Active Polymer Brushes

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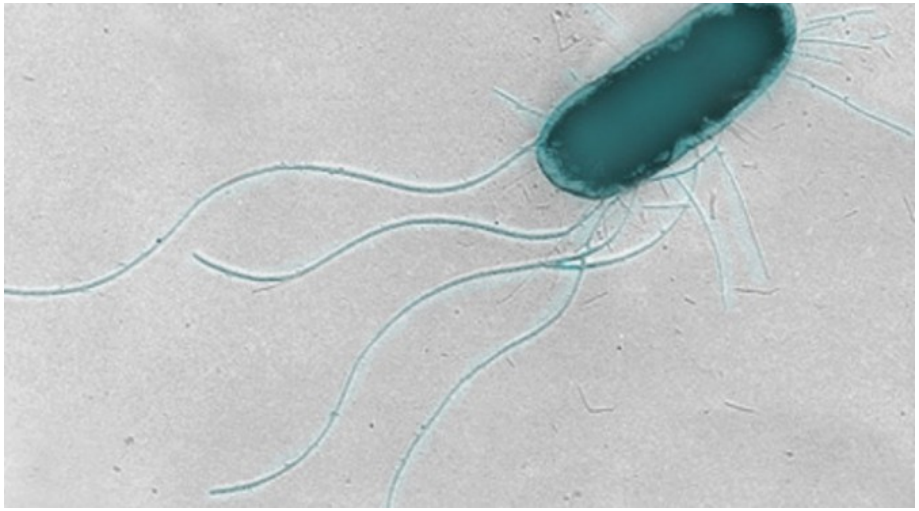
Introduction

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

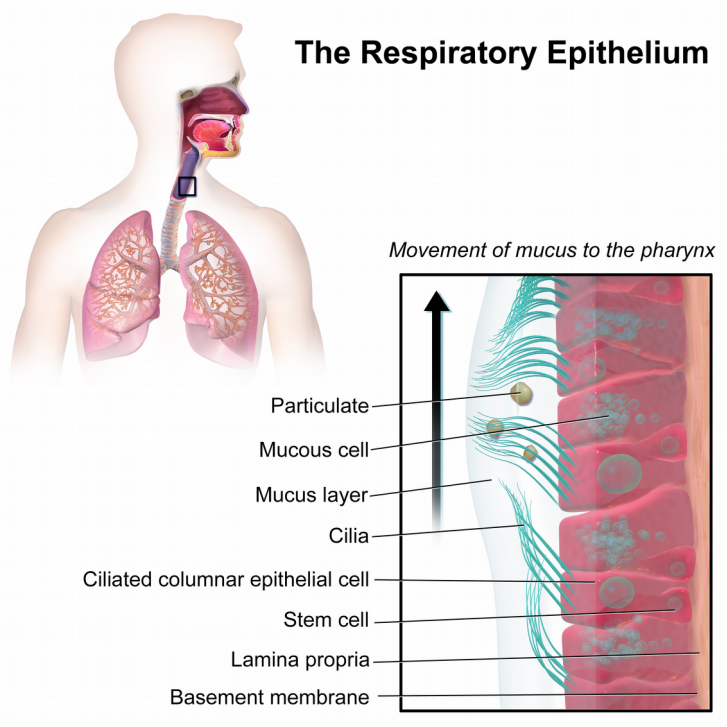


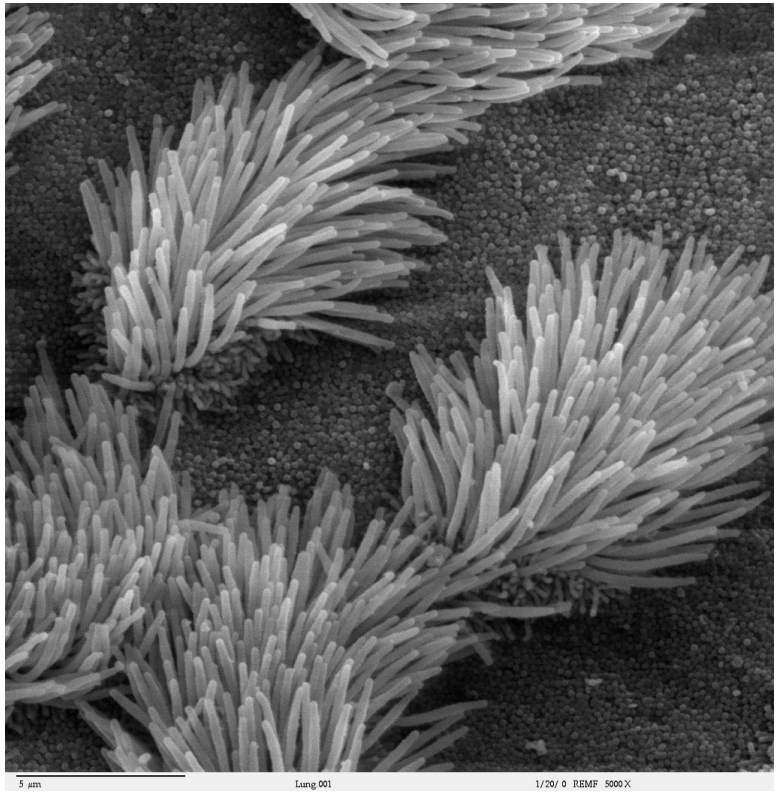
Some cells use flagella (hairs) to propel themselves

