation of effective coefficients

We will compare these two approaches on the transport of photons and suprathermal particles in binary (random) mixtures.

Application to slowing down

We consider the following PDE in random media:

$$\partial_t f + v \cdot \nabla f + k(x)\partial_v(a(v)f) = 0, \ \ k(x) = k_f \chi_f(x,\omega) + k_p \chi_p(x,\omega)$$
$$f(x,v,t=0) = 1_{x \in \text{ fuel}} \delta(v - v_0)$$

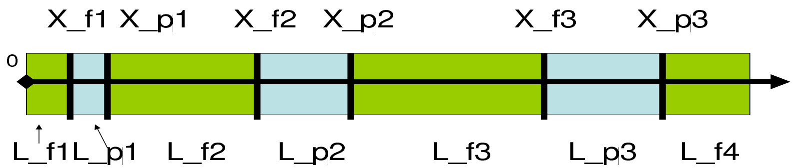
This is really a 1D problem: renewal theory can be rigorously applied if we assume that along each line, chords of pusher and fuel are independent random variables with same distribution.
Particular interpretation of this PDE is simple:

- Characteristic curves are

$$\left\{ \begin{array}{l} \dfrac{dX(t)}{dt} = V(t) \\ \dfrac{dV(t)}{dt} = -k(X(t))a(V(t)) \end{array} \right. \Longrightarrow \left\{ \begin{array}{l} dH(V(t)) = -k(X(t))dX(t), \\ H(V) = \displaystyle\int_0^V \frac{v}{a(v)} dv \end{array} \right.$$

- Particle is created at $x = 0$ in the fuel with "energy" $H_0 = H(v_0)$.
- When crossing a chord of length $L_i (i = f, p)$, "energy" decreases by $k_i L_i$
- Particle stops when energy is 0.

Question is: what is the probability P that particle stops in fuel (and may react again) or in pusher.



Let X^e be the end of the trajectory defined by

$$H_0 = k_f \underbrace{(X_f^1 - 0)}_{L_f^1} + k_p \underbrace{(X_p^1 - X_f^1)}_{L_p^1} + k_f \underbrace{(X_f^2 - X_p^1)}_{L_f^2} + \ldots + k_i(X^e - X_i^n)$$

Distribution of L_f^1 is slightly different[a] from other lengths because $x = 0$ is not necessary the beginning of a chord.

Homogenization scaling requires that mean chord lengths l_f and l_p are small in front of slowing distances in homogenous materials H_0/k_f and H_0/k_p.

Let $\varepsilon = \dfrac{k_p l_l}{H_0}$. We introduce the scaling $X \to X/\varepsilon$ and $H_0 \to H_0/\varepsilon$.

In this scaling, chord lengths are of order 1 and initial energy of particle goes to infinity.

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[a] except for markovian distribution

$$P = P\left(X^e \in \bigcup_{n\geq 1}(X_p^n, X_f^{n+1})\right)$$
$$= \bigsqcup_{n\geq 1} P\left(\sum_{j=1}^{n-1}(k_f L_f^j + k_p L_p^j) < H_0 < \sum_{j=1}^{n-1}(k_f L_f^j + k_p L_p^j) + k_f L_f^{n+1}\right)$$

We introduce the renewal measure

$$U(x, dx) = \bigsqcup_{n\geq 1} P\left(\sum_{j=1}^{n-1}(k_f L_f^j + k_p L_p^j) \in (x, x+dx)\right)$$

$$\Rightarrow P = \int_0^\infty U(x, dx) P(x < H_0 < x + k_f L_f^{n+1})$$

Let $F(u) = P(k_f L_f^{n+1} > u) 1_{u>0}$, $P = \int_{-H_0}^{\infty} U(x + H_0, dx) F(-x)$.

