STOCHASTIC TRANSITION MATRIX APPROACH

TO

STOCHASTIC TRANSPORT

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EXAMPLES OF STOCHASTIC TRANSPORT

There are a number of areas in neutron and photon transport where the medium is spatially random.

Typical of such problems are 1) disposition of sources in a radioactive drum, 2) the fuel lumps in a pebble-bed reactor, 3) absorbing materials in reactors which use burnable poisons, 4) clouds containing randomly dispersed water droplets, and 5) boron lumps in concrete shields.

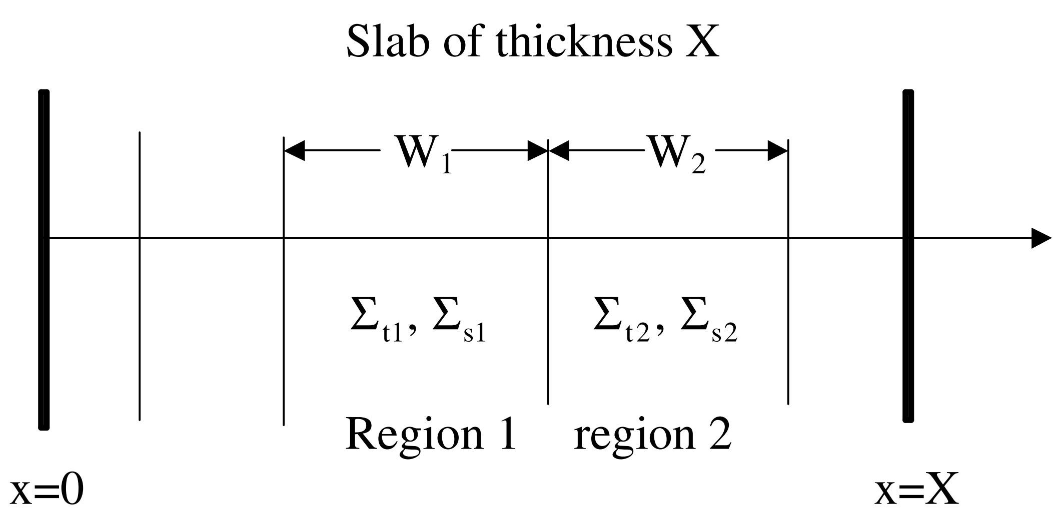
In each of these problems, the spatial distribution of the absorbers and scatterers are no longer known deterministically but rather in the form of a statistical distribution.

STOCHASTIC TRANSPORT IN 1-D

- The steady state one-dimensional transport equation with isotropic scattering:

$$\mu \frac{\partial \Psi(x,\mu)}{\partial x} + \Sigma_t(x)\Psi = \frac{\Sigma_s(x)}{2} \int_{-1}^{+1} d\mu' \Psi(x,\mu')] + Q(x,\mu)$$

- The cross-sections are spatially random



Transport equation in matrix form (S_N description)

$$\frac{d\boldsymbol{\Psi}(x)}{dx} = -\mathbf{A}(x)\boldsymbol{\Psi}(x) + \mathbf{S}(x)$$

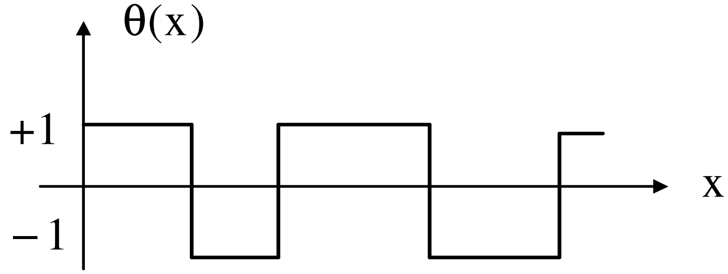
where

$\Psi_j(x) = \Psi(x, \mu_j)$ with j=1ÉN,

$\mathbf{A}(x) = \mathbf{A}_0 + \theta(x)\mathbf{A}_1$

θ (x)=+1 when x is in the material region Ò1Ó

$\theta(x) = -1$ in the material region Ò2Ó



A particular realization of $\{\theta(x)\}$

$P(W_j) = e^{-W_j\lambda_j}\lambda_j$ ((j=1,2)

$P[\theta(x)=1] = p_1 = \lambda_2/(\lambda_1+\lambda_2)$

$P[\theta(x)=-1] = p_2 = \lambda_1/(\lambda_1+\lambda_2)$

$\{\theta(x)\}$ is *a Dichotomic (or binary) Markov processes* with transition probability per unit increment in the positive x-direction Òλ_1Ófrom θ=+1 to $\theta=-1$, and Òλ_2Ófrom $\theta=-1$ (*Generalized Telegraph Signal)*

