Determining the units of the thermal conductivity calculation

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We wish to know the units of the thermal conductivity values that our programs spit out. In essence, we are calculating the transfered power from atom coordinate i to atom coordinate j:

$$P_{i\to j} = 2\gamma_0 k_B (T_h - T_c) K_{ij} \sum_{\sigma,\tau} \left[c_{\sigma,1} c_{\tau,1} a_{i,\sigma} a_{j,\tau} \frac{\lambda_\sigma - \lambda_\tau}{\lambda_\sigma + \lambda_\tau} \right] \tag{1}$$

In practice our calculation is a sum of these power terms corresponding to atom interactions that cross the molecular interfaces, including the 3D nature of the interactions. The units of some of these variables are implied; others come from the particular molecular forcefield used in the calculation. For each of the forcefields there is an associated energy and length unit, which we will refer to as E and L respectively. Separate from the energy minimization calculation is the mass unit M.

Quickly we understand that forces have units of EL^{-1} and spring constants are EL^{-2}. Regarding the eigenvalues, they correspond to the square of their mode frequency:

$$\lambda = \omega^2 \propto \frac{k}{m} \tag{2}$$

$$[\lambda] = EL^{-2}M^{-1} \tag{3}$$

While the eigenvalue factor in Equation 1 is canceled, its units is related to the time scale, t, of our calculation:

$$t = [\lambda]^{-1/2} = E^{-1/2}\, L\, M^{1/2} \tag{4}$$

The units of power will be given by $E_k\, t^{-1}$ where E_k is the implied unit of $k_B T$ in Equation 1. Let us confirm that the expression (without the $k_B T$ factor) gives us the inverse time unit.

Firstly, we understand the components of the eigenvectors to be dimensionless. Next, we relate the damping factor γ_0 to force units via the units of velocity:

$$F_{\text{drag}} = -\gamma v \tag{5}$$

$$[\gamma] = [F][v]^{-1} = EL^{-2}\, t = E^{1/2}\, L^{-1}\, M^{1/2} \tag{6}$$

From the Green's function definition

$$q(t) = \int G(t,t')F(t')dt' \tag{7}$$

we see the coefficients c have units:

$$[c] = E^{-1}\, L^2\, t^{-1} = E^{-1/2}\, L\, M^{-1/2} = [\gamma]^{-1} \tag{8}$$

Finally we hope to retrieve the inverse time unit:

$$\left[\frac{P_{i\to j}}{k_B T}\right] = [\gamma_0][c]^2[K_{ij}] = [c]E\,L^{-2} = t^{-1} \tag{9}$$

The numbers I have generated up to this point actually do not factor in the drag constant γ_0. I have been calculating:

$$\frac{P_{i\to j}}{2\gamma_0 k_B \Delta T}$$

so our grid values have units of

$$[\text{grid}] = [\gamma]^{-1}t^{-1} = E^{-1}L^2\,t^{-2} = M^{-1} \tag{10}$$

Our forcefields typically have

$$E = \text{kcal/mol}$$
$$L = \text{angstroms}$$

while our programs use

$$M = \text{atomic mass unit (amu)}$$

We keep in mind these conversion factors:

$$1\,\text{kcal/mol} = 6.8894\times 10^{-21}\,\text{J}$$
$$1\,\text{Å} = 10^{-10}\,\text{m}$$
$$1\,\text{amu} = 1.6605\times 10^{-27}\,\text{kg}$$

Our time unit t is therefore:

$$t = \frac{10^{-10}\,\text{m}\sqrt{1.6605\times 10^{-27}\,\text{kg}}}{\sqrt{6.8894\times 10^{-21}\,\text{J}}} = 4.9094\times 10^{-14}\,\text{s} \tag{11}$$

We want to finish with the SI units for thermal conductivity W/m/K.