Using renewal theorem

$$\lim_{H_0\to\infty} P = \int_{-\infty}^{\infty} \frac{F(x)dx}{k_f l_f + k_p l_p} = \frac{k_f c_f}{k_f c_f + k_p c_p}$$

Same result can be proved using homogenization theory [Gol04] ($k^\varepsilon(x) \rightharpoonup k_f c_f + k_p c_p$).
Interest of renewal method is that it provides a result without assumption on the characteristic length scale[LZ93]. Denote

$$\begin{aligned} P_f(H) &= P(\text{particle starting from fuel with energy } H \text{ will stop in fuel}) \\ P_p(H) &= P(\text{particle starting from pusher with energy } H \text{ will stop in fuel}) \end{aligned}$$

We establish renewal equation:

$$\begin{aligned} P_f(H) &= \int_0^\infty P_f(H/L_f = l)P(L_f = l)dl \\ &= \int_0^{H/k_f} P_f(H/L_f = l)P(L_f = l)dl + \int_{H/k_f}^\infty P_f(H/L_f = l)P(L_f = l)dl \\ &= \int_0^H P_p(H-h)P(k_f L_f = h)dh + P(k_f L_f > H) \end{aligned}$$

Similarly

$$
\begin{aligned}
P_p(H) &= \int_0^{\infty} P_p(H/L_p = l)P(L_p = l)dl \\
&= \int_0^{H/k_p} P_p(H/L_p = l)P(L_p = l)dl + \int_{H/k_p}^{\infty} P_p(H/L_p = l)P(L_f = l)dl \\
&= \int_0^{H} P_f(H-h)P(k_p L_p = h)dh
\end{aligned}
$$

Knowing distribution functions for L_p and L_f we can solve this two coupled convolution equations.
Simplest case is markovian distribution
$P(L_f = l) = \exp(-l/l_f)/l_f, \; P(L_p = l) = \exp(-l/l_p)/l_p$.
Equations are solved by taking Laplace

$$
\begin{cases}
\hat{P}_f(s) = \int_0^{\infty} e^{-hs} P_f(h)dh \\
\hat{P}_p(s) = \int_0^{\infty} e^{-hs} P_p(h)dh
\end{cases}
$$

$$\begin{cases} \hat{P}_f(s) = \dfrac{\hat{P}_p(s)}{k_f l_f (s + 1/(k_f l_f))} + \dfrac{1}{s + 1/(k_f l_f)} \\ \hat{P}_p(s) = \dfrac{\hat{P}_f(s)}{k_p l_p (s + 1/(k_p l_p))} \end{cases}$$

Solving the system and taking inverse Laplace transform gives

$$P_f(H) = \frac{k_f l_f + k_p l_p \exp\left(-H(1/(k_f l_f) + 1/(k_p l_p))\right)}{k_f l_f + k_p l_p}$$

All calculations based on renewal equation use the same technique:

- Take conditional expectation with respect to the length of the first chord.
- Obtain a system of coupled convolution equations
- Solve by taking Laplace transform

Extension to 3D geometries

Previous formula in only valid for markovian random medium: how does it behave on arbitrary random medium?
We study slowing down in a random medium given by spherical inclusions of pusher in the fuel (given radius r and with overlapping).
The approach used is:

- Find asymptotic values for $P(H)$ when $rk_p/H \ll 1$ and $rk_p/H \gg 1$.
- Propose a generic formula depending on weight function $\exp(-rk_p/H)$ and having the correct limiting behavior.
- Fit the formula on numerical simulations

For $rk_p/H \ll 1$, homogenization applies,

$$P(H) \sim \frac{k_f c_f}{k_f c_f + k_p c_p}.$$

For $rk_p/H \gg 1$, slowing power of spheres is large.
Probability of stopping in a sphere $\sim$ probability that distance $d(X^0, \mathcal{S})$ between the starting point X^0 and the spheres $\mathcal{S}$ is less than H/k_f.

$$P(H) \sim 1 - \mathbb{P}(d(X^0, \mathcal{S}) \leq \frac{H}{k_f} / X^0 \in \mathcal{S}^c) = 1 - \frac{\mathbb{P}(d(X^0, \mathcal{S}) \leq \frac{H}{k_f})}{c_f}$$

$\mathbb{P}(d(X^0, \mathcal{S}) \leq \frac{H}{k_f})$ is just the probability that at least one center lies in a cylinder C of radius r and length $\frac{H}{k_f}$
Number of centers in a volume $V = \pi r^2 \frac{H}{k_f}$ is a random variable N
$\mathbb{P}(N = n) = e^{-\frac{3c_p|V|}{4\pi r^3}} \frac{1}{n!} (\frac{3c_p|V|}{4\pi r^3})^n$. Hence

