Párováni bazí, hybridizace a denaturace DNA/RNA

hraje důležitou roli v přírodě i aplikacích:

- struktura DNA a duplikace genetické informace
- transkripce a translace
- rekombinace DNA
- struktura RNA a její aktivita

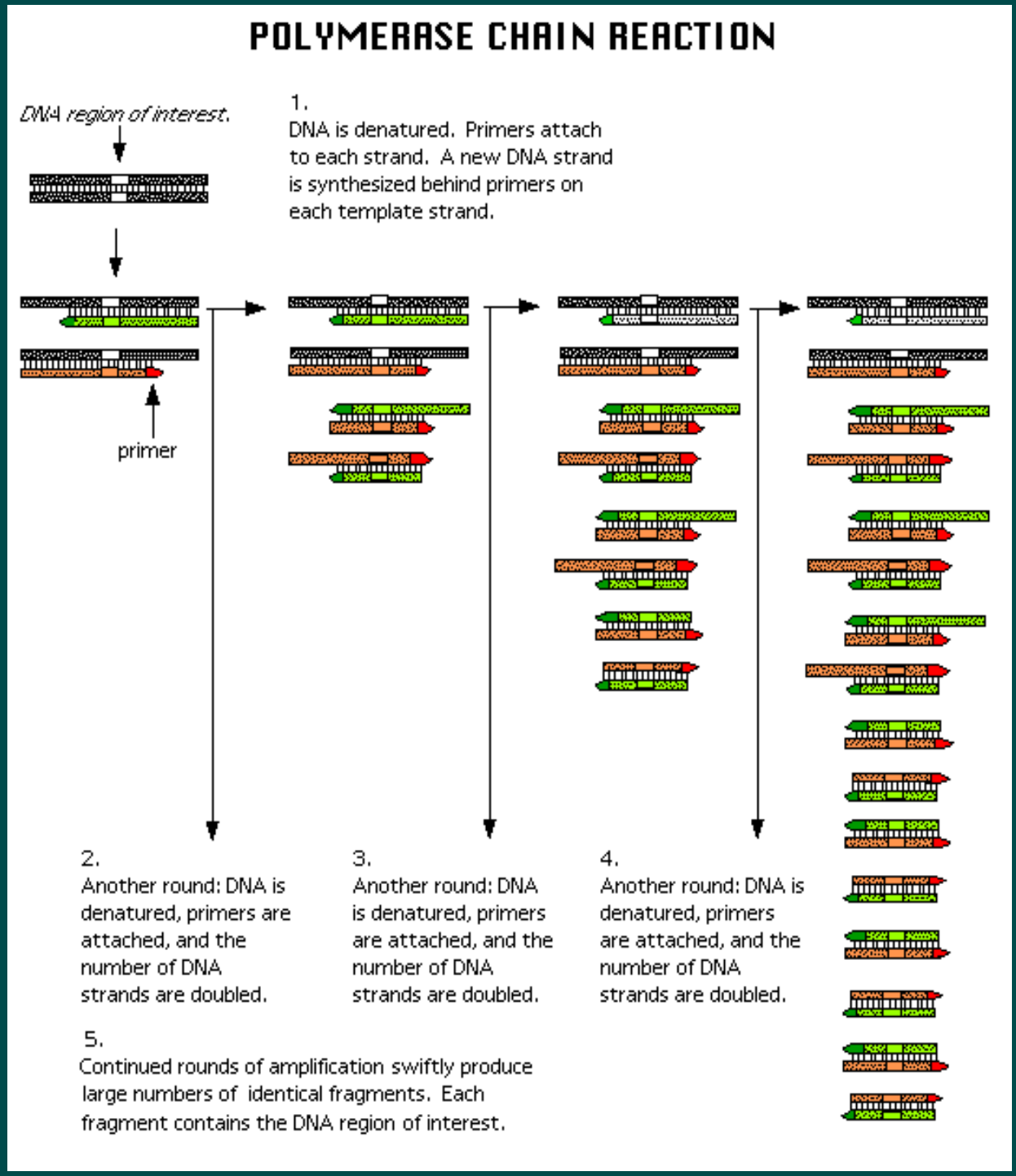
- klonování, rekombinantní DNA
- polymerázová reakce (PCR)
- DNA čipy, microarrays
- DNA výpočty

