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Monte Carlo vs. Deterministic Calculations (or Lagrangian vs. Eulerian Formulations) in Neutron Transport Analysis

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References

1. Eugene P. Wigner, "Mathematical Problems of Nuclear Reactor Theory," *Proceedings of Symposium in Applied Mathematics*, American Mathematical Society, Providence, Vol. 11, pp. 89-104 (1961).
2. R. Sanchez and N. J. McCormick, "A Review of Neutron Transport Approximations," *Nucl. Sci. Eng.*, **80**, 481 (1982).
3. E. E. Lewis, W. F. Miller, *Computational Methods of Neutron Transport*, American Nuclear Society, Inc., IL (1993).
4. Rudi J. J. Stamm'ler, Maximo J. Abbate, *Methods of Steady-State Reactor Physics in Nuclear Design*, Academic Press Inc. (1983).
5. I. Lux and L. Koblinger, *Monte Carlo Particle Transport Methods: Neutron and Photon Calculations*, CRC Press (1990).
6. L. B. Miller, "Monte Carlo Analysis of Reactivity Coefficients in Fast Reactors; General Theory and Applications," ANL-7307 (TID-4500), Argonne National Laboratory, IL (1967).

Contents of Comparisons between MC and Det.

1. Mathematician's Viewpoint

> … As Wigner pointed out, **neutron transport can be analyzed from two distinct points of view, analgous to the Lagrangian and Eulerian formulations of hydrodynamics**. One can either consider the particle density in a unit volume of phase space or one can focus attention on the individual particles and consider their motion. …

<Laurence B. Miller, 1967>

2. Code-User's Viewpoint

> An estimate of a physical quantity calculated by the Monte Carlo method **inevitably** has its statistical uncertainty.

Motivation

… Nowadays the trend in the development of general-purpose transport methods is to **combine the use of both the integrodifferential and integral equations**. …

<Sanchez and McCormick , 1982>

- M&C 2013, Monte Carlo Transport – Hybrid Methods
  - UM, *Improved Convergence of Monte Carlo Generated Multi-Group Scattering Moments*
  - NCSU, *Extending the Subspace Hybrid Method for Eigenvalue Problems in Reactor Physics Calculations*
  - NCSU/LANL, *A Hybrid Approach to the Neutron Transport k-Eigenvalue Problem Using NDA-based Algorithms*
  - KAIST, *Refinement of the Overlapping/Global Iteration Method based on Monte Carlo/p-CMFD Calculations*
  - UNIST, *Hybrid Method of Deterministic and Probabilistic Approaches for the Continuous Energy Neutron Transport Problem*
  - UM, *A New "Implicit Correlation" Method for Cross-Correlation Sampling in MCNPX-PoliMi*
  - …
  - KAIST, *Feasibility of a Monte Carlo-Deterministic Hybrid Method for Fast Reactor Analysis*

Objective of Reactor Theory

… When we speak about reactor theory, we still mean only that comparatively narrow set of problems the solution of which immediately preceded and made possible the establishment of the chain reaction and which concerns itself with the calculation of the neutron densities or neutron fluxes as functions of the position, time, and energy of the neutron. …

<Wigner, 1961>

$$N^i(\mathbf{r},t), \sigma_r^i(E),$$
$$f_r^i(E',\mathbf{\Omega}' \to E,\mathbf{\Omega})$$

$$\frac{1}{v}\frac{\partial \Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} = -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t) - \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$
$$+\int_{E'} dE' \int_{4\pi} d\mathbf{\Omega}' \Sigma_s(\mathbf{r},E') f_s(E',\mathbf{\Omega}' \to E,\mathbf{\Omega})\Phi(\mathbf{r},E',\mathbf{\Omega}',t)$$
$$+\int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \frac{\chi(E)}{4\pi} \nu_f(E)\Sigma_f(\mathbf{r},E')\Phi(\mathbf{r},E',\mathbf{\Omega}',t)$$
$$+Q_{ex}(\mathbf{r},E,\mathbf{\Omega},t)$$

$$k,$$
$$\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$

Boltzmann Equation

- The transport theory which permits one to calculate the neutron densities or fluxes is **an essentially statistical theory** because the behavior of individual neutrons is subject to statistical laws. Note that the theory goes back to the Boltzmann's book on the kinetic theory of gases.

  (L. Boltzmann, *Vorlesungen über Gastheorie*, Leipzig, J. A. Barth (1896)).

- The fundamental concept of the Boltzmann equation is the neutron flux $\Phi(\mathbf{r},E,\Omega,t)$ which gives for the time t the number of neutrons, multiplied by their speed, which satisfy the following conditions:

  (a) They are in unit volume at $\mathbf{r}$.

  (b) Their energy is in unit range at E.

