Environmental transport phenomena: Lecture II

Benoît Crouzy
(benoit.crouzy@meteoswiss.ch)

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

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**

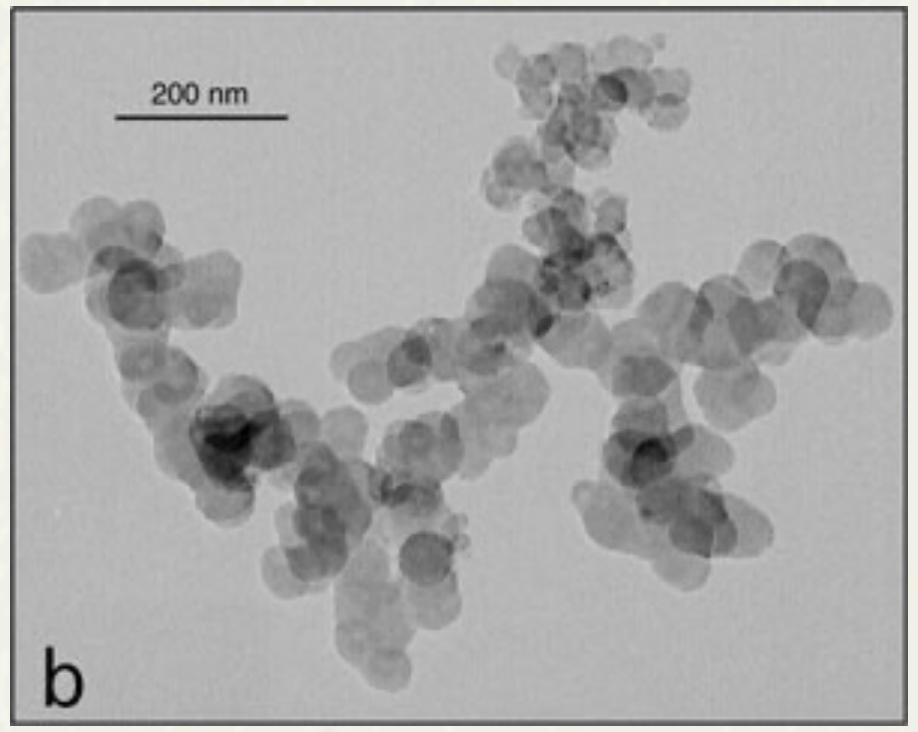
- Sediment (e.g. rivers)

Increased deposition (positive interaction) or sediment anchoring

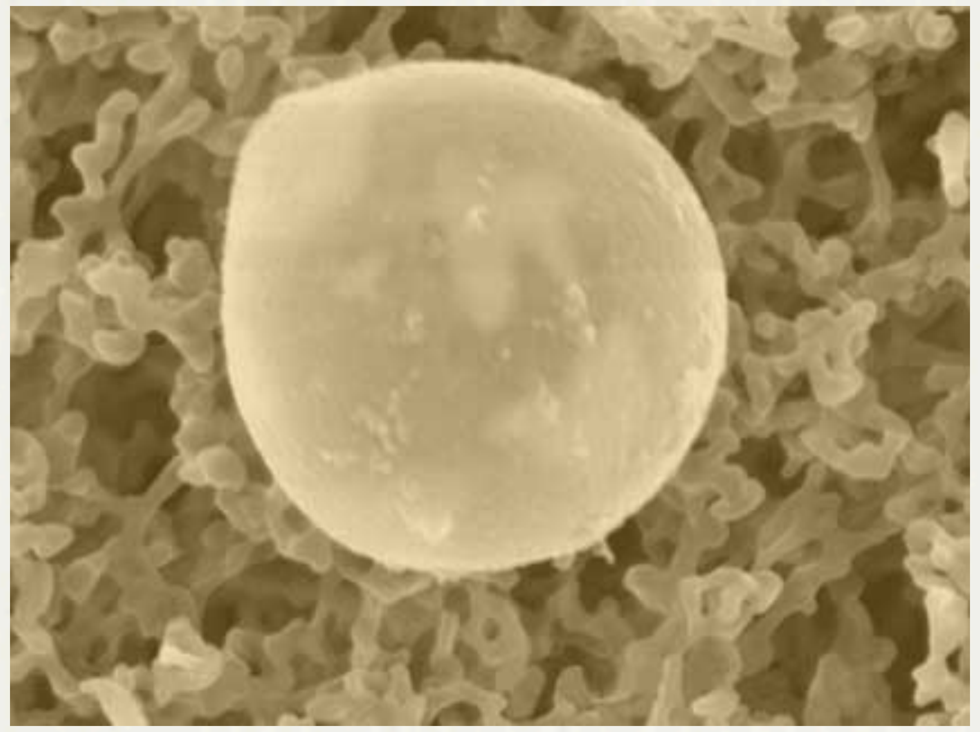
Increased scouring due to flow deflection (negative interaction)

