

Active Polymer Brushes

K. Speyer, C. Pastorino and M. Müller

Introduction

Active Matter: Agents that consume energy in order to move or exert mechanical forces



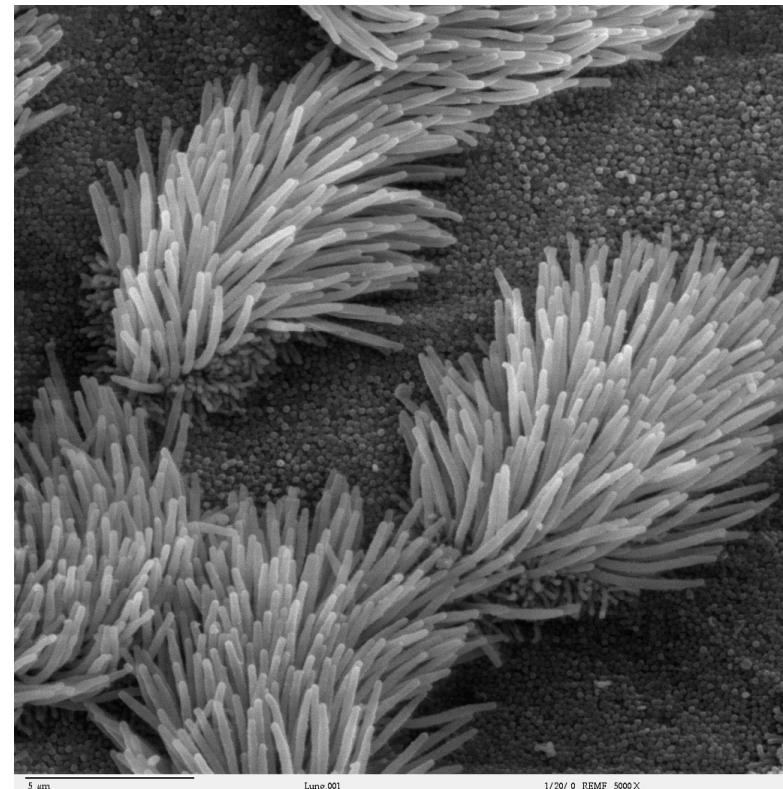
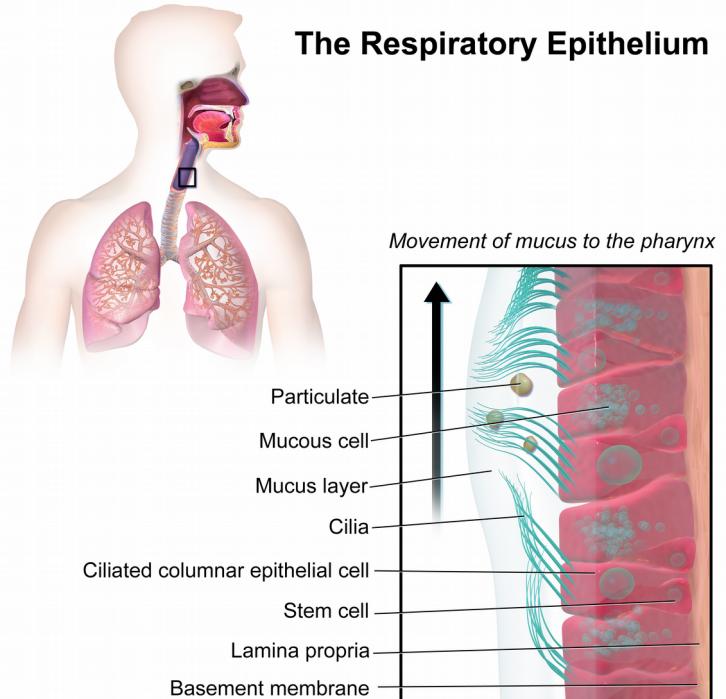
Some cells use flagella (hairs) to propel themselves



