Dynamics of Chromosome Movements During Meiosis in Fission Yeast

--- Simulation using bead-rod model

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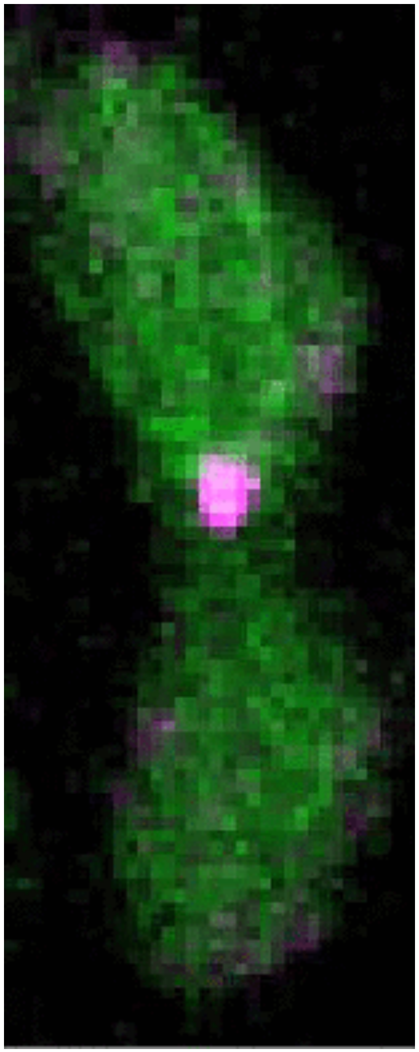
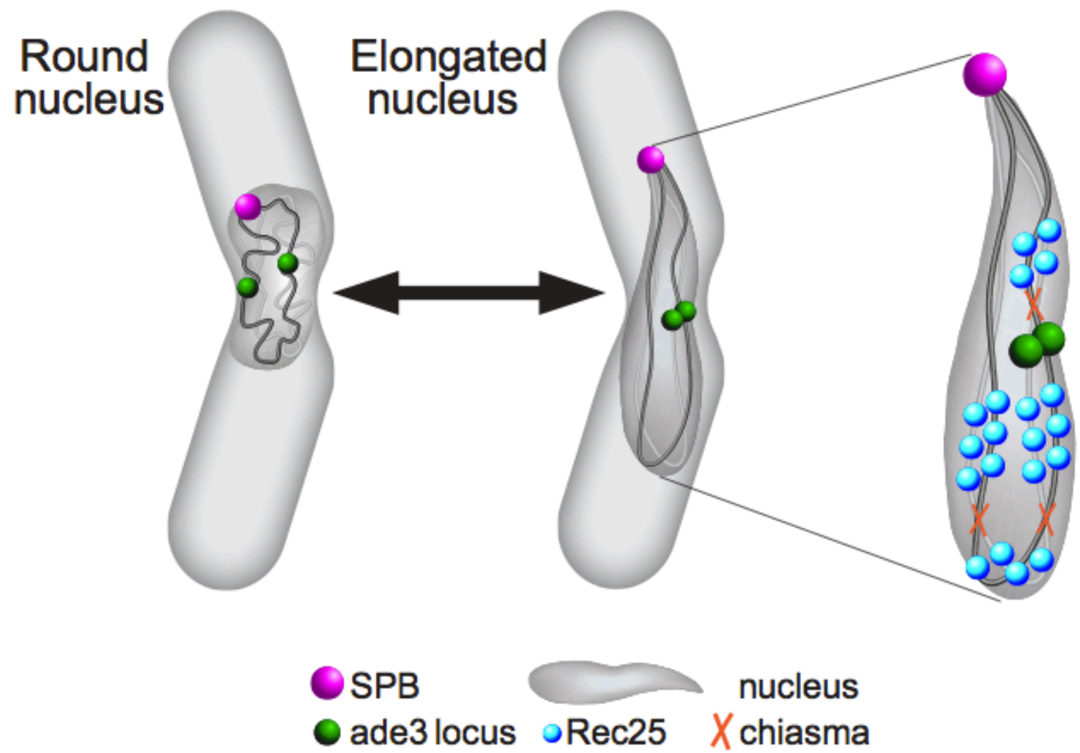
Outline

