Notes on Dynamic Mapping

$$\mathbf{R}_I = \sum_i C_{Ii}(t)\mathbf{r}_i$$

$$\dot{\mathbf{R}}_I = \sum_i \left(\frac{\partial C_{Ii}(t)}{\partial t}\mathbf{r}_i + C_{Ii}(t)\frac{\partial \mathbf{r}_i}{\partial t} \right)$$

$$\mathbf{V}_I = \sum_i \left[C_{Ii}\mathbf{v}_i + \mathbf{r}_i \left(\sum_j \sum_m \frac{\partial C_{Ii}(t)}{\partial r_{jm}} v_{jm} + \sum_J \sum_m \frac{\partial C_{Ii}(t)}{\partial R_{Jm}} V_{Jm} \right) \right] = \sum_i C_{Ii}\mathbf{v}_i + \sum_j \sum_m \sum_i \mathbf{r}_i \frac{\partial C_{Ii}(t)}{\partial r_{jm}} v_{jm} + \sum_J \sum_m \sum_i \mathbf{r}_i \frac{\partial C_{Ii}(t)}{\partial R_{Jm}} V_{Jm}$$

$$\begin{aligned} V_{In} &= \sum_i C_{Ii} v_{in} + \sum_j \sum_m \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial r_{jm}} v_{jm} + \sum_J \sum_m \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial R_{Jm}} V_{Jm} \\ &= \sum_i C_{Ii} v_{in} + \sum_j \sum_m N_{Ij}^{nm} v_{jm} + \sum_J \sum_m M_{IJ}^{nm} V_{Jm} \end{aligned}$$

$$N_{Ij}^{nm} = \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial r_{jm}}$$

$$M_{IJ}^{nm} = \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial R_{Jm}}$$

If we align the matrix elements as shown below, this equation can be solved by standard linear

algebra libraries.