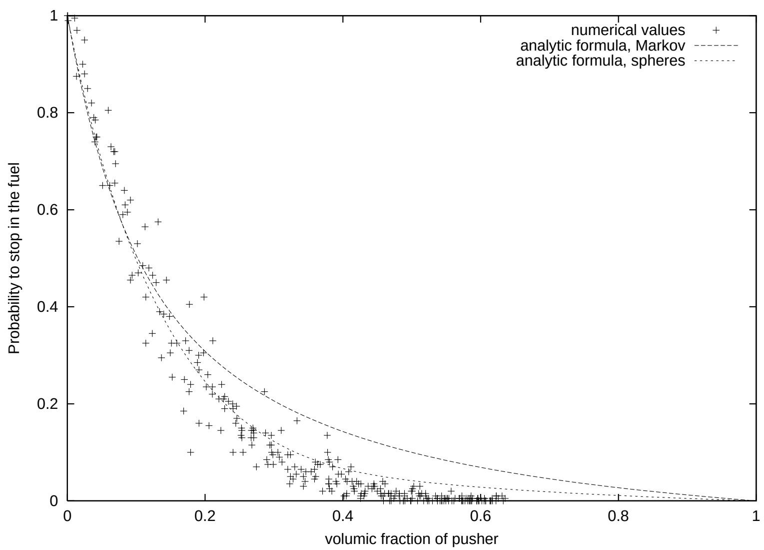
$$\mathbb{P}(H) \sim 1 - \frac{1 - e^{-\frac{3Hc_p}{4k_f r}}}{c_f} \sim 1 - \frac{3Hc_p}{4rc_f k_f} \sim \exp(-\frac{3Hc_p}{4rc_f k_f})$$

Finally, we propose the formula (with A to be fitted)

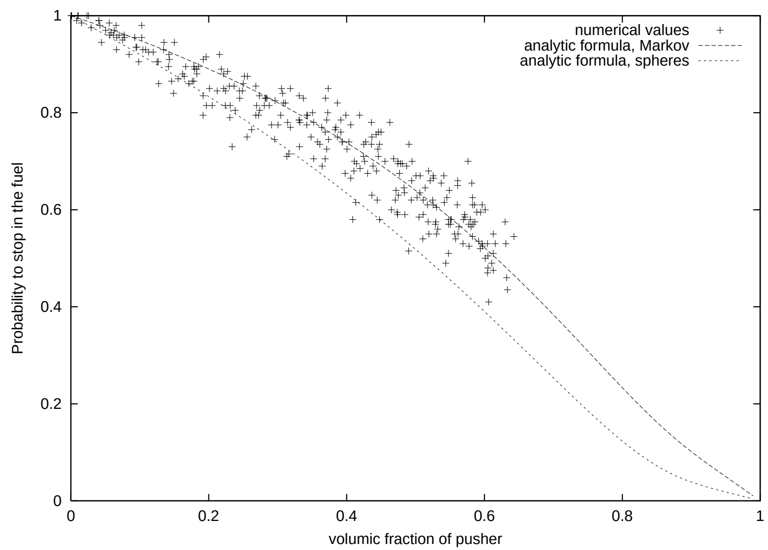
$$P = \exp(-\frac{3Hc_p}{4rc_f k_f})(1 - exp(-Ark_p/H)) + \frac{k_f c_f}{k_f c_f + k_p c_p} exp(-Ark_p/H).$$

Extension to 3D geometries

Numerical simulations are detailed in [CPS04]: $A \sim 1$ gives correct results.
We now compare results from renewal theory (on a non-markovian geometry), numerical simulations and fitted analytical formula in planar geometry.
We set $l_p = \pi/2r,\ l_f = l_p c_f/c_p$



$k_p r = 0.1, k_p = 9k_f$



$k_p r = 1, k_p = k_f$

The two formulas share the same asymptotical behavior and do not differ so much in intermediate cases (compared to numerical results).

Application to linear transport

The transport process is solution of

$$\partial_t \phi + \overrightarrow{\Omega} \cdot \nabla \phi + (\sigma_p \chi_p(\tau_x \omega) + \sigma_f \chi_f(\tau_x \omega))(\phi - \int \phi \frac{d\overrightarrow{\Omega}}{4\pi}) = 0.$$

Rescaling for homogenization theory:

- small scale hypothesis $\varepsilon = \frac{d}{\delta} \ll 1$.
- High contrast ratio between fuel and pusher opacity $q = \frac{\sigma_f}{\sigma_p} \ll 1$.

