

# Workshop: Modeling of chemically powered nanomotors

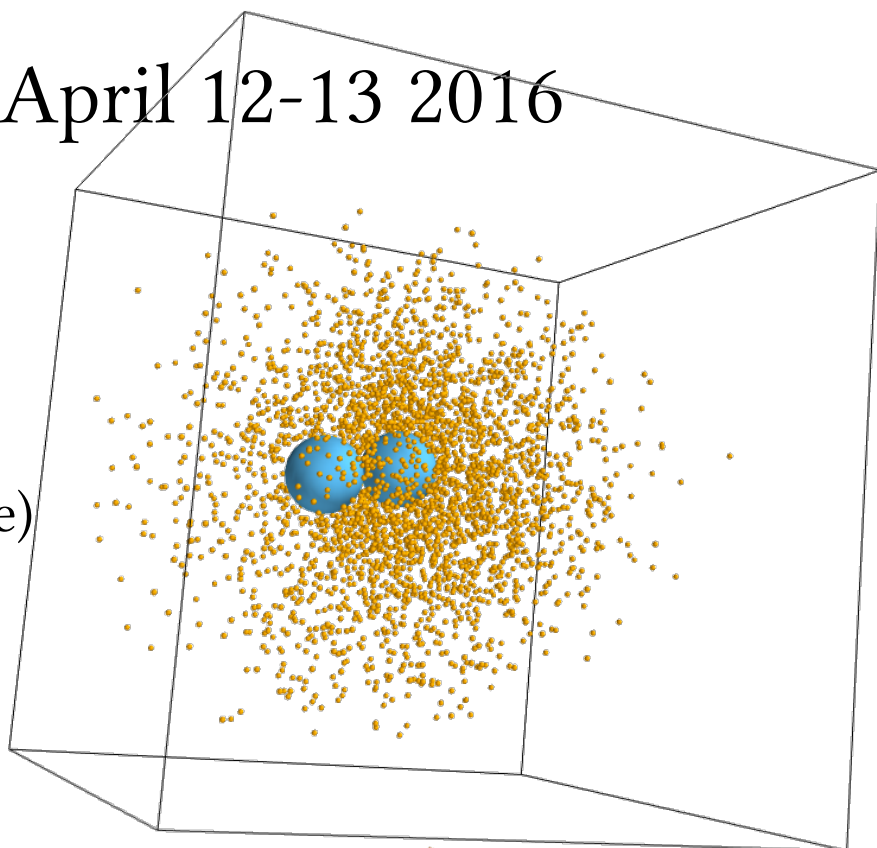
Leuven - April 12-13 2016

## Speakers

Steve Ebbens (Sheffield)  
Ray Kapral (Toronto)  
Marisol Ripoll (Jülich)  
Ayusman Sen (Penn State)

## Hands-on simulation

Pierre de Buyl (Leuven)  
Mu-Jie Huang (Toronto)



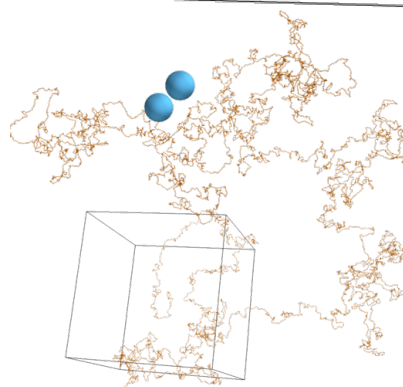
```
write(*,*) 'Running for', N_loop, 'loops'
call main$tic()
do i = 1, N_loop
  if (modulo(i,5) == 0) write(*, '(i05)', ac
md_loop: do j = 1, N_MD_steps
  call md_pos(solvent, dt)

! Extra copy for rattle
colloids% pos_rattle = colloids% pos
do k=1, colloids% Nmax
  colloids% pos(:,k) = colloids% pos
  dt**2 * colloids% force(:,k)
end do

call rattle_dimer_pos(colloids, d, dt

so_max = solvent% maximum_displacem
co_max = colloids% maximum_displacem

$ ./single_dimer_pbc dimer.parameters
$ ./h5md_view_dimer.py dimer.h5
```



<http://lab.pdebuyl.be/2016-nanomotor/>

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