Mesoscopic simulations of anisotropic chemically-powered nanomotors

Pierre de Buyl

Instituut voor Theoretische Fysica, KU Leuven

Stuttgart - Institute for Computational Physics - 24 june 2019

0000-0002-6640-6463
@pdebuyl
`http://pdebuyl.be/`

Acknowledgments

Nanomotor and enzyme modeling

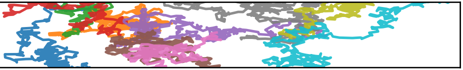
- Raymond Kapral (University of Toronto)

Funding

- Fonds Wetenschappelijk Onderzoek – Vlaanderen

About the slides

- The slides are downloadable `http://pdebuyl.be/`
- You can click on the references to go the bibliography.
- There, you can click on the doi to go to the article.



Introduction

What are nanomotors?

- 9mm disks Ismagilov *et al* (2002)
- Bimetalic nanorods Paxton *et al* (2004)
- Janus particles Howse *et al* (2007)
- Janus particles Ke *et al* (2010)
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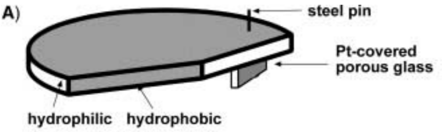

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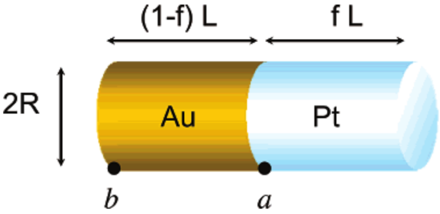

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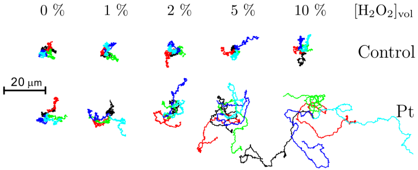

FIG. 1 (color online). Trajectories over 25 sec for ×5 particles of the control (blank) and platinum-coated particles in water and varying solutions of hydrogen peroxide.

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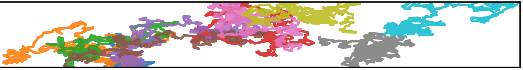

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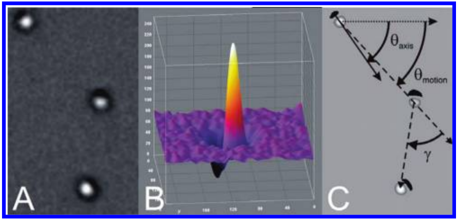

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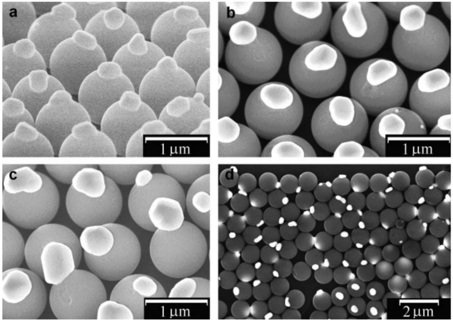
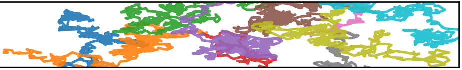


Circle swimmers



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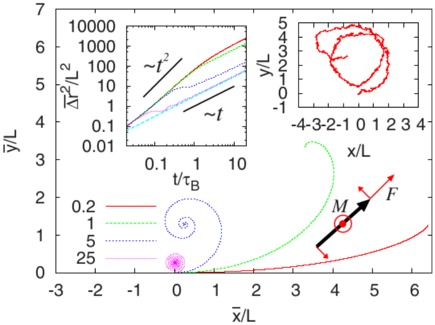

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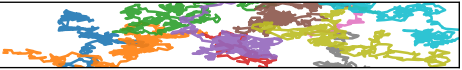

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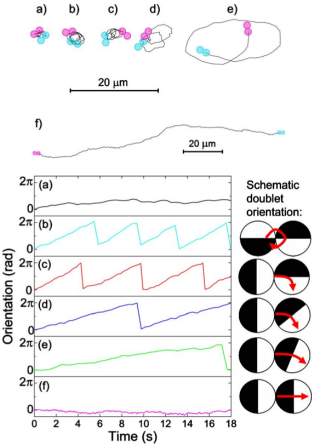

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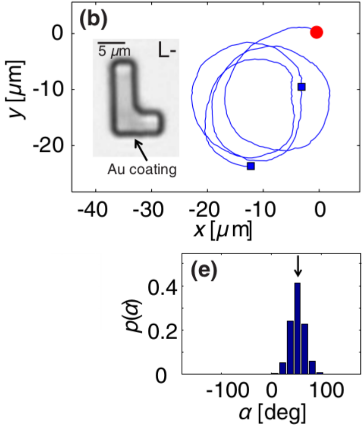

