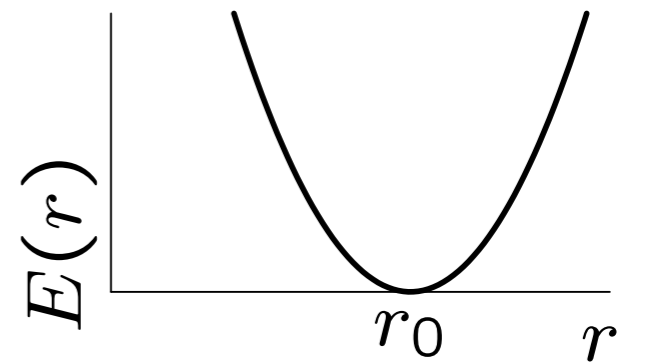
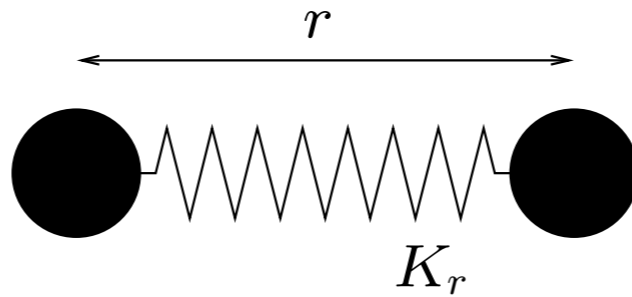
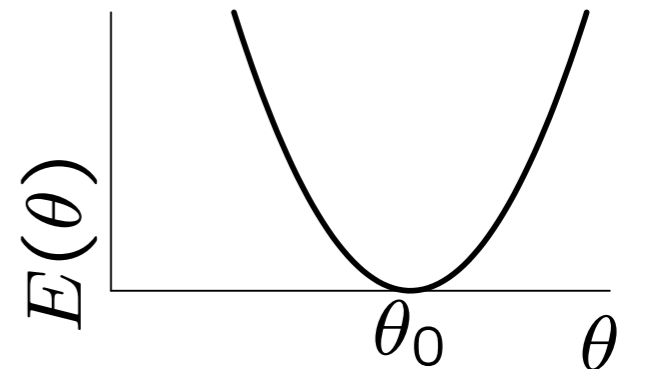
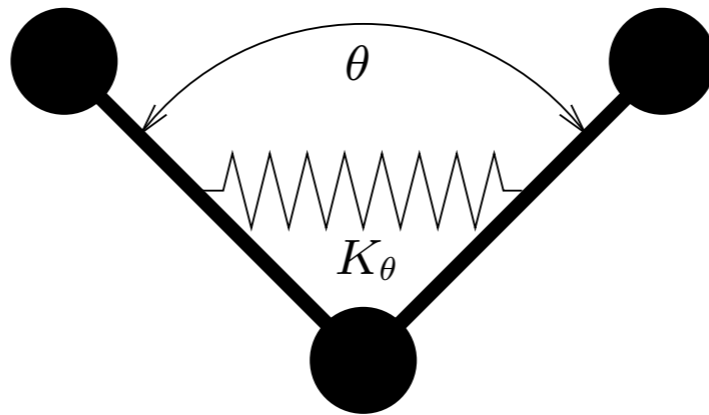


VÝPOČETNÍ METODY

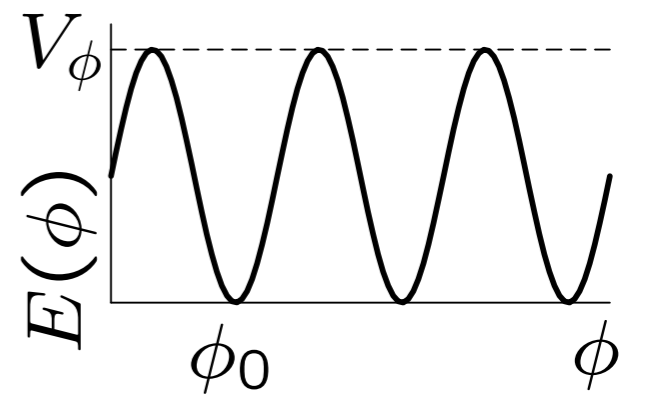
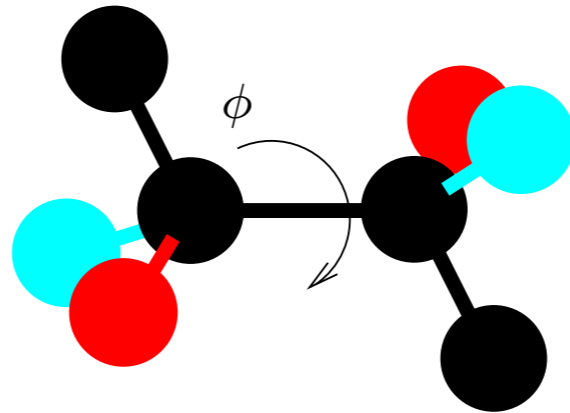
$$E = K_r(r - r_0)^2$$