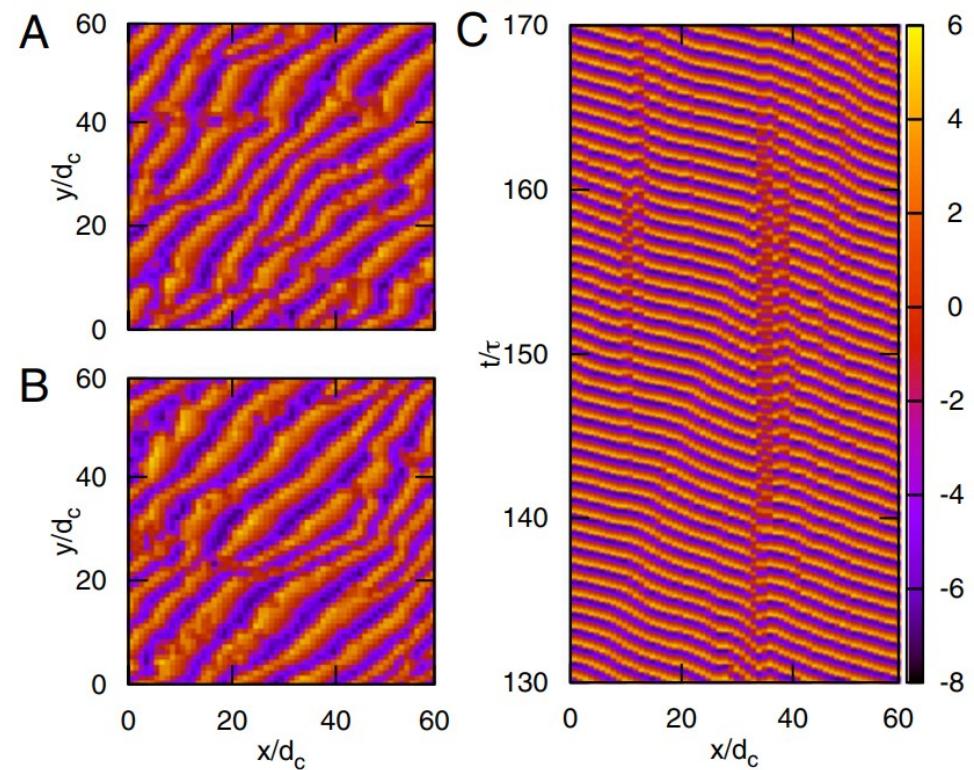
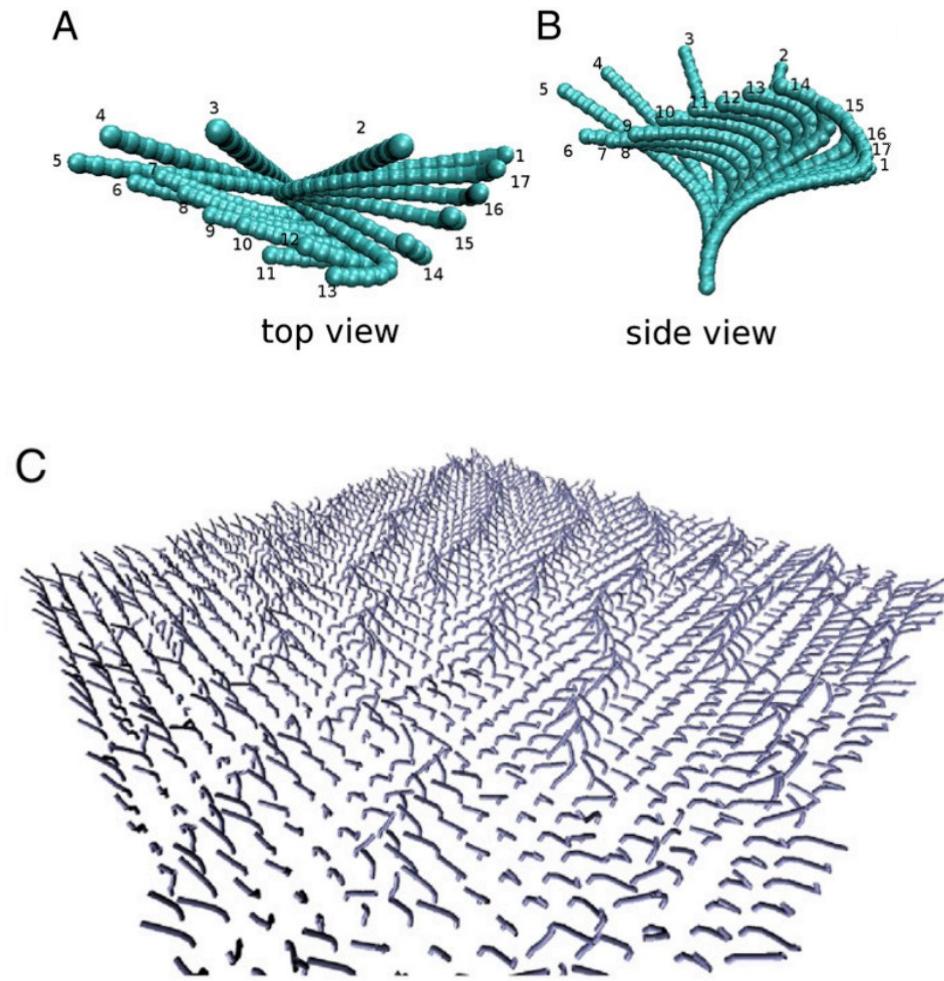
A flock of starlings acting as a swarm