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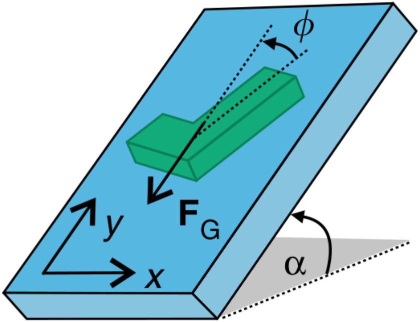

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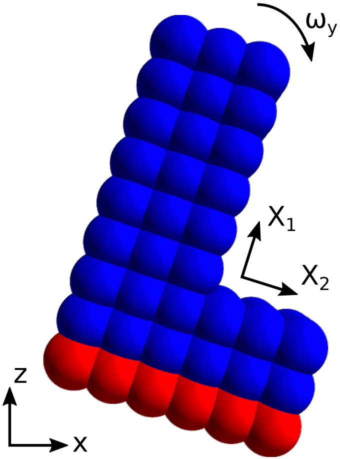
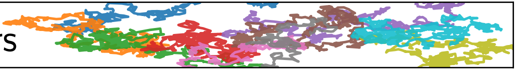


Perspectives for nanomotors



Applications

- Biotechnology
- Chemical processes
- New phases of matter

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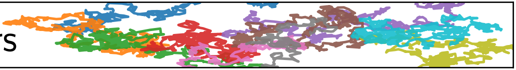

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Statistical Physics

- “Ideal” nonequilibrium device

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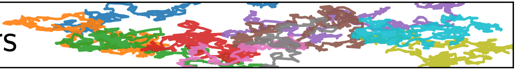


Applications

- Biotechnology
- Chemical processes
- New phases of matter

Statistical Physics

- “Ideal” nonequilibrium device

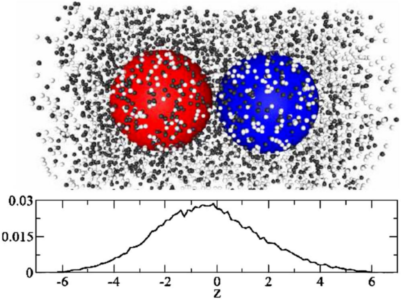
Reviews

- Wang (2013): general review (book)
- Kapral (2013): phoretic propulsion and applications of nanomotors
- Ebbens (2016): the special role of *chemical* nanomotors

Simulations of nanomotors

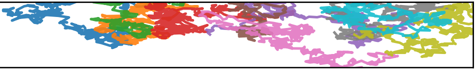
Methods

- Molecular Dynamics
- The solvent is coarse-grained using “Multiparticle Collision Dynamics”.
    - Thermal fluctuations
    - Hydrodynamics
    - Conservation of energy and momentum
- Chemical kinetics



From Rückner and Kapral (2007)

How do nanomotors move?



Phoretic theory

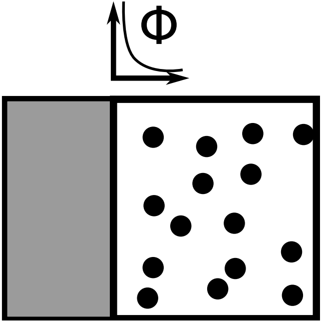
- Stokes equation in the boundary layer returns the slip velocity

$$v^s(\vec{r}) = -\frac{k_B T}{\eta} \Lambda \nabla c(\vec{r})$$

$$\Lambda = \int_0^\infty r[e^{-\Phi(r)/k_B T} - 1] dr$$

- Potential

$$V(r) = \epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \frac{1}{4} \right)$$



References

- Anderson (1989); Brady (2011); Kapral (2013)

RMPCDMD

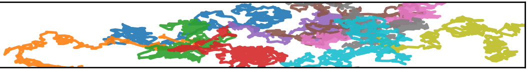
RMPCDMD

Core features

- MPCD fluid particles with optional Andersen thermostat.
- Walls with reflective or bounce-back collisions.
- Molecular dynamics for spheres, dimers, and bead assemblies.
- Chemistry for the fluid.

