Transport in Media and Geometry

SNU/NUKE/EHK

Interaction/Survival Probability in medium

- ✓ A particle starts at position $\vec{x}_o$ in an arbitrary infinite scattering medium and the particle is directed along an axis with unit direction vector $\vec{\mu}$.

- ✓ The probability that a particle exists at position $\vec{x}$ relative to $\vec{x}_o$ without having collided is $p_s(\vec{\mu}\cdot(\vec{x}-\vec{x}_o))$, the survival probability.

- ✓ The change in survival probability due to interaction is characterized by an interaxtion coefficient $\mu(\vec{\mu}\cdot(\vec{x}-\vec{x}_o))$ (in unit L^{-1}). This interaction coefficient can change along the particle flight path.

- ✓ The change in survival probability is expressed by the following equation :

$$\mathrm{d}p_{\mathrm{s}}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0)) = -p_{\mathrm{s}}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))\mu(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))\mathrm{d}(\vec{\mu}\cdot(\vec{x}-\vec{x}_0))$$

Interaction Probability in an infinite medium

- To simplify, let $\vec{x}_o$ = (0, 0, 0) and $\vec{x}$ = (0, 0, 1) .

  Then,

$$\frac{\mathrm{d}p_\mathrm{s}(z)}{p_\mathrm{s}(z)} = -\mu(z)\mathrm{d}z$$

- We can integrate this for z = 0 where we assume that p(0) = 1 to z and obtain the survival probability at z :

$$p_\mathrm{s}(z) = \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)$$

- The probability that a particle has interacted <u>within a distance z</u> is simply 1 − p_s(z), the cumulative probability c(z) :

$$c(z) = 1 - p_\mathrm{s}(z) = 1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)$$

- Since the medium is <u>infinite</u>, c(∞) = 1 and p_s(∞), = 0.

Interaction Probability in an infinite medium (cont)

- *The differential (per unit length) probability, p(z), for interaction at z can be obtained by p(z) = dc(z)/dz;*

$$p(z) = \frac{\mathrm{d}}{\mathrm{d}z}\left[1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)\right] = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) = \mu(z)p_{\mathrm{s}}(z)$$

- *With constant μ (homogeneous medium),*

$$p_{\mathrm{s}}(z) = e^{-\mu z} \quad \textit{and} \quad c(z) = 1 - p_{\mathrm{s}}(z) = 1 - e^{-\mu z} \ .$$

- *Thus,* $p(z) = \frac{\mathrm{d}}{\mathrm{d}z}[1 - e^{-\mu z}] = \mu e^{-\mu z} = \mu p_{\mathrm{s}}(z)$

Interaction Probability in a finite medium

✓ When the medium is finite with a boundary at $z = z_b$,

$$\underline{c(\infty)} = 1 - p_s(\infty) = 1 - \exp\left(-\int_0^\infty dz'\mu(z')\right) \underline{< 1}$$

that is, the cumulative probability at infinity is less than one because either the particle escapes a finite geometry or $\mu(z) = 0$ beyond some limit.

✓ Rewrite the cumulative probability as

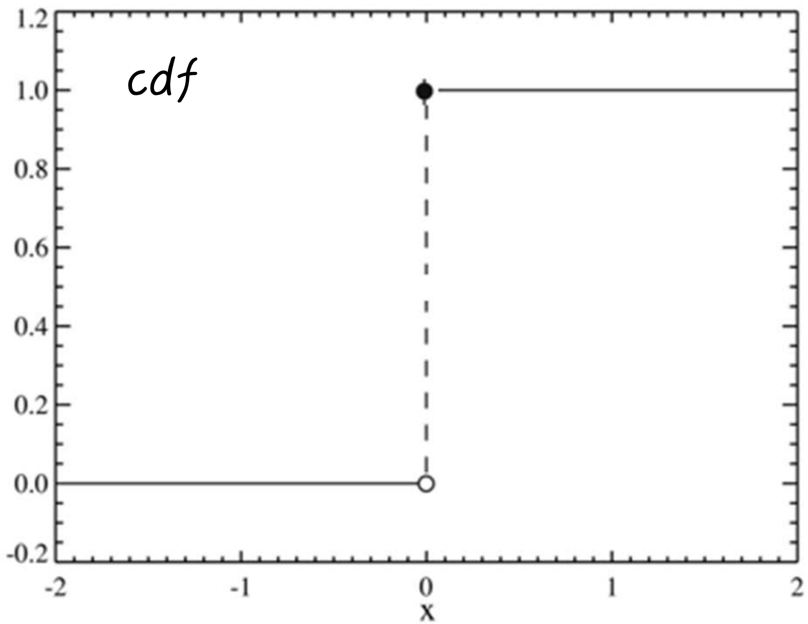
$$c(z) = 1 - p_s(z) = 1 - \exp\left(-\int_0^z dz'\mu(z')\right) + \exp\left(-\int_0^{z_b} dz'\mu(z')\right)\theta(z - z_b)$$

