Estimation of coincidence and correlation in non-analogous Monte Carlo particle transport

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Coincidence and correlation in transport

- Basis of many measurement methods
  → need for simulation in full-scale systems
- Coincidence: a sequence of events (deterministic)
  - e.g: energy deposition in detector (pulse height tally)
- Correlation: measure of interdependence of events (stochastic)
  - general definition: $\rho(\xi,\eta)=\frac{\sigma_{\xi\eta}}{\sigma_{\xi}\sigma_{\eta}}$
  - higher moments of distributions is involved
  - e.g.: neutron noise
- Transport implications: multiple contributions from a single source event
  - non-stopping detection (e.g.: scattering)
  - multiplication (e.g. fission, pair production)

Monte Carlo transport

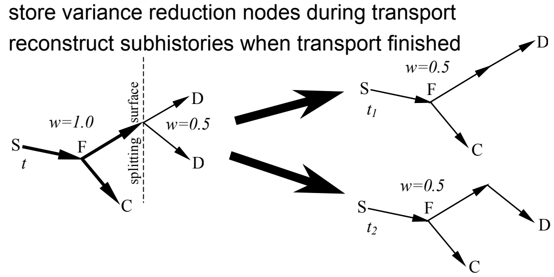
- Analogous Monte Carlo is suitable: independent tracking of particles and events
- Problem: huge calculation time, not feasible for full-scale problems
- Variance reductions methods are needed
  → non-analogous Monte Carlo
- Difficulties with non-analogous Monte Carlo:

collective effect of particles (non-Boltzmann estimator) ↔ particle splitting methods

results influenced by the higher moments ↔ introduction of particle weights

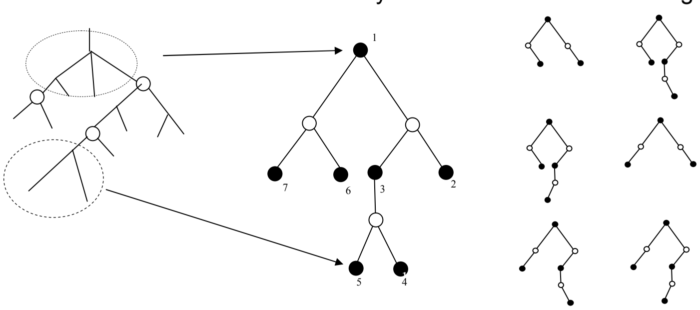
History splitting

- Removal of the artifical multiplications introduced by particle splitting methods by creating independent, analogous histories
- Different approaches (Thomas E. Booth)
  - supertrack:
    - supertracks (subhistories) are followed instead of tracks
    - not compatible with the structure of MC codes
    - implemented in MCNP5 for pulse height tally
  - deconvolution:
    - store variance reduction nodes during transport
    - reconstruct subhistories when transport finished



Generation of subhistories

- Non-analogous history tree has to be divided into analogous subtrees
- Simplification of the tree: physical (●) and variance reduction (○) nodes has to be distinguished:
  - physical: contains all analogous (physical) steps between variance reduction steps, physical multiplication
  - variance reduction: can have only one child node in the analogous case



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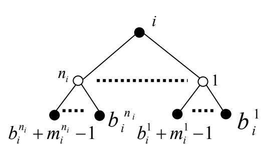
Algorithm for the generation of subhistories

- An S subtree is defined by a subset of physical nodes satisfying Boolean expression B_1
  - physical node: logical conjunction ($\wedge$)
  - variance reduction node: logical exclusive disjunction ($\oplus$)

$$B_i = (i \in S) \wedge (B_{b_i^1} \oplus \ldots \oplus B_{b_i^1+m_i^1}) \wedge \ldots \wedge (B_{b_i^n} \oplus \ldots \oplus B_{b_i^n+m_i^n})$$