We obtain

$$\partial_t \phi^{\varepsilon,q} + \overrightarrow{\Omega} \cdot \nabla \phi^{\varepsilon,q} + (\frac{\sigma_p}{q} \chi_p(\tau_{x/\varepsilon} \omega) + \sigma_f \chi_f(\tau_{x/\varepsilon} \omega))(\phi^{\varepsilon,q} - \int \phi^{\varepsilon,q} \frac{d\overrightarrow{\Omega}}{4\pi}) = 0.$$

and we let $\varepsilon, q \to 0$.
The result depends on the optical depth of heterogeneities.

Application to linear transport

There are three cases

- $\varepsilon \ll q$. First apply homogenization theory[DG00]

$$\phi^q \rightharpoonup \phi^q, \ \ \partial_t \phi^q + \overrightarrow{\Omega} \cdot \nabla \phi^q + \tilde{\sigma}(\phi^q - \int \phi^q \frac{d\overrightarrow{\Omega}}{4\pi}) = 0.$$

  with effective opacity $\tilde{\sigma} = \frac{\sigma_p}{q} c_p + \sigma_f c_f$. It is then possible to apply diffusion approximation after proper time rescaling:

$$\phi^q(t/q) \to \Phi, \ \ \partial \Phi = \frac{1}{3 c_p \sigma_p} \Delta \Phi.$$

- $q \ll 1$.
  First apply diffusion approximation in the pusher without time rescaling[RS91].
  $\phi^{\varepsilon,q} \sim \chi_p(\tau_{x/\varepsilon} \phi_p^q + \chi_f(\tau_{x/\varepsilon}\omega))\phi_f$ where (ϕ_f, ϕ_p^q) are solution of a coupled system of PDE

$$\begin{cases} \partial_t \phi_f + \overrightarrow{\Omega} \cdot \nabla \phi_f + \sigma_f(\phi_f - \int \phi_f \frac{d\overrightarrow{\Omega}}{4\pi}) = 0 \text{ in fuel} \\ \partial_t \phi_p^q = \frac{q}{3\sigma_p} \Delta \phi_p^q \text{ in pusher} \end{cases}$$

Finding effective behavior of this system when $\varepsilon \to 0$ is an open problem (related studies are billiard problems with finite horizon hypothesis).

- $\varepsilon \sim q$. Diffusion approximation and homogenization operate at the same scale: classical techniques apply[BLP78][Cl98].

The rescaled equation writes as

$$\partial_t \phi^\varepsilon + \overrightarrow{\Omega} \cdot \nabla \phi^\varepsilon + (\frac{\sigma_p}{\varepsilon} \chi_p(\tau_{x/\varepsilon}\omega) + \sigma_f \chi_f(\tau_{x/\varepsilon}\omega))(\phi^\varepsilon - \int \phi^\varepsilon \frac{d\overrightarrow{\Omega}}{4\pi}) = 0.$$

We rescale time and insert formal asymptotic expansion
$\phi^\varepsilon = \phi^0(x,t) + \varepsilon\phi^1(x, \overrightarrow{\Omega}, \tau_{x/\varepsilon}\omega, t) + \varepsilon^2\phi^2(x, \overrightarrow{\Omega}, \tau_{x/\varepsilon}\omega, t) + \ldots$
Under suitable technical assumption on the random field[Cl98], one can prove that $\phi^\varepsilon \to \Phi(x,t)$ (deterministic function) solution of $\partial_t \Phi = \dfrac{1}{3\tilde{\sigma}} \Delta\Phi$ where $\tilde{\sigma}$ is obtained by solving a cell problem.
We note also $\tilde{D} = \frac{1}{3\tilde{\sigma}}$ the effective diffusion coefficient.

The cell problem

In periodic medium ($\chi(y)$ $T-$periodic), find $\overrightarrow{g}(y, \overrightarrow{\Omega})$ solution of

$$\overrightarrow{\Omega}.\nabla\overrightarrow{g} + \sigma_p \chi(y)(\overrightarrow{g} - \int \overrightarrow{g}\frac{d\overrightarrow{\Omega}}{4\pi}) = \overrightarrow{\Omega},\ 3\tilde{\sigma} = \left(\frac{1}{|T|}\int_T dy \int \overrightarrow{g}_i \cdot \overrightarrow{\Omega}_i \frac{d\overrightarrow{\Omega}}{4\pi}\right)^{-1}$$

