Environmental transport phenomena: Lecture II

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Federal Department of Home Affairs FDHA
Federal Office of Meteorology and Climatology MeteoSwiss

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Introduction: transported components

Fluid motion is associated to the transport of **various components**

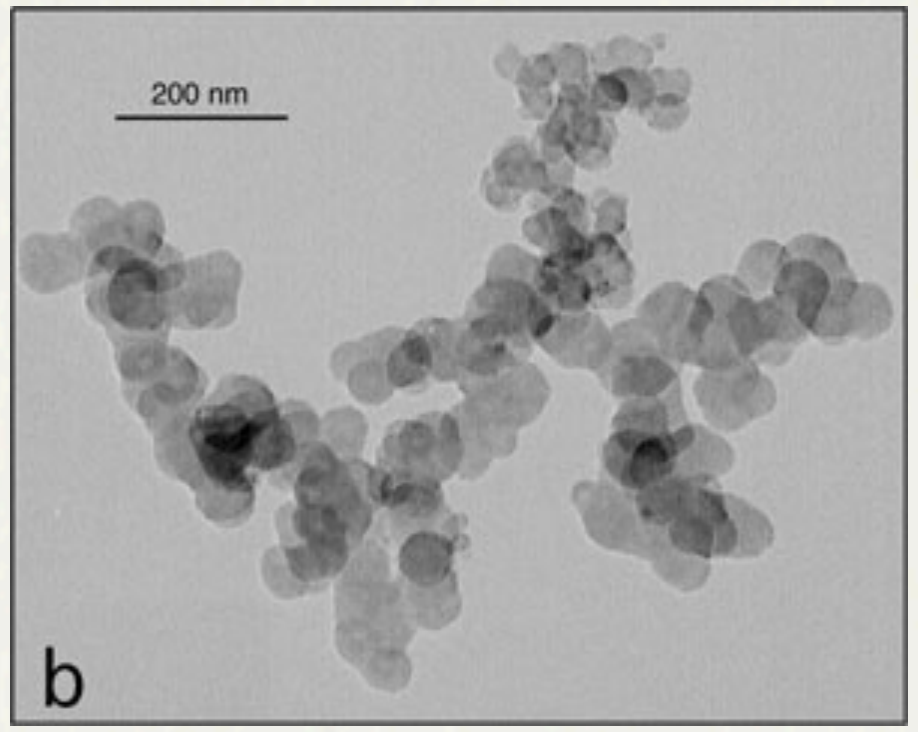
- Sediment (e.g. rivers)

Increased deposition (positive interaction) or sediment anchoring

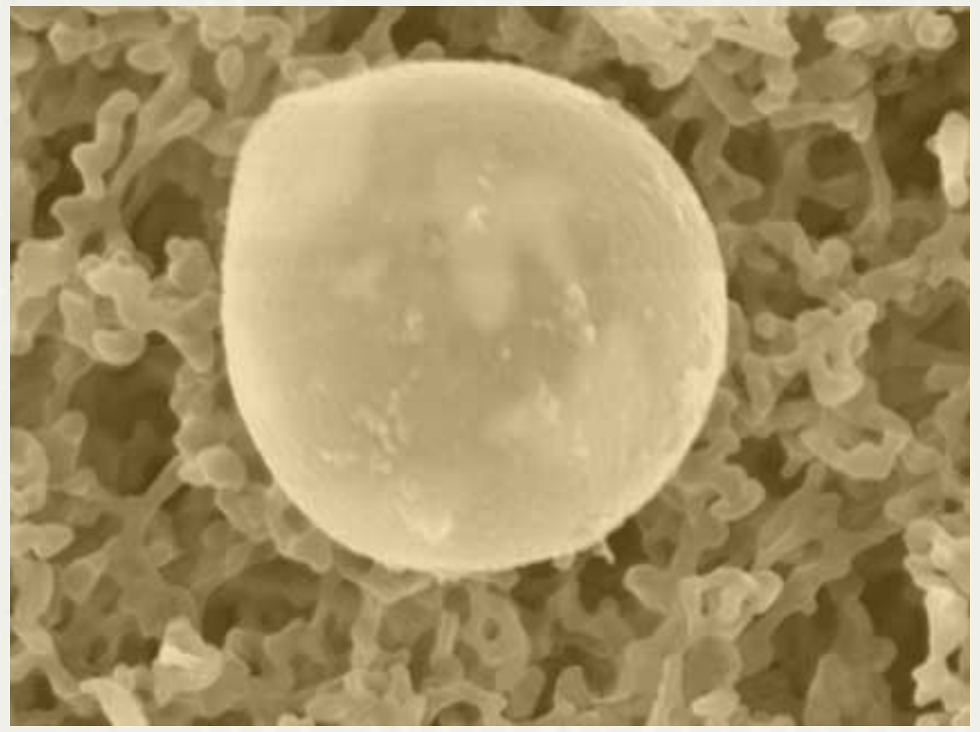
Increased scouring due to flow deflection (negative interaction)

Introduction: transported components

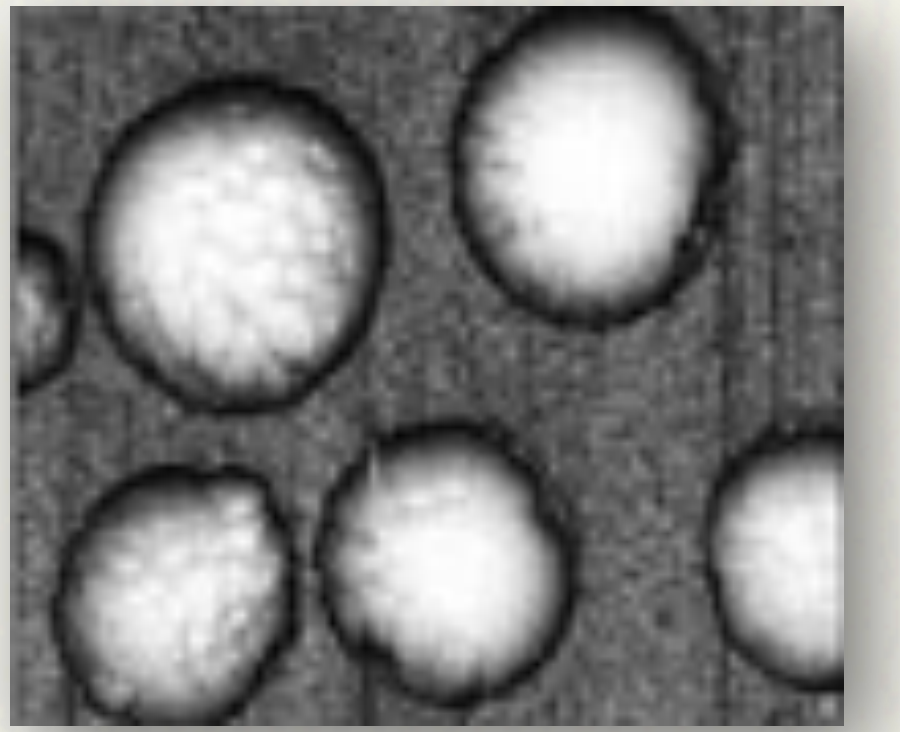
- Huge variety of aerosol (particles in suspension in the air)



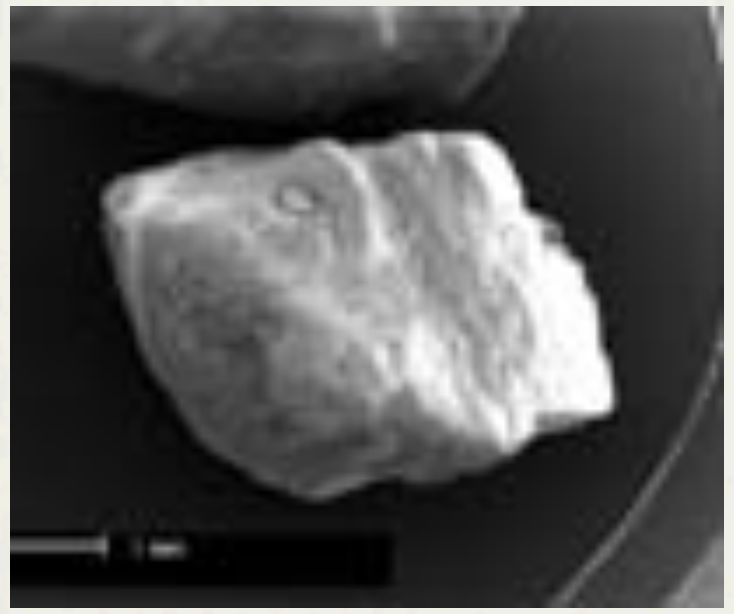
Soot (Diesel):
ca. 0.1 µm



Mineral dust
0.2 - 10 µm



Amonium sulfate:
ca. 0.1 µm

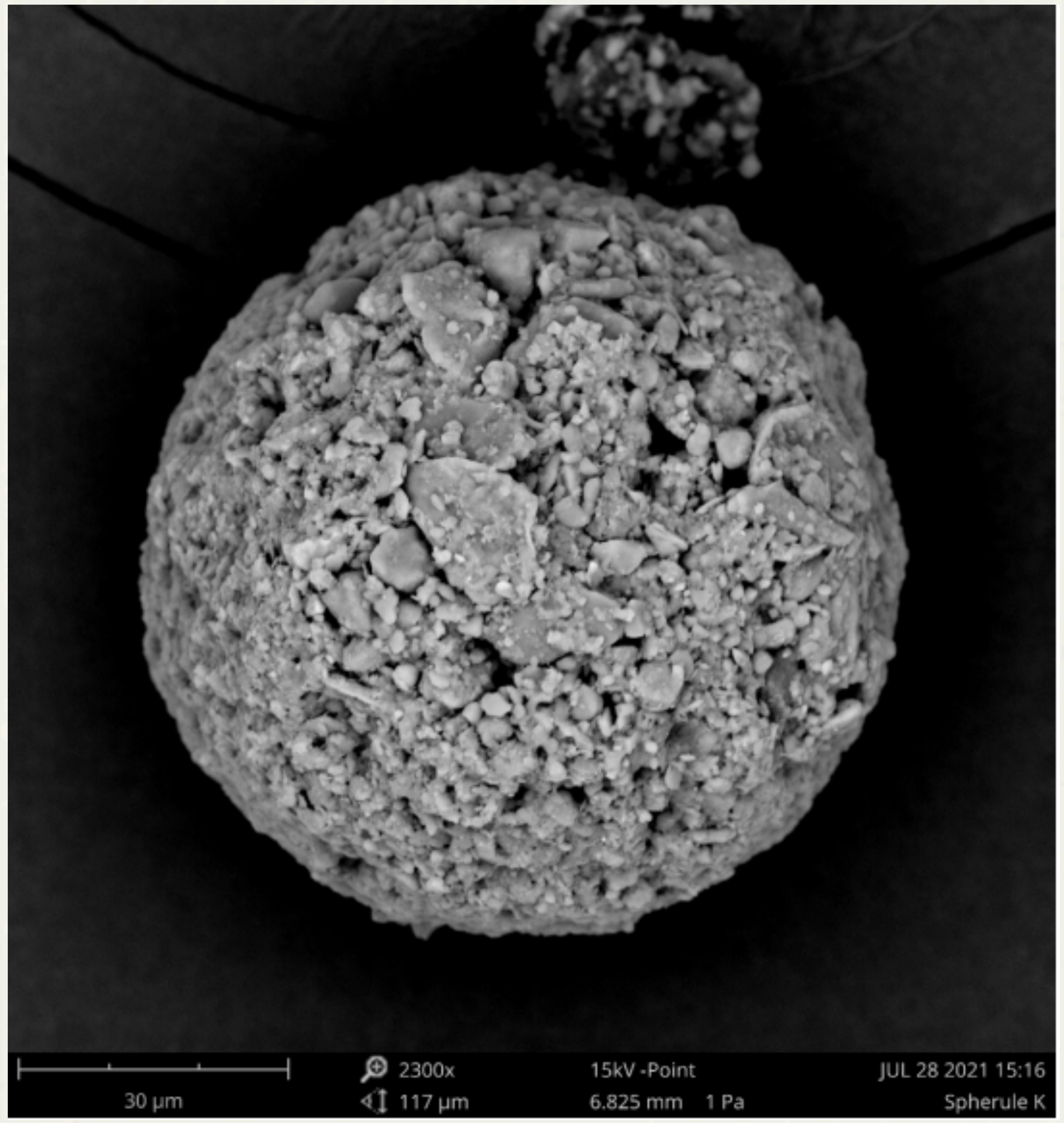


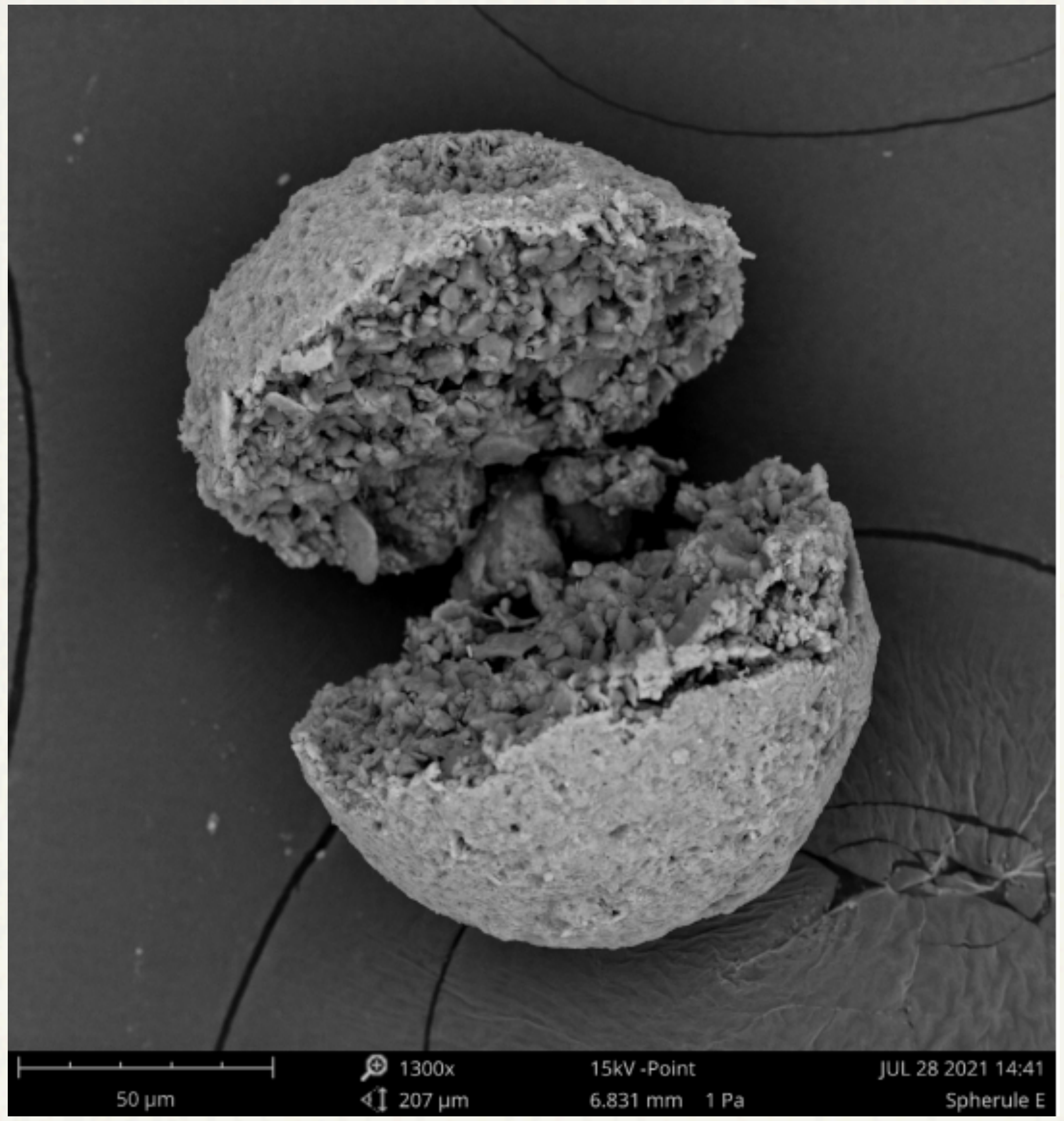
Marine salt:
0.2 - 10 µm

+ secondary aerosol from volatile organic compounds

Introduction: transported components

- Transport of Saharan dust: aggregate formation (iberulites, Switzerland 2021)

