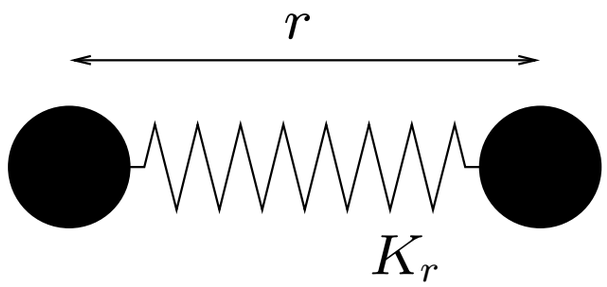
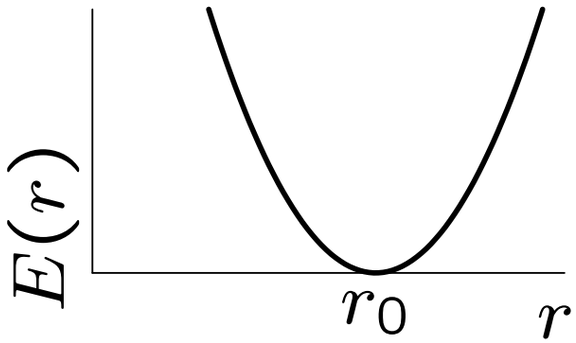
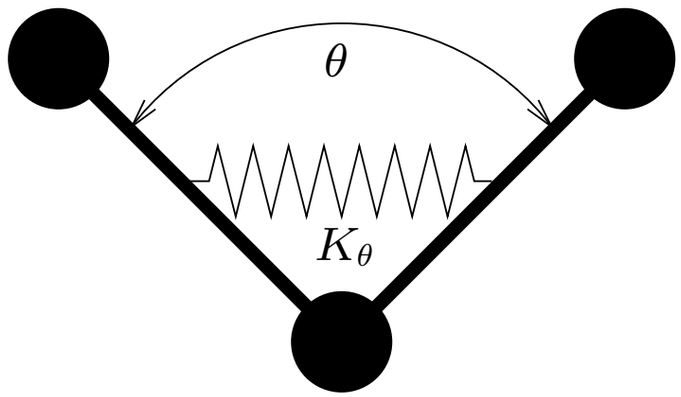
VYPOČETNÍ METODY