Stochastic Transition Matrix (STM) formalism

- The solution of

$$\frac{d\boldsymbol{\Psi}(x)}{dx} = -\mathbf{A}(x)\boldsymbol{\Psi}(x) + \mathbf{S}(x)$$

$$\boxed{\boldsymbol{\Psi}(x) = \mathbf{U}(x)\boldsymbol{\Psi}(0) + \int_0^x dx'\,\mathbf{U}(x,x')\mathbf{S}(x')}$$

where $\mathbf{U}(x)$ and $\mathbf{U}(x,x')$ are the solutions of

$$\boxed{\frac{d\mathbf{U}(x)}{dx} = -\mathbf{A}(x)\mathbf{U}(x)}$$

Initial conditions $\mathbf{U}(0) = \mathbf{I}$ and $\mathbf{U}(x',x') = \mathbf{I}$, respectively.

$\mathbf{U}(x)$ is stochastic. $\{\mathbf{U}(x)\}$ with the initial value $\mathbf{U}(0) = \mathbf{I}$

is not a Markov process.

However, the joint matrix process

$\{\Theta(x), \mathbf{U}(x)\}$ *is Markov!*

- The averaged STM: $<\mathbf{U}(x)>$

$$<\mathbf{U}(x)> = <\mathbf{U}(x)>_1 + <\mathbf{U}(x)>_2$$

$$\frac{d}{dx}<\mathbf{U}(x)>_1 = -(\mathbf{A}_0 + \mathbf{A}_1)<\mathbf{U}>_1 - \lambda_1<\mathbf{U}>_1 + \lambda_2<\mathbf{U}>_2$$

$$\frac{d}{dx}<\mathbf{U}(x)>_2 = -(\mathbf{A}_0 - \mathbf{A}_1)<\mathbf{U}>_2 - \lambda_2<\mathbf{U}>_2 + \lambda_1<\mathbf{U}>_1$$

Initial conditions $<\mathbf{U}(x)>_1 = p_1\mathbf{I}$ and $<\mathbf{U}(x)>_2 = p_2\mathbf{I}$.

- Conclusion: <U(x)> is *exactly* calculable.

A special case: The density n(x) of the medium is random.

- In this case **U**(x) satisfies

$$\boxed{\frac{d\mathbf{U}(x)}{dx} = -n(x)\mathbf{A}\,\mathbf{U}(x),}$$

where **A** depends only on the microscopic cross-sections.

$$\mathbf{U}(x) = e^{-z(x)\mathbf{A}}, \quad \text{with } z(x) \equiv \int_0^x dx'\, n(x').$$

The calculation of $<\mathbf{U}(x)>$ is considerably simplified by expanding **A** as

$$\mathbf{A} = \sum_{j=1}^{N} \gamma_j \mathbf{E_j}, \quad \text{where} \quad \mathbf{E}_j\mathbf{E}_k = \delta_{j,k}\mathbf{E}_j$$

where γ_j are the eigen-values of $\mathbf{A}$.

Then $<\mathbf{U}(x)>$ is expressed as

$$\boxed{<\mathbf{U}(x)>=\sum_{j=1}^{N}<e^{-z(x)\gamma_j}>\mathbf{E}_j=\sum_{j=1}^{N}<u(x)>_j\mathbf{E}_j},$$

where u(x) satisfies, generically,

$$\frac{du(x)}{dx}=-\gamma\, n(x)u(x).$$

Its mean $<u(x)>=\ <u(x)>_1+<u(x)>_2$ is calculated from

$$\frac{d<u(x)>_1}{dx}=-(\gamma n_1+\lambda_1)<u>_1+\lambda_2<u>_2,$$

$$\frac{d<u(x)>_2}{dx}=-(\gamma n_2+\lambda_2)<u>_2+\lambda_1<u>_1,$$

with $<u(0)>_1=p_1$ and $<u(0)>_2=p_2$.