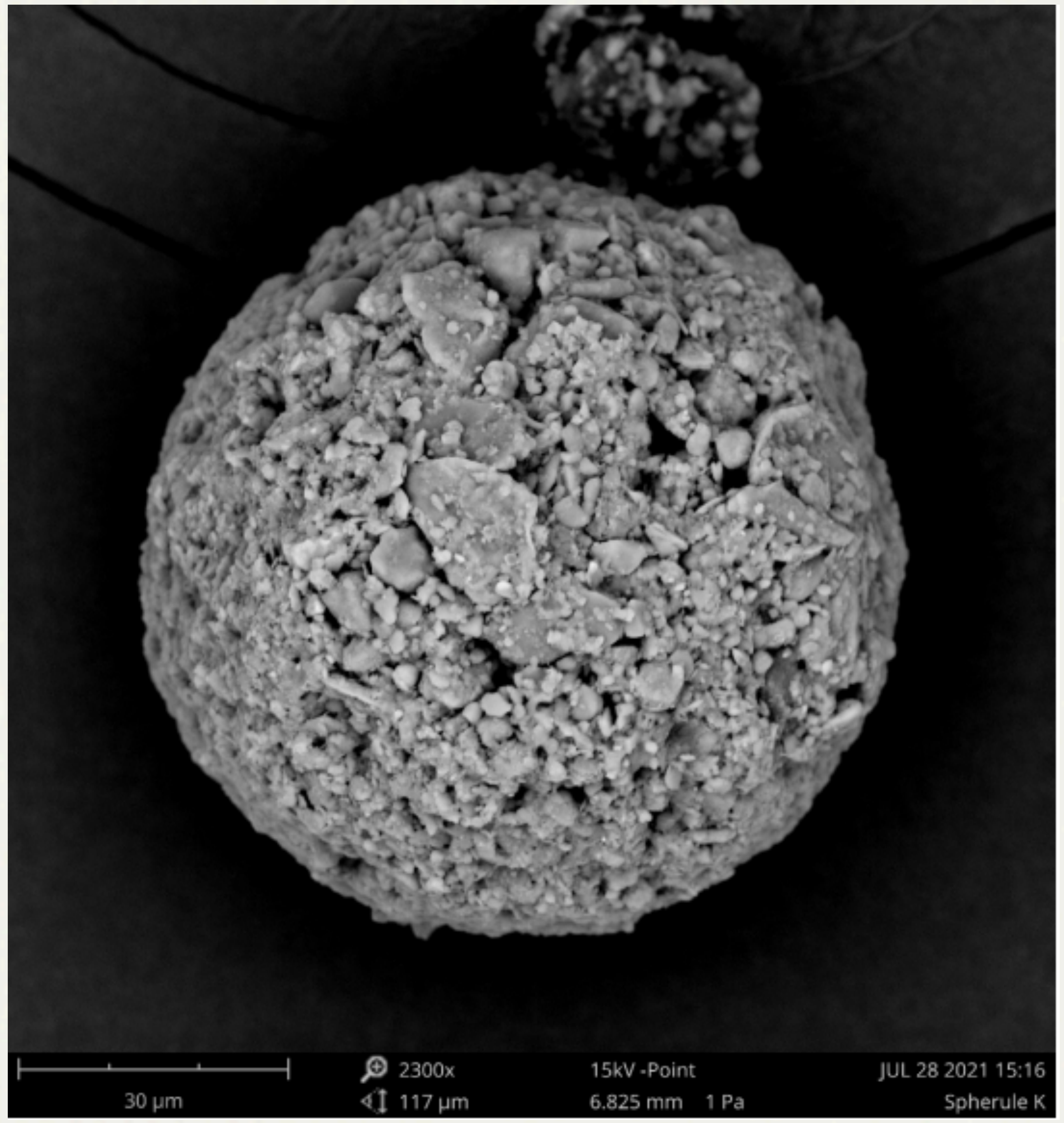


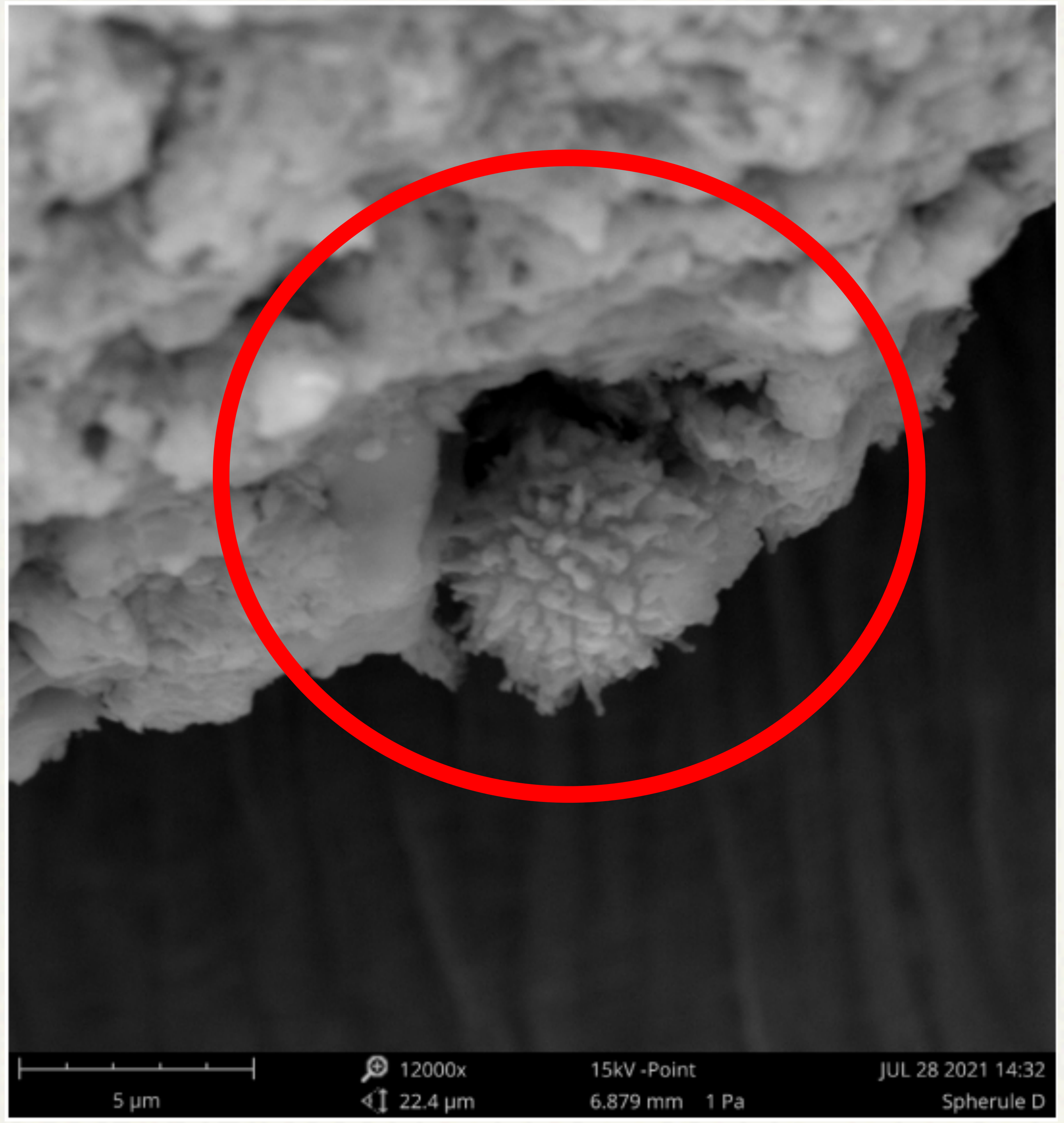


Iberulites from Saharan dust

Introduction: transported components

- Transport of Saharan dust: aggregate formation (iberulites, Switzerland 2021)

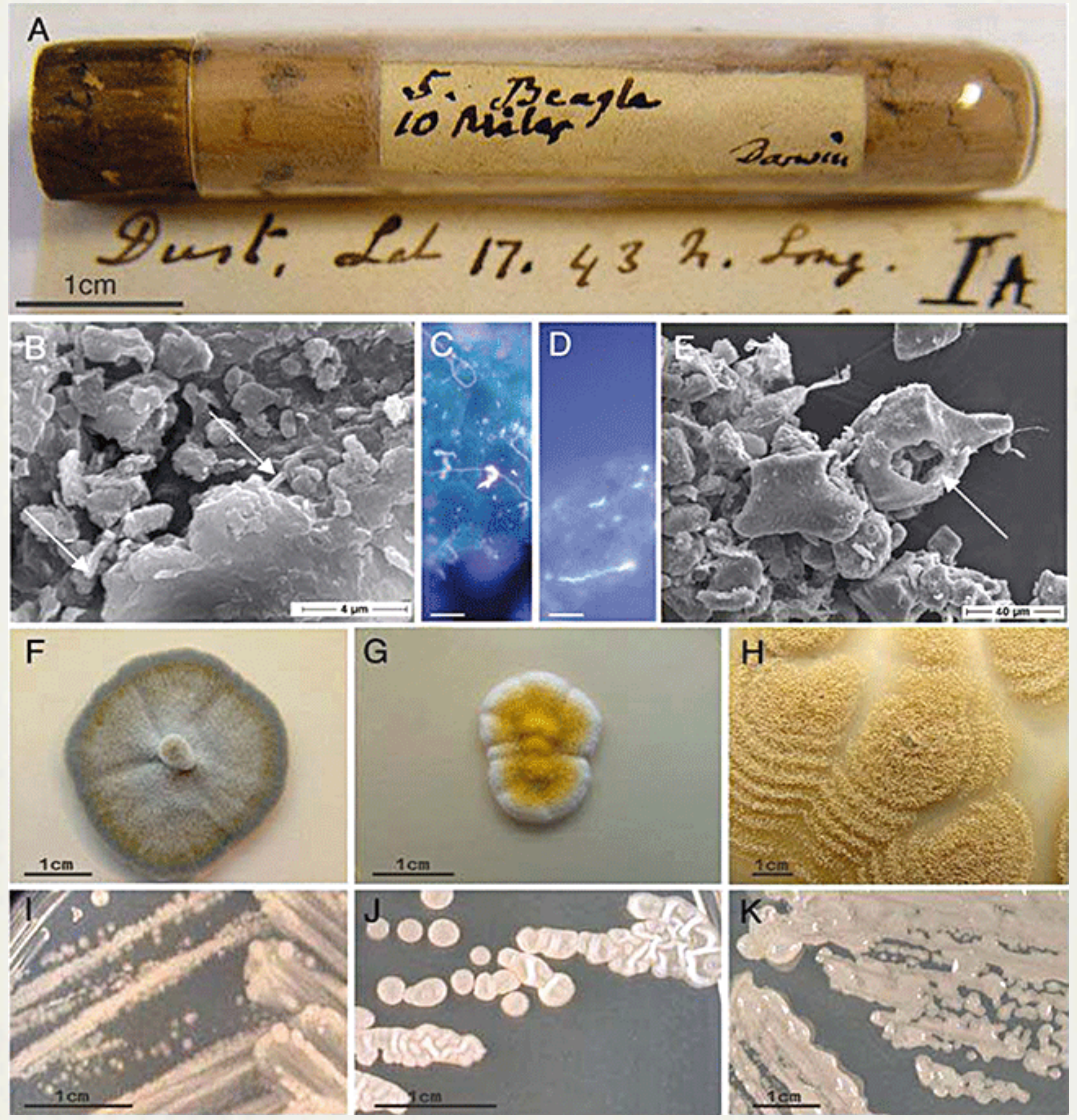




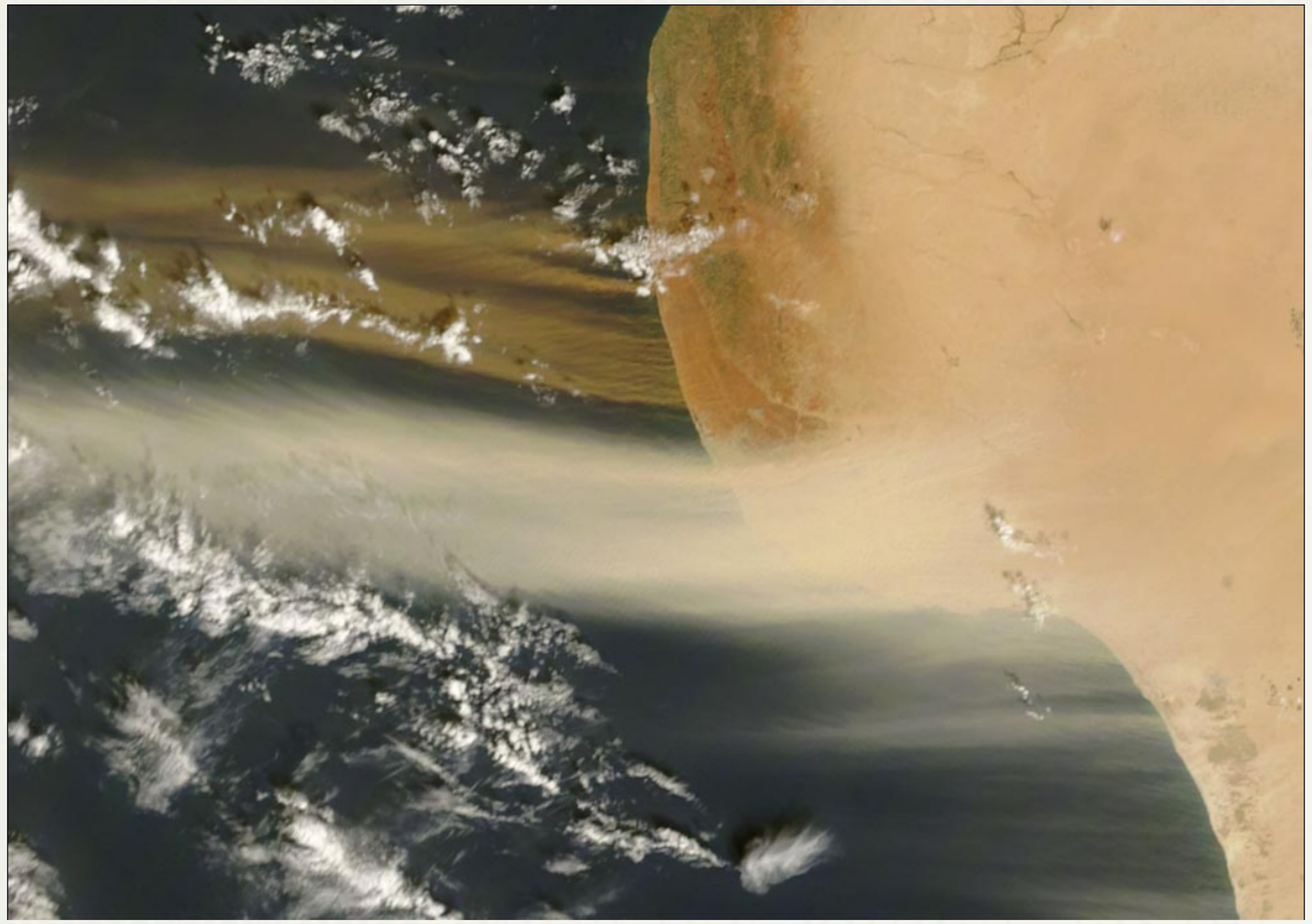
?

Introduction: transported components

- Flow of life in the atmosphere !

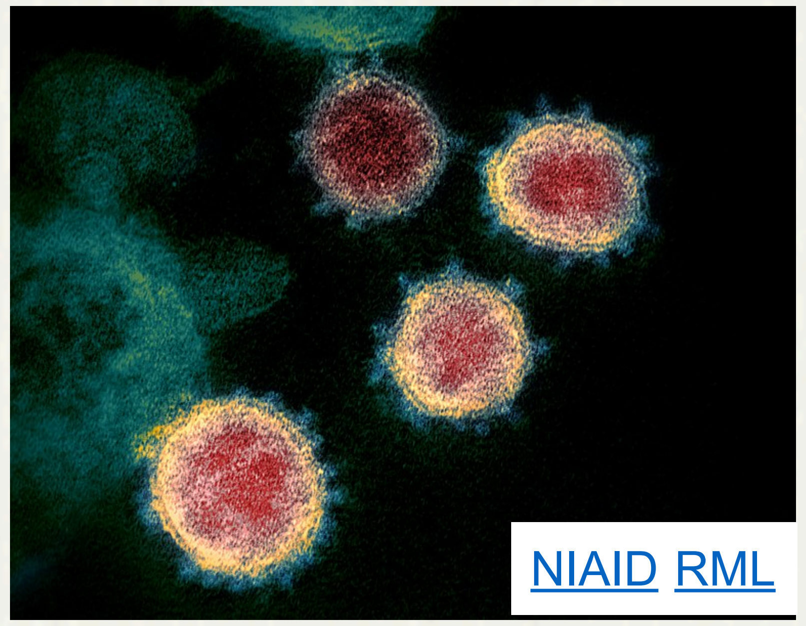


Environmental Microbiology, Volume: 9, Issue: 12, Pages: 2911-2922, First published: 23 October 2007, DOI: (10.1111/j.1462-2920.2007.01461.x)