  (c) The direction of their velocity lies within a unit solid angle about the direction defined by the unit vector Ω.

The Assumptions of Transport Theory

1. Φ is a continuous function.
   - The number of neutrons is so large that they can be considered to form a statistical assembly and a continuous flux function Φ can describe them adequately. This appears to imply such high neutron densities that the time behavior of Φ is governed by the law of averages.
2. Linearity
   - The neutron fluxes do not affect the medium of the reactor so that the transport equation for the flux is linear. This also implies the neglect of neutron-neutron collisions.
3. Disregard of the wave nature of the neutrons
   - Classical mechanics forms the basis of the transport equation disregarding the wave nature of the neutrons, for example, the simultaneous specification of energy and position in flux. The only case in which the wave nature of the neutrons plays a macroscopic role is the diffraction in crystalline media which can be overcome by the use of anisotropic cross sections.
4. Disregard of the spin dependency of the flux
   - It is assumed that Φ_r and Φ_l, the fluxes due to neutrons of spin parallel and antiparallel, respectively, to velocity are equal.

Two Methods of Transport Theory

The great variety of methods used to solve the transport equations can be divided, from the point of view of the mathematician, into two groups, which are analogous to the **Eulerian and Lagrangian formulations of hydrodynamics**. <Wigner, 1961>

- The **Lagrangian** specification is a way of looking at fluid motion where the observer **follows an individual fluid parcel**.
- The **Eulerian** specification of the flow field is a way **of looking at fluid motion that focuses on specific locations** in the space as time passes.

- For the mathematical representations of fluid flow, in the Lagrangian picture we keep track of the locations of individual fluid particles while coordinates are fixed in space in the Eulerian picture.
- The Euler's and Lagrange's equations are in the same relation as the story of the man, who describes the contents of his chest of drawers by starting at the left side of his top drawer and going down to the right side of the bottom drawers, is related to the story of the man who tells where his shirts are, where his socks are, and so on.

Material Derivative (Lagrangian Derivative)

- The link between the Eulerian and Lagragian descriptions of fluid motion is the "material derivative"

$$\boxed{\begin{aligned}\frac{df}{dt} &= \frac{\partial f}{\partial t} + v\Omega_x \frac{\partial f}{\partial x} + v\Omega_y \frac{\partial f}{\partial y} + v\Omega_z \frac{\partial f}{\partial z} \\ &= \frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f\end{aligned}}$$

which represents the time rate of change of the property *f following a fluid element*.

- In the neutron transport equation, the above relation for the angular neutron density N is expressed as

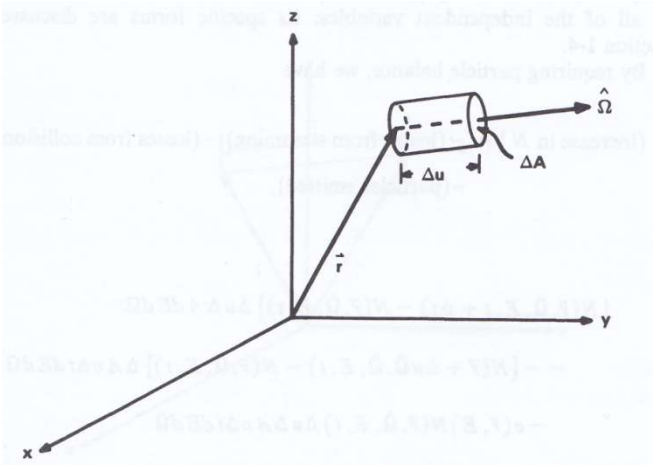
$$\frac{dN}{dt} = \frac{\partial N}{\partial t} + \mathbf{v}\cdot\nabla N$$

$$\Phi = vN \longrightarrow \boxed{\frac{1}{v}\frac{d\Phi}{dt} = \frac{d\Phi}{ds} = \frac{1}{v}\frac{\partial \Phi}{\partial t} + \boldsymbol{\Omega}\cdot\nabla\Phi}$$

where s means the travel distance along the characteristic curve.

Two ways for Derivations of the Streaming Term

< Lagrangian Viewpoint >



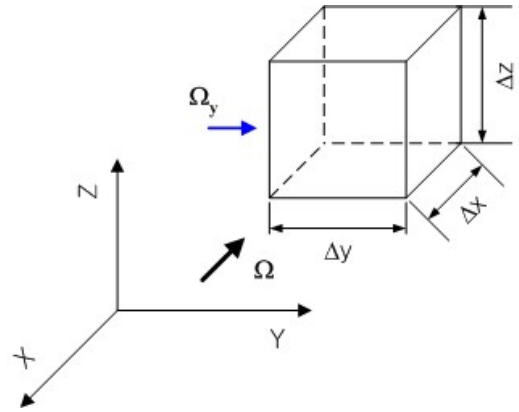
increase in the number of particles in $\Delta u \Delta A dE d\mathbf{\Omega}$ during Δt