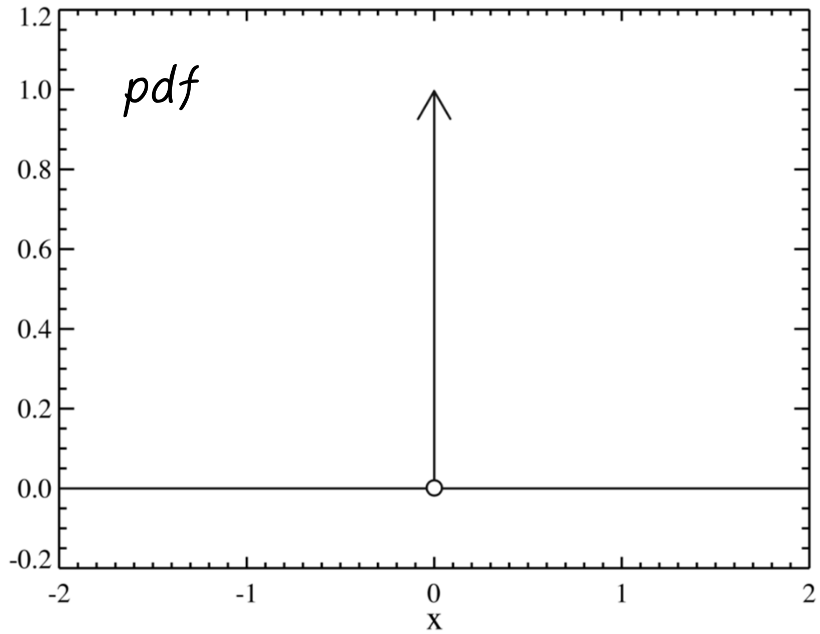
by drawing a boundary at $z = z_b$, and assuming that $\mu(z) = 0$ for $z \geq z_b$, where $\theta(x) = 1$ if $x \geq 0$ and $= 0$ if $x < 0$.

– The probability distribution becomes

$$\frac{d}{dz}c(z) = p(z) = \mu(z)\exp\left(-\int_0^z dz'\mu(z')\right) + p_s(z_b)\delta(z - z_b) \quad (Eq.\ 1)$$

$$\theta(x), \quad \delta(x) = \frac{d}{dx}\theta(x)$$





Interaction Probability in a finite medium (cont.)

$$c(z) = 1 - p_{\mathrm{s}}(z) = 1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) + \exp\left(-\int_0^{z_{\mathrm{b}}} \mathrm{d}z'\mu(z')\right)\theta(z - z_{\mathrm{b}})$$

$$p(z) = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) + p_{\mathrm{s}}(z_{\mathrm{b}})\delta(z - z_{\mathrm{b}}) \qquad \text{(Eq. 1)}$$

- ✓ Once the particle reaches the boundary, it reaches it overcoming a cumulative probability equal to one minus its survival probability. Probability is conserved.
- ✓ If a particle reaches the boundary, it is absorbed and transport discontinues. (This is exactly what is done in a MC simulation.)
- ✓ If this were not the case, an attempt at particle transport simulation would put the logic into an infinite loop. (This is exactly what happens in nature!)

$$c(z) = 1 - p_{\mathrm{s}}(z) = 1 - \exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) \quad \text{and} \quad p(z) = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)$$

, for $z < z_b$.