Introduction: transported components

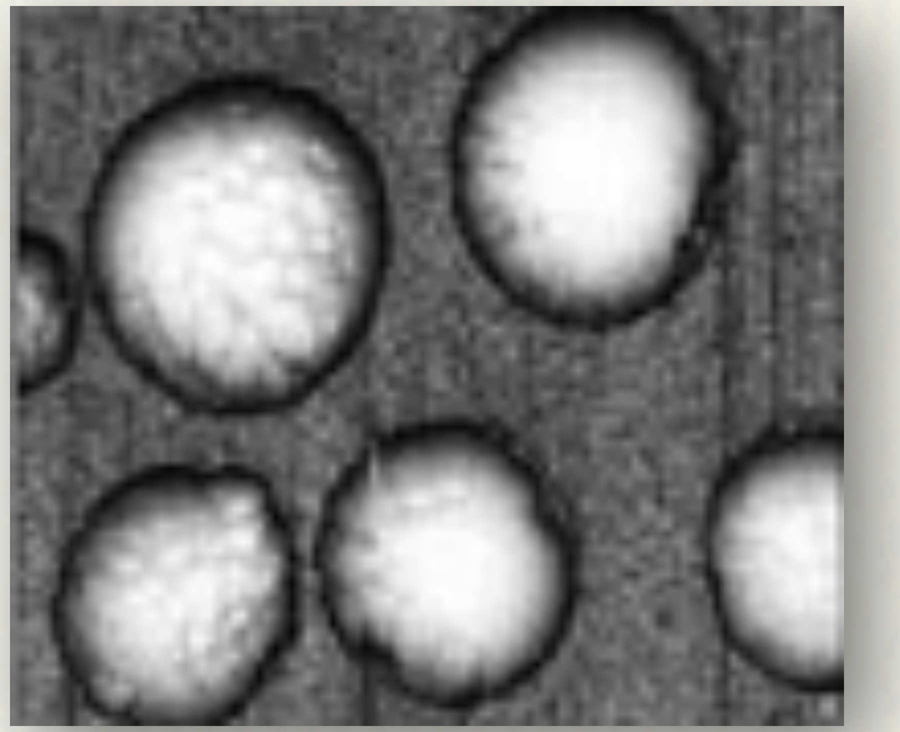
- Huge variety of aerosol (particles in suspension in the air)