$$= \left[N(\mathbf{r}, E, \mathbf{\Omega}, t + \Delta t) - N(\mathbf{r}, E, \mathbf{\Omega}, t) \right] \Delta u \Delta A dE d\mathbf{\Omega}$$

$$= \left[N(\mathbf{r}, E, \mathbf{\Omega}, t + \Delta t) - N(\mathbf{r}, E, \mathbf{\Omega}, t) \right] v \Delta t \Delta A dE d\mathbf{\Omega}$$

$$\Rightarrow \frac{d\Phi}{du}$$

< Eulerian Viewpoint >



increase in the number of particles in $\Delta V dE d\mathbf{\Omega}$ during Δt

$$= \left[N(x, y + \Delta y, z, E, \mathbf{\Omega}, t + \Delta t) - N(x, y, z, E, \mathbf{\Omega}, t) \right] v \Omega_y \Delta t \Delta x \Delta z dE d\mathbf{\Omega}$$

$$\Rightarrow \mathbf{\Omega} \cdot \nabla \Phi$$

Eulerian & Lagrangian Formulations

- Eulerian Form
  - One can focus one's attention on a volume element and an energy-direction range, and obtain the change of the number of neutrons in this volume element and energy-direction range in unit time.

$$\frac{1}{v}\frac{\partial\Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} = -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t) - \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$
$$+\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E')f_s(E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega})\Phi(\mathbf{r},E',\mathbf{\Omega}',t)$$
$$+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\frac{\chi(E)}{4\pi}\nu_f(E)\Sigma_f(\mathbf{r},E')\Phi(\mathbf{r},E',\mathbf{\Omega}',t) \quad \cdots\cdots (1)$$
$$+Q_{ex}(\mathbf{r},E,\mathbf{\Omega},t)$$

- Lagrangian Form
  - Alternatively, one can focus one's attention on a neutron balance along with its characteristic curve.

$$\frac{d}{ds}\Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega},t)=Q(\mathbf{r},E,\mathbf{\Omega},t) \quad \cdots\cdots (2)$$

Third Form of Transport Equation

- A third form of the transport equation, namely, its spherical harmonics form, can be obtained by expanding the angular flux as

$$\Phi(\mathbf{r},E',\mathbf{\Omega}') = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\sum_{m=-l}^{l}\phi_l^m(\mathbf{r},E')Y_{lm}(\mu',\varphi');$$

$$\Rightarrow \frac{1}{2l+1}\left[\frac{1}{2}\sqrt{(l+m+2)(l+m+1)}\left(-\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\phi_{l+1}^{m+1}(\mathbf{r},E)\right.$$

$$+\frac{1}{2}\sqrt{(l-m+2)(l-m+1)}\left(+\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\phi_{l+1}^{m-1}(\mathbf{r},E)$$

$$+\frac{1}{2}\sqrt{(l-m)(l-m-1)}\left(+\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\phi_{l-1}^{m+1}(\mathbf{r},E)$$

$$+\frac{1}{2}\sqrt{(l+m)(l-m+1)}\left(-\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\phi_{l-1}^{m-1}(\mathbf{r},E)$$

$$\left.+\sqrt{(l+m+1)(l-m+1)}\frac{\partial}{\partial z}\phi_{l+1}^{m}(\mathbf{r},E)+\sqrt{(l+m)(l-m)}\frac{\partial}{\partial z}\phi_{l-1}^{m}(\mathbf{r},E)\right]$$

$$+\Sigma_t(\mathbf{r},E)\phi_l^m(\mathbf{r},E)$$

$$=\int_{E'}dE'\;\Sigma_s^l(\mathbf{r},E'\to E)\phi_l^m(\mathbf{r},E')+\delta_{l0}\chi(\mathbf{r},E)\int_{E'}dE'\nu\Sigma_f(\mathbf{r},E')\phi_0^0(\mathbf{r},E')+Q_{ex,l}^m(\mathbf{r},E) \quad \cdots\cdots (3)$$

Discrete Ordinate Multi-group Transport Eq.

