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Isotopic Depletion with Monte Carlo

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This work considers a method to deplete isotopes during a time-dependent Monte Carlo simulation of an evolving system. The method is based on explicitly combining a conventional estimator for the scalar flux with the analytical solutions to the isotopic depletion equations. There are no auxiliary calculations done and the method is an integral part of the Monte Carlo calculation. The method eliminates negative densities and reduces the variance in the estimates for the isotopic densities, compared to existing methods. Moreover, existing methods are shown to be special cases of the general method described in this work, as they can be derived by combining a high variance estimator for the scalar flux with a low-order approximation to the analytical solution to the depletion equation.

There are several methods currently in use to deplete isotopes during a time-dependent Monte Carlo simulation, including analog depletion and pathlength depletion and variants on these basic approaches. These methods share the characteristic that for each appropriate "event" Monte Carlo simulation (e.g., absorption by isotope N_i in the zone or a pathlength traversed in the zone) during the timestep, the density tally for isotope N_i is decremented (or incremented). For example, for analog depletion, the zone density of isotope N_i would be decremented by one (or more, depending on the "weight" of the neutron) for every neutron absorption by that isotope during the timestep.

There are several drawbacks to these conventional schemes including substantial fluctuations due to low isotopic densities with analog depletion and negative densities with either method, but particularly so with analog depletion. The new method eliminates negative densities, improves the accuracy considerably, and substantially reduces the fluctuations.

The method utilizes the analytical solution to the isotopic depletion equation with an appropriate estimator for the average scalar flux over the timestep. For example, one might choose the pathlength estimator or the last event estimator to estimate the average scalar flux over the timestep. It is straightforward to show that both analog depletion and pathlength depletion are special cases of the new method:

- pathlength depletion corresponds to a first order Taylor series expansion to the analytical solution combined with the pathlength estimator.
- analog depletion is similar except the first order approximate solution is combined with a restricted last event estimator, namely one that is only scored for absorptions on the particular isotope in question

A simple Monte Carlo code was written to test this method. The test problem is an infinite, homogeneous medium with an initial neutron flux ϕ_0 neutrons $/ \mathrm{cm}^2 \bullet \mathrm{s}$ and a known time-dependent source of neutrons for $t > 0$ that for convenience is assumed to be constant with magnitude S_0 neutrons $/ \mathrm{cm}^3 \bullet \mathrm{s}$. In addition, there is a depleting isotope with number density X(t) cm^{-3}. The isotope is assumed to be *dilute*, in that it does not affect the cross section of the mixture, hence allowing one to obtain analytical solutions for X(t) and $\phi(t)$. This system can be solved using Monte Carlo at a *point*, taking into account absorption, scattering, census (end of timestep), and number of initial particles and the number of source particles emitted during the timestep.

A medium with the following properties was analyzed:

Δt = 1.0 s
$\phi(0)$ = 5.0 neutrons / $\mathrm{cm}^2 \bullet \mathrm{s}$
V = 1.0 cm^3
v = 2.0 cm/s

$S_0 = 10.0$ neutrons / $cm^3 \bullet s$
$\Sigma_t = 1.0\ cm^{-1}$
$\Sigma_s = 0.5\ cm^{-1}$
$X(0) = .05$ / $b \bullet cm$
$\sigma_{ax} = .01\ b$

Three simulations , each with ten timesteps, were performed and the number of source particles emitted during each timestep varied from 10,000 to 160,000.

Table 1 is a compilation of the average scalar flux as a function of time, as predicted by the pathlength, isotopic absorption, and collision estimators, for each of the simulations. Only selected timesteps are shown. Table 2 tabulates the density of the depleting isotope X(t) for these simulations. The expression "exponential" depletion corresponds to the use of the new method while "linear depletion" corresponds to the use of existing methods to deplete X(t). When used with "analog", the term "exponential" means that the exact analytical solution (which is exponential) is combined with the restricted last event estimator.

Conclusions

1. Negative densities are caused by the low order Taylor series expansion which is inherent in the existing methods for depleting isotopes.
2. Fluctuations in the isotopic densities are caused by the use of a poor estimator for the scalar flux, such as is implicitly used for analog depletion.
3. Both analog depletion and pathlength depletion can be improved by the simple expedient of using the correct exponential attenuation over the timestep versus a linear attenuation, and this change is easy to implement.
4. Other results which are not presented here indicate that the new method is quite robust, capable of predicting isotopic densities with excellent accuracy with very large timesteps and extreme variations in the particle weights.

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Table 1. Scalar Flux Edits for Pathlength, Analog, and Collision Estimators.

