

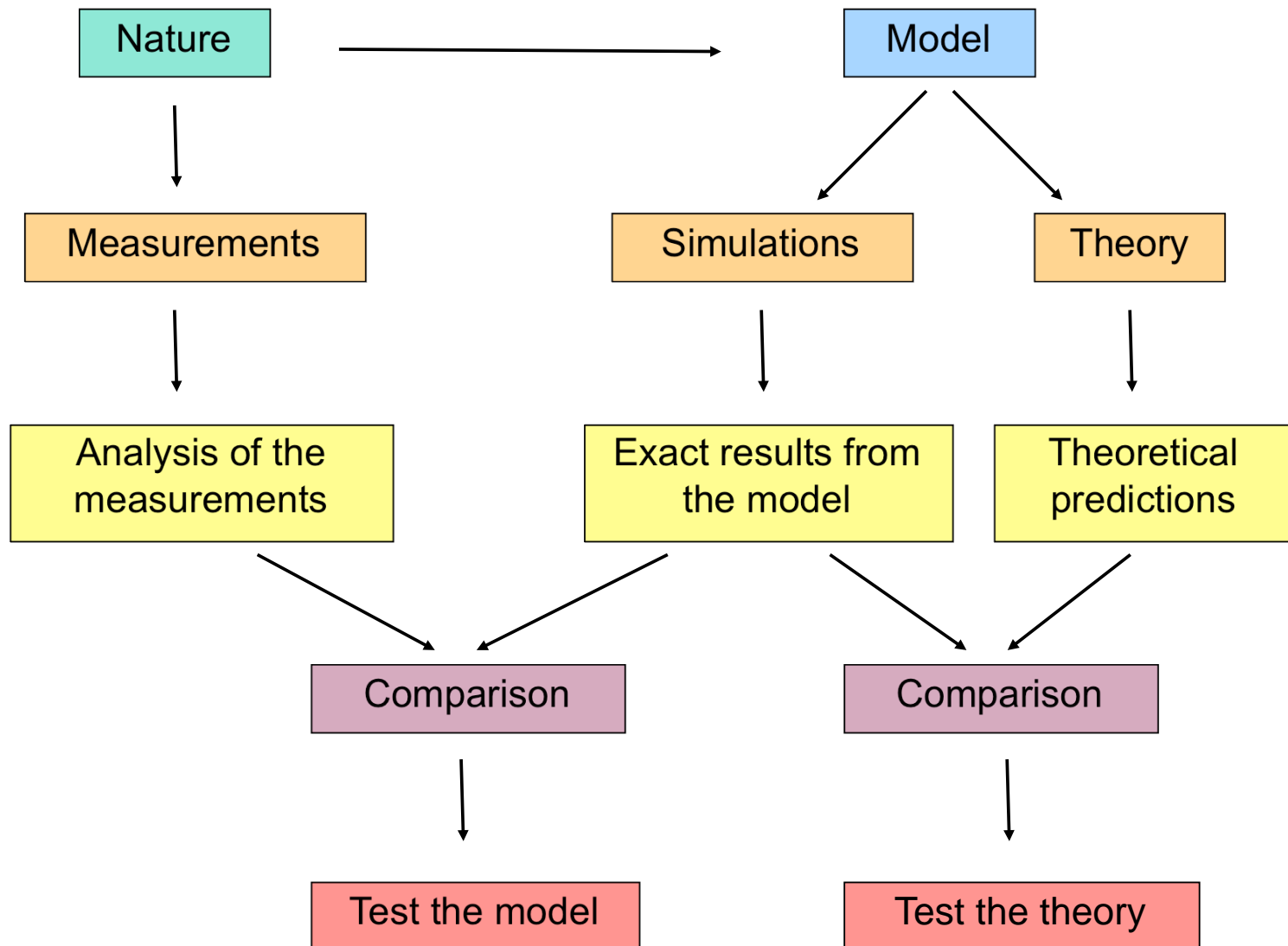


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# Models vs experiments

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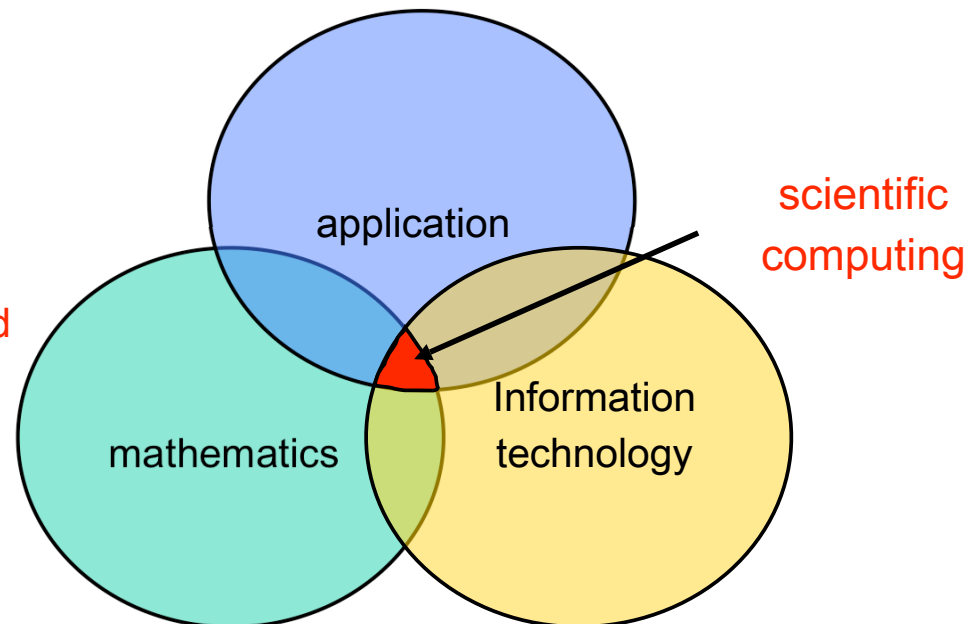


Computational science or scientific computing? It is difficult to give a precise definition.

An a relatively restricted sense we can think of the above as a collection of techniques and theoreis which can be used to solve scientific and engineering problems using computers.

According to Kenneth Wilson (Nobel Prize in Physics) a problem in scientific computing (-86):

1. is mathematically well defined
2. cannot be solved using traditional methods
3. requires in-depth knowledge of the field of application



According to Webster's dictionary:

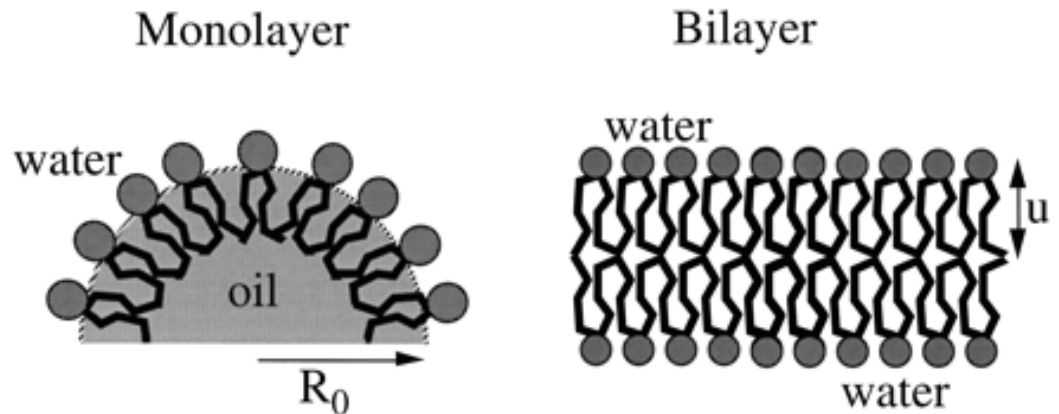
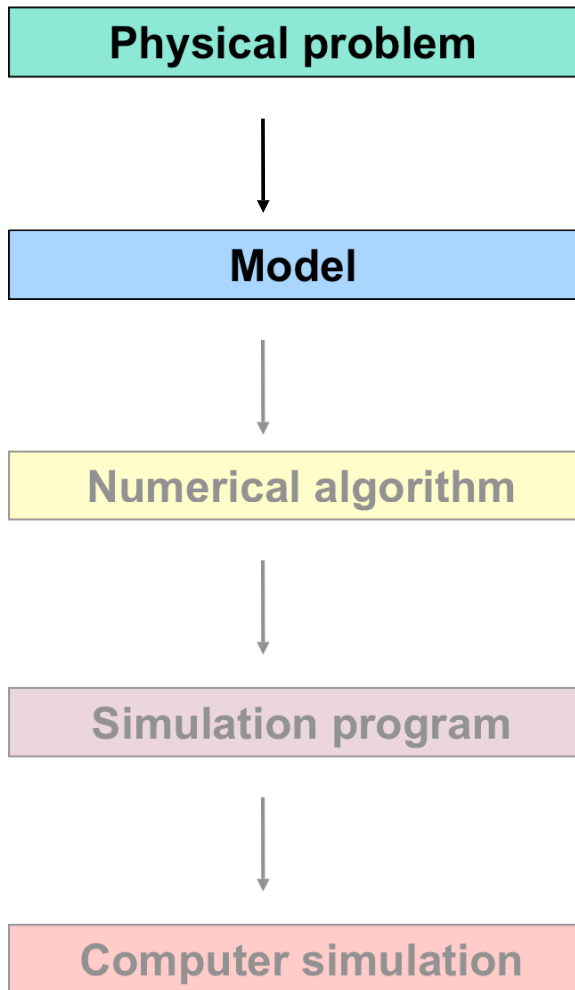
**sim·u·la·tion** *n.*

1. The act or process of simulating.
2. An imitation; a sham.
3. Assumption of a false appearance.
4.
  - a. Imitation or representation, as of a potential situation or in experimental testing.
  - b. Representation of the operation or features of one process or system through the use of another: *computer simulation of an in-flight emergency*

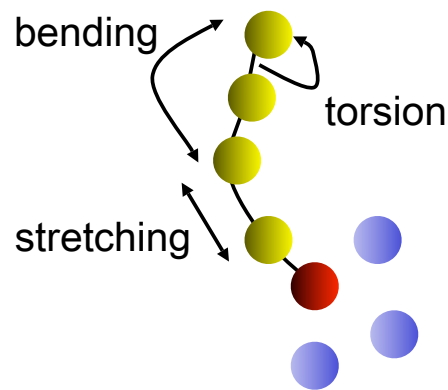
- Simulation is an algorithmic approach
- Simulation is not a stairway to heaven, it has its own advantages and disadvantages

# Constructing a model

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Model: a lipid (fat) molecule in water



