Supplementary materials: DNA overstretching modeled at the base pair level

Attila Kocsis[a], David Swigon[b]

[a]*Department of Structural Mechanics, Budapest University of Technology and Economics*
[b]*Department of Mathematics, University of Pittsburgh*

---

1. Parametrization of matrices $\boldsymbol{D}^n$ and $\widetilde{\boldsymbol{D}}^n$

Components of orthogonal matrix $\boldsymbol{D}^n$ employing the Euler-angle system ζ^n, κ^n, η^n are

$$D^n_{ij} = \boldsymbol{d}^n_i \cdot \boldsymbol{d}^{n+1}_j = Z_{ij}(\zeta^n) Y_{kl}(\kappa^n) Z_{lj}(\eta^n),$$

where

$$\zeta^n = \frac{\theta^n_3}{2} - \gamma^n, \qquad \eta^n = \frac{\theta^n_3}{2} + \gamma^n,$$
$$\kappa^n = \sqrt{(\theta^n_1)^2 + (\theta^n_2)^2}, \quad \tan\gamma^n = \frac{\theta^n_1}{\theta^n_2}$$

and

$$\boldsymbol{Y}(\alpha) = \begin{bmatrix} \cos\alpha & 0 & \sin\alpha \\ 0 & 1 & 0 \\ -\sin\alpha & 0 & \cos\alpha \end{bmatrix},$$
$$\boldsymbol{Z}(\alpha) = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The mid-basis $\widetilde{\boldsymbol{d}}^n_i$ for step n is defined by

$$\widetilde{D}^n_{ij} = \boldsymbol{d}^n_i \cdot \widetilde{\boldsymbol{d}}^n_j = Z_{ik}(\zeta^n) Y_{kl}(\kappa^n/2) Z_{lj}(\gamma^n).$$

2. Explicit expressions of matrices $\boldsymbol{\Gamma}$ and $\boldsymbol{\Lambda}$

Matrix $\boldsymbol{\Gamma}$ is given by

$$\boldsymbol{\Gamma}(\alpha) = \begin{bmatrix} -\dfrac{\theta^n_1}{\kappa^n}\sin\zeta^n + \dfrac{\theta^n_2\cos\zeta^n}{2\tan\left(\dfrac{\kappa^n}{2}\right)} & -\dfrac{\theta^n_2}{\kappa^n}\sin\zeta^n - \dfrac{\theta^n_1\cos\zeta^n}{2\tan\left(\dfrac{\kappa^n}{2}\right)} & \tan\left(\dfrac{\kappa^n}{2}\right)\cos\zeta^n \\ \dfrac{\theta^n_1}{\kappa^n}\cos\zeta^n + \dfrac{\theta^n_2\sin\zeta^n}{2\tan\left(\dfrac{\kappa^n}{2}\right)} & \dfrac{\theta^n_2}{\kappa^n}\cos\zeta^n - \dfrac{\theta^n_1\sin\zeta^n}{2\tan\left(\dfrac{\kappa^n}{2}\right)} & \tan\left(\dfrac{\kappa^n}{2}\right)\sin\zeta^n \\ -\dfrac{\theta^n_2}{2} & \dfrac{\theta^n_1}{2} & 1 \end{bmatrix}.$$

Skew matrix $[{}_j\Lambda^n_{kl}]$ is defined when $j = 1$ as

$$
{}_1\Lambda^n_{12} = \frac{\theta^n_2 \left(1 - \cos\left(\frac{\kappa^n}{2}\right)\right)}{(\kappa^n)^2},
$$

$$
{}_1\Lambda^n_{13} = \frac{\theta^n_1 \theta^n_2 \left(2\sin\left(\frac{\kappa^n}{2}\right) - \kappa^n\right)}{2(\kappa^n)^3},
$$

$$
{}_1\Lambda^n_{23} = \frac{1}{2} + \left(\frac{\theta^n_2}{\kappa^n}\right)^2 \frac{2\sin\left(\frac{\kappa^n}{2}\right) - \kappa^n}{2\kappa^n},
$$

when $j = 2$ as

$$
{}_2\Lambda^n_{12} = \frac{\theta^n_1 \left(\cos\left(\frac{\kappa^n}{2}\right) - 1\right)}{(\kappa^n)^2},
$$

$$
{}_2\Lambda^n_{13} = \left(\frac{\theta^n_1}{\kappa^n}\right)^2 \frac{\kappa^n - 2\sin\left(\frac{\kappa^n}{2}\right)}{2\kappa^n} - \frac{1}{2},
$$

$$
{}_2\Lambda^n_{23} = \frac{\theta^n_1 \theta^n_2 \left(\kappa^n - 2\sin\left(\frac{\kappa^n}{2}\right)\right)}{2(\kappa^n)^3}
$$

and when $j = 3$ as

$$
{}_3\Lambda^n_{12} = \frac{1}{2}\cos\left(\frac{\kappa^n}{2}\right), \quad {}_3\Lambda^n_{13} = -\frac{\theta^n_1}{2\kappa^n}\sin\left(\frac{\kappa^n}{2}\right), \quad {}_3\Lambda^n_{23} = -\frac{\theta^n_2}{2\kappa^n}\sin\left(\frac{\kappa^n}{2}\right).
$$