- Background
- Bead-rod model
  (dynamical equations, numerical scheme, parameters)
- Simulation Result
  (animation movie, compare with theory)
- Discussion

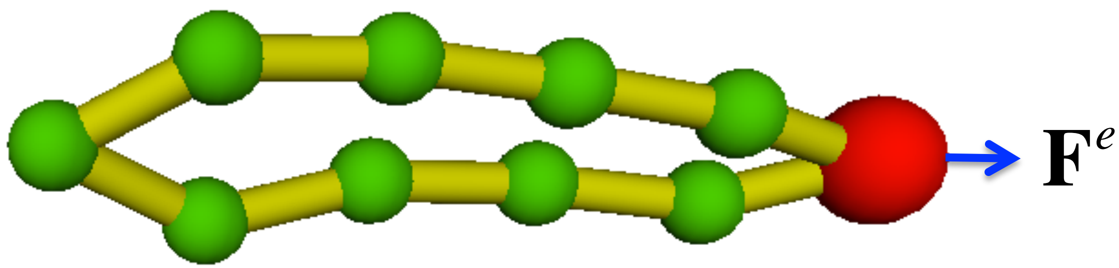
Nuclear Oscillation





Nuclear oscillation

Bead-Rod Ring Model



- Bead:
  position ---- $\mathbf{r}_i$

- Rod:
  length --- a

Ring driven by a periodic force

Brownian Dynamics:

Inertia-less assumption $\mathbf{F}_i = \mathbf{0}$

$$\mathbf{F}_i = \mathbf{F}_i^h + \mathbf{F}_i^\phi + \mathbf{F}_i^c + \mathbf{F}_i^b + \mathbf{F}_i^e$$

i is the index of bead

$\mathbf{F}_i^h$ is hydrodynamic force

$\mathbf{F}_i^\phi$ represents force generate from potential

$\mathbf{F}_i^c$ is constraint force to keep the rod length

$\mathbf{F}_i^b$ is brownian force

$\mathbf{F}_i^e$ is external force

Brownian Dynamics:

$$\mathbf{F}_i = \mathbf{F}_i^h + \mathbf{F}_i^\phi + \mathbf{F}_i^c + \mathbf{F}_i^b + \mathbf{F}_i^e = \mathbf{0}$$

$$\mathbf{F}_i^h = -\zeta \dot{\mathbf{r}}_i$$

$$\mathbf{F}_i^\phi = -\nabla U(\mathbf{r})$$

$$\mathbf{F}_i^c = T_i \mathbf{u}_i - T_{i-1}\mathbf{u}_{i-1}; \mathbf{u}_i = (\mathbf{r}_{i+1} - \mathbf{r}_i)/a$$

$$\left\langle \mathbf{F}_i^b(t) \right\rangle = \mathbf{0}; \left\langle \mathbf{F}_i^b(t)\mathbf{F}_j^b(t+\Delta t) \right\rangle = 2k_B T \zeta \delta_{ij} \delta(\Delta t)$$

$$\mathbf{F}_i^e = f(\mathbf{r}_i, t)$$

- Dynamical differential equation:

$$\frac{d\mathbf{r}_i}{dt} = \zeta^{-1}(\mathbf{F}_i^\phi + \mathbf{F}_i^c + \mathbf{F}_i^b + \mathbf{F}_i^e)$$

Numerical Scheme

- Predictor-corrector algorithm:

Step 1: predict using known forces

$$\mathbf{r}_i^*(t+\Delta t) = \mathbf{r}_i(t) + \zeta^{-1}(\mathbf{F}_i^h + \mathbf{F}_i^\phi + \mathbf{F}_i^b + \mathbf{F}_i^e)\Delta t$$