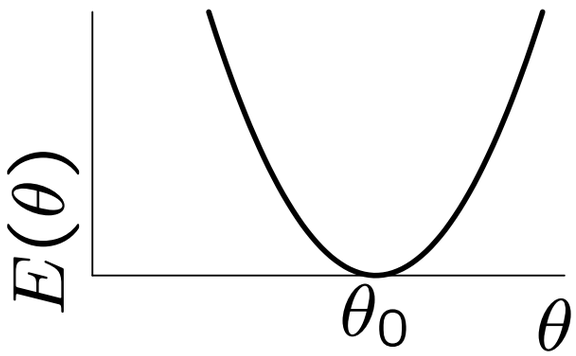
$$E = K_r(r - r_0)^2$$



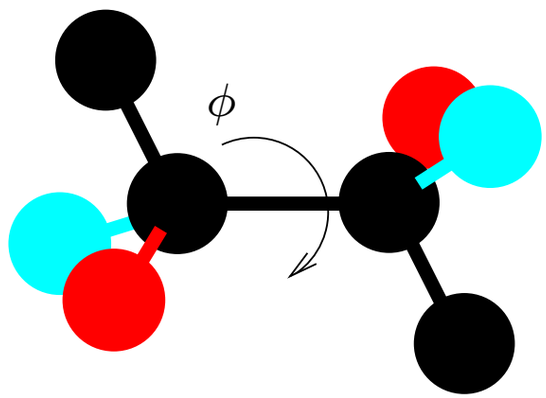


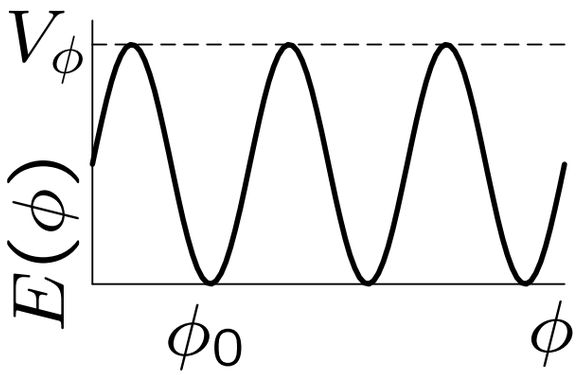
$$E = K_\theta(\theta - \theta_0)^2$$





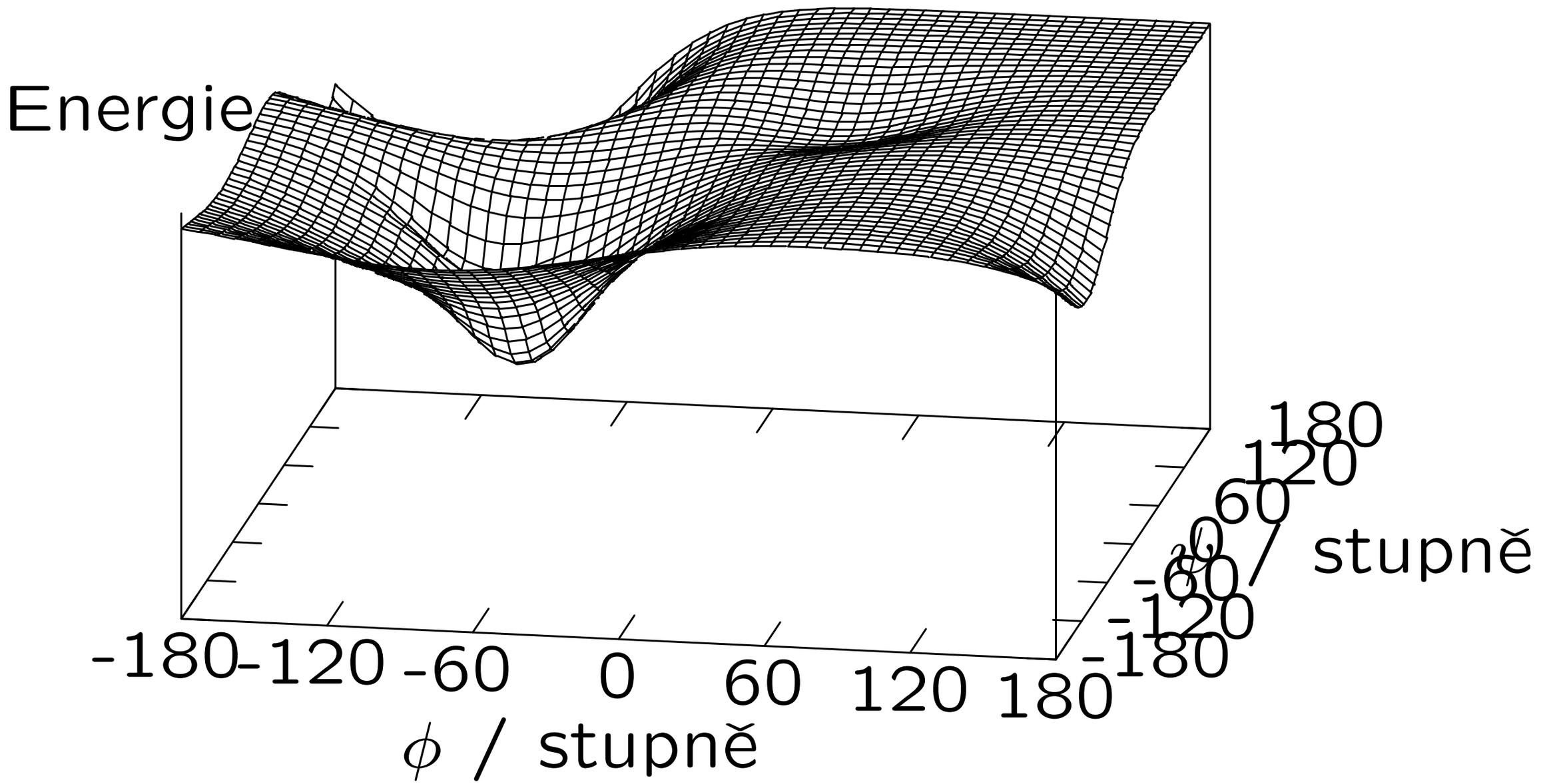
$$E = \frac{V_\phi}{2}(1 + \cos n(\phi - \phi_0))$$