$$(\mathbf{I} - \mathbf{M})\mathbf{V} = (\mathbf{C} + \mathbf{N})\mathbf{v}$$

$$\begin{pmatrix} V_1^x \\ V_2^x \\ \ldots \\ V_p^x \\ V_1^y \\ V_2^y \\ \ldots \\ V_p^y \\ V_1^z \\ V_2^z \\ \ldots \\ V_p^z \end{pmatrix} = \left(\begin{pmatrix} C_{11} & \ldots & C_{1q} & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & 0 & 0 & 0 & 0 & 0 \\ C_{p1} & \ldots & C_{pq} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{11} & \ldots & C_{1q} & 0 & 0 & 0 \\ 0 & 0 & 0 & \vdots & \ddots & \vdots & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{p1} & \ldots & C_{pq} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & C_{11} & \ldots & C_{1q} \\ 0 & 0 & 0 & 0 & 0 & 0 & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & C_{p1} & \ldots & C_{pq} \end{pmatrix} \begin{pmatrix} v_1^x \\ v_2^x \\ \ldots \\ v_p^x \\ v_1^y \\ v_2^y \\ \ldots \\ v_p^y \\ v_1^z \\ v_2^z \\ \ldots \\ v_p^z \end{pmatrix} + \begin{pmatrix} N_{11}^{xx} & \ldots & N_{1q}^{xx} & N_{11}^{xy} & \ldots & N_{1q}^{xy} & N_{11}^{xz} & \ldots & N_{1q}^{xz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ N_{p1}^{xx} & \ldots & N_{pq}^{xx} & N_{p1}^{xy} & \ldots & N_{pq}^{xy} & N_{p1}^{xz} & \ldots & N_{pq}^{xz} \\ N_{11}^{yx} & \ldots & N_{1q}^{yx} & N_{11}^{yy} & \ldots & N_{1q}^{yy} & N_{11}^{yz} & \ldots & N_{1q}^{yz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ N_{p1}^{yx} & \ldots & N_{pq}^{yx} & N_{p1}^{yy} & \ldots & N_{pq}^{yy} & N_{p1}^{yz} & \ldots & N_{pq}^{yz} \\ N_{11}^{zx} & \ldots & N_{1q}^{zx} & N_{11}^{zy} & \ldots & N_{1q}^{zy} & N_{11}^{zz} & \ldots & N_{1q}^{zz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ N_{p1}^{zx} & \ldots & N_{pq}^{zx} & N_{p1}^{zy} & \ldots & N_{pq}^{zy} & N_{p1}^{zz} & \ldots & N_{pq}^{zz} \end{pmatrix} \right) \begin{pmatrix} v_1^x \\ v_2^x \\ \ldots \\ v_p^x \\ v_1^y \\ v_2^y \\ \ldots \\ v_p^y \\ v_1^z \\ v_2^z \\ \ldots \\ v_p^z \end{pmatrix} + \begin{pmatrix} M_{11}^{xx} & \ldots & M_{1q}^{xx} & M_{11}^{xy} & \ldots & M_{1q}^{xy} & M_{11}^{xz} & \ldots & M_{1q}^{xz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ M_{p1}^{xx} & \ldots & M_{pq}^{xx} & M_{p1}^{xy} & \ldots & M_{pq}^{xy} & M_{p1}^{xz} & \ldots & M_{pq}^{xz} \\ M_{11}^{yx} & \ldots & M_{1q}^{yx} & M_{11}^{yy} & \ldots & M_{1q}^{yy} & M_{11}^{yz} & \ldots & M_{1q}^{yz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ M_{p1}^{yx} & \ldots & M_{pq}^{yx} & M_{p1}^{yy} & \ldots & M_{pq}^{yy} & M_{p1}^{yz} & \ldots & M_{pq}^{yz} \\ M_{11}^{zx} & \ldots & M_{1q}^{zx} & M_{11}^{zy} & \ldots & M_{1q}^{zy} & M_{11}^{zz} & \ldots & M_{1q}^{zz} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ M_{p1}^{zx} & \ldots & M_{pq}^{zx} & M_{p1}^{zy} & \ldots & M_{pq}^{zy} & M_{p1}^{zz} & \ldots & M_{pq}^{zz} \end{pmatrix} \begin{pmatrix} V_1^x \\ V_2^x \\ \ldots \\ V_p^x \\ V_1^y \\ V_2^y \\ \ldots \\ V_p^y \\ V_1^z \\ V_2^z \\ \ldots \\ V_p^z \end{pmatrix}$$

Partial Derivatives needed for generating matrix M:

$$\frac{\partial \ln C_{Ii}}{\partial X_J} = -\frac{\partial w_{Ji} / \partial X_J}{\sum_K w_{Ki}} - \frac{1}{\sum_j \frac{w_{Ij}}{\sum_K w_{Kj}}} \cdot \sum_j w_{Ij} - \frac{\partial w_{Jj} / \partial X_J}{\left(\sum_K w_{Kj}\right)^2} = -\frac{\partial w_{Ji} / \partial X_J}{\sum_K w_{Ki}} + \frac{\sum_j w_{Ij} \frac{\partial w_{Jj} / \partial X_J}{\left(\sum_K w_{Kj}\right)^2}}{\sum_j w_{Ij} \frac{1}{\sum_K w_{Kj}}}$$

$$= -\frac{\partial w_{Ji} / \partial X_J}{\sum_K w_{Ki}} + \frac{\sum_j \frac{w_{Ij}}{\sum_K w_{Kj}} \times \frac{\partial w_{Jj} / \partial X_J}{\sum_K w_{Kj}}}{\sum_j \frac{w_{Ij}}{\sum_K w_{Kj}}}$$

$$= -\frac{\partial w_{Ji} / \partial X_J}{\sum_K w_{Ki}} + \sum_j C_{Ij} \times \frac{\partial w_{Jj} / \partial X_J}{\sum_K w_{Kj}}$$

$$\frac{\partial \ln C_{Ii}}{\partial X_I} = \frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} - \frac{\partial w_{Ii} / \partial X_I}{\sum_K w_{Ki}} - \frac{1}{\sum_j \frac{w_{Ij}}{\sum_K w_{Kj}}} \cdot \sum_j \left(\frac{\partial w_{Ij}}{\partial X_I} \frac{1}{\sum_K w_{Kj}} - w_{Ij} \frac{\partial w_{Ij} / \partial X_I}{\left(\sum_K w_{Kj}\right)^2} \right)$$