A flock of starlings acting as a swarm

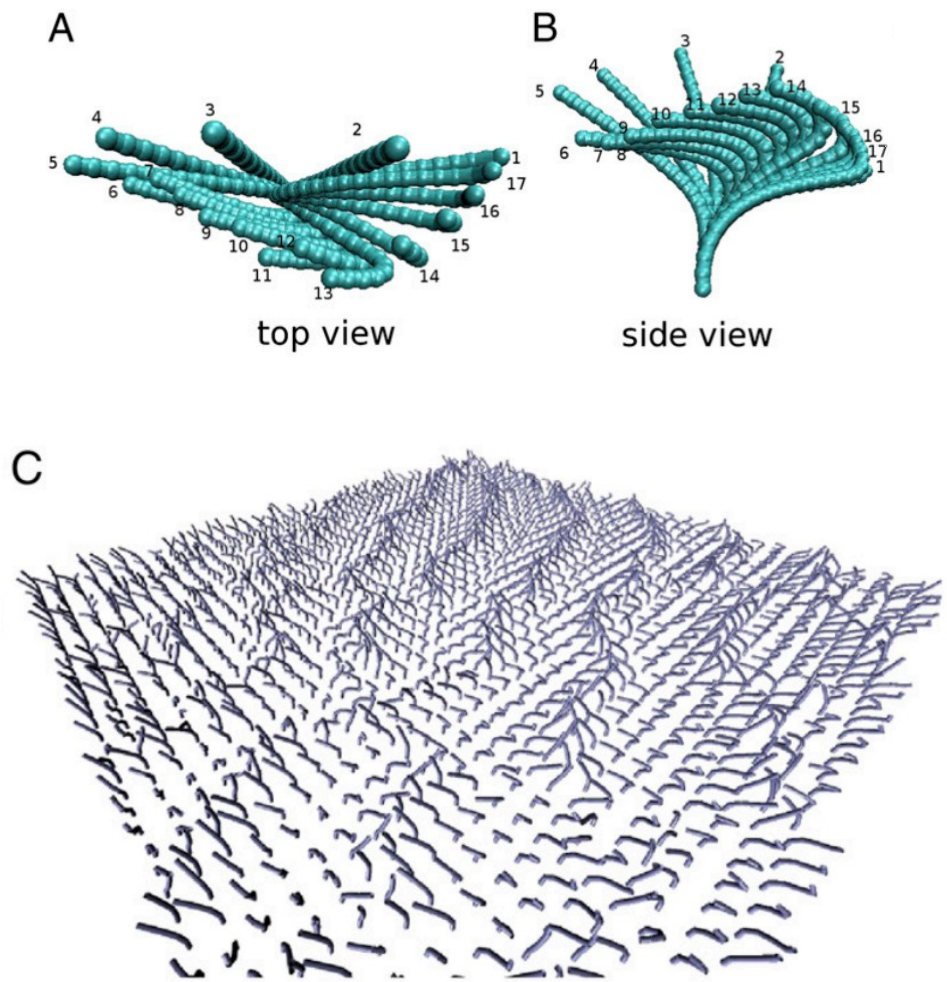
Introduction

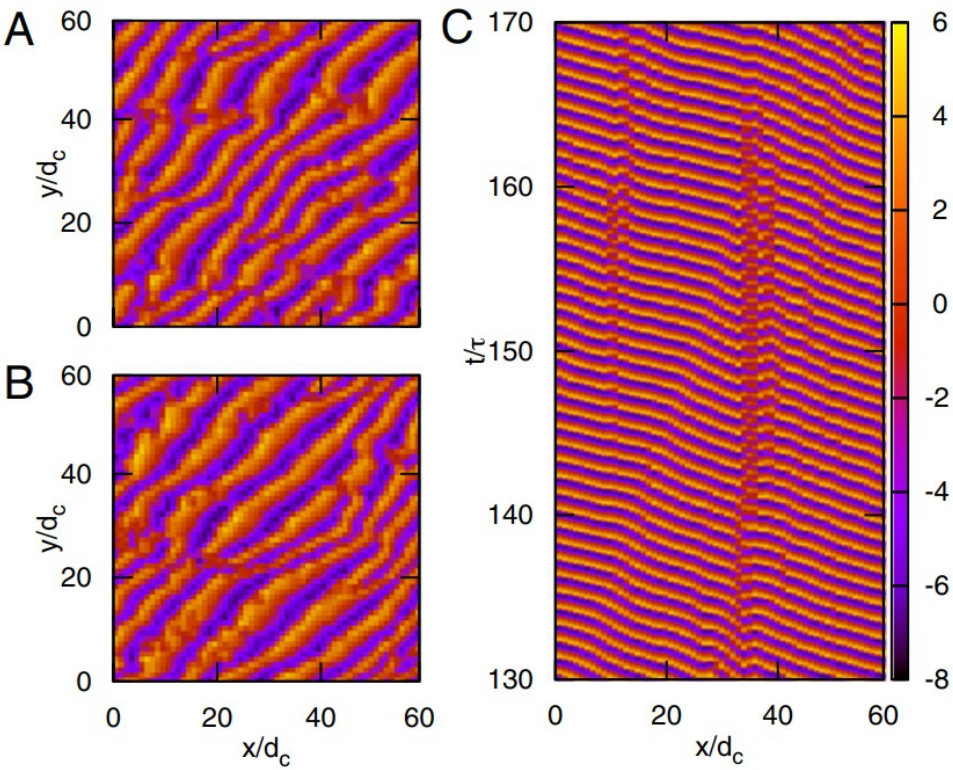
Case of study: Cilia





Literature Overview





Elgeti & Gomper; *PNAS*; 2013

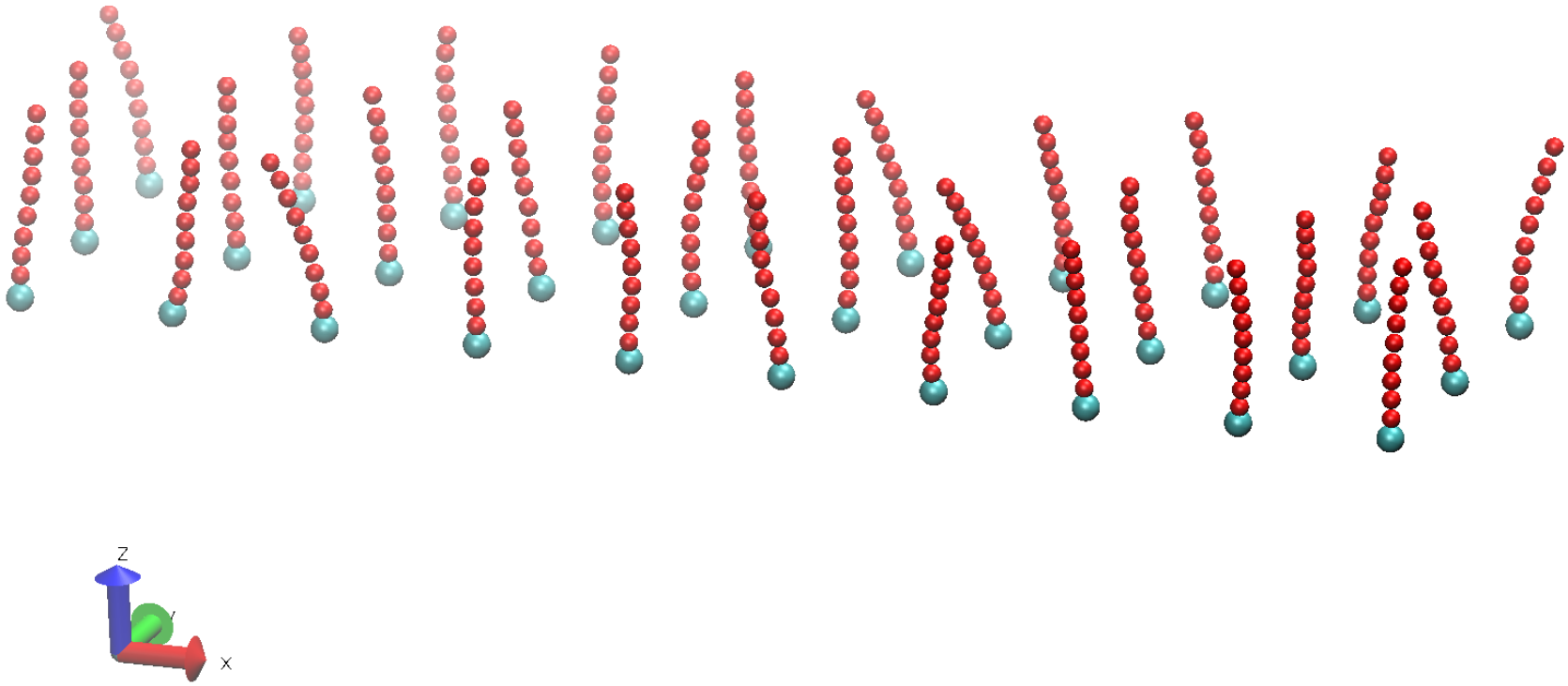
Objectives and Workplan

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 (conectivity)**
- **Lennard-Jonnes (excluded voume)**
- **Bending (flexibility)**
- **Activation**

Solvent forces:

- **Soft Potential**

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

Thermostat:

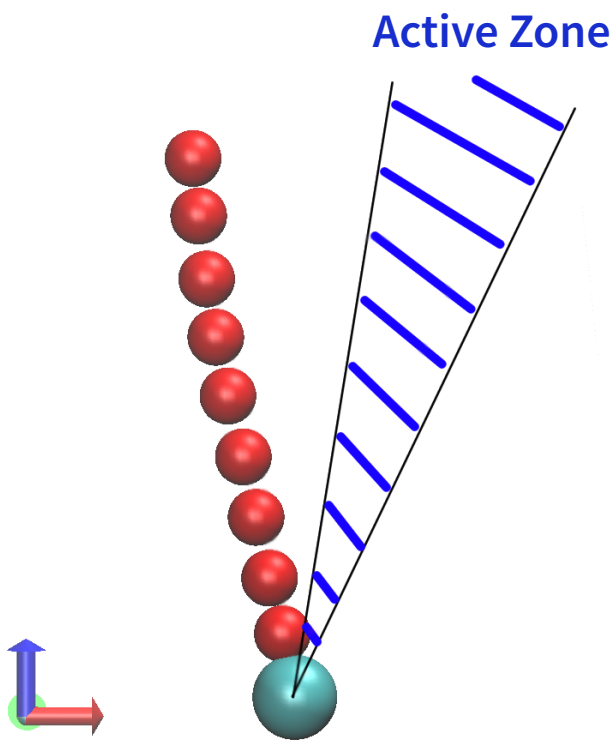
- DPD (correct hydrodynamic behaviour)

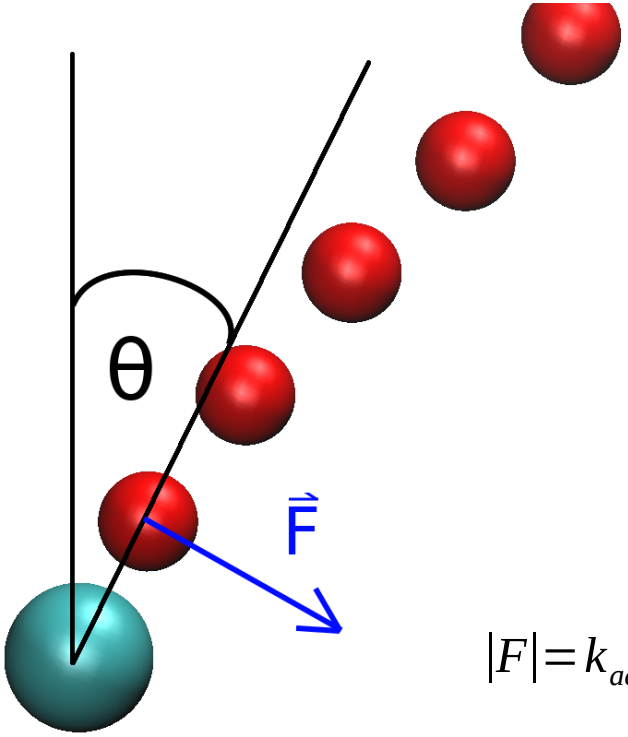
Wall – Particles Interaction:

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

Activation Model

2D Model

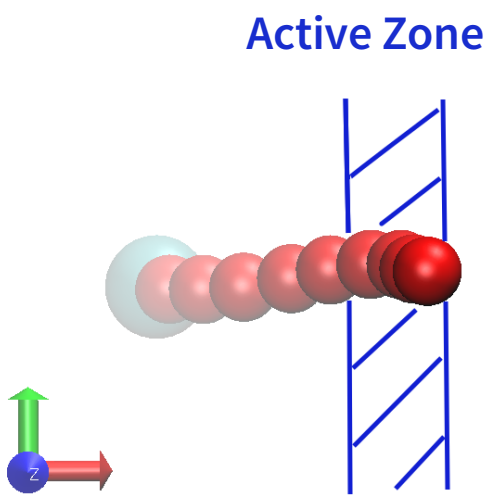


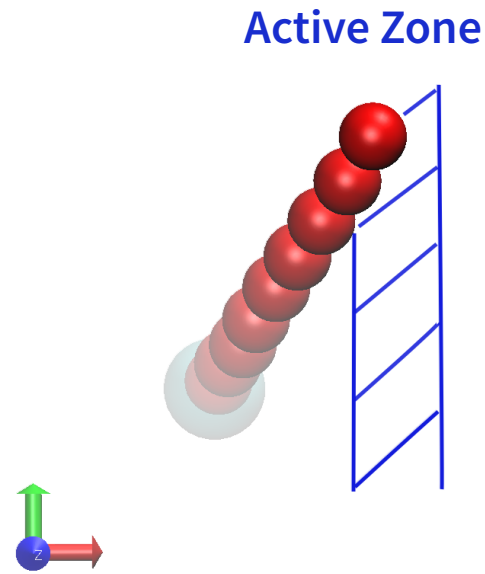


$$|F| = k_{act}\,\theta$$

Activation Model

Straightforward 3D Model



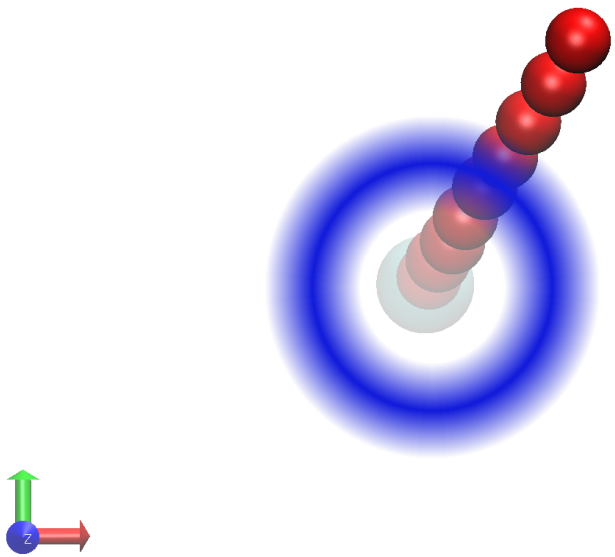


At different oscillation angles, the time spent in the Active Zone differs → Oscillation frequency varies

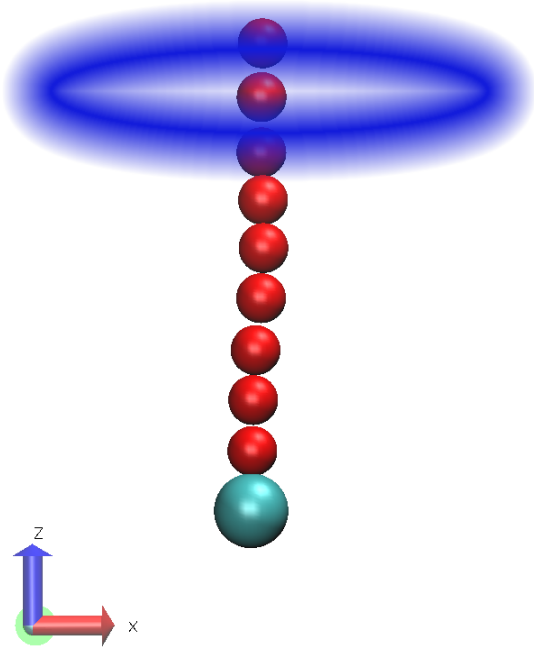
Activation Model

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

Speedup:

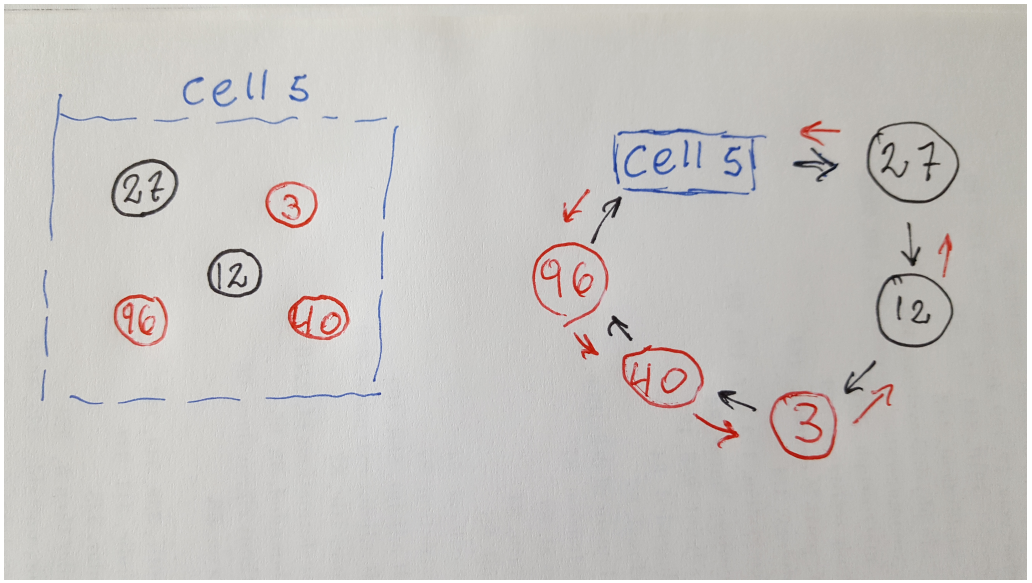
x6 with RESPA

x14 with RESPA + OpenMP

```
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
            *dt2_short*FX_short(i)
Y(i) = Y(i) + dt_short*VY(i) + 0.5
            *dt2_short*FY_short(i)
Z(i) = Z(i) + dt_short*VZ(i) + 0.5
            *dt2_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
```

Ordered cell linked list

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



r_neigh(27) = 12

r_neigh(3) = 40

l_neigh(3) = 12

l_neigh(96) = 40

head(5) = 27

tail(5) = 96

GPU acceleration

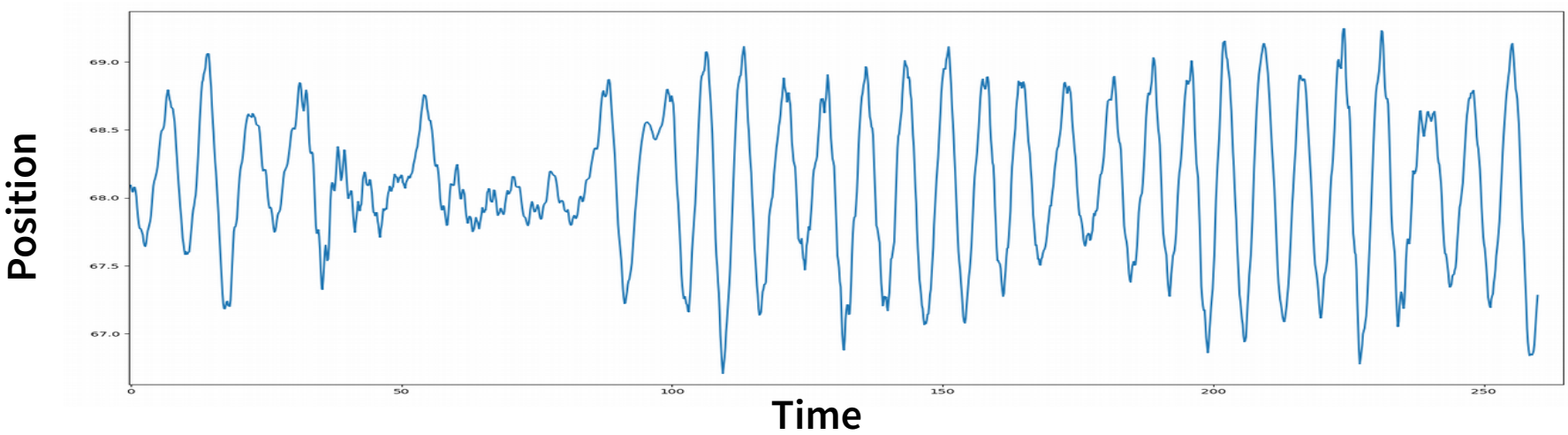
OpenAcc parallelization was attempted, but unsuccessful due to time constrains.

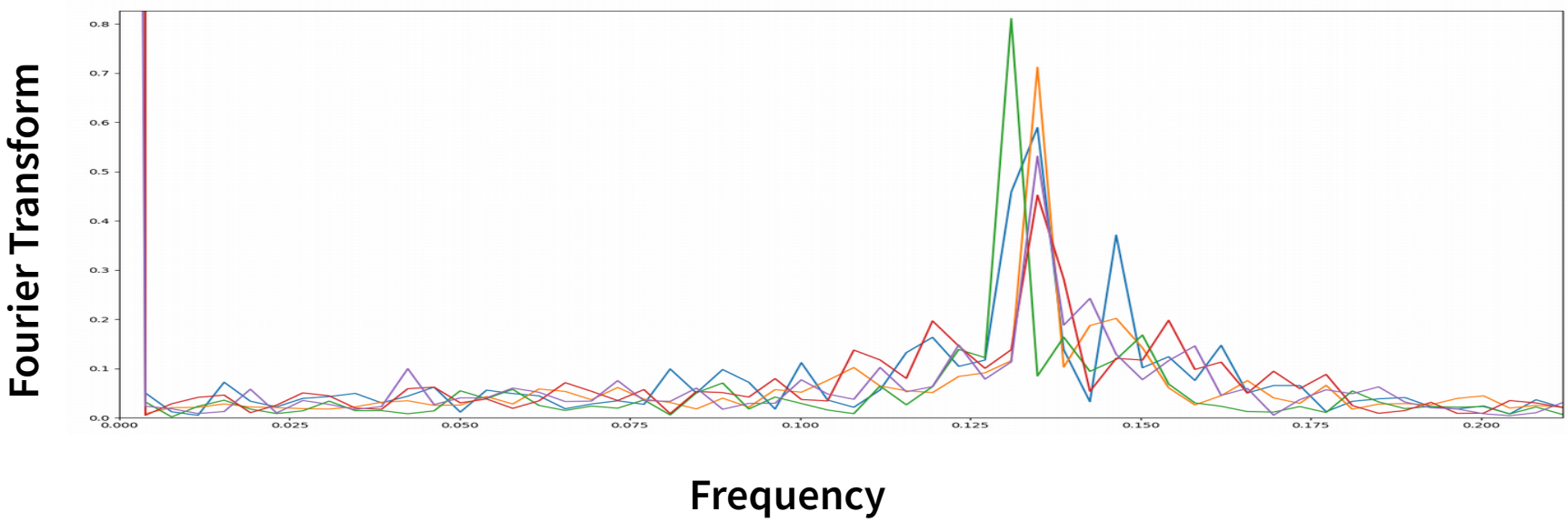
Data transfer between host and device is time-wise expensive.

Routines called often should be parallelized.