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

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


Energie
-180
-120
-60
0
60
120
180
ϕ / stupně
180
120
60
0
-60
-120
-180
ϑ / stupně

Parametry silového pole AMBER (parm94.dat)

```
PARM94 for DNA, RNA and proteins with TIP3P Water. USE SCEE=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)
```

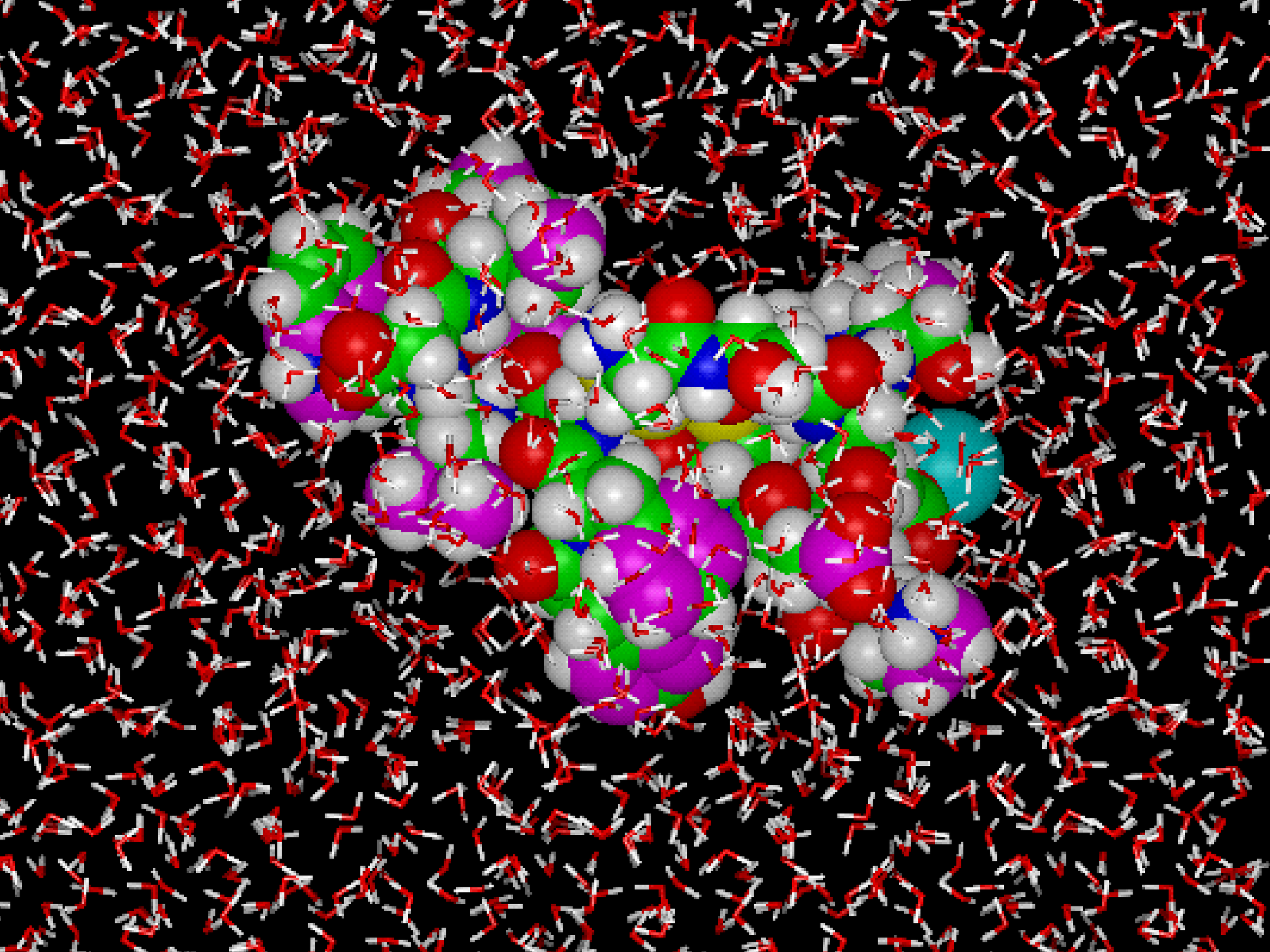
definice atomových typů