$$= \frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} - \frac{\partial w_{Ii} / \partial X_I}{\sum_K w_{Ki}} - \frac{\sum_j \left(\frac{\partial w_{Ij} / \partial X_I}{\sum_K w_{Kj}} - \frac{\partial w_{Ij} / \partial X_I}{\sum_K w_{Kj}} \times w_{Ij} / \sum_K w_{Kj} \right)}{\sum_j w_{Ij} / \sum_K w_{Kj}}$$

$$= \frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} - \frac{\partial w_{Ii} / \partial X_I}{\sum_K w_{Ki}} - \sum_j C_{Ij} \left(\frac{\partial w_{Ij} / \partial X_I}{w_{Ij}} - \frac{\partial w_{Ij} / \partial X_I}{\sum_K w_{Kj}} \right)$$

N matrix:

$$\frac{\partial \ln C_{Ii}}{\partial x_j} = -\frac{1}{\sum_k \frac{w_{Ik}}{\sum_J w_{Jk}}} \frac{\frac{\partial w_{Ij}}{\partial x_j}\sum_J w_{Jj} - w_{Ij}\sum_J \frac{\partial w_{Jj}}{\partial x_j}}{\left(\sum_J w_{Jj}\right)^2} = \frac{1}{\sum_k \frac{w_{Ik}}{\sum_J w_{Jk}}} \frac{\frac{\partial w_{Ij}}{\partial X_I}\sum_J w_{Jj} - w_{Ij}\sum_J \frac{\partial w_{Jj}}{\partial X_J}}{\left(\sum_J w_{Jj}\right)^2}$$

$$= C_{Ij}\left(\frac{\partial w_{Ij} / \partial X_I}{w_{Ij}} - \frac{\sum_J \frac{\partial w_{Jj}}{\partial X_J}}{\sum_J w_{Jj}}\right)$$

$$\frac{\partial \ln C_{Ii}}{\partial x_i} = \frac{\partial w_{Ii} / \partial x_i}{w_{Ii}} - \frac{\sum_J \frac{\partial w_{Ji}}{\partial x_i}}{\sum_J w_{Ji}} - \frac{1}{\sum_k \frac{w_{Ik}}{\sum_J w_{Jk}}} \frac{\frac{\partial w_{Ii}}{\partial x_i}\sum_J w_{Ji} - w_{Ii}\sum_J \frac{\partial w_{Ji}}{\partial x_i}}{\left(\sum_J w_{Ji}\right)^2}$$

$$= -\frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} + \frac{\sum_J \partial w_{Ji} / \partial X_J}{\sum_J w_{Ji}} + \frac{1}{\sum_k \frac{w_{Ik}}{\sum_J w_{Jk}}} \frac{\frac{\partial w_{Ii}}{\partial X_I}\sum_J w_{Ji} - w_{Ii}\sum_J \frac{\partial w_{Ji}}{\partial X_J}}{\left(\sum_J w_{Ji}\right)^2}$$

$$= -\frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} + \frac{\sum_J \partial w_{Ji} / \partial X_J}{\sum_J w_{Ji}} + C_{Ii}\frac{\partial w_{Ii} / \partial X_I}{w_{Ii}} - C_{Ii}\sum_J \frac{\partial w_{Ji} / \partial X_J}{\sum_J w_{Ji}}$$

$$= (1 - C_{Ii})\left(\frac{\sum_J \partial w_{Ji} / \partial X_J}{\sum_J w_{Ji}} - \frac{\partial w_{Ii} / \partial X_I}{w_{Ii}}\right)$$

$$N_{Ij}^{nm} = \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial r_{jm}}$$

$$M_{IJ}^{nm} = \sum_i r_{in} \frac{\partial C_{Ii}(t)}{\partial R_{Jm}}$$

Mass Constraints

In order to keep the mass of CG particles nearly constant, we add a mass dependent Gaussian width that decreases width while mass is large and increases otherwise. Adding this mass constraint will make the evaluation of partial derivatives dw/dx much more complicated. Because mass of CG particle I will also be a function of other CG particles. Starting from the definition of weighting functions and mapping coefficients, it's straightforward to write that:

$$\frac{\partial w_{Ii}}{\partial R_J} = \frac{\partial w_{Ii}}{\partial M_I} \cdot \frac{\partial M_I}{\partial R_J} + \delta_{IJ} \frac{\partial w_{Ii}}{\partial R_J}$$

$$\frac{\partial M_I}{\partial R_J} = \sum_i m_i \frac{\partial}{\partial R_J} \frac{C_{Ii}}{\sum_J C_{Ji}} = \sum_i m_i \frac{\frac{\partial C_{Ii}}{\partial R_J} \sum_J C_{Ji} - C_{Ii} \sum_K \frac{\partial C_{Ki}}{\partial R_J}}{\left(\sum_i C_{Ji} \right)^2}$$

$$\frac{\partial \ln C_{Ii}}{\partial R_J} = \frac{1}{w_{Ii}} \frac{\partial w_{Ii}}{\partial R_J} - \frac{1}{\sum_J w_{Ji}} \sum_K \frac{\partial w_{Ki}}{\partial R_J} - \frac{\sum_\alpha \frac{\frac{\partial w_{I\alpha}}{\partial R_J} \sum_J w_{Ja} - w_{I\alpha} \sum_M \frac{\partial w_{M\alpha}}{\partial R_J}}{\left(\sum_J w_{Ja} \right)^2}}{\sum_\alpha \frac{w_{I\alpha}}{\sum_J w_{J\alpha}}}$$

These three equations can lead to a linear equation solving dw/dR, plugging the definition of mapping function into the dM/dR matrices,

$$\sum_K \frac{\partial C_{Ki}}{\partial R_J} = \sum_K \left\{ \frac{C_{Ki}}{w_{Ki}} \frac{\partial w_{Ki}}{\partial R_J} - \frac{C_{Ki}}{\sum_J w_{Ji}} \sum_M \frac{\partial w_{Mi}}{\partial R_J} - \frac{C_{Ki}}{\sum_\alpha \frac{w_{I\alpha}}{\sum_J w_{J\alpha}}} \sum_\alpha \frac{\frac{\partial w_{I\alpha}}{\partial R_J} \sum_J w_{J\alpha} - w_{I\alpha} \sum_N \frac{\partial w_{N\alpha}}{\partial R_J}}{\left(\sum_J w_{J\alpha} \right)^2} \right\}$$

$$\frac{\partial M_I}{\partial R_J} = \sum_i m_i \frac{\frac{\partial C_{Ii}}{\partial R_J}\sum_J C_{Ji} - C_{Ii}\sum_K \frac{\partial C_{Ki}}{\partial R_J}}{\left(\sum_J C_{Ji}\right)^2}$$

$$= \sum_i \frac{m_i}{\sum_J C_{Ji}} \left\{ \frac{C_{Ii}}{w_{Ii}} \frac{\partial w_{Ii}}{\partial R_J} - \frac{C_{Ii}}{\sum_J w_{Ji}} \sum_K \frac{\partial w_{Ki}}{\partial R_J} - \frac{C_{Ii}}{\sum_\alpha \frac{w_{I\alpha}}{\sum_J w_{J\alpha}}} \sum_\alpha \frac{\frac{\partial w_{I\alpha}}{\partial R_J}\sum_J w_{J\alpha} - w_{I\alpha}\sum_M \frac{\partial w_{M\alpha}}{\partial R_J}}{\left(\sum_J w_{J\alpha}\right)^2} \right\}$$

$$-\sum_K \sum_i \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \left\{ \frac{C_{Ki}}{w_{Ki}} \frac{\partial w_{Ki}}{\partial R_J} - \frac{C_{Ki}}{\sum_J w_{Ji}} \sum_M \frac{\partial w_{Mi}}{\partial R_J} - \frac{C_{Ki}}{\sum_\alpha \frac{w_{K\alpha}}{\sum_J w_{J\alpha}}} \sum_\alpha \frac{\frac{\partial w_{K\alpha}}{\partial R_J}\sum_J w_{J\alpha} - w_{K\alpha}\sum_N \frac{\partial w_{N\alpha}}{\partial R_J}}{\left(\sum_J w_{J\alpha}\right)^2} \right\}$$

