

Time-resolved force distribution analysis

Additional file 1

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Notation

$\vec{F}_i$ – force on atom i as vector

F_i – magnitude of $\vec{F}_i$

$\vec{U}_i$ – unit vector in the direction of $\vec{F}_i$

such that $\vec{F}_i = F_i \cdot \vec{U}_i$.

Forces decomposition for 3-body potentials

For an angle formed by atoms i, j, k (bonds i - j and j - k , see Figure 1), the sum of the atomic forces is zero:

$$\vec{F}_i + \vec{F}_j + \vec{F}_k = 0 \quad (1)$$

The atomic forces $\vec{F}_i$ and $\vec{F}_k$ can be decomposed into a component in the direction of $\vec{F}_j$ and a perpendicular component. The perpendicular components cancel each other out because of Equation 1.

The components in the direction of $\vec{F}_j$ can be written as:

$$\vec{F}_{ij} = -\vec{F}_{ji} = F_i \cos(\vec{F}_i, -\vec{F}_j) \cdot \vec{U}_j \quad (2)$$

$$\vec{F}_{kj} = -\vec{F}_{jk} = F_k \cos(\vec{F}_k, -\vec{F}_j) \cdot \vec{U}_j \quad (3)$$

The pairwise force between atoms i and k can be obtained by a vector difference:

$$\vec{F}_{ki} = \vec{F}_i - \vec{F}_{ji} = -\vec{F}_{ik} = -(\vec{F}_k - \vec{F}_{jk}) \quad (4)$$

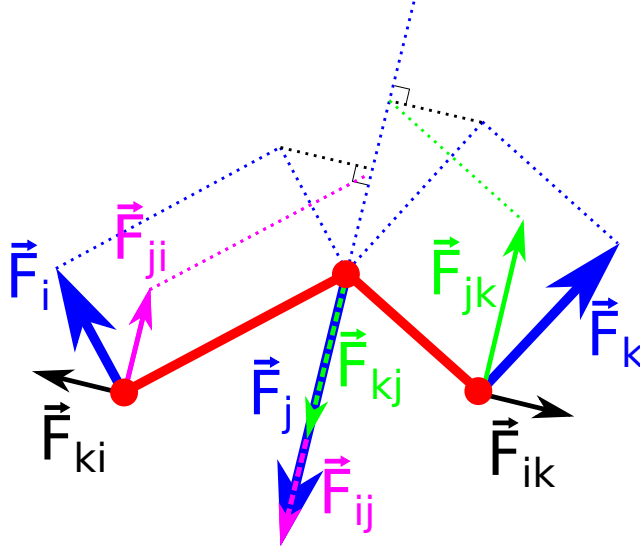


Figure 1: Force decomposition for an angle potential. $\vec{F}_i$ and $\vec{F}_k$ are decomposed into a component in the direction opposite to $\vec{F}_j$ and a component in the perpendicular direction.

Forces decomposition for 4-body potentials

For a dihedral angle formed by atoms i, j, k, l (bonds $i-j, j-k$ and $k-l$, see Figure 2), the sum of the atomic forces is zero:

$$\vec{F}_i + \vec{F}_j + \vec{F}_k + \vec{F}_l = 0 \quad (5)$$

which can also be written as:

$$\vec{F}_i + \vec{F}_l = -(\vec{F}_j + \vec{F}_k) \quad (6)$$

Atoms j and k can be considered to form a single body on which a combined force:

$$\vec{F}_{j+k} = \vec{F}_j + \vec{F}_k \quad (7)$$

acts as shown in Figure 2a. Similar to the force decomposition for an angle, $\vec{F}_i$ and $\vec{F}_l$ can be decomposed in a component in the direction of $\vec{F}_{j+k}$ and a component in the perpendicular direction. The components in the perpendicular direction cancel each other out because of Equation 6. The components in the direction of $\vec{F}_{j+k}$ can be written as:

$$\vec{F}_{i(j+k)} = F_i \cos(-\vec{F}_i, \vec{F}_{j+k}) \cdot \vec{U}_{j+k} \quad (8)$$

$$\vec{F}_{l(j+k)} = F_l \cos(-\vec{F}_l, \vec{F}_{j+k}) \cdot \vec{U}_{j+k} \quad (9)$$

The pairwise forces acting on atoms j and k can be written in a generic way as:

$$\vec{F}_j = \vec{F}_{ij} + \vec{F}_{kj} + \vec{F}_{lj} \quad (10)$$

$$\vec{F}_k = \vec{F}_{ik} + \vec{F}_{jk} + \vec{F}_{lk} \quad (11)$$

and, because $j+k$ is considered a single body, j and k do not move with respect to each other, so the pairwise force between them is zero:

$$\vec{F}_{kj} = -\vec{F}_{jk} = 0 \quad (12)$$

such that:

$$\vec{F}_{j+k} = \vec{F}_{ij} + \vec{F}_{lj} + \vec{F}_{ik} + \vec{F}_{lk} \quad (13)$$