3. Stability analysis

Elements of the n^{th} diagonal block of the *Hessian* are

$$\begin{aligned}
\frac{\partial^2\psi}{\partial\boldsymbol{w}_i\partial\boldsymbol{w}_j} =& \frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{P}_i\boldsymbol{P}_j\boldsymbol{B}^n,\boldsymbol{x}^n,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&+\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},(\boldsymbol{P}_i)^T(\boldsymbol{P}_j)^T\boldsymbol{B}^n,\boldsymbol{x}^n,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},(\boldsymbol{P}_i)^T\boldsymbol{P}_j\boldsymbol{B}^n,\boldsymbol{x}^n,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{P}_i(\boldsymbol{P}_j)^T\boldsymbol{B}^n,\boldsymbol{x}^n,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}=\boldsymbol{H}(i,j),
\end{aligned}$$

$$\begin{aligned}
\frac{\partial^2\psi}{\partial\boldsymbol{x}^n_i\partial\boldsymbol{x}^n_j} =& \frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{B}^n,\boldsymbol{x}^n+\varepsilon\boldsymbol{d}^n_i+\varepsilon\boldsymbol{d}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&+\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{B}^n,\boldsymbol{x}^n-\varepsilon\boldsymbol{d}^n_i-\varepsilon\boldsymbol{d}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{B}^n,\boldsymbol{x}^n+\varepsilon\boldsymbol{d}^n_i-\varepsilon\boldsymbol{d}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{B}^n,\boldsymbol{x}^n-\varepsilon\boldsymbol{d}^n_i+\varepsilon\boldsymbol{d}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}=\boldsymbol{H}(i+3,j+3),
\end{aligned}$$

$$\begin{aligned}
\frac{\partial^2\psi}{\partial\boldsymbol{w}_i\partial\boldsymbol{x}^n_j} =& \frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{P}_i\boldsymbol{B}^n,\boldsymbol{x}^n+\varepsilon\boldsymbol{B}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&+\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},(\boldsymbol{P}_i)^T\boldsymbol{B}^n,\boldsymbol{x}^n-\varepsilon\boldsymbol{B}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},\boldsymbol{P}_i\boldsymbol{B}^n,\boldsymbol{x}^n-\varepsilon\boldsymbol{d}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}\\
&-\frac{\psi\left(\boldsymbol{B}^{n-1},\boldsymbol{x}^{n-1},(\boldsymbol{P}_i)^T\boldsymbol{B}^n,\boldsymbol{x}^n+\varepsilon\boldsymbol{B}^n_j,\boldsymbol{B}^{n+1},\boldsymbol{x}^{n+1}\right)}{4\varepsilon^2}=\boldsymbol{H}(i,j+3)=\boldsymbol{H}(j+3,i),
\end{aligned}$$

for $i,j=1,2,3$, where

$$\boldsymbol{P}_i=\left(\boldsymbol{I}+\frac{\boldsymbol{w}_i}{2}\right)\left(\boldsymbol{I}-\frac{\boldsymbol{w}_i}{2}\right)^{-1},\quad i=1,2,3,$$

$$\boldsymbol{w}_1=\begin{bmatrix}0&0&0\\0&0&\varepsilon\\0&-\varepsilon&0\end{bmatrix},\ \boldsymbol{w}_2=\begin{bmatrix}0&0&-\varepsilon\\0&0&0\\\varepsilon&0&0\end{bmatrix},\ \boldsymbol{w}_3=\begin{bmatrix}0&\varepsilon&0\\-\varepsilon&0&0\\0&0&0\end{bmatrix},\ \boldsymbol{I}=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}.$$

Off-diagonal blocks are constructed in a similar way.

4. Force constants and intrinsic step parameters

Force constants F_{ij} [kT/deg^2], H_{ij} [kT/Å^2], G_{ij} [kT/deg/Å] and intrinsic step parameters $\overline{\theta}_i$ [deg], $\overline{\rho}_j$ [Å] obtained from [1] shown in Table 1. The constants for the 6 steps not explicitly listed here can be obtained by symmetry considerations [2].

References

[1] `http://dnaserver.rutgers.edu/database.php`.

[2] B. Coleman, W. Olson, D. Swigon, Theory of sequence-dependent dna elasticity, Journal of Chemical Physics 118 (2003) 7127–7140.

