Report
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June 1 – July 31, 2011

This visit was dedicated to the activities set within the task **T.1.1 A molecular level modeling of fluid-brush-solid systems.**

Since this was my initial visit to UMCS Lublin within this project, the first few days we spent to arrange accommodation, opening the bank account and setting up the office place in the Laboratory of computer modeling at the Chemistry department.

To perform molecular modeling of fluid-brush-solid system, it was decided to use the molecular dynamics and, in particular, the package LAMMPS. Since I newer was working with LAMMPS before, I spent two weeks learning about the LAMMPS - a classical molecular dynamics code.

We also were discussing with Stefan Sokolowski the set up of the system that we will model. It has been decided that model system will include the rectangular box elongated in *z* direction and with periodic boundary conditions in *x* and *y* directions. On each of two sides of the rectangle in z direction, i.e., at z=0 and z=L_z we placed a wall of the size L_x x L_y, that supposes to be covered by brushes with varied surface density $N_{brush}/ (L_x \text{ x } L_y)$. The box itself is filled with a model Lennard-Jones fluid of the total density $N_{fluid}/ (L_x \text{ x } L_y \text{ x } L_z)$.

To model the brushes we are using the tangent Lennard-Jones spheres. The length of brushes is the same and is determined by the number N_B of the segments within each brush. All segments of each brush are equivalent except the first one – wall segment - that keeps brush to be fixed at the wall. In general there is a possibility to let for the wall segments to move within the *xy* plane, however, on the initial stage we will keep them fixed.

The next step was to prepare the initial configuration for both surface brushes and fluid subsystems. As for brushes we decided first to place and fix them at the sites of the squared lattice on *xy* surface, where the lattice constant depends and is defined by the desired value of surface density $N_{brush}/ (L_x \text{ x } L_y)$.

```
          program CHAINSONLY
c-----------------------------------------------------------------
c         startring configuration: ONLY CHAINS
c-----------------------------------------------------------------
        implicit none
        real*4 x(11111),y(11111),z(11111)
        real*4 xl,yl,sig,dx,dy,xx,yy,zz,zl,zeroplane
        integer nx,ny,n,i,j,k,ikind,ipart,nseg,np(1111111)
        integer izero,imol,ibond,nb
        write(*,*) 'enter xl,yl,zl and the site-site dist, zeroplane'
```

```
c-------------------------------------------------
      read(*,*)xl,yl,zl,sig,zeroplane
      write(*,*) ' enter nx, ny, (n=nx*ny)) and nseg'
      read(*,*)nx,ny,nseg
c-------------------------------------------------
      dx=xl/float(nx)
      dy=yl/float(ny)
      n=nx*ny
      ipart=0
      do i=1,nx
      xx=float(i-1)*dx
      do j=1,ny
      yy=float(j-1)*dy
      ikind=0
      do k=1,nseg
      zz=(k-1)*sig+zeroplane
      ipart=ipart+1
      ikind=ikind+1
      x(ipart)=xx
      y(ipart)=yy
      z(ipart)=zz
      np(ipart)=ikind
      enddo
      enddo
      enddo
      open(14,file='c.dat')
      write(14,*)' LAMMPS data file from restart file'
      write(14,*) ' '
      write(14,*) ipart,'  atoms'
      write(14,*) nx*ny*(nseg-1),'  bonds'
      write(14,*) ' '
      write(14,*) nseg,' atom types'
      write(14,*) ' 1 bond types '
      write(14,*) ' '
      write(14,*)'0   ',xl,'  xlo xhi'
      write(14,*)'0   ',yl,'  ylo yhi'
      write(14,*)'0   ',zl,'  zlo zhi'
      write(14,*) ' '
      write(14,*)' Masses '
      write(14,*) ' '
      do i=1,nseg
      write(14,*)i,' 1 '
      enddo
      write(14,*) ' '
      write(14,*) ' Atoms '
      write(14,*) ' '
      izero=0
114   format(1x,i4,1x,i2,1x,i2,1x,i2,1x,3(f10.6,1x),3(i2,1x))
      ipart=0
      do i=1,nx
      do j=1,ny
      ikind=0
      do k=1,nseg
      ikind=ikind+1
      ipart=ipart+1
```

```
        imol=1
        if(ikind.eq.1)imol=1
        write(14,114)ipart,imol,ikind,x(ipart),y(ipart),z(ipart),izero,izero,izero
        enddo
        enddo
        enddo
        write(14,*) ' '
        write(14,*) ' Bonds '
        write(14,*) ' '
c---------------------------------------
        ibond=0
        nb=0
        do i=1,nx*ny
        do j=1,nseg-1
        nb=nb+1
        ibond=ibond+1
        write(14,*)nb,' 1 ',ibond,ibond+1
        enddo
        ibond=ibond+1
        enddo
        write(14,*)
        stop
        end
```