Step 2: correct using constraint force

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i^*(t+\Delta t) + \zeta^{-1}\mathbf{F}_i^c\Delta t \qquad (*)$$

Step 3: substitute eq. (*) to constraint equations

$$(\mathbf{r}_{i+1} - \mathbf{r}_i)^2 - a^2 = 0$$

Solve a set of nonlinear algebraic equations $\Rightarrow$ $\mathbf{F}_i^c$

Step 4: re-substitute $\mathbf{F}_i^c$ to (*) obtain the final $\mathbf{r}_i(t+\Delta t)$

Parameter Estimation

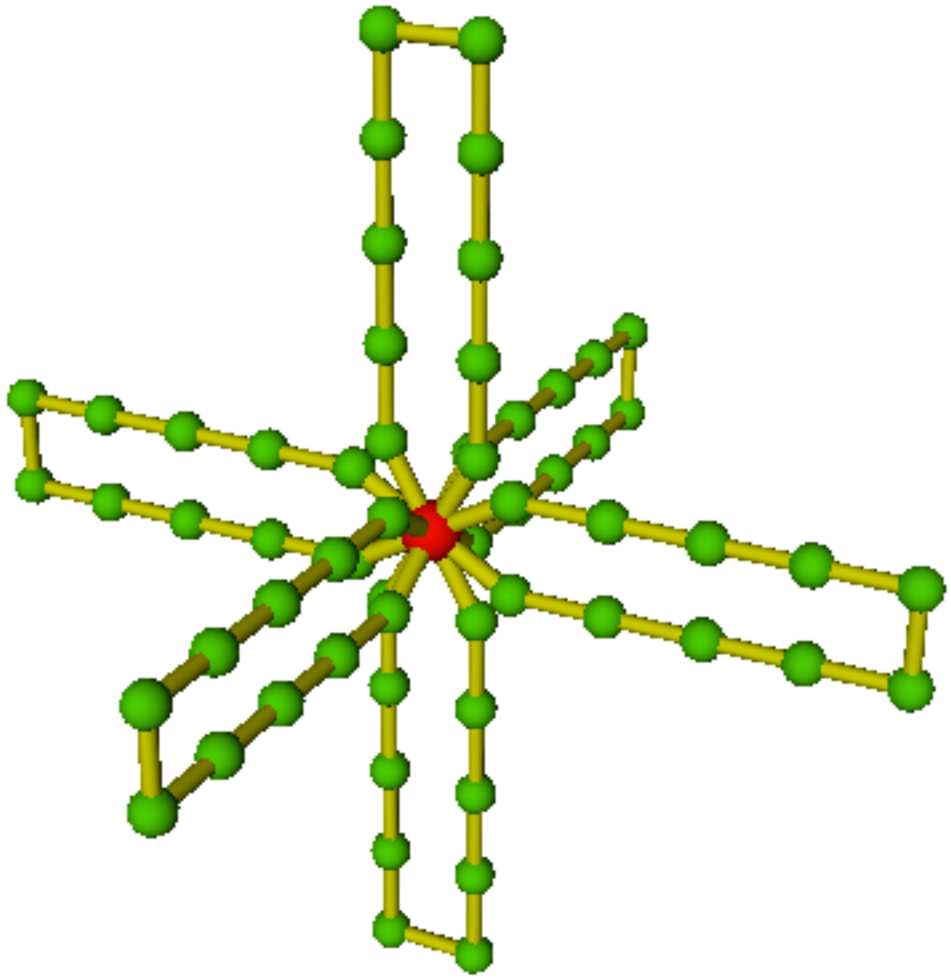
- Length of Chromosomes in base pairs:
  Chromosome I: 5.579.133 bp ~ 5,6Mbp
  Chromosome II: 4.539.804 bp ~ 4,5Mbp
  Chromosome III: 2.452.833 bp ~ 2,5Mbp

- Compaction ratio of chromosomes: ~ 100bp/nm

- Kuhn length: ~ 100nm

- System size for 3 pairs of chromosomes: ~ 2000-3000
  monomers in one ring : 200 ~ 600