Kombinatorický charakter nukleových kyselin vytváří problémy, které nejsou zvládnutelné bez matematického aparátu a výpočetní techniky

PCR

HRÁČI
- primer
- templát
- DNA polymeráza

CYKLY
- denaturace
- annealing
- polymerizace



Přibližný výpočet bodu topení oligonukleotidu

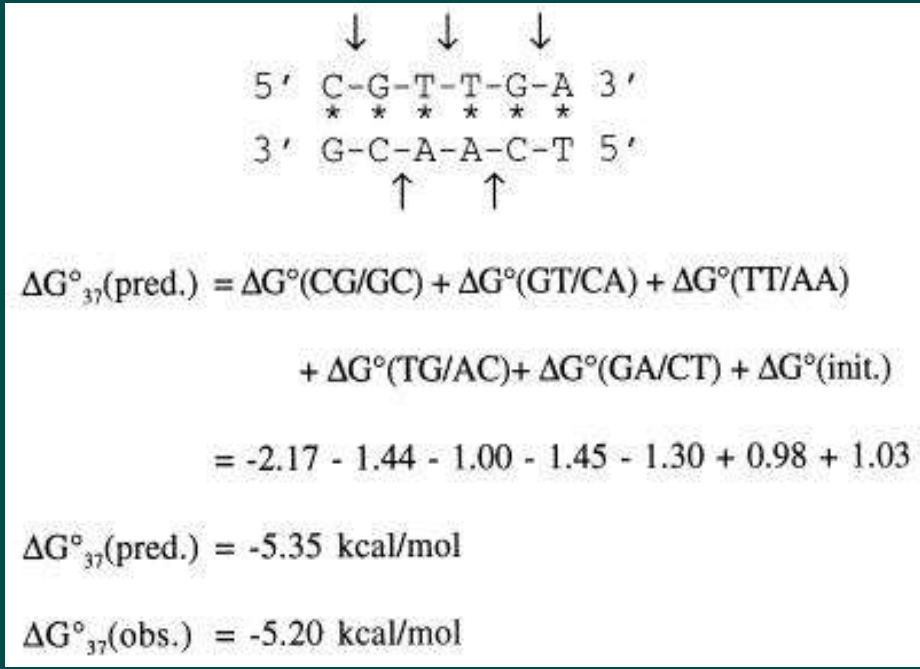
```
5'-ACGTAGAT     denaturace
   ::::::::    <---------->    5'-ACGTAGAT + ATCTACGT-3'
3'-TGCATCTA     hybridizace
```

Tm – teplota, při niž je 50% oligonukleotidu denaturováno

$$Tm = 2*(n(A)+n(T)) + 4*(n(C)+n(G))$$

$$Tm = 2AT+4CG$$

Metoda NN (Nearest Neighbor)