Extension to random case uses the infinitesimal generator defined on random functions

$$Df(\omega) = \nabla_x f(\tau_x \omega)_{|x=0}.$$

Poisson equation for $\overrightarrow{g}(\omega, \overrightarrow{\Omega})$ becomes

$$\overrightarrow{\Omega}.D\overrightarrow{g} + \sigma_p \chi(\omega)(\overrightarrow{g} - \int \overrightarrow{g}\frac{d\overrightarrow{\Omega}}{4\pi}) = \overrightarrow{\Omega},\ \tilde{D} = 3\tilde{\sigma} = \left(\int P(d\omega) \int \overrightarrow{g}_i \cdot \overrightarrow{\Omega}_i \frac{d\overrightarrow{\Omega}}{4\pi}\right)^{-1}$$

Effectively solving this problem requires to reduce it to a periodic problem([BP04] for a proof for elliptic equations, not proven for kinetic equations?):

- Generate a sample of random medium of size L
- Solve Poisson equation with periodic boundary conditions
- Let $L \to \infty$

Consequence: Solving the cell problem is as difficult as solving the original one.

Alternative expression for D: Kubo's formula

Consider the markov process $(X(t), \overrightarrow{\Omega}(t))$:

$$\frac{dX(t)}{dt} = \overrightarrow{\Omega}(t) \quad \overrightarrow{\Omega}(t) \text{ jump process with intensity } \sigma(X(t))$$

Then

$$\overrightarrow{g}_i(x, \overrightarrow{\Omega}) = \int_0^\infty \mathbb{E}(\overrightarrow{\Omega}_i(t)/X(0) = x, \overrightarrow{\Omega}(0) = \overrightarrow{\Omega})dt$$
$$\tilde{D} = \frac{1}{3}\int_0^\infty \mathbb{E}(\overrightarrow{\Omega}(0) \cdot \overrightarrow{\Omega}(t))dt$$

For computational purpose, we notice that

$$\begin{aligned} \mathbb{E}X_i(t)^2 &= \int_0^t \int_0^t \mathbb{E}\mathbb{E}(\overrightarrow{\Omega}_i(s)\overrightarrow{\Omega}_i(u))dsdu = 2\int_0^t \int_0^s \mathbb{E}\mathbb{E}(\overrightarrow{\Omega}_i(s)\overrightarrow{\Omega}_i(u))dsdu \\ &= 2t\int_0^t \mathbb{E}(\overrightarrow{\Omega}(0)_i \overrightarrow{\Omega}_i(s))ds - 2\int_0^t s\mathbb{E}(\overrightarrow{\Omega}_i(0)\overrightarrow{\Omega}_i(s))ds \end{aligned}$$

Hence $D = \lim_{t \to \infty} \frac{\mathbb{E}X_i(t)^2}{2t}$.

$\Rightarrow$ Need to simulate Random walk in random media.

Solution of the cell problem

It is enough to consider periodic case: note $\sigma(y)$ the periodized sample of the random opacity and T its period.
There is an analytic solution in stratified medium (1D case): cell problem is

$$\mu\partial_y g + \sigma(y)(g - \int_{-1}^{1} g\frac{d\mu}{2}) = \mu,\ 3\tilde{\sigma} = \left(\frac{1}{|T|}\int_T dy \int_{-1}^{1} \mu g \frac{d\mu}{2}\right)^{-1}$$

- integrate with respect to μ: $\partial_y \int_{-1}^{1} \mu g d\mu = 0 \Rightarrow \int_{-1}^{1} \mu g d\mu$ does not depend on y.
- Multiply by μ: $\mu^2\partial_y g + \sigma(y)(\mu g - \mu\int_{-1}^{1} g\frac{d\mu}{2}) = \mu^2$
- Integrate with respect to μ: $\int_{-1}^{1} \mu^2\partial_y g d\mu + \sigma(y)\int_{-1}^{1} \mu g d\mu = \frac{2}{3}$
- Integrate with respect to y: $\tilde{\sigma} = \frac{1}{|T|}\int_T \sigma(y)dy = \langle\sigma\rangle$

Hence in 1D geometry, effective opacity is always an arithmetic mean $\langle\sigma\rangle$.

