Computational biophysics

Protein's geometry

Centre of mass $\vec{R}_{cm} = \frac{\sum_{i=1}^{N} m_i \vec{r}_i}{\sum_{i=1}^{N} m_i}$

Radius of gyration $r_g = \sqrt{\frac{\sum_{i=1}^{N} m_i (\vec{r}_i - \vec{R}_{cm})^2}{\sum_{i=1}^{N} m_i}}$

$RMSD(t) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\vec{r}_i(t) - \vec{r}_i(0))^2}$

$RMSF_i = \sqrt{\langle \Delta r_i^2 \rangle} = \sqrt{\frac{1}{M} \sum_{f=1}^{M} (\vec{r}_{i,f} - \langle \vec{r}_i \rangle)^2}$

$B_i = \frac{8\pi^2}{3} RMSF_i^2$

Semi-empirical force fields

Bond stretching

Harmonic $U(r_{AB}) = \frac{1}{2} k_{AB} (r_{AB} - r_{AB,eq})^2$

Anarmonic $U(r_{AB}) = \frac{1}{2} \left[k_{AB} + k_{AB}^{(3)} (r_{AB} - r_{AB,eq}) \right] (r_{AB} - r_{AB,eq})^2$

Quartic correction $U(r_{AB}) = \dfrac{1}{2} \left[k_{AB} + k_{AB}^{(3)} (r_{AB} - r_{AB,eq}) + k_{AB}^{(4)} (r_{AB} - r_{AB,eq})^2 \right] \cdot$
$\cdot (r_{AB} - r_{AB,eq})^2$

Morse $U(r_{AB}) = D_{AB} \left[1 - e^{-\alpha_{AB}(r_{AB} - r_{AB,eq}^2)} \right]$

Valence angle bending

Potential $U(\theta_{ABC}) = \dfrac{1}{2} [k_{ABC} + k_{ABC}^{(3)} (\theta_{ABC} - \theta_{ABC,eq}) +$
$+ k_{ABC}^{(4)} (\theta_{ABC} - \theta_{ABC,eq})^2 + \cdots](\theta_{ABC} - \theta_{ABC,eq})^2$

Fourier
$$U(\theta_{ABC}) = \sum_{\{j\}_{ABC}} k_{j,ABC}^{fourier} [1 + \cos(j\theta_{ABC} + \psi_j)]$$
$$k_{j,ABC}^{fourier} = \frac{2k_{ABC}^{harmonic}}{j^2}$$

Torsions

Potential $U(\omega_{ABCD}) = \frac{1}{2} \sum_{\{j\}_{ABCD}} V_{j,ABCD} \left[1 + (-1)^{j+1} \cos(j\omega_{ABCD} + \psi_{j,ABCD}) \right]$

Improper $U(\omega_{ABCD}) = \frac{1}{2} \sum_{\{j\}_{ABCD}} V_{j,ABCD} [1 + (-1)^{j+1} \cos(j\omega_{ABCD} + \psi_{j,ABCD})]$

Van der Waals

Lennard-Jones $U(r_{AB}) = 4\epsilon_{AB} \left[\left(\frac{\sigma_{AB}}{r_{AB}} \right)^{12} - \left(\frac{\sigma_{AB}}{r_{AB}} \right)^6 \right]$

Morse $U(r_{AB}) = D_{AB} \left[1 - e^{-\alpha_{AB}(r_{AB} - r_{AB,eq}^2)} \right]^2$

Hill $U(r_{AB}) = \epsilon \left[\frac{6}{\beta_{AB} - 6} e^{\beta_{AB} \frac{1 - r_{AB}}{r_{AB}^*}} - \frac{\beta_{AB}}{\beta_{AB} - 6} \left(\frac{r_{AB}^*}{r_{AB}} \right)^6 \right]$

Electrostatic interactions

Distribution of charges $U_{AB} = \sum_{A} \sum_{B>A} \vec{M}^{(A)} \vec{V}^{(B)}$

Point like $U_{AB} = \frac{q_A q_B}{\epsilon_{AB} r_{AB}}$

Dipolar interactions $U_{AB/CD} = \frac{\mu_{AB} \mu_{CD}}{\epsilon_{AB/CD} r_{AB/CD}^3} (\cos \chi_{AB/CD} - 3 \cos \alpha_{AB} \cos \alpha_{CD})$

Parameterization

Parameters $Z = \sqrt{\sum_{i}^{observables} \sum_{j}^{occurrences} \frac{(calc_{i,j} - expt_{i,j})^2}{w_i^2}}$

$\sigma_{AB} = \sigma_A + \sigma_B$ $\quad \epsilon_{AB} = \sqrt{\epsilon_A \epsilon_B}$

Classical mechanics

Newton's laws

$\vec{F} = m\vec{a}$ $\quad \vec{F}_{BA} = -\vec{F}_{AB}$

$\vec{v}(t) = \frac{d\vec{r}}{dt}$ $\quad \vec{a}(t) = \frac{d\vec{v}}{dt} = \frac{d^2\vec{r}}{dt^2}$ $\quad m\frac{d^2\vec{r}}{dt^2} = \vec{F}$