$c(z_b) = 1$ and $p(z_b) = p_s(z_b)\cdot\delta(0) = \infty$; $c(z) = 1$ and $p(z) = 0$, for $z > z_b$.

Crossing boundary of different media

✓ The μ_i's in their own domains are

$$\begin{aligned} \mu(z) &= \mu_1(z)\theta(z)\theta(b_1 - z) \\ &+ \mu_2(z)\theta(z-b_1)\theta(b_2 - z) \\ &+ \mu_3(z)\theta(z-b_2)\theta(b_3 - z) \\ &\vdots \end{aligned}$$

where $\theta(x) = 1$ if $x \geq 0$, and $= 0$ if $x < 0$.

✓ The interaction probability at z is $\boxed{p(z) = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right)}$

$$\begin{aligned} p(z) &= \theta(z)\theta(b_1 - z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')} \\ &+ \theta(z-b_1)\theta(b_2 - z)\mu_2(z)e^{-\int_0^{b_1} \mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^z \mathrm{d}z'\mu_2(z')} \\ &+ \theta(z-b_2)\theta(b_3 - z)\mu_3(z)e^{-\int_0^{b_1} \mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^{b_2} \mathrm{d}z'\mu_2(z')}e^{-\int_{b_2}^z \mathrm{d}z'\mu_3(z')} \\ &\vdots \end{aligned}$$

Crossing boundary of different media (cont.)

✓ The interaction probability at z is

$$
\begin{aligned}
p(z) &= \theta(z)\theta(b_1 - z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')} \\
&+ \theta(z-b_1)\theta(b_2 - z)\mu_2(z)e^{-\int_0^{b_1} \mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^{z} \mathrm{d}z'\mu_2(z')} \\
&+ \theta(z-b_2)\theta(b_3 - z)\mu_3(z)e^{-\int_0^{b_1} \mathrm{d}z'\mu_1(z')}e^{-\int_{b_1}^{b_2} \mathrm{d}z'\mu_2(z')}e^{-\int_{b_2}^{z} \mathrm{d}z'\mu_3(z')} \\
&\vdots
\end{aligned}
$$

Or

$$
\begin{aligned}
p(z) &= \theta(z)\theta(b_1 - z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')} \\
&+ p_\mathrm{s}(b_1)\theta(z-b_1)\theta(b_2 - z)\mu_2(z)e^{-\int_{b_1}^{z} \mathrm{d}z'\mu_2(z')} \\
&+ p_\mathrm{s}(b_2)\theta(z-b_2)\theta(b_3 - z)\mu_3(z)e^{-\int_{b_2}^{z} \mathrm{d}z'\mu_3(z')} \\
&\vdots
\end{aligned}
$$

where $\theta(x) = 1$ if $x \geq 0$, and $= 0$ if $x < 0$.

Crossing boundary of different media (cont.)

- Now consider a change of variables $b_{i-1} \le z_i \le b_i$ and introduce the conditional survival probability $p_s(b_i|b_{i-1})$ which is the probability that a particle does not interact in the region $b_{i-1} \le z_i \le b_i$ given that it has not interacted in a previous region either.
- By conservation of probability:

$$p_{\mathrm{s}}(b_i) = p_{\mathrm{s}}(b_{i-1})p_{\mathrm{s}}(b_i|b_{i-1})$$

then, we can rewrite

$$\begin{aligned} p(z) &= \theta(z)\theta(b_1 - z)\mu_1(z)e^{-\int_0^z \mathrm{d}z'\mu_1(z')} \\ &+ p_{\mathrm{s}}(b_1)\theta(z - b_1)\theta(b_2 - z)\mu_2(z)e^{-\int_{b_1}^z \mathrm{d}z'\mu_2(z')} \\ &+ p_{\mathrm{s}}(b_2)\theta(z - b_2)\theta(b_3 - z)\mu_3(z)e^{-\int_{b_2}^z \mathrm{d}z'\mu_3(z')} \\ &\vdots \end{aligned}$$

into

$$\begin{aligned} p(z) &= p(z_1, z_2, z_3 \cdots) \\ &= p(z_1) + p_{\mathrm{s}}(b_1)[p(z_2) + p_{\mathrm{s}}(b_2|b_1)[p(z_3) + p_{\mathrm{s}}(b_3|b_2)[\cdots \end{aligned}$$

Crossing boundary of different media (cont.)

