

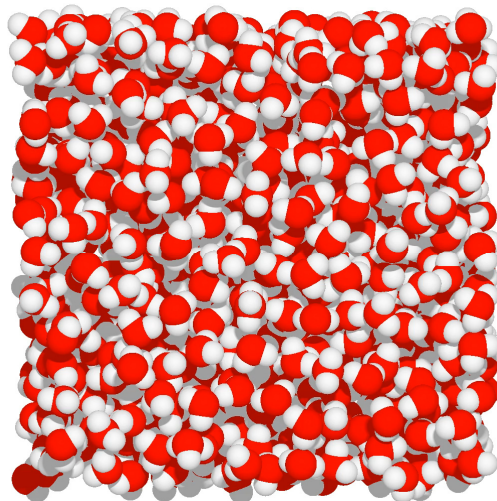
Verhandlungen der Deutschen Physikalischen Gesellschaft,
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Entfernte Partikel haben einen starken und schnellen Einfluss auf das Molekülverhalten

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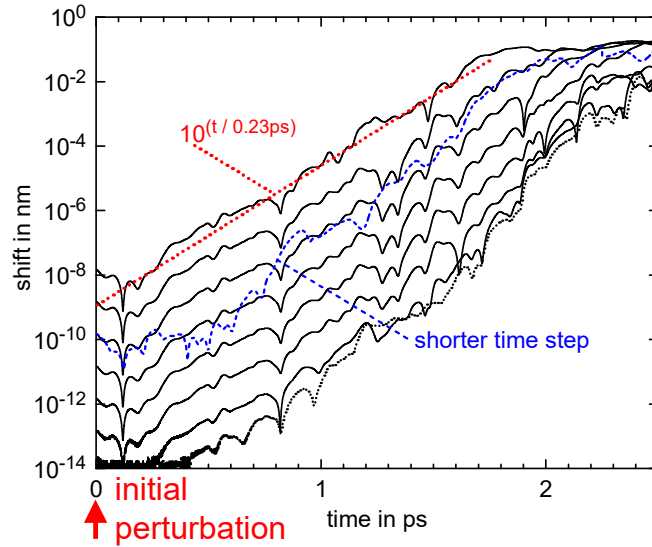
liquid water, 37°C, periodic boundaries



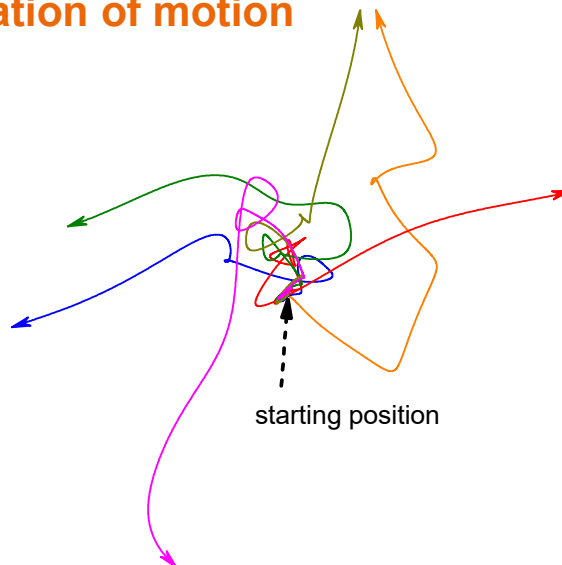
2



Lyapunov instability in liquid water at 37°C



randomization of motion



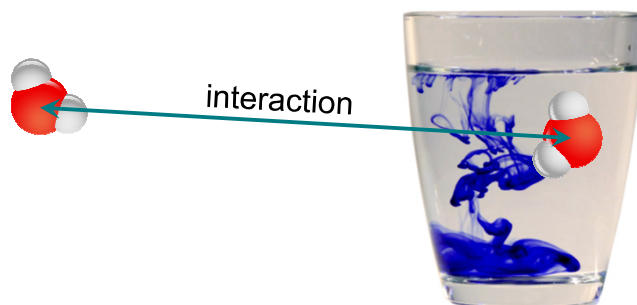
consequences

- deterministic chaos, Lyapunov time
- prediction every 0.23 ps further into the future requires one more decimal digit in start coordinates and calculations
- thus: cannot be predicted over intermediate times
- this is statement only about prediction, not about reality itself

thought experiment

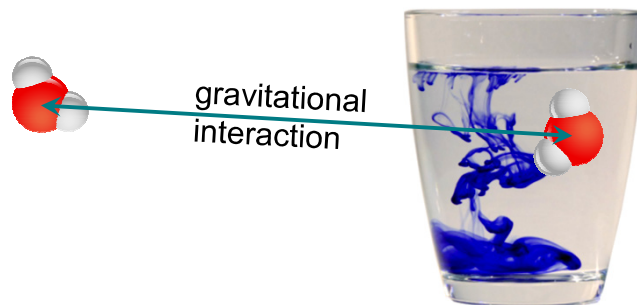
distant
interacting
molecule

nearby
observed
molecule



question:

- How long does it take until the interaction leads to an observable bifurcation?
- bifurcation = shift by molecular diameter



interaction of distant particle 1 for $\Delta t_{interaction}$

$$F = G \frac{m_1 m_2}{r_{1,2}^2}$$

m_1 – mass of distant particle
 m_2 – mass of observed particle

$$F = m_2 a$$

$r_{1,2}$ – distance between particles

$$a = \frac{\partial^2 s}{\partial t^2}$$

F – force acting between particles

t – time

Δs_0 – initial shift of observed particle

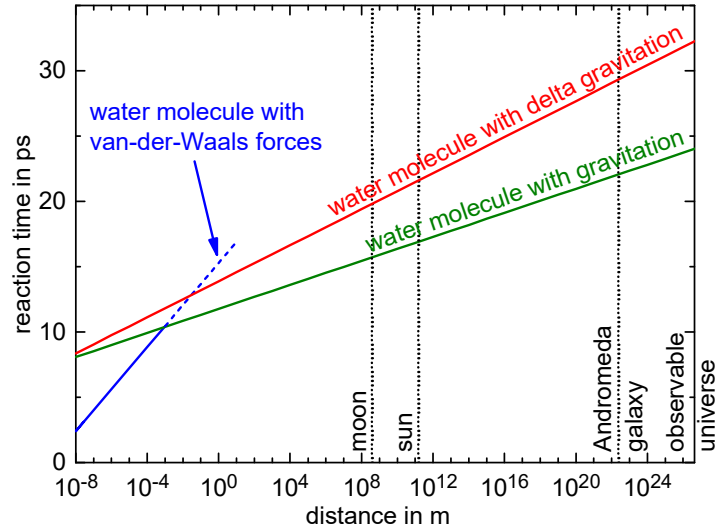
t_{scale} – 0.23 ps

$$\Delta t_{interaction} \Rightarrow \Delta s_0$$

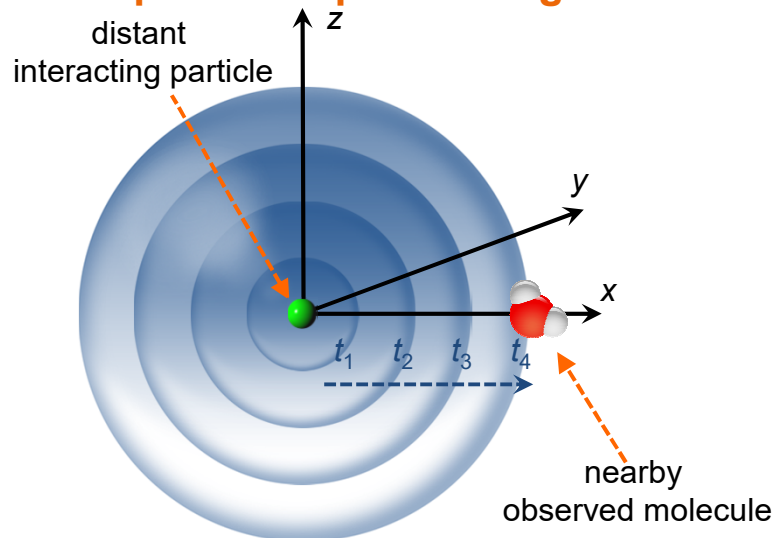
$$\Delta s = \Delta s_0 10^{t/t_{scale}}$$

$$\Delta t_{reaction} = t_{scale} \left(\log_{10} \frac{2\Delta s}{Gm_1} + 2 \log_{10} r_{1,2} - 2 \log_{10} \Delta t_{interaction} \right)$$

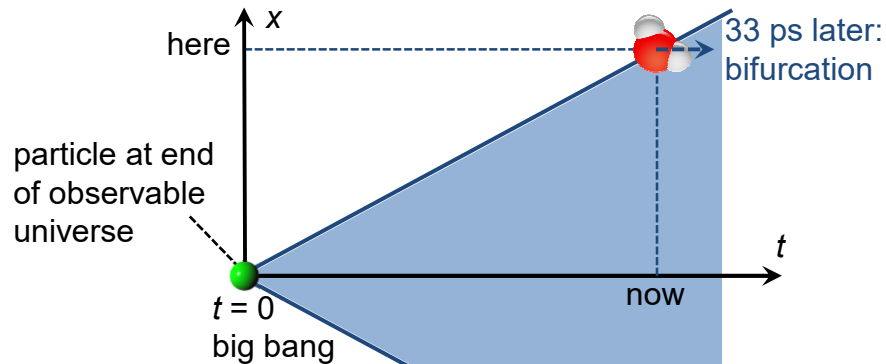
influence between two water molecules



interaction spheres at proceeding time



cone of interaction



picture

- all particles send information
- travels with speed of light
- any particle experiences at every moment the sum of all interactions with all particles
- interactions superimpose linearly
- reacts to this interaction
- if any faraway particle would have been in a slightly different place, after at most 33 ps the observed particle would react differently at any multi-furcation

consequences

- all particles influence each other within 0 to 33 ps on universal scale (possibly much faster)
- but: speed of light
- this is about **interaction in reality**, not only about prediction
- randomizing effect
- even in a fully deterministic world view
- characterizes reality properly or model deficient
- state at big bang not only initial condition but all particles since then exert a current randomizing influence
- molecules behave random (strictly unpredictable) after few ps at most
- applies to all deterministically chaotic systems

Ernst Mach

There is no cause nor effect in nature;
nature has but an individual existence;
nature simply is.

Ernst Mach: The Science of Mechanics.
A Critical and Historical Account of its Development.
Translated by Thomas J. McCormack.
The Open Court Publishing Co., Chicago, 1919.

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