Force acting on atom $\vec{F}_i(\vec{r}_1, \ldots, \vec{r}_N, \dot{\vec{r}}_i) = \sum_{j \neq i} \vec{F}_{ij}(\vec{r}_i - \vec{r}_j) + \vec{F}^{(ext)}(\vec{r}_i, \dot{\vec{r}}_i)$

Bond stretching: $U = \frac{k_l}{2}(l - l^0)^2$

Bond bending: $U = \frac{k_\theta}{2}(\theta - \theta^0)^2$

Bond torsion: $U = k_\phi[1 + \cos(n\phi - \phi^0)]$

Van der Waals interactions: $U = \left[\frac{a_{ij}}{r_{ij}^{12}} - \frac{b_{ij}}{r_{ij}^6} \right]$

Electrostatic interactions: $U = \frac{332 q_i q_j}{\epsilon r_{ij}}$

$\vec{p}_i = m_i \vec{v}_i = m\dot{\vec{r}}_i$ $\quad \vec{F}_i = m_i \ddot{\vec{r}}_i = \dot{\vec{p}}_i$

$\vec{x}(t) = \{\vec{r}_1(t), \ldots, \vec{r}_N(t), \vec{p}_1(t), \ldots, \vec{p}_N(t)\}$

Lagrangian formulation

$\vec{F}_i(\vec{r}_1, \ldots, \vec{r}_N) = -\Delta_i U(\vec{r}_1, \ldots, \vec{r}_N)$

$W_{AB} = \int_A^B \vec{F}_i d\vec{l} = U_A - U_B = -\Delta U_{AB}$ $\quad \oint \vec{F}_i d\vec{l} = 0$

Kinetic energy $K(\dot{\vec{r}}_1, \ldots, \dot{\vec{r}}_N) = \frac{1}{2} \sum_i m_i \dot{\vec{r}}_i^2$

$\mathcal{L}(\vec{r}_1, \ldots, \vec{r}_N, \dot{\vec{r}}_1, \ldots, \dot{\vec{r}}_N) = K(\dot{\vec{r}}_1, \dot{\vec{r}}_N) - U(\vec{r}_1, \ldots, \vec{r}_N)$

Euler-Lagrange $\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}_i} \right) - \frac{\partial \mathcal{L}}{\partial \vec{r}_i} = 0$

$E = \frac{1}{2} \sum_i m_i \dot{\vec{r}}_i^2 + U(\vec{r}_1, \ldots, \vec{r}_N)$

$quad \frac{dE}{dt} = 0$

Generalized coordinates

$q_\alpha = f_\alpha(\vec{r}_1, \ldots, \vec{r}_N)$ $\quad \alpha = 1, \ldots, 3N$ $\quad \vec{r}_i = \vec{g}_i(q_1, d \ldots, q_{3N})$ $\quad i = 1, \ldots, N$

$\dot{\vec{r}}_i = \sum_{\alpha=1}^{3N} \frac{\partial \vec{r}_i}{\partial q_\alpha} \dot{q}_\alpha$ $\quad \mathcal{L}(q, \dot{q}) = \frac{1}{2} \sum_{\alpha=1}^{3N} \sum_{\beta=1}^{3N} G_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta - U(q_1, \ldots, q_{3N})$

Legendre transforms

$s = f'(x) \equiv g(x)$ $\quad f'(x) = g(x) = s \Rightarrow x = g^{-1}(s)$

$b(g^{-1}(s)) = f(g^{-1}(s)) - sg^{-1}(s) \equiv \tilde{f}(s) = f(x(s)) - sx(s)$

$\tilde{f}(s_1, \ldots, s_n) = f(x_1(s_1, \ldots, s_n), \ldots x_n(s_1, \ldots, s_n)) - \sum_i s_i x_i(s_1, \ldots, s_n)$

Hamiltonian formulation

$\mathcal{H}(\vec{r}_1, \ldots, \vec{r}_N, \vec{p}_1, \ldots, \vec{p}_N) = -\tilde{\mathcal{L}}(\vec{r}_1, \ldots, \vec{r}_N, \vec{p}_1, \ldots, \vec{p}_N)$

$\mathcal{H}(\vec{r}_1, \ldots, \vec{r}_N, \vec{p}_1, \ldots, \vec{p}_N) = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m_i} + U(\vec{r}_1, \ldots, \vec{r}_N)$

$\mathcal{H}(q_1, \ldots, q_{3N}, p_1, \ldots, p_{3N}) = \frac{1}{2} \sum_\alpha \sum_\beta p_\alpha G_{\alpha\beta}^{-1} p_\beta + U(q_1, \ldots, q_{3N})$

Hamilton equations $\dot{q}_\alpha = \frac{\partial \mathcal{H}}{\partial p_\alpha}$ $\quad \dot{p}_\alpha = -\frac{\partial \mathcal{H}}{\partial q_\alpha}$ $\quad \frac{\mathcal{H}}{dt} = 0$ $\quad \mathcal{H} = const$

Some properties

Conservation laws $\frac{da}{dt} = \frac{\partial a}{\partial x_t} \dot{x}(t) = \{a, \mathcal{H}\} = 0$

Incompressibility $\nabla_x \dot{(x)} = 0$

Symplectic structure $M = J^T M J$ $\quad J_{kl} = \frac{\partial x_k(t)}{\partial x_l(0)}$