IMPLEMENTATION OF THE BOUNDARY CONDITIONS

Start with

$$\mathbf{\Psi}(x) = \mathbf{U}(x)\mathbf{\Psi}(0) + \int_0^x dx'\,\mathbf{U}(x,x')\mathbf{S}(x')$$

Average both sides

$$<\mathbf{\Psi}(x)> = <\mathbf{U}(x)\mathbf{\Psi}(0)> + \int_0^x dx' <\mathbf{U}(x,x')> \mathbf{S}(x')\,.$$

Approximate

$$<\mathbf{U}(x)\mathbf{\Psi}(0)> \approx <\mathbf{U}(x)><\mathbf{\Psi}(0)>$$

(The only approximation needed in the STM approach).

$$\boxed{<\mathbf{\Psi}(x)> \approx <\mathbf{U}(x)><\mathbf{\Psi}(0)> + \int_0^x dx' <\mathbf{U}(x,x')> \mathbf{S}(x')}\,.$$

Only half of the components of $\mathbf{\Psi}(0)$ are specified at x=0, and half of $\mathbf{\Psi}(X)$ is specified at the second boundary at x=X.

$$<\mathbf{\Psi}(X)> \approx <\mathbf{U}(X)><\mathbf{\Psi}(0)> + \int_0^X dx' <\mathbf{U}(X,x')> \mathbf{S}(x')$$

to determine the unknown components $<\mathbf{\Psi}(0)>$ and $<\mathbf{\Psi}(X)>$.

Summary of the STM Approach:

$$<\boldsymbol{\Psi}(x)>\approx<\mathbf{U}(x)><\boldsymbol{\Psi}(0)>+\int_0^x dx'<\mathbf{U}(x,x')>\mathbf{S}(x'),$$

$$<\boldsymbol{\Psi}(X)>\approx<\mathbf{U}(X)><\boldsymbol{\Psi}(0)>+\int_0^X dx'<\mathbf{U}(X,x')>\mathbf{S}(x'),$$

where $<U(x)>$ is calculated exactly for a given set of cross-sections.

□ CONNECTION WITH THE ŅMODIFIED-LEVERMORE-POMRANINGÓEQUATIONS

Write the first equation using

$$<\boldsymbol{\Psi}(x)>=<\boldsymbol{\Psi}(x)>_1+<\boldsymbol{\Psi}(x)>_2$$

$$<\mathbf{U}(x)>=<\mathbf{U}(x)>_1+<\mathbf{U}(x)>_2,$$

Connection with the MLP equations:

$$<\mathbf{\Psi}(x)>_j \approx <\mathbf{U}(x)>_j <\mathbf{\Psi}(0)> + \int_0^x dx' <\mathbf{U}(x,x')>_j \mathbf{S}(x'), \qquad \text{(j=1,2)}.$$

We differentiate with respect x:

$$\frac{d<\mathbf{\Psi}(x)>_j}{dx} \approx \frac{d<\mathbf{U}(x)>_j}{dx} <\mathbf{\Psi}(0)> + \int_0^x dx' \frac{<\mathbf{U}(x,x')>_j}{dx} \mathbf{S}(x') + p_j \mathbf{S}(x) \; ,$$

MLP equations:

$$\mu \frac{\partial}{\partial x} <\Psi(x,\mu)>_1 + \Sigma_{t1} <\Psi>_1 = \frac{\Sigma_{s1}}{2} \int_{-1}^{1} d\mu' <\Psi(x,\mu')>_1$$

$$+\mu[\lambda_2 <\Psi>_2 - \lambda_1 <\Psi>_1] + p_1 Q(x,\mu) \, ,$$

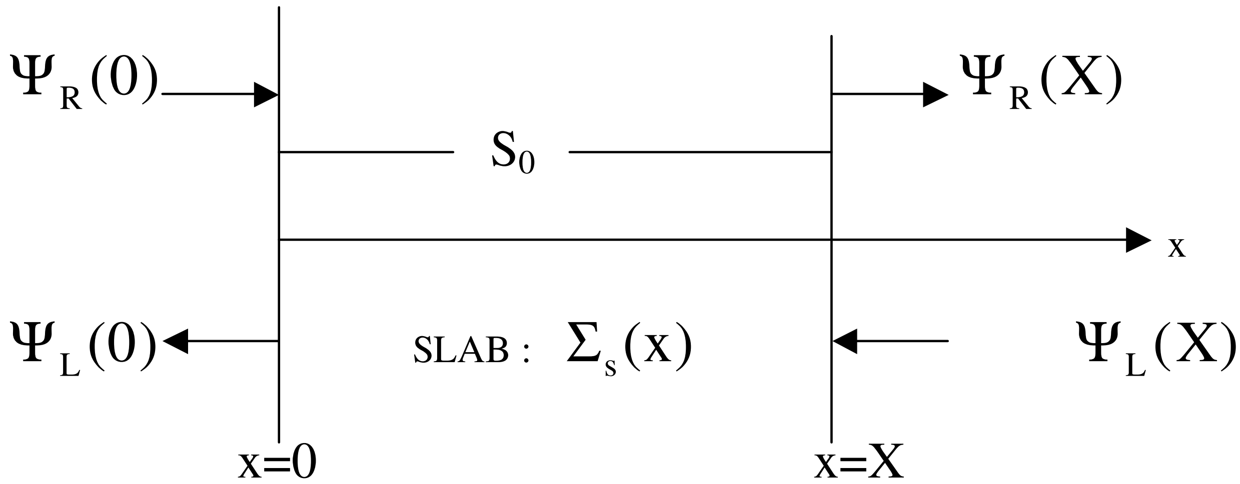
$$\mu \frac{\partial}{\partial x} <\Psi(x,\mu)>_2 + \Sigma_{t2} <\Psi>_2 = \frac{\Sigma_{s2}}{2} \int_{-1}^{1} d\mu' <\Psi(x,\mu')>_2$$