Introduction: transported components

- Bioaerosol affecting crops, health and cloud formation



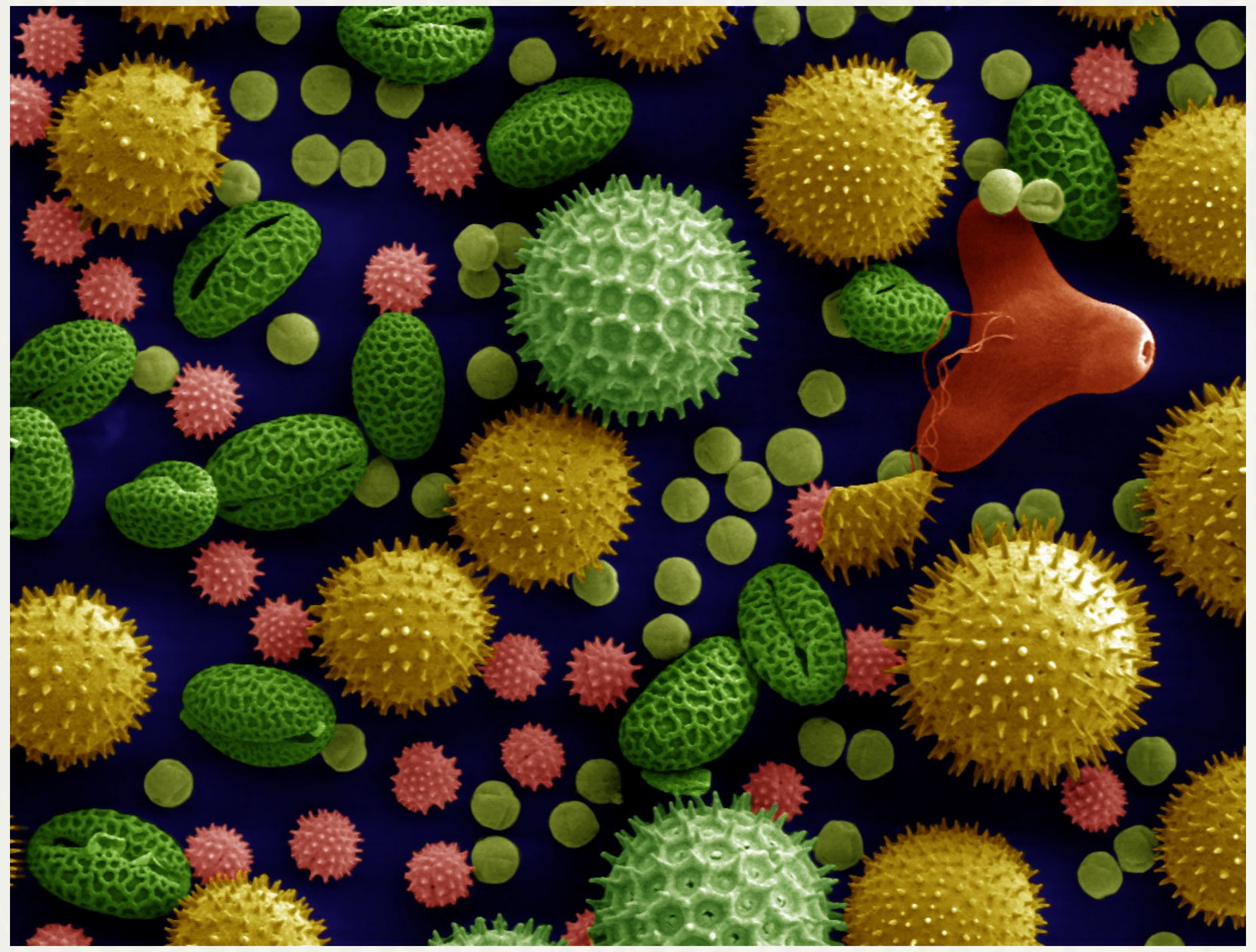
viruses

<

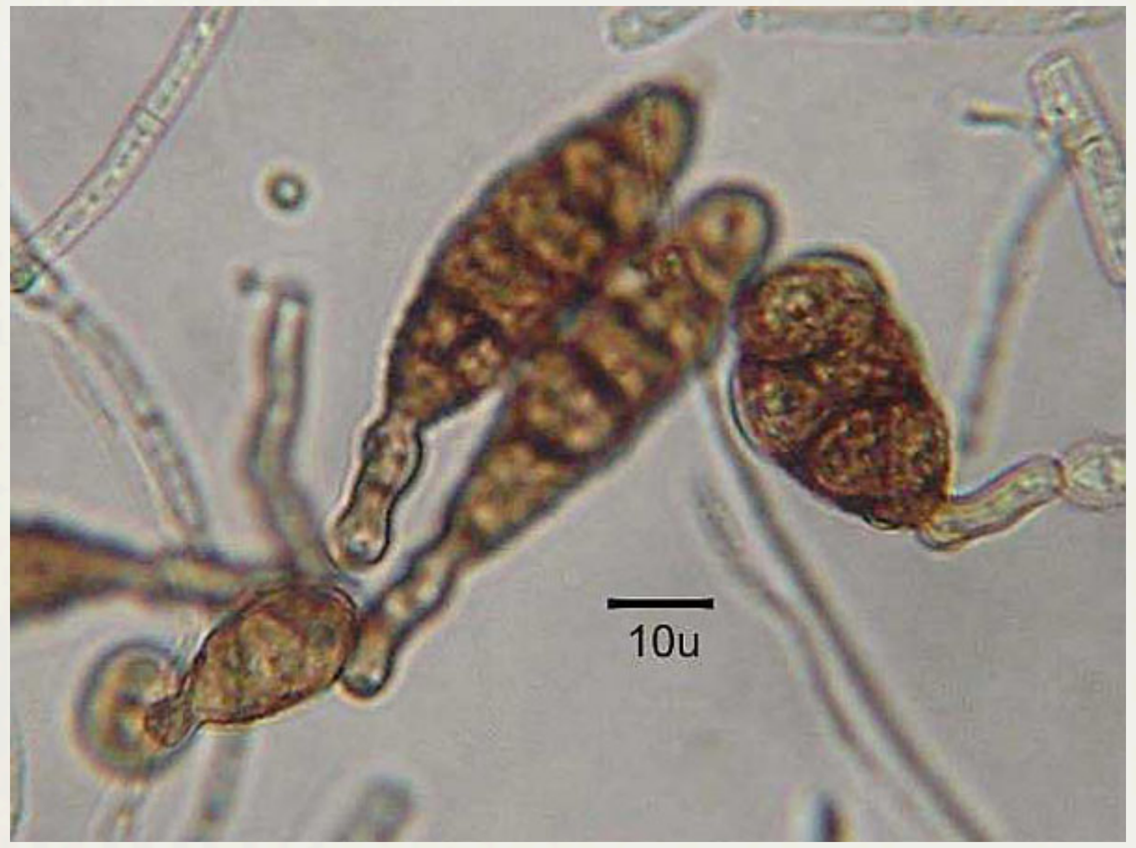
bacteria

1 μm

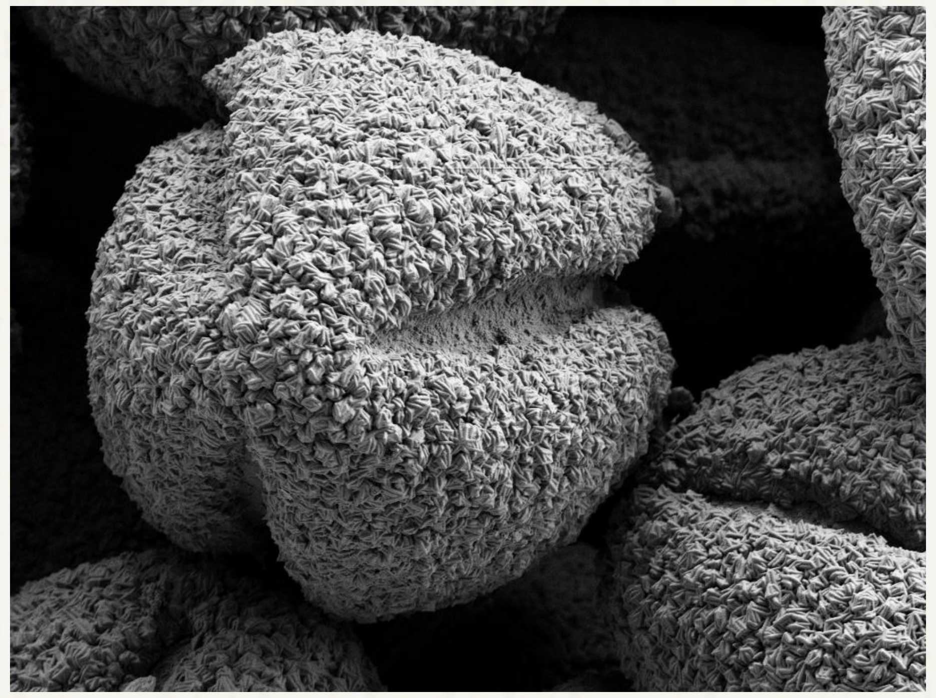
<



Fungal spores



Pollen



Introduction: transported components

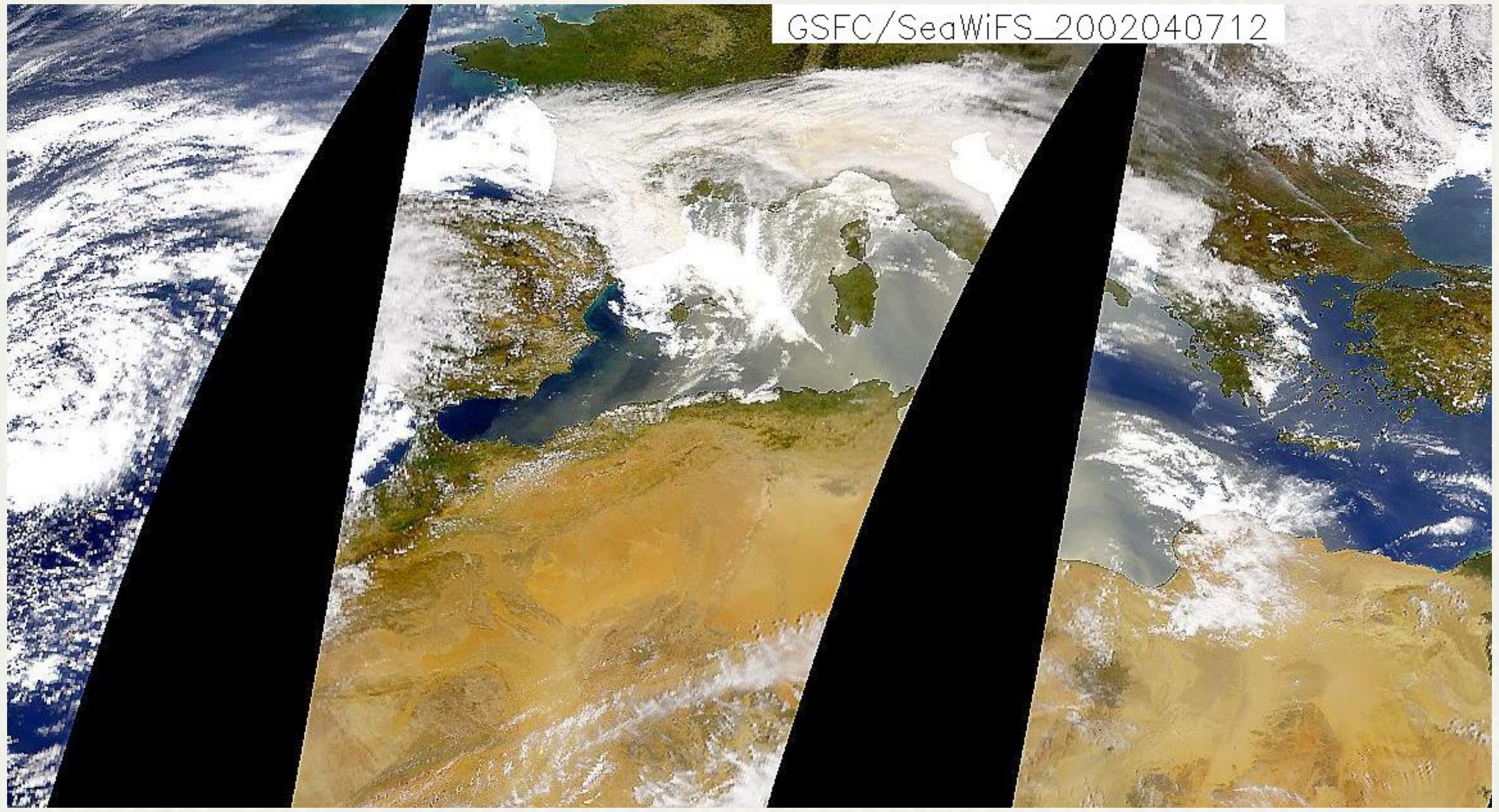
- Contaminants (organic and inorganic)

- Chemicals (gases)

Scales

Environmental transport occurs over a **huge range of scales**.

Saharan dust event

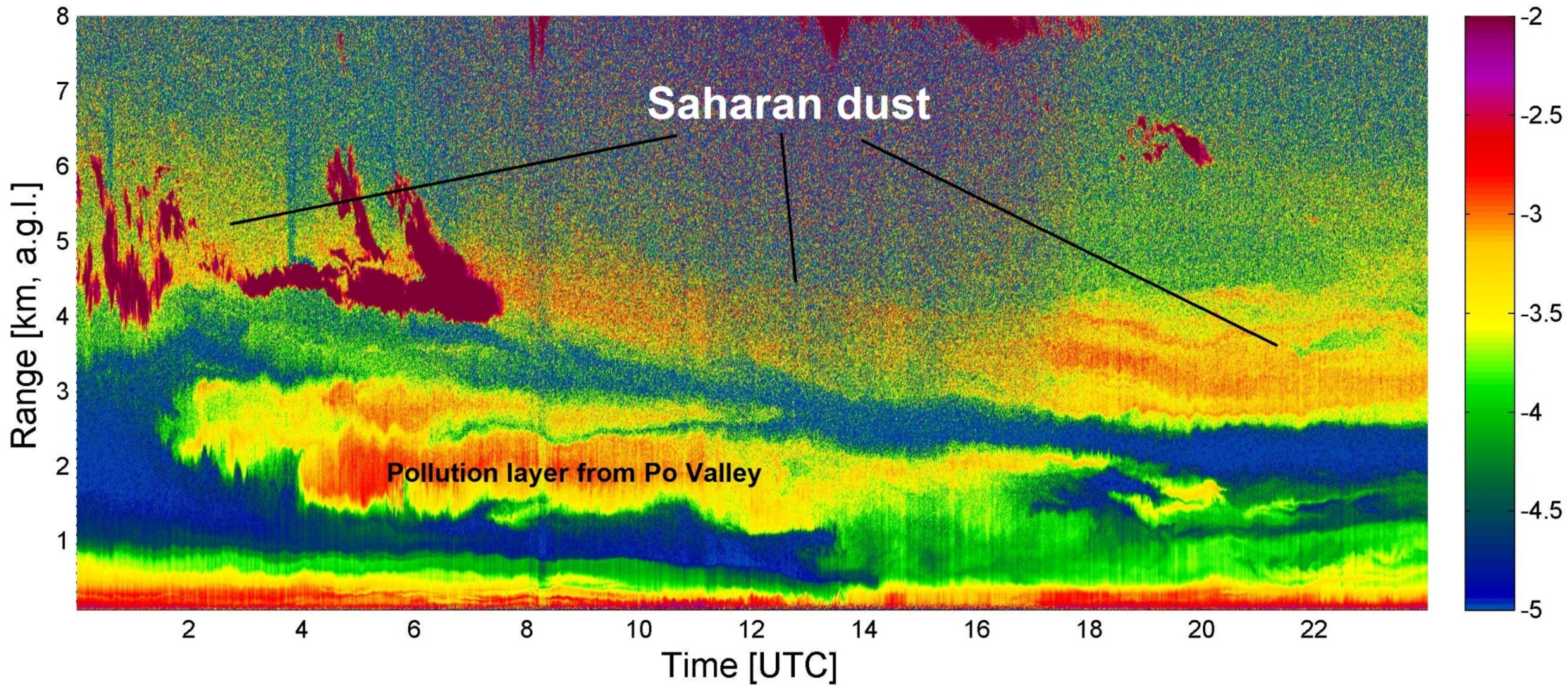


vs

Tracer diffusion

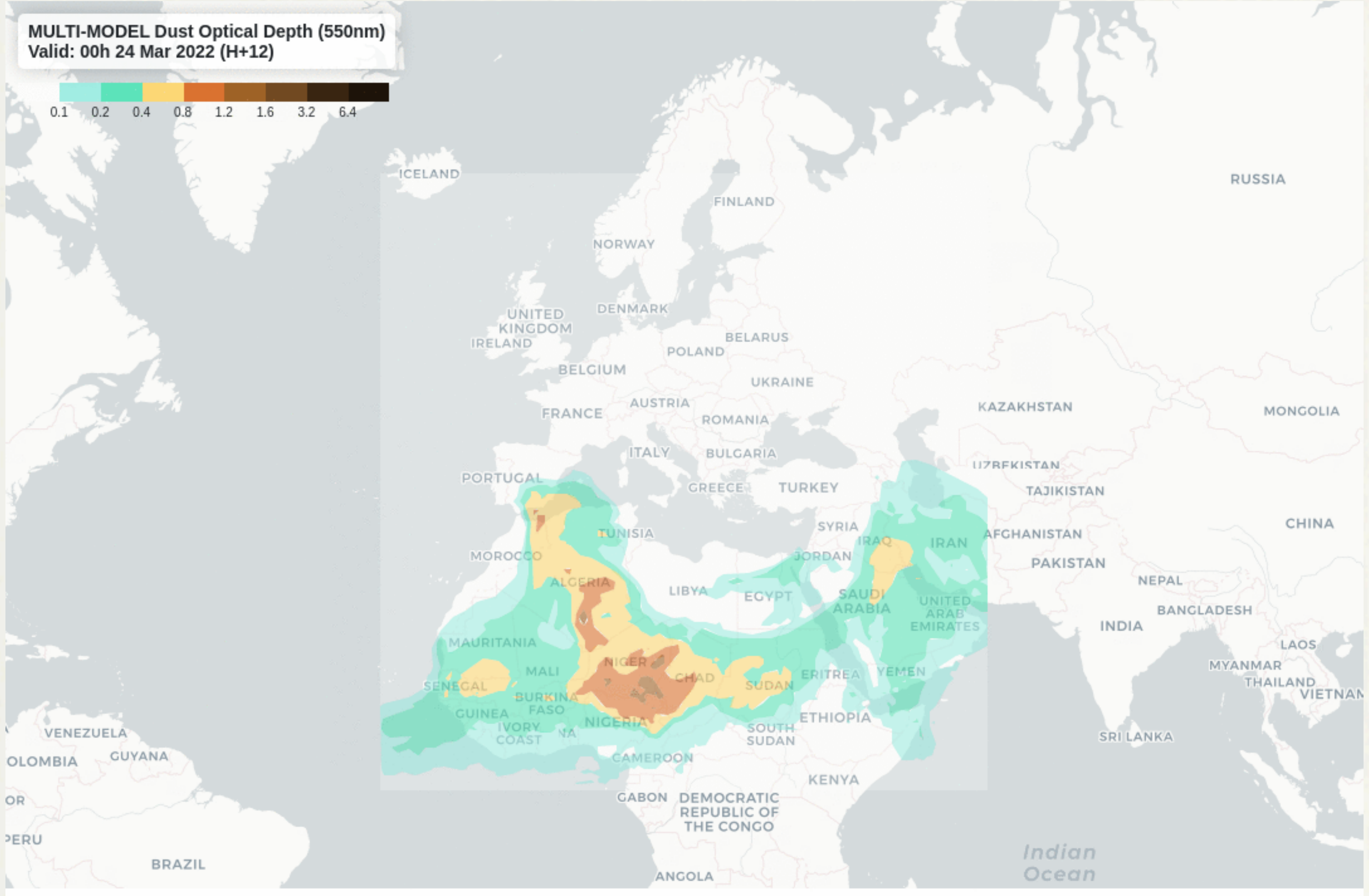
Scales

Transport of Saharan dust: LIDAR measurement in Payerne



Scales

Transport of **Saharan dust**: numerical forecasts (Copernicus Atmosphere Monitoring Service)