Development

- Open-source: BSD 3-clause
- Fortran 2008, OpenMP
- `https://github.com/pdebuyl-lab/RMPCDMD`
- `http://lab.pdebuyl.be/rmpcdmd/`

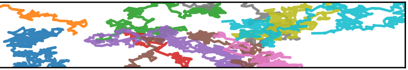


Trajectory data

- HDF5 trajectory files: `http://nongnu.org/h5md/`
- Contains named data. Sample:

```
particles
 \-- <group1>
      \-- box
      \-- (position)
      |    \-- step: Integer[variable]
      |    \-- time: Float[variable]
      |    \-- value: <type>[variable][N][D]
      \-- (image)
      |    \-- step: Integer[variable]
      |    \-- time: Float[variable]
      |    \-- value: <type>[variable][N][D]
      \-- (species: Enumeration[N])
      \-- ...
```

RMPCDMD usage: chemotaxis



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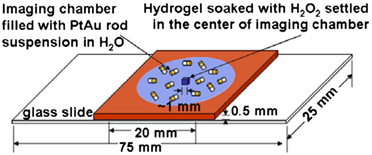
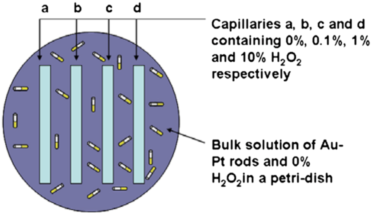
(a)



(b)



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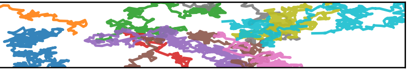

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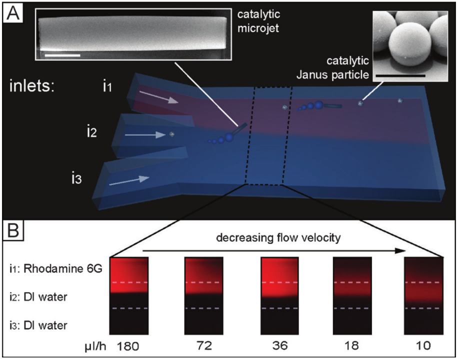

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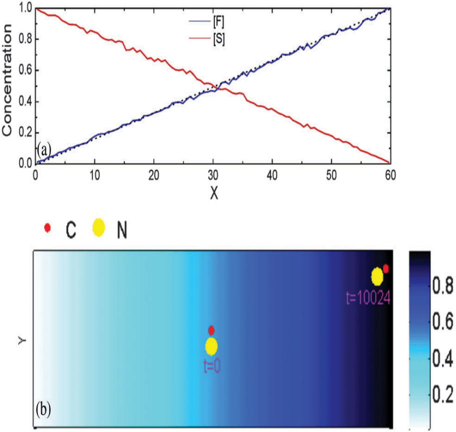

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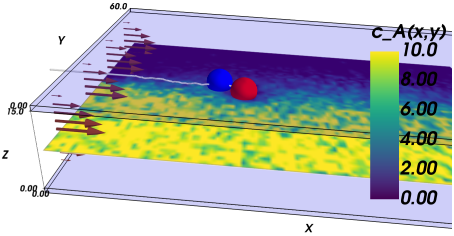
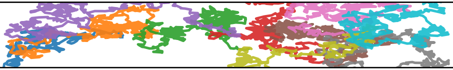


Mesoscopic simulations of L particles

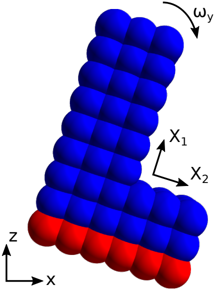
Anisotropic nanomotors



Stochastic model

$$\begin{pmatrix} \dot{X}_1 \\ \dot{X}_2 \\ \dot{X}_3 \equiv \theta \end{pmatrix} = \sqrt{2D^L}\zeta + \beta D^L F \ ,$$

- D^L is the diffusion matrix
- ζ is a vector white noise
- F is an external force



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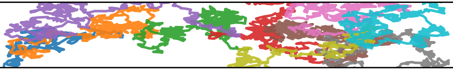

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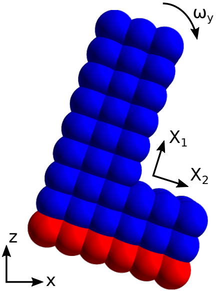


Hydrodynamics [Happel and Brenner (1983)]

