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memorandum

Computational Physics

XCP-5

Multigroup Free-atom Doppler-broadening Approximation: Theory

Summary

Multigroup cross sections at a one target temperature can be Doppler-broadened to multigroup cross sections at a higher target temperature by matrix multiplication if the group structure sufficiently resolves the original temperature continuous energy cross section. Matrix elements are the higher temperature group weighted averages of the integral over the lower temperature group boundaries of the free-atom Doppler-broadening kernel. The results match theory for constant and $1/v$ multigroup cross sections at 618_lanl group structure resolution.

Background

With the release of NDI 2.0.3 (November 2005) the nuclear data team provided 618 group libraries[1] which offered the possibility for higher fidelity simulations at the cost of increased disk space. The original high fidelity libraries occupy 2,239 MiB, an order of magnitude more than all previous lower fidelity libraries combined (219 MiB).

In NDI 2.0.10 (February 2009) we provided the `mtmg08`[2] library at ten Doppler-broadened temperatures and another order of magnitude increase in library size (27,165 MiB). In NDI 2.0.18 we provided `mtmg01`[3] at fifteen Doppler-broadened temperatures and a doubling of size over `mtmg08` (54,049 MiB). This year we plan to release `mt71x` at twenty-three Doppler-broadened temperatures occupying 176,035 MiB.

The read time for high fidelity multi-temperature data is already of concern to our users and, with the advent of small memory per core future architecture machines, its memory footprint has become an issue for our management. This memo explores the possibility of Doppler-broadening high fidelity multigroup data “on the fly”.

Discussion

Derivation

Evaluated nuclear data models the scattering of energetic projectiles by cold ($kT = 0$ MeV) nuclei. Processing codes, such as NJOY[4], Doppler-broaden cold cross sections to model the effect of energetic projectiles scattered by thermally energetic target nuclei. The Doppler-broadened cross sections are defined to preserve the reaction rate per volume. Thus[5, Eq. 1]:

$$\rho_p \rho_t v \sigma(E, T) \doteq \rho_p \rho_t \int |\vec{v} - \vec{W}| \sigma(E', 0) p(\vec{W}) d^3W, \quad (1)$$

where ρ_p is the density of projectiles with lab velocity $\vec{v}$, ρ_t is the density of the targets with lab velocity $\vec{W}$, $E \doteq \frac{1}{2}mv^2$ is the kinetic energy of the incident particles, $E' \doteq \frac{1}{2}m|\vec{v} - \vec{W}|^2$ is the relative energy of the projectile as seen by the target, and $p(\vec{W}) d^3W$ is the fraction of targets with velocity in d^3W around $\vec{W}$.

If the Maxwell-Boltzmann velocity distribution is used for $p(\vec{W})$ in Equation 1, the result is the free-atom Doppler-broadening equation. Generalizing to an unspecified lower temperature, choosing spherical coordinates, integrating over angular variables, and changing from velocity to energy variables, the free-atom Doppler-broadening equation becomes[5, Eq. 5],[6, Eq. 17]:

$$\sqrt{E} \sigma(E, T_2) = \sqrt{\frac{\alpha}{4\pi}} \int_0^\infty \frac{\sqrt{E'}}{\sqrt{E}} \sigma(E', T_1) \left(e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \right) dE', \quad (2)$$

where E is the projectile energy, $\sigma(E, T)$ is the Doppler-broadened effective cross section of projectile with energy E on target with temperature T , $\alpha \doteq \frac{M}{mk(T_2 - T_1)}$ (M the target mass and m the projectile mass), and E' is the relative energy of the projectile as seen by the target.

Multiplying this equation by the temperature dependent weight function over the square root of projectile energy and integrating over the group i energies of the (decreasing) group boundary set $\{E_i\}$ gives:

$$w_i(T_2) \sigma_i(T_2) \doteq \int_{E_{i+1}}^{E_i} w(E, T_2) \sigma(E, T_2) dE = \int_{E_{i+1}}^{E_i} w(E, T_2) \times \sqrt{\frac{\alpha}{4\pi}} \int_0^\infty \frac{\sqrt{E'}}{E} \sigma(E', T_1) \left(e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \right) dE' dE, \quad (3)$$

where $w_i(T_2) \doteq \int_{E_{i+1}}^{E_i} w(E, T_2) dE$. Equation 3 describes the processing done by the BROADR and GROUPR modules in NJOY.