- A subhistories can be described by row of a matrix telling which physical nodes are included
- The matrix can be generated by a recursive tree-search algorithm:



$$\underline{\underline{\mathbf{A}}} = \mathrm{f}_1\left(\underline{\mathbf{0}}^T\right)$$

$$\mathrm{f}_i\left(\underline{\underline{\mathbf{A}}}\right) = \mathrm{g}_i^{n_i}\left(\underline{\underline{\mathbf{A}}}\right) + \underline{\underline{\mathbf{1}}}_i$$

$$\mathrm{g}_i^j\left(\underline{\underline{\mathbf{A}}}\right) = \begin{pmatrix} \mathrm{f}_{b_i^j}\left[\mathrm{g}_i^{j-1}\left(\underline{\underline{\mathbf{A}}}\right)\right] \\ \vdots \\ \mathrm{f}_{b_i^j+m_i^j-1}\left[\mathrm{g}_i^{j-1}\left(\underline{\underline{\mathbf{A}}}\right)\right] \end{pmatrix}$$

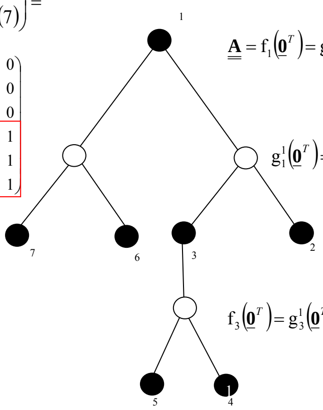
$$\underline{\underline{\mathbf{1}}}_k = \begin{pmatrix} a_{11} & \cdots & a_{i1} & \cdots & a_{m1} \\ \vdots & & \vdots & & \vdots \\ a_{1j} & \cdots & a_{ij} & \cdots & a_{mj} \\ \vdots & & \vdots & & \vdots \\ a_{1n} & \cdots & a_{in} & \cdots & a_{mn} \end{pmatrix} \qquad a_{ij} = \delta_{ik}$$

$$\mathrm{g}_i^0\left(\underline{\underline{\mathbf{A}}}\right) = \underline{\underline{\mathbf{A}}}$$

Example for the evaluation of the subhistory generating algorithm

$$g_1^2(\underline{\mathbf{0}}^T)=\begin{pmatrix} f_6\left[g_1^1(\underline{\mathbf{0}}^T)\right] \\ f_7\left[g_1^1(\underline{\mathbf{0}}^T)\right]\end{pmatrix}=\begin{pmatrix} g_1^1(\underline{\mathbf{0}}^T)+\underline{\underline{\mathbf{1}}}(6) \\ g_1^1(\underline{\mathbf{0}}^T)+\underline{\underline{\mathbf{1}}}(7)\end{pmatrix}=$$

$$=\begin{pmatrix} 0&1&0&0&0&1&0\\ 0&0&1&1&0&1&0\\ 0&0&1&0&1&1&0\\ 0&1&0&0&0&0&1\\ 0&0&1&1&0&0&1\\ 0&0&1&0&1&0&1 \end{pmatrix}$$



$$\underline{\underline{\mathbf{A}}}=f_1(\underline{\mathbf{0}}^T)=g_1^2(\underline{\mathbf{0}}^T)+\underline{\underline{\mathbf{1}}}(1)=\begin{pmatrix} 1&1&0&0&0&1&0\\ 1&0&1&1&0&1&0\\ 1&0&1&0&1&1&0\\ 1&1&0&0&0&0&1\\ 1&0&1&1&0&0&1\\ 1&0&1&0&1&0&1 \end{pmatrix}$$

$$g_1^1(\underline{\mathbf{0}}^T)=\begin{pmatrix} f_2\left[g_1^0(\underline{\mathbf{0}}^T)\right] \\ f_3\left[g_1^0(\underline{\mathbf{0}}^T)\right]\end{pmatrix}=\begin{pmatrix} \underline{\mathbf{0}}^T+\underline{\underline{\mathbf{1}}}(2) \\ f_3\left[\underline{\mathbf{0}}^T\right]\end{pmatrix}=$$