Initial configuration

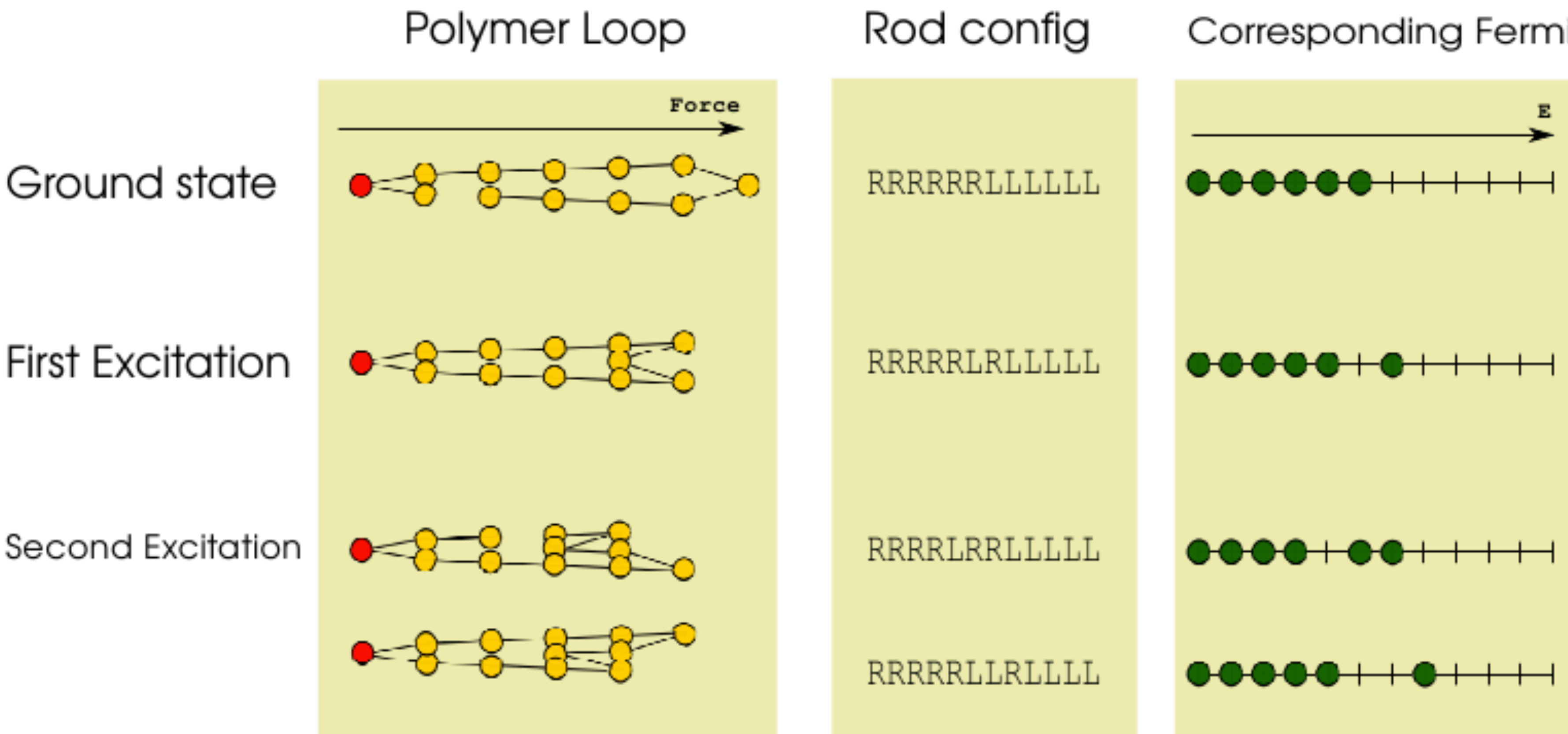


Animation Movie

Theoretical Stories (Yen Ting Lin)