- The discrete ordinate equation is derived by considering a particle balance equation in an infinitesimal volume for neutrons moving in the direction ($\mathbf{\Omega}_m$) in energy group g.

$$\mathbf{\Omega}_m \cdot \nabla \Phi_{g,m}(\mathbf{r}) + \Sigma_{tg}(\mathbf{r}) \Phi_{g,m}(\mathbf{r}) = Q_{g,m}(\mathbf{r}),$$
$$\Phi_{g,m}(\mathbf{r}) = f_{g,m}(\mathbf{r}), \quad \mathbf{\Omega} \cdot \mathbf{n} < 0, \quad \mathbf{r} \in \Gamma \qquad \text{(4)}$$

- An application of the finite difference method for the one-dimensional S_N equation yields

$$\mu_m \frac{\partial}{\partial z} \Phi_{g,m}(z) + \Sigma_{tg}(z) \Phi_{g,m}(z) = Q_{g,m}$$

$$\Rightarrow \quad \mu_m \frac{\Phi_{k+1,g,m} - \Phi_{k,g,m}}{h_k} + \Sigma_{tg,k} \Phi_{g,m}(z_{k+1/2}) = Q_{k,g,m}$$

$$\left. \frac{\partial \Phi_{g,m}(z)}{\partial z} \right|_{z=z_{k+1/2}} \cong \frac{\Phi_{k+1,g,m} - \Phi_{k,g,m}}{h_k};$$
$$\Phi_{k,g,m} \equiv \Phi_{g,m}(z_k), \; h_k = z_{k+1} - z_k$$

Integral Equation

$$\frac{d}{ds}\Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega},t)=Q(\mathbf{r},E,\mathbf{\Omega},t) \quad \cdots\cdots (2)$$

- Note that the derivative in the Lagrangian form of Eq. (2) is a derivative along a characteristic curve.
- Eq. (2) is seen to be a linear first-order ordinary differential equation of which integration yields

$$\Phi(\mathbf{r},E,\mathbf{\Omega},t)=\int_0^{\infty} e^{-\eta(s')}\cdot Q(\mathbf{r}-s'\mathbf{\Omega},E,\mathbf{\Omega},t-\frac{s'}{v})ds'; \quad \cdots\cdots (5)$$

$$\eta(s')=\int_0^{s'}\Sigma_t(\mathbf{r}-s''\mathbf{\Omega},E)ds''$$

- The most widely used technique for solving integral transport equations is the method of collision probabilities.

Method of Characteristics

- Complicated geometry can be easily treated in the integral transport method.
- However, in the case of standard treatment (i.e., collision probability method), the integral transport method has drawbacks due to its formulation in which the transport equation is integrated for the angle. Especially in the collision probability method, the treatment of anisotropic scattering is very difficult.

- The method of characteristics first proposed by Askew combining desirable features of the integral transport and S_N methods has been considered as an effective method for the complicated geometry problems.

  (J. R. Askew, "A Characteristics Formulation of the Neutron Transport Equation in Complicated Geometries," AEEW-M-1108, U.K. Atomic Energy Authority.)

$$\mathbf{\Omega}_m \cdot \nabla \Phi_{g,m}(\mathbf{r}) + \Sigma_{tg}(\mathbf{r}) \Phi_{g,m}(\mathbf{r}) = Q_{g,m}(\mathbf{r}),$$

projection to x-y plane ➡

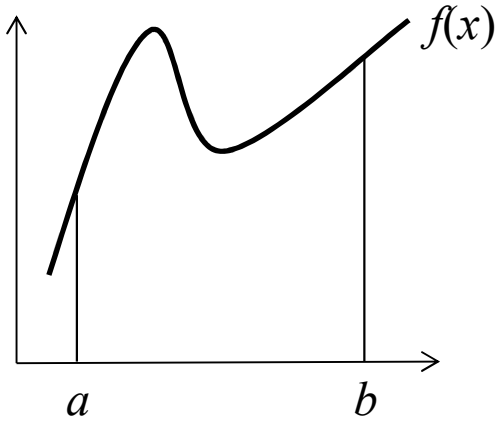
$$\sin\theta_m \frac{d}{dp_m} \Phi_{g,m}(\mathbf{r}) + \Sigma_{tg}(\mathbf{r}) \Phi_{g,m}(\mathbf{r}) = Q_{g,m}(\mathbf{r})$$

$$p_m = u_m \sin\theta_m \quad \Rightarrow \quad dp_m = \sin\theta_m du_m$$

Derivation of Monte Carlo Solution

… let's first note that **all problems solved by Monte Carlo are essentially equivalent to integrations**. …

F. James, *Monte Carlo Phase Space*, CERN 68-15 report (1968).
Lux and Koblinger, (1990).



$$\bar{I} = (b-a)\bar{f} = (b-a)\left[\frac{1}{N}\sum_{i=1}^{N} f(x_i)\right],$$

$$\sigma^2\left[\bar{I}\right] = (b-a)^2\left[\frac{1}{N(N-1)}\sum_{i=1}^{N}\left(f(x_i)-\bar{f}\right)^2\right]$$