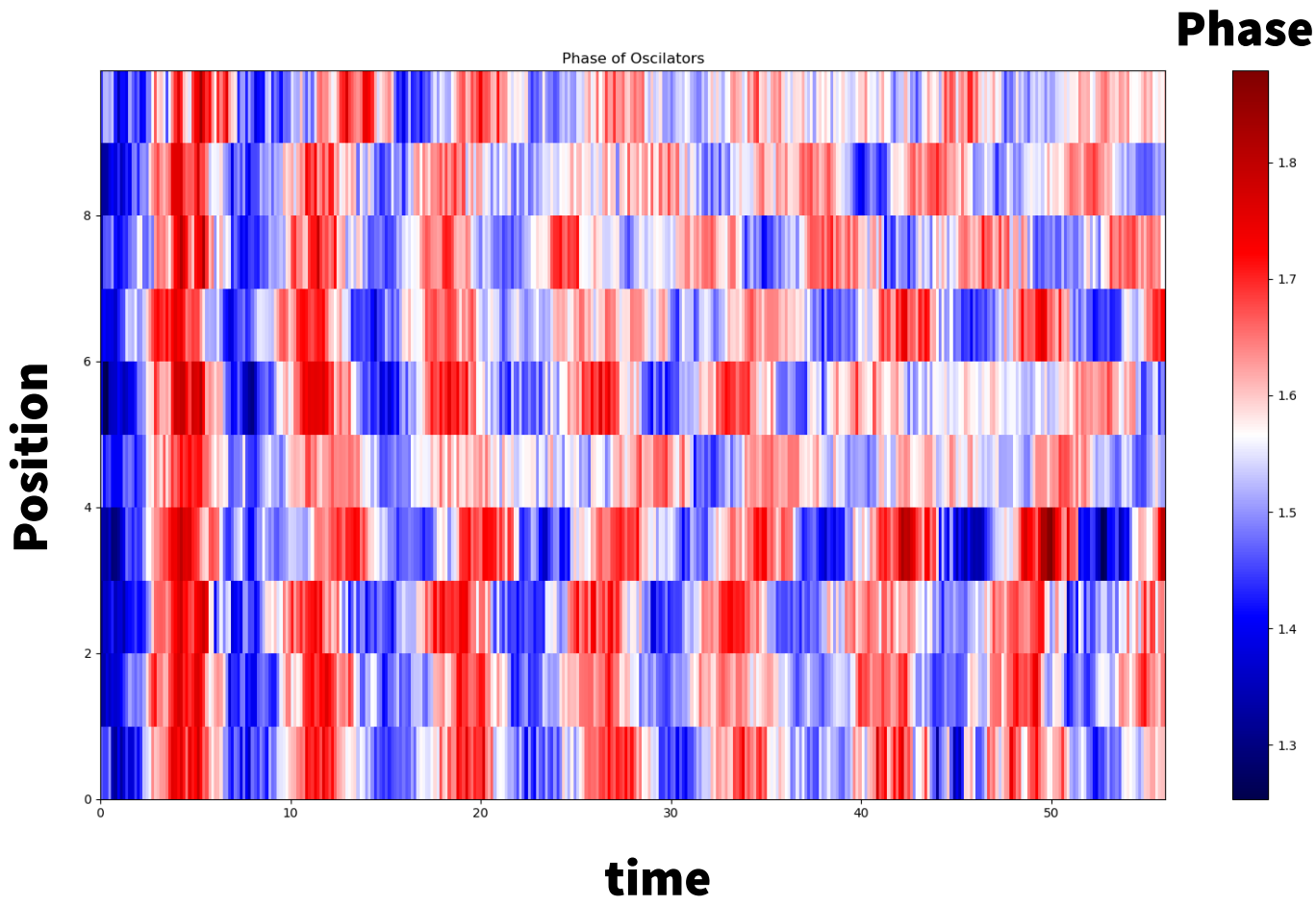
Cell linked list algorithm is not trivial to parallelize.