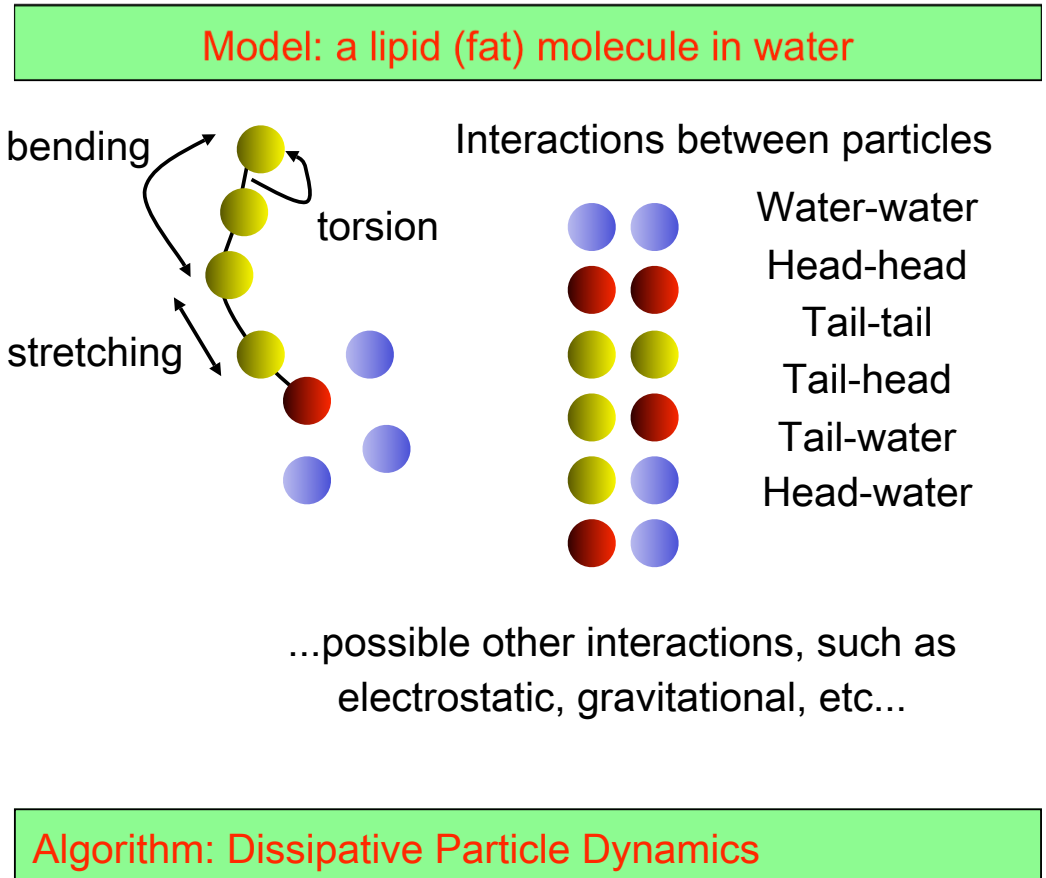
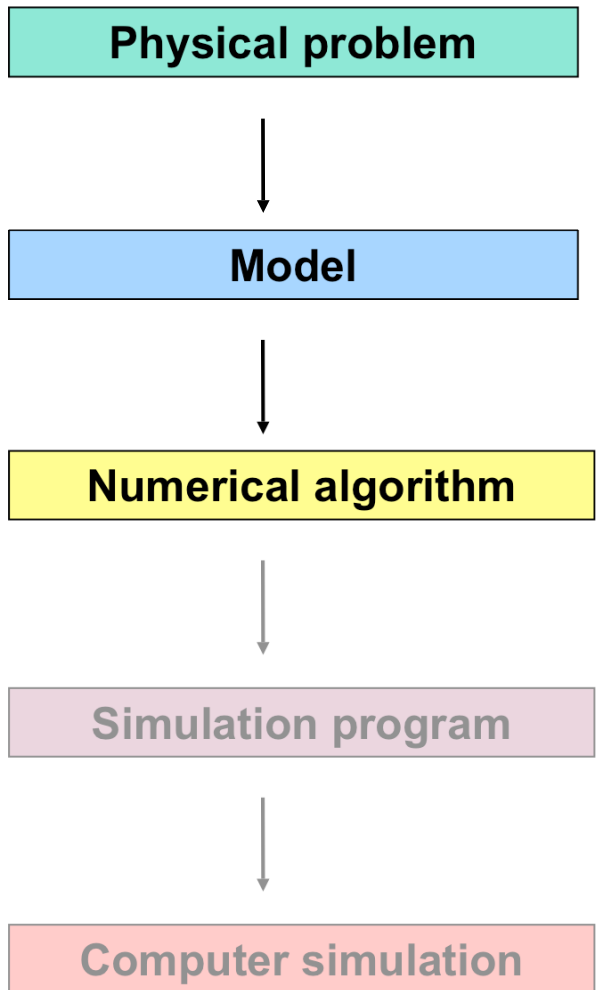
Interactions between particles

- Water-water (two blue circles)
- Head-head (two red circles)
- Tail-tail (two yellow circles)
- Tail-head (one yellow and one red circle)
- Tail-water (one yellow and one blue circle)
- Head-water (one red and one blue circle)

...possible other interactions, such as electrostatic, gravitational, etc...