Extension to 3D geometries (isotropic case)

For arbitrary geometry, cell problem cannot be solved analytically but bounds can be exhibited[Cl98].

$$\tilde{D} = D_0 - f_p \sigma_p \mathbb{E} \sum_{n=0}^{\infty} F(\kappa_0) F(\kappa_n) \quad \begin{cases} (\kappa_n)_{n \geq 0} \text{ Ergodic markov chain} \\ F \text{ centered random variable} \end{cases}$$

$$2\mathbb{E} \sum_{n=0}^{\infty} F(\kappa_0) F(\kappa_n) = \mathbb{E} F(\kappa_0)^2 + \lim_{N \to \infty} \mathbb{E} \left(\frac{1}{\sqrt{N}} \sum_{n=0}^{N} F(\kappa_n) \right)^2 \geq 0,$$

Hence $\tilde{\sigma} \geq \sigma_{vdh} = \dfrac{1}{3D_0}$.

$$D_0 = \int \frac{d\overrightarrow{\Omega}}{4\pi} \int P(d\omega) \int_0^{\infty} dt e^{-\int_0^t \sigma(\overrightarrow{\Omega} s, \omega) ds}.$$

Integration takes place only along straight lines (no scattering): knowing chord length distributions of fuel and pusher, it can be computed using renewal techniques (see [Vdh88]).

Renewal effective opacity

Replace scattering by absorption:

$$\partial_t \phi + \overrightarrow{\Omega} \cdot \nabla \phi + \sigma(x)\phi = 0.$$

Solve along characteristics: $s = x + \overrightarrow{\Omega} t$

$$\partial_s \phi + \sigma(s)\phi = 0 \Rightarrow \phi(s) = e^{-\int_0^s \sigma(y)dy}$$

Effective opacity is defined by $e^{-\tilde{\sigma} s} = \mathbb{E} e^{-\int_0^s \sigma(y)dy}$.

$$\tilde{\sigma} = \left(\int_0^\infty e^{-\tilde{\sigma} s} ds \right)^{-1} = \left(\int_0^\infty \mathbb{E} e^{-\int_0^s \sigma(y)dy} ds \right)^{-1}$$

Define $g_f(x) = \mathbb{E}(e^{-\int_0^x \sigma(y)dy}/0 \in f),\ g_p(x) = \mathbb{E}(e^{-\int_0^x \sigma(y)dy}/0 \in p)$.
Effective diffusion is

$$D_0 = c_f \int_0^\infty g_f(x)dx + c_p \int_0^\infty g_p(x)dx = c_f \hat{g}_f(0) + c_p \hat{g}_p(0)$$ (Laplace transform)

Renewal equations are (for markovian statistics)

$$\begin{cases} g_f(x) = \int_0^x g_p(x-y)e^{-\sigma_f y}\frac{e^{-y/l_f}}{l_f}dy + \frac{e^{-(\sigma_f+1/l_f)x}}{l_f(\sigma_f+1/l_f)} \\ g_p(x) = \int_0^x g_f(x-y)e^{-\sigma_p y}\frac{e^{-y/l_p}}{l_p}dy + \frac{e^{-(\sigma_p+1/l_p)x}}{l_p(\sigma_p+1/l_p)} \end{cases}$$

Taking Laplace transform and solving gives

$$\frac{1}{3D_0} = \sigma_{vdh} = \frac{\langle\sigma\rangle + c_f l_p \sigma_p \sigma_f}{1 + c_f l_p(\sigma_f + \sigma_p - \langle\sigma\rangle)}.$$

Extension to 3D geometries

We consider imbedding of pusher spheres in the fuel and use the same approach as for slowing down problem. We neglect opacity in fuel $\sigma_f = 0$.

- Find asymptotic values for $\tilde{\sigma}$ when $\sigma_p r \ll 1$ and $\sigma_p r \gg 1$ (optical depth of one single sphere).
- Propose a generic formula depending on weight function $\exp(-c_f^2 \sigma_p r)$ and having the correct limiting behavior.
- Fit the formula on numerical simulations

For $\sigma_p r \ll 1$, $\tilde{\sigma} \sim \langle \sigma \rangle = c_p \sigma_p$
For $\sigma_p r \gg 1$ and $\sigma_f = 0$:
Effective diffusion coefficient writes as

$$D = c_p \int_0^\infty \mathbb{E}(\overrightarrow{\Omega}(0)\overrightarrow{\Omega}(t)/0 \in p)dt + c_f \int_0^\infty \mathbb{E}(\overrightarrow{\Omega}(0)\overrightarrow{\Omega}(t)/0 \in f)dt$$