If we write the inner integral as a sum of integrals over groups and approximate each inner group integral by the multigroup cross section times group integral of the Doppler-broadening kernel, we have a multigroup approximation to the free-atom Doppler-broadening formula:

$$w_i(T_2) \sigma_i(T_2) \approx \int_{E_{i+1}}^{E_i} w(E, T_2) \times \sum_{j=0}^{N_g} \sigma_j(T_1) \sqrt{\frac{\alpha}{4\pi}} \int_{E_{j+1}}^{E_j} \frac{\sqrt{E'}}{E} \left(e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \right) dE' dE, \quad (4)$$

where $\sigma_i(T_2)$ is the broadened effective multigroup cross section in group i at temperature T_2 and $\sigma_j(T_1)$ is the effective multigroup cross section in group j at temperature T_1 .

The inner integral in Equation 4 can be evaluated in closed form. After changes of variables, integration by parts, and much tedious algebra, the indefinite inner integral is:

$$I(x, y) = \frac{1}{2} \left[\left(1 + \frac{1}{2x^2}\right) \text{erf}(y - x) - \frac{y + x}{\sqrt{\pi}x^2} \exp(-(y - x)^2) + \frac{y - x}{\sqrt{\pi}x^2} \exp(-(y + x)^2) - \left(1 + \frac{1}{2x^2}\right) \text{erf}(y + x) \right], \quad (5)$$

where $x^2 \doteq \alpha E$ and $y^2 \doteq \alpha E'$. The definite inner integral is then:

$$I_j(\alpha, E) = I(\alpha E, \alpha E_j) - I(\alpha E, \alpha E_{j+1}) \quad (6)$$

Defining the elements of the multigroup free-atom Doppler-broadening matrix by:

$$\mathbf{D}_{i,j}(T_2, T_1) \doteq \int_{E_{i+1}}^{E_i} \frac{w(E, T_2)}{w_i(T_2)} I_j(\alpha, E) dE, \quad (7)$$

the multigroup free-atom Doppler-broadening approximation becomes:

$$\sigma_i(T_2) \approx \sum_{j=0}^{N_g} \mathbf{D}_{i,j}(T_2, T_1) \sigma_j(T_1). \quad (8)$$

Characterization

Figure 1 plots Equation 5 for $1 \leq x \leq 10^6$. Its value is increasing in y , a necessary condition for the Doppler-broadening matrix elements to be positive; for $x \gg 1$ the $\text{erf}(y - x)$ and $\exp(-(y - x)^2)$ terms dominate to produce its change primarily along the diagonal. These terms produce non-zero values around $y = x$ and zero values elsewhere in the Equation 7 integrand. The resulting Doppler-broadening matrix preserves cross sections for $\sqrt{\alpha E} \gg 1$.

Figure 2 plots Equation 5 for $10^{-6} \leq x \leq 1$ scaled by x . Its value is also increasing in y , a necessary condition for the Doppler-broadening matrix elements to be positive; for $1 \gg x$ the $\text{erf}(y + x)$ and $\exp(-(y + x)^2)$ terms dominate to produce its change primarily along $y = 1$. These terms produce zero values above $y \gg 1$ and non-zero values around and below $y = 1$ in the Equation 7 integrand. The resulting Doppler-broadening matrix averages values around and below $\sqrt{\alpha E'} = 1$ for $1 \gg \sqrt{\alpha E}$.

Figure 1: The indefinite integral $I(x, y)$ for $x \geq 1$ from Equation 5. For $x \gg 1$ the major contribution to the definite integral is along the diagonal line $y = x$. Since $I(x, y)$ is strictly increasing in y , the definite integral is positive.

Figure 2: The indefinite integral $I(x, y)$ times x for $x \leq 1$ from Equation 5. The major contribution to the definite integral is along the line $y = 1$. Since $I(x, y)$ is strictly increasing in y , the definite integral is positive.

The multigroup free-atom Doppler-broadening approximation has the following properties:

Property 1 (Nonnegative Matrix). *If $T_2 > T_1$ and $w(E, T_2) \geq 0$ then $\mathbf{D}_{i,j}(T_2, T_1) \geq 0$.*

Proof. Since $E \geq 0$ and $E' \geq 0$:

$$0 \leq |\sqrt{E'} - \sqrt{E}| \leq \sqrt{E'} + \sqrt{E}.$$

Since $T_2 > T_1$, $\alpha > 0$; thus:

$$\begin{aligned} 0 &\leq |\sqrt{\alpha}(\sqrt{E'} - \sqrt{E})| \leq \sqrt{\alpha}(\sqrt{E'} + \sqrt{E}), \\ 0 &\leq \alpha(\sqrt{E'} - \sqrt{E})^2 \leq \alpha(\sqrt{E'} + \sqrt{E})^2, \\ 0 &\geq -\alpha(\sqrt{E'} - \sqrt{E})^2 \geq -\alpha(\sqrt{E'} + \sqrt{E})^2. \end{aligned}$$