Assuming that $\frac{\partial w_{Ii}}{\partial R_J} = A_{IJi}$, the partial derivative can be summarized as:

$$A_{IJi} - \delta_{IJ}\frac{\partial w_{Ii}}{\partial r_{Ii}}\frac{R_I}{r_{Ii}} = \frac{\partial w_{Ii}}{\partial M_I}\left[\sum_i \beta_{Ii}A_{IJi} - \sum_i\sum_K \chi_{Ii}A_{KJi} - \sum_i\sum_\alpha \varepsilon_{Ii\alpha}A_{IJ\alpha} + \sum_i\sum_\alpha\sum_M \phi_{Ii\alpha}A_{MJ\alpha}\right]$$
$$-\frac{\partial w_{Ii}}{\partial M_I}\left[\sum_K\sum_i \eta_{IKi}A_{KJi} - \sum_K\sum_i\sum_M \mu_{IKi}A_{MJi} - \sum_K\sum_i\sum_\alpha \theta_{IKi\alpha}A_{KJ\alpha} + \sum_K\sum_i\sum_\alpha\sum_N \rho_{IKi\alpha}A_{NJ\alpha}\right]$$

The coefficients are:

$$\beta_{Ii} = \frac{m_i}{\sum_J C_{Ji}}\cdot\frac{C_{Ii}}{w_{Ii}} \qquad \chi_{Ii} = \frac{m_i}{\sum_J C_{Ji}}\cdot\frac{C_{Ii}}{\sum_J w_{Ji}} \qquad \varepsilon_{Ii\alpha} = \frac{m_i}{\sum_J C_{Ji}}\frac{C_{Ii}}{\sum_\beta \frac{w_{I\beta}}{\sum_J w_{J\beta}}}\frac{1}{\sum_J w_{J\alpha}}$$

$$\phi_{Ii\alpha} = \frac{m_i}{\sum_J C_{Ji}}\frac{C_{Ii}}{\sum_\beta \frac{w_{I\beta}}{\sum_J w_{J\beta}}}\frac{w_{I\alpha}}{\left(\sum_J w_{J\alpha}\right)^2} \qquad \eta_{IKi} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2}\frac{C_{Ki}}{w_{Ki}} \qquad \mu_{IKi} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2}\frac{C_{Ki}}{\sum_J w_{Ji}}$$

$$\theta_{IKi\alpha} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2}\frac{C_{Ki}}{\sum_\beta \frac{w_{K\beta}}{\sum_J w_{J\beta}}}\frac{1}{\sum_J w_{J\alpha}} \qquad \rho_{IKi\alpha} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2}\frac{C_{Ki}}{\sum_\beta \frac{w_{K\beta}}{\sum_J w_{J\beta}}}\frac{w_{K\alpha}}{\left(\sum_J w_{J\alpha}\right)^2}$$

Theoretically, solving this complex tensor equation can give us the answer of all the derivatives that we need. The next step is to simplify this formula.

First of all, notice that:

$$\sum_K \mu_{IKi} = \sum_K \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Ki}}{\sum_J w_{Ji}} = \frac{m_i}{\sum_J C_{Ji}} \frac{C_{Ii}}{\sum_J w_{Ji}} = \chi_{Ii}$$

These two terms just cancels out. The self-consistent equation can be written as:

$$A_{IJi} - \delta_{IJ} \frac{\partial w_{Ii}}{\partial r_{Ii}} \frac{R_I}{r_{Ii}} = \frac{\partial w_{Ii}}{\partial M_I} \left[\sum_i \beta_{Ii} A_{IJi} - \sum_i \sum_\alpha \varepsilon_{Ii\alpha} A_{IJ\alpha} + \sum_i \sum_\alpha \sum_M \phi_{Ii\alpha} A_{MJ\alpha} \right]$$

$$- \frac{\partial w_{Ii}}{\partial M_I} \left[\sum_K \sum_i \eta_{IKi} A_{KJi} - \sum_K \sum_i \sum_\alpha \theta_{IKi\alpha} A_{KJ\alpha} + \sum_K \sum_i \sum_\alpha \sum_N \rho_{IKi\alpha} A_{NJ\alpha} \right]$$