$$E = K_\theta(\theta - \theta_0)^2$$

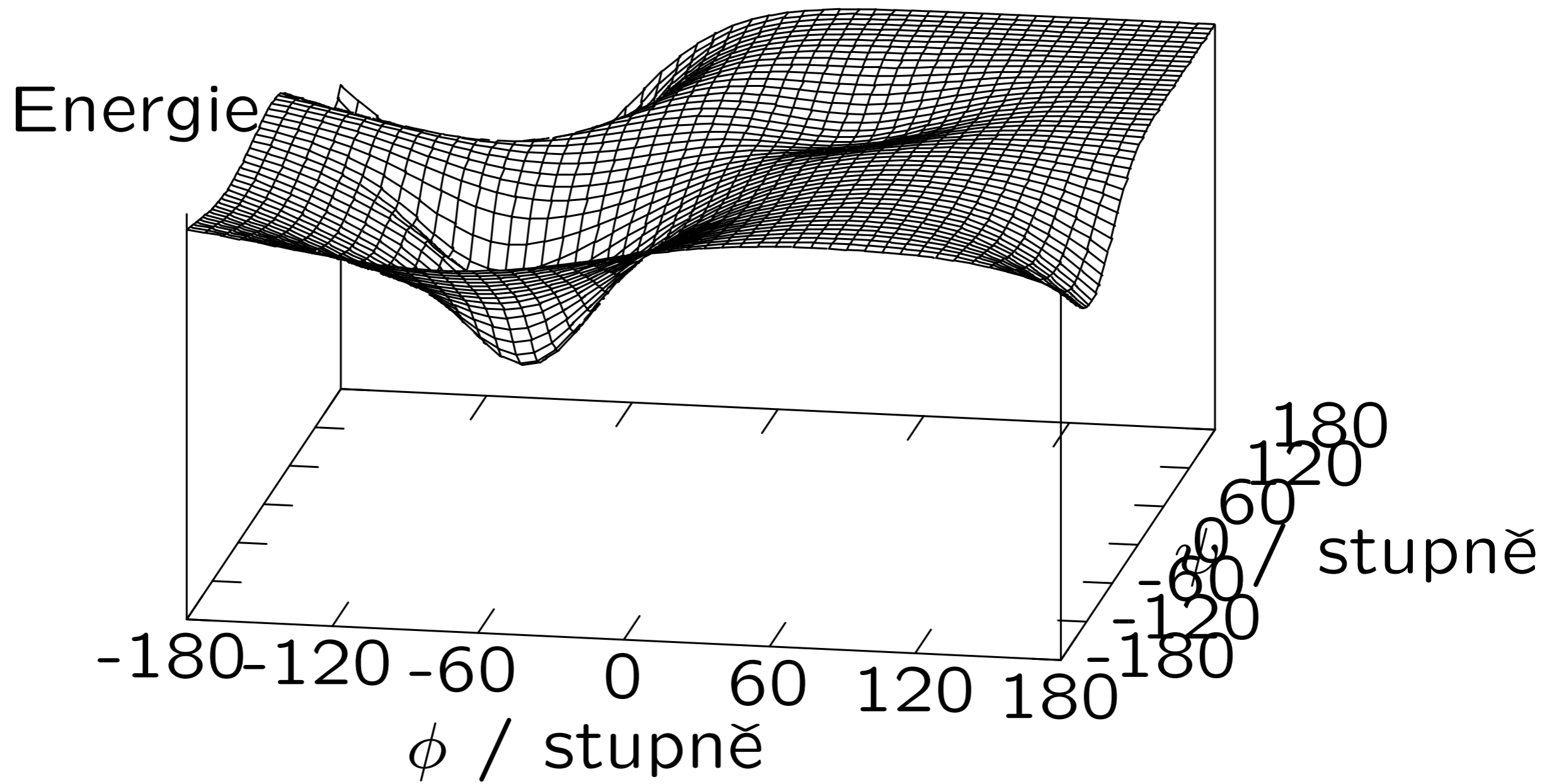


$$E = \frac{V_\phi}{2}(1 + \cos n(\phi - \phi_0))$$



$$E = C \frac{Q_1 Q_2}{r}$$

$$E = \frac{A}{r^{12}} - \frac{B}{r^6}$$



Parametry silového pole AMBER (parm94.dat)

