

# Numerical realization of helicoidal DNA model

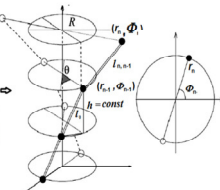
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## MECHANICAL DNA MODEL



The parameter\*

Parameter	Symbol	Value
Morse potential range	$a$	6.3 Å <sup>-1</sup>
Stacking interaction range	$b$	0.5 Å <sup>-1</sup>
Morse potential depth	$D$	0.15 eV
Stacking interaction coupling	$s$	0.65 eV Å <sup>-2</sup>
Interplane distance	$h$	3.4 Å
Elastic coupling	$K$	0.04 eV Å <sup>-2</sup>
Equilibrium distance	$R_0$	10 Å
Twist angle	$\theta$	0.60707 rad
Base masses	$m$	300 amu

## LAGRANGIAN of DNA MODEL\*\*

$$L = m \sum_n \dot{r}_n^2 + r_n^2 \dot{\Phi}_n^2 - \sum_n [D(e^{-a(r_n-R)})^2 + K(l_{n,n-1} - l_0)^2 + S(r_n - r_{n-1})^2 e^{-b(r_n+r_{n-1})}]$$

$$l_0 = \sqrt{h^2 + 4R^2 \sin^2(\theta/2)}, \quad l_{n,n-1} = \sqrt{h^2 + r_n^2 + r_{n-1}^2 - 2r_n r_{n-1} \cos(\Phi_n - \Phi_{n-1})}$$

## DIMENSIONLESS VARIABLES

$$y_n = (r_n - R)a, \quad r = Ra, \quad \varphi_n = (\Phi_n - n\theta), \quad \tilde{l} = \sqrt{Da^2/m}, \quad k = K/(Da^2), \quad s = St/(Da^2), \quad \beta = b/a, \quad \sqrt{m}/Da = 0.07ps, \quad 1/a = 0.16 \text{ \AA}$$

$$\tilde{L} = \sum_n \dot{y}_n^2 + (y_n + r)^2 \dot{\varphi}_n^2 - \left[ (e^{-y_n} - 1)^2 + k(\tilde{l}_{n,n-1} - \tilde{l}_0)^2 + s(y_n - y_{n-1})^2 e^{-\beta(y_n + y_{n-1})} \right]$$

$$\tilde{l}_{n,n-1} = a l_{n,n-1} = \sqrt{h^2 + (y_n + r)^2 + (y_{n-1} + r)^2 - 2(y_n + r)(y_{n-1} + r) \cos(\varphi_n - \varphi_{n-1})}, \quad \tilde{l}_0 = a l_0 = \sqrt{h^2 + 4r^2 \sin^2(\theta/2)}, \quad \tilde{h} = ah$$

\* M. Barbi, S. Lepri, M. Peyrard, N. Theodorakopoulos Phys. Rev. 68, 061909 (2003)

\*\* M. Barbi, S. Cocco, M. Peyrard, and S. Ruffo, J. Biol. Phys. 24, 97 (1999)

## LAGRANGE EQUATIONS

$$I) \frac{d}{dt} \frac{\partial \tilde{L}}{\partial \dot{y}_n} = \frac{\partial \tilde{L}}{\partial y_n}$$

$$y_n = (y_n + r) \dot{\varphi}_n^2 + (e^{-y_n} - 1) e^{-y_n} - k \left[ (\tilde{l}_{n,n-1} - \tilde{l}_0) \frac{\partial \tilde{l}_{n,n-1}}{\partial y_n} + (\tilde{l}_{n,n+1} - \tilde{l}_0) \frac{\partial \tilde{l}_{n,n+1}}{\partial y_n} \right] - s \left[ (y_n - y_{n-1}) e^{-\beta(y_n + y_{n-1})} + (y_n - y_{n+1}) e^{-\beta(y_n + y_{n+1})} \right] + \beta s \left[ (y_n - y_{n-1})^2 e^{-\beta(y_n + y_{n-1})} + (y_n - y_{n+1})^2 e^{-\beta(y_n + y_{n+1})} \right]$$

$$II) \frac{d}{dt} \frac{\partial \tilde{L}}{\partial \dot{\varphi}_n} = \frac{\partial \tilde{L}}{\partial \varphi_n}$$

$$(y_n + r)^2 \dot{\varphi}_n = -2(y_n + r) \dot{\varphi}_n - k \left[ (\tilde{l}_{n,n-1} - \tilde{l}_0) \frac{\partial \tilde{l}_{n,n-1}}{\partial \varphi_n} + (\tilde{l}_{n,n+1} - \tilde{l}_0) \frac{\partial \tilde{l}_{n,n+1}}{\partial \varphi_n} \right]$$

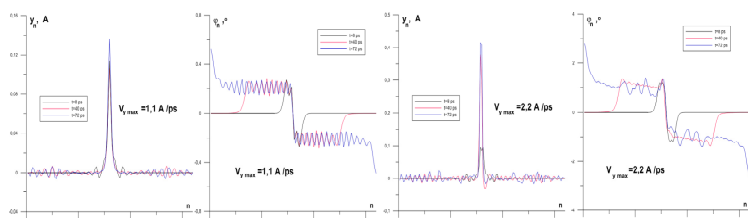
$$\frac{\partial \tilde{l}_{n,n\pm 1}}{\partial y_n} = \frac{y_n + r}{\tilde{l}_{n,n\pm 1}} \left( 1 - \frac{y_{n\pm 1} + r}{y_n + r} \cos(\varphi_n - \varphi_{n\pm 1}) \right), \quad \frac{\partial \tilde{l}_{n,n\pm 1}}{\partial \varphi_n} = \frac{(y_n + r)(y_{n\pm 1} + r)}{\tilde{l}_{n,n\pm 1}} \sin(\varphi_n - \varphi_{n\pm 1})$$

with initial conditions:  $y_n(0) = y_{n0}, \quad \dot{y}_n(0) = v_{n0}, \quad \varphi_n(0) = \varphi_{n0}, \quad \dot{\varphi}_n(0) = \omega_{n0}$