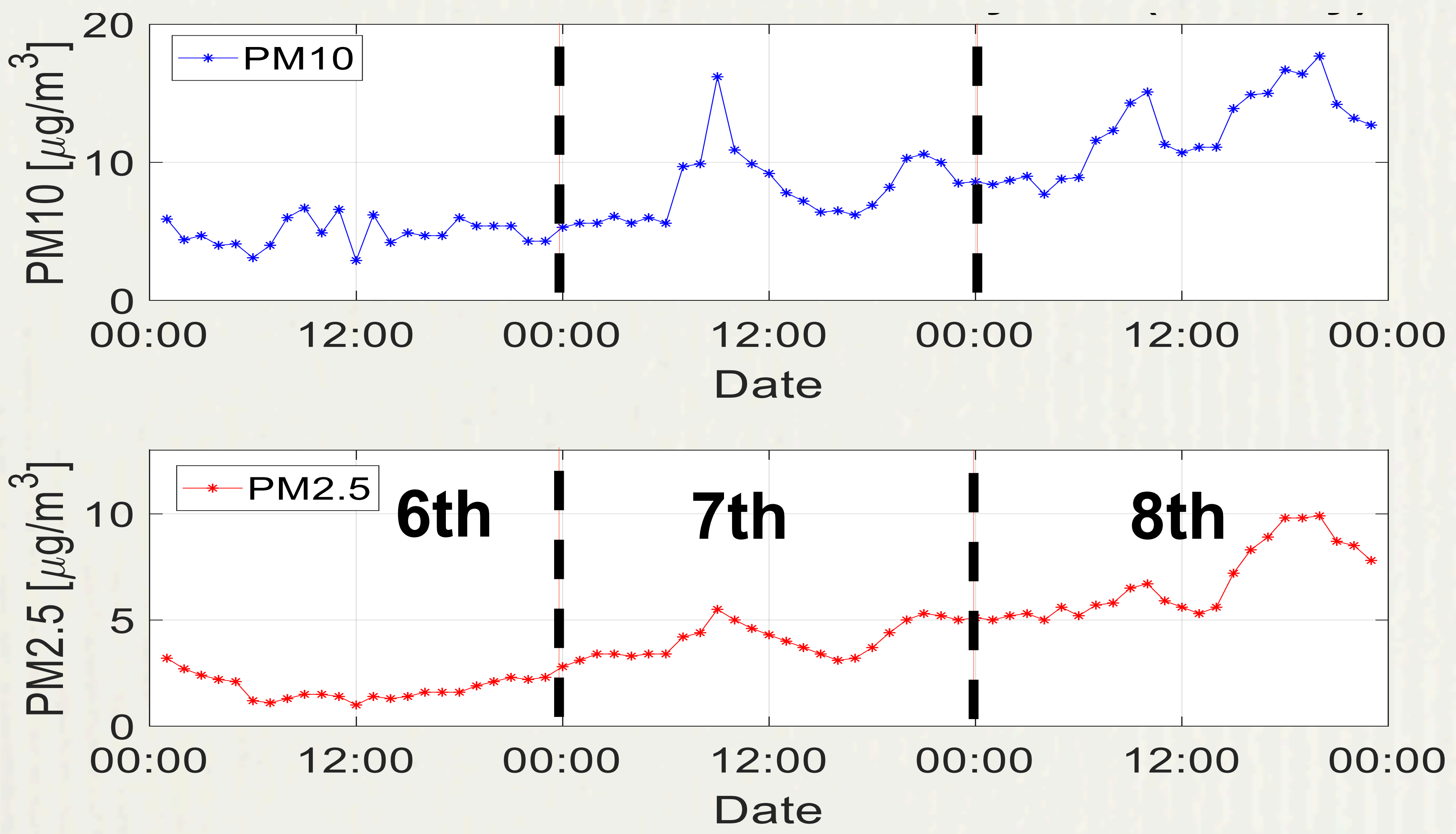
https://atmosphere.copernicus.eu/global-forecast-plots

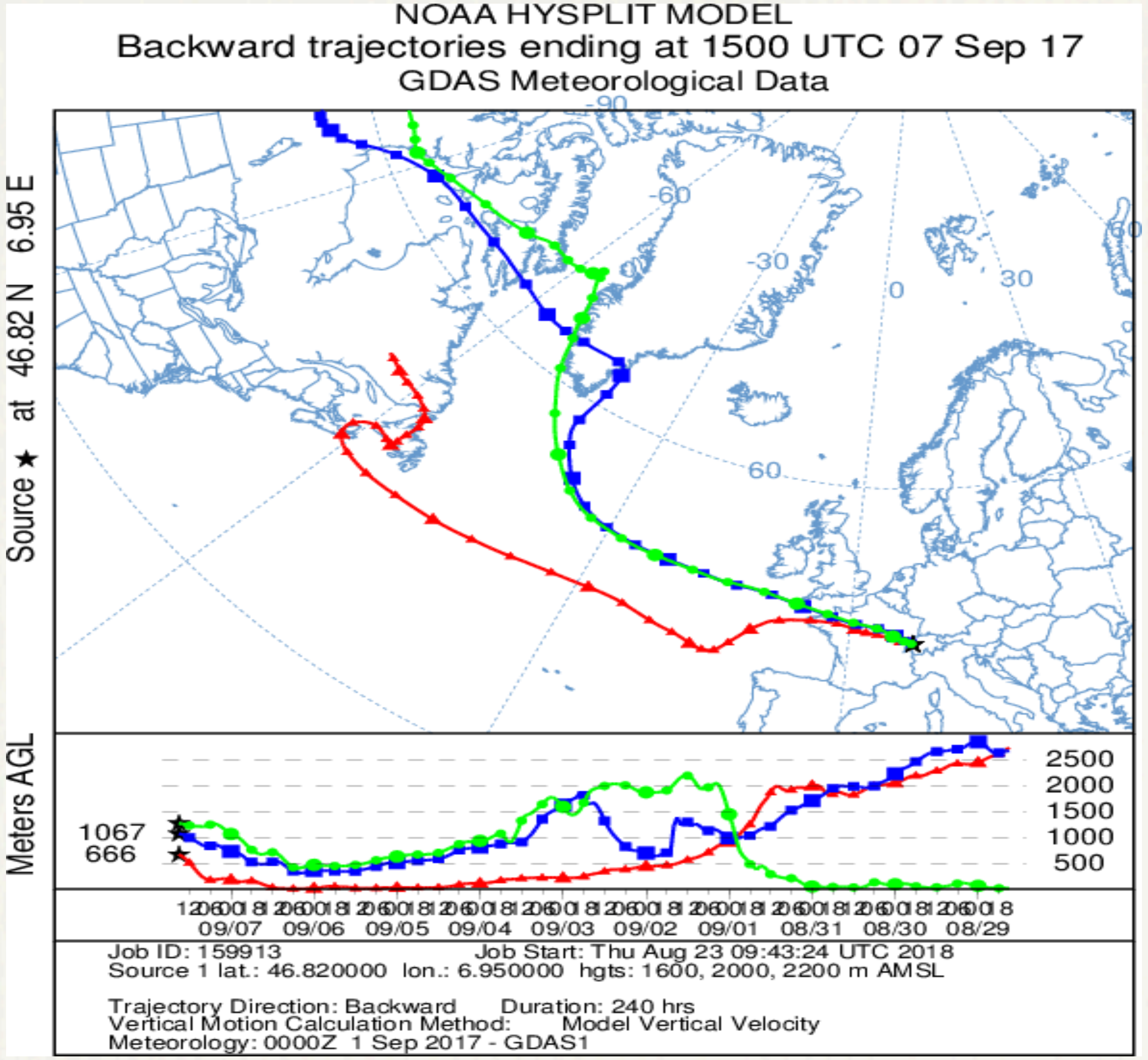
https://atmosphere.copernicus.eu/charts/packages/cams/products/fire-activity?base_time=202309270000&projection=classical_global

Scales

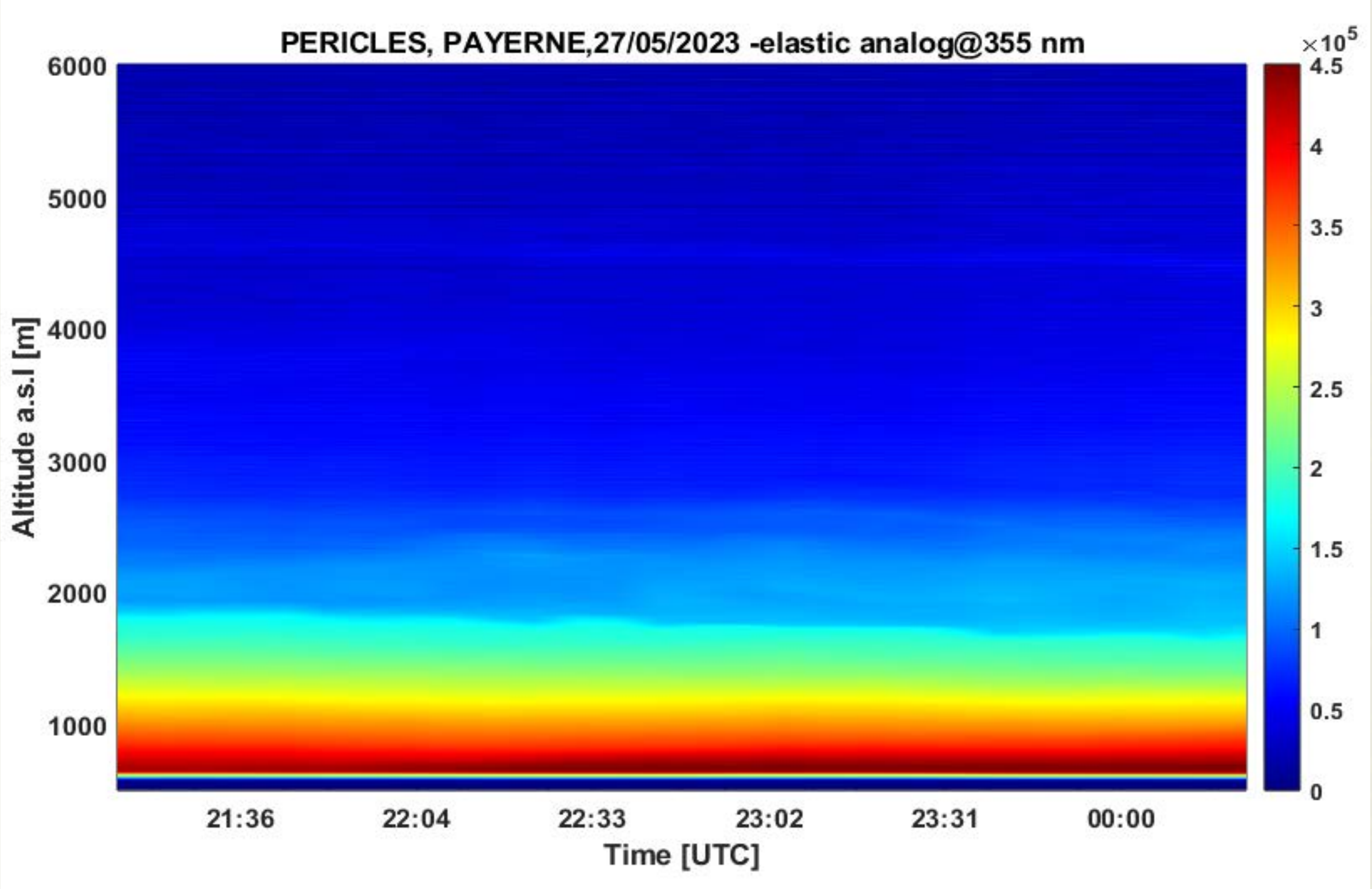
2017 north America fires

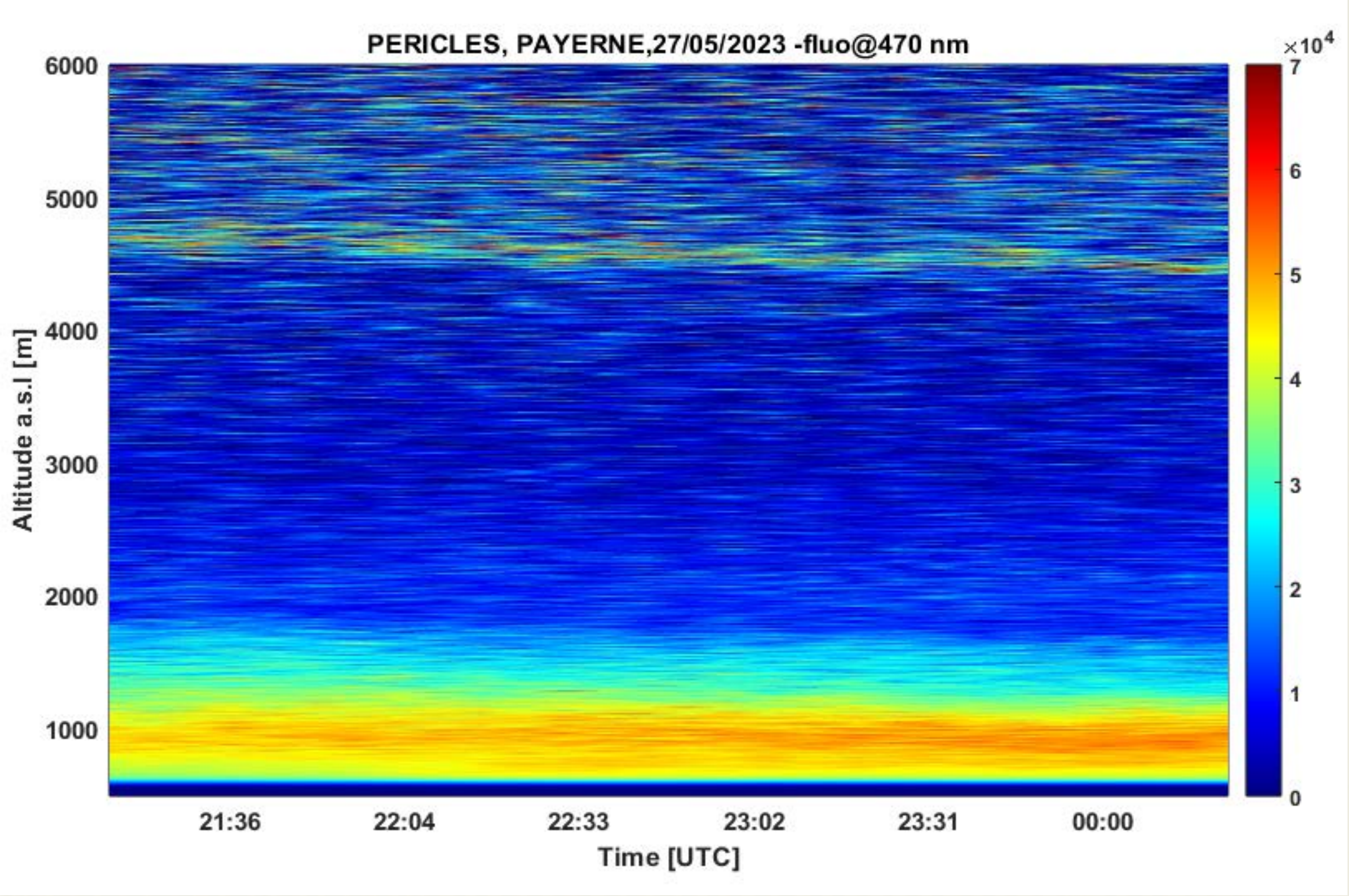
Surface PM concentration (Payerne, CH)