1. Flow-induced self-propulsion
2. Hydrodynamic friction on all coupled degrees of freedom
3. (Also a direct torque)

Cross displacements

Definition

- As in Kraft *et al* (2013):

$$C_{ij}(\tau) = \langle (X_i(\tau) - X_i(0))\,(X_j(\tau) - X_j(0)) \rangle$$

Cross displacements

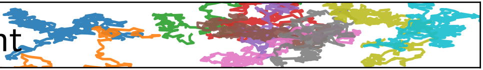
Definition

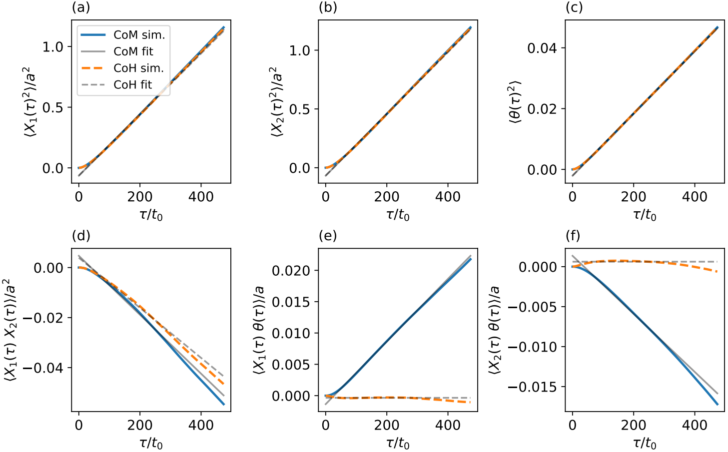
- As in Kraft *et al* (2013):

$$C_{ij}(\tau) = \langle (X_i(\tau) - X_i(0))\,(X_j(\tau) - X_j(0)) \rangle$$

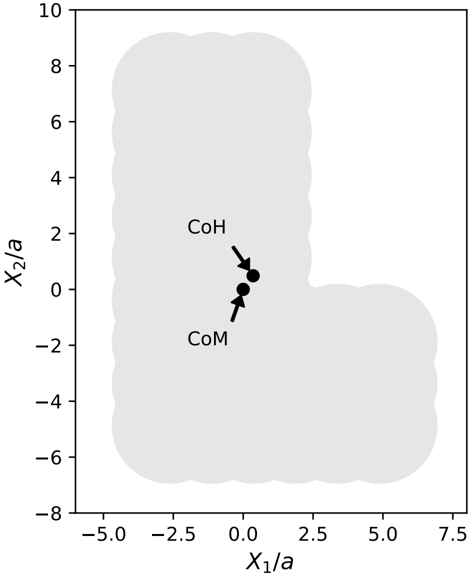
- The diagonal entries are the mean-square displacement.

Equilibrium cross-displacement

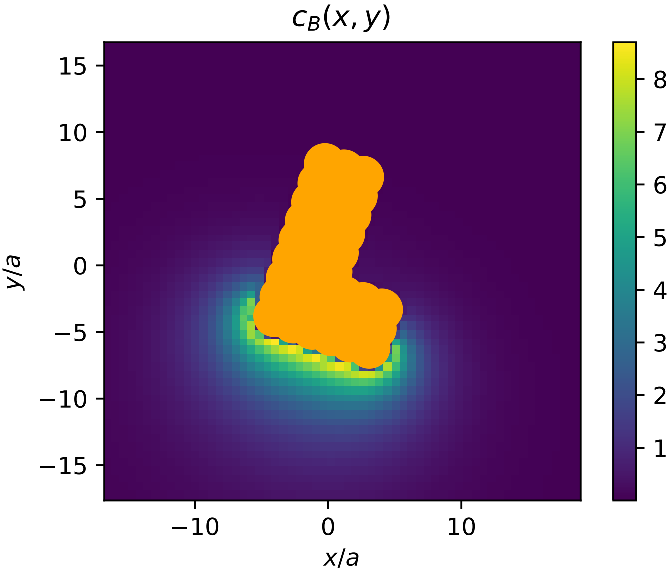




Center of hydrodynamics



Anisotropic nanomotors



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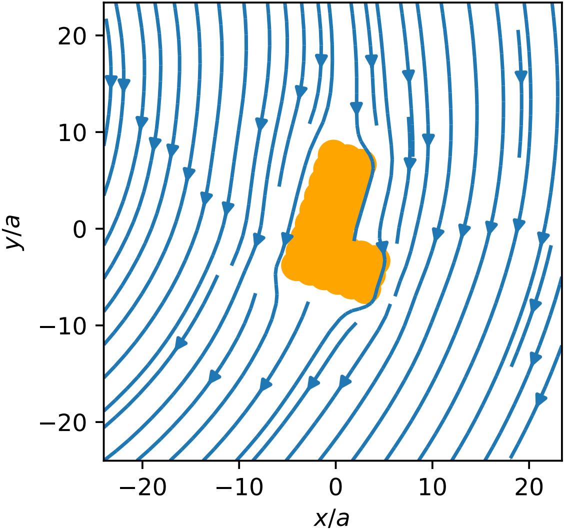