Collision Density Equation

- The collision density can be written, from its definition, as

$$\psi(\mathbf{r},E,\mathbf{\Omega},t) \equiv \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$

$$= \Sigma_t(\mathbf{r},E)\int_0^\infty e^{-\eta(s')}\cdot Q(\mathbf{r}-s'\mathbf{\Omega},E,\mathbf{\Omega},t-\frac{s'}{v})ds' \quad \cdots\cdots (6)$$

$$\Phi(\mathbf{r},E,\mathbf{\Omega},t) = \int_0^\infty e^{-\eta(s')}\cdot Q(\mathbf{r}-s'\mathbf{\Omega},E,\mathbf{\Omega},t-\frac{s'}{v})ds'; \quad \cdots\cdots (5)$$

- Then introducing the transport kernels into Eq. (6) gives

$$\boxed{\psi(\mathbf{P}) = \hat{Q}(\mathbf{P}) + \int d\mathbf{P}'K(\mathbf{P}'\rightarrow\mathbf{P})\psi(\mathbf{P}');} \quad \cdots\cdots (7)$$

$$\hat{Q}(\mathbf{r},E,\mathbf{\Omega},t) = \int T(E,\mathbf{\Omega};\mathbf{r}'\rightarrow\mathbf{r})Q(\mathbf{r}',E,\mathbf{\Omega},t')d\mathbf{r}'$$

$$K(\mathbf{r}',E',\mathbf{\Omega}'\rightarrow\mathbf{r},E,\mathbf{\Omega}) = T(E',\mathbf{\Omega}';\mathbf{r}'\rightarrow\mathbf{r})C(\mathbf{r};E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega})$$

$$T(E,\mathbf{\Omega};\mathbf{r}'\rightarrow\mathbf{r}) = \frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2}\exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|}\Sigma_t(\mathbf{r}-s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|},E)ds\right]\delta\left(\mathbf{\Omega}\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}-1\right)$$

$$C(\mathbf{r}';E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega}) = \sum_\alpha \frac{\Sigma_\alpha(\mathbf{r}';E',\mathbf{\Omega}')}{\Sigma_t(\mathbf{r}',E')}f_\alpha(E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega})$$

Series Solution

$$\psi(\mathbf{P}) = \hat{Q}(\mathbf{P}) + \int d\mathbf{P}' K(\mathbf{P}' \to \mathbf{P})\psi(\mathbf{P}') \qquad \cdots\cdots (7)$$

- Consider the solution of Eq. (7) obtained by iteration; thus

$$\psi_0(\mathbf{P}) = \hat{Q}(\mathbf{P})$$
$$\psi_1(\mathbf{P}) = \int d\mathbf{P}' K(\mathbf{P}' \to \mathbf{P}) \cdot \psi_0(\mathbf{P}')$$
$$\vdots \qquad\qquad \vdots$$
$$\psi_n(\mathbf{P}) = \int d\mathbf{P}' K(\mathbf{P}' \to \mathbf{P}) \cdot \psi_{n-1}(\mathbf{P}')$$

Clearly ψ_0 is the first-collision source. ψ_1 means the collision density from the second-collision neutrons. Similarly, ψ_2 indicates the contribution of the third-collision neutrons, and so on. If the series $\boxed{\sum_{j=0}^{\infty} \psi_j(\mathbf{P})}$ converges, it represents a solution to Eq. (7).

Neumann Series Solution

- From the Neumann series solution for the integral transport equation, the neutron flux can be written as

$$\Phi(\mathbf{r},E,\mathbf{\Omega}) = \frac{1}{\Sigma_t(\mathbf{r},E)} \sum_{j=0}^{\infty} \int d\mathbf{r}' \int dE_0 \int d\mathbf{\Omega}_0 K_j(\mathbf{r}', E_0, \mathbf{\Omega}_0 \rightarrow \mathbf{r}, E, \mathbf{\Omega}) \times \int d\mathbf{r}_0 T(E_0, \mathbf{\Omega}_0; \mathbf{r}_0 \rightarrow \mathbf{r}') S(\mathbf{r}_0, E_0, \mathbf{\Omega}_0) \,, \quad \cdots\cdots (8)$$

$$K_j(\mathbf{r}', E_0, \mathbf{\Omega}_0 \rightarrow \mathbf{r}, E, \mathbf{\Omega}) = \int d\mathbf{r}_1 \int dE_1 \int d\mathbf{\Omega}_1 \cdots \int d\mathbf{r}_{j-1} \int dE_{j-1} \int d\mathbf{\Omega}_{j-1} \times K(\mathbf{r}_{j-1}, E_{j-1}, \mathbf{\Omega}_{j-1} \rightarrow \mathbf{r}, E, \mathbf{\Omega}) \cdots K(\mathbf{r}', E_0, \mathbf{\Omega}_0 \rightarrow \mathbf{r}_1, E_1, \mathbf{\Omega}_1)$$

2. Statistical Uncertainty in Monte Carlo Calculations

Error vs. Uncertainty

- When we measure a physical quantity with an instrument or obtain a numerical value, we want to **know how close the estimated value is to the true value**.

