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#include <iostream>
#include "io.h"
#include "analysis.h"
#include "container.h"
#include "potentials.h"
#include "countdown.h"
typedef pot_coulomb T_pairpot;           // Specify pair potential
#include "markovmove.h"

using namespace std;

int main() {
    cell::cell con(100.);                // Use a spherical container
    canonical nvt;                        // Use the canonical ensemble
    pot_setup cfg;                       // Setup pair potential (default)
    interaction<T_pairpot> pot(cfg);      // Functions for interactions
    countdown<int> clock(10);            // Estimate simulation time
    macromolecule protein;              // Group for the protein
    ioaam aam(con);                      // Protein input file format is AAM
    protein.add( con, aam.load(
        "calbindin.aam" ) );            // Load protein from disk
    protein.move(con, -protein.cm);      // ..translate it to origo (0,0,0)
    protein.accept(con);                 // ..accept translation
    group salt;                          // Group for salt and counter ions
    salt.add( con, particle::NA, 34+19); // Insert sodium ions
    salt.add( con, particle::CL, 34 );   // Insert chloride ions
    saltmove sm(nvt, con, pot);          // Class for salt movements

    aam.load(con, "confout.aam");        // Load old config (if present)
    chargereg tit(nvt,con,pot,salt,7.6); // Prepare titration. pH 7.6
    systemenergy sys(pot.energy(con.p)); // System energy analysis
    cout << con.info() << tit.info();   // Some information

    for (int macro=1; macro<=10; macro++) { // Markov chain
        for (int micro=1; micro<=1e3; micro++) {
            switch (rand() % 2) {         // Randomly chose move
                case 0:
                    sys+=sm.move(salt);   // Displace salt particles
                    break;
                case 1:
                    sys+=tit.titrateall(); // Titrate sites on the protein
                    protein.charge(con.p); // Re-calc. protein charge
                    protein.dipole(con.p); // Re-calc. dipole moment
                    break;
            }
        } // END of micro loop
        sys.update(pot.energy(con.p));    // Update system energy averages
        aam.save("confout.aam", con.p);  // Save configuration to disk
        cout << "Macro step " << macro
            << " completed. ETA: " << clock.eta(macro);
    } // END of macro loop
    cout << sys.info() << sm.info()      // Print results
        << tit.info() << salt.info() << protein.info();
}

```