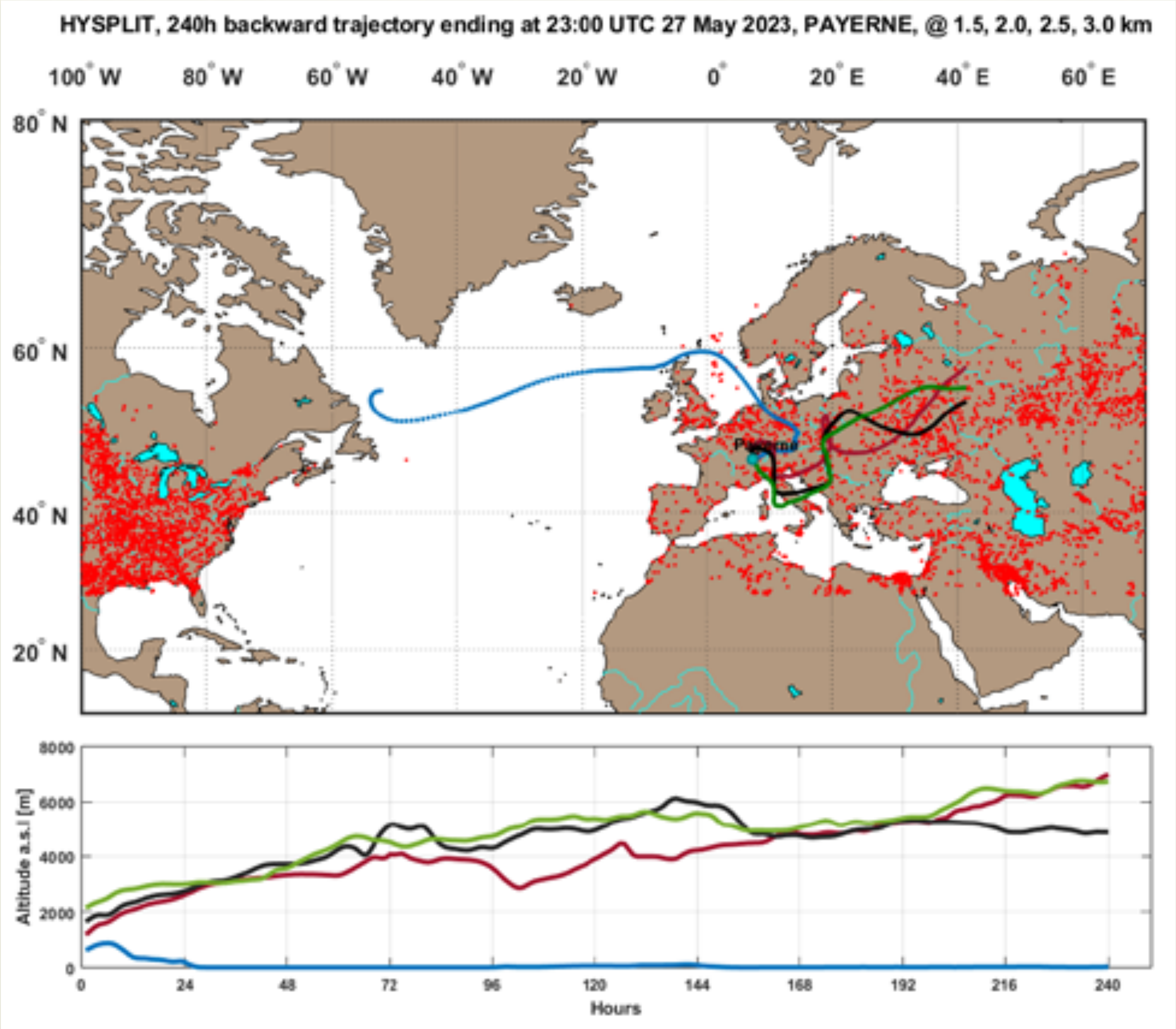


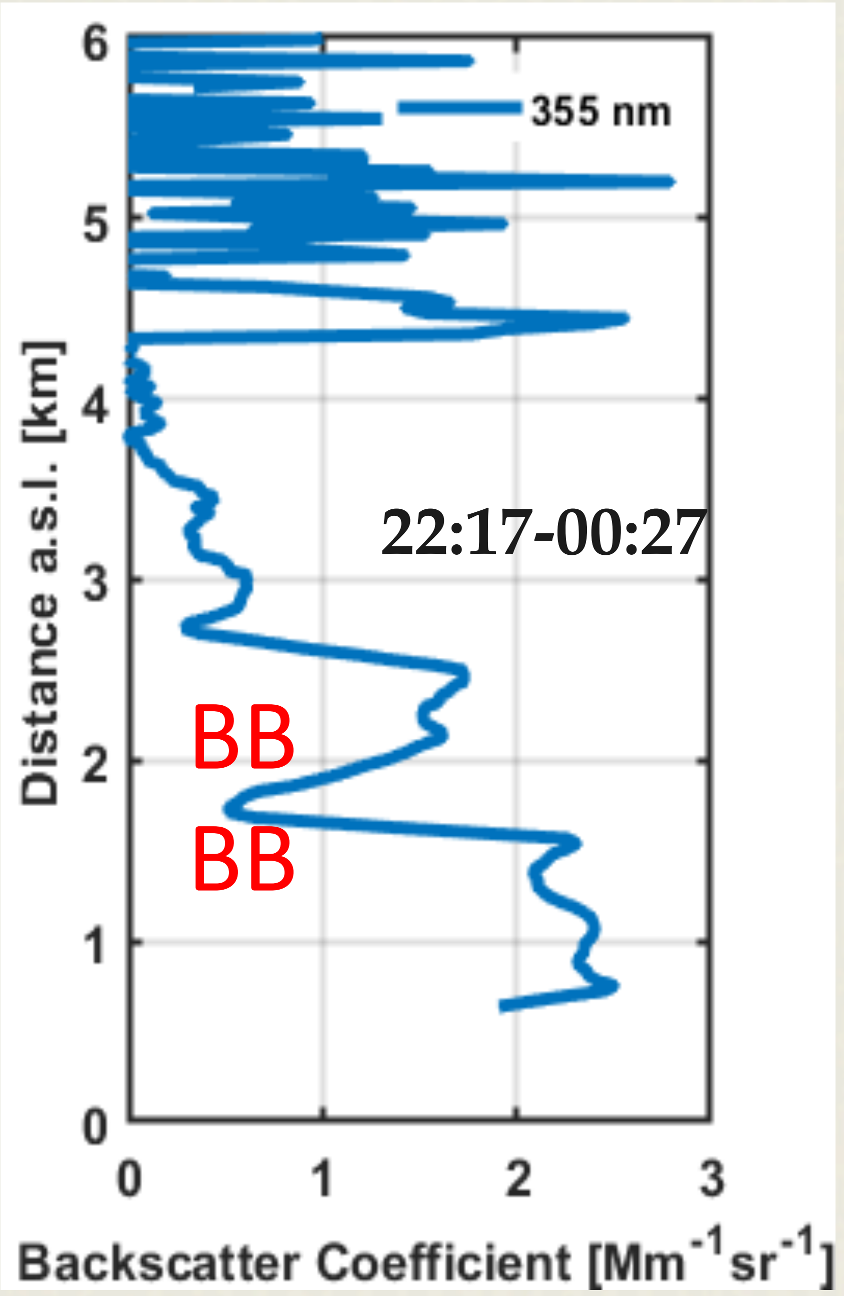


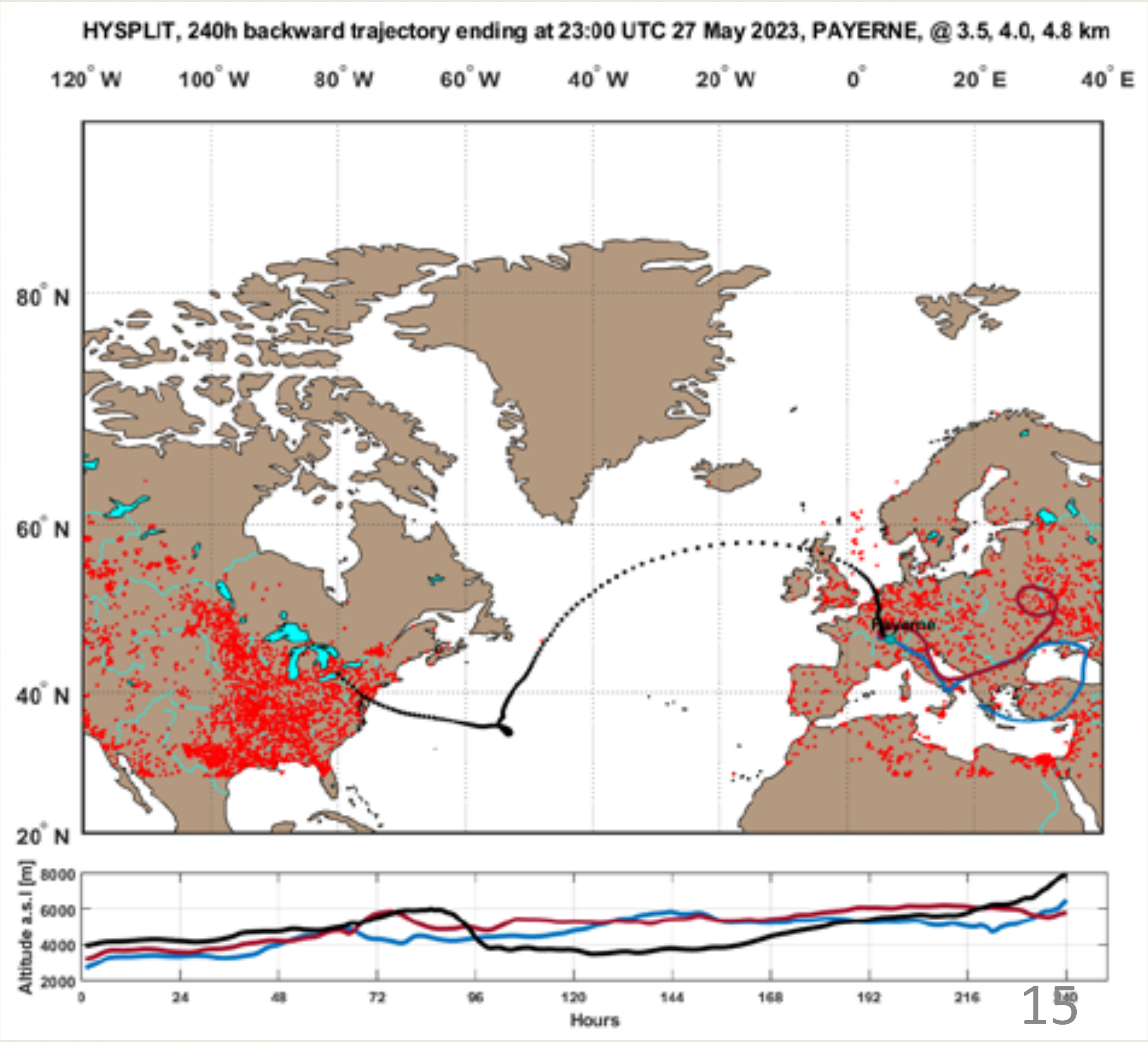
Scales: 2023 Canada fires











Methods

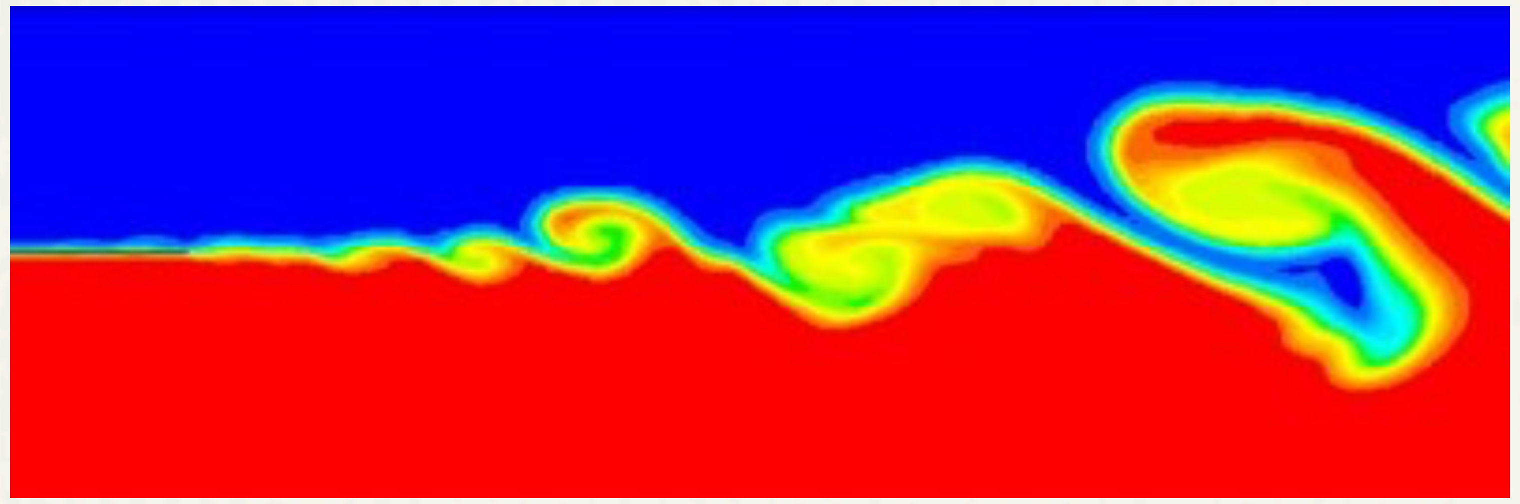
Depending on the scale and on the substance, various approaches are applied

- **Large scale**, compute air parcel trajectories and dispersion/deposition of atmospheric pollutants e.g. Hysplit, SILAM, ICON ART

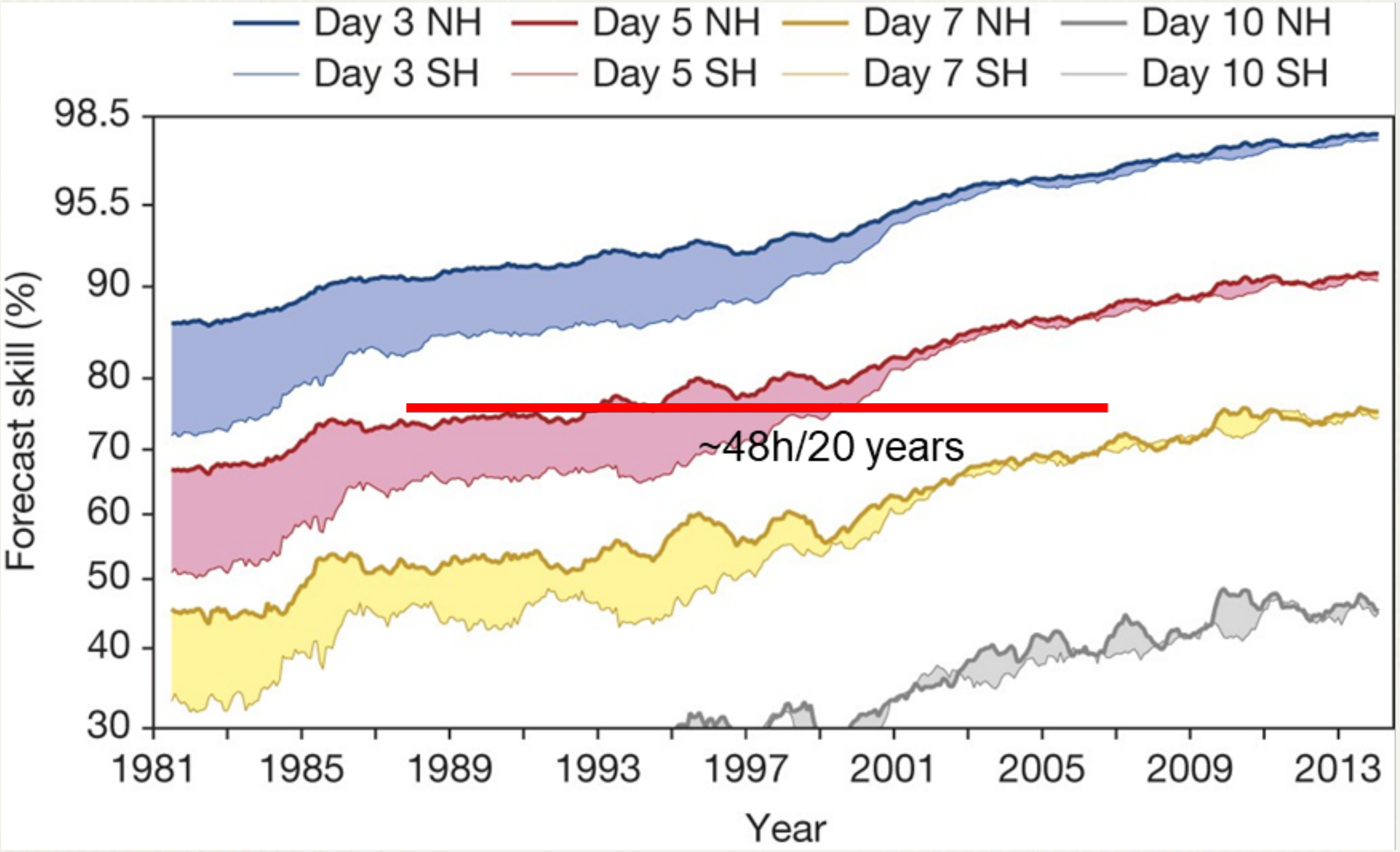
https://www.ready.noaa.gov/HYSPLIT_traj.php

- Shorter or intermediate scale: **CFD software** (e.g. FLUENT)

- Simplified **physical models**



The quiet revolution of traditional weather models



ECMWF

Partnership of European Countries since 1975 including Switzerland

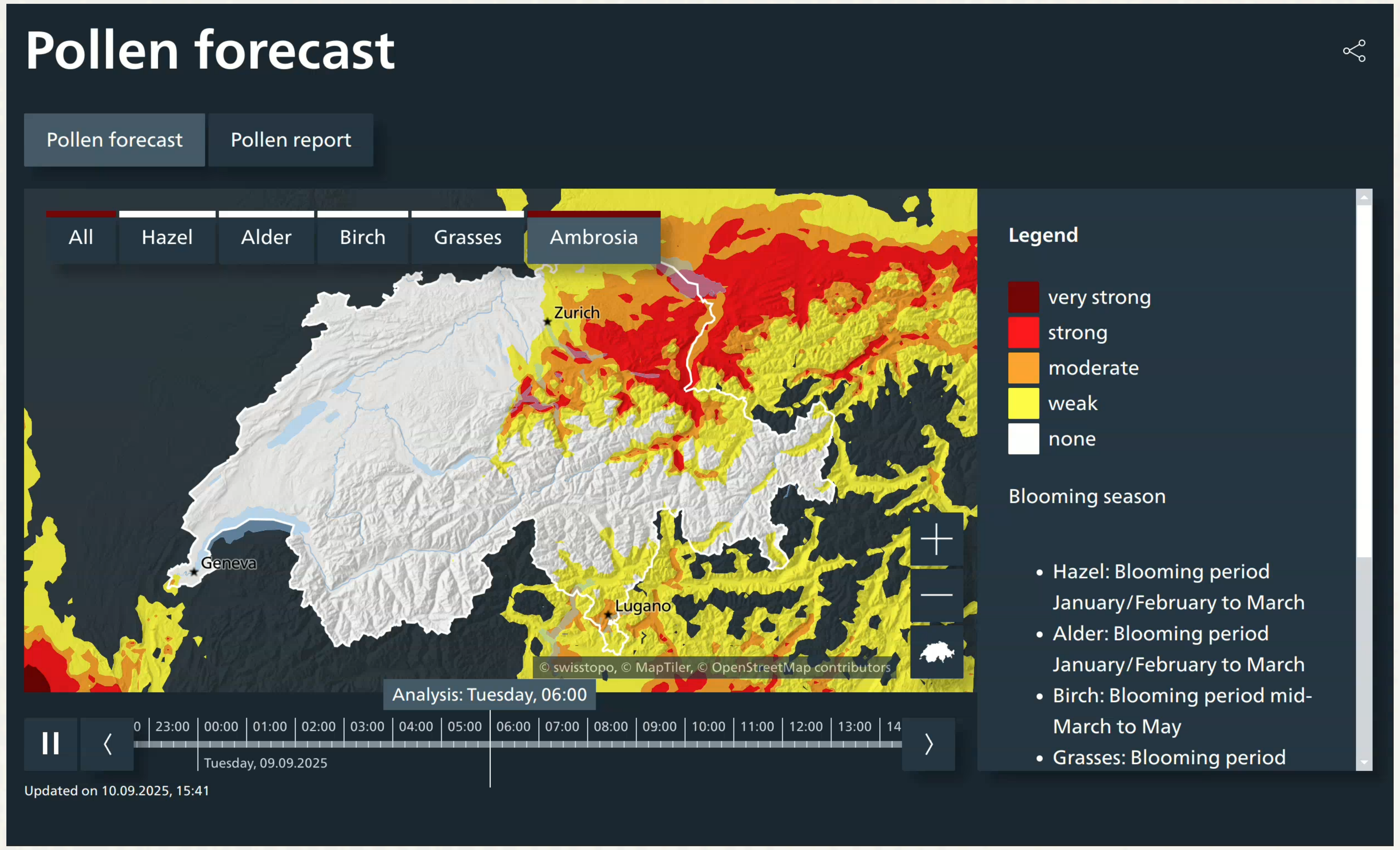
The loud revolution of AI weather models


Collaboration
MeteoSchweiz
NVIDIA
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

Issues

- **Black box** models, output always look "nice", **little effort** to run

- Processes may be **forgotten**: e.g. pollen measurement on the side of GMO maize field



Necessary to understand processes to avoid pitfalls

What are the relevant transport processes ?

- **Advection**: movement of a substance driven by the bulk flow. Mathematically described by a continuity equation (we assume a solenoidal flow $\nabla \cdot \mathbf{v} = 0$)

General expression (continuity equation) $$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

$\mathbf{J} \longrightarrow$ Amount of substance transferred per unit area and unit of time

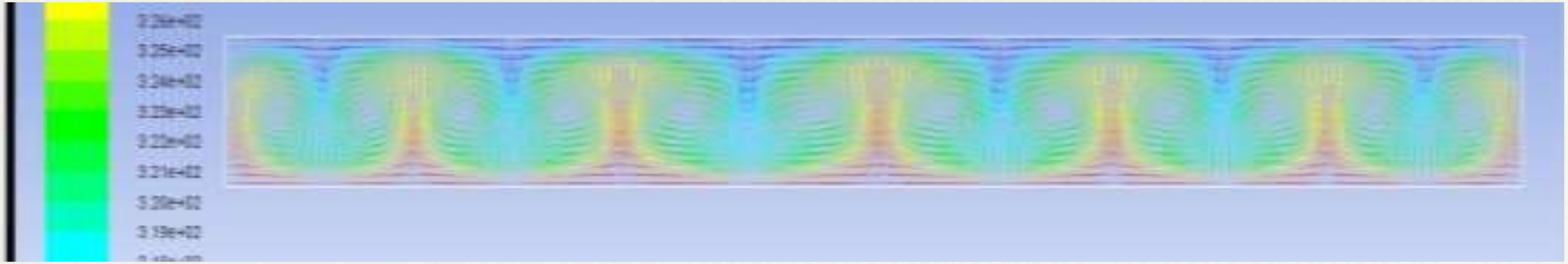
If we have only transport by advection

$$\mathbf{J}(x, y, z, t) = C(x, y, z, t)\mathbf{u}(x, y, z, t)$$

$$\Rightarrow \quad \frac{\partial C}{\partial t} + \mathbf{u}\nabla C = 0$$

What are the relevant transport processes ?