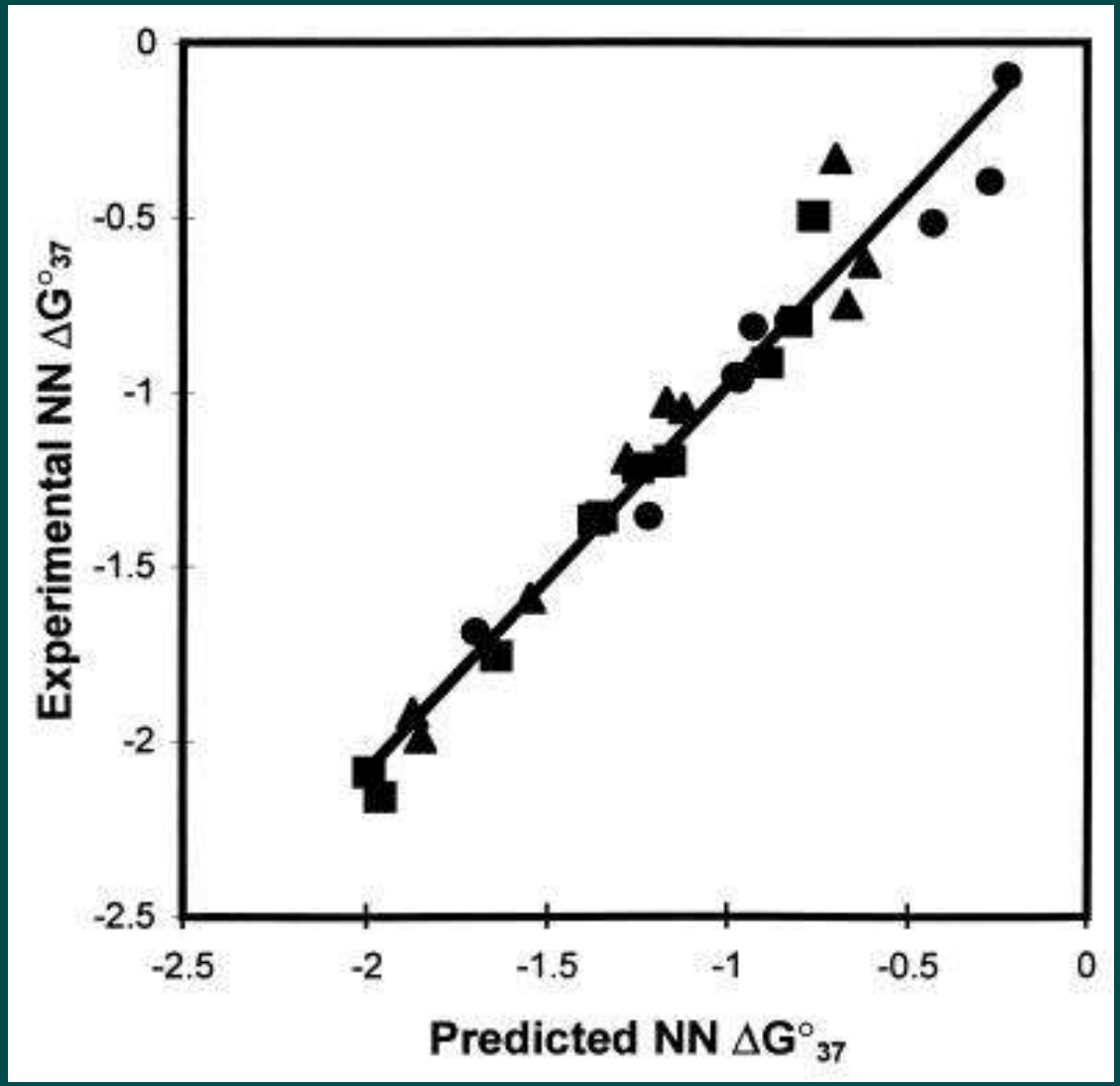

```
deltaG   = deltaH – deltaS.T

deltaG   – volna energie
H        – entalpie
S        – entropie
T        - teplota
```