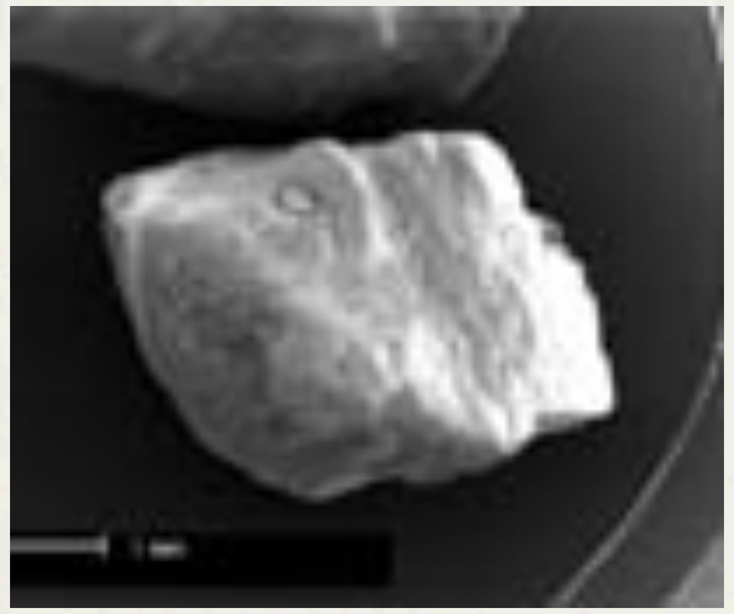
Soot (Diesel):
ca. 0.1 μm



Mineral dust
0.2 - 10 μm



Amonium sulfate:
ca. 0.1 μm

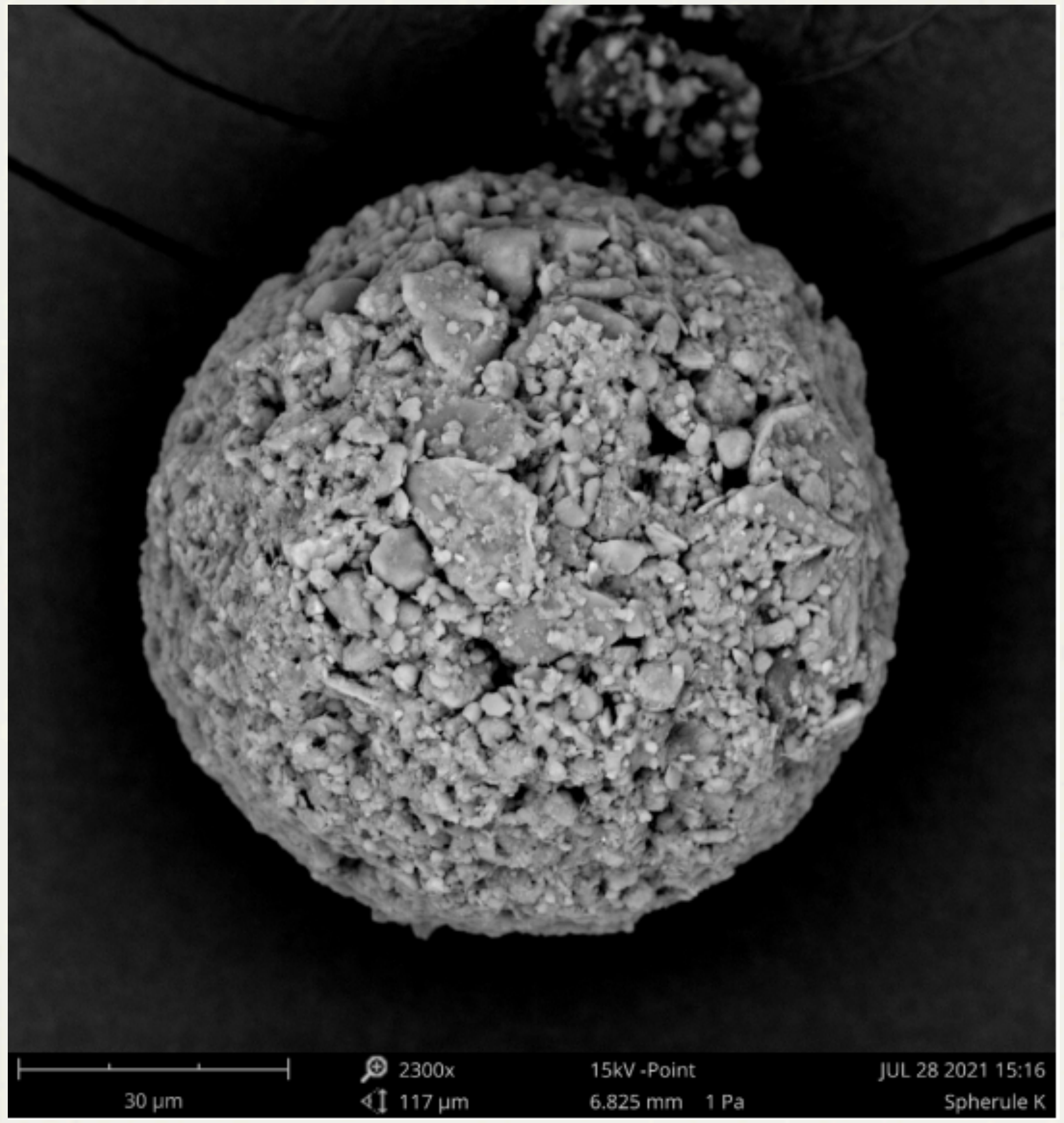


