MATH0488 – Elements of stochastic processes

Molecular dynamics: from Brownian motion to polymeric fluids

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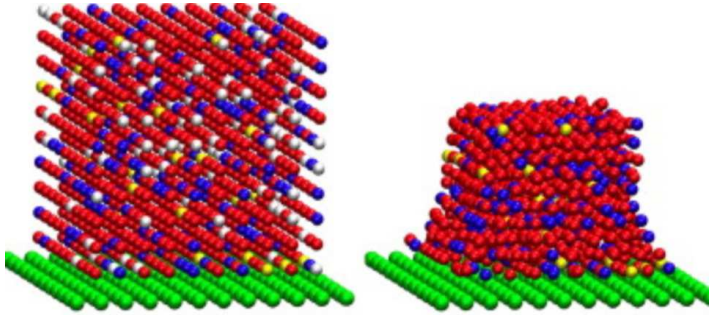
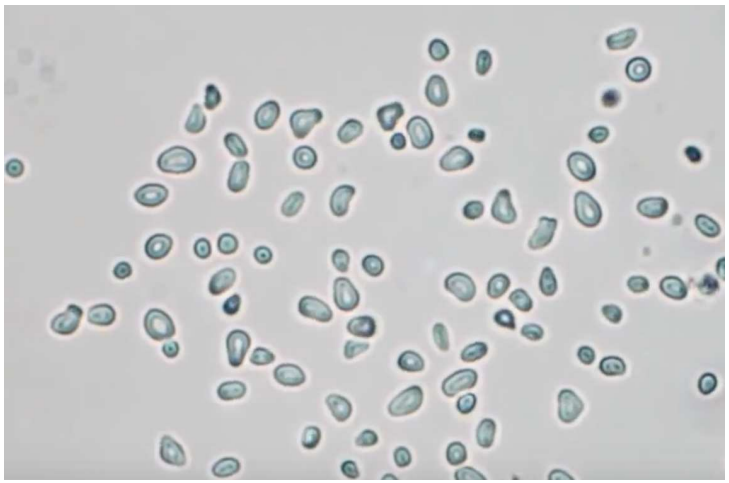
March 1, 2016

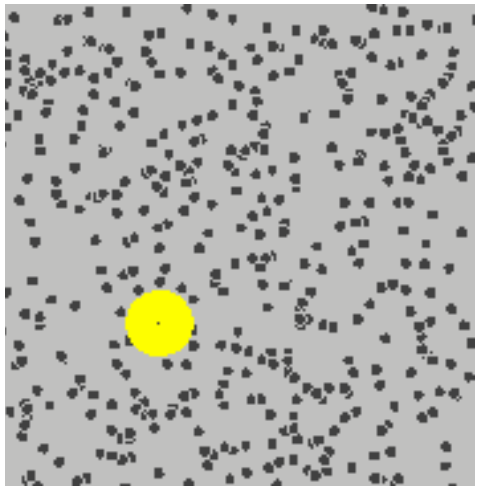
Introduction



- Matter is made out of a great many interacting atoms, or elementary parts. Thus, macroscale behavior (mechanical, electrical,...) of matter should be explainable in terms of the microscopic behavior and motion of the atoms, or the elementary parts.
- Realistic physical bodies are composed of a huge number of atoms; for example, 1 mm^3 of bulk metal contains about 10^{19} atoms. We are not going to be able or want to know how every atom is actually behaving or where it is actually moving. A deterministic approach is not feasible.
- Systems of vast numbers of atoms are governed by principles that call for a probabilistic description. We are going to want to know about average behavior and what the odds are for different effects occurring. We are going to want to describe the motion of atoms as a random motion.
- A probabilistic description can also be motivated by the behavior of atoms being not according to classical mechanics, but rather quantum mechanics, but this is beyond the scope of this course.