$$\beta_{Ii} = \frac{m_i}{\sum_J C_{Ji}} \cdot \frac{C_{Ii}}{w_{Ii}}$$

$$\eta_{IKi} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Ki}}{w_{Ki}}$$

$$\varepsilon_{Ii\alpha} = \frac{m_i}{\sum_J C_{Ji}} \frac{C_{Ii} \times C_{I\alpha}}{w_{I\alpha}}$$

$$\phi_{Ii\alpha} = \frac{m_i}{\sum_J C_{Ji}} \frac{C_{Ii} \times C_{I\alpha}}{\sum_J w_{J\alpha}}$$

$$\theta_{IKi\alpha} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Ki} \times C_{K\alpha}}{w_{K\alpha}}$$

$$\rho_{IKi\alpha} = \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Ki} \times C_{K\alpha}}{\sum_J w_{J\alpha}}$$

This equation can further be summarized in a more compact form:

$$A_{IJi} - \delta_{IJ} \frac{\partial w_{Ii}}{\partial r_{Ii}} \frac{R_I}{r_{Ii}} = \frac{\partial w_{Ii}}{\partial M_I} \left(\sum_\alpha \Gamma_{I\alpha} A_{IJ\alpha} - \sum_K \sum_\alpha \Delta_{IK\alpha} A_{KJ\alpha} \right)$$

The coefficient matrices are linear combinations of the above coefficients:

$$\Gamma_{I\alpha} = \beta_{I\alpha} - \sum_i \varepsilon_{Ii\alpha}$$

$$\Delta_{IK\alpha} = \eta_{IK\alpha} - \sum_i \theta_{IKi\alpha} + \sum_i \sum_M \rho_{IMi\alpha} - \sum_i \phi_{Ii\alpha}$$

Expanding these coefficients, one can derive that:

$$\Gamma_{I\alpha} = \beta_{I\alpha} - \sum_i \varepsilon_{Ii\alpha} = \frac{m_\alpha}{\sum_J C_{J\alpha}} \cdot \frac{C_{I\alpha}}{w_{I\alpha}} - \sum_i \frac{m_i}{\sum_J C_{Ji}} \frac{C_{Ii} \times C_{I\alpha}}{w_{I\alpha}}$$

$$\begin{aligned}
\Delta_{IK\alpha} &= \eta_{IK\alpha} - \sum_i \theta_{IKi\alpha} + \sum_i \sum_M \rho_{IMi\alpha} - \sum_i \phi_{Ii\alpha} \\
&= \frac{m_\alpha C_{I\alpha}}{\left(\sum_J C_{J\alpha}\right)^2} \frac{C_{K\alpha}}{w_{K\alpha}} - \sum_i \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Ki} \times C_{K\alpha}}{w_{K\alpha}} + \sum_i \sum_M \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \frac{C_{Mi} \times C_{M\alpha}}{\sum_J w_{J\alpha}} - \sum_i \frac{m_i}{\sum_J C_{Ji}} \frac{C_{Ii} \times C_{I\alpha}}{\sum_J w_{J\alpha}} \\
&= \frac{m_\alpha C_{I\alpha}}{\left(\sum_J C_{J\alpha}\right)^2} \frac{C_{K\alpha}}{w_{K\alpha}} - \sum_i \frac{m_i C_{Ii}}{\left(\sum_J C_{Ji}\right)^2} \left\{ \frac{C_{Ki} \times C_{K\alpha}}{w_{K\alpha}} - \frac{\sum_M C_{Mi} \times C_{M\alpha}}{\sum_J w_{J\alpha}} + \frac{\sum_J C_{Ji} \times C_{I\alpha}}{\sum_J w_{J\alpha}} \right\}
\end{aligned}$$

Explicitly solving this linear equation requires huge amount of computation, assuming that *m* equals to the number of CG particles and *n* the number of FG particles, evaluating $\Gamma_{I\alpha}$ has time complexity O(n), $\Delta_{IK\alpha}$ has complexity O(mn), then, overall, the complexity of generating these coefficients will be O(m^3n^2), and solving this linear equation will take time O(m^6n^3) , which is extremely demanding.