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c
c       This is a documnet on the pair potential molecular dynamics (MD)
c       program. The program is self explanatory and the best way to
understand
c       how it works is to read it. The general outline and a
c       sample input follow below. There are 2 kinds of potentials
c       implemented: Lennard-Jones (LJ) and a pair-potential for Si (Hafner's
c       given on a regular grid. Four (X2) kinds of dynamics are possible:
c       a) simple MD w/ fixed cell shape, b) Parrinello/Rahman dynamics,
c       and both (sets of eq.'s of motion) dynamics proposed in PRB 44, 2358
c       (1991), i.e., c) Eq's (3-a) and (8), and d) Eq.'s (3-a) and (9).
c       These dynamics can be used as minimization strategies too
c       (see description inside TPAGE).
c
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MAIN PROGRAM
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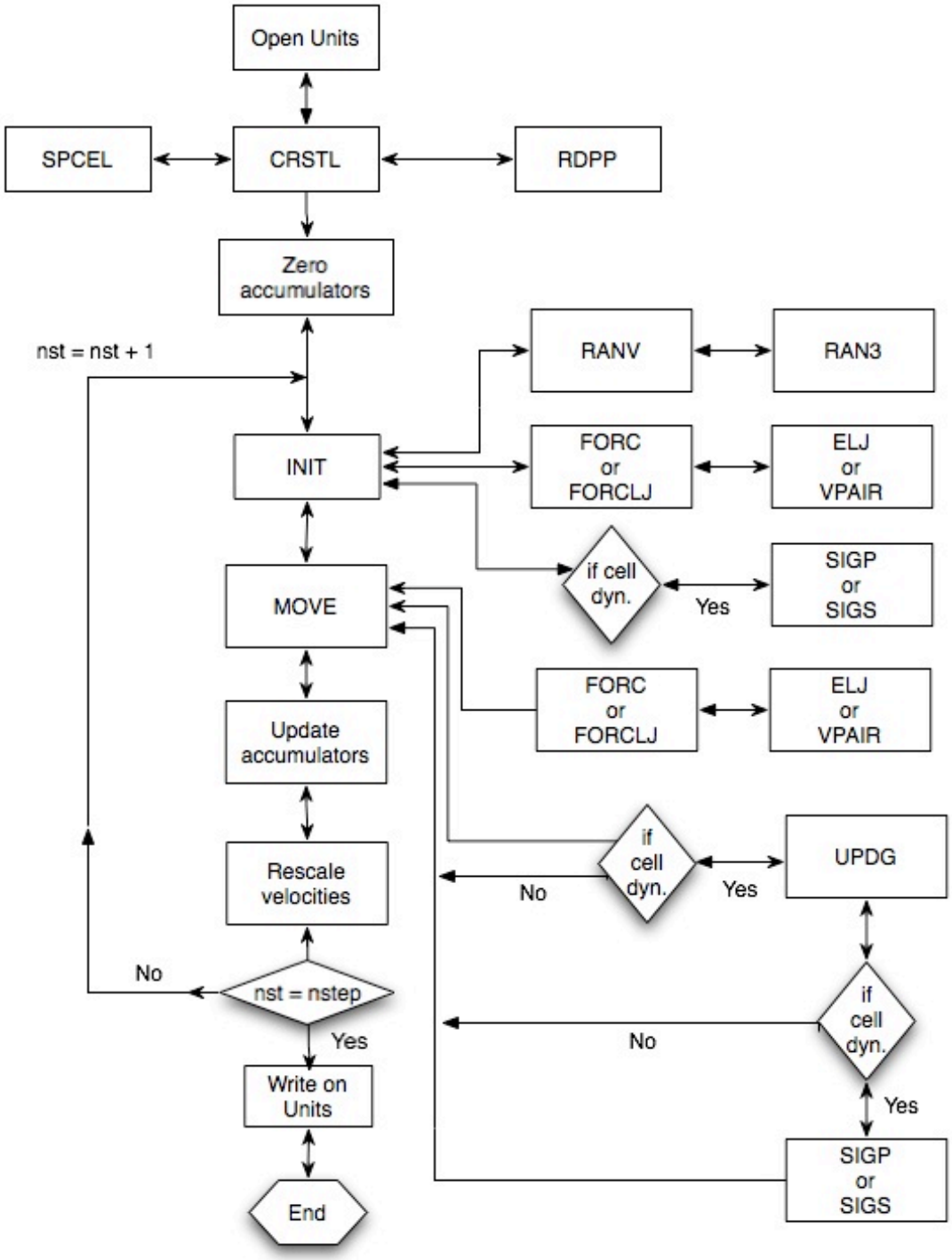

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c      The subroutines are listed approximately according with callin order.
c      They are well documented and a description of variables is
c      provided in their begining. The basics goes as follows: input is read
c      inside TPAGE and CRSTL (which calls RDPP - to read some pair-
potential).
c      SPCEL constructs supercells.
c      INIT initializes the atomic (and cell vectors) positions, velocities
c      and forces (and also some intermediate values necessary for the
c      integration of Eq.'s of motion according to the Beeman algorithm.
c      J. Comp. Phys. 20, 130 (1976).
c      It calls RANV which provides the initial velocity distribution.