If starting point 0 is in p, collision immediatly takes place:

$$\lim_{\sigma_p r \to \infty} \mathbb{E}(\overrightarrow{\Omega}(0)\overrightarrow{\Omega}(t)/0 \in p)dt = 0.$$

If starting point 0 is in f, $X(t)$ follows a straight line until it hits a sphere and then $\mathbb{E}(\overrightarrow{\Omega}(0)\overrightarrow{\Omega}(t)) = 0, t \geq T$.

$$D \sim \frac{c_f l_f}{3} \; l_f \text{ mean chord length between two spheres}$$

From ergodicity

$$l_f = l_p \frac{c_f}{c_p} = \frac{3c_f}{4c_p r}$$

Hence $\tilde{\sigma} \sim \frac{4c_p}{3c_f^2 r}$ (Rigorous proof ?).

We look for a fitting formula:

$$\tilde{\sigma} = c_p \sigma_p (1 - \frac{4\alpha}{3}) e^{-\alpha c_f^2 \sigma_p r} + \frac{4c_p}{3} \frac{1 - e^{-\alpha c_f^2 \sigma_p r}}{c_f^2 r}$$

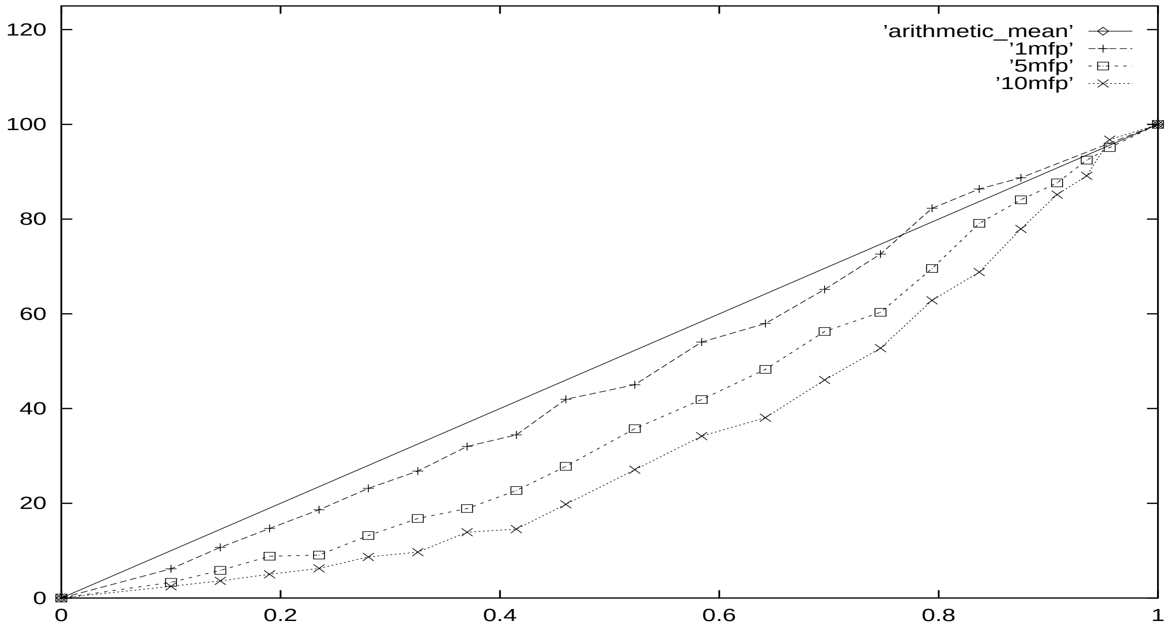
α being fitted on numerical simulations.

For $\sigma_f = 0$, renewal theory gives (with same mean chord length)