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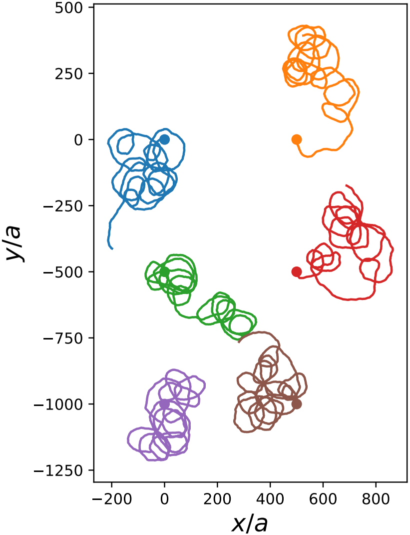

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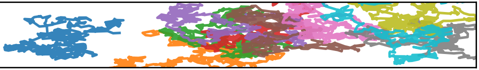


Average velocity

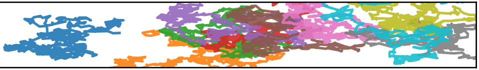
- $$\begin{pmatrix} \dot{X}_1 \\ \dot{X}_2 \\ \dot{X}_3 \equiv \dot{\theta} \end{pmatrix} = \beta D^{L@CoH} F$$

  where F is the vector force in X_1, X_2 and θ
- Radius from equilibrium $D^{L@CoH}$

  $$R = \frac{\sqrt{\dot{X}_1^2 + \dot{X}_2^2}}{\dot{X}_3} \approx 33$$
- Radius from simulations

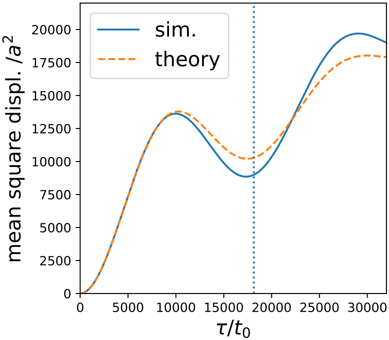
  $$R \approx 56$$

Anisotropic nanomotors



Mean-square displacement

- Numerical data from the simulations
- Theory from Brownian model Ebbens *et al* (2010) with simulated value for velocity and angular velocity.



Fast Correlation Algorithm

Fast Correlation Algorithm (FCA)

How to compute efficiently correlation functions?

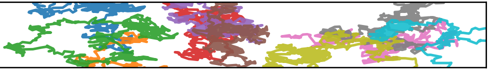
- Compute correlations with the convolution theorem.
- Same value as direct computation (up to rounding errors).
- Benefit: Fast Fourier Transforms require $O(N \log N)$ [vs $O(N^2)$ for direct comput.]
- Allen & Tildesley already use the FCA. Python implementation in nmoldyn.
- No standalone FCA code for easy reuse.

tidynamics

A solution

- Python package for the Fast Correlation Algorithm: tidynamics
- Published in the Journal of Open Source Software (JOSS) doi:10.21105/joss.00877
- Define the correlation functions as in the fields of stochastic and molecular dynamics.
- Handles data in NumPy arrays.

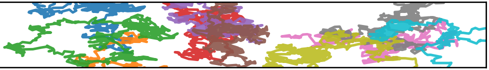
tidynamics



Installation

-
  ```
  pip install --user tidynamics
  ```
- Requires NumPy

tidynamics



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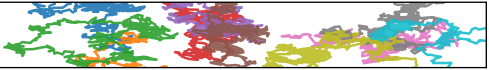
Usage

- `tidynamics.acf(velocity)`
- `tidynamics.msd(position)`

tidynamics



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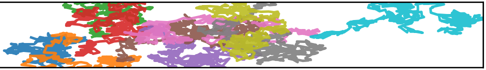
Documentation

- `http://lab.pdebuyl.be/tidynamics/`



Conclusions & perspectives

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Computational modeling of anisotropic colloids

- Study of shapes not amenable to theoretical “solutions”
- Computational screening of shapes
- Control of trajectories

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- Inclusion of external fields (chemical gradients or gravity)

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Thank you

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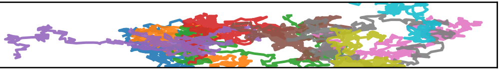

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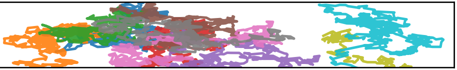

Introduction: what are nanomotors and why are they interesting?

RMPCDMD

Mesoscopic simulations of L particles

Fast Correlation Algorithm

Conclusions & perspectives