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1: #include <iostream>
2: #include "analysis.h"
3: #include "container.h"
4: #include "potentials.h"
5: #include "countdown.h"
6: typedef pot_coulomb T_pairpot;           // Specify pair potential
7: #include "markovmove.h"
8:
9: using namespace std;
10:
11: int main() {
12:     cell::cell con(100.);                // Use a spherical container
13:     canonical nvt;                        // Use the canonical ensemble
14:     pot_setup cfg;                       // Setup pair potential (default)
15:     interaction<T_pairpot> pot(cfg);      // Functions for interactions
16:     countdown<int> clock(10);             // Estimate simulation time
17:     macromolecule protein;              // Group for the protein
18:     ioaam aam(con);                      // Protein input file format is AAM
19:     protein.add( con, aam.load(
20:         "calbindin.aam" ) );             // Load protein from disk
21:     protein.move(con, -protein.cm);       // ..translate it to origo (0,0,0)
22:     protein.accept(con);                 // ..accept translation
23:     group salt;                          // Group for salt and counter ions
24:     salt.add( con, particle::NA, 34+19); // Insert sodium ions
25:     salt.add( con, particle::CL, 34 );   // Insert chloride ions
26:     saltmove sm(nvt, con, pot);          // Class for salt movements
27:     aam.load(con, "confout.aam");        // Load old config (if present)
28:     chargereg tit(nvt,con,pot,salt,7.6); // Prepare titration. pH 7.6
29:     systemenergy sys(pot.energy(con.p)); // System energy analysis
30:     cout << con.info() << tit.info();   // Some information
31:
32:     for (int macro=1; macro<=10; macro++) { // Markov chain
33:         for (int micro=1; micro<=1e3; micro++) {
34:             switch (rand() % 2) {         // Randomly chose move
35:                 case 0:
36:                     sys+=sm.move(salt);   // Displace salt particles
37:                     break;
38:                 case 1:
39:                     sys+=tit.titrateall(); // Titrate protein sites
40:                     protein.charge(con.p); // Re-calc. protein charge
41:                     protein.dipole(con.p); // Re-calc. dipole moment
42:                     break;
43:             }
44:         }                                // END of micro loop
45:         sys.update(pot.energy(con.p));    // Update system energy
46:         aam.save("confout.aam", con.p);   // Save config. to disk
47:         cout << "Macro step " << macro
48:             << " completed. ETA: " << clock.eta(macro);
49:     }                                    // END of macro loop
50:     cout << sys.info() << sm.info()      // Print results
51:         << tit.info() << salt.info() << protein.info();
52: }

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