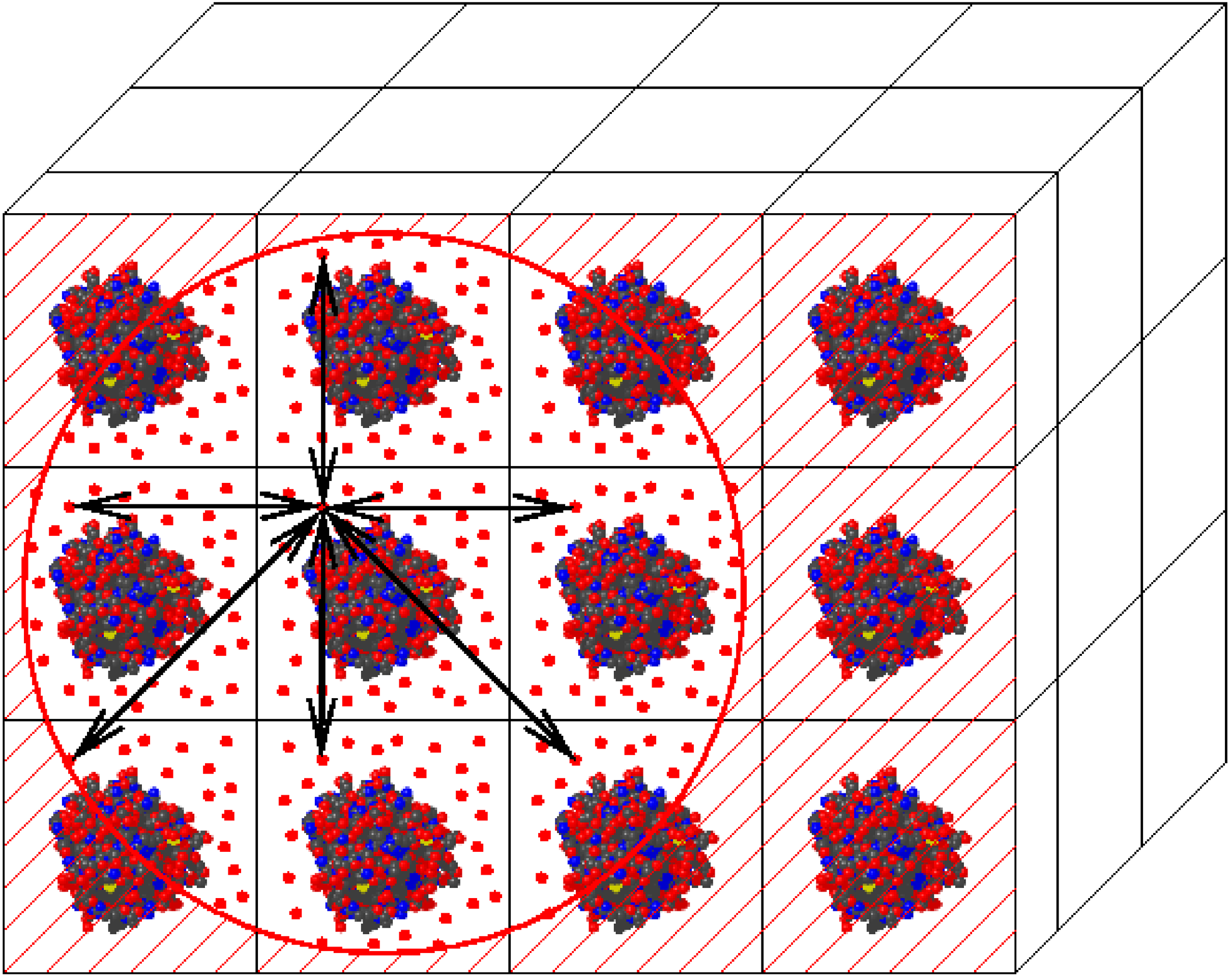
vazby

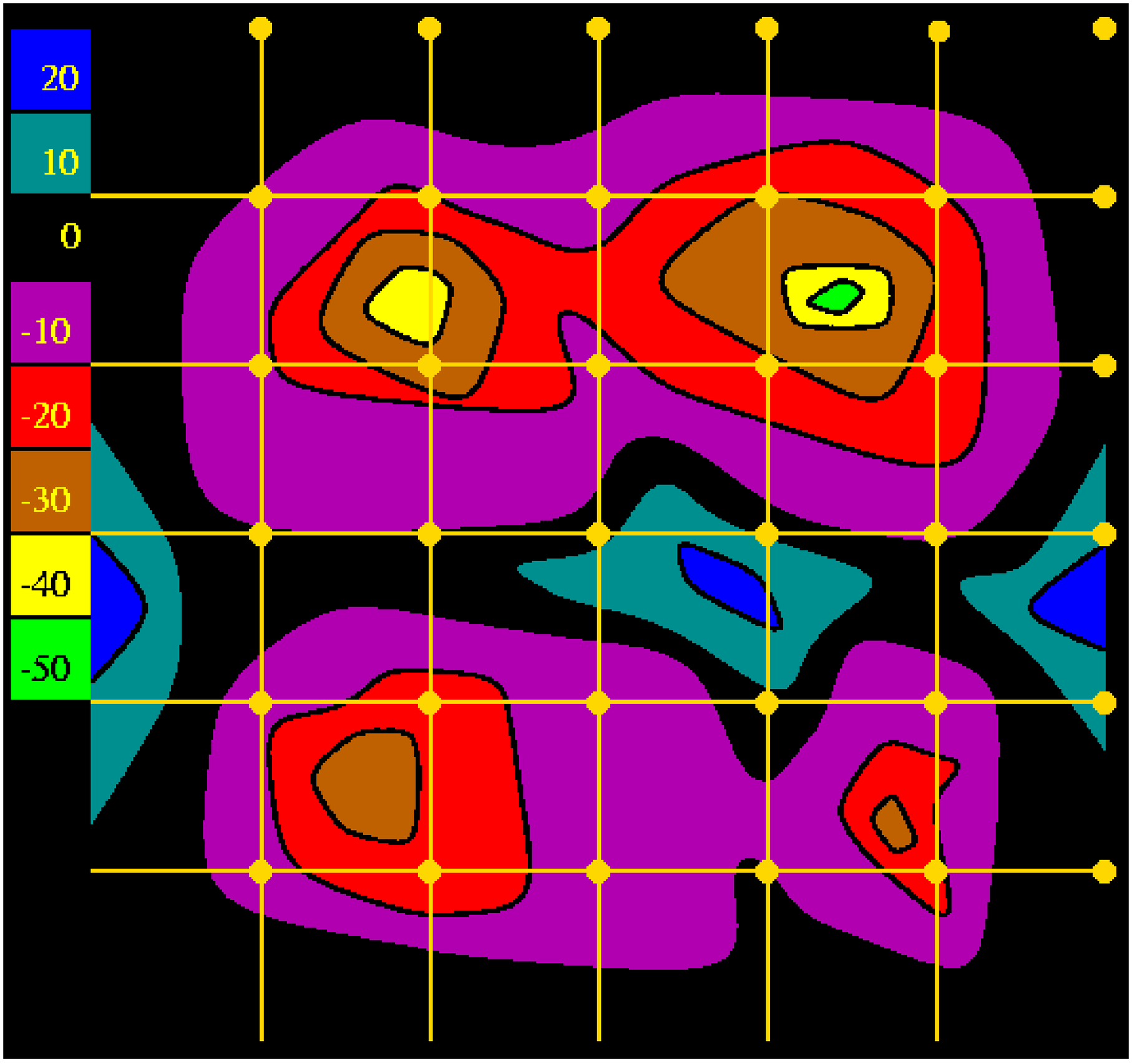
úhly

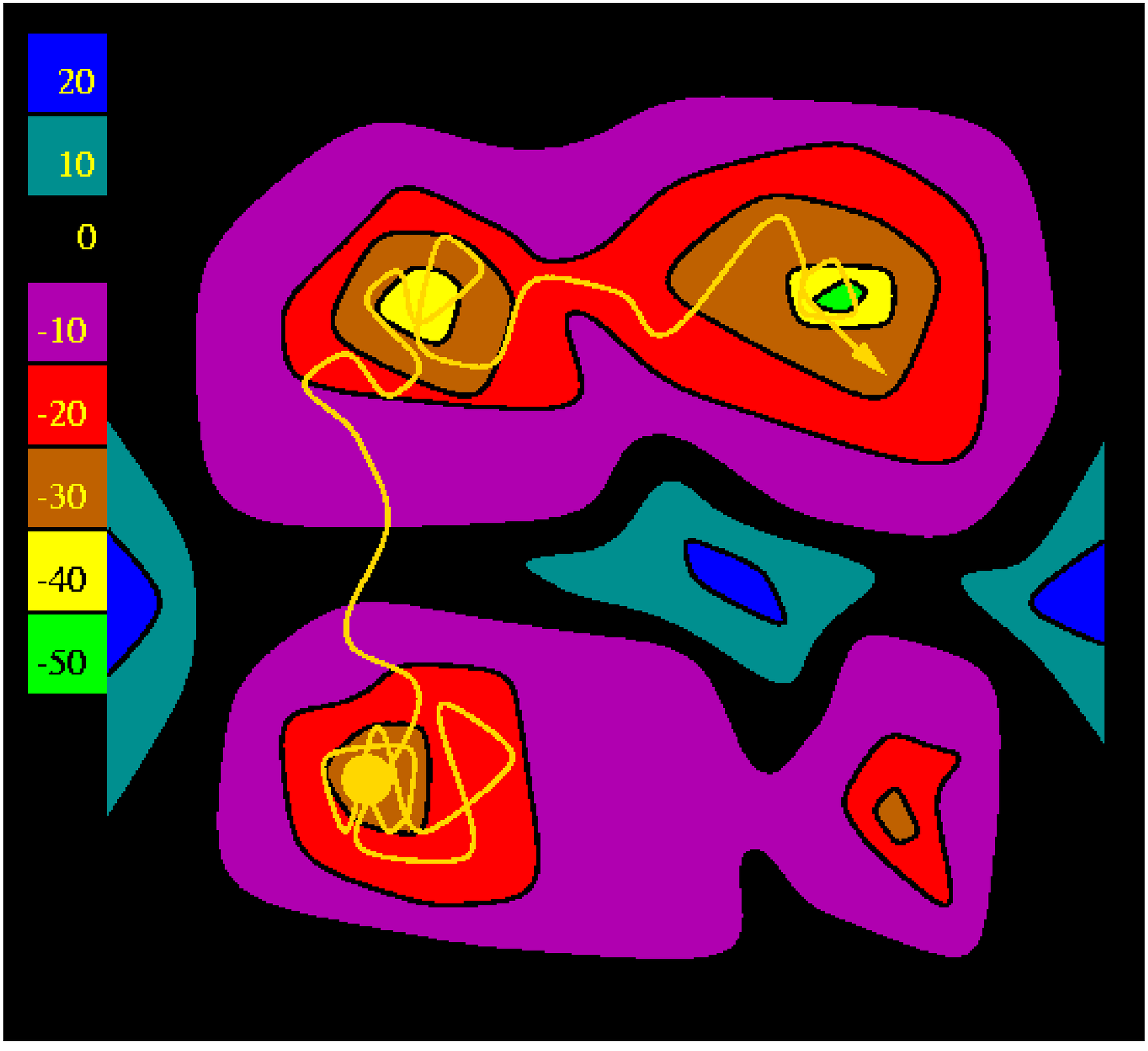
torze

