BROWNIAN MOTION OF AN ELLIPSOID

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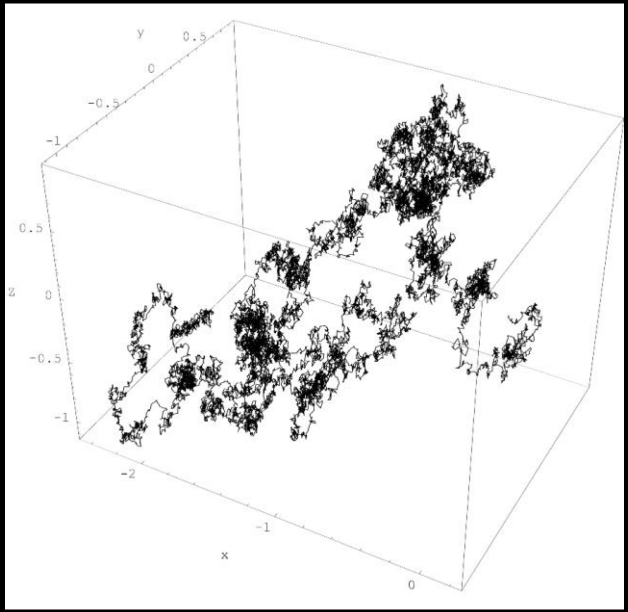
OUTLINE

- INTRODUCTION
- LITERATURE REVIEW
- PROBLEM OUTLINE
- GOVERNING EQUATIONS & NUMERICAL METHOD
- RESULTS

BROWNIAN MOTION

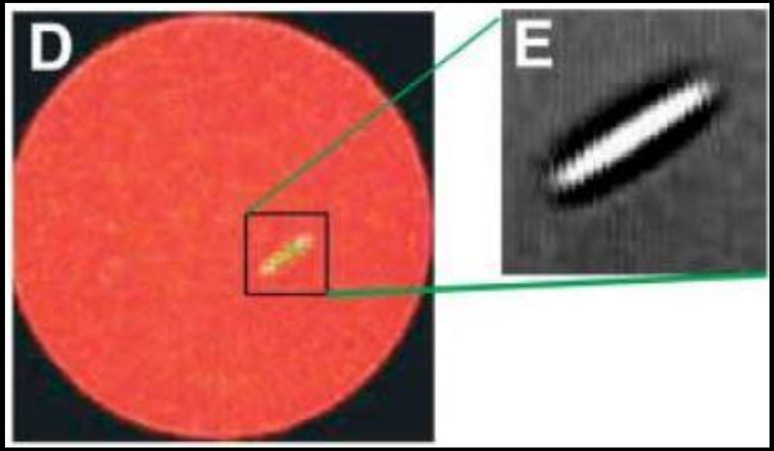
- Suspended particles below the micrometer size.
- Thermal fluctuations of the fluid molecules surrounding.

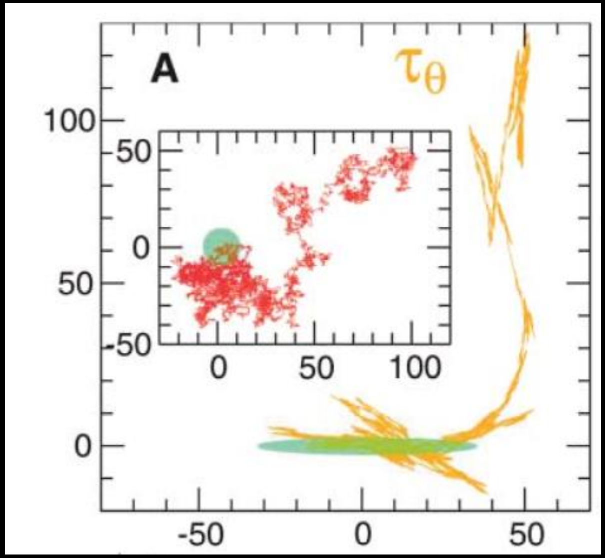


- Random motion paths.
- In this presentation we focus on the Brownian motion of ellipsoidal particles.

LITERTURE REVIEW

- Brownian motion of an ellipsoid was firstly studied by Perrin [1-2].
- The anisotropic shape gives raise to rotation and translation coupling.
- Recent experiments measure diffusion coefficients in quasi-2D geometries [3-4].