$$+\boxed{\mu}[\lambda_1 <\Psi>_1 - \lambda_2 <\Psi>_2] + p_2 Q(x,\mu) \, .$$

with $<\Psi(0,\mu)>_1 = p_1 <\Psi(0,\mu)>$ and $<\Psi(0,\mu)>_2 = p_2 <\Psi(0,\mu)>$.

Applications: **Two-Stream Transport**

- **Pure**ly **Scattering slab**



Two-stream transport equations read

$$\boxed{\frac{d\Phi(x)}{dx} = -\Sigma_s(x)J(x)} \quad \text{and} \quad \boxed{\frac{dJ(x)}{dx} = S_0}\ .$$

where $\Phi(x) = \Psi_R(x) + \Psi_L(x)$ and $J(x) = \Psi_R(x) - \Psi_L(x)$.

Introducing $\mathbf{\Psi}(x) = [\Phi(x), J(x)]^T$ and $\mathbf{S} = [0,1]^T S_0$ we write this as

Purely Scattering Slab: Continued

$$\boxed{\frac{d\boldsymbol{\Psi}(x)}{dx} = -\Sigma_s(x)\mathbf{A}\boldsymbol{\Psi}(x) + \mathbf{S}}, \qquad \text{with} \quad \mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

$$\mathbf{U}(x) = e^{-z(x)\mathbf{A}}, \qquad \text{with } z(x) = \int_0^x dx' \Sigma_s(x').$$

Using the property $\mathbf{A}^2 = \mathbf{0}$, we find the delightfully simple result

$$\mathbf{U}(x) = \mathbf{I} - z(x)\mathbf{A}.$$

$<\mathbf{U}(x)>$ immediately follows from this as $<\mathbf{U}(x)> = \mathbf{I} - <z(x)>\mathbf{A}$,

$$\boxed{<\mathbf{U}(x)> = \mathbf{I} - x\bar{\Sigma}_s\mathbf{A}} \quad \text{with} \qquad \bar{\Sigma}_s = <\Sigma_s(x)> = p_1\Sigma_{s1} + p_2\Sigma_{s2}.$$

The STM equation reads

$$<\boldsymbol{\Psi}(x)> \approx [\mathbf{I} - x\bar{\Sigma}_s\mathbf{A}] <\boldsymbol{\Psi}(0)> + \int_0^x dx'[\mathbf{I} - (x - x')\bar{\Sigma}_s\mathbf{A}]\mathbf{S}$$

$$\boxed{<\Phi(x)> \approx <\Phi(0)> - x\bar{\Sigma}_s J(0) - S_0\bar{\Sigma}_s\frac{x^2}{2}} \quad \text{and} \quad \boxed{<J(x> = <J(0)> + xS_0}.$$

- Implementation of the boundary conditions:

$$< \Phi(X) > \approx < \Phi(0) > - X\bar{\Sigma}_s J(0) - S_0 \bar{\Sigma}_s \frac{X^2}{2}$$

$$< J(X >=< J(0 > + XS_0$$

Using

$$< \Phi(0) >= \Psi_R(0) + < \Psi_L(0) > \text{ and } < J(0) >= \Psi_R(0) - < \Psi_L(0) >$$

one obtain $< \Psi_L(0) >$ and $< \Psi_R(X) >$, the exit current at x=X.