$$=\begin{pmatrix} 0&1&0&0&0&0&0\\ 0&0&1&1&0&0&0\\ 0&0&1&0&1&0&0 \end{pmatrix}$$

$$f_3(\underline{\mathbf{0}}^T)=g_3^1(\underline{\mathbf{0}}^T)+\underline{\underline{\mathbf{1}}}(3)=\begin{pmatrix} 0&0&1&1&0&0&0\\ 0&0&1&0&1&0&0 \end{pmatrix}$$

$$g_3^1(\underline{\mathbf{0}}^T)=\begin{pmatrix} f_4\left[g_4^0(\underline{\mathbf{0}}^T)\right] \\ f_5\left[g_5^0(\underline{\mathbf{0}}^T)\right]\end{pmatrix}=\begin{pmatrix} \underline{\mathbf{0}}^T+\underline{\underline{\mathbf{1}}}(4) \\ \underline{\mathbf{0}}^T+\underline{\underline{\mathbf{1}}}(5)\end{pmatrix}=\begin{pmatrix} 0&0&0&1&0&0&0\\ 0&0&0&0&1&0&0 \end{pmatrix}$$

Detector contributions

- Weight of a subhistory equals the product of the physical nodes

$$W_i=\prod_{j\in S_i} w_j$$

- Detection events corresponds to a physical node

$$f_i(t)=\sum_j \delta(t-t_j)$$

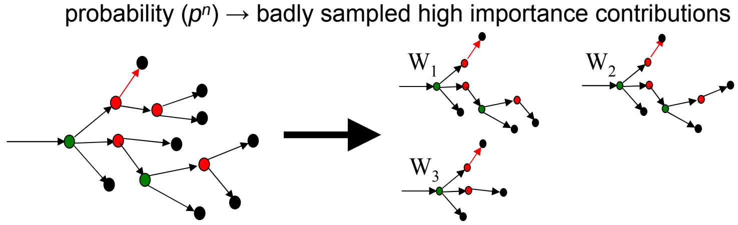
- A dot product with matrix A selects the detections for the subhistories
- With a convolution one can have the response in a time window (Θ) assuming a given source distribution (S)

$$N(T,t)=\underline{\mathbf{W}}^{\mathbf{T}}\int_{-\infty}^{\infty} S(u)\underline{\underline{\mathbf{A}}}\underline{\mathbf{f}}(u)\Theta(T,t-u)du$$

- The convolution can be done by Monte Carlo method:
  - sample a source time for each subhistory
  - calculate the detection time and collect into time bins

Replacement of Russian roulette

- RR: a track is removed (*w=0*) or survived with increased weight (*w'=w/p*)
- Problems:
  - RR game is played on every subhistory containing the branch
  - several (*n*) RR games are played on a subhistory → low survival probability (p^n) → badly sampled high importance contributions



variance reduction node · physical multiplication · termination

- Alternative history control method: switch back to analogue transport

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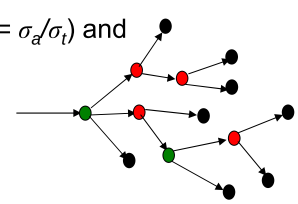
Applied variance reduction methods

- Splitting
  - Geometrical splitting
    - a particle is split into *n* pieces when enters a region with higher importance, *w=1/n*
    - played only when the particle enters a region for the first time
  - Implicit capture
    - the particle is split into absorbed ($w=\sigma_a/\sigma_t$) and unabsorbed ($w=1-\sigma_a/\sigma_t$) parts
    - switched off below weight cutoff
    - limit for number of implicit captures on a track



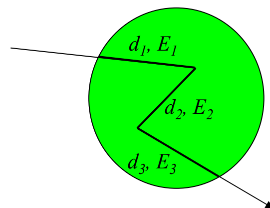
Detection with the track length estimator