1. F. Perrin, J. Phys. Radium V, 497 (1934).
2. F. Perrin, J. Phys. Radium V, 497 (1936).
3. Y. Han et al. Science (2006)
4. Y. Han et al. Physical Review E, (2009)

LITERATURE REVIEW

- Different approaches exist in the modelling of Brownian particles.
- The Langevin approach models the random molecules collisions as a rapidly fluctuating force on the particle.
- The Fluctuating hydrodynamics approach models the thermal fluctuations by adding a fluctuating stress tensor inside the fluid dynamics equations [1].
- In this presentation we will model the Brownian motion of our particle by means of the fluctuating hydrodynamics.

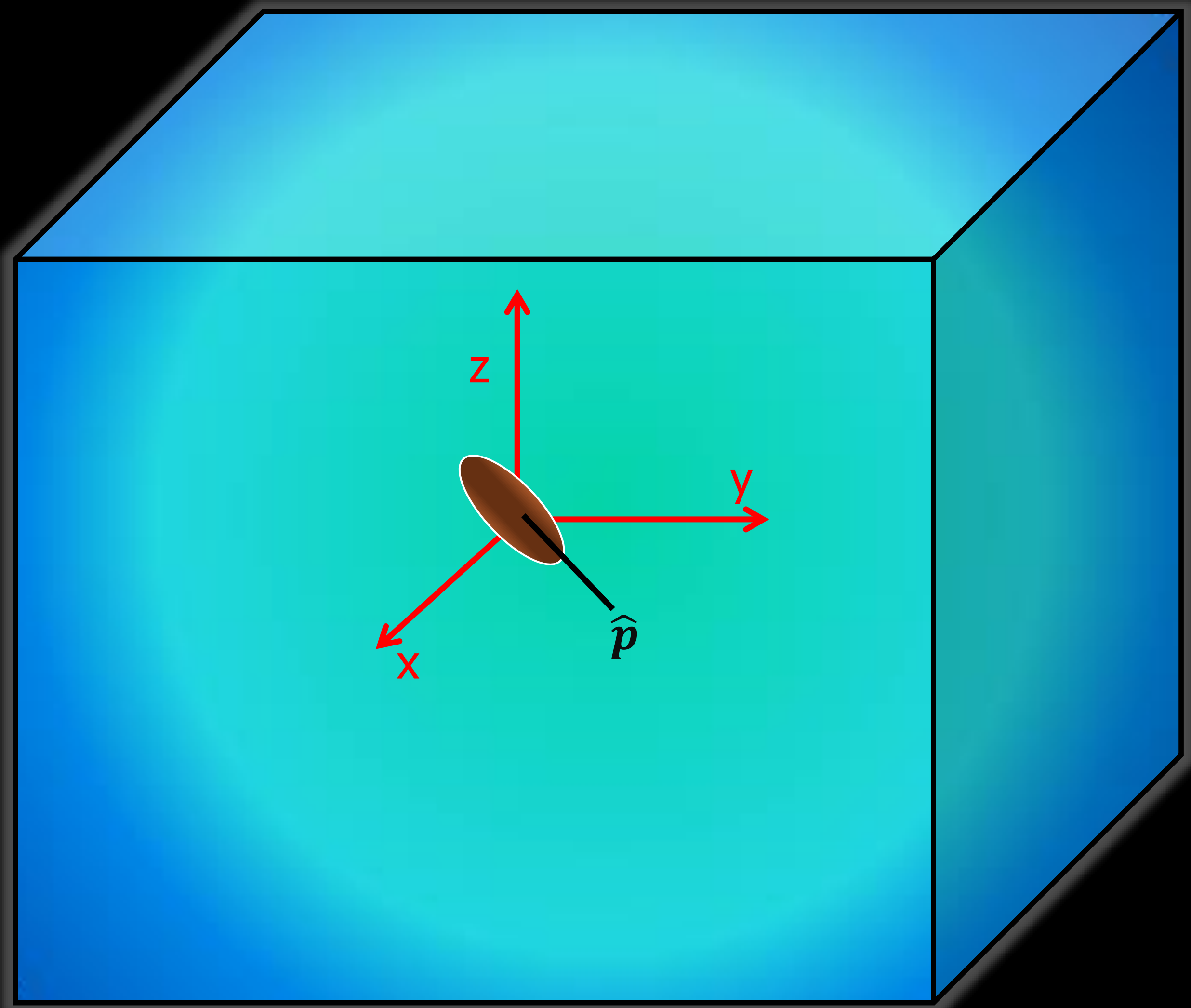
1. B. Uma et al. Phys. Fluids **23**, 073602 (2011)

OBJECTIVE

- Our goal is to develop a code that is able to:
  - Track center of mass and orientation of an ellipsoid.
  - Resolve the instantaneous particle-wall and particle-particle hydrodynamics interactions.