N= 10000			pathlength		analog		collision	
n	time	scalar flux [a]	rsd [b]	error [c]	rsd	error	rsd	error
1	1.00	0.1052E+02	0.84%	0.45%	46.45%	71.13%	1.16%	-1.46%
5	5.00	0.1983E+02	0.78%	0.35%	57.73%	-31.22%	0.87%	0.24%
10	10.00	0.2000E+02	0.80%	-1.01%	44.72%	257.16%	0.89%	-1.12%

N= 160000			pathlength		analog		collision	
n	time	scalar flux	rsd	error	rsd	error	rsd	error
1	1.00	0.1052E+02	0.21%	0.23%	15.86%	-8.49%	0.29%	-0.30%
5	5.00	0.1983E+02	0.20%	0.05%	12.44%	1.13%	0.22%	0.08%
10	10.00	0.2000E+02	0.20%	-0.15%	17.96%	28.11%	0.22%	-0.26%

Notes:

[a] scalar flux from analytical solution

[b] relative standard deviation (standard deviation/mean)

[c] relative error compared with analytical solution

Table 2. Isotopic (X) Density at End of Timestep for Test Problem 1.

N = 10,000

LINEAR depletion

n	time	analytical[a]	pathlength		analog		collision	
1	1.00	0.4501E-01	0.4472E-01	(-0.6%)	0.4100E-01	(-8.9%)	0.4482E-01	(-0.4%)
5	5.00	0.2135E-01	0.1955E-01	(-8.4%)	0.1900E-01	(-11.0%)	0.1963E-01	(-8.0%)
10	10.0	0.7862E-02	0.6426E-02	(-18.2%)	0.2000E-02	(-74.5%)	0.6467E-02	(-17.7%)

EXPONENTIAL depletion

n	time	analytical	pathlength		analog		collision	
1	1.00	0.4501E-01	0.4499E-01	(-0.05%)	0.4176E-01	(-7.2%)	0.4508E-01	(0.15%)
5	5.00	0.2135E-01	0.2132E-01	(-0.16%)	0.2091E-01	(-2.0%)	0.2139E-01	(0.20%)
10	10.0	0.7862E-02	0.7860E-02	(-0.02%)	0.5566E-02	(-29.2%)	0.7902E-02	(0.51%)

N=160,000

LINEAR depletion

n	time	analytical	pathlength		analog		collision	
1	1.00	0.4501E-01	0.4473E-01	(-0.62%)	0.4519E-01	(0.40%)	0.4476E-01	(-0.56%)
5	5.00	0.2135E-01	0.1957E-01	(-8.33%)	0.1969E-01	(-7.78%)	0.1959E-01	(-8.24%)
10	10.0	0.7862E-02	0.6430E-02	(-18.2%)	0.5625E-02	(-28.4%)	0.6432E-02	(-18.1%)

EXPONENTIAL depletion

n	time	analytical	pathlength		analog		collision	
1	1.00	0.4501E-01	0.4500E-01	(-0.02%)	0.4541E-01	(0.90%)	0.4502E-01	(0.03%)
5	5.00	0.2135E-01	0.2133E-01	(-0.08%)	0.2136E-01	(0.04%)	0.2135E-01	(0.01%)
10	10.0	0.7862E-02	0.7865E-02	(0.04%)	0.7421E-02	(-5.60%)	0.7867E-02	(0.06%)

Note: [a] number density in nuclei/b•cm

Table 3. Density of Isotope X as a Function of Timestep.

LINEAR Depletion

n	time	analytical	pathlength		analog		collision	
nominal timestep								
1	1.00	0.4645E-01	0.4631E-01	(-0.30%)	0.4525E-01	(-2.59%)	0.4635E-01	(-0.22%)
5	5.00	0.2244E-01	0.2071E-01	(-7.68%)	0.1950E-01	(-13.09%)	0.2075E-01	(-7.53%)
10	10.00	0.8265E-02	0.6807E-02	(-17.64%)	0.5000E-02	(-39.50%)	0.6817E-02	(-17.52%)
10 x timestep								
1	10.00	0.8265E-02	0.0000E+00	(******%)	0.0000E+00	(******%)	0.0000E+00	(******%)
.1 x timestep								
100	10.00	0.8265E-02	0.8129E-02	(-1.64%)	0.7700E-02	(-6.83%)	0.8123E-02	(-1.71%)

Exponential Depletion

n	time	analytical	pathlength		analog		collision	
nominal timestep								
1	1.00	0.4645E-01	0.4644E-01	(-0.02%)	0.4547E-01	(-2.12%)	0.4648E-01	(0.06%)
5	5.00	0.2244E-01	0.2242E-01	(-0.06%)	0.2103E-01	(-6.29%)	0.2246E-01	(0.09%)
10	10.00	0.8265E-02	0.8268E-02	(0.04%)	0.6900E-02	(-16.51%)	0.8279E-02	(0.17%)
10 x timestep								
1	10.00	0.8265E-02	0.8204E-02	(-0.74%)	0.9602E-02	(16.18%)	0.8302E-02	(0.44%)
.1 x timestep								
100	10.00	0.8265E-02	0.8270E-02	(0.07%)	0.7837E-02	(-5.18%)	0.8264E-02	(0.00%)