Introduction

Case of study: Cilia



Literature Overview



Elgeti & Gomper; PNAS; 2013

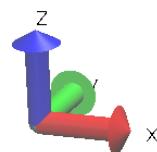
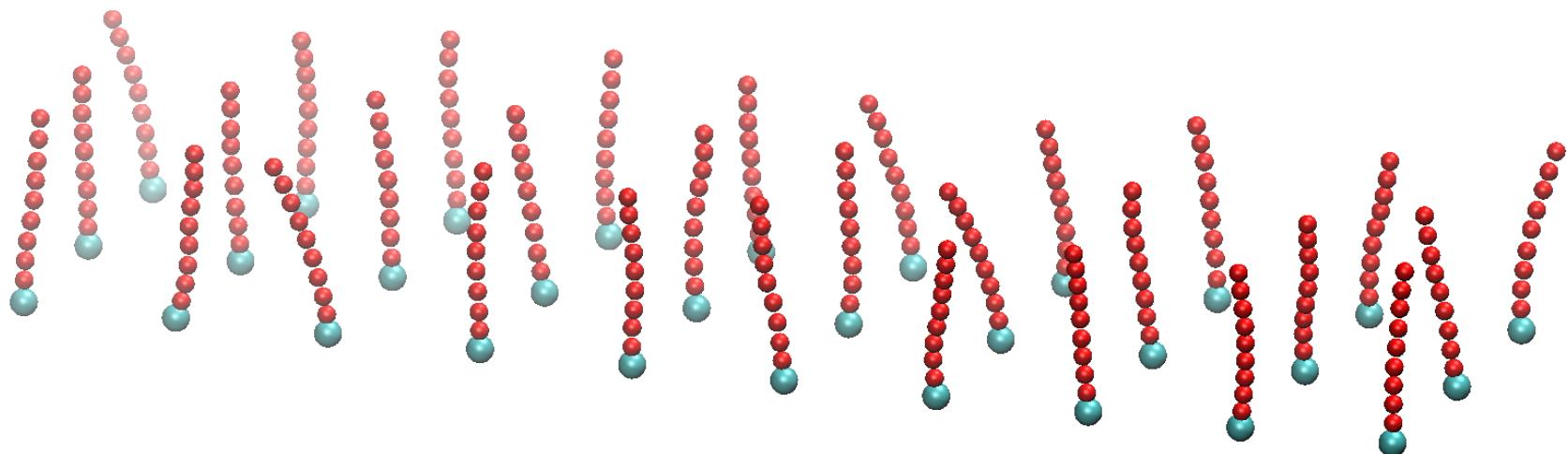
Objectives and Workplan

Implement a simple activation model for coarse grain polymer brushes in explicit solvent, and observe hydrodynamic coupling between polymers.

- Adapt a 3D activation model
- Implement Multiple Time Scale MD (RESPA)
- Rewrite cell linked list algorithm
- Add Soft Potentials
- OpenAcc speedup
- Analyze data

System Studied

Active grafted Polymers + Liquid (not shown)



Forces

Intramolecular forces:

- FENE (connectivity)
- Lennard-Jonnes (excluded volume)
- Bending (flexibility)
- Activation

Solvent forces:

- Soft Potential

$$F(r) = a_{\alpha\beta} \left(1 - \frac{r}{r_{cut}}\right)^{\hat{r}}$$

Thermostat:

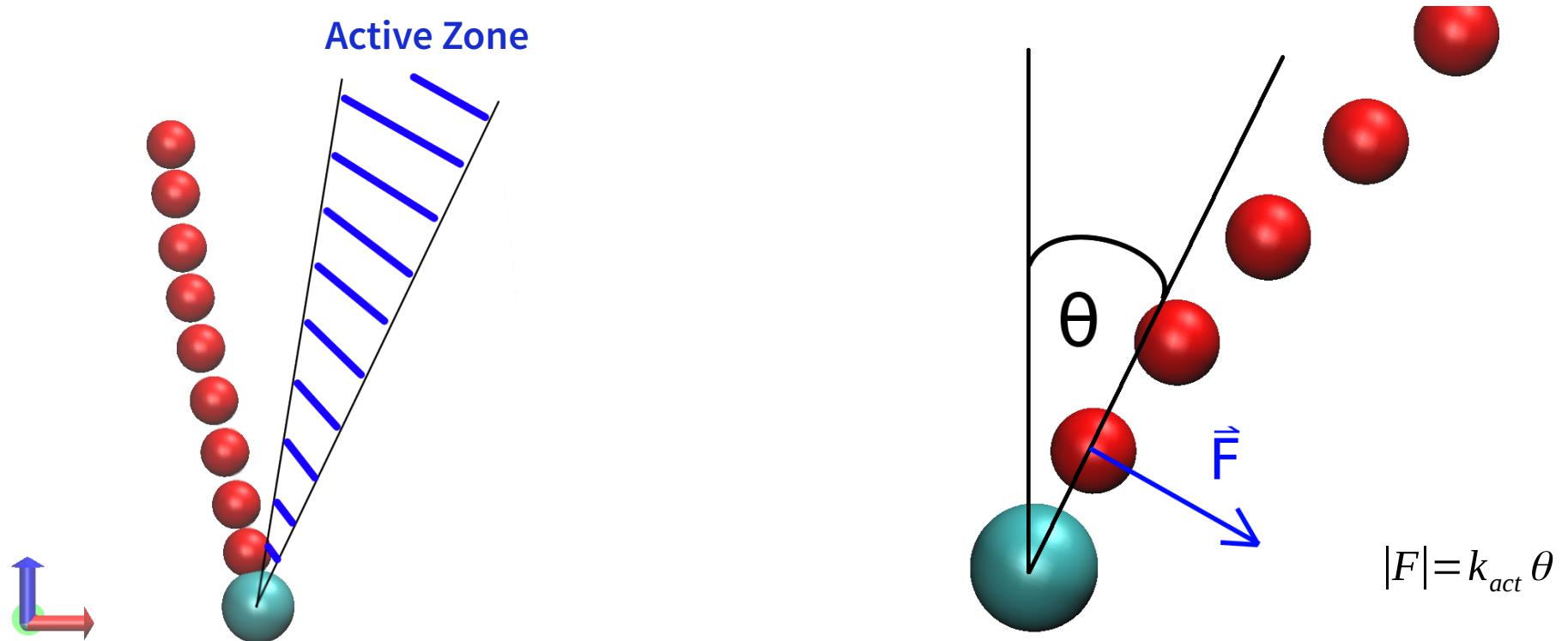
- DPD (correct hydrodynamic behaviour)