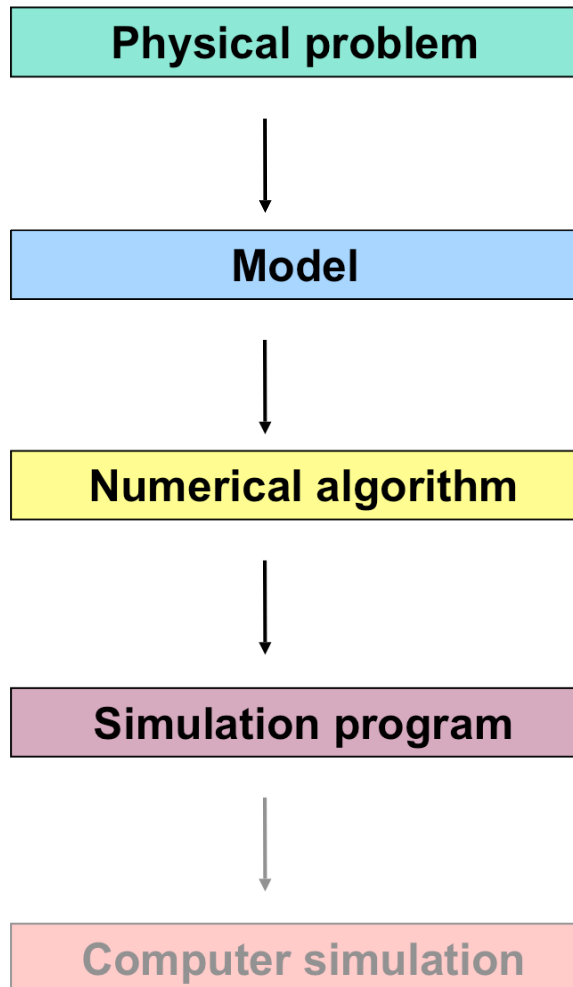
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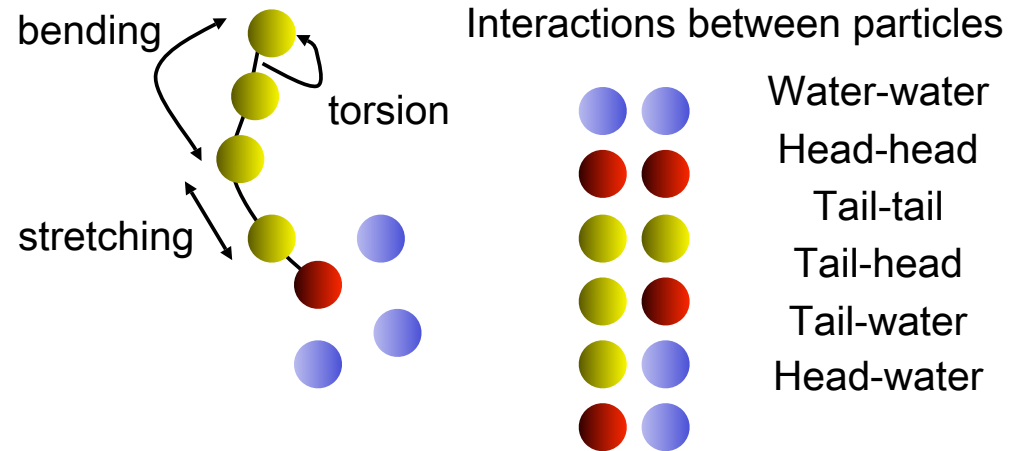


# Constructing a model

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Model: a lipid (fat) molecule in water