The Hamiltonian of the system: $$H = E_0 + 2m\Phi\delta \sum_{j=1}^{N} j\, Z_j$$

Equivalent to N/2 Fermions in N energy levels



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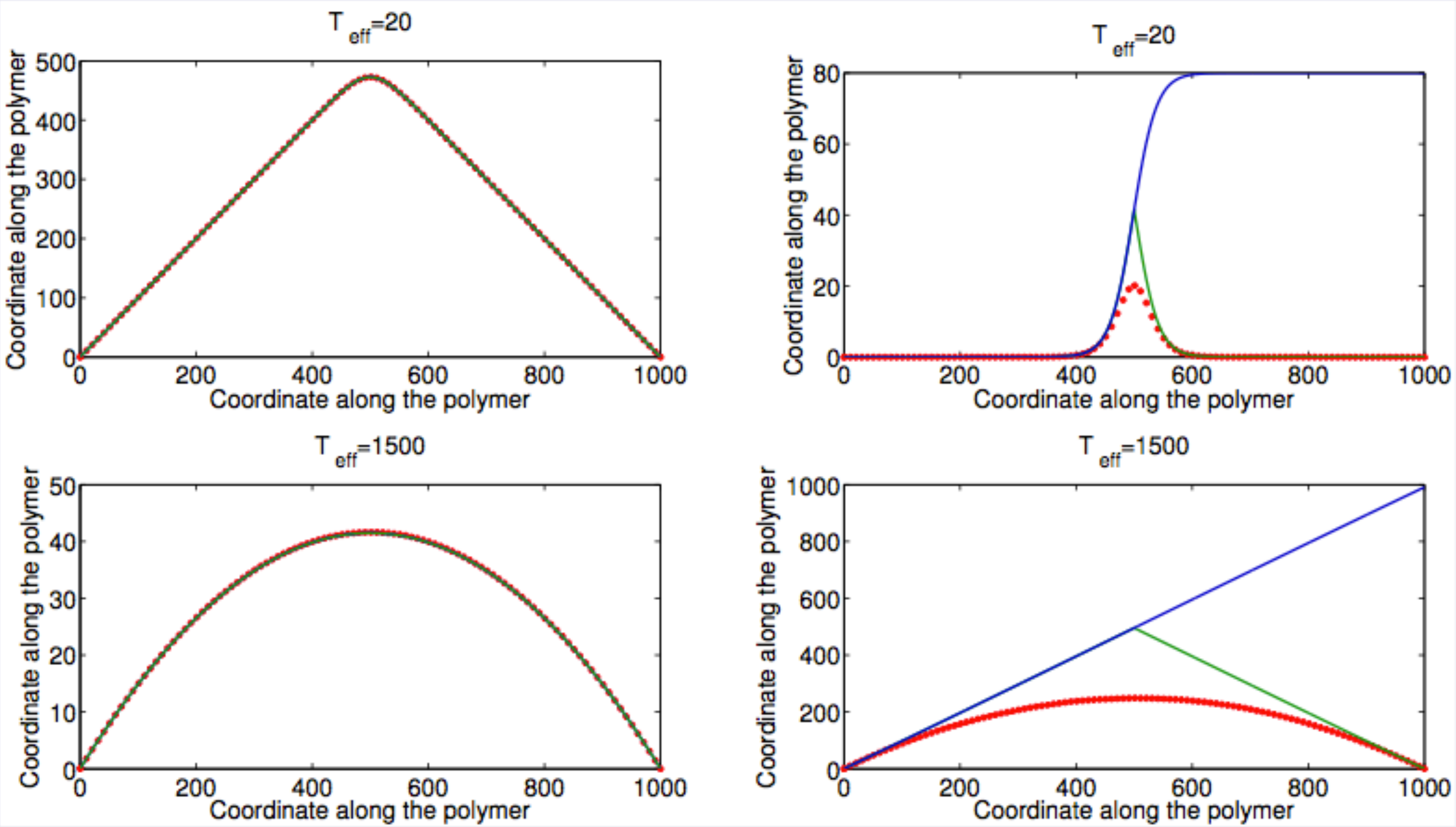
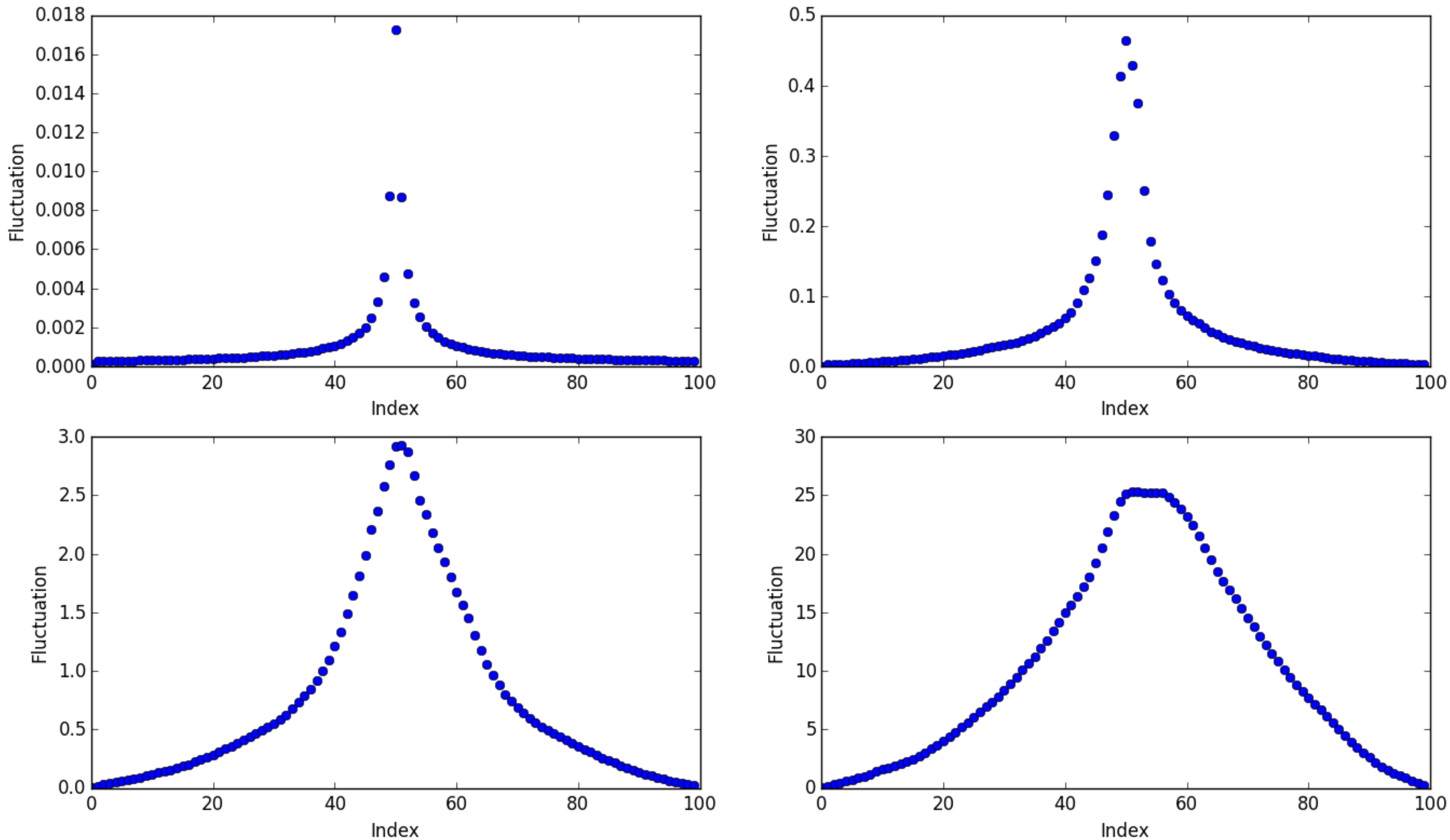