Wall – Particles Interaction:

- Integrated 9-3 Potential on Bottom Wall
- Specular Wall on Top

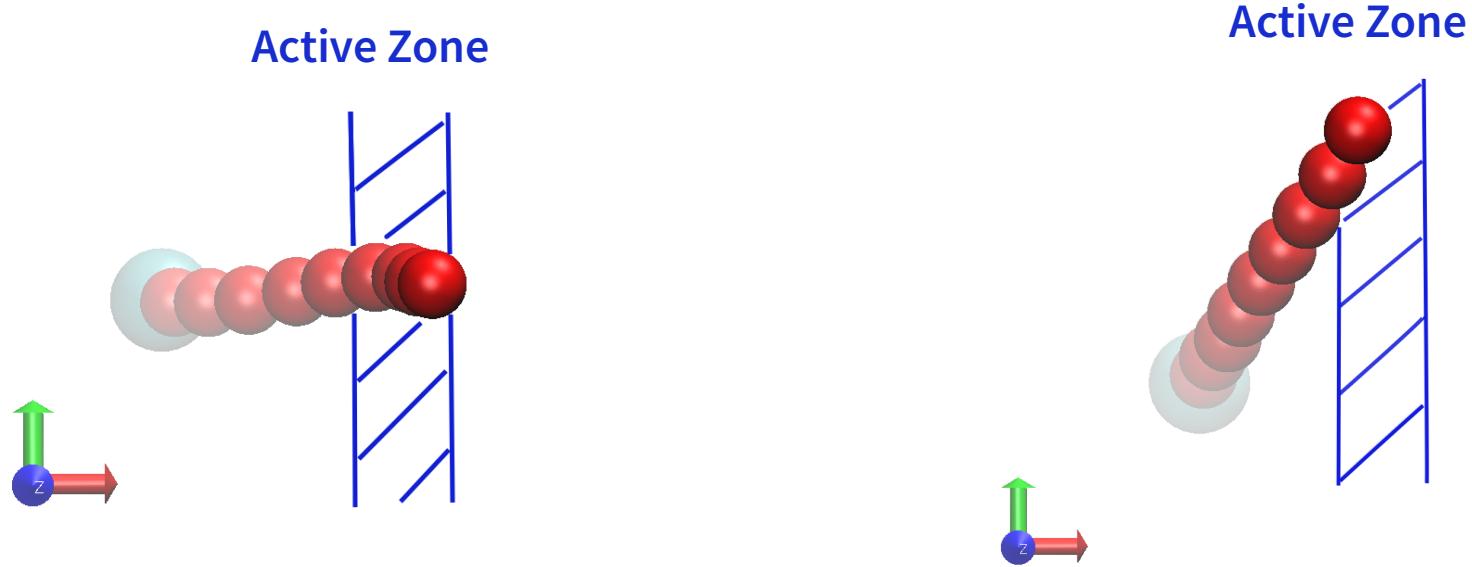
Activation Model

2D Model



Activation Model

Straightforward 3D Model

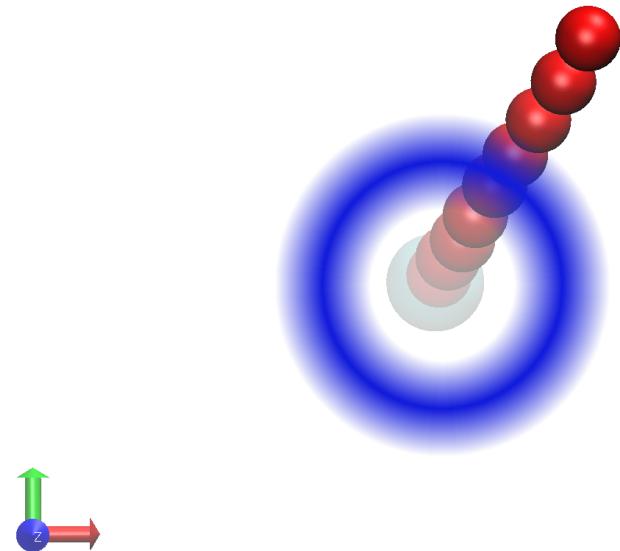


At different oscillation angles, the time spent in the **Active Zone** differs → Oscillation frequency varies