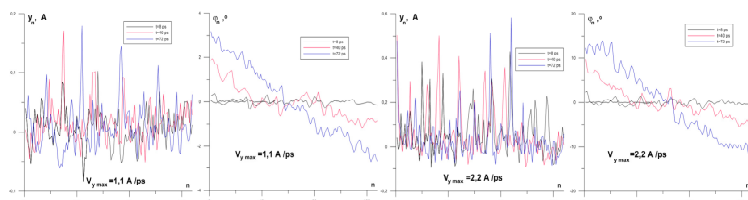
The system of ordinary differential equations (I) - (II) is solved numerically by the Runge-Kutta method of the fifth order of accuracy with a variable automatically selectable time step

## DYNAMICS OF SINGLE DISTURBANCE (N=128)

VELOCITY DISTURBANCE IN CENTER BY FIVE PAIRS IN BOTH DIRECTIONS ( $v_{y_{max}} \cos^2((n-N/2)\pi/10)$ )



UNIFORM RANDOM VELOCITY DISTURBANCE IN ALL PAIRS ( $v_{y_{max}} \times \xi_n, \xi_n \in (0, 1]$ )



## RANDOM DISTRIBUTIONS GENERATORS TESTING

BOX-MULLER TRANSFORMATION

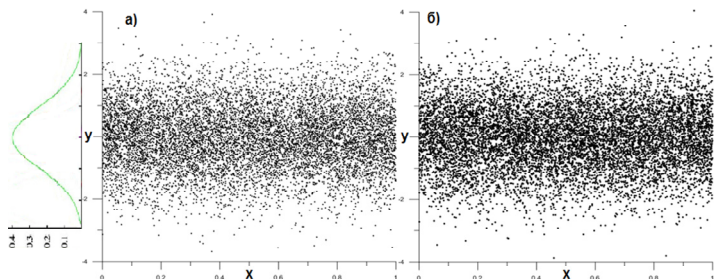
$$1) \xi_1 = \cos(2\pi\varphi) \sqrt{-2 \ln(r)}, \quad \xi_2 = \sin(2\pi\varphi) \sqrt{-2 \ln(r)},$$

$$\varphi \in (0, 1), \quad r \in (0, 1)$$

$$2) s = x^2 + y^2, \quad s \leq 1 \Rightarrow \xi_1 = x \sqrt{-2 \ln(s)/s}, \quad \xi_2 = y \sqrt{-2 \ln(s)/s},$$

$$x \in [-1, 1], \quad y \in [-1, 1]$$

$$\zeta = \mu + \sigma \xi \Rightarrow \zeta \sim N(\mu, \sigma^2)$$



## MOLECULAR DYNAMICS (MICROCANONICAL ENSEMBLE)

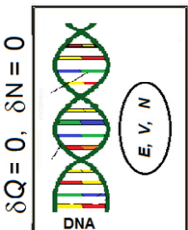
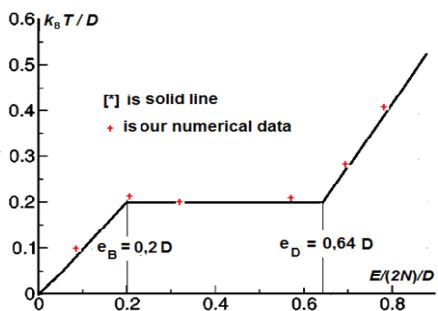
$$E = const, \quad N = const, \quad P - M_{\theta}|_{\theta=L,N}, \quad V - \Phi|_{\theta=L,N} = const$$

PARAMETRIC REPRESENTATION OF CURVE T (e)

$$T = T(e), \quad \frac{k_B T}{D} = \frac{E_{bin}}{DN}, \quad e = \frac{E}{D2N} \Rightarrow \begin{cases} k_B T / D = f(\sigma), \\ e = \psi(\sigma) \end{cases}$$

INITIAL CONDITIONS FOR EACH RANDOM VARIANT OF DNA STATE

$$y_n = 0, \quad \dot{y}_n = \zeta_n, \quad \varphi_n = 0, \quad \dot{\varphi}_n = 0, \quad \zeta \sim N(\mu = 0, \sigma^2)$$



COMPARISON WITH EXPERIMENT

$$\left( \frac{k_B T_D}{D} \right)_{\text{theor.}} \approx 0.2 \Rightarrow T_D \approx \frac{0.2D}{k_B} \approx 350K \approx 77^\circ C$$

$$(T_D)_{\text{experimental}} = 75...85^\circ C$$

$$\Delta s = 2 \frac{e_D - e_n}{T_D} \approx 3.7 \times 10^{-4} eV / K$$

$$(\Delta s)_{\text{theoretical}} \approx 3.8 \times 10^{-4} eV / K^*$$

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## CONCLUSIONS

- Model by M. Barbi et al. well describes the denaturation of homogeneous DNA with single T-A bonds between bases. Satisfactory DMDM results require at least 10<sup>4</sup> implementations of DNA random states with dimensionless time increments  $\Delta t < 0.02$  up to  $t = 10^5$ .
- Good agreement was obtained with the experimental data and calculations for the denaturation temperature.
- DMDM with a large number of base pairs requires the development and implementation of a parallel numerical algorithm.
- It is necessary to generalize the model for a heterogeneous DNA molecule and continue DMDM.