Abstract
For both fundamental and technological reasons, there is a strong
desire to understand the overall behavior of complex macro-

cellular and biological soft-matter systems.
From theoretical point of view, this task is highly nontrivial since

processes in these systems occur over a wide range of length and
time scales, while current modeling and analytical techniques are

time consuming and frequently limited only.
To fill this gap, one has to develop new methods, an idea which has

lead to concepts known as multiscale modeling and coarse-graining.

The idea of multiscale modeling gives rise to the fundamental
problem that there is no unique way to perform coarse-graining. We

employ a method that allows us to perform controlled spatial

course-graining followed by corresponding temporal coarse-
graining in a systematic well-defined fashion.

Problem
The diffusion constant for typical lipids is about

The time needed to diffuse around the sample shown in the centre is:

It would take about 20 years to see a particle ex-
duced from the head to the tail.

We replace a group of several “microscopic” atoms by a larger

“effective” particle.
We want softer potentials!

A fixed particle has a fixed potential.

Dynamics in biophysical systems has characteristic time scales.
The kind of dynamics that can be investigated depends on the

power of the molecular-dynamics methods.
Past: Traditional MD can “see” the movement of only small
groups of atoms.
Now: Coarse-grained dynamics brings the dynamics in lipid
membranes into the reach.
Future: Better coarse-graining techniques might be able to solve

the protein folding problem “holily grail” of theoretical biophysics.

Outlook

Spatial coarse-graining

Aim: Reduce the number of particles

We can describe the collision of two billiard balls by just two par-
ticles — instead of 10^N atoms.
We replace a group of several “microscopic” atoms by a larger

“effective” particle.

Temporal coarse-graining

The integration time step in a MD simulation is limited by the

slope of the internal potentials.
A potential can be softened by coarse-graining (watering) over time.
All particles fluctuate somewhat so their potential does, too.

A fixed particle has a fixed potential.

If the particle can move, so does the potential. The red line marks the av-
erage over time.

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