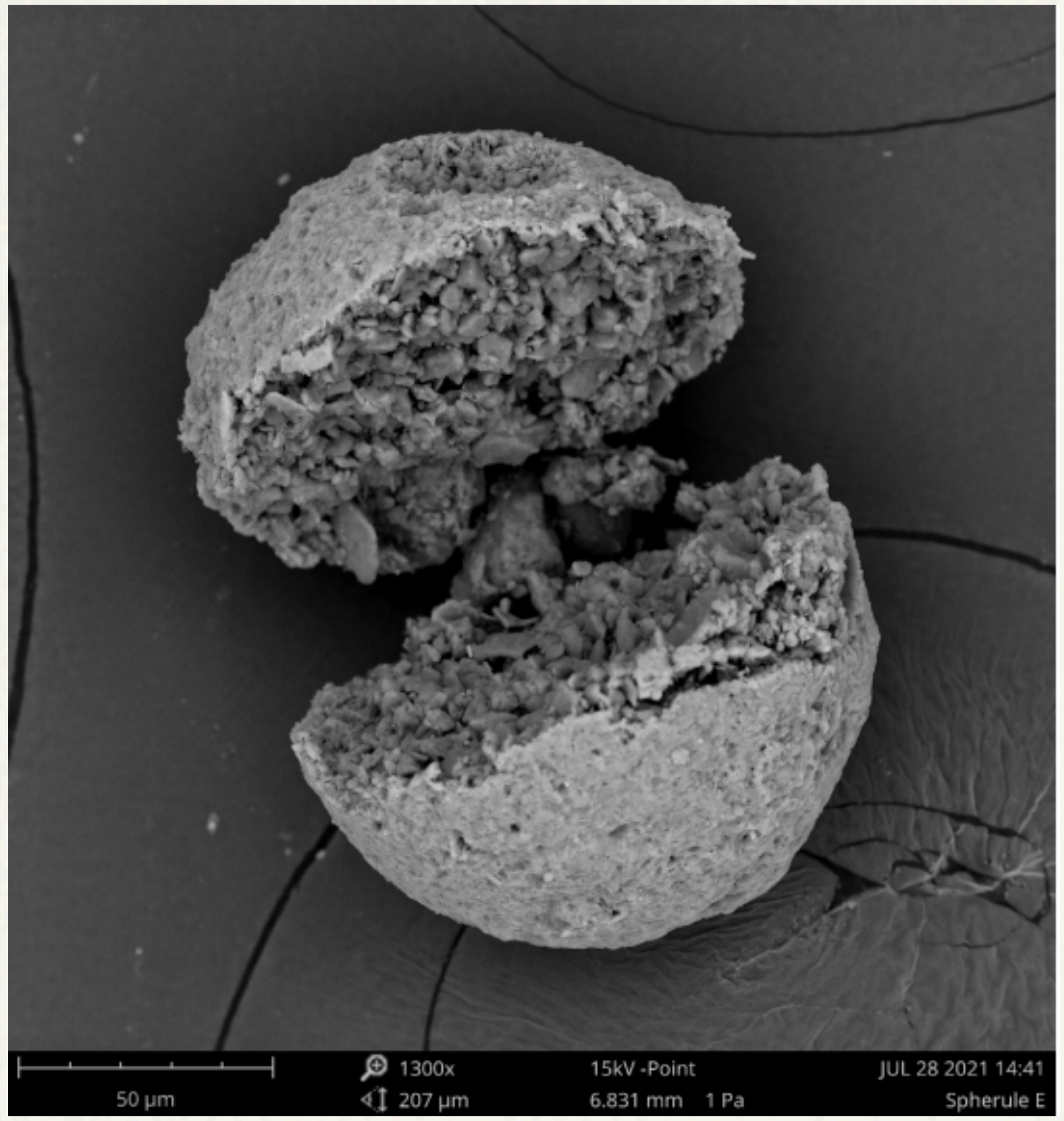
Marine salt:
0.2 - 10 μm

+ secondary aerosols from volatile organic compounds