A decomposition of $\vec{F}_{i(j+k)}$ and $\vec{F}_{l(j+k)}$ can be made in the direction of $\vec{F}_j$ and $\vec{F}_k$, as shown in Figure 2b, such that:

$$\vec{F}_{i(j+k)} = \vec{F}_{ij} + \vec{F}_{ik} \quad (14)$$

$$\vec{F}_{l(j+k)} = \vec{F}_{lj} + \vec{F}_{lk} \quad (15)$$

Defining α as the angle between $\vec{F}_{j+k}$ and $\vec{F}_j$ and β as the angle between $\vec{F}_{j+k}$ and $\vec{F}_k$, these vectors can be written as:

$$\vec{F}_{ij} = -\vec{F}_{ji} = \frac{F_{i(j+k)} \sin \beta}{\sin \alpha \cos \beta + \sin \beta \cos \alpha} \cdot \vec{U}_j \quad (16)$$

$$\vec{F}_{lj} = -\vec{F}_{jl} = \frac{F_{l(j+k)} \sin \beta}{\sin \alpha \cos \beta + \sin \beta \cos \alpha} \cdot \vec{U}_j \quad (17)$$

$$\vec{F}_{ik} = -\vec{F}_{ki} = \frac{F_{i(j+k)} \sin \alpha}{\sin \alpha \cos \beta + \sin \beta \cos \alpha} \cdot \vec{U}_k \quad (18)$$

$$\vec{F}_{lk} = -\vec{F}_{kl} = \frac{F_{l(j+k)} \sin \alpha}{\sin \alpha \cos \beta + \sin \beta \cos \alpha} \cdot \vec{U}_k \quad (19)$$

Finally, the pairwise force between atoms i and l can be obtained by a vector difference:

$$\vec{F}_{li} = \vec{F}_i - \vec{F}_{ji} - \vec{F}_{ki} = -\vec{F}_{il} = -(\vec{F}_l - \vec{F}_{jl} - \vec{F}_{kl}) \quad (20)$$

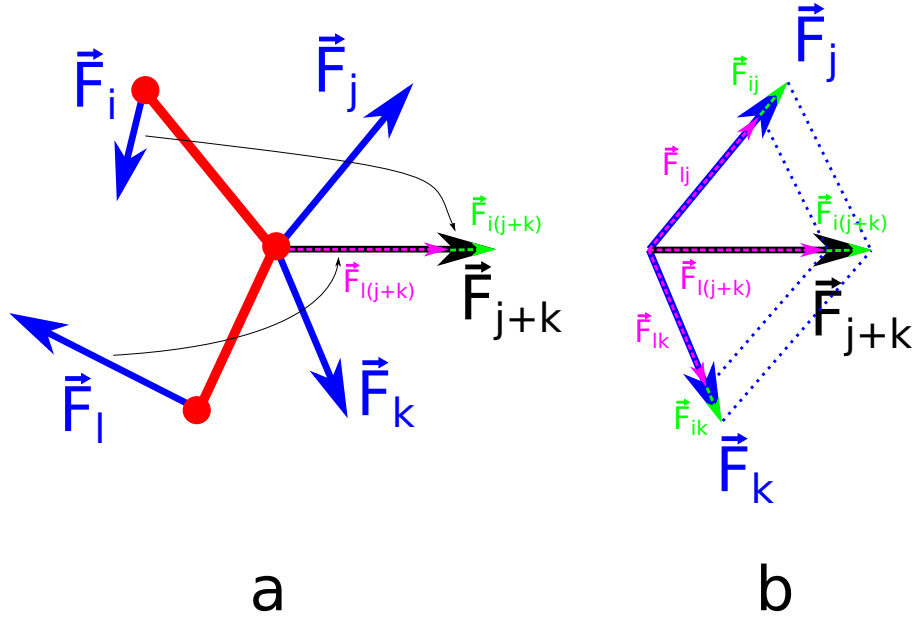


Figure 2: Force decomposition for a dihedral angle potential. a) Atoms j and k are considered a single body on which a combined $\vec{F}_{j+k}$ acts. Forces are then decomposed similar to Figure 1. b) The pairwise forces between the atoms i and l and the $j+k$ single body are decomposed into components in directions of $\vec{F}_j$ and $\vec{F}_k$.