PARM94 for DNA, RNA and proteins with TIP3P Water. USE SCCE=1.2 in energy progs									
C	12.01								sp2 C carbonyl group
CA	12.01								sp2 C pure aromatic (benzene)
H	1.008								H bonded to nitrogen atoms
HC	1.008								H aliph. bond. to C without electrwd.group
NB	14.01								sp2 N in 5 memb.ring w/LP (HIS,ADE,GUA)
P	30.97								phosphate
S	32.06								sulphur in disulfide linkage
...									
OW-HW	553.0	0.9572		!	TIP3P water				
C-CA	469.0	1.409		JCC,7,(1986),230;	TYR				
C-CB	447.0	1.419		JCC,7,(1986),230;	GUA				
C-N*	424.0	1.383		JCC,7,(1986),230;	CYT,URA				
...									
HW-OW-HW	100.	104.52		TIP3P water					
HW-HW-OW	0.	127.74		(found in crystallographic water with 3 bonds)					
CB-C-NA	70.0	111.30		NA					
CB-C-O	80.0	128.80							
...									
X-C-CA-X	4	14.50	180.0	2.					intrpol.bsd.on C6H6
X-C-CB-X	4	12.00	180.0	2.					intrpol.bsd.on C6H6
CT-CT-OS-CT	1	0.383	0.0	-3.					
N-CT-C-N	1	0.40	180.0	-4.					
...									
H	0.6000	0.0157			!Ferguson base pair geom.				
HW	0.0000	0.0000			TIP3P water model				
O	1.6612	0.2100			OPLS				
S	2.0000	0.2500			W. Cornell CH3SH and CH3SCH3 FEP's				
IP	1.8680	0.00277			Na+ Aqvist JPC 1990,94,8021. (adapted)				