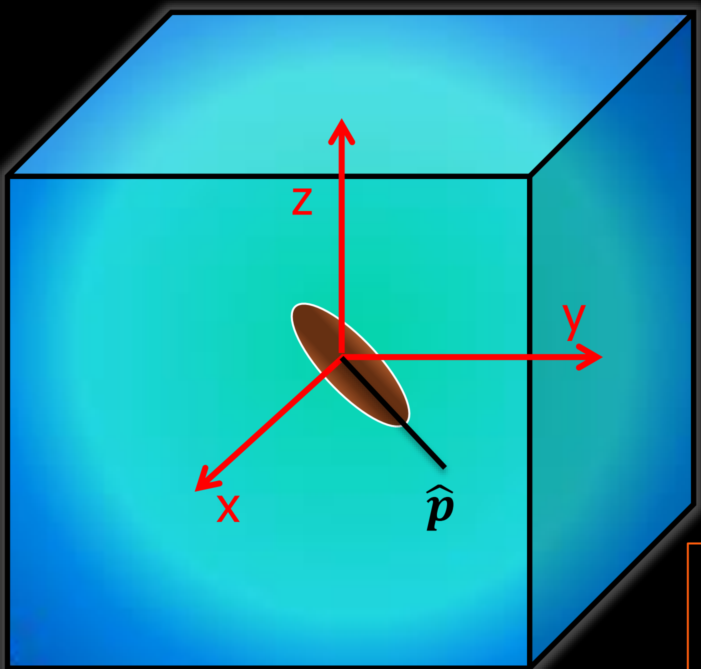
- We decided to test our code for an unconfined ellipsoid.

PROBLEM OUTLINE



- Inertialess ellipsoid
- Inertialess and quiescent fluid
- Newtonian fluid
- Unbounded fluid

PROBLEM DEFINITION



Governing Equations:

- $\nabla \cdot \boldsymbol{u} = \mathbf{0} \qquad \nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$
- $\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\mathbf{D} + \mathbf{S}$

Stochastic properties of **S**:

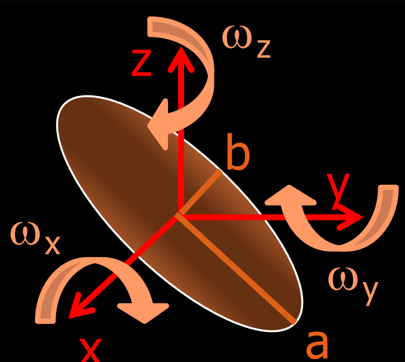
- $\langle S_{ij}(\mathbf{X}, t) \rangle = 0$
- $\langle S_{ik}(\mathbf{X}, t) S_{lm}(\mathbf{X}', t') \rangle = 2 k_B T \mu (\delta_{il}\delta_{km} + \delta_{im}\delta_{kl}) \delta(\mathbf{X} - \mathbf{X}') \delta(t - t')$

Parameters:

- $k_B T = 1$
- $\mu = 1$
- $\phi = {}^{a}/_{b}$

Initial and boundary conditions:

- $\mathbf{x}_c(0) = \mathbf{0}$
- $\hat{\boldsymbol{p}}(0) = [1,0,0]$
- $\mathbf{u} = \mathbf{u}_p + \boldsymbol{\omega} \times (\mathbf{x}_c - \mathbf{X})$ on $\partial\Sigma_p$
- $\mathbf{u} = \mathbf{0}$ on the external boundaries