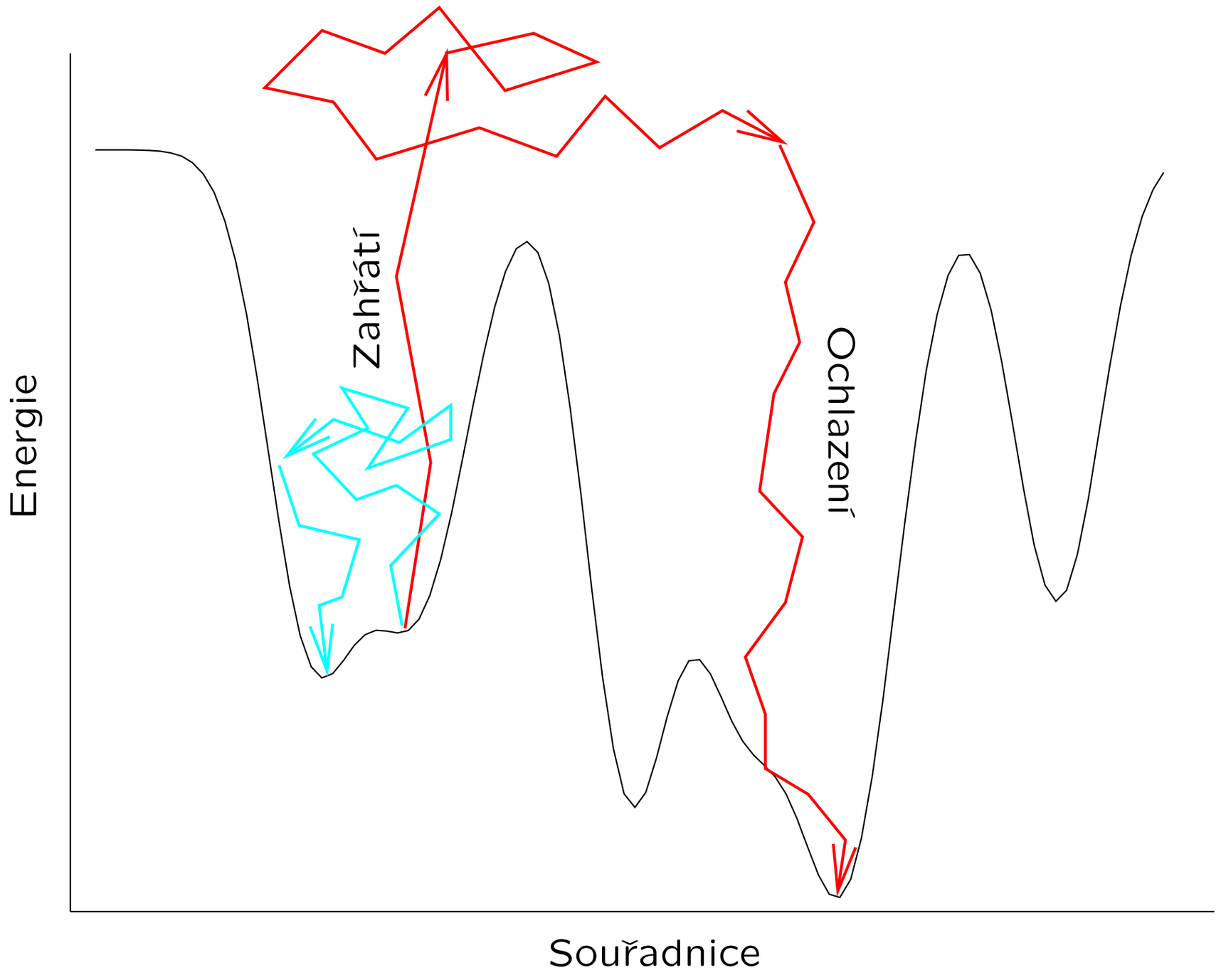
vdW poloměry






20
10
0
-10
-20
-30
-40
-50


20
10
0
-10
-20
-30
-40
-50


Energie
Zahřátí
Ochlazení
Souřadnice