As for the fluid – we were using the way, when the fluid particles are randomly placed into the box avoiding the overlap of their cores.

```
          PROGRAM  FLUIDSTART
c-------------------------------------------------------------------------
c         startring configuration: BRUSHES plus FLUID      I
c-------------------------------------------------------------------------
       implicit none
       real*4 x(11111),y(11111),z(11111)
       real*4 xa(11111),ya(11111),za(11111)
       real*4 xl,yl,sig,dx,dy,xx,yy,zz,zl,zeroplane
       integer nx,ny,n,i,j,k,ikind,ipart,nseg,np(1111111)
       integer izero,imol,ibond,nb,ipartt,ncreate,idum,icrea
       real*4 zl2,yl2,xl2,dz,odl1,ran2,zk,yk,xk
       write(*,*) 'enter xl,yl,zl and the site-site dist between
     > bonded seg, zeroplane'
       read(*,*)xl,yl,zl,sig,zeroplane
        write(*,*) ' enter nx, ny, (n=nx*ny)) and nseg'
        read(*,*)nx,ny,nseg
        dx=xl/float(nx)
        dy=yl/float(ny)
        n=nx*ny
        ipart=0
        do i=1,nx
        xx=float(i-1)*dx
        do j=1,ny
        yy=float(j-1)*dy
        ikind=0
        do k=1,nseg
        zz=(k-1)*sig+zeroplane
        ipart=ipart+1
```

```
        ikind=ikind+1
        x(ipart)=xx
        y(ipart)=yy
        z(ipart)=zz
        np(ipart)=ikind
        enddo
        enddo
        enddo
        ipartt=ipart
        write(*,*)' how many atoms?'
        read(*,*)ncreate
        open(14,file='c.dat')
        write(14,*)' LAMMPS data file from restart file'
        write(14,*) ' '
        write(14,*) ipart+ncreate,'  atoms'
        write(14,*) nx*ny*(nseg-1),'  bonds'
        write(14,*) ' '
        write(14,*) nseg+1,' atom types'
        write(14,*) ' 1 bond types '
        write(14,*) ' '
        write(14,*)'0   ',xl,'  xlo xhi'
        write(14,*)'0   ',yl,'  ylo yhi'
        write(14,*)'0   ',zl,'  zlo zhi'
        write(14,*) ' '
        write(14,*)' Masses '
        write(14,*) ' '
        do i=1,nseg+1
        write(14,*)i,' 1 '
        enddo
        write(14,*) ' '
        write(14,*) ' Atoms '
        write(14,*) ' '
        izero=0
114  format(1x,i4,1x,i2,1x,i2,1x,3(f10.6,1x),3(i2,1x))
        ipart=0
          do i=1,nx
          do j=1,ny
          ikind=0
          do k=1,nseg
          ikind=ikind+1
          ipart=ipart+1
          imol=1
          if(ikind.eq.1)imol=1
       write(14,114)ipart,imol,ikind,x(ipart),y(ipart),z(ipart),izero,izero,izero
          enddo
          enddo
          enddo
c-------------------------------------------------
           xl2=xl/2.
           yl2=yl/2.
           idum=-121315
           icrea=0
           do  i=1,ncreate
           write(*,*) ' I create the ',i,' -th atom'
101        xk=xl*ran2(idum)
           yk=xl*ran2(idum)
           zk=zeroplane+(zl-zeroplane)*ran2(idum)
c-------------------  with chains -----------------
            do j=1,ipartt
            dx=x(j)-xk
```

```
            dx=xl2-abs(xl2-abs(dx))
            dy=y(j)-yk
            dy=yl2-abs(yl2-abs(dy))
            dz=z(j)-zk
            dz=zl2-abs(zl2-abs(dz))
            odl1=dx*dx+dy*dy+dz*dz
            if(odl1.le.1) goto 101
            enddo
            do j=1,icrea
            dx=xa(j)-xk
            dx=xl2-abs(xl2-abs(dx))
            dy=ya(j)-yk
            dy=yl2-abs(yl2-abs(dy))
            dz=za(j)-zk
            dz=zl2-abs(zl2-abs(dz))
            odl1=dx*dx+dy*dy+dz*dz
            if(odl1.le.1) goto 101
            enddo
            icrea=icrea+1
            xa(icrea)=xk
            ya(icrea)=yk
            za(icrea)=zk
            enddo
c-----------------------------------------------
        do i=1,ncreate
        imol=2
        write(14,114)ipartt+i,imol,nseg+1,xa(i),ya(i),
     > za(i),izero,izero,izero
        enddo
c-----------------------------------------------
         write(14,*) ' '
         write(14,*) ' Bonds '
         write(14,*) ' '
         ibond=0
         nb=0
         do i=1,nx*ny
         do j=1,nseg-1
           nb=nb+1
           ibond=ibond+1
        write(14,*)nb,' 1 ',ibond,ibond+1
        enddo
           ibond=ibond+1
         enddo
         write(14,*)
         stop
         end
```

After the system set up was finished, the next stage was to choose the proper ensemble, thermostat, etc.

The input script for the main LAMMPS program **lmp_openmpi** is as follows:

```
# LJ brush
echo screen
units          lj
atom_style   bond
boundary     p p f
```

```
#read_data  c.dat
read_restart restart.1

#declare bonds and interactions
reset_timestep 0
pair_style      lj/cut  3
pair_coeff      * *  1.0  1.0

bond_style fene
bond_coeff 1  30.0 1.3 1.0 1.0

group pinned type 1
group flexible subtract all pinned
group spherical type 9

# assign arbitrary velocities and a NVE ensemble
#velocity     flexible create 3.0 2349852
velocity all zero linear
neighbor     0.5 bin
lattice fcc 0.2

fix         no1 flexible nve
fix         no2 flexible temp/rescale 1 3 3 0.000001 1.0
fix         no3 all wall/reflect zlo zhi

#thermo_style custom step temp epair ebond vol
thermo_style custom step epair ebond
thermo      500

#dump       1 all custom 20 dump.lammpstrj &
#               tag type x y z
timestep    0.00005
dump           d1 all custom 100 dump.lammpstrj id mol type x y z

run 10000

write_restart restart.1
```

Besides the activities related to the modeling of fluid-brush-solid systems I had numerous discussions with local researchers – participants of the projects – who were working on other project tasks.

On June 22, 2011 I made presentation entitled “Excluded volume and physics of phase transitions in soft matter” at the Laboratory of Computer Modeling of Physico-Chemical Processes Seminar.