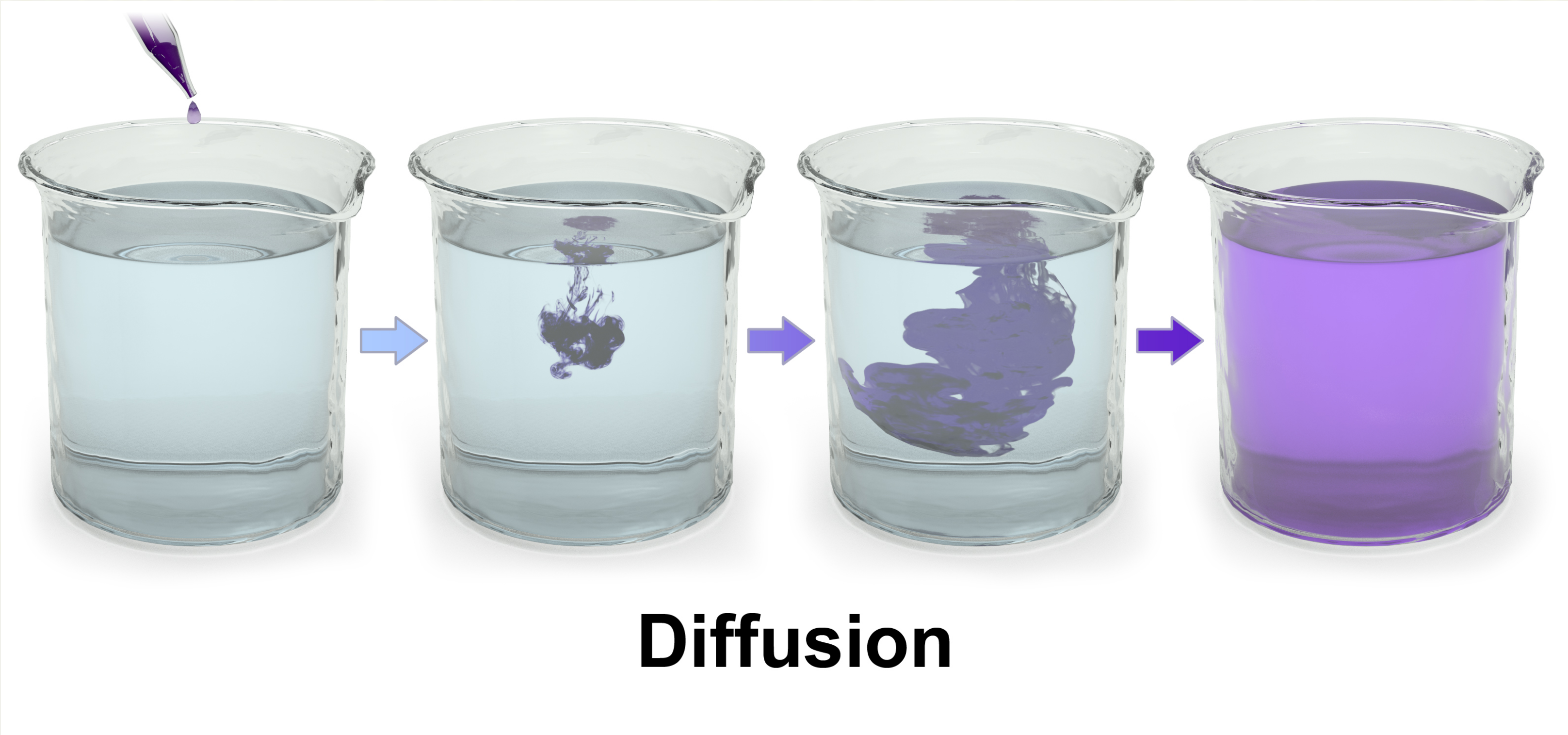
- **Convection**: buoyancy-driven motion. Not directly treated in this lecture,

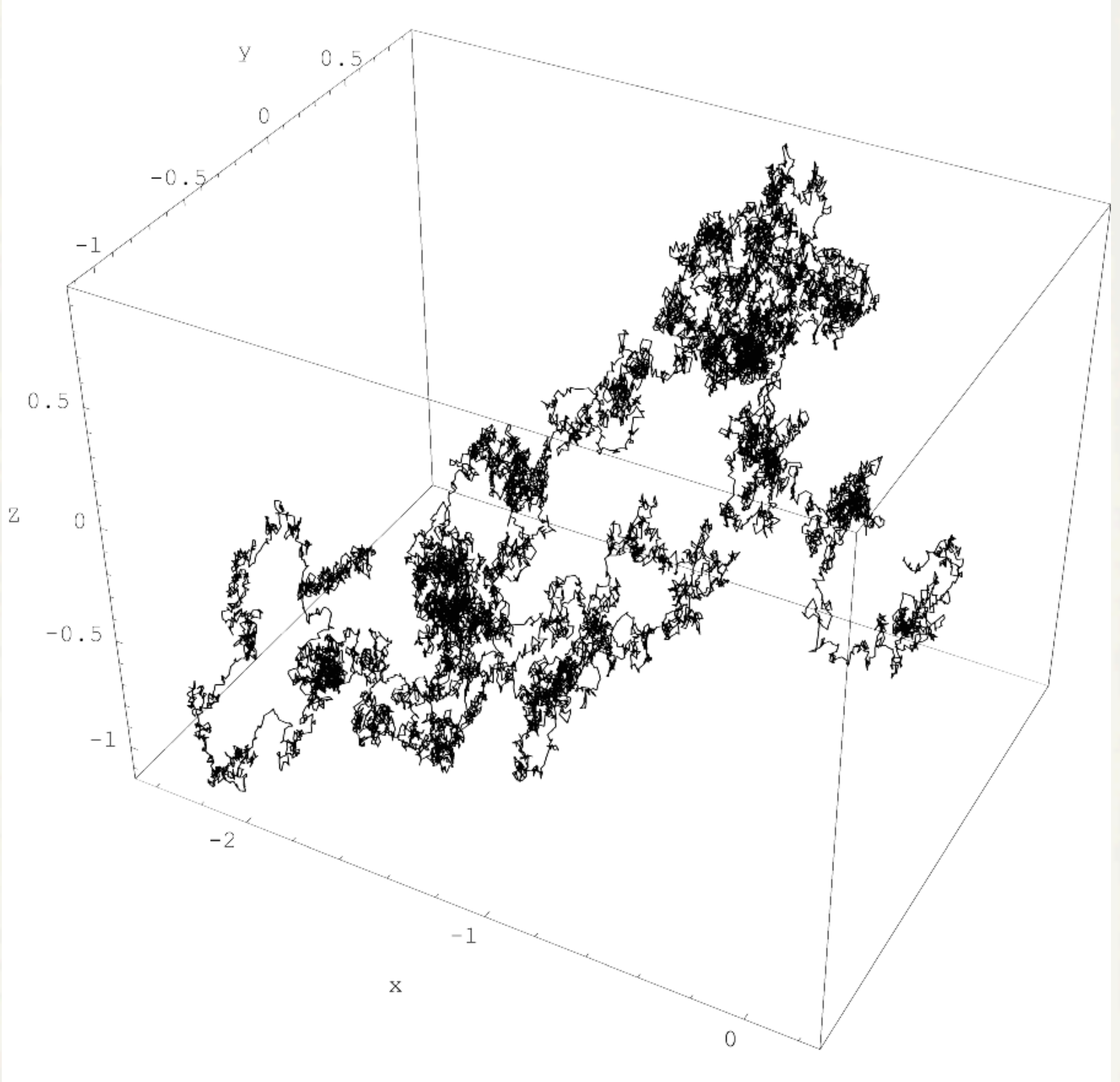


Rayleigh-Bénard instability

What are the relevant transport processes ?

- **Molecular** diffusion: occurs in a fluid at rest or in a laminar flow, due to the thermal excitation of fluid molecules.

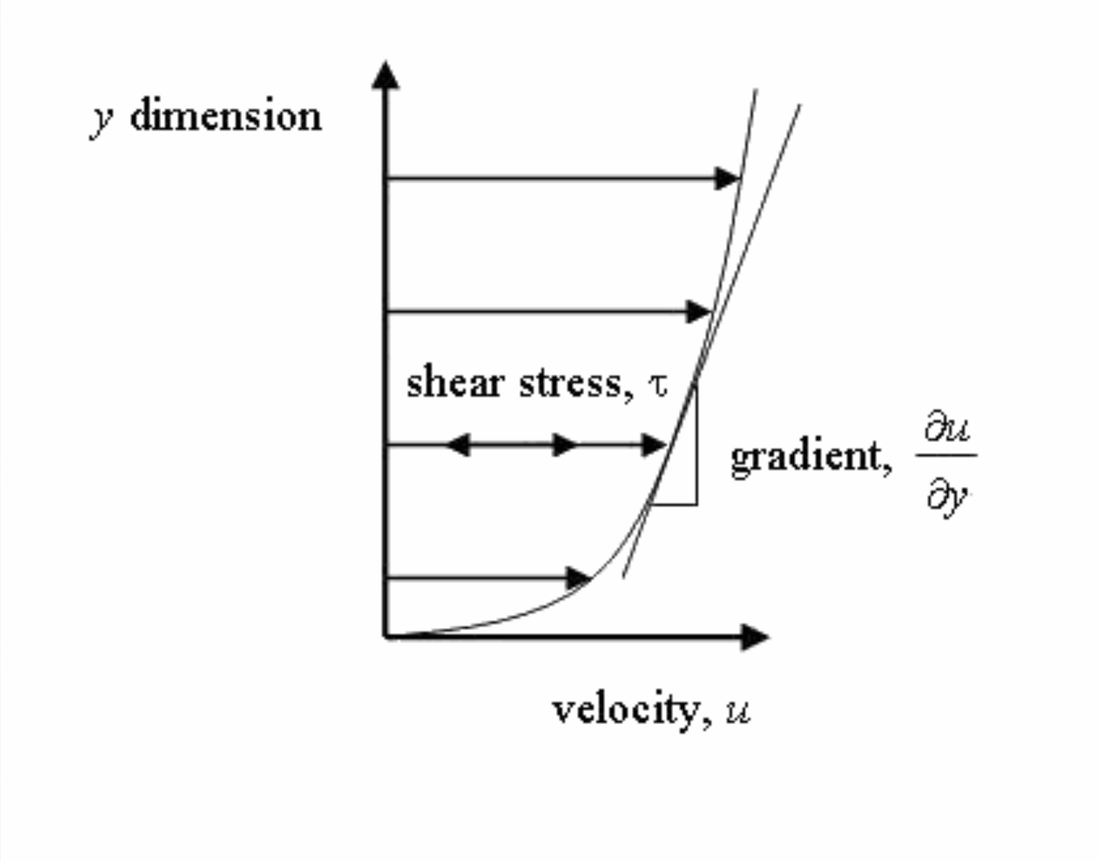




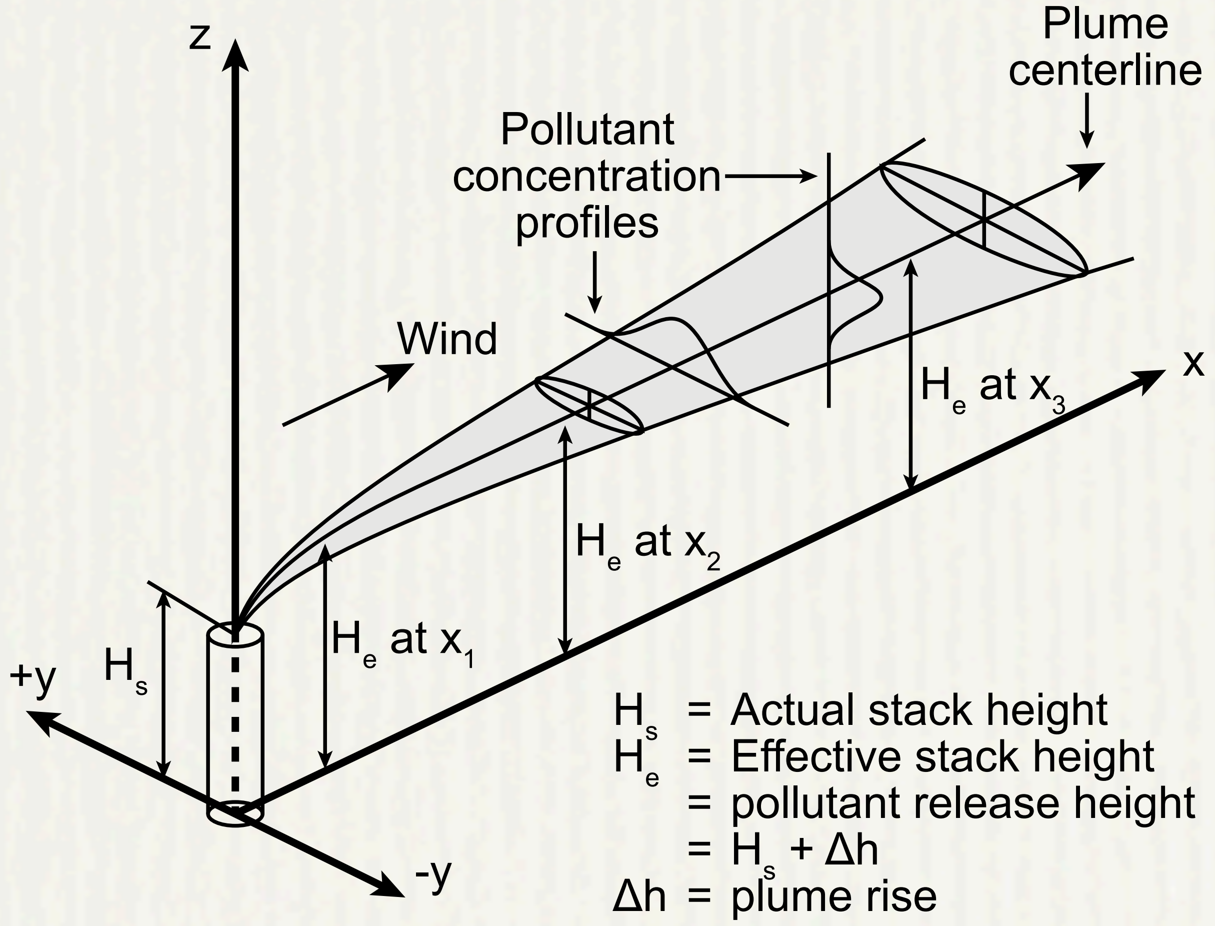
- **Turbulent** diffusion: similar to molecular diffusion but occurs in a turbulent flow. Similar mathematical description, but diffusion coefficient typically orders of magnitude larger.

Introduction

- Shear: Advection with a gradient velocity profile (e.g. log-profile in the boundary layer)



- Dispersion: Combined effect of shear and transverse (turbulent) diffusion



Movement of center of mass: advection, convection, shear

Mixing, spreading: diffusion, dispersion

III) Molecular diffusion

Molecular diffusion

Basic concept: **random migration** of molecules or small particles due to thermal energy (solute in solvent, e.g. benzene in water)

Simple example: ideal gas ("randomly" moving point particles that do not interact except when they collide elastically)

Kinetic energy (average !): $\langle \frac{1}{2} m v_x^2 \rangle = \frac{1}{2} k_B T$

In three dimensions: $\langle \frac{1}{2} (m v_x^2 + m v_y^2 + m v_z^2) \rangle = \frac{3}{2} k_B T$

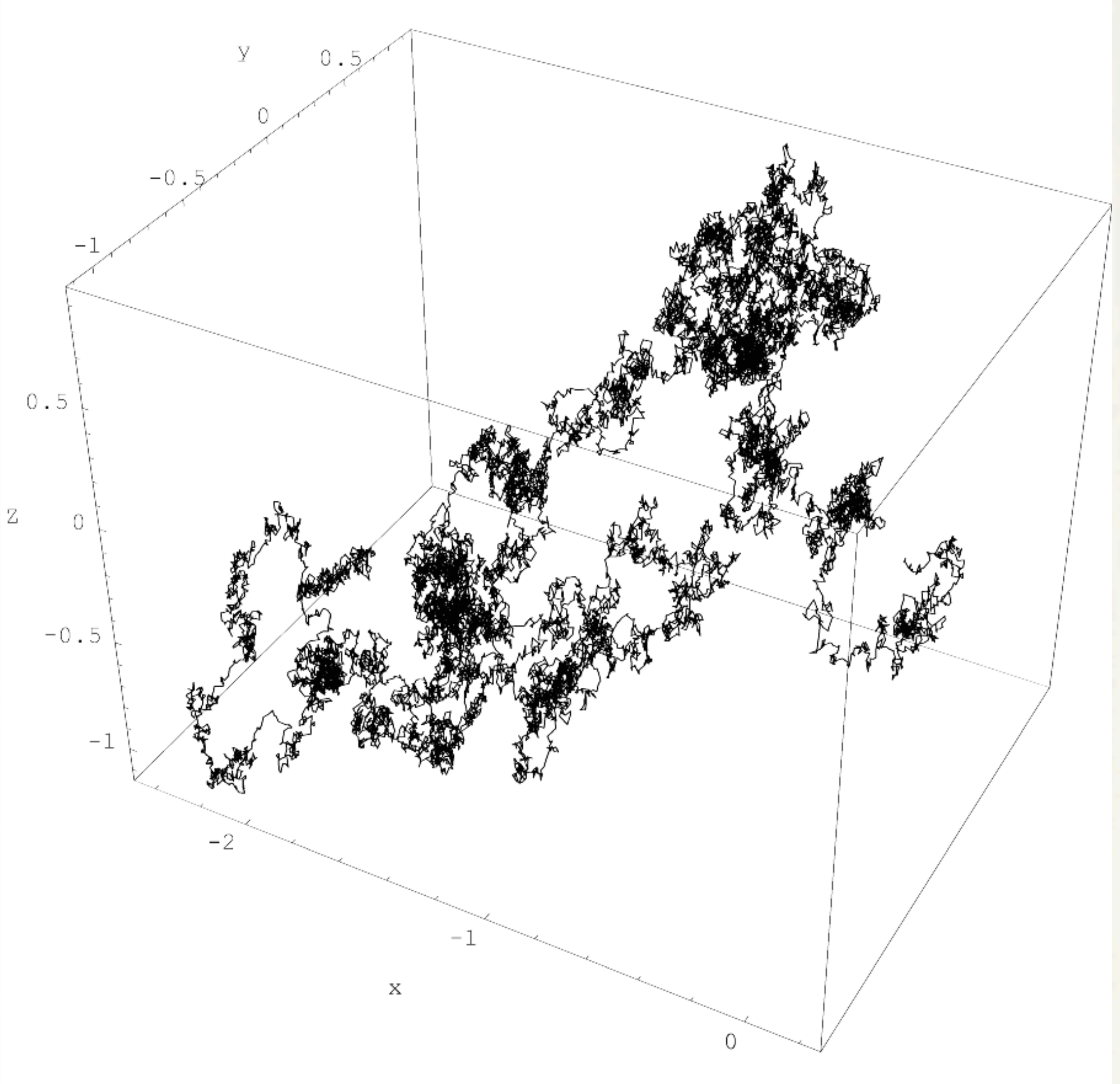
Boltzmann constant: $k_B = 1.38 \; 10^{-23}$ J/K

Molecular diffusion

The typical average thermal velocities are **very large**.