Numerical comparison

With Lennard-Jones potential



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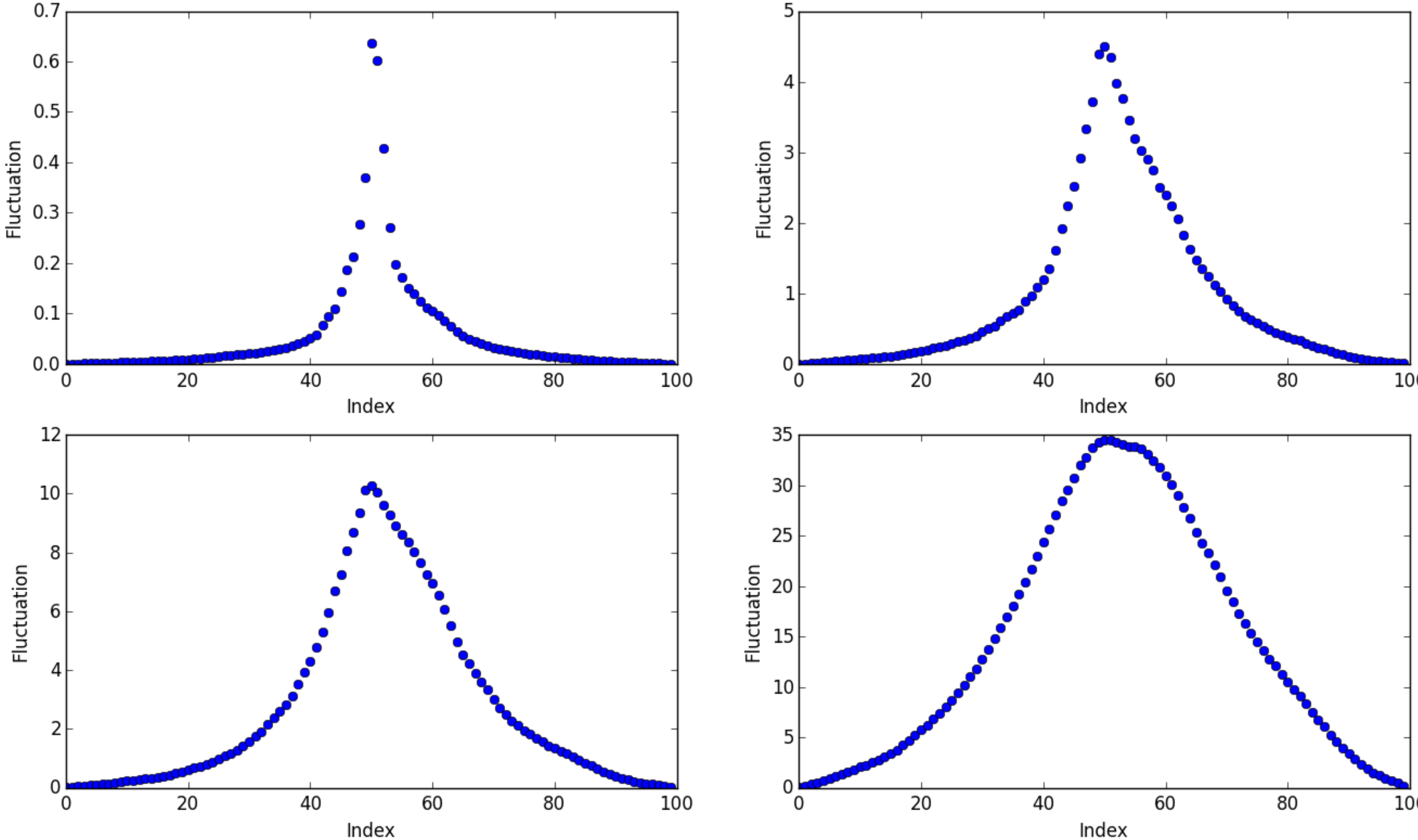
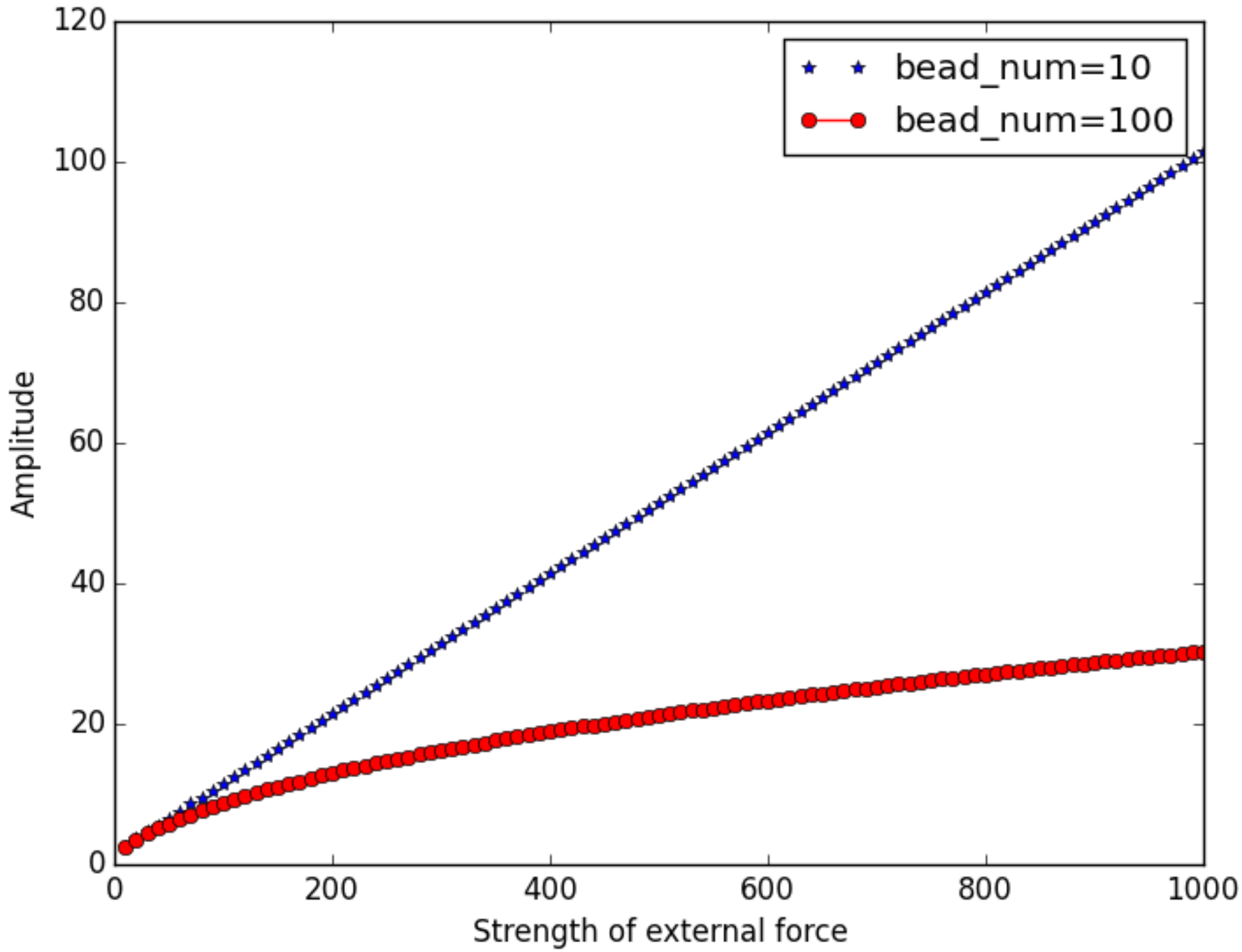


Driven Force & Oscillation Amplitude



Thank you!