Introduction: transported components

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

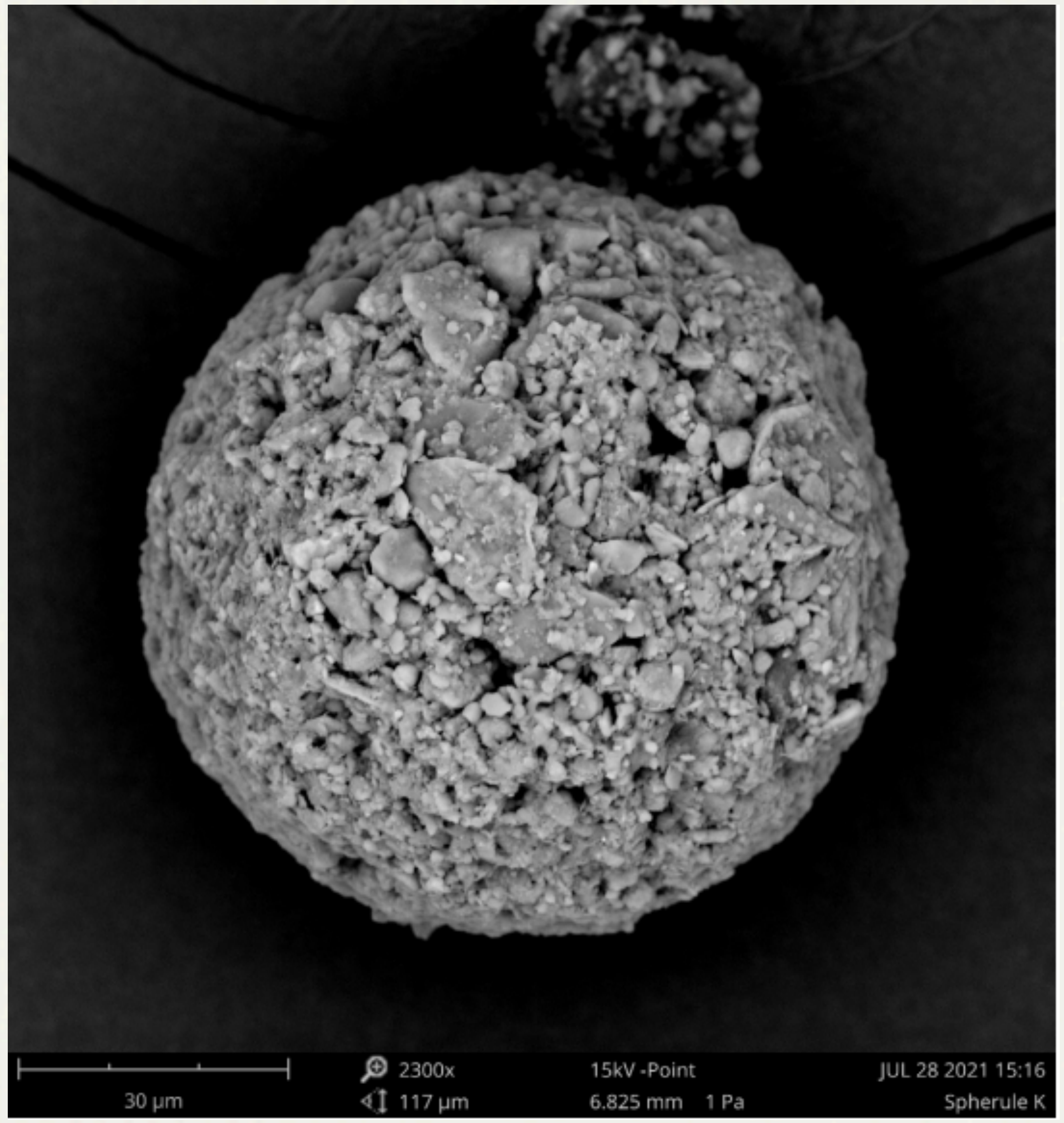


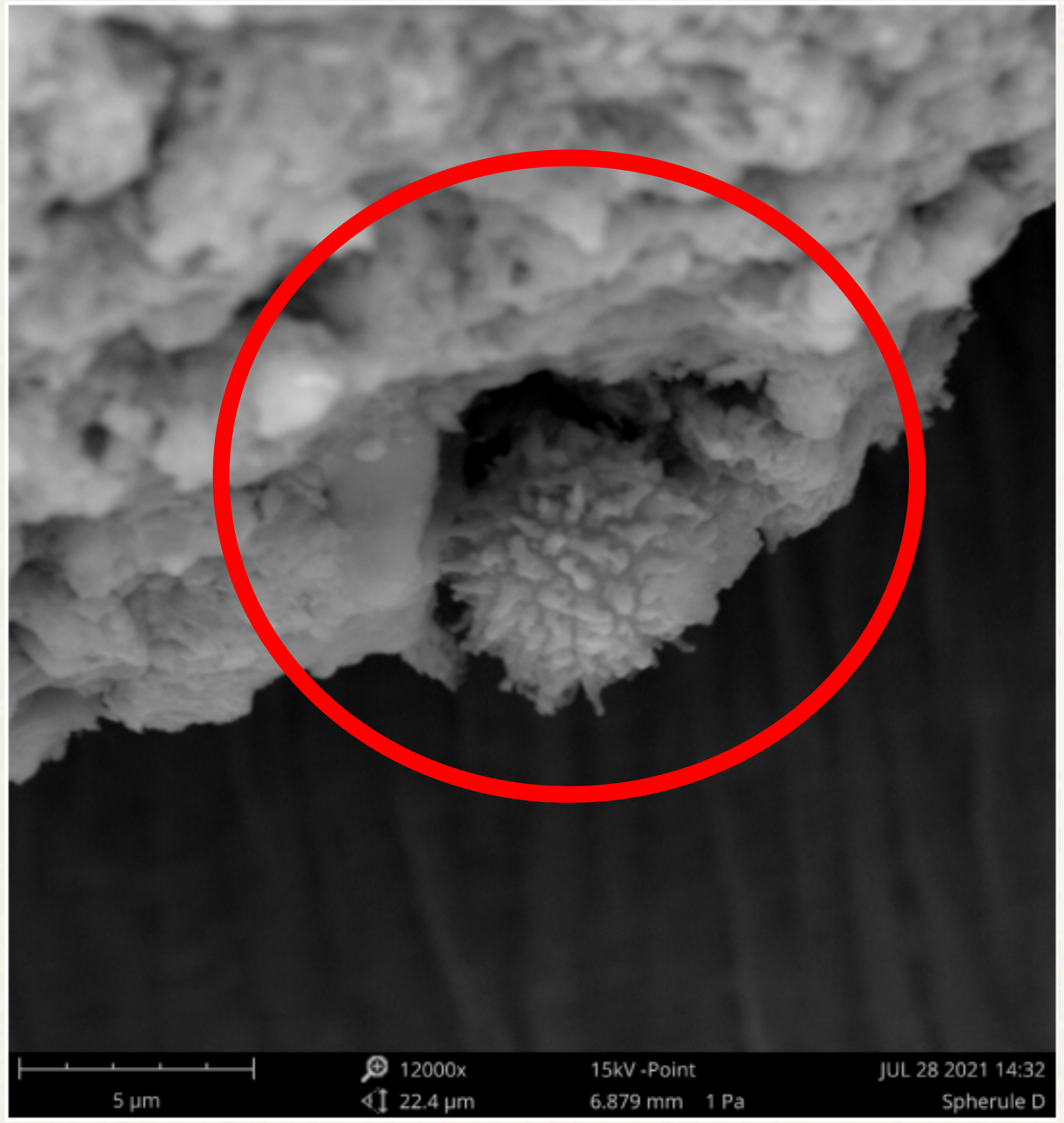