Introduction





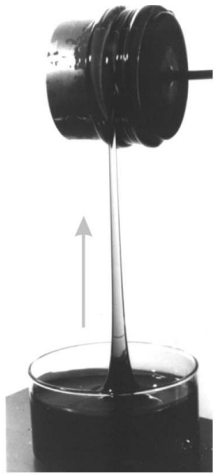
Macroscale behavior: little particles
of plant pollens jiggle around in a liquid.

Robert Brown.
(botanist, experimentalist).

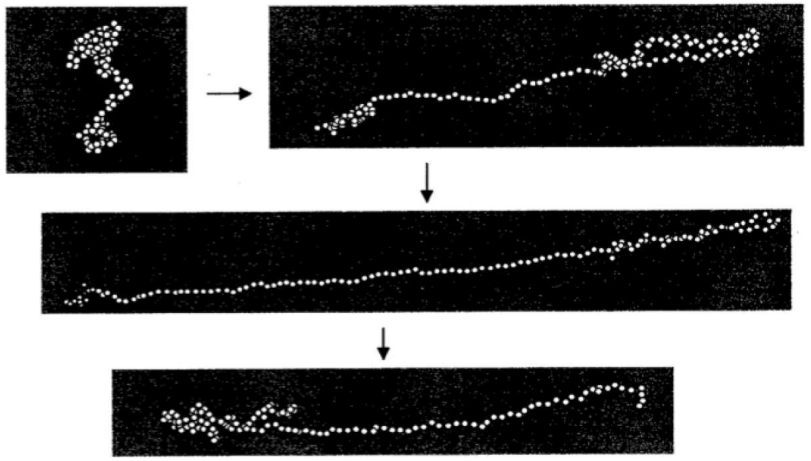
Microscale origin: effect of collisions
with smaller liquid molecules in thermal motion.

Albert Einstein.
(theoretical physicist).

We will first look at foundational discoveries of Brown and Einstein.



Macroscale behavior: adding polymers to a fluid increases viscosity.



Microscale origin: effect of intermolecular forces and collisions with smaller liquid molecules in thermal motion.

We will then look at an engineering application relevant to polymeric fluids.

Agenda

- We will be meeting in building B37 room Amphi 2 from 10h45 to 12h45 at the following dates:

1	2	**3**	4	5	6
08/03	15/03	**22/03**	12/04	19/04	26/04
lecture	Q&A	**lecture**	Q&A	Q&A	Q&A

- Your presence is strongly recommended for the lectures:
  - Tuesday March 8, 10h45–12h45,
  - Tuesday March 22, 10h45–12h45,

- If you should need some help, please attend the Q&A sessions or contact A. Crovato or M. Arnst by email to ask a question by email or schedule an appointment.

- Please work in groups of 2 or 3 people. Send the first and last names of all the group members (2 or 3 people), as well as their email addresses, by email to M. Arnst before/on Monday March 14.

- The project report must be sent in PDF format by email to M. Arnst before/on Thursday April 28.

- Project presentations will be scheduled between Tuesday May 3 and Tuesday May 10.

Grading

- Report:
  - The report should collect your solutions to all the exercises that you worked on.
  - One report per group is required. The group is responsible for ensuring that work is fairly distributed among group members and that a high-quality report is written.
  - The report must be neat, well organized, and professionally presented. All graphs must be computer plots. Label all graph axes and include proper units.
  - Please include a list of all the references that you will have consulted.
  - Length of 15 to 30 pages (including figs. and list of refs., single spacing, font size of 12 pt).
  - The report must be sent in PDF format by email to M. Arnst before/on Thursday April 28. Please attach to your email a file with any code that you will have written.
- Presentation:
  - Please prepare a creative presentation. Be original and thoughtful in your selection of material that you include. The presentation need not collect all the solutions to all the exercises that you worked on because the report already does that. The presentation should collect only those solutions that you consider the most important or the most interesting ones.
  - Be original and thoughtful in how you present the material that you include. Slides offer opportunities that the report may not, such as displaying animations. Graphs in slides typically require larger axis and tick labels than graphs in the report.
  - Length of about 10 slides. The first slide must include the group members names, and the last slide must list conclusions.

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