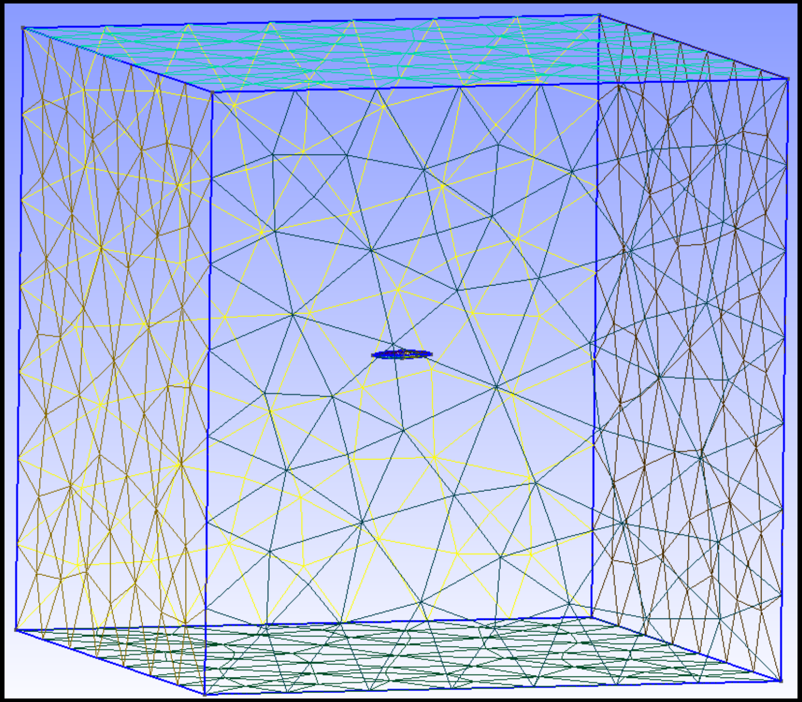
Force and Torque on the particle:

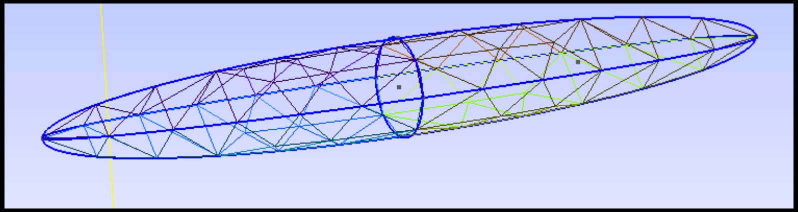
- $\mathbf{T} = \int_{\partial\Sigma_p} (\mathbf{x}_c - \mathbf{X}) \times \boldsymbol{\sigma} \cdot \mathbf{n}\, ds = \mathbf{0}$
- $\boldsymbol{F} = \int_{\partial\Sigma_p} \boldsymbol{\sigma} \cdot \mathbf{n}\, ds = \mathbf{0}$

Particle equations of motion:

- $\frac{d\boldsymbol{x}_c}{dt} = \boldsymbol{u}_p \qquad \frac{d\boldsymbol{\theta}}{dt} = \boldsymbol{\omega}$