- The difference between the estimated and true values is the **error**.

$$\text{Error} = Q_{\text{est}} - Q_{\text{true}}$$

Unfortunately, the true value is unknown and unknowable.

- We can only **estimate** the error.
- The estimate of the error is called the **uncertainty**.

Uncertainty can be expressed in either absolute or percentage terms for typically 95% confidence interval, for example,

5 Volts ±0.5 Volts, 5 Volts ±10%, etc.

Types of Errors: Bias & Random Error

- **Random, Stochastic or Precision Error**
  - tend to be random in nature by effects of uncontrolled variables

- **Bias or Systematic Error (Accuracy)**
  - Error that remains with repeated measurements by a faulty equipment or consistent human errors
  - difference between your measurement (mean value) and the truth.

$$\sigma^2\left[\bar{Q}\right] = E\left[\left(\bar{Q} - Q_{\text{true}}\right)^2\right]$$

$$= E\left[\left\{\left(\bar{Q} - E\left[\bar{Q}\right]\right) + \left(E\left[\bar{Q}\right] - Q_{\text{true}}\right)\right\}^2\right]$$

$$= E\left[\left(\bar{Q} - E\left[\bar{Q}\right]\right)^2\right] + E\left[\left(E\left[\bar{Q}\right] - Q_{\text{true}}\right)^2\right] + 2\,\cancel{E\left[\left(\bar{Q} - E\left[\bar{Q}\right]\right)\left(E\left[\bar{Q}\right] - Q_{\text{true}}\right)\right]}$$

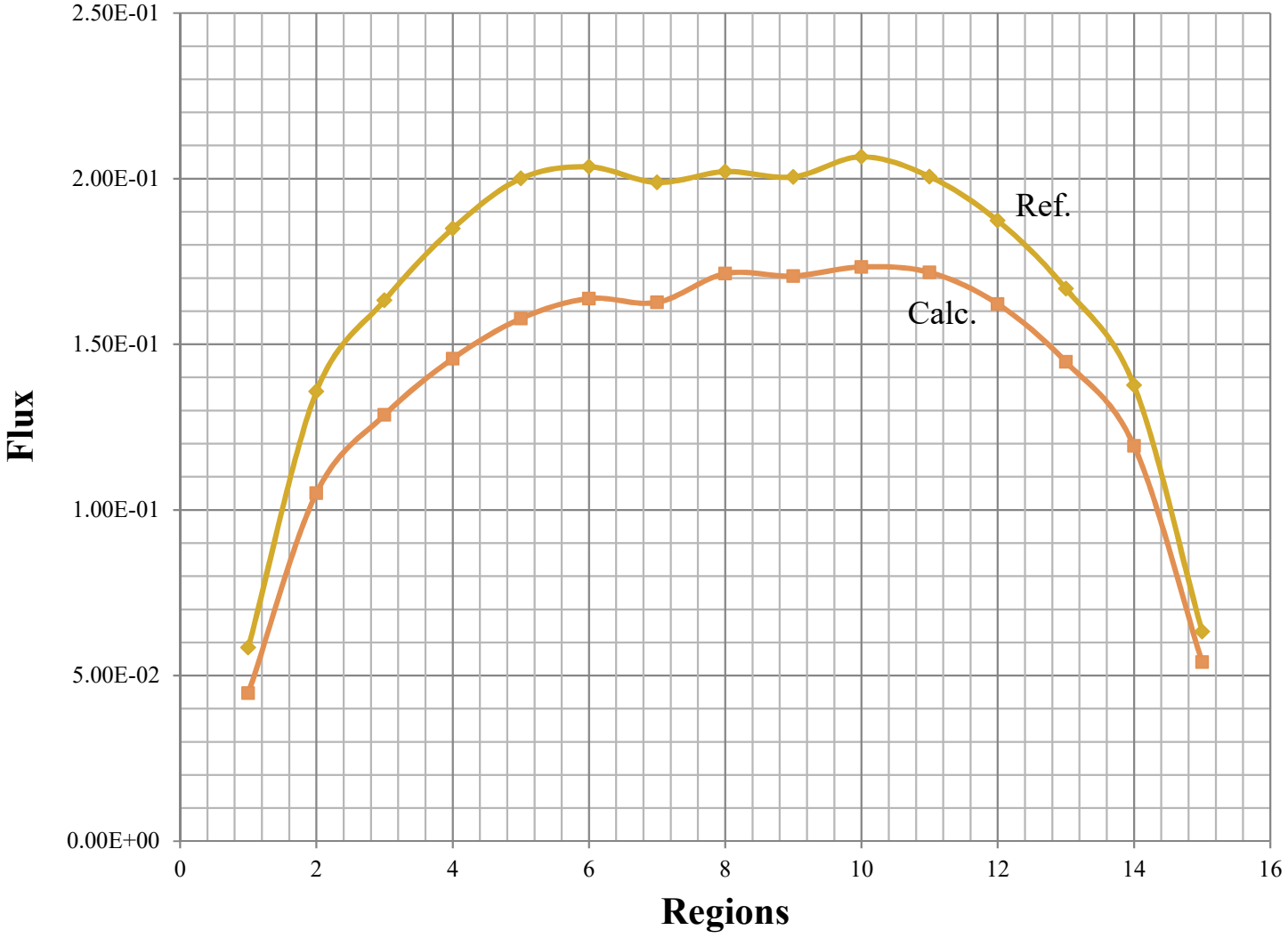
$$= \sigma_S^2\left[\bar{Q}\right] + Bias^2$$