Results: Single Chain Dynamics





Results: Phase Field Dynamics



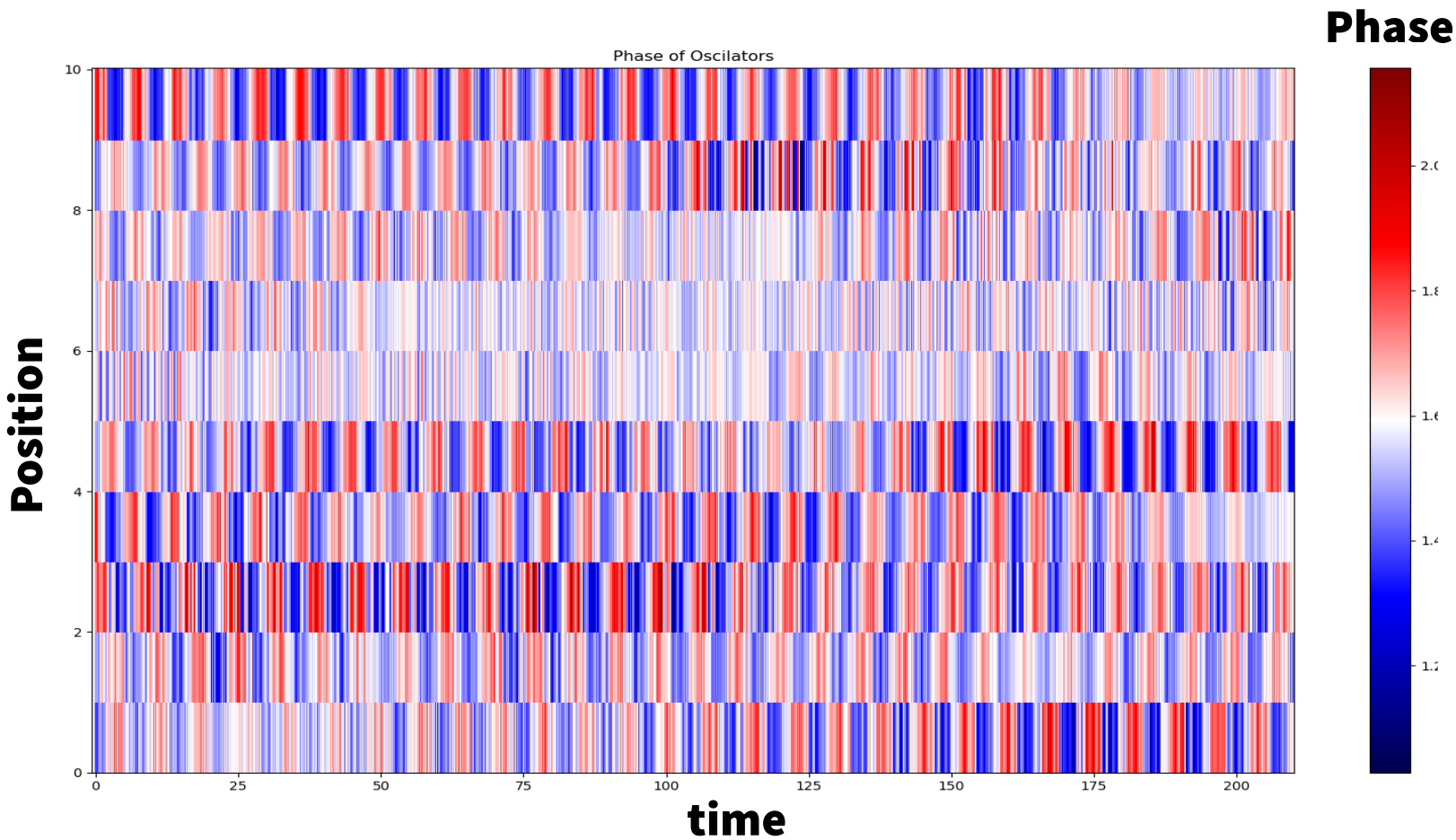
Parameters

$a_{sb} = 0.4\ k_B T$

$a_{ss} = 0.04\ k_B T$

$\gamma = 0.03$

Results: Phase Field Dynamics



Parameters

$a_{sb} = 1\ k_B T$

$a_{ss} = 0.04\ k_B T$

$\gamma = 0.005$

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

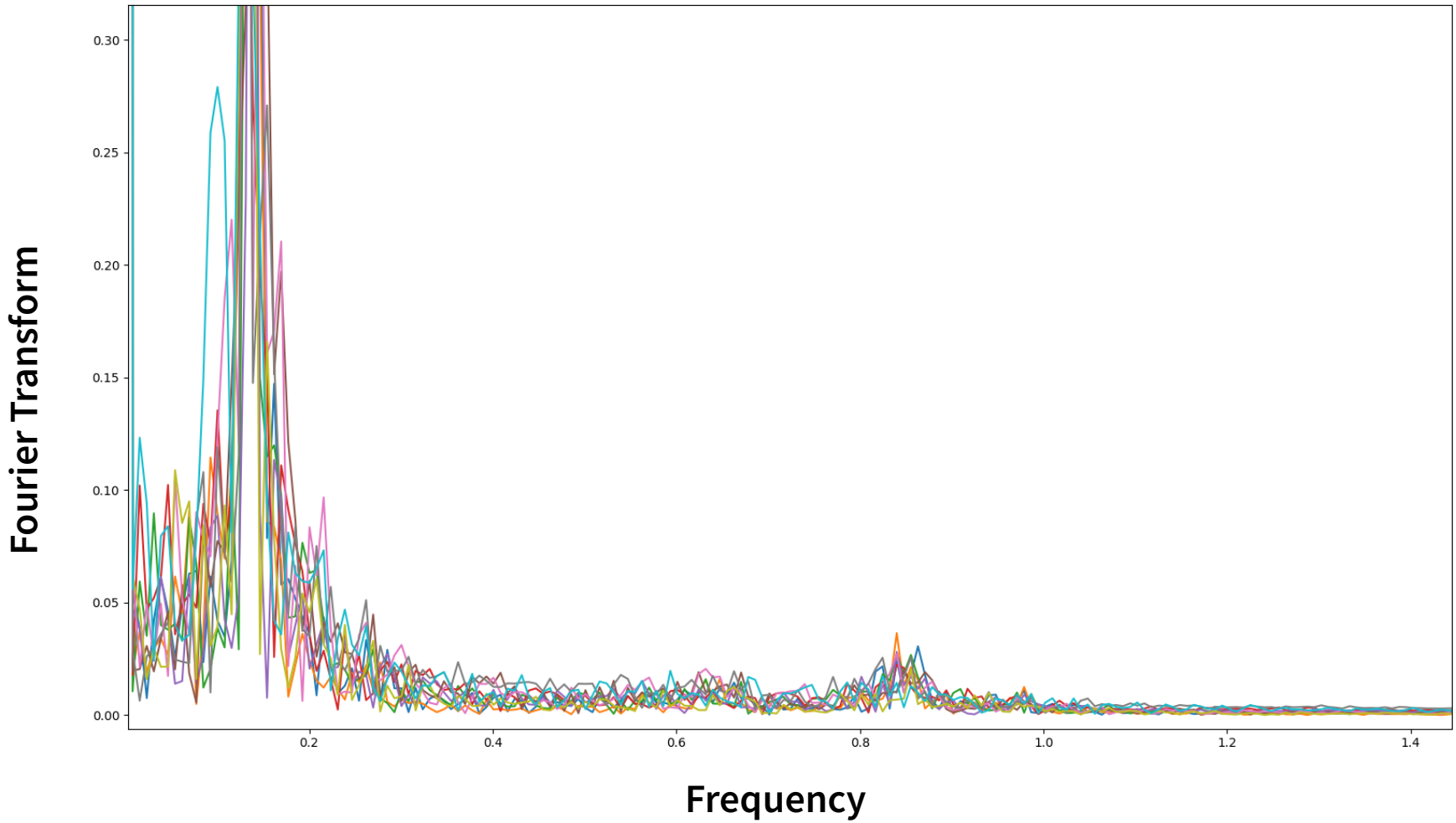
Higher k_{act} → more power pumped into the system → higher friction coefficient (& lower time step) → loss of phase coherence

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

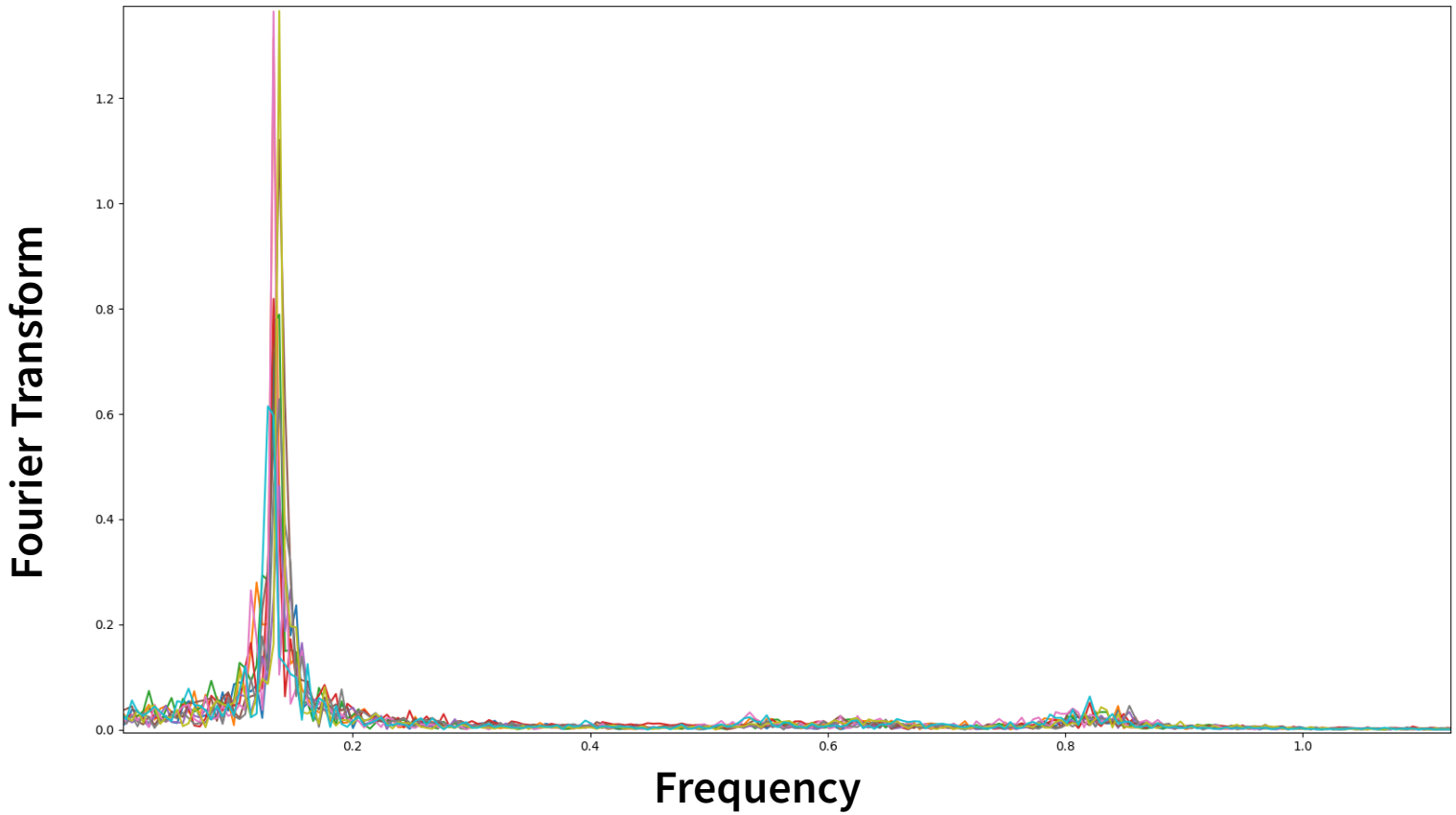
End

Thank you for your hospitality!