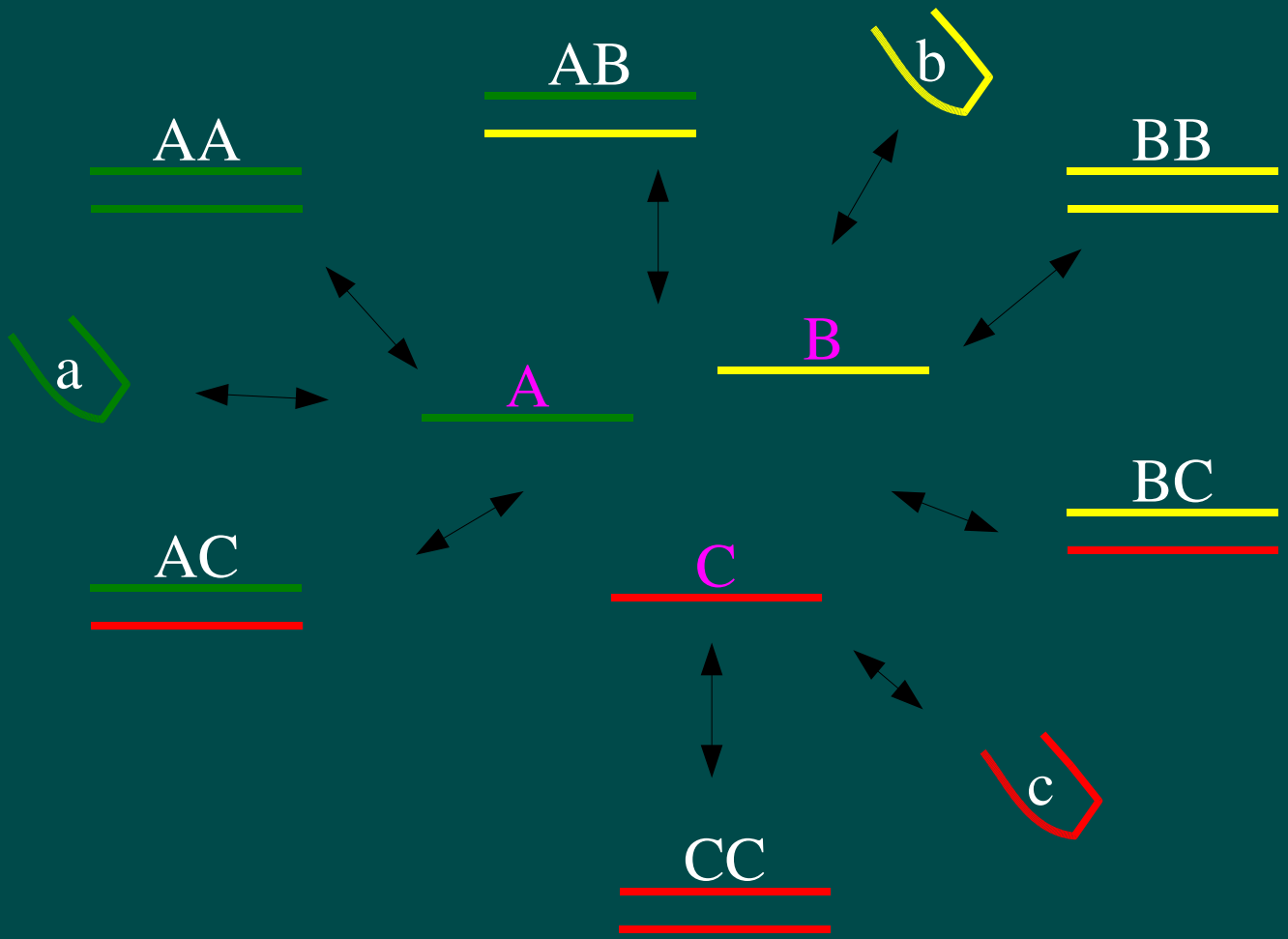
Sequence	Parameter kcal/mol Unified (ref. 22)
AA/TT	–1.00
AT/TA	–0.88
TA/AT	–0.58
CA/GT	–1.45
GT/CA	–1.44
CT/GA	–1.28
GA/CT	–1.30
CG/GC	–2.17
GC/CG	–2.24
GG/CC	–1.84
Average	–1.42
Init. w/term. G·C–	0.98
Init. w/term. A·T–	1.03
Sodium concentration, M	1.0
Rank of stacking matrix	12