Deterministic vs. Monte Carlo

- Aside from uncertainties in the cross section data, the computing errors of the deterministic methods are **systematic** from
  - discretization of the time-space-angle-energy phase space,
  - simplified representation of 3D configuration with rare exceptions.

- In contrast, the Monte Carlo method is capable of directly treating the very complex 3D configuration as well as the continuous-energy cross section data.
- However the stochastic simulation of particle histories inevitably produce the **stochastic uncertainties**.

Importance of Considering the Uncertainty



Uncertainty Quantification – Sampling Method

$$\bar{x} \pm \sigma_x, \quad \bar{y} \pm \sigma_y \;\Rightarrow\; \boxed{z = f(x,y)} \;\Rightarrow\; \bar{z}, \sigma_z \;??$$

- Because of the input data uncertainties, there can be an infinitely different set of inputs, (x_i,y_i) (i=1,2,…). This may result in different z's as many as the number of input sets.

$$\begin{array}{ccccc}
(x_1,y_1) & \longrightarrow & z = f(x,y) & \longrightarrow & z_1 \\
(x_2,y_2) & \longrightarrow & z = f(x,y) & \longrightarrow & z_2 \\
\vdots & & & & \vdots \\
(x_i,y_i) & \longrightarrow & \boxed{z_i = f(x_i,y_i)} & \longrightarrow & z_i \\
\vdots & & \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots & & \vdots
\end{array} \qquad \text{(B.1)}$$

- Then from the results, the variance of z can be estimated by

$$\sigma_z^2 \equiv \sigma^2[\bar{z}] = \frac{1}{N(N-1)} \sum_i^N (z_i - \bar{z})^2; \; \bar{z} = \frac{1}{N} \sum_i^N z_i \qquad \cdots\cdots\cdots \text{(B.2)}$$

- This methodology is called the **stochastic sampling method** or Brute force method.

Uncertainty Quantification – S/U Analysis

- Let's assume that $\bar{z}$ is determined from the best estimates of input variables as

$$\bar{z} = f(\bar{x}, \bar{y}) \qquad \text{(B.3)}$$

- The Taylor series expansion of Eq. (B.1), $z_i = f(x_i, y_i)$ to the first order of input variations about their mean values, $(z_i - \bar{z})$ in Eq. (B.2), the sample variance formulation, leads to

$$z_i - \bar{z} \cong (x_i - \bar{x})\left(\frac{\partial f}{\partial x}\right) + (y_i - \bar{y})\left(\frac{\partial f}{\partial y}\right) \qquad \text{(B.4)}$$

- The substitution of Eq. (B.4) into Eq. (B.2) results in

$$\sigma_z^2 \cong \frac{1}{N(N-1)} \sum_i^N \left((x_i - \bar{x})\left(\frac{\partial f}{\partial x}\right) + (y_i - \bar{y})\left(\frac{\partial f}{\partial y}\right) \right)^2$$

$$= \frac{1}{N(N-1)} \left\{ \sum_i^N (x_i - \bar{x})^2 \left(\frac{\partial f}{\partial x}\right)^2 + \sum_i^N (y_i - \bar{y})^2 \left(\frac{\partial f}{\partial y}\right)^2 + 2\sum_i^N (x_i - \bar{x})(y_i - \bar{y})\left(\frac{\partial f}{\partial x}\right)\left(\frac{\partial f}{\partial y}\right) \right\}$$

$$= \sigma_x^2 \left(\frac{\partial f}{\partial x}\right)^2 + \sigma_y^2 \left(\frac{\partial f}{\partial y}\right)^2 + 2\,\mathrm{cov}[x, y]\left(\frac{\partial f}{\partial x}\right)\left(\frac{\partial f}{\partial y}\right) \qquad \text{(B.5)}$$

3. Monte Carlo Hybrid Methods

Approaches to Combine MC and Det. Methods

1. **Monte Carlo variance reduction using deterministic adjoint**
   - J. C. Wagner, A. Haghighat, "Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function," *Nucl. Sci. Eng.,* **128**, 186 (1998).