c      Forces, energies and certain quantities required for stress
c      calculations are obtained inside subroutines FORCLJ and ELJ if LJ
c      potentials are used. Otherwise subroutines FORC and VPAIR are called.
c      The choice for LJ type potentials is set inside the program.
c      There is one variable called "ilj" which is set equal to "1"
c      if LJ potentials are to be used and "0" otherwise.
c      This is the only variable set "manually" inside. Search for this
c      variable throughout and check if it is properly set.
c      The choice of LJ parameters is done inside ELJ.
c      UPDG updates structure related quantites (volume etc) in case of
c      variable cell shape dynamics (VCSD).
c      Subroutines SIGS and SIGP, calculate lattice vectors accelerations
c      according to Eq.'s (8) and (9)
c      of PRB 44, 2358 (1991) respectively.
c
c      It is important to read  PRB 44, 2358 (1991) to know what is going on
c      inside the program if VCSD is being performed.
c      The statndard input goes as follows:
c

 Test: md of Ar atom in fcc cell                          (title)
nd                                                        (calc)
 s   n                                                    (ic,iio)
     8.000000                                             (alatt)
    1    1    1                                          (nsc)
       1.000000       0.000000       0.000000           (avec)
       0.000000       1.000000       0.000000
       0.000000       0.000000       1.000000
     0.00400                                               (cmass)
     0.00000     0.00000     0.00000                       (press)
     0.00000     0.00000     0.00000
    1                                                     (ntype)
    4   Ar    40.00000                                    (natom,nameat,atmass)
       0.000000       0.000000       0.000000           (rat)
       0.500000       0.500000       0.000000
       0.000000       0.500000       0.500000
       0.500000       0.000000       0.500000
      40.000000                                           (rcut)
    4    4    4                                         (ncell)
  100  110   10                                         (nstep,ntcheck,ntimes
    000.00000     0.00100   250.00000                   (temp,ttol,dt)
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c       Those familiar with Berkeley/UMN type versions of plane wave
c       pseudopotential codes will notice the similarity of variable names
c       and program structure. The input goes as follows:
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c       title: run title (read inside TPAGE)
c       calc: type of calculation (see TPAGE)
c       ic: initialization "ID" (see CRSTL)
c       iio: output "ID" (see CRSTL)
c       alatt: lattice cte in a.u. (Bohr radii)
c       nsc: # of primitive cells along the 3 directions used to
c            build the supercell (see CRSTL and SPCEL)
c       avec: (trully) primitive cell vectors (see CRSTL)
c       cmass: fictitious cell mass (see PRB 44, 2358 (1991)). If "nd nm" or
c              "sd or sm" type of dynamics are used, this mass should vary
c              inversely with supercell volume.
c       press: external stress tensor in Mbar (see CRSTL).
c              The order is: xx     yy      zz
c                            xy     xz      yz
c       ntype: # of atom types (see CRSTL)
c       natom(nt): # of atoms of same type
c       nameat(nt): name of this atom type
c       atmass(nt): atomic mass in proton units
c       rat(na,nt): "reduced" atomic position for na atom of type nt
c       rcut: radius beyond which interatomic interactions are ignored
c       ncell: # of neighboring "supercells" along the 3 primitive directions
c              which should completely contain the interaction sphere. If
c              this choice is not carefully made, particles may "drift away"
c              and the dynamical energy may not conserve.
c       nstep: # of MD timesteps
c       ntcheck: # of steps taken before temperature is checked or rescaled.
c       ntimes: # of times the temperature is checked.
c       temp: chosen temperature
c       ttol: relative temperature deviation tolerated for temperature
c             rescaling
c       dt: time step in Rydberg-like units. This unit is twice that in the
c           Hartree system which is approx. equal to 2.48D-17 sec's.
c
c       The io is essentially obvious:
c       unit=5,file='inp': standard input (above)
c       unit=6,file='out': standard output (trivial except for error messages)
c       unit=7,file='io': contains the final atomic and cell configuration and
c                         it may be used as input for subsequent runs (see the
c                         role played by variables "ic" and "iio" above.
c       unit=20,file='car': this file shoud record the history of the MD run,
c                           i.e. the position, velocity, acceleration of atoms
c                           and cell vectors at every timestep. From this file
c                           the trajectory should be reproduced in order any
c                           kind of analysis to be done separately later.
c                           It can be (very) large and should be unformatted.
c       unit=21,file='e': "Total" potential, kinetic, total energy, and
c                              PV."Total" means ionic plus cell-like energies.
c       unit=22,file='eal': Potential, kinetic, and total energies
c                                decomposed in ionic and cell contributions.
c       unit=23,file='ave': accumulated average values for "Total"
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c       unit=24,file='p': (cte) external, internal and "run averaged"
c                              pressures.
c       unit=25,file='avec': Lengths and angles between primitive cell
c                                  vectors.
c       unit=26,file='tv': "Instantaneous" temperature and volume.
c       unit=31,file='sip': Pair potential for Si (sample input).
c
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c
c       Final observations:
c       a) The new VCSD's should conserve symmetries. If it
c          does not, it is sign that something is not working. Bad energy
c          conservation, i.e. bad dynamics is the usual cause, and decreasing
c          time steps or increasing cell mass can improve this aspect.
c
c       b) Don't forget to turn off double precision when running this code
c          on Crays.
c
c
c                           Renata M. Wentzcovitch
c
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