Porovnání metod AT2CG4 a NN

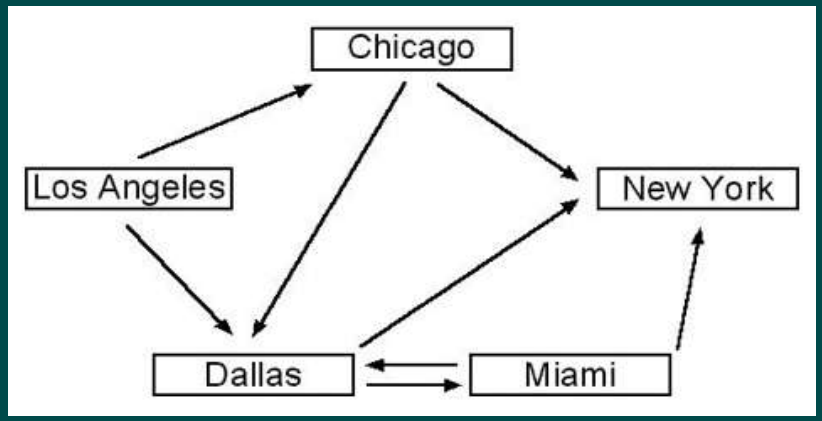
Primer Name	Sequence	Melting Tm (AT=2,CG=4)	Melting Tm Nearest Neighbor
KS	5'- CGAGGTCGACGGTATCG	56 °C	57 °C
M13 (-20) (Universal)	5'-GTAAAACGACGGCCAGT	52 °C	55 °C
M13 (-40)	5'-GTTTTCCCAGTCACGAC	52 °C	53 °C
M13 forward	5'-GTTTTCCCAGTCACGACGTTG	64 °C	59 °C
M13 reverse	5'-TGAGCGGATAACAATTTCACACAG	68 °C	58 °C
M13 Reverse	5'-CAGGAAACAGCTATGAC	50 °C	50 °C
M13 Reverse (-40)	5'-GTTGTGTGGAATTGTG	46 °C	48 °C
Neomycin forward	5'-AGGATCTCCTGTCATCTCACCTTGCTCCTG	92 °C	66 °C
Neomycin reverse	5'-AAGAACTCGTCAAGAAGGCGATAGAAGGCG	90 °C	65 °C