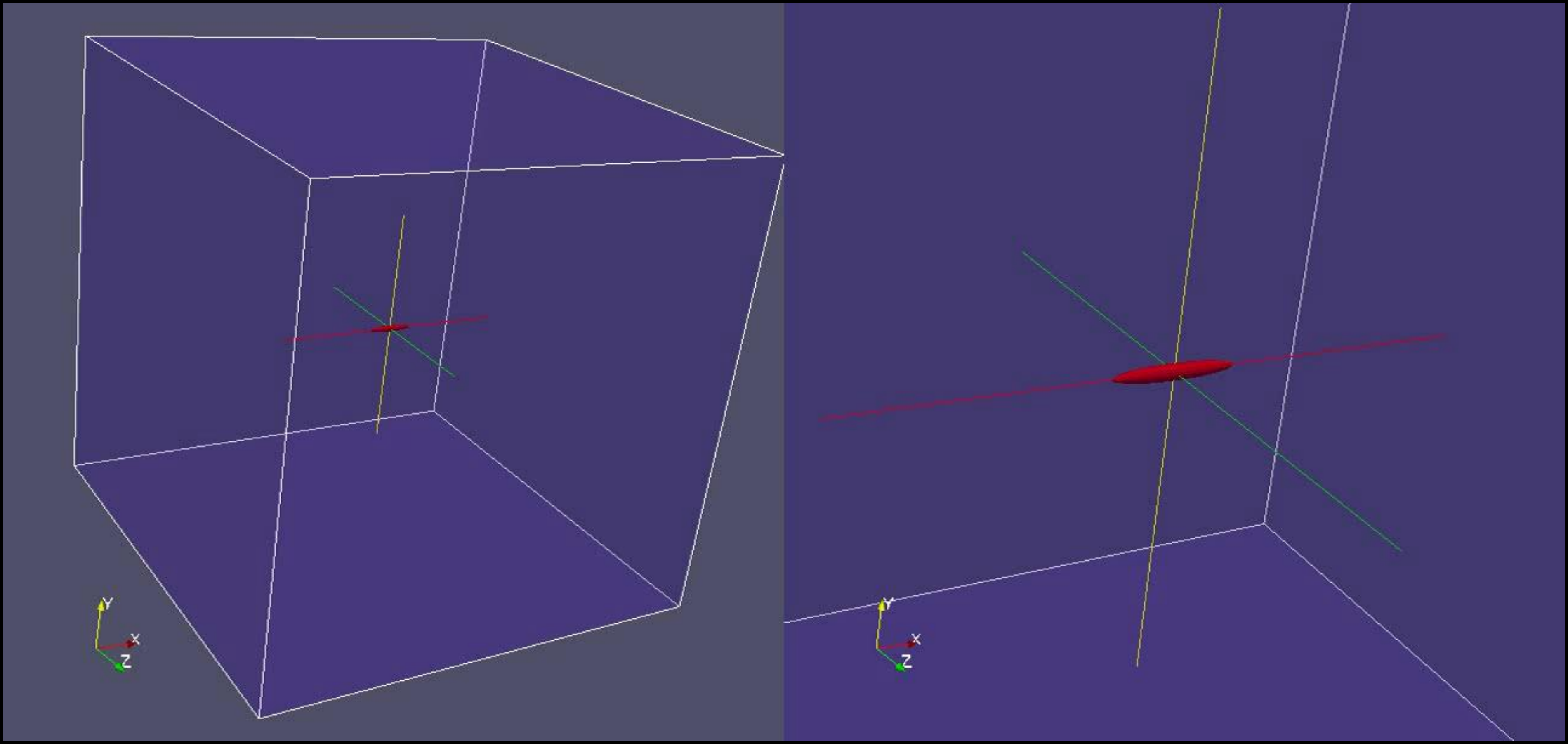
NUMERICAL METHOD





- We used a FEM along with an ALE treatment of the mesh.
- The box lenght L >> a
- The ellipsoid moving inside the domain is distorting the mesh.
- Remesh was applied everytime an element aspect ratio was bigger than a treshold value.
- Fluctuating-hydrodynamics finite element discretization is very sensitive to elements aspect ratios.

RESULTS

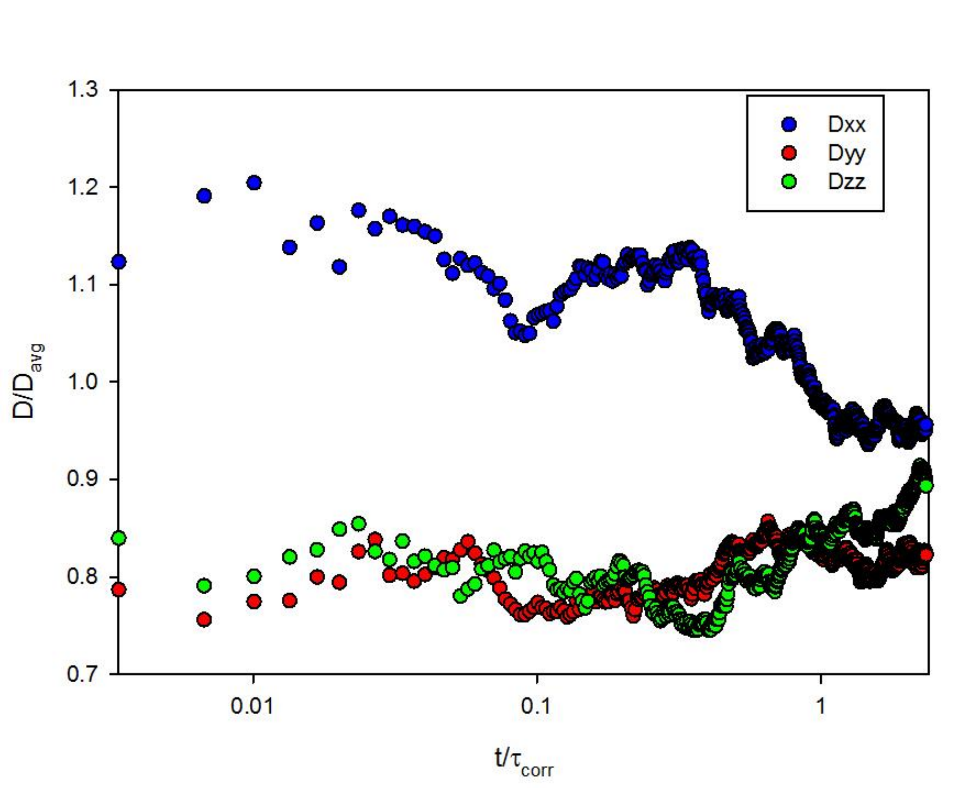


DIFFUSION

- Because of the anisotropic shape an ellipsoid diffuses faster along its major axis.
- At starting times we will see a preferential diffusion direction.
- But as the ellipsoid orientation changes the memory of the initial orientation is lost.
- From a fixed frame we would see no more a preferential diffusion direction.