Table 1: Force constants F_{ij} [kT/deg^2], H_{ij} [kT/Å^2], G_{ij} [kT/deg/Å] and intrinsic step parameters $\overline{\theta}_i$ [deg], $\overline{\rho}_j$ [Å].

	CG	CA	TA	AG	GG	AA	GA	AT	AC	GC	MN	MN_{st}	MN^{dg}	MN^{dg}_{st}
F_{11}	0.107	0.121	0.135	0.197	0.157	0.149	0.133	0.190	0.130	0.120	0.116	0.116	0.116	0.116
F_{12}	0.000	-0.004	0.000	0.014	0.010	0.007	-0.003	0.000	0.011	0.000	0.000	0.000	0.000	0.000
F_{13}	0.000	-0.003	0.000	0.034	0.003	0.002	0.019	0.000	0.011	0.000	0.000	0.000	0.000	0.000
F_{22}	0.038	0.061	0.053	0.067	0.068	0.064	0.044	0.068	0.077	0.095	0.047	0.047	0.047	0.047
F_{23}	0.018	0.020	0.031	0.024	0.014	0.034	0.024	0.024	0.021	0.012	0.018	0.018	0.000	0.000
F_{33}	0.103	0.066	0.056	0.080	0.086	0.101	0.086	0.091	0.099	0.069	0.066	0.066	0.066	0.066
G_{11}	-0.352	-0.316	-0.164	-0.282	-0.330	-0.263	-0.369	-0.162	-0.113	-0.248	-0.250	-0.250	0.000	0.000
G_{21}	0.000	0.028	0.000	0.038	0.063	0.017	0.028	0.000	0.065	0.000	0.000	0.000	0.000	0.000
G_{31}	0.000	-0.029	0.000	0.137	0.125	0.168	-0.038	0.000	0.018	0.000	0.000	0.000	0.000	0.000
G_{12}	0.000	-0.038	0.000	-0.080	0.009	0.086	-0.021	0.000	0.175	0.000	0.000	0.000	0.000	0.000
G_{22}	0.038	0.029	-0.014	-0.088	0.116	-0.211	-0.071	0.047	-0.051	0.355	-0.049	-0.049	0.000	0.000
G_{32}	-0.117	-0.127	-0.088	-0.068	-0.104	-0.254	-0.237	-0.122	-0.118	-0.227	-0.173	-0.173	0.000	0.000
G_{13}	0.000	0.019	0.000	-1.411	-0.867	-0.673	-0.679	0.000	0.057	0.000	0.000	0.000	0.000	0.000
G_{23}	0.003	-0.008	-0.163	-0.403	-0.026	-0.120	0.141	0.229	0.240	0.724	-0.095	-0.095	0.000	0.000
G_{33}	-0.357	-0.310	-0.514	-0.803	-0.587	-0.254	-0.383	-0.350	-0.566	-0.635	-0.431	-0.431	0.000	0.000
H_{11}	2.510	3.167	3.459	2.963	3.106	7.161	5.158	4.063	4.077	2.449	3.010	3.010	3.010	3.010
H_{12}	0.000	0.725	0.000	0.128	0.081	0.783	1.840	0.000	1.476	0.000	0.000	0.000	0.000	0.000
H_{13}	0.000	0.074	0.000	0.656	1.177	2.772	3.285	0.000	-0.047	0.000	0.000	0.000	0.000	0.000
H_{22}	3.521	2.262	2.007	4.498	3.841	8.107	4.162	8.886	11.452	5.582	2.961	2.961	2.961	2.961
H_{23}	3.214	2.362	2.330	3.732	4.365	1.777	2.124	5.428	6.243	6.349	2.096	2.096	0.000	0.000
H_{33}	22.628	20.875	37.210	34.532	33.325	37.297	24.466	38.484	32.711	31.530	23.560	23.560	23.560	23.560
$\overline{\theta}_1$	0.00	-0.02	0.00	-1.31	-0.04	-1.30	-1.51	0.00	0.46	0.00	0.00	0.00	0.00	0.00
$\overline{\theta}_2$	4.32	4.98	2.93	3.79	5.04	0.43	1.83	1.01	1.79	0.70	2.79	2.79	0.00	0.00
$\overline{\theta}_3$	34.73	34.98	37.08	32.65	33.06	35.18	35.49	29.86	31.36	33.58	33.79	33.79	33.79	33.79
$\overline{\rho}_1$	0.00	-0.05	0.00	0.09	-0.04	0.02	-0.29	0.00	0.26	0.00	0.00	0.00	0.00	0.00
$\overline{\rho}_2$	0.3	0.3	0.1	-0.3	-0.4	-0.2	-0.1	-0.7	-0.6	-0.2	-0.2	-0.2	0.0	0.0
$\overline{\rho}_3$	3.4	3.4	3.3	3.3	3.4	3.3	3.3	3.2	3.3	3.3	3.3	3.3	3.3	3.3