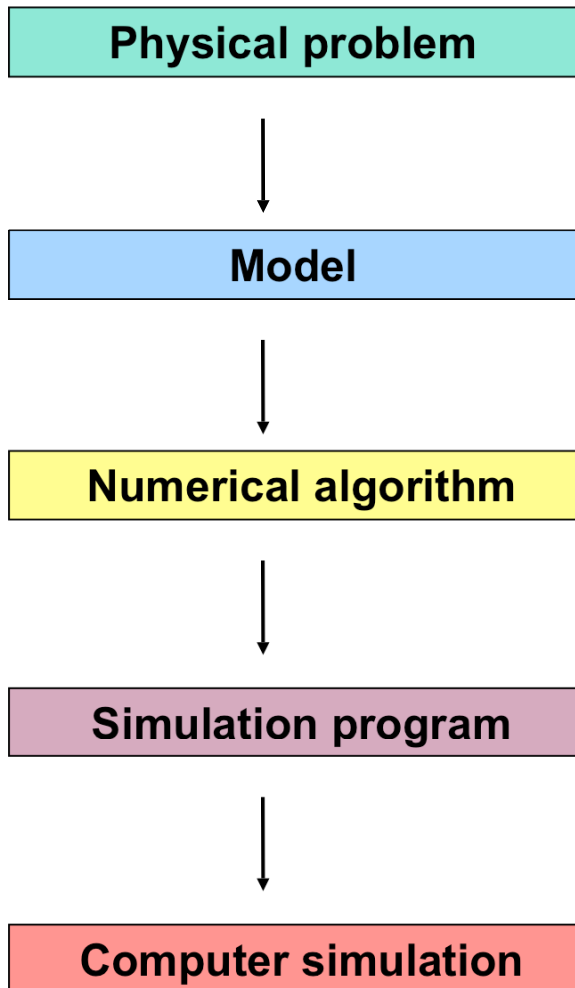
...possible other interactions, such as electrostatic, gravitational, etc...

Algorithm: Dissipative Particle Dynamics

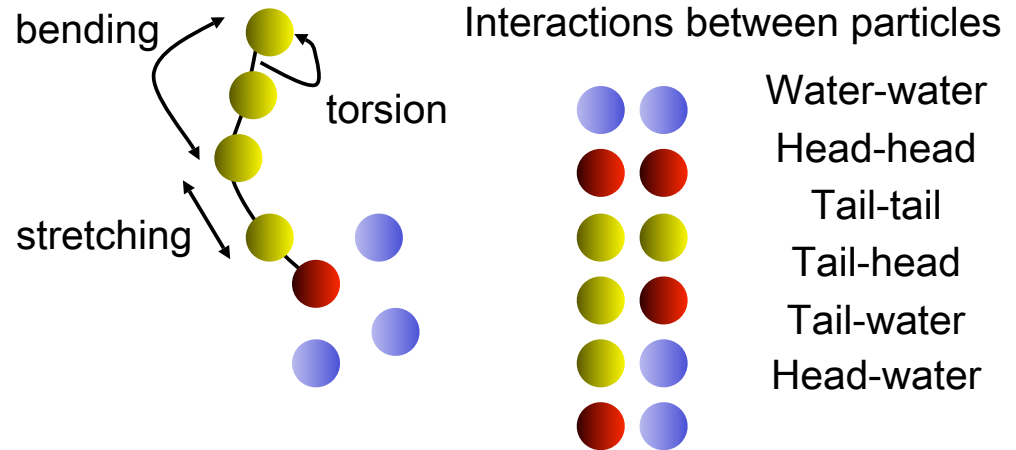
Simulation program: Programing and debugging. Test the code using theoretical models for validation.

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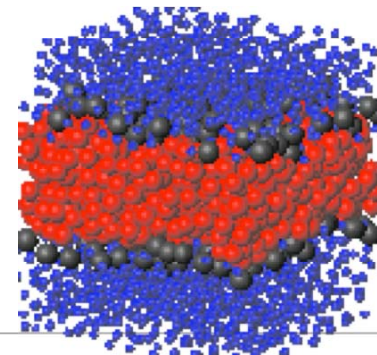
Model: a lipid (fat) molecule in water



...possible other interactions, such as electrostatic, gravitational, etc...

Algorithm: Dissipative Particle Dynamics

Simulation: collect data & analyze



Next, I will show you a real-world example of a specific application.