✓ $p(z) = p(z_1, z_2, z_3 \cdots) = p(z_1) + p_s(b_1)[p(z_2) + p_s(b_2|b_1)[p(z_3) + p_s(b_3|b_2)[\cdots$

, which means that the variables z_1, z_2, $z_3 \cdots$ ($z_i = z - b_{i-1}$) can be treated as independent.

– If we consider the interactions over z_1 as independent, then from (Eq. 1) we have:

$$p(z_1) = \mu_1(z_1)\exp\left(-\int_0^{z_1} dz'\mu_1(z')\right) + p_s(b_1)\delta(z_1 - b_1)$$

– If the particle makes it to $z = b_1$, consider z_2 as an independent variable and sample from:

$$p(z_2) = \mu_2(z_2)\exp\left(-\int_0^{z_2} dz'\mu_2(z')\right) + p_s(b_2|b_1)\delta(z_2 - b_2)$$

– If the particle makes it to $z = b_2$, consider z_3 as an independent variable and sample from

$$p(z_3) = \mu_3(z_3)\exp\left(-\int_0^{z_3} dz'\mu_3(z')\right) + p_s(b_3|b_2)\delta(z_3 - b_3)$$

and so on.

$$p(z) = \mu(z)\exp\left(-\int_0^{z} dz'\mu(z')\right) + p_s(z_b)\delta(z - z_b) \quad \text{(Eq. 1)}$$

Crossing boundary of different media (cont.)

<u>Example</u>

$$p(z) = \mu(z)\exp\left(-\int_0^z \mathrm{d}z'\mu(z')\right) + p_\mathrm{s}(z_\mathrm{b})\delta(z - z_\mathrm{b})$$

- ✓ Consider only two regions of space on either side of z = b with different interaction coefficients. That is:

$$\mu(z) = \mu_1\theta(b - z) + \mu_2\theta(z - b)$$

- ✓ The interaction probability for this example is:

$$p(z) = \theta(b - z)\mu_1 e^{-\mu_1 z} + \theta(z - b)\mu_2 e^{-\mu_1 b} e^{\mu_2(z-b)} \quad \text{(Eq. 2)}$$

- ✓ Now, treat z_1 as independent, that is

$$p(z_1) = \mu_1 e^{-\mu_1 z_1} + e^{-\mu_1 b}\delta(z_1 - b)$$

- ✓ If the particle makes it to z = b, we consider z_2 as an independent variable and sample from:

$$p(z_2) = \mu_2 e^{-\mu_2 z_2}$$

which is the identical probability distribution implied by (Eq. 2)

Crossing boundary of different media (cont.)

<u>Example</u>

- ✓ The importance of this proof is as follows:
  - The interaction of a particle is dependent only on the local scattering conditions.
  - If space is divided up into regions of locally constant interaction coefficients, then we may sample the distance to an interaction by considering the space to be uniform in the local interaction coefficient.
  - We sample the distance to an interaction and transport the particle.
  - If a boundary demarcating a region of space with different scattering characteristics interrupts the particle transport, we may stop at that boundary and
  - resample using the new interaction coefficient of the region beyond the boundary.

Crossing boundary of different media (cont.)

Example

- The alternative approach would be to invert the cumulative probability distribution implied by

$$c(z) = 1 - p_s(z) = 1 - \exp\left(-\int_0^z dz'\mu(z')\right) \quad ; \quad \int_0^z dz'\mu(z') = -\log_e(1-r)$$

where r is a uniform random number between 0 and 1.

$$z = \sum_{i=1}^{k}(b_i) + z_{k+1} \quad \text{from} \quad \sum_{i=1}^{k}(\mu_i \cdot b_i) + (\mu_{k+1} \cdot z_{k+1}) = -\log_e(1-r);$$

- The interaction distance z would be determined by summing the interaction coefficient until the equality in the Eq. is satisfied.
- In some applications it may be efficient to do the sampling directly according to the above. In other applications it may be more efficient to resample every time the interaction coefficient changes.
- It is simply a trade-off between the time taken to index the look-up table for μ(z) and recalculating the logarithm in a resampling procedure.