Spolehlivost metody NN

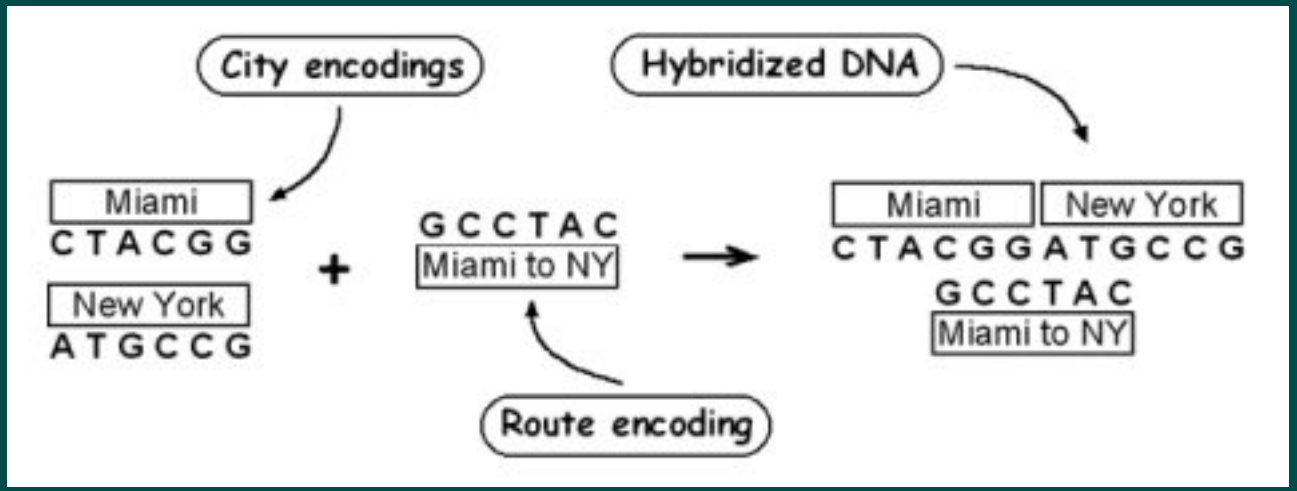



AB
b
AA
BB
a
B
A
BC
AC
C
c
CC

DNA computing – DNA-based computing



Los Angeles	GCTACG
Chicago	CTAGTA
Dallas	TCGTAC
Miami	CTACGG
New York	ATGCCG



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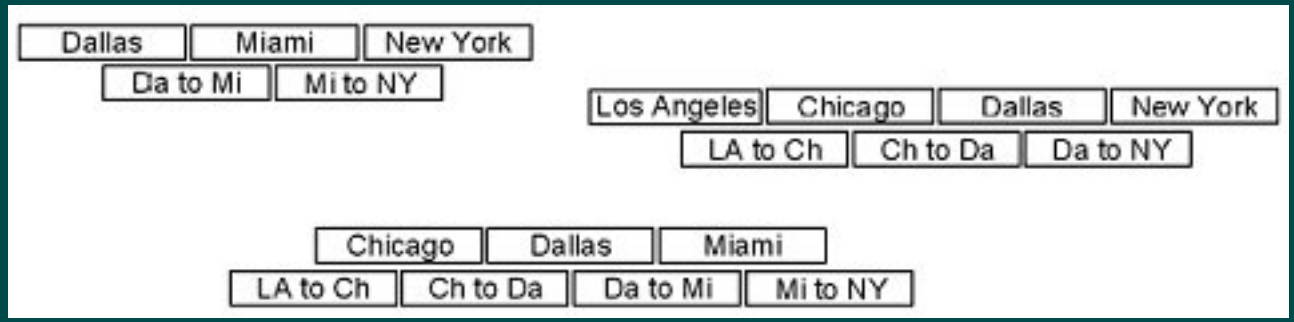
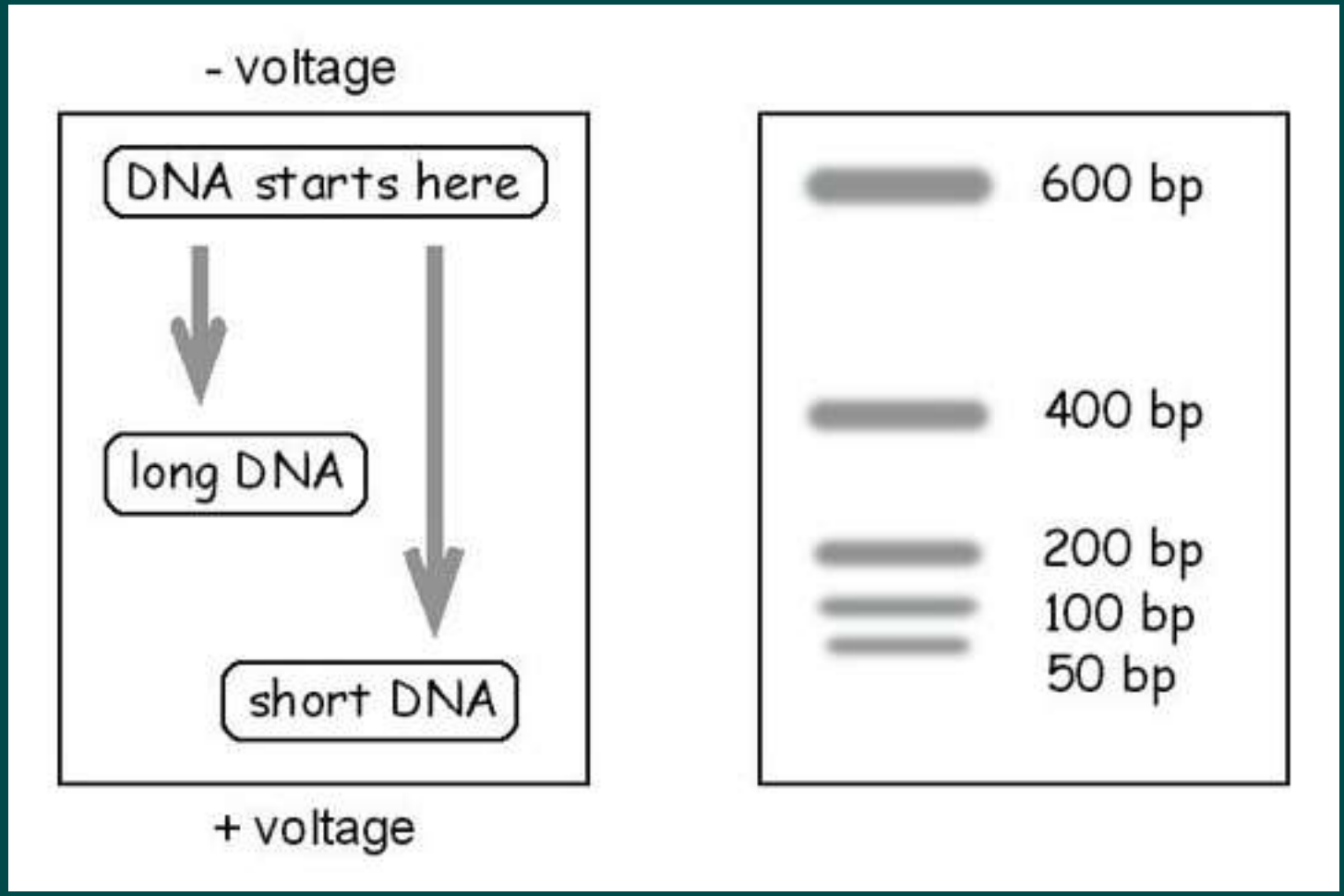