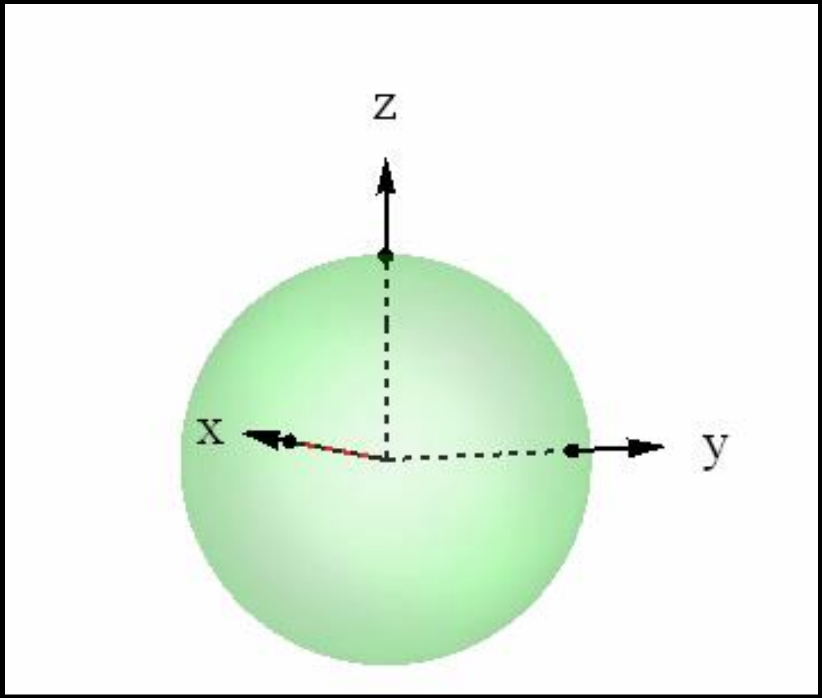
RESULTS $\phi = 8$

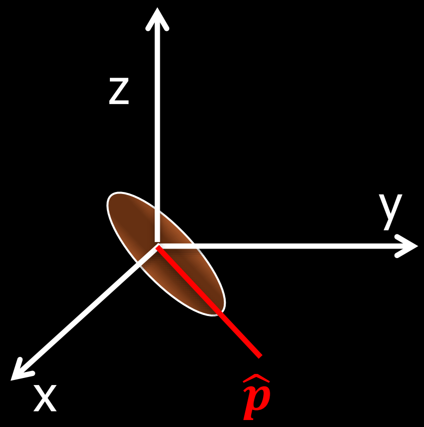
- The translational diffusion coefficients in the fixed frame are computed from the particle displacements.
- $D_{xx}(t) = \langle x_c(t)^2 \rangle / 2t \quad D_{yy}(t) = \langle y_c(t)^2 \rangle / 2t \quad D_{zz}(t) = \langle z_c(t)^2 \rangle / 2t$



RESULTS $\phi = 8$

- One could look at the probability distribution of the orientation vector $\hat{\boldsymbol{p}}$.
- $\hat{\boldsymbol{p}}$ is a vector describing a random walk in the unit sphere.