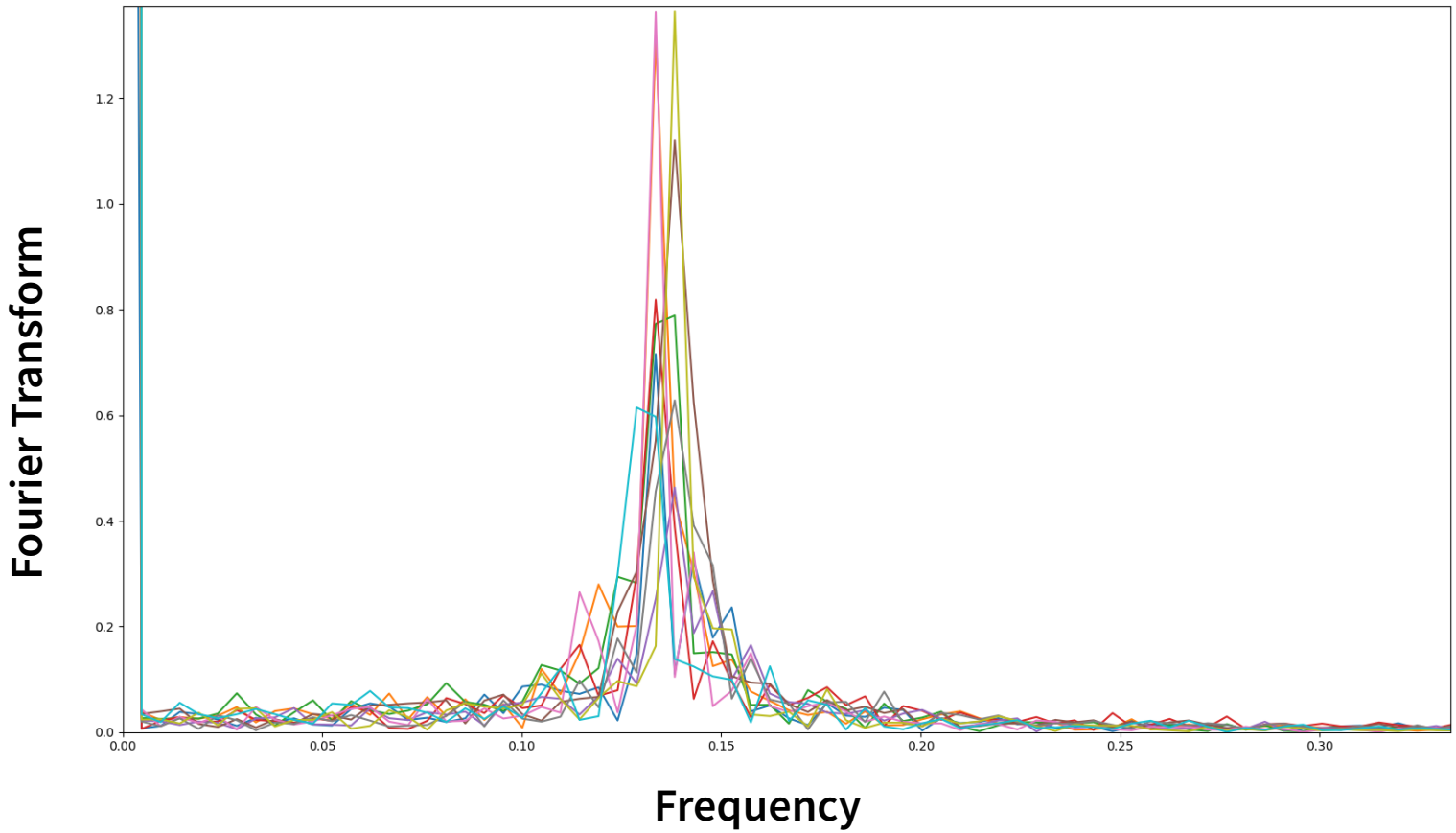
Higher Modes FFT



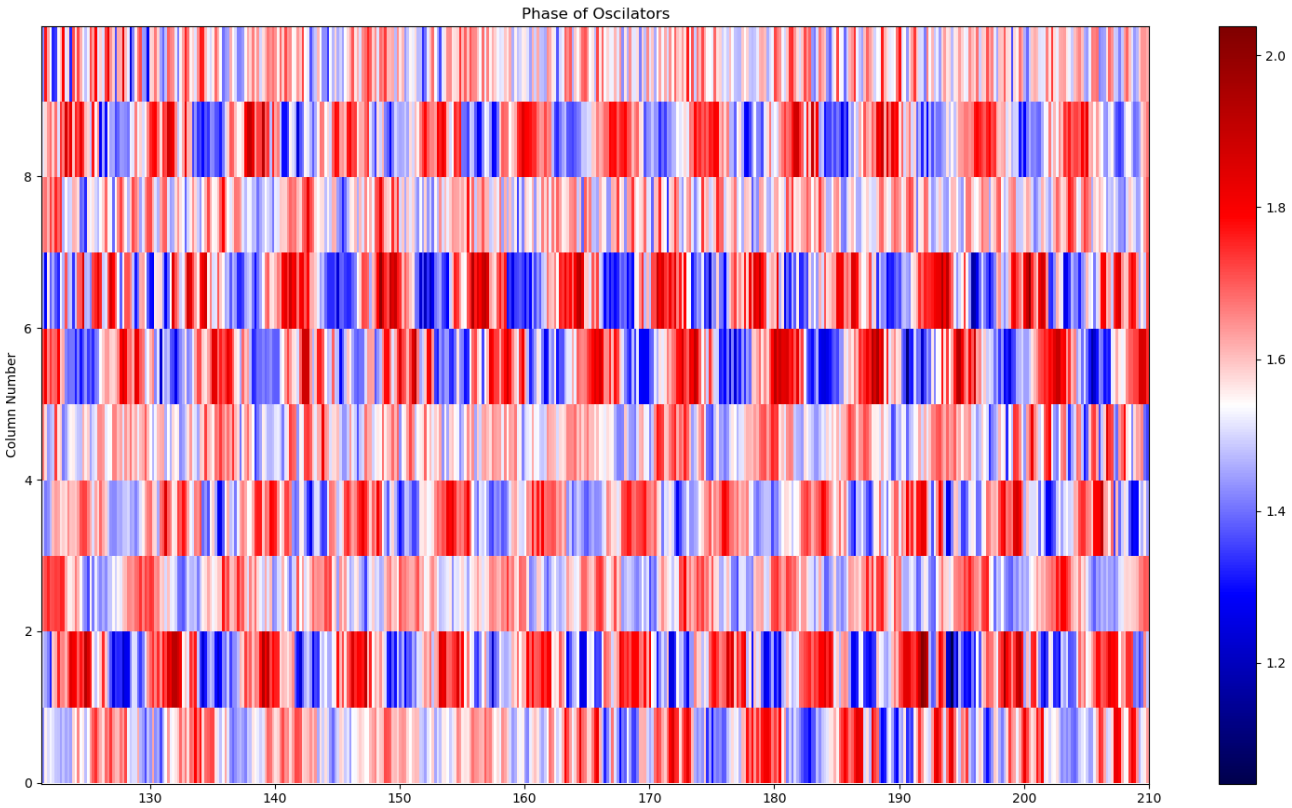
Higher Modes FFT



FFT


Fourier Transform
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Frequency

Kimogram



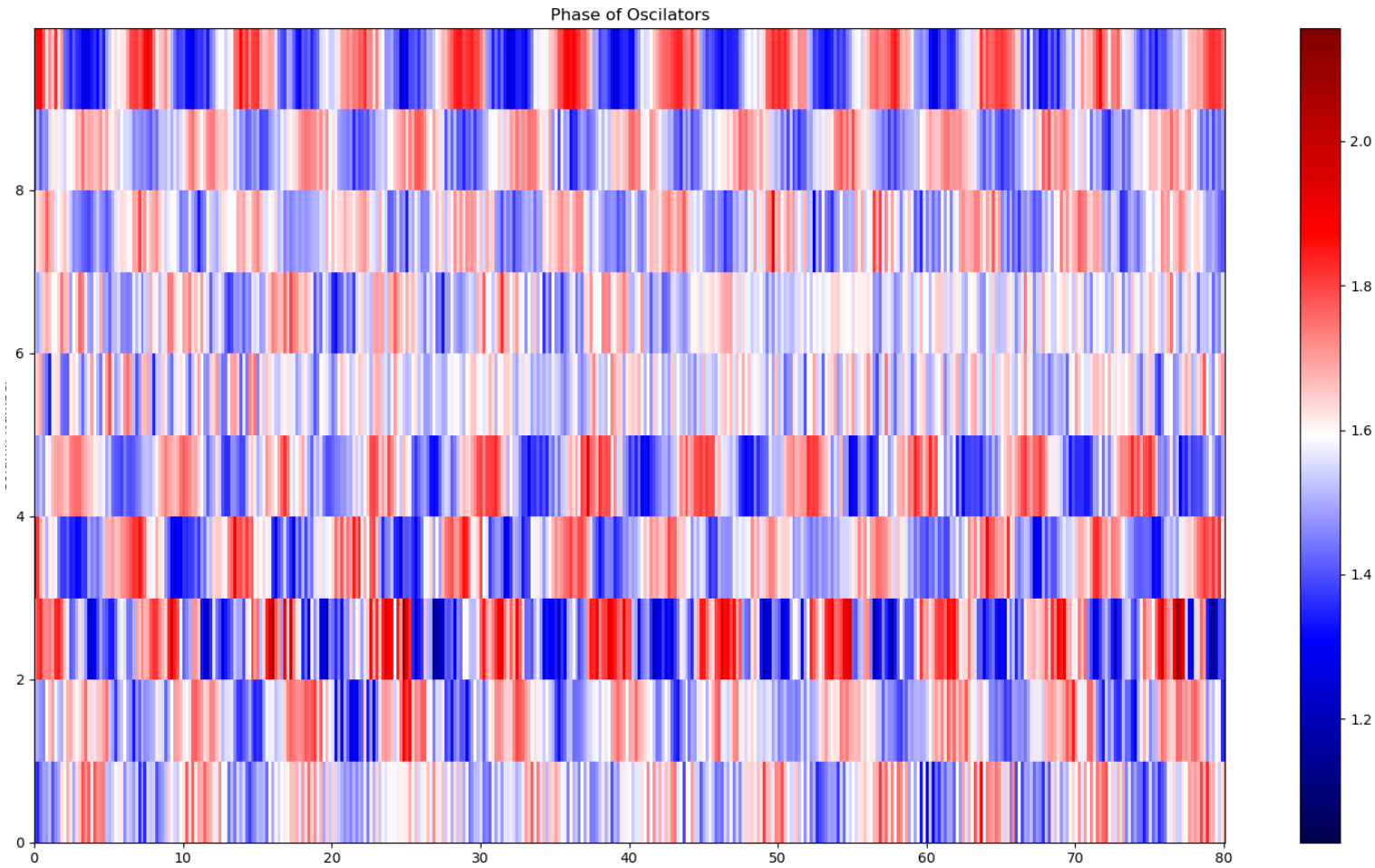
Parameters