- Aim: split every incoming particle into detected and undetected part
- Solution: track length estimator with implicit capture along the flight path
  - distance to next scattering is sampled *(d_i)*, capture excluded

$$w_{abs} = \sum_i \frac{\Sigma_a(E_i) - \Sigma_d(E_i)}{\Sigma_a(E_i)} \left(1 - e^{-\Sigma_a(E_i) d_i}\right) \prod_{j=1}^{i-1} e^{-\Sigma_a(E_j) d_j}$$

$$w_{det} = \sum_i \frac{\Sigma_d(E_i)}{\Sigma_a(E_i)} \left(1 - e^{-\Sigma_a(E_i) d_i}\right) \prod_{j=1}^{i-1} e^{-\Sigma_a(E_j) d_j}$$

$$w_{undet} = \prod_i e^{-\Sigma_a(E_i) d_i}$$



Test calculation: number-of-detections estimator

- One-dimensional, monoenergetic Monte Carlo code has been produced to test the history splitting algorithms
- Infinite, homogeneous media
  - detection (non-stopping)
  - absorption
- Estimator: number of detections from a source event
  - analog to pulse height tally
- Theoretically: $P(N = k) = \left(\frac{\Sigma_d}{\Sigma_t}\right)^k \left(\frac{\Sigma_a}{\Sigma_t}\right)$
- Variance reduction: splitting into 2 after the 5th detection
- Number of variance reduction nodes (n) limited
- Results obtained with the same running time are compared

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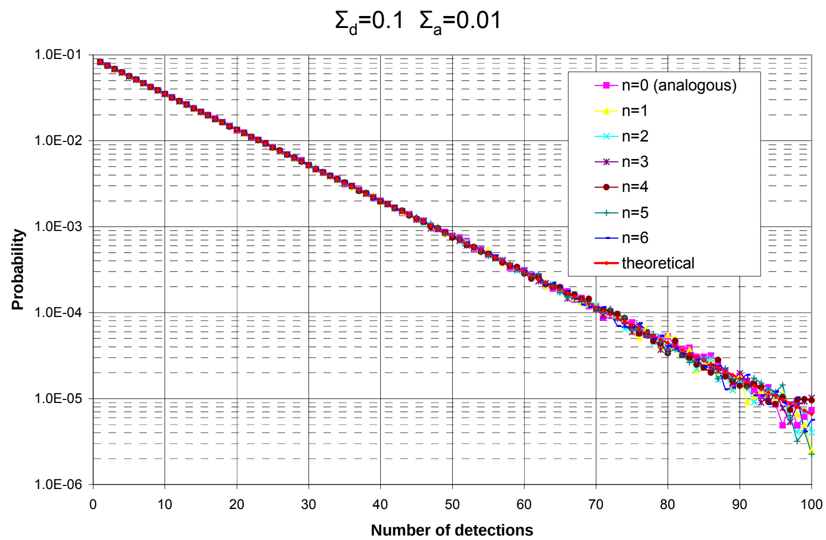
Number-of-detections spectra



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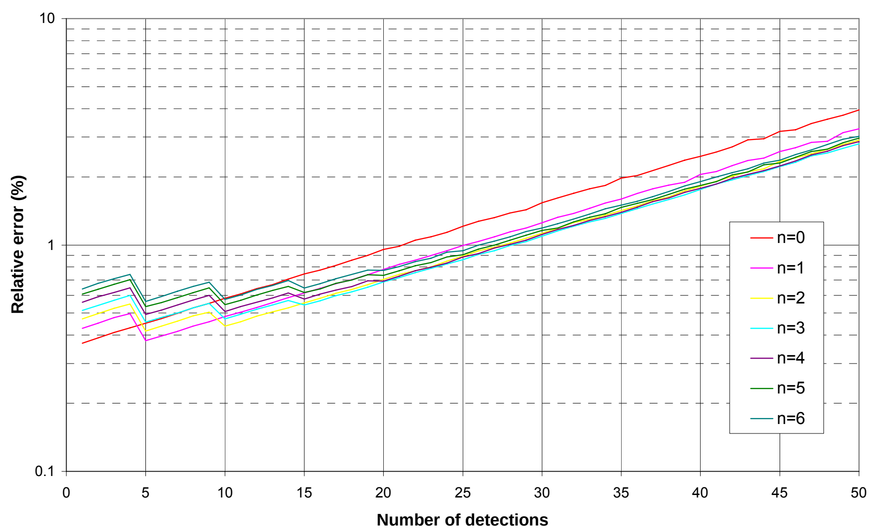
Relative error of the Monte Carlo estimator