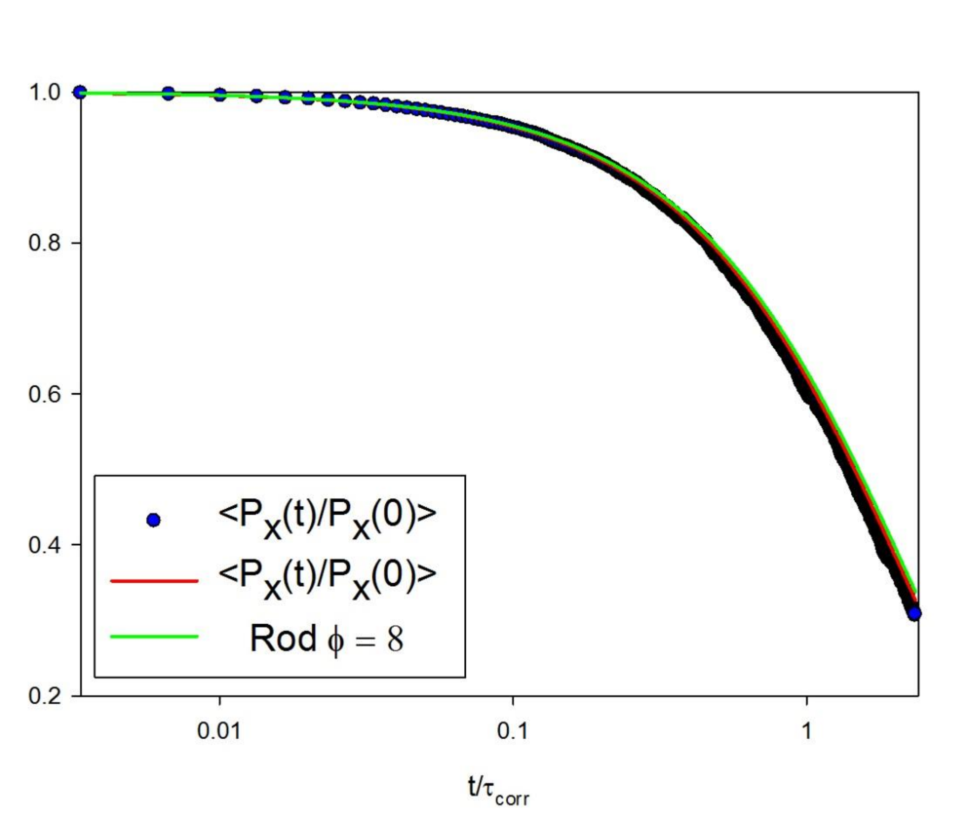




RESULTS $\phi = 8$

- The average of the orientation vector $\hat{\boldsymbol{p}}$ components is an exponential decreasing function.
- Red line is the Langevin equation analytical solution.

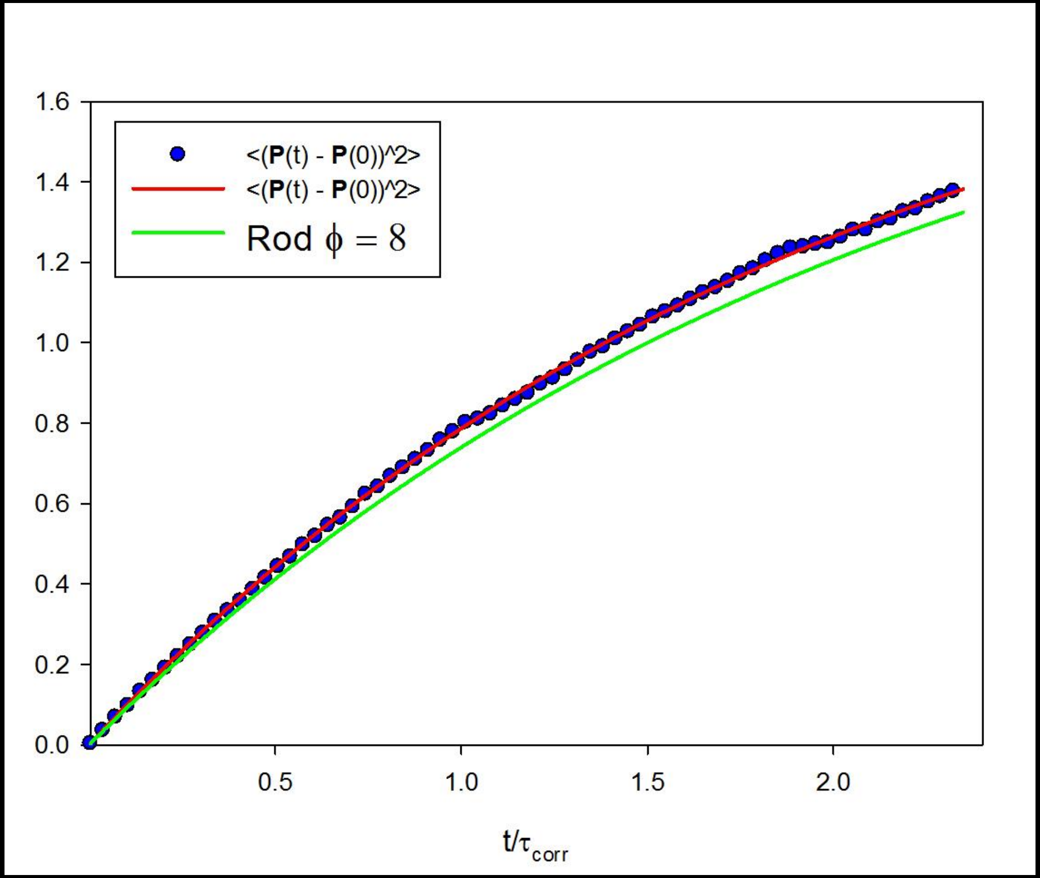
- Components other than x are zero.
- Green line is the analytical solution for a rigid rod of the same aspect ratio.
- Excellent match is found between numerical and analytical solution.