2. **Solving an equivalent equation with phase discretization**
   - T. Kitada, T. Takeda, "Effective Convergence of Fission Source Distribution in Monte Carlo Simulation," *J. Nucl. Sci. Technol.*, **38** [5] (2001).
   - M. J. Lee, H. G. Joo, D. Lee, K. Smith, "Coarse Mesh Finite Difference Formulation for Accelerated Monte Carlo Eigenvalue Calculation," *Ann. Nucl. Energy*, **65**, 101 (2014).

3. **Unbiased modification of the neutron simulation**
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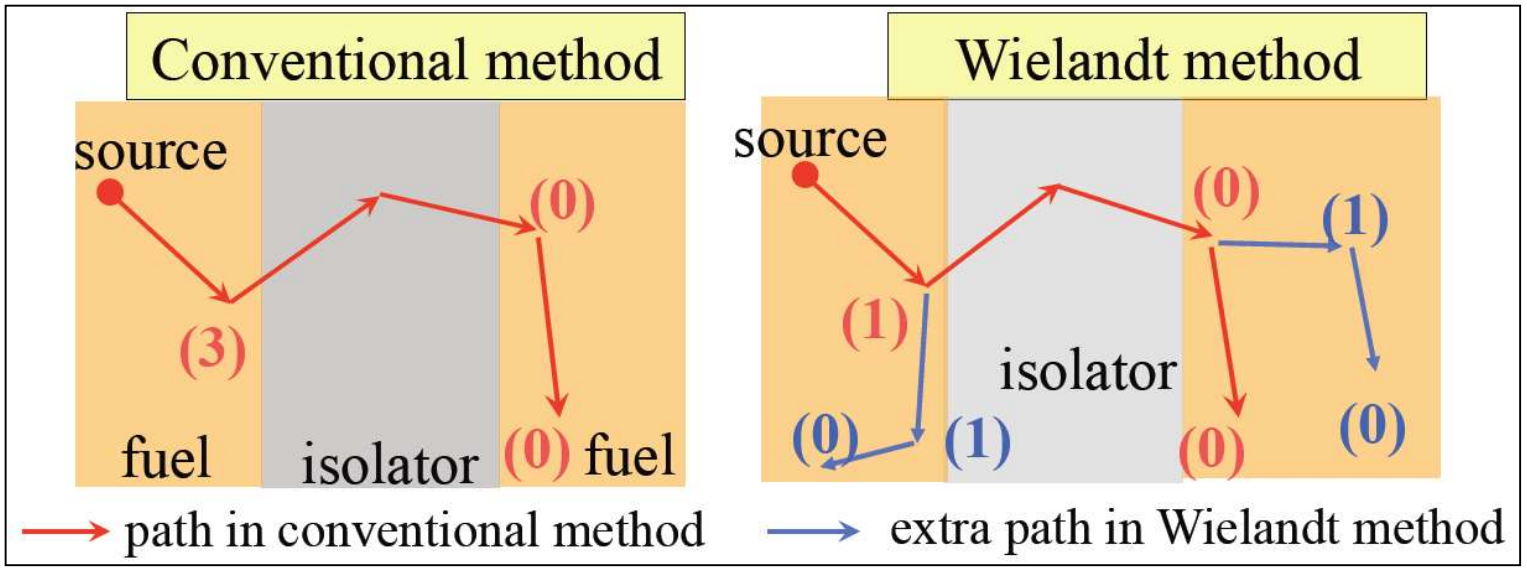
Monte Carlo Wielandt Method

< Integro-differential Eq. > < Integral Eq. >

$$\mathbf{T}\phi - \frac{1}{k_e}\mathbf{F}\phi = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{F}\phi \quad \Rightarrow \quad S^i = \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}S^{i-1} + \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}\left(\left(\frac{\mathbf{H}}{k_e}\right)S^{i-1}\right)$$

$$+\left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}\left(\left(\frac{\mathbf{H}}{k_e}\right)^2 S^{i-1}\right) + \cdots + \varepsilon^i; \quad \mathbf{H} = \mathbf{F}\mathbf{T}^{-1}$$



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Conclusion in Monte Carlo vs. Deterministic Methods

- Mathematician's viewpoints

Neutron Balance in Volume:
Eulerian Formulation

Neutron Balance in CC:
Lagrangian Formulation

→ Integral Formulation

↓ *Monte Carlo method as an integrator*

Neumann Series
Solution of CDE

- An estimate of a tallied mean should be interpreted considering its statistical uncertainty.
- Uncertainty (random error and bias) in new Monte Carlo methods should be carefully examined.