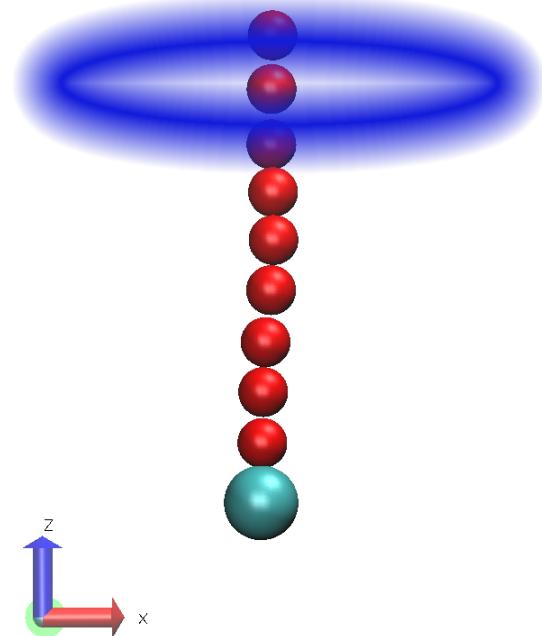
Activation Model

Symetric 3D Model

Active Zone



Active Zone



Multiple Time Scale MD

Tuckerman, Berne and Martyna; *J. Chem. Phys.*; 1992

DO i = 1, Natoms

$$VX(i) = VX(i) + 0.5*dt_long*FX_long(i)$$

$$VY(i) = VY(i) + 0.5*dt_long*FY_long(i)$$

$$VZ(i) = VZ(i) + 0.5*dt_long*FZ_long(i)$$

ENDDO

DO inner = 1, Ninner

DO i = 1, Natoms

$$X(i) = X(i) + dt_short*VX(i) + 0.5 *dt 2_short*FX_short(i)$$

$$Y(i) = Y(i) + dt_short*VY(i) + 0.5 *dt 2_short*FY_short(i)$$

$$Z(i) = Z(i) + dt_short*VZ(i) + 0.5 *dt 2_short*FZ_short(i)$$

$$VX(i) = VX(i) + 0.5*dt_short*FX_short(i)$$

$$VY(i) = VY(i) + 0.5*dt_short*FY_short(i)$$

$$VZ(i) = VZ(i) + 0.5*dt_short*FZ_short(i)$$

ENDDO

CALL FORCES_short

DO i = 1, Natoms

$$VX(i) = VX(i) + 0.5*dt_short*FX_short(i)$$

$$VY(i) = VY(i) + 0.5*dt_short*FY_short(i)$$

$$VZ(i) = VZ(i) + 0.5*dt_short*FZ_short(i)$$

ENDDO

ENDDO

CALL FORCES_long

DO i = 1, Natoms

$$VX(i) = VX(i) + 0.5*dt_long*FX_long(i)$$

$$VY(i) = VY(i) + 0.5*dt_long*FY_long(i)$$

$$VZ(i) = VZ(i) + 0.5*dt_long*FZ_long(i)$$

ENDDO

Multiple Time Scale MD

Tuckerman, Berne and Martyna; *J. Chem. Phys.*; 1992

```
DO i = 1,Natoms
  VX(i) = VX(i) + 0.5*dt_long*FX_long(i)
  VY(i) = VY(i) + 0.5*dt_long*FY_long(i)
  VZ(i) = VZ(i) + 0.5*dt_long*FZ_long(i)
ENDDO
DO inner = 1, Ninner
  DO i = 1,Natoms
    X(i) = X(i) + dt_short *VX(i) + 0.5
      *dt 2_short *FX_short(i)
    Y(i) = Y(i) + dt_short *VY(i) + 0.5
      *dt 2_short *FY_short(i)
    Z(i) = Z(i) + dt_short *VZ(i) + 0.5
      *dt 2_short *FZ_short(i)
  VX(i) = VX(i) + 0.5*dt_short *FX_short(i)
  VY(i) = VY(i) + 0.5*dt_short *FY_short(i)
  VZ(i) = VZ(i) + 0.5*dt_short *FZ_short(i)
ENDDO
```