Iberulites from Saharan dust

Introduction: transported components

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

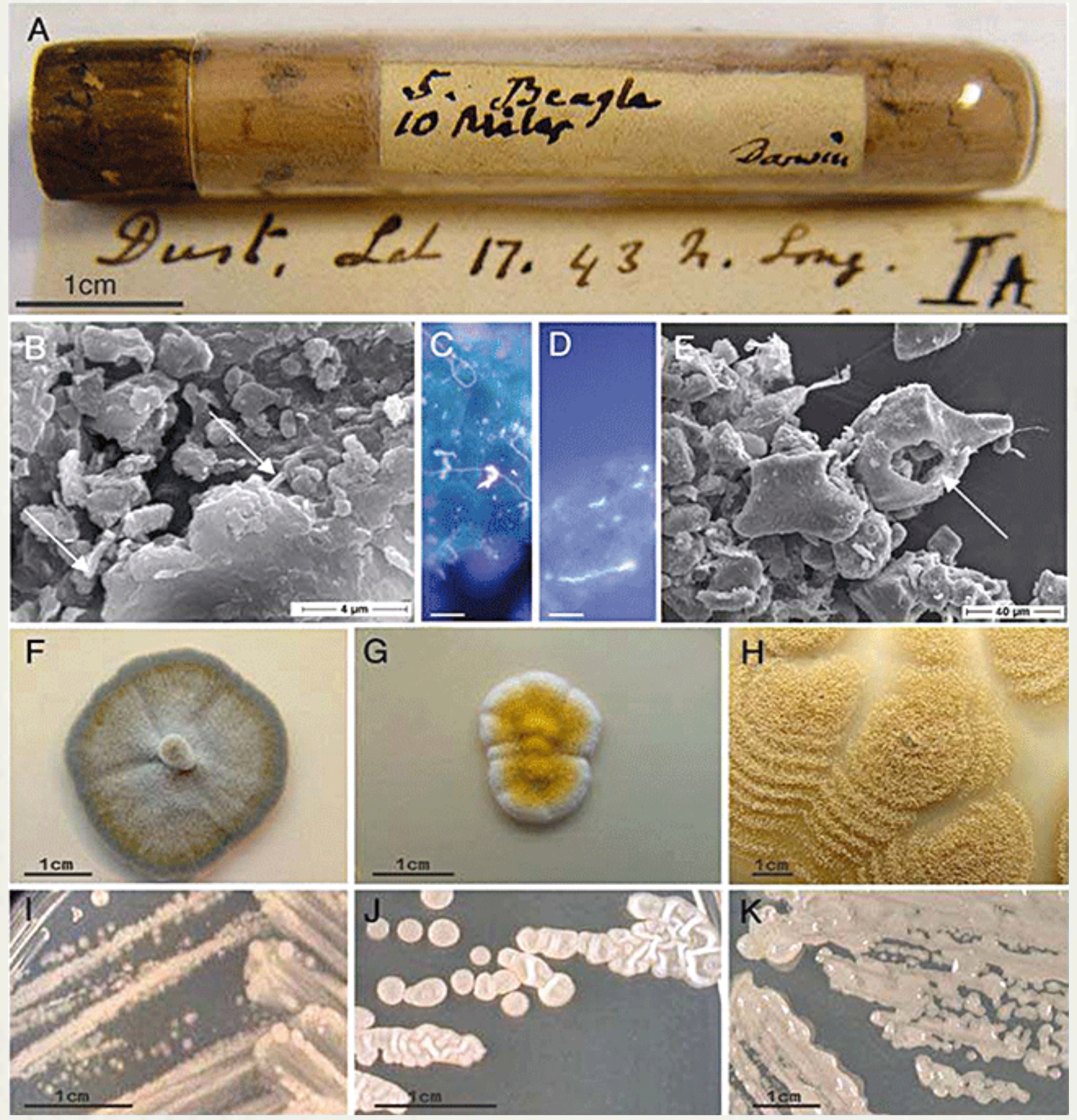




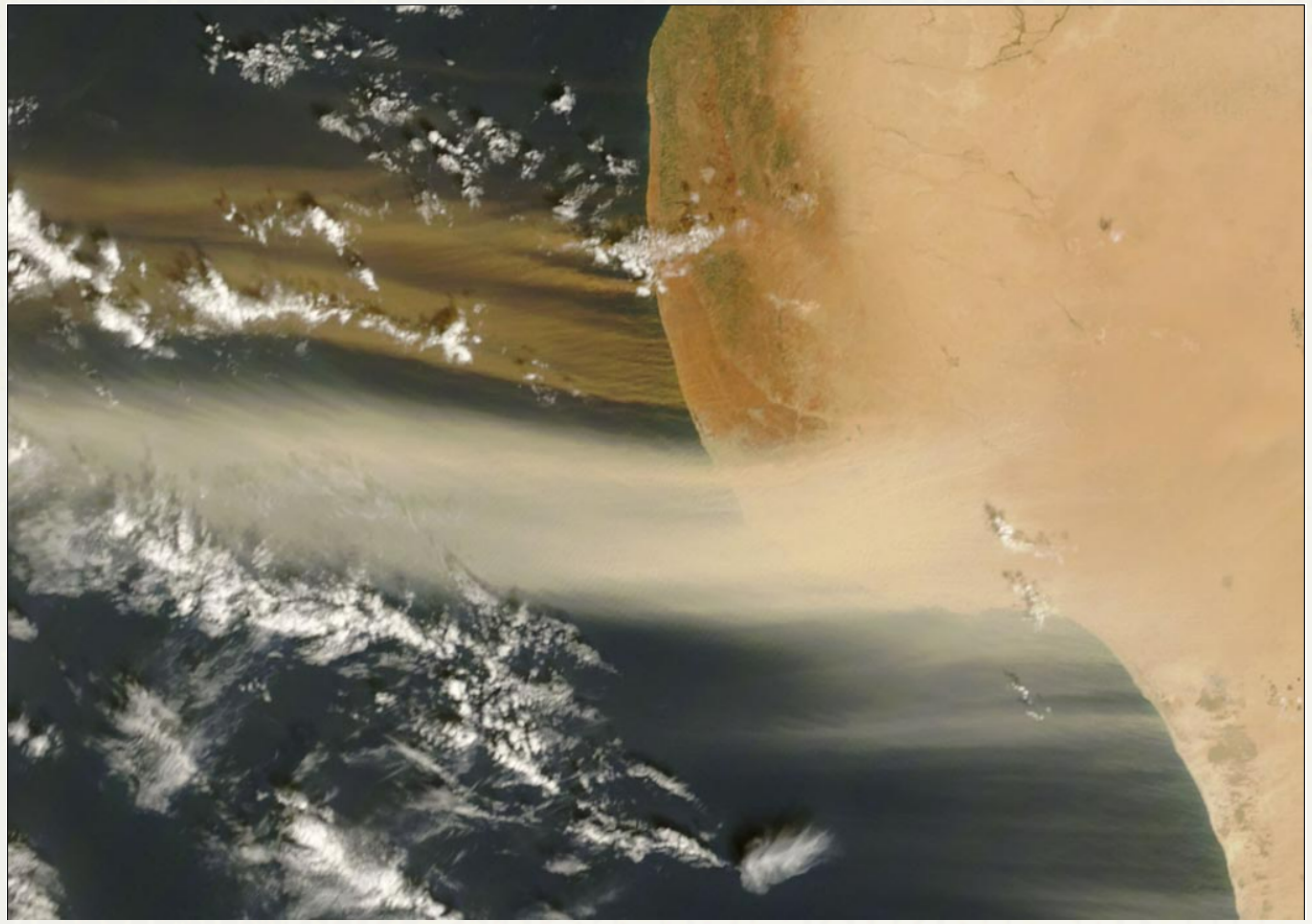
?

Introduction: transported components

- Flow of life in the atmosphere !