Average velocity of N_2 molecules at room temperature: 464 m/s !

The trajectories of molecules are however not straight (**collisions**) !



Air at ambient temperature (2.7 10^{25} molecules / m^3)

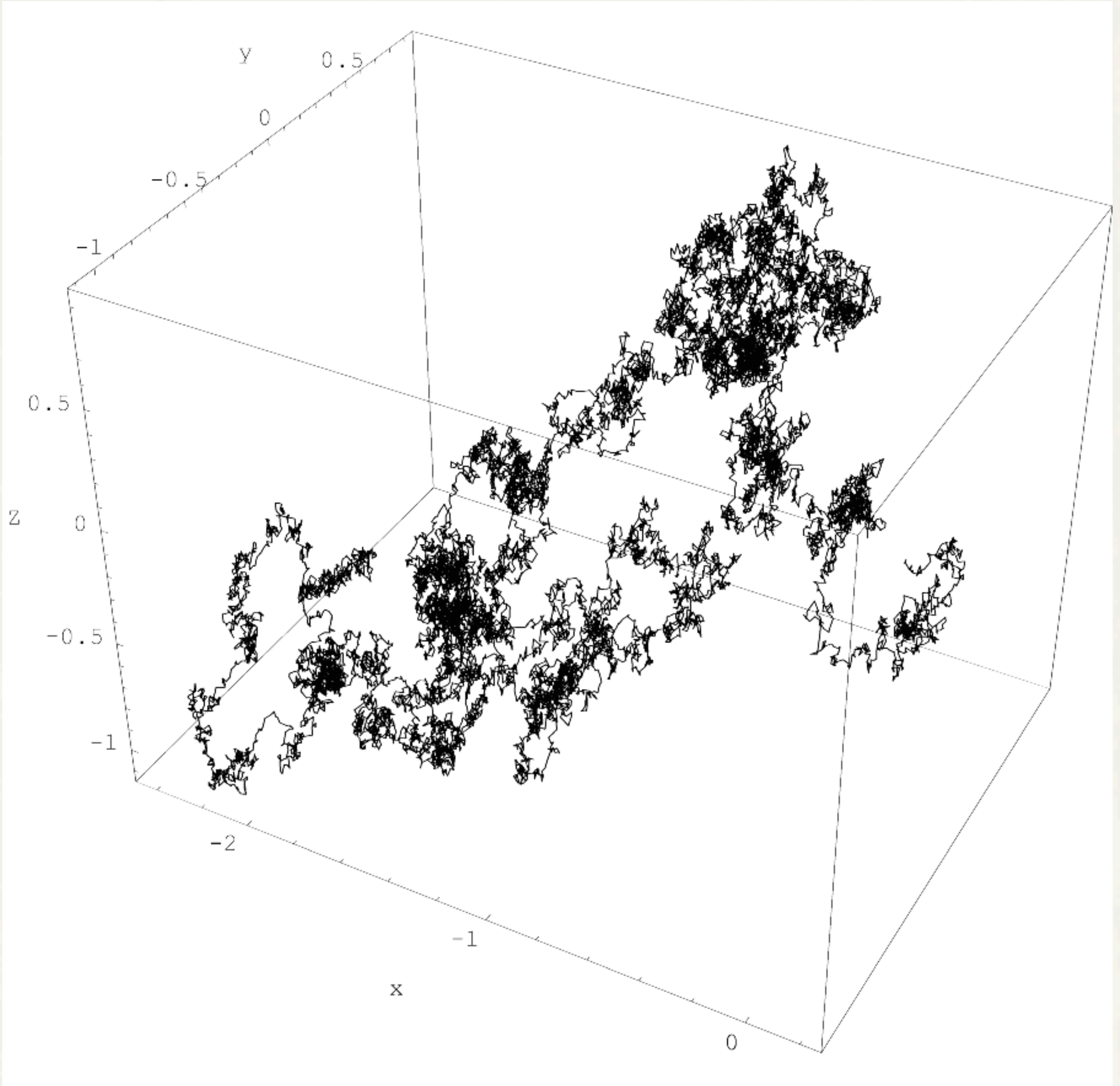
Mean free path between two collisions (air, ambient pressure): 68 nm.

Diffusion: random walk description

Trajectories of molecules in solvent are extremely complex (**chaotic**).

No chance to solve the equation of motion for all the particles.

Use a **statistical approach**: probability to have the particle at a given position p(x,y,z,t).



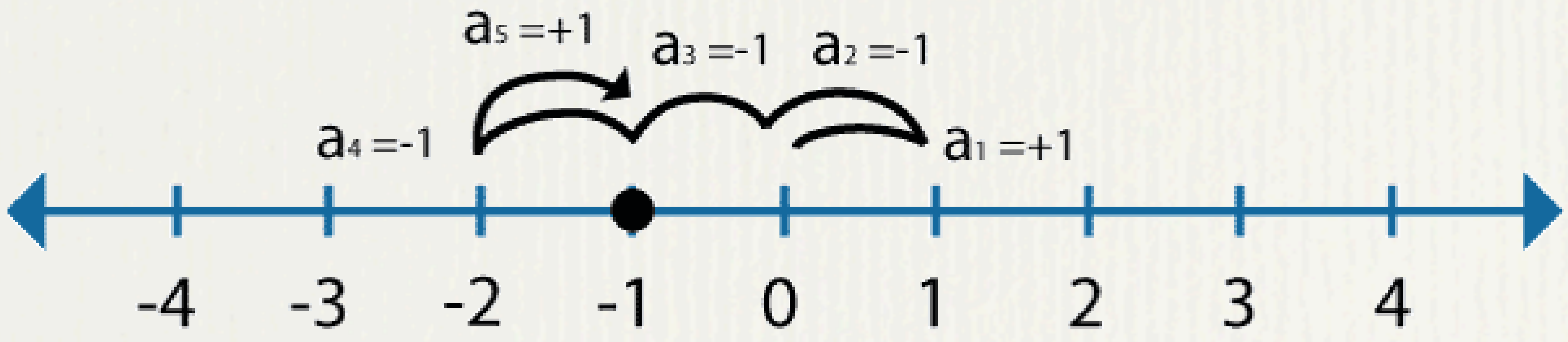
Many particles (N): probability density p(x,y,z,t) proportional to concentration.

$$C(x, y, z, t) = Np(x, y, z, t)$$

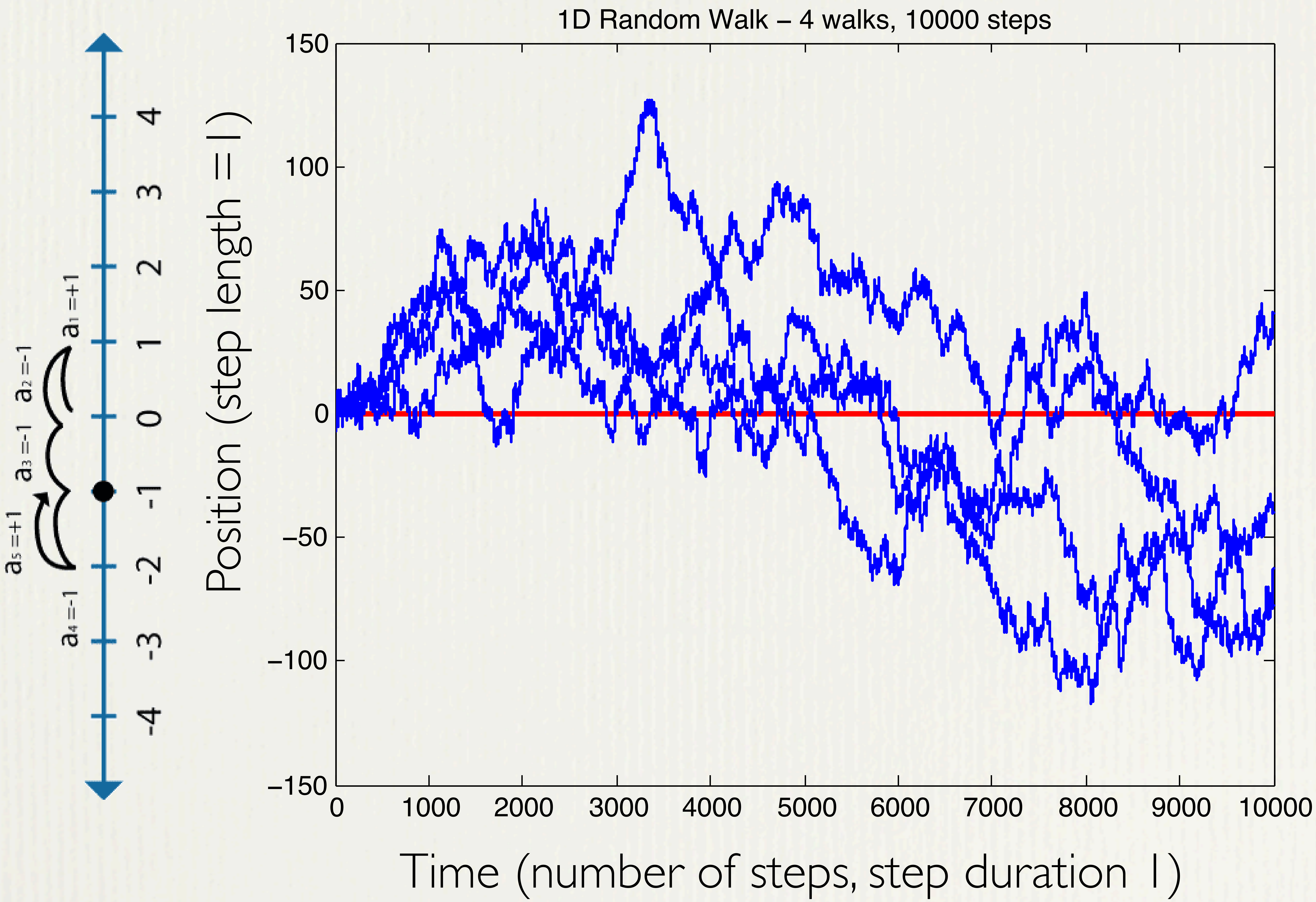
1D random walk

Simple **model** for diffusion: the 1D random walk (example diffusion of tracer molecules in a narrow pipe).

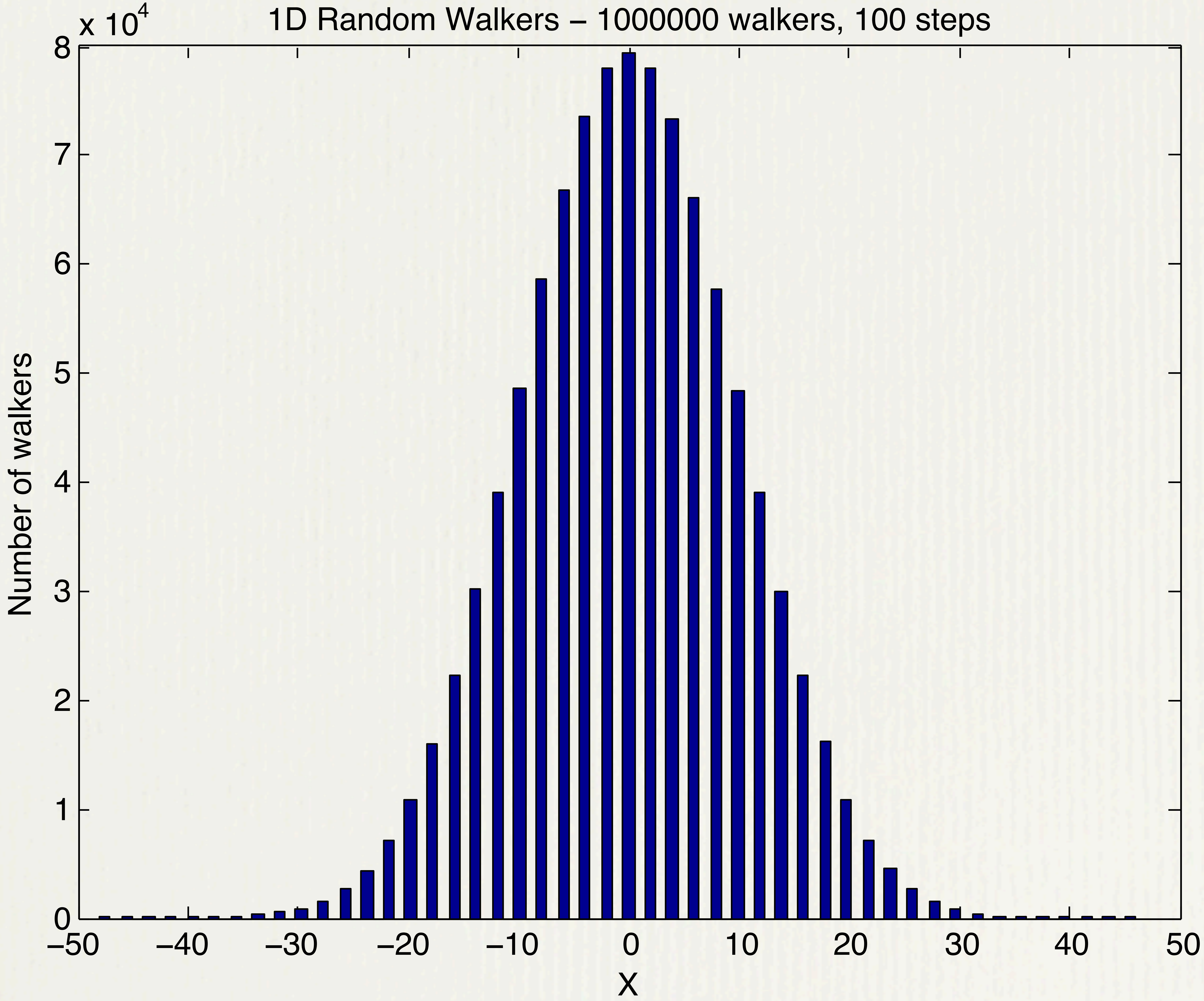
- Repeated steps to the **left** or to the **right** with equal probability, **no memory**
- Step n corresponds to displacement $$\delta_n = a_n v_x \tau = a_n u \tau = a_n \delta$$
- τ and δ depend on particle size and shape, liquid properties and temperature