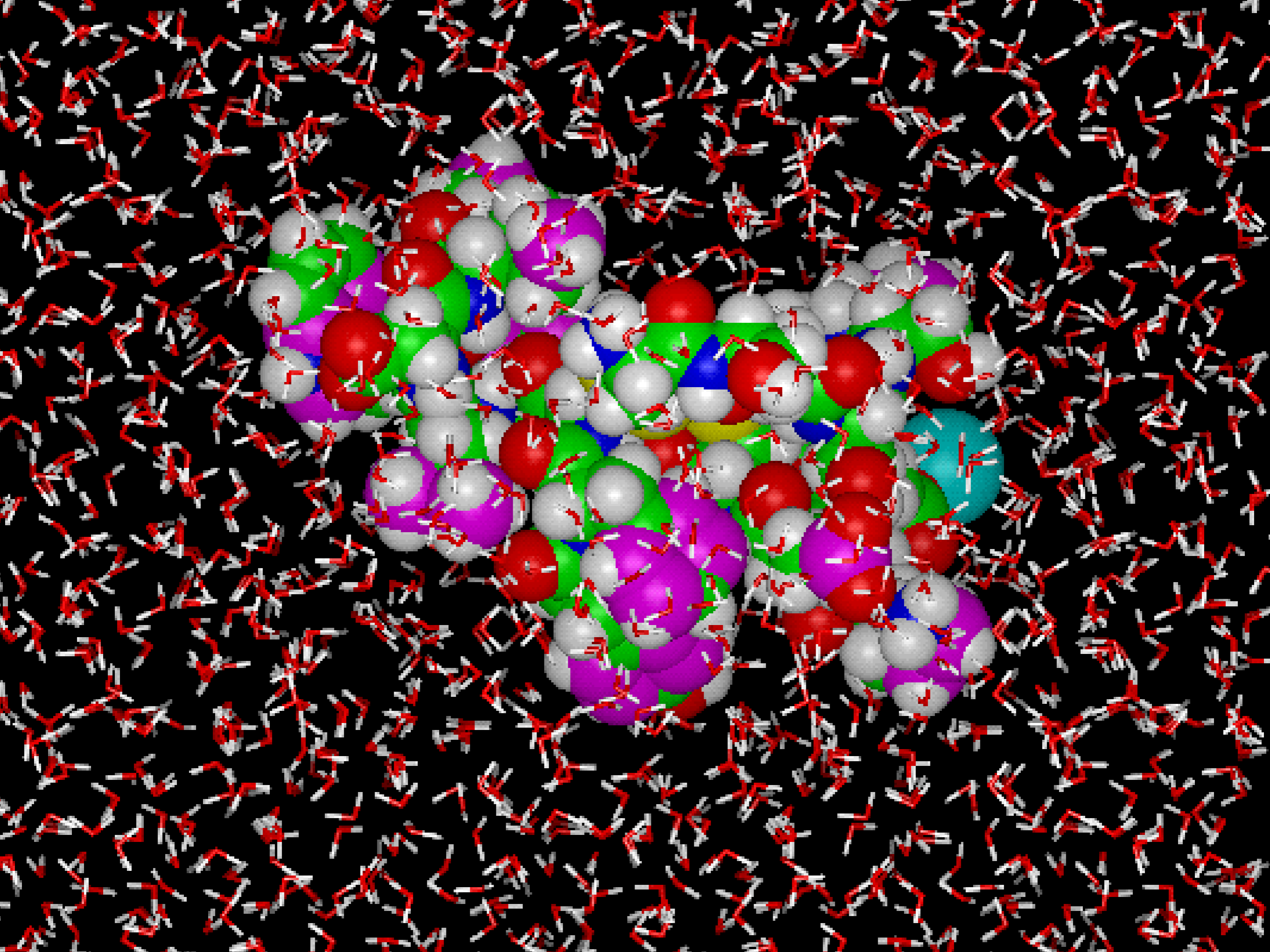
definice
atomových typů