DNA computing – DNA-based computing



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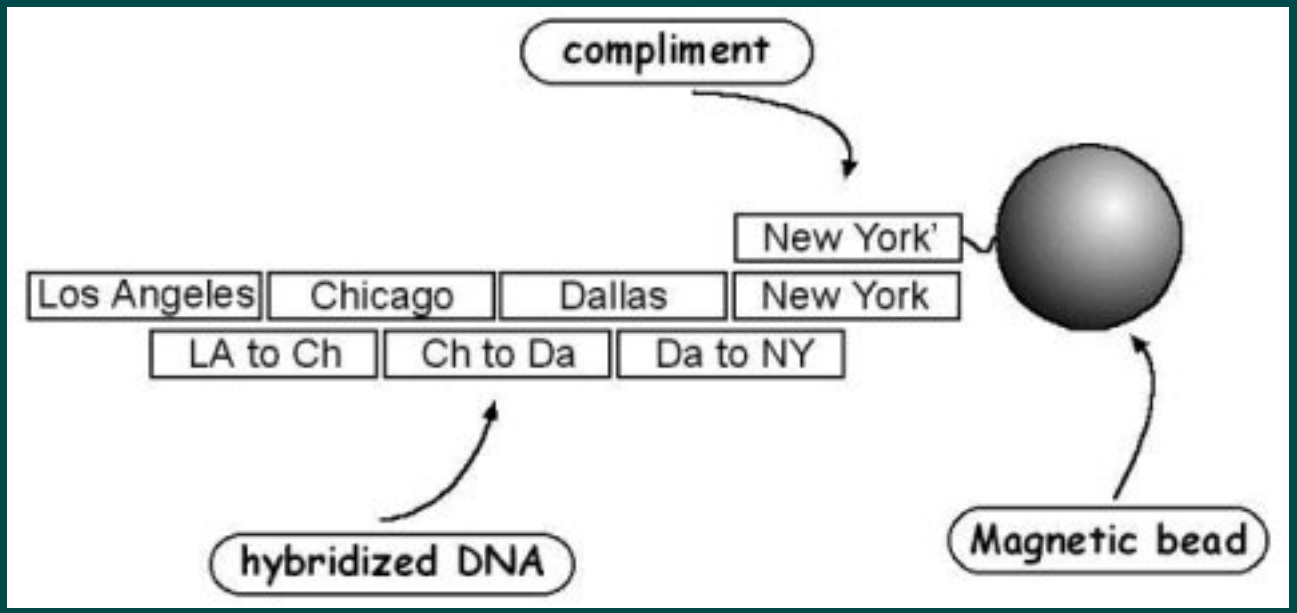

DNA computing – DNA-based computing