Since e^x is a strictly increasing function:

$$e^0 = 1 \geq e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} \geq e^{-\alpha(\sqrt{E'} + \sqrt{E})^2},$$

and since it is positive for all x :

$$1 \geq 1 - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \geq e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \geq 0.$$

Since the inner integrand in Equation 4 is non-negative and its upper limit is greater than its lower limit, the inner integral (area under the curve) is non-negative. And since $w(E, T_2) \geq 0$ the outer integrand is non-negative, and thus since its upper limit is greater than its lower limit the outer integral is non-negative. $\square$

The fact that $I_j(\alpha, E)$ is positive even though its closed form expression in Equation 5 has negative second and fourth terms, together with the large range for α , E and E' , suggests that the closed form solution might be susceptible to catastrophic cancellation and require further numerical analysis before it is computationally useful.

Property 2 (Identity Limit). $\lim_{T_2 \rightarrow T_1} \mathbf{D}_{i,j}(T_2, T_1) = \delta_{i,j}$

Proof. From the definition of $\mathbf{D}$ in Equation 7 the result follows if we show that:

$$\lim_{\alpha \rightarrow \infty} I_j(\alpha, E) = H(E - E_j) - H(E - E_{j+1}),$$

where $H(x)$ is the unit (Heaviside) step function. From the definition of I_j :

$$\begin{aligned} \lim_{\alpha \rightarrow \infty} I_j(\alpha, E) = & \frac{1}{2} \left[\lim_{\alpha \rightarrow \infty} \left(\frac{\sqrt{\alpha}(\sqrt{E'} + \sqrt{E})}{\sqrt{\pi}\alpha E} \exp(-\alpha(\sqrt{E'} - \sqrt{E})^2) \right) \right. \\ & - \lim_{\alpha \rightarrow \infty} \left(\left(1 + \frac{1}{2\alpha E} \right) \operatorname{erf}(\sqrt{\alpha}(\sqrt{E'} - \sqrt{E})) \right) \\ & - \lim_{\alpha \rightarrow \infty} \left(\frac{\sqrt{\alpha}(\sqrt{E'} - \sqrt{E})}{\sqrt{\pi}\alpha E} \exp(-\alpha(\sqrt{E'} + \sqrt{E})^2) \right) \\ & \left. + \lim_{\alpha \rightarrow \infty} \left(\left(1 + \frac{1}{2\alpha E} \right) \operatorname{erf}(\sqrt{\alpha}(\sqrt{E'} + \sqrt{E})) \right) \right]_{E'=E_{j+1}}^{E_j}, \end{aligned}$$

The exponential and $1/(2\alpha E)$ terms go to zero, leaving the error functions:

$$\begin{aligned}
\lim_{\alpha \rightarrow \infty} I_j(\alpha, E) &= \\
&= \frac{1}{2} \lim_{\alpha \rightarrow \infty} \left[-\operatorname{erf}(\sqrt{\alpha}(\sqrt{E'} - \sqrt{E})) + \operatorname{erf}(\sqrt{\alpha}(\sqrt{E'} + \sqrt{E})) \right]_{E'=E_{j+1}}^{E_j} \\
&= \frac{1}{2} \left\{ \lim_{\alpha \rightarrow \infty} \left[-\operatorname{erf}(\sqrt{\alpha}(\sqrt{E} - \sqrt{E_j})) + \operatorname{erf}(\sqrt{\alpha}(\sqrt{E} + \sqrt{E_{j+1}})) \right] \right. \\
&\quad \left. + \lim_{\alpha \rightarrow \infty} \left[\operatorname{erf}(\sqrt{\alpha}(\sqrt{E} + \sqrt{E_j})) - \operatorname{erf}(\sqrt{\alpha}(\sqrt{E} + \sqrt{E_{j+1}})) \right] \right\} \\
&= \frac{1}{2} \left\{ -(1 - 2H(\sqrt{E} - \sqrt{E_j})) + (1 - 2H(\sqrt{E} - \sqrt{E_{j+1}})) \right\}.
\end{aligned}$$

Since E , E_j , and E_{j+1} are all positive:

$$\lim_{\alpha \rightarrow \infty} I_j(\alpha, E) = H(E - E_j) - H(E - E_{j+1})$$

□

Since the multigroup free-atom Doppler-broadening approximation proper limit for zero temperature change, it should be a good approximation if the group structure resolves the cross section at least for sufficiently small temperatures.