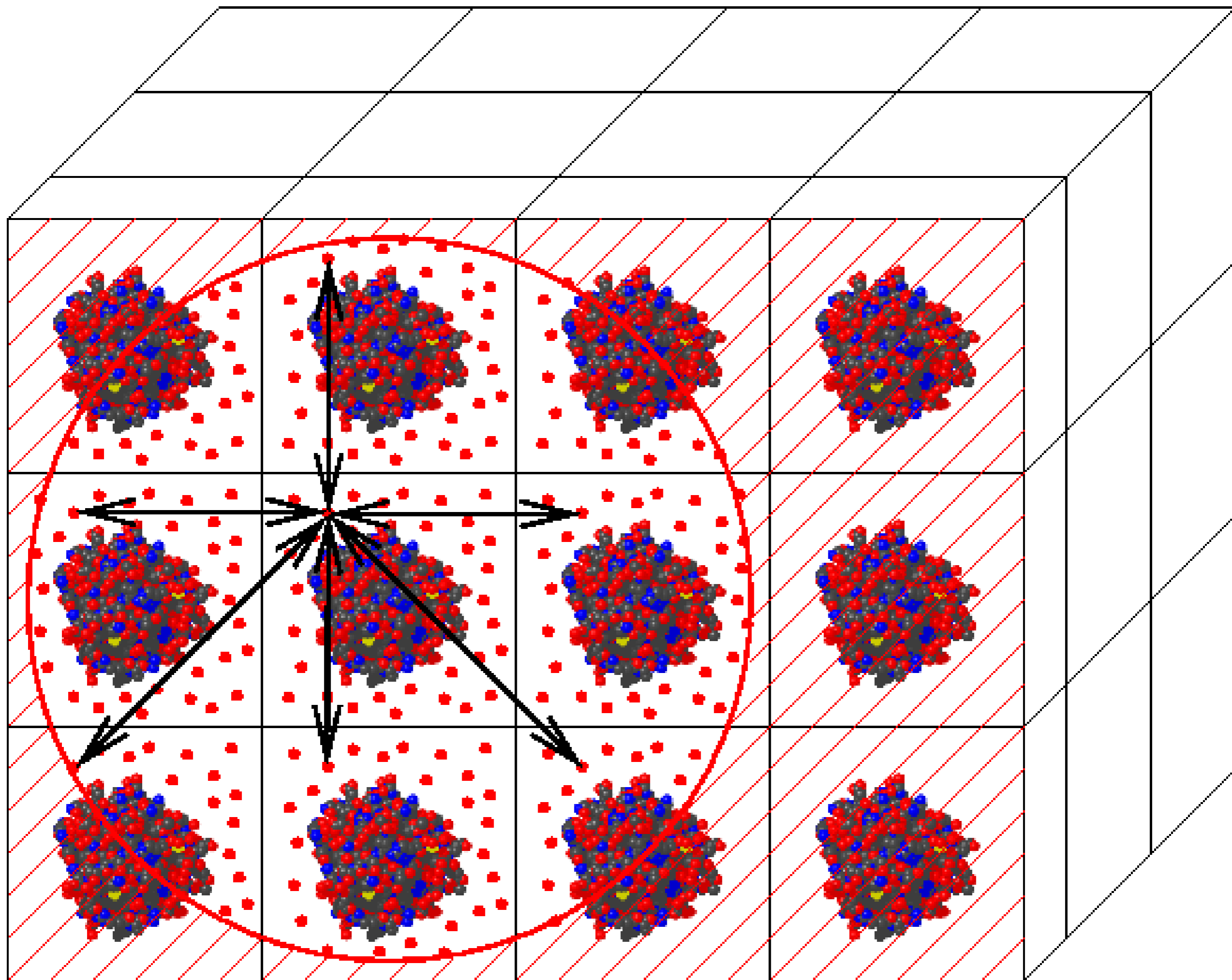
vazby

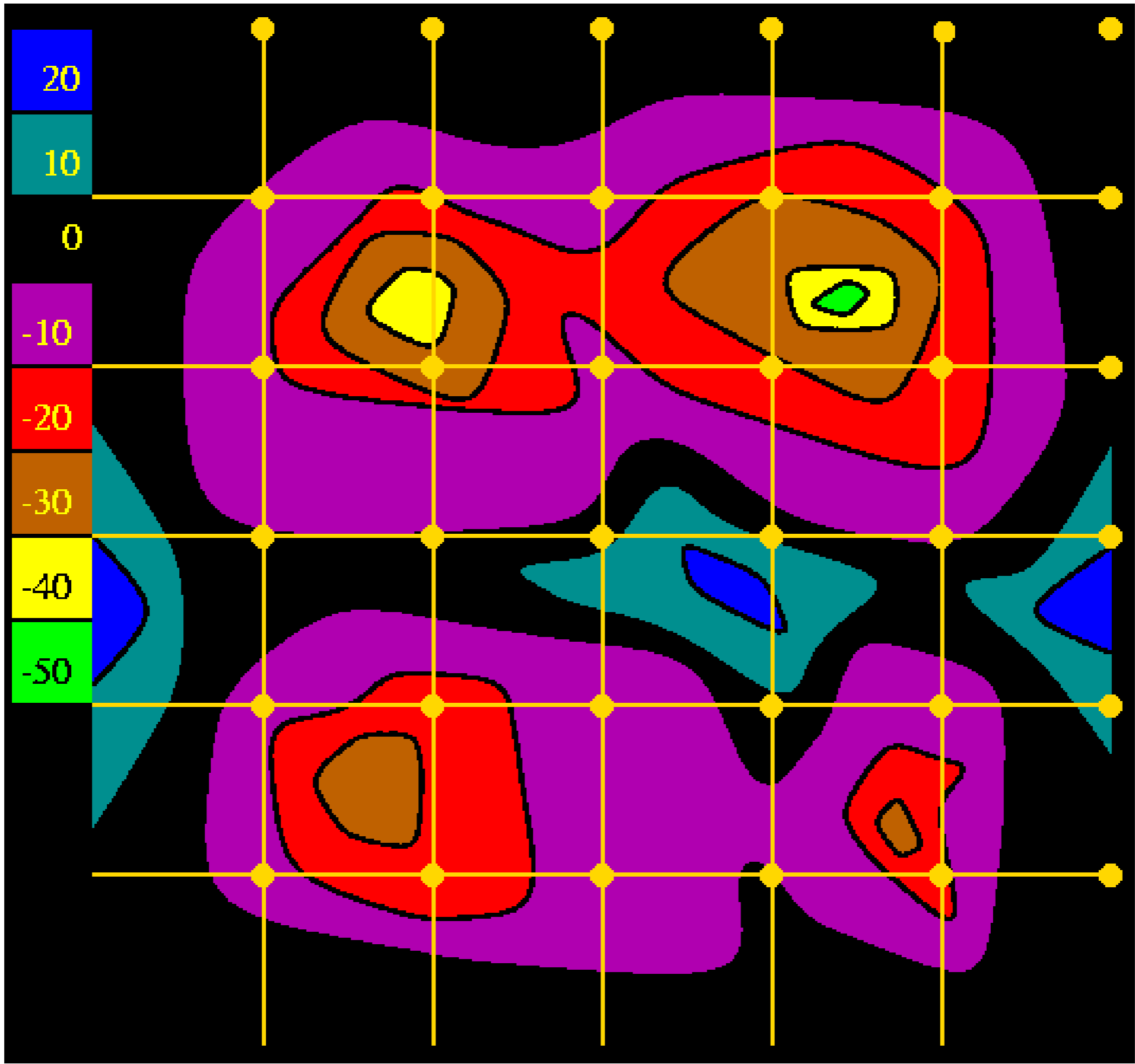