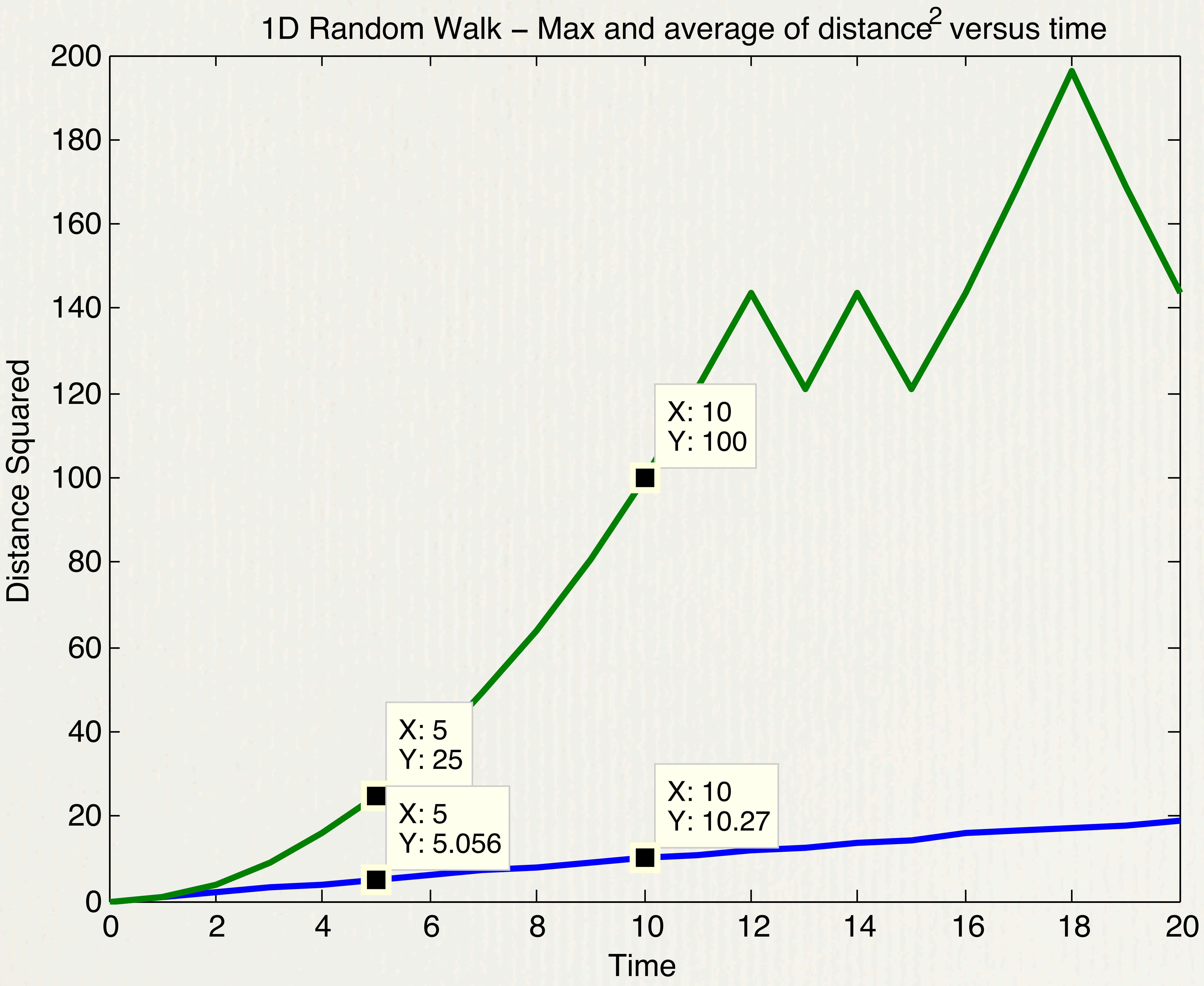
1D random walk: example trajectories



1D random walk: histograms of positions

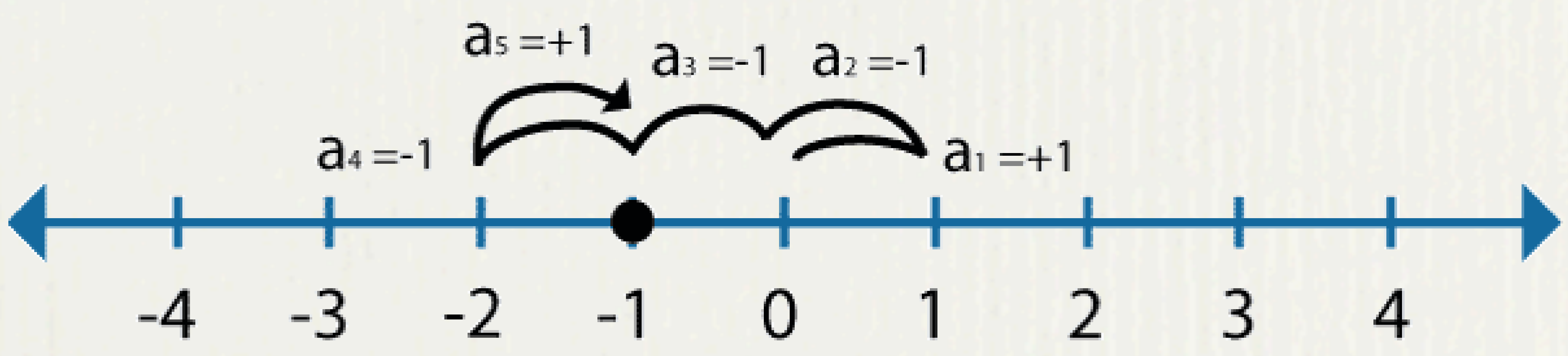


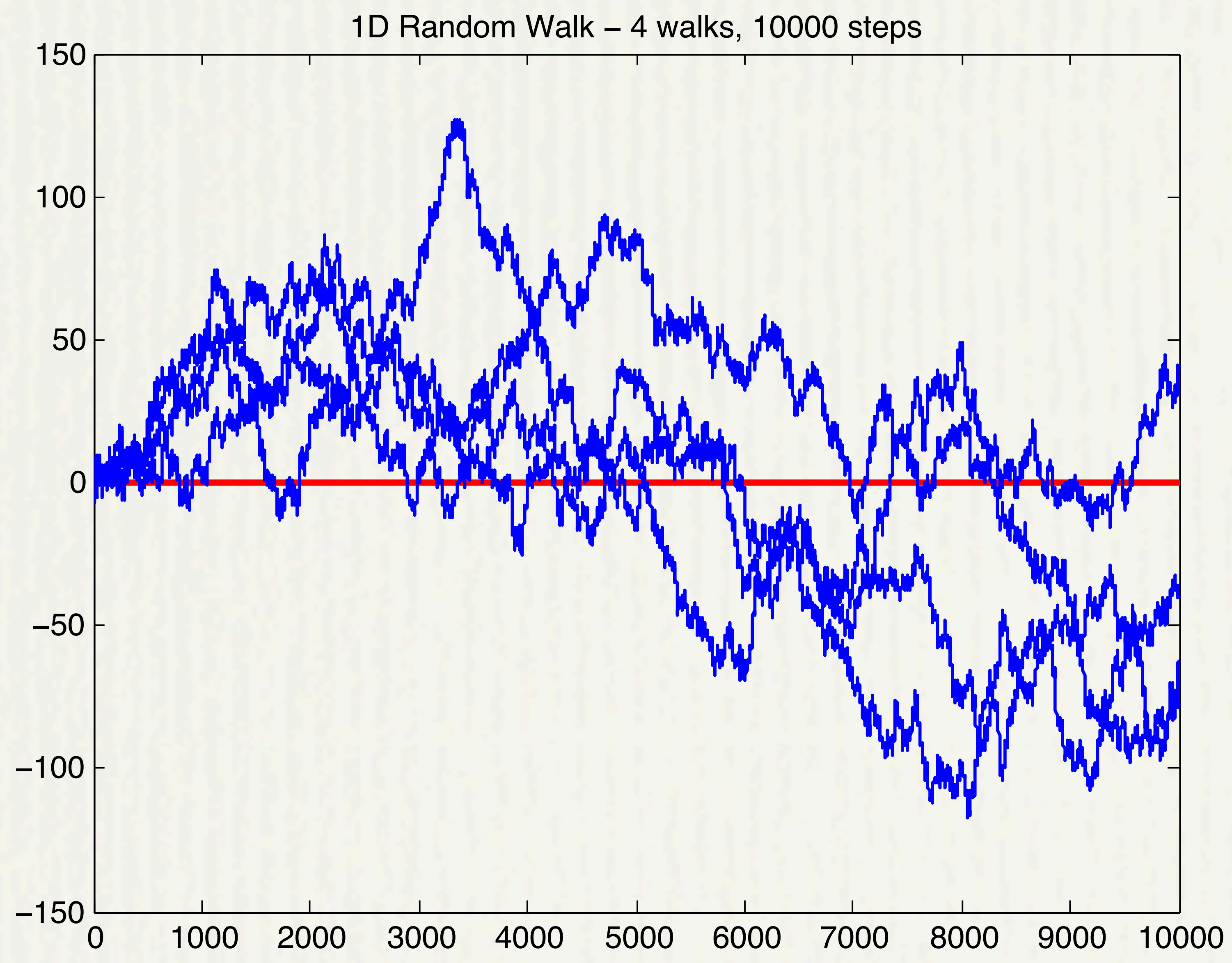
1D random walk: average and max distance^2



1D random walk: first observations

- In one dimension all the trajectories come **back to the origin**
- As time increases the particles explore a larger domain (**dispersion**)
- Average (root-mean-squared) distance from he starting point proportional to the **square root** of time





1D random walk: microscopic description

- Discrete **evolution equation** (particle label i, timestep label n):

$$x_i(n+1) = x_i(n) + a_n\delta$$

- Large number of particles, **average spreading** given by the standard deviation σ(t) on the position at the time t

$$\sigma^2(t = n\tau) = \langle (x(n) - \langle x(n) \rangle)^2 \rangle = \langle x(n)^2 \rangle - \langle x(n) \rangle^2 = \frac{\delta^2}{\tau} t$$

- **Diffusion coefficient** as a dimensional parameter characterizing the spreading

$$2D = \frac{\delta^2}{\tau} \qquad \sigma(t) = \sqrt{(2Dt)}$$

Diffusion coefficient

- Dimension [D]=**L^2/T**, unit m^2/s, often expressed in cm^2/s
- Typical values for **solutes** in water (ambient temperature) $\sim 10^{-5} cm^2/s$
- Typical values for dispersed **gases** (ambient temperature) $\sim 10^{-1} cm^2/s$
- In **solids** much lower values (example: gas in metal, or helium leaking out of a balloon)
- Increases with temperature and decreases with density.

How fast is diffusion ?

- Thermal velocities are extremely large, does this result in a fast spreading ?

- Time for spreading over one meter with $D=10^{-5} cm^2/s$? **116 days !!**

- Common experience (e.g. cigarette smoke in a room), the process is much faster.

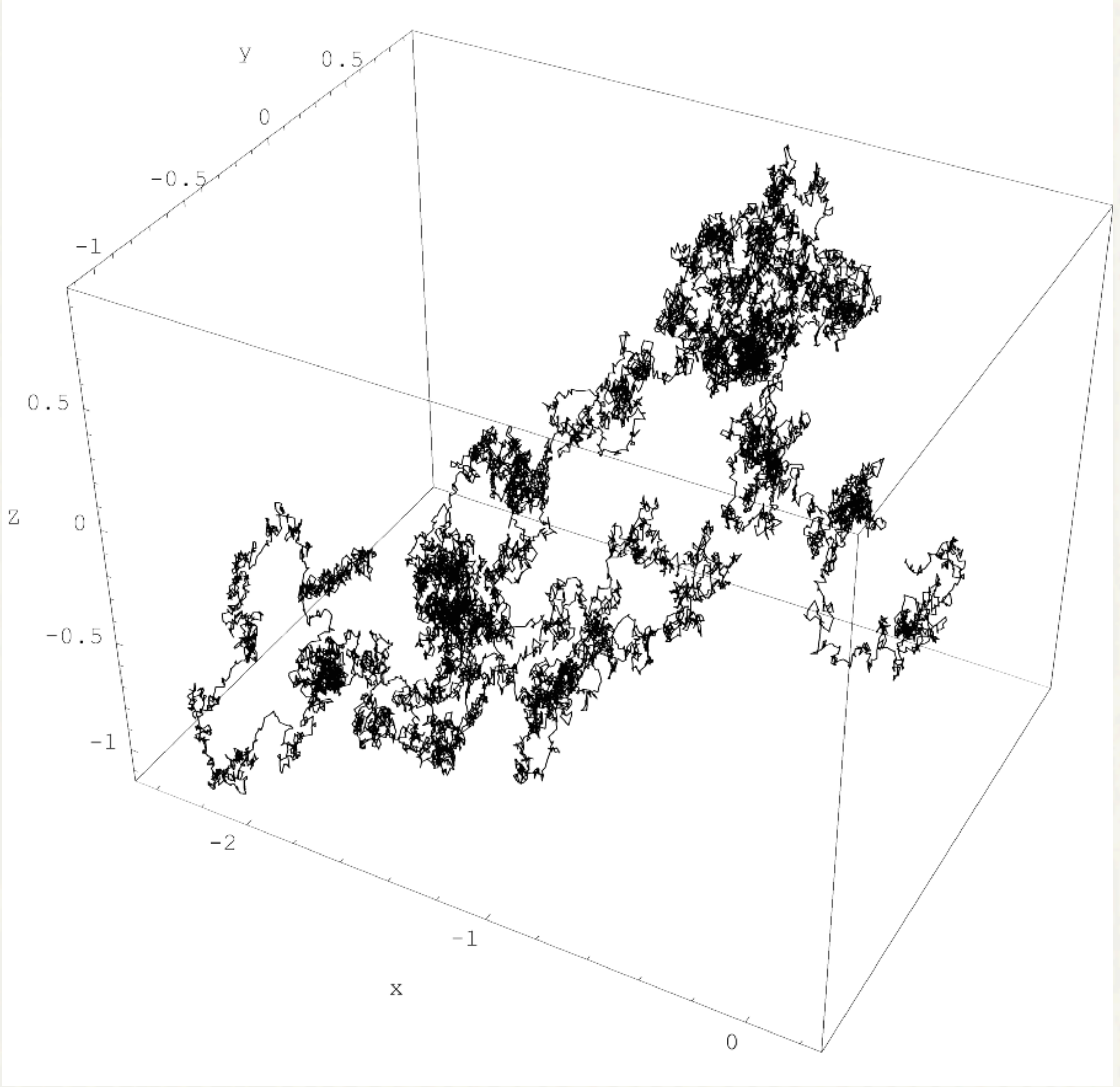
- **Turbulence** results in a diffusion coefficient orders of magnitude larger.

Generalization to 2D and 3D

- All we have learned for 1D can be **generalized** to 2D and 3D.

- We allow the particle to explore the thee dimensions at each time step.

$$\langle r^2 \rangle = \langle x^2 + y^2 + z^2 \rangle = 6Dt$$



- Non-trivial effect: probability never to return at origin is 0 in 1D and 2D. However, a drunk bird only has a 34% chance to return home (3D diffusion).

Macroscopic description: Fick's first law

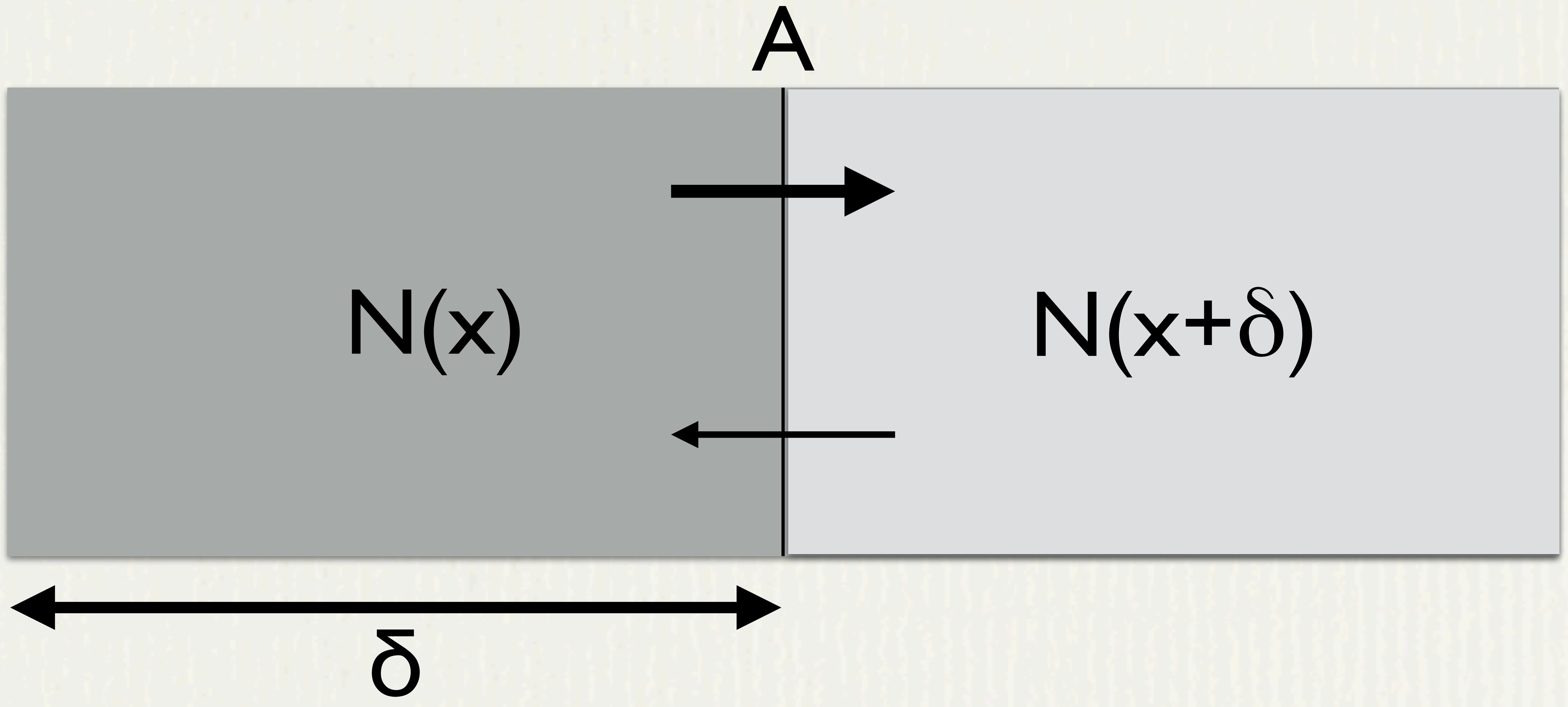
- Microscopic -> Macroscopic by $C(x,y,z,t) = Np(x,y,z,t)$

- Assumption: steady state (**fixed concentration profile**)

- The solute moves from regions of high concentration to a region of low concentration

- **J**(x,y,z) (bold letter -> vector) the diffusion flux. Amount of substance transferred per unit area and unit of time (typical units mole m^{-2} s^{-1})

Derivation of Fick's first law



- At each timestep τ each particle close to the border between two regions of different concentrations (space divided in boxes of length δ and section A) has a probability 1/2 to cross the border.

- Across the barrier the net number of crossing particles is given by

$$\frac{N(x)}{2} - \frac{N(x+\delta)}{2}$$

Derivation of Fick's first law

- Over a barrier of section A and per time unit we have a **flux**

$$j_x = -\frac{1}{2}\left(\frac{N(x+\delta) - N(x)}{A\tau}\right)$$

$$= -\frac{\delta^2}{2\tau}\left(\frac{N(x+\delta)/\delta - N(x)/\delta}{A\delta}\right)$$

$$= -\frac{\delta^2}{2\tau}\left(\frac{N(x+\delta)/(A\delta) - N(x)/(A\delta)}{\delta}\right)$$

Derivation of Fick's first law

- We then use the fact that $C(x) = N(x)/(A\delta)$

$$j_x = -\frac{\delta^2}{2\tau}\left(\frac{C(x+\delta) - C(x)}{\delta}\right)$$

- In the **macroscopic** description, we consider that δ<<1

$$J(x) = -D\frac{dC(x)}{dx} \quad \text{1D}$$

$$\mathbf{J}(x,y,z) = -D\nabla C(x,y,z) \quad \text{3D}$$

No time dependence, fixed concentration profile

valid only in the **isotropic** case !

- Application: exercise set 2, diffusion in a lake

Derivation of Fick's second law

- We start from the continuity equation

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

- We assume that at each time the concentration profile results in a flux coming from diffusion (no advection)

$$\mathbf{J}(x, y, z) = -D\nabla C(x, y, z)$$

- We combine the two relations and use the fact that $(\nabla \cdot \nabla f) = \nabla^2 f$

$$\frac{\partial C(x, y, z, t)}{\partial t} = D\nabla^2 C(x, y, z, t) \qquad \text{3D}$$

Diffusion equation

$$\frac{\partial C(x, t)}{\partial t} = D\frac{\partial^2 C(x, t)}{\partial x^2} \qquad \text{1D}$$