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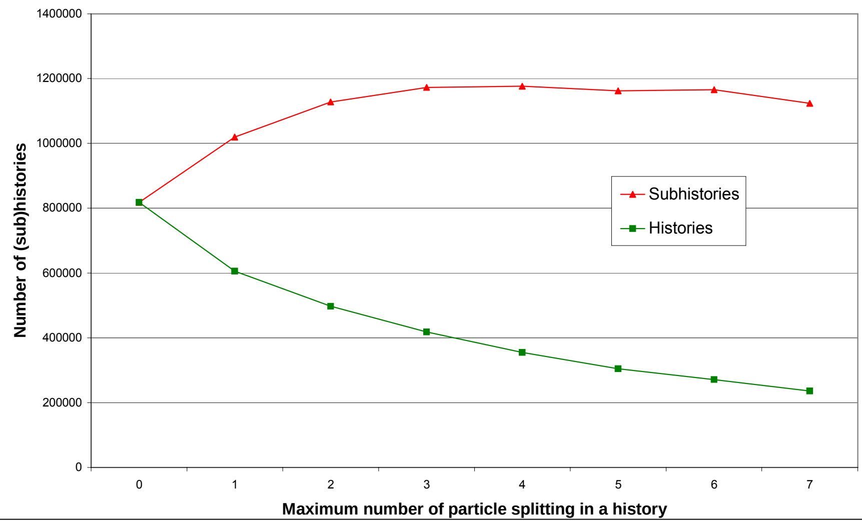
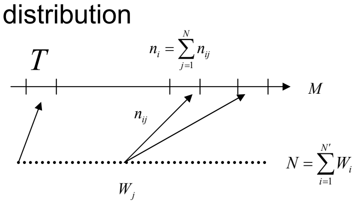
Number of (subhistories)



Recontruction of the variance

- Subhistory weights preserves only the first moment of the distribution



$$\sigma^2(n_i) = \frac{1}{M}\sum_{j=1}^{M}\left(\frac{1}{M}\sum_{k=1}^{M} n_k - n_j\right)^2 = \overline{n_i^2} - \overline{n}_i^2$$

$$\sigma^2(n_i) = N\sigma^2(n_{ij}) = N\left(\overline{n_{ij}^2} - \overline{n}_{ij}^2\right)$$

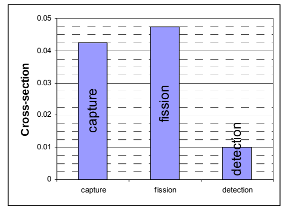
$$\overline{n_{ij}^2} = E\{n_{ij}^2\} = \sum_{k=0}^{\infty} P(n_{ij} = k)k^2 = \sum_{k=0}^{\infty}\frac{1}{MN}\sum_{i=1}^{M}\sum_{j=1}^{N'} W_j \delta_{k,n_{ij}} k^2 = \boxed{\frac{1}{MN}\sum_{i=1}^{M}\sum_{j=1}^{N'} W_j n_{ij}^2}$$

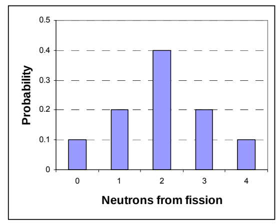
- Second moment can be calculated from the distribution of the contributions from independent subhistories
- Subhistory weights should be interpreted as probabilities