úhly

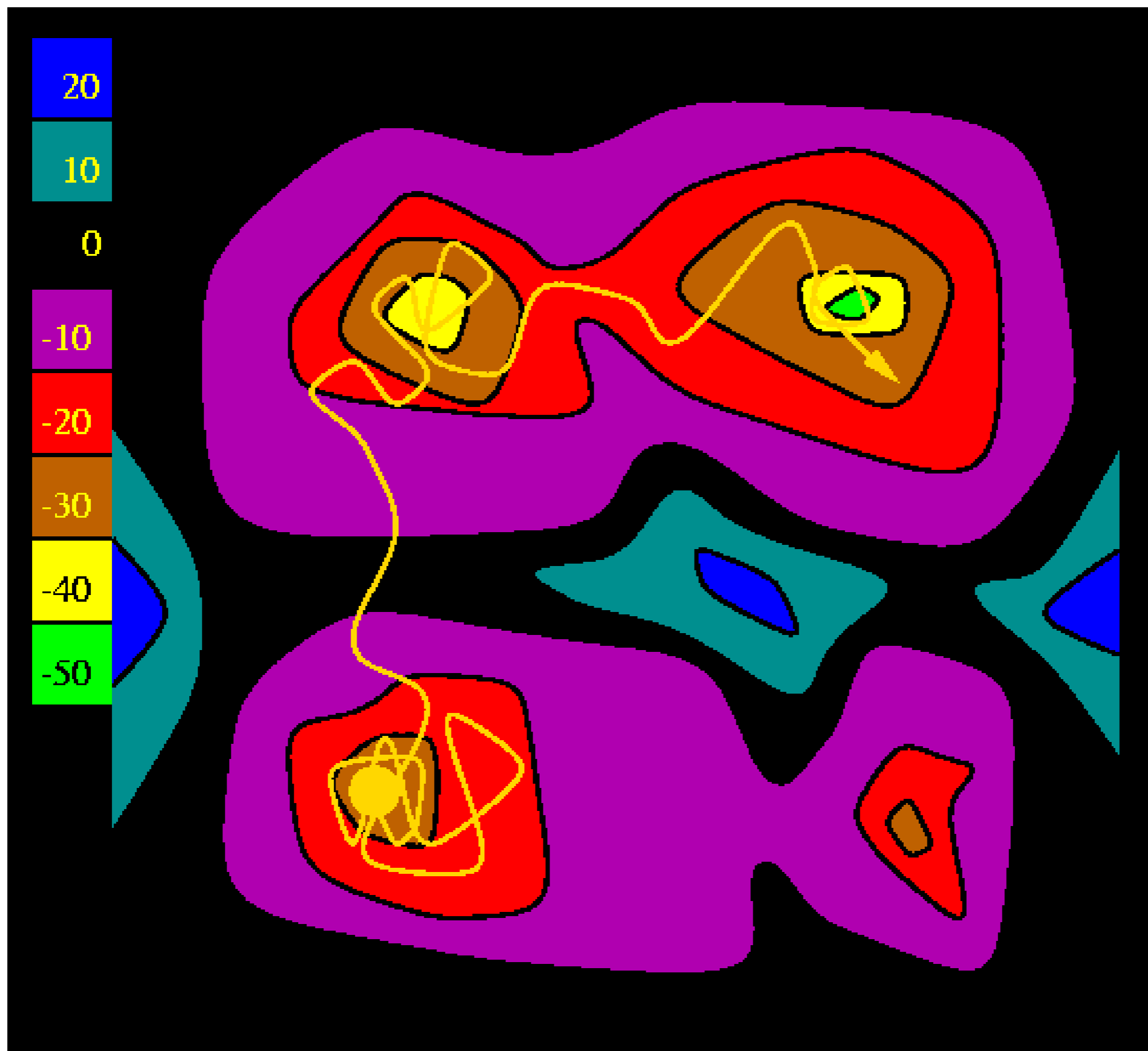
torze

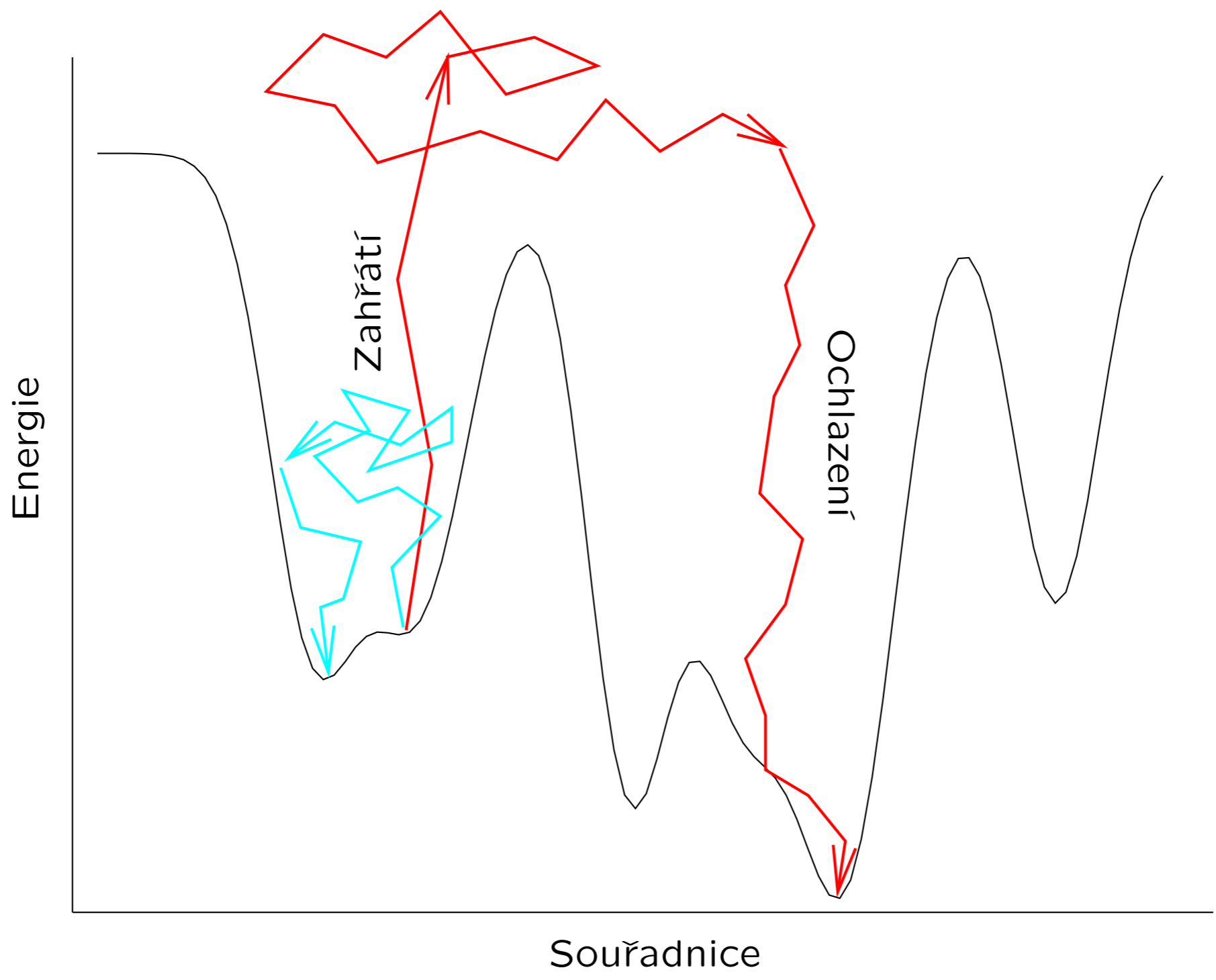
vdW
poměry











Energie

Souřadnice

Zahřátí

Ochlazení