Two cases:

a) *External source, no incident particles*: $\Psi_R(0) = 0$, $\Psi_L(X) = 0$

$$\boxed{< \Phi(x) > \approx \frac{XS_0}{2}[1 + \bar{\Sigma}_s x(1 - \frac{x}{X})]}$$

b) *No source, incident fluxes* $\Psi_R(0)$ *and* $\Psi_L(X)$ *are given.*

$$\boxed{<\Phi(x)> \approx \Psi_R(0)[1 - x\bar{\Sigma}] + <\Psi_L(0)>[1 + x\bar{\Sigma}_s]}$$

where

$$<\Psi_L(0)> = \frac{(1/2)X\bar{\Sigma}_s\Psi_R(0) + \Psi_L(X)}{1 + (1/2)X\bar{\Sigma}_s}$$

$$<\Psi_R(X)> = \frac{\Psi_R(0) + 1/2)X\bar{\Sigma}\Psi_L(X)}{1 + (1/2)X\bar{\Sigma}_s} .$$

Observe:

(1) When $\Psi_R(0) = \Psi_L(X)$, $\quad <\Psi_L(0)> = <\Psi_R(X)> = \Psi_R(0)$

(2) When $\Psi_L(X) = 0$,

$$\text{Albedo} = \frac{<\Psi_L(0)>}{\Psi_R(0)} \approx \frac{X\bar{\Sigma}_s}{2 + X\bar{\Sigma}_s} ,$$

$$\text{Attenuation} = \frac{<\Psi_R(X)>}{\Psi_R(0)} \approx \frac{1}{1 + (1/2)X\bar{\Sigma}_s}$$

- **Purely absorbing Slab**

$$\frac{d\Psi(x)}{dx} = -\Sigma_a(x)\mathbf{A}\Psi(x)\text{, where } \mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \qquad \Psi(x) = [\Psi_R(x), \Psi_L(x)]^T$$

The eigen-values of $\mathbf{A}$ are $\gamma_1 = 1$ and $\gamma_2 = -1$.

$$\mathbf{A} = \gamma_1\mathbf{E}_1 + \gamma_2\mathbf{E}_2\text{, where } \mathbf{E}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \text{ and } \mathbf{E}_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

$$\boxed{< \mathbf{U}(x) >=< \exp[-z(x)\mathbf{A}] >=< u_1(x) > \mathbf{E}_1 + < u_2(x) > \mathbf{E}_2}$$

$$u_1(x) = e^{-z(x)}, \quad u_2(x) = e^{z(x)}, \quad z(x) \equiv \int_0^x dx'\Sigma_a(x') \ .$$

$$\boxed{< \Psi_R(x) >=< u_1(x) > \Psi_R(0)} \ ,$$

$$\boxed{< \Psi_L(x) >=< u_2(x) >< \Psi_L(0) >= \frac{< u_2(x) >}{< u_2(X) >}\Psi_L(X)}$$

$$< \Psi_R(X) >=< u_1(X) > \quad \text{and} \quad < \Psi_L(0) >= 1/ < u_2(X) > .$$

- Remark

The above derivation can also be carried out using $\mathbf{U}(x)$ directly, rather than $<\mathbf{U}(x)>$.

Then, *for each realization*

$$\Psi_R(x) = u_1(x)\Psi_R(0),$$

$$\Psi_L(x) = u_2(x)\Psi_L(0).$$

Evaluating the latter at x=X, $\Psi_L(0)$ would be calculated as

$$\Psi_L(0) = \Psi_L(X)/u_2(X) = u_1(X)\Psi_L(X),$$

thus satisfying the boundary condition in each realization. Then $\Psi_L(x)$ would read

$$\Psi_L(x) = u_1(X)u_2(x)\Psi_L(X),$$

and the symmetry condition $\Psi_R(X) = \Psi_L(0)$ would be satisfied at each realization, as well as with the average fluxes $<\Psi_R(x)> = <u_1(x)> \Psi_R(0)$ and $<\Psi_L(x)> = <u_1(X)u_2(x)> \Psi_L(X)$ without any particular model for the spatial randomness of $\Sigma_a(x)$.

conclusions

1. The stochastic transition matrix approach to stochastic transport proves to be more straightforward to implement than implementing the MLP equations. The main reason is that it does not involve the partial averages $<\Psi(x)>_1$ and $<\Psi(x)>_2$, and hence the difficulty associated with the implementation of their boundary conditions, as encountered when working with the MLP equations, is avoided.

2. When the density of the medium is spatially random, the calculation of the *average* of stochastic transition matrix is reduced to the calculation of the a scalar $<u(x)>=<\exp[\gamma z(x)]>$, which involves solving two MLP equations for $<u(x)>_1$ and $<u(x)>_2$ with well-defined initial conditions. This aspect of STM reduces the computational burden considerably.