Interpolation scheme

Adam J. Jackson

As part of the application of the ΔV_{xc} method, it is necessary to generate a unit cell of target volume. While the parameters may be optimised with an *ab initio* calculation, the goal of ΔV_{xc} is to reduce computational cost and hence we should use the available information to minimise this. Therefore we suggest linear interpolation between the surrounding minimised cells on the precalculated E-V curve. The unit cell matrix contains a set of lattice vectors:

$$\mathbf{R} = \begin{bmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{bmatrix} = \begin{bmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{bmatrix} \tag{1}$$

If we are to interpolate between two precalculated lattices $\mathbf{R}'$ and $\mathbf{R}''$, then we label their lattice vectors $\vec{a}', \vec{b}', \vec{c}'$ and $\vec{a}'', \vec{b}'', \vec{c}''$. The interpolated lattice $\mathbf{R} = \mathbf{R}' + \lambda(\mathbf{R}'' - \mathbf{R}')$, where λ is the shared scaling parameter for interpolation. When lambda has been determined, the same process might be applied to atomic positions for an improved estimate.

The challenge then becomes to determine $\lambda = f(V, \mathbf{R}', \mathbf{R}'')$. The volume of a lattice unit cell,

$$V = \left| \vec{a} \cdot \left(\vec{b} \times \vec{c} \right) \right| . \tag{2}$$

For the interpolated cell, therefore:

$$V = \left|((1-\lambda)\vec{a}' + \lambda\vec{a}'') \cdot \left[\left((1-\lambda)\vec{b}' + \lambda\vec{b}''\right) \times ((1-\lambda)\vec{c}' + \lambda\vec{c}'')\right]\right| \tag{3}$$

$$V = \left|((1-\lambda)\vec{a}' + \lambda\vec{a}'') \cdot \left[\begin{array}{ll} & (1-\lambda)\vec{b}' \times (1-\lambda)\vec{c}' + (1-\lambda)\vec{b}' \times \lambda\vec{c}'' \\ + & \lambda\vec{b}'' \times (1-\lambda)\vec{c}' + \lambda\vec{b}'' \times \lambda\vec{c}'' \end{array}\right]\right| \tag{4}$$

$$V = \left|((1-\lambda)\vec{a}' + \lambda\vec{a}'') \cdot \left[\begin{array}{ll} & (1-\lambda)^2\vec{b}' \times \vec{c}' + \lambda(1-\lambda)\vec{b}' \times \vec{c}'' \\ + & \lambda(1-\lambda)\vec{b}'' \times \vec{c}' + \lambda^2\vec{b}'' \times \vec{c}'' \end{array}\right]\right| \tag{5}$$

$$V = \left|\begin{array}{ll} & (1-\lambda)\vec{a}' \cdot \left[\begin{array}{ll} & (1-\lambda)^2\vec{b}' \times \vec{c}' + \lambda(1-\lambda)\vec{b}' \times \vec{c}'' \\ + & \lambda(1-\lambda)\vec{b}'' \times \vec{c}' + \lambda^2\vec{b}'' \times \vec{c}'' \end{array}\right] \\ + & \lambda\vec{a}'' \cdot \left[\begin{array}{ll} & (1-\lambda)^2\vec{b}' \times \vec{c}' + \lambda(1-\lambda)\vec{b}' \times \vec{c}'' \\ + & \lambda(1-\lambda)\vec{b}'' \times \vec{c}' + \lambda^2\vec{b}'' \times \vec{c}'' \end{array}\right] \end{array}\right| \tag{6}$$

$$V = \left|\left[\begin{array}{c} (1-\lambda)^3 \\ \lambda(1-\lambda)^2 \\ \lambda(1-\lambda)^2 \\ \lambda^2(1-\lambda) \\ \lambda(1-\lambda)^2 \\ \lambda^2(1-\lambda) \\ \lambda^2(1-\lambda) \\ \lambda^3 \end{array}\right] \cdot \left[\begin{array}{c} \vec{a}' \cdot \vec{b}' \times \vec{c}' \\ \vec{a}' \cdot \vec{b}' \times \vec{c}'' \\ \vec{a}' \cdot \vec{b}'' \times \vec{c}' \\ \vec{a}' \cdot \vec{b}'' \times \vec{c}'' \\ \vec{a}'' \cdot \vec{b}' \times \vec{c}' \\ \vec{a}'' \cdot \vec{b}' \times \vec{c}'' \\ \vec{a}'' \cdot \vec{b}'' \times \vec{c}' \\ \vec{a}'' \cdot \vec{b}'' \times \vec{c}'' \end{array}\right]\right| \tag{7}$$

If we denote the right-hand vector containing all the volume permutations as $\vec{x}$, we can express this as a simple (albeit cumbersome) cubic equation.

$$V = \left|\begin{array}{c} x_1(1-\lambda)^3 + (x_2+x_3+x_5)\lambda(1-\lambda)^2 \\ +(x_4+x_6+x_7)\lambda^2(1-\lambda) + x_8\lambda^3 \end{array}\right| \tag{8}$$

$$V = \left|\begin{array}{ll} & x_1(-\lambda^3 + 3\lambda^2 - 3\lambda + 1) \\ + & (x_2+x_3+x_5)(\lambda^3 - 2\lambda^2 + \lambda) \\ + & (x_4+x_6+x_7)(\lambda^2 - \lambda^3) \quad + x_8(\lambda^3) \end{array}\right| \tag{9}$$

$$V = \left|\begin{array}{ll} & (-x_1+x_2+x_3-x_4+x_5-x_6-x_7+x_8)\lambda^3 \\ + & (3x_1 - 2x_2 - 2x_3 + x_4 - 2x_5 + x_6 + x_7)\lambda^2 \\ + & (-3x_1 + x_2 + x_3 + x_5)\lambda \\ + & (x_1) \cdot 1 \end{array}\right| \tag{10}$$

This equation is solved by standard numerical methods to provide the suggested lattice vectors. A real value of λ is required for a physically-meaningful solution, and a positive value is preferred.