$a_{sb} = 1\ k_B T$

$a_{ss} = 0.04\ k_B T$

$\gamma = 0.005$

Kimogram



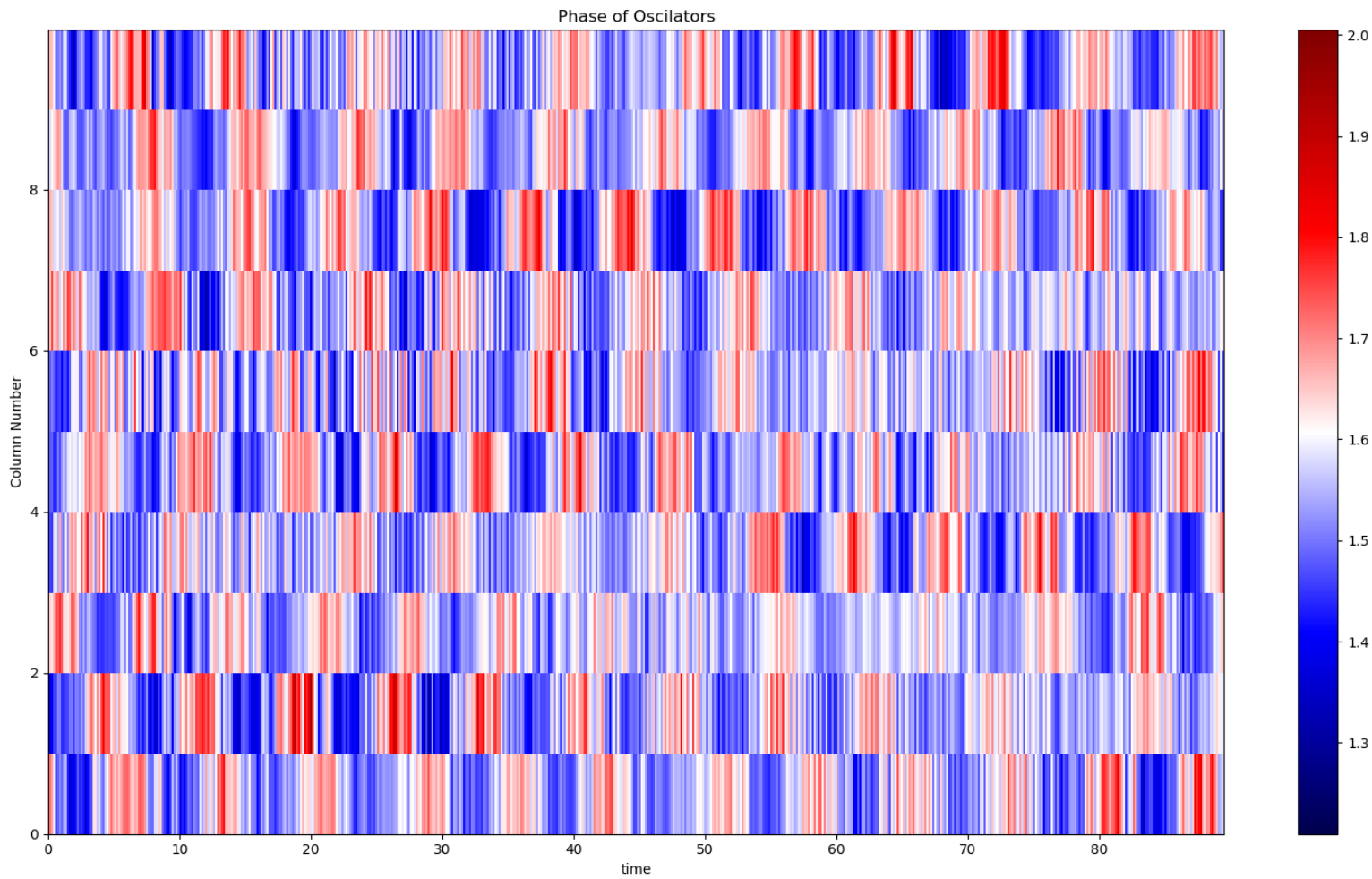
Parameters

$a_{sb} = 1\ k_B T$

$a_{ss} = 0.04\ k_B T$

$\gamma = 0.005$

Kimogram 2D Model



Parameters

$A_{sb} = 1.3\ k_B T$

$a_{ss} = 0.4\ k_B T$

$\gamma = 0.01$