Property 3 (Multiplicative Composition). *If the group structure is sufficiently fine for multigroup free-atom Doppler broadening then $\mathbf{D}(T_3, T_1) = \mathbf{D}(T_3, T_2)\mathbf{D}(T_2, T_1)$.*

Proof. Let $\sigma(T)$ be the multigroup cross section at temperature T , $\mathbf{D}(T, T')$ be the multigroup free-atom Doppler-broadening matrix from temperature T' to temperature T . Then by Equation 8 and the assumption of sufficiently fine groups:

$$\begin{aligned}
\sigma(T_3) &\doteq \mathbf{D}(T_3, T_2)\sigma(T_2), \\
\sigma(T_2) &\doteq \mathbf{D}(T_2, T_1)\sigma(T_1).
\end{aligned}$$

Inserting the second equation in the first equation gives:

$$\begin{aligned}
\sigma(T_3) &= \mathbf{D}(T_3, T_2) (\mathbf{D}(T_2, T_1)\sigma(T_1)), \\
&= (\mathbf{D}(T_3, T_2)\mathbf{D}(T_2, T_1)) \sigma(T_1).
\end{aligned}$$

Since the multigroup free-atom Doppler-broadened approximation is assumed:

$$\sigma(T_3) \doteq \mathbf{D}(T_3, T_1)\sigma(T_1);$$

which implies that:

$$\mathbf{D}(T_3, T_2)\mathbf{D}(T_2, T_1) = \mathbf{D}(T_3, T_1).$$

□

Property 4 (Bootstrap Case). *If the weight function is independent of temperature, the multigroup free-atom Doppler-broadening matrix depends only on the temperature difference.*

Proof. From the definition of the multigroup free-atom Doppler-broadening matrix in Equation 7, if the weight function is independent of temperature:

$$\mathbf{D}_{i,j}(T_2, T_1) \doteq \int_{E_{i+1}}^{E_i} \frac{w(E)}{w_i} I_j(\alpha, E) dE.$$

Since the only temperature dependence on the right hand side is through $\alpha \doteq \frac{M}{mk(T_2 - T_1)}$, $\mathbf{D}$ must be dependent only on the temperature difference. $\square$

Continuous energy free-atom Doppler-broadening can be bootstrapped[6, p. 7]: cross sections at one temperature can be broadened to a higher temperature with a kernel dependent only on the temperature difference. Bootstrapping also works for multigroup free-atom Doppler-broadening in the special case where the weight function is **not** temperature dependent; for example in this case to step from any T_0 to $T_0 + n\Delta T$ requires n applications of a single Doppler-broadening matrix:

$$\mathbf{D}(T_0 + n\Delta T, T_0) = \mathbf{D}^n(\Delta T),$$

where the right hand side matrix depends only on the temperature difference. If the weight function **is** temperature dependent, then the Multiplicative Composition property requires stepping with n different Doppler-broadening matrices:

$$\mathbf{D}(T_0 + n\Delta T, T_0) = \prod_{i=n}^1 \mathbf{D}(T_0 + i\Delta T, T_0 + (i-1)\Delta T).$$

Property 5 (Balance Preserving). *If the cross sections for an isotope balance and all are broadened using the multigroup free-atom Doppler-broadening approximation, the resulting cross sections balance.*

Proof. Matrix multiplication distributes over vector addition. $\square$

Property 6 (Collapse Compatible). *If the group structure used in the outer integral in the multigroup free-atom Doppler-broadening matrix is a subset of the group structure used in the inner integral, then multiplication by this matrix approximates temperature broadening followed by collapse.*

Proof. Let the coarse (decreasing) group boundary set $\{E_j\}$ be collapse compatible with the fine (decreasing) group boundary set $\{E_i\}$, i.e. $\{E_i\} \subseteq \{E_j\}$ and let $\sigma_i(T_2)$ and $\sigma_{i'}(T_1)$ be cross sections in the fine group structure. If the fine group structure is sufficient for the multigroup approximation then from Equation 8:

$$\sigma_i(T_2) = \sum_{i'=0}^{N_f} \mathbf{D}_{i,i'}(T_2, T_1) \sigma_{i'}(T_1),$$

The collapse from the fine to the coarse group structure is given by:

$$\begin{aligned}\sigma_j(T_2) &= \sum_{E_i \in [E_j, E_{j+1}]} \frac{w_i(T_2)}{w_j(T_2)} \left(\sum_{i'=0}^{N_f} \mathbf{D}_{i,i'}(T_2, T_1) \sigma_{i'}(T_1) \right) \\ &= \sum_{i'=0}^{N_f} \left(\sum_{E_i \in [E_j, E_{j+1}]} \frac{w_i(T_2)}{w_j(T_2)} \mathbf{D}_{i,i'}(T_2, T_1) \right) \sigma_{i'}(T_1).\end{aligned}$$