$$\tilde{\sigma} = \frac{c_p \sigma_p}{1 + \frac{3}{4} c_f^2 \sigma_p r}$$

Numerical computation of $\tilde{\sigma}$

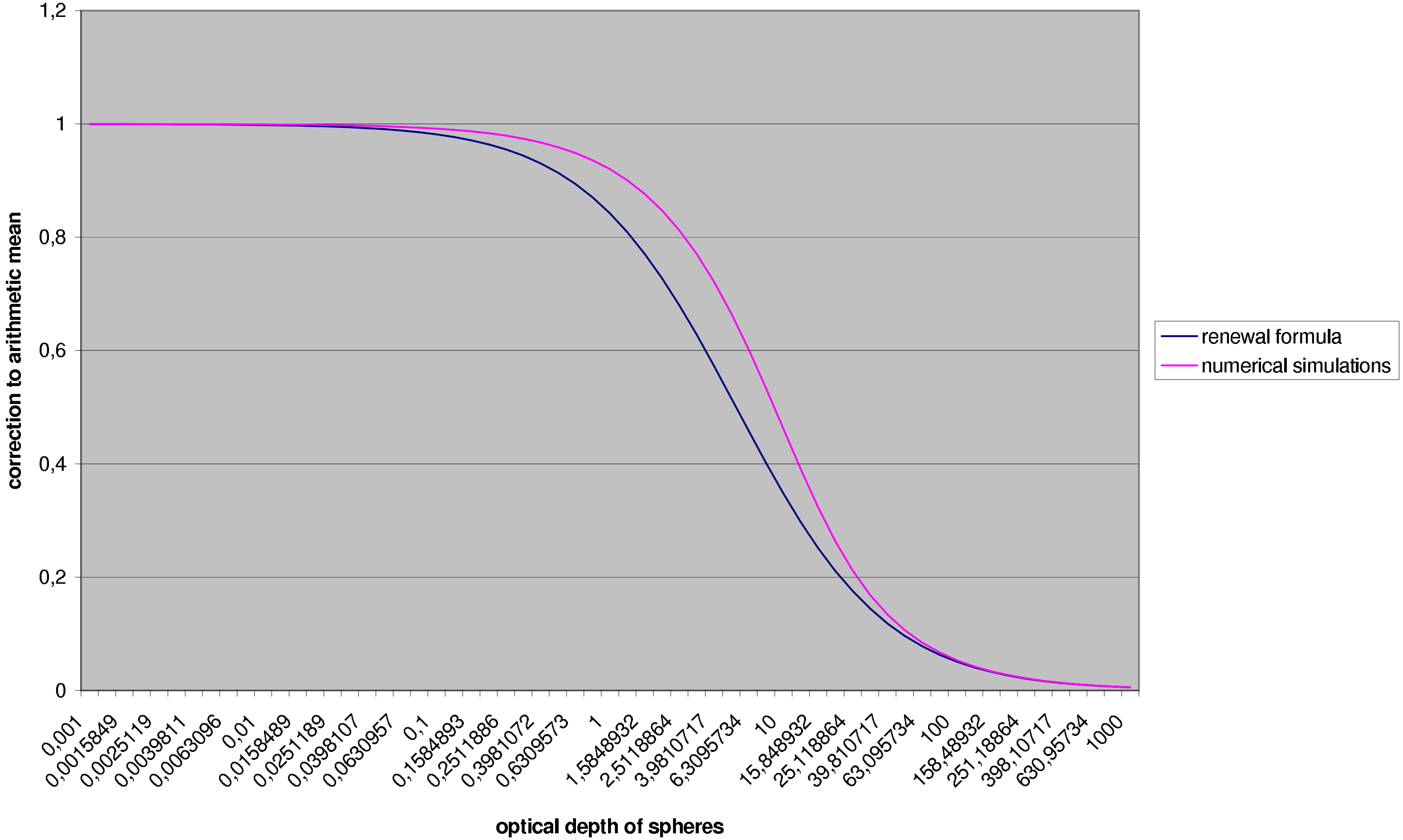
We use the probabilistic representation of the PDE and perform simulations of $\mathbb{E}X(t)^2/2t$ for random inclusions of spheres with different optical depth of spheres



Effective opacity as a function of volume fraction c_p

Comparison between the two formulas

We compare the two formulations: main difference appear for optical depth of spheres of order 1.



Why does renewal effective opacity (transport on a line without scattering) compare well with homogenization effective opacity (with scattering in 3D geometry)??

Concluding remarks

- Particle transport through binary mixtures must be simplified if used in hydrocode simulations.
- Homogenization theory gives the theoretical framework for proving that effective behavior exists but is of limited interest for computing explicitly effective coefficients
- Although not always applicable, renewal theory gives simplified coefficients which compare well with numerical simulations in 3D geometries
- Renewal computations can easely be extended to more complex mixtures (more than two phases).
- Knowledge of the details of the random medium (i.e. chord length distribution functions) is not necessary

One of the main issue that we did not address is how to obtain the characteristic length scale of the mixture from a statistical hydrodynamical model (two-point turbulence models).

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