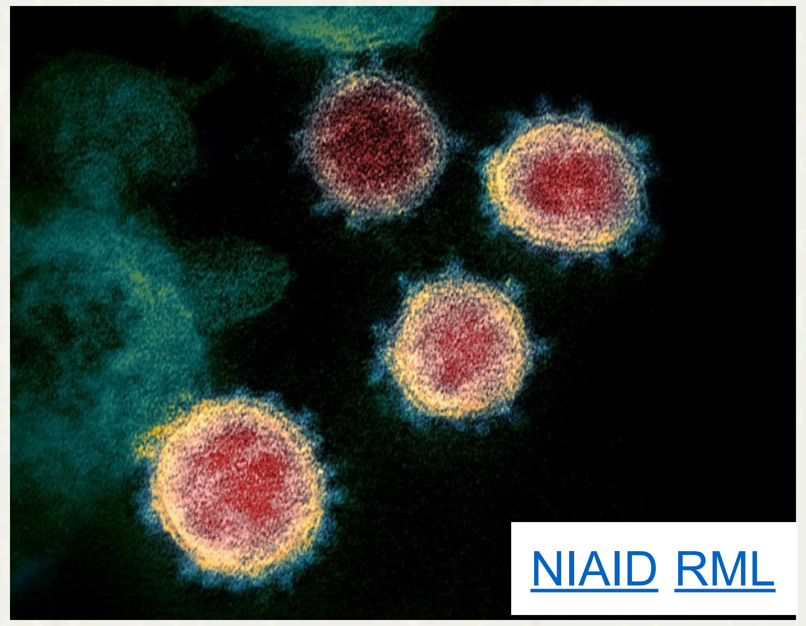


Environmental Microbiology, Volume: 9, Issue: 12, Pages: 2911-2922, First published: 23 October 2007, DOI: (10.1111/j.1462-2920.2007.01461.x)



Introduction: transported components

- Bioaerosol affecting crops, health and cloud formation



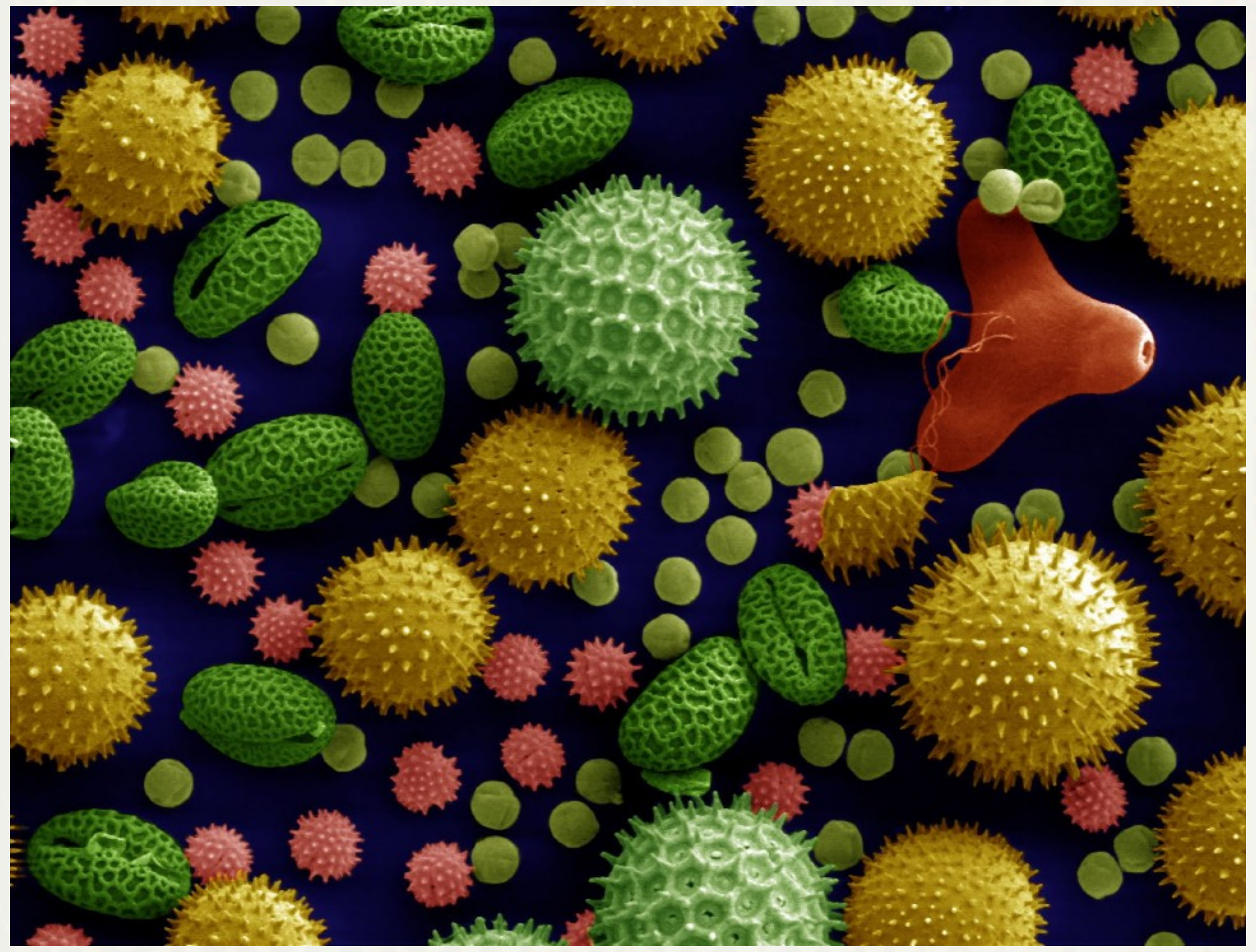
viruses

<