From the definition of $\mathbf{D}$ in Equation 7:

$$\begin{aligned}\sum_{E_i \in [E_j, E_{j+1}]} \frac{w_i(T_2)}{w_j(T_2)} \mathbf{D}_{i,i'}(T_2, T_1) &= \sum_{E_i \in [E_j, E_{j+1}]} \frac{w_i(T_2)}{w_j(T_2)} \int_{E_{i+1}}^{E_i} \frac{w(E, T_2)}{w_i(T_2)} I_{i'}(\alpha, E) dE \\ &= \int_{E_{j+1}}^{E_j} \frac{w(E, T_2)}{w_j(T_2)} I_{i'}(\alpha, E) dE \\ &\doteq \mathbf{D}_{j,i'}(T_2, T_1)\end{aligned}$$

□

The collapse property offers the possibility of using a sufficiently fine group structure for the multi-group free-atom Doppler-broadening approximation to hold and collapsing in place the broadened cross sections to a computationally usable group structure. Since multigroup collapse can also be represented by matrix multiplication, the collapse compatible property can be written as:

$$\mathbf{D} = \mathbf{C} \mathbf{D}',$$

where $\mathbf{D}$ is the Doppler-broadening matrix from low to high temperature and fine to coarse groups, $\mathbf{C}$ is the collapse matrix from fine to coarse groups, and $\mathbf{D}'$ is the Doppler-broadening matrix from low to high temperature at fine groups.

Verification

The multigroup free-atom Doppler-broadening approximation can be verified against the well known analytic Doppler-broadening of constant and $1/v$ cross sections. With the choice of a sufficiently fine group structures we expect the constant cross section to develop a $1/v$ tail below the target temperature and the $1/v$ cross section to remain unchanged. Using the 618_lanl energy boundaries[7], flat weights, and the quad integration routine from SciPy[8] to evaluate Equation 7, we calculated the Doppler-broadening matrix for seven temperatures between a 1 eV and 1 MeV.

Figure 3 show the results of multiplying those matrices by a constant one barn multigroup cross section initially at $kT = 0$ eV. The results agree with the development of a $1/v$ tail below the target temperature predicted by theory.

Figure 3: Doppler-broadening of a constant multigroup cross section at $T = 0$ eV to temperatures from 1 eV to 1 MeV. The results agree with theoretical predictions over the entire energy range. Compare with [6, Fig. 4].

Figure 4: Doppler-broadening of a multigroup $1/v$ cross section at $T = 0$ eV to temperatures from 1 eV to 1 MeV. The result should be temperature-independent: to the scale of the figure, it is. Compare with [6, Fig. 5].

Figure 4 show the results of multiplying those matrices by a multigroup cross section proportional to $1/v$ initially at $T = 0$ eV. For flat weights, the $1/v$ multigroup cross section is an eigen-vector of the Doppler-broadening matrix with eigen-value one.

Based on the excellent agreement of these test cases with theory, it appears that the 618_lanl group structure may indeed be fine enough for this approximation.

Conclusion

Multigroup cross sections at a one target temperature can be Doppler-broadened to multigroup cross sections at a higher target temperature by matrix multiplication if the group structure sufficiently resolves the original temperature continuous energy cross section. Matrix elements are the high temperature group weighted averages of the integral over the low temperature group boundaries of the free-atom Doppler-broadening kernel. The results match theory for constant and $1/v$ multigroup cross sections at 618_lanl group structure resolution.

If this approximation proves sufficient for actual cross sections at 618_lanl resolution, it could reduce the disk and memory footprint for high-fidelity multi-temperature data: each high temperature data table, currently represented by a complete replica of the low temperature table including several 618×618 matrices, could be replaced by a single 618×618 Doppler-broadening matrix for a savings approaching an order of magnitude. If the resolution of the simulation multigroup data used is some $n < 618$, then the the Doppler-broadening matrices could be smaller ($618 \times n$) including both broadening and collapse for more memory savings and a better, i.e. more averaged, approximation. Further, since the matrix multiplication, and possibly the matrix creation, could be done “on the fly”, this approximation trades memory for computation and is hence future architecture friendly.

The next step is to calculate Doppler-broadening matrices with the temperature dependent TD weight function and compare the result of using them on real data to the data Doppler-broadened by NJOY.

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