RESULTS $\phi = 8$

- The mean square displacement of $\hat{\boldsymbol{p}}$ is $\langle(\hat{\boldsymbol{p}}(t) - \hat{\boldsymbol{p}}(0))^2\rangle$

- At small times the MSD is linear in time.
- At longer time $\hat{\boldsymbol{p}}$ experiences the sphere's curvature.
- Red line is the analytical solution of the Langevin equation.
- Green line is the MSD of a rigid rod of the same aspect ratio.
- Again an excellent match is found between numerical and analytical solution.

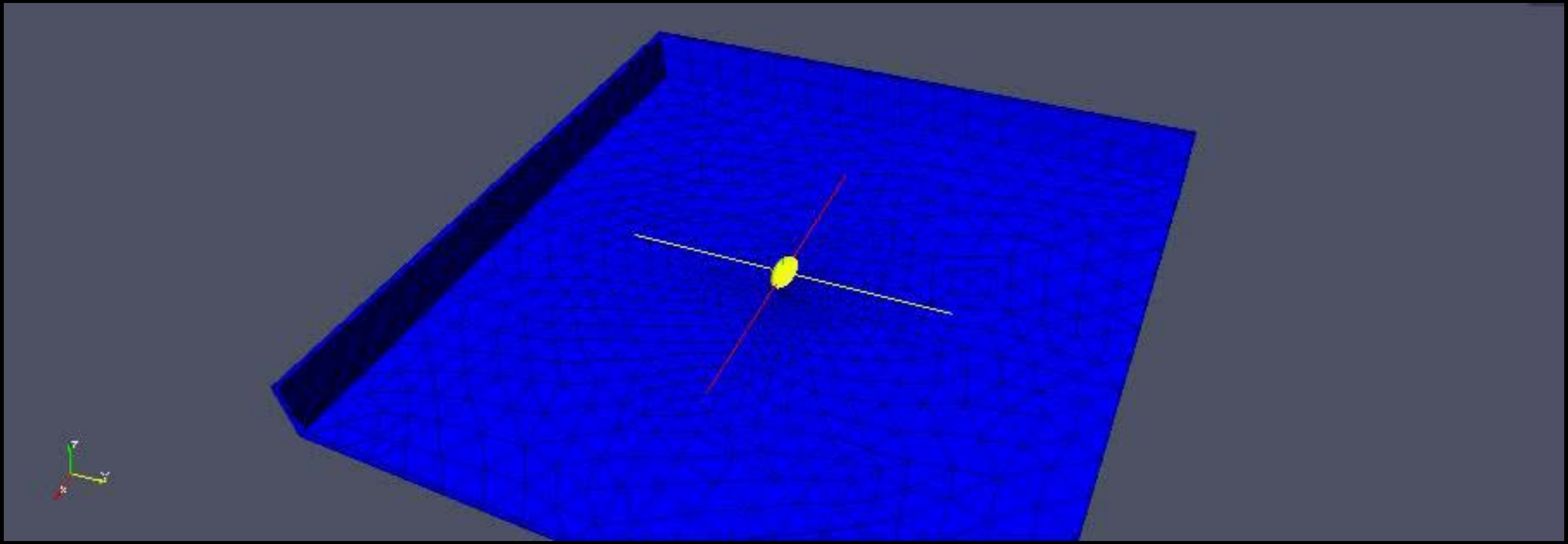


CONCLUSIONS

- Particles undergoing Brownian motion show random-like paths.
- Ellipsoidal particles diffusion is anisotropic at small times but shifts to isotropic at longer times.
- The diffusion of the orientation vector shows an excellent match with analytical solutions.
- Fluctuating hydrodynamics proves to be a very flexible way to model Brownian motion of particles.

FUTURE WORK

- Part of the future work will be to investigare the dynamics of ellipsoidal particles near walls.
- A first step in this direction has already been done.



THANKS FOR THE ATTENTION