Test calculation: Feynman-α method

$$\frac{\sigma^2(N)}{\langle N \rangle} = 1 + \frac{\varepsilon D_\nu}{\rho_p^2}\left(1 - \frac{1-e^{-\alpha T}}{\alpha T}\right) = 1 + Y$$

- Variance-to-mean ratio:
- Measures the deviation from Poisson-distribution
- Infinite, homogeneous media
  - absorption
  - fission
  - detection (stoping)
- Analytic solution can be calculated
- Implicit capture and time splitting





$$k_\infty = \frac{\nu \Sigma_f}{\Sigma_t} = 0.95$$

$$\rho = \frac{1-k_\infty}{k_\infty} = -0.05263$$

$$\alpha = -\frac{\rho}{\Lambda} = 0.005$$

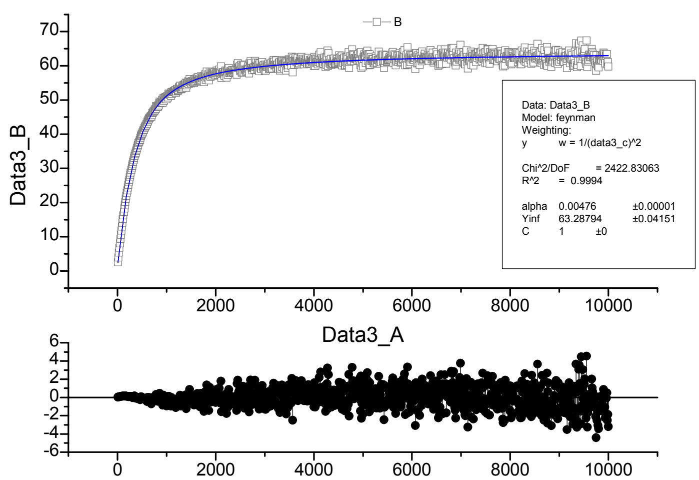
$$\Lambda = \frac{1}{\nu \Sigma_f} = 10.5263$$

$$D_\nu = \overline{\nu(\nu-1)} = 0.8$$

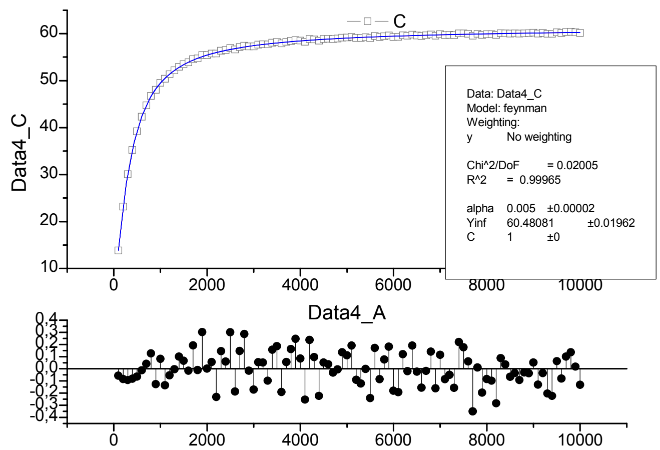
$$\varepsilon = \frac{\Sigma_d}{\Sigma_f} = 0.2105$$

$$Y_\infty = \frac{\varepsilon D_\nu}{\rho^2} = 60.8$$

Analogous Monte Carlo



Variance reduction with history splitting



Conclusions

- A history spliting algorithm has been developed and tested for simple problems
- History splitting is suitable to remove artificial multiplications and make correct estimation of coincidence with a wide variety of variance reduction techniques
- Instead of RR alternative history control methods are suggested
- Variance reduction techniques has to be used with caution as the increase in the calculation time can overwhelm the improvement in the statistics
- A higher moments can be reconstructed by interpreting weights as probability of subhistories and correlations can be estimated
- The method has been implemented in MCNP4C3 and validation calculations are in hand for neutron noise measurements on several subcritical assemblies (Delphi, Yalina, KUCA)