Speedup:

x6 with RESPA

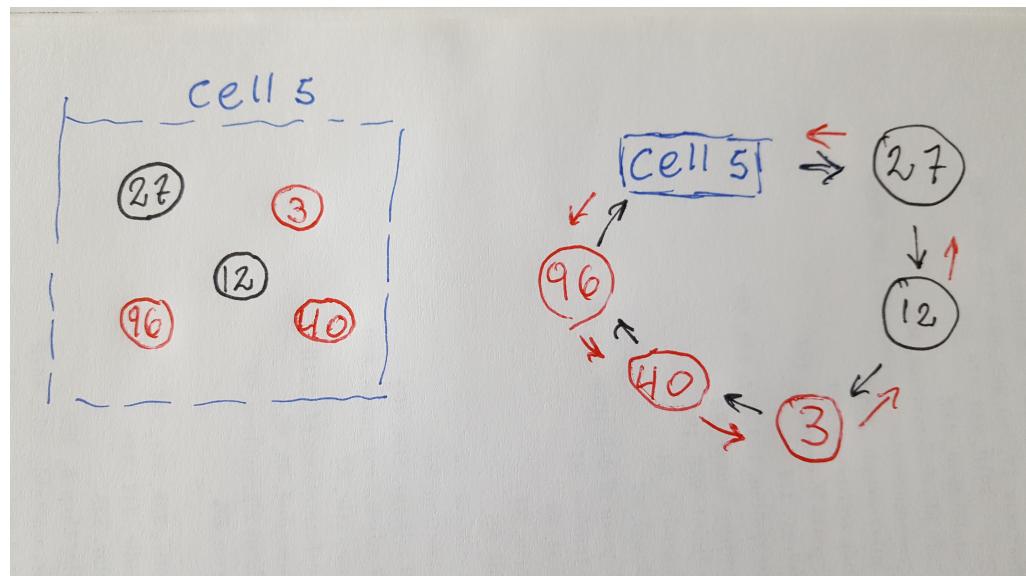
x14 with RESPA + OpenMP

CALL FORCES_short

```
DO i = 1,Natoms
  VX(i) = VX(i) + 0.5*dt_short *FX_short(i)
  VY(i) = VY(i) + 0.5*dt_short *FY_short(i)
  VZ(i) = VZ(i) + 0.5*dt_short *FZ_short(i)
ENDDO
ENDDO
CALL FORCES_long
DO i = 1,Natoms
  VX(i) = VX(i) + 0.5*dt_long*FX_long(i)
  VY(i) = VY(i) + 0.5*dt_long*FY_long(i)
  VZ(i) = VZ(i) + 0.5*dt_long*FZ_long(i)
ENDDO
```

Ordered cell linked list

An ordered cell-linked list allows to loop over the liquid particles (or monomers) alone.



$$r_{\text{neigh}}(27) = 12$$

$$r_{\text{neigh}}(3) = 40$$

$$l_{\text{neigh}}(3) = 12$$

$$l_{\text{neigh}}(96) = 40$$

$$\text{head}(5) = 27$$

$$\text{tail}(5) = 96$$

GPU acceleration

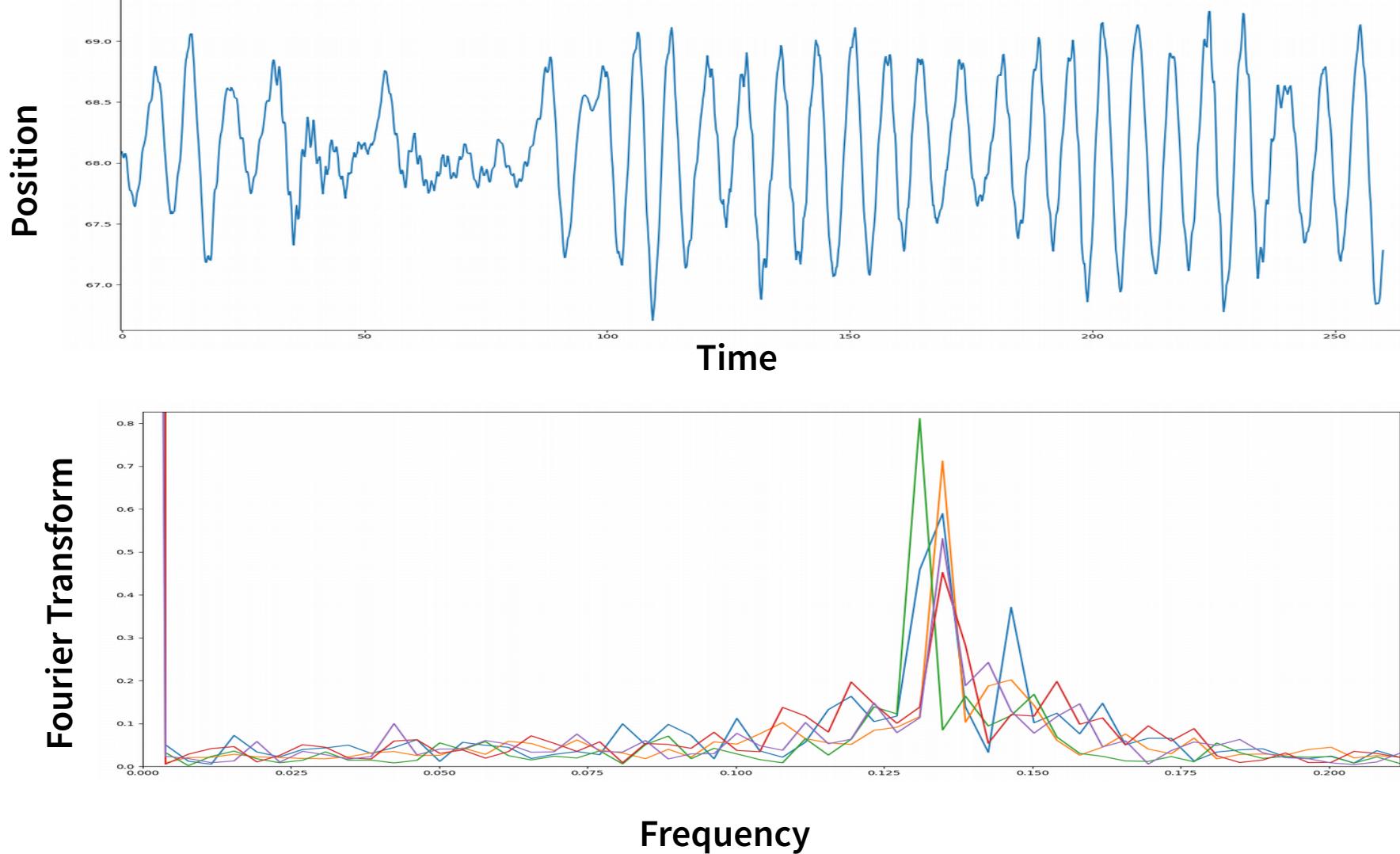
OpenAcc parallelization was attempted, but unsuccessful due to time constrains.

Data transfer between host and device is time-wise expensive.

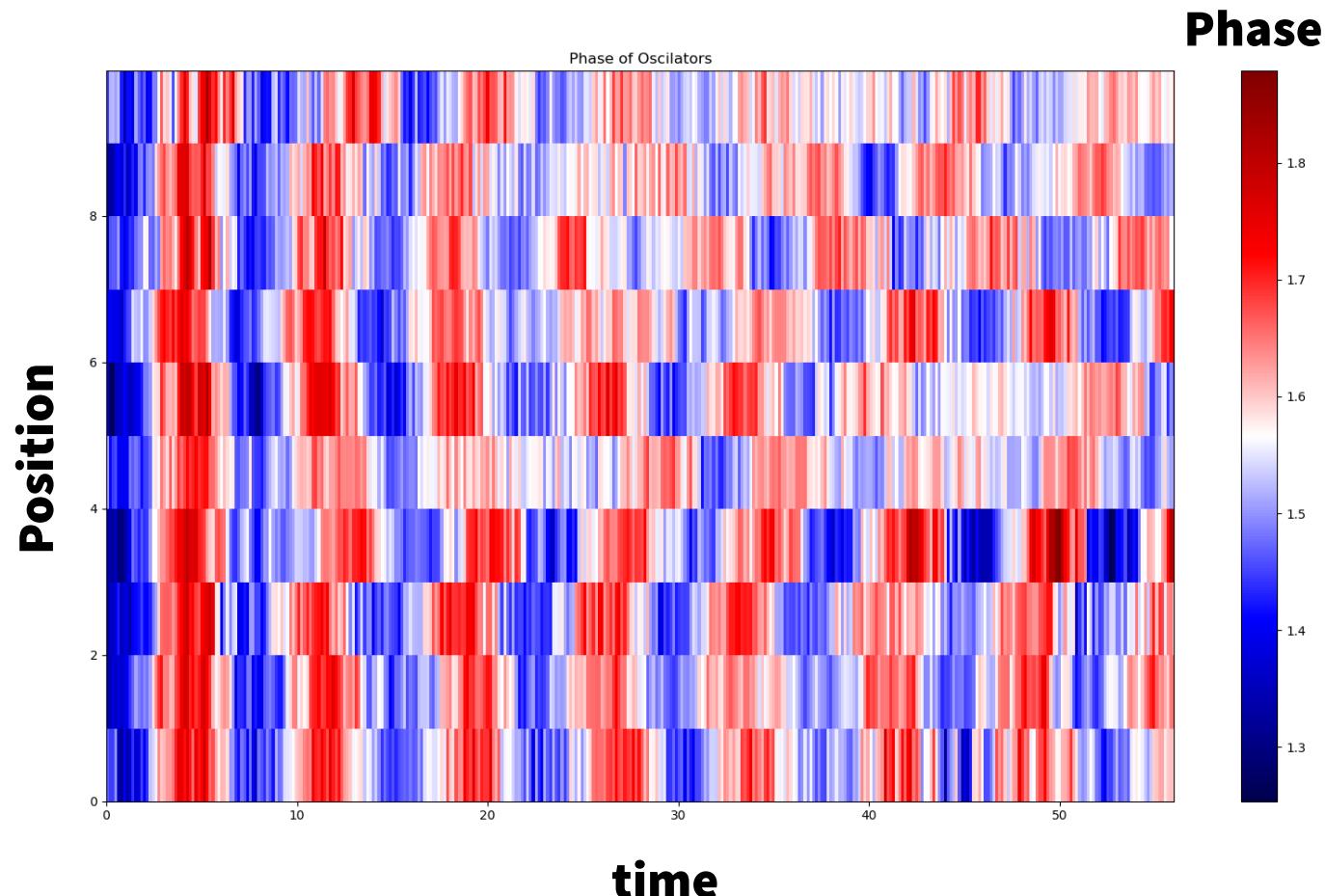
Routines called often should be parallelized.

Cell linked list algorithm is not trivial to parallelize.

Results: Single Chain Dynamics

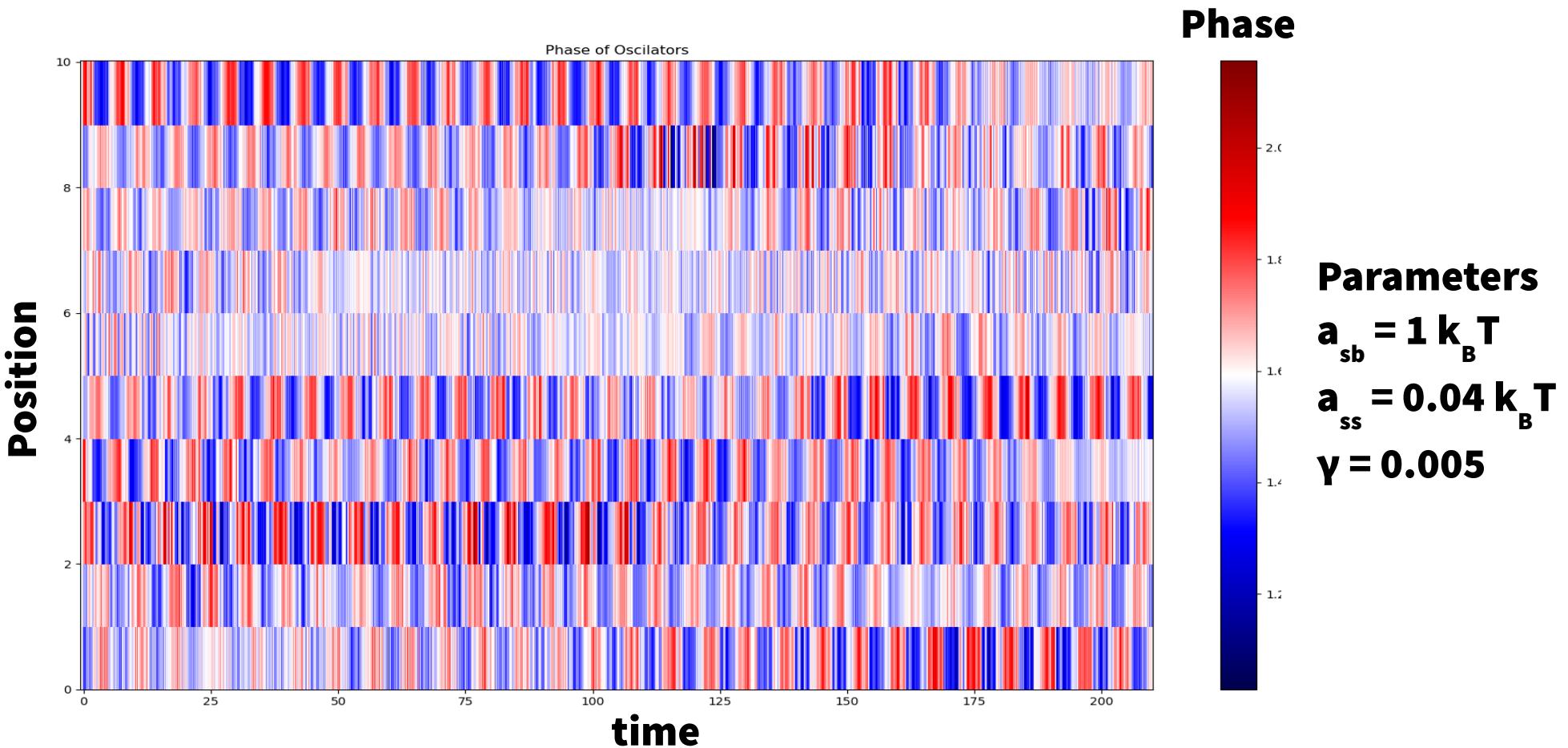


Results: Phase Field Dynamics



Parameters
 $a_{sb} = 0.4 k_B T$
 $a_{ss} = 0.04 k_B T$
 $\gamma = 0.03$

Results: Phase Field Dynamics



Why was there no synchronization?

1) Complex Interplay between parameters:

A low a_{sb} gives no coupling, while a high value hinders the self sustained oscillations

A low γ doesn't thermalize the system, while a high value hinders the self sustained oscillations

Higher k_{act} → more power pumped into the system → higher friction coefficient (& lower time step) → loss of phase coherence

2) The activation model enhances the excitation of Internal modes which are unnecessary for the system description and require a higher friction coefficient and lower time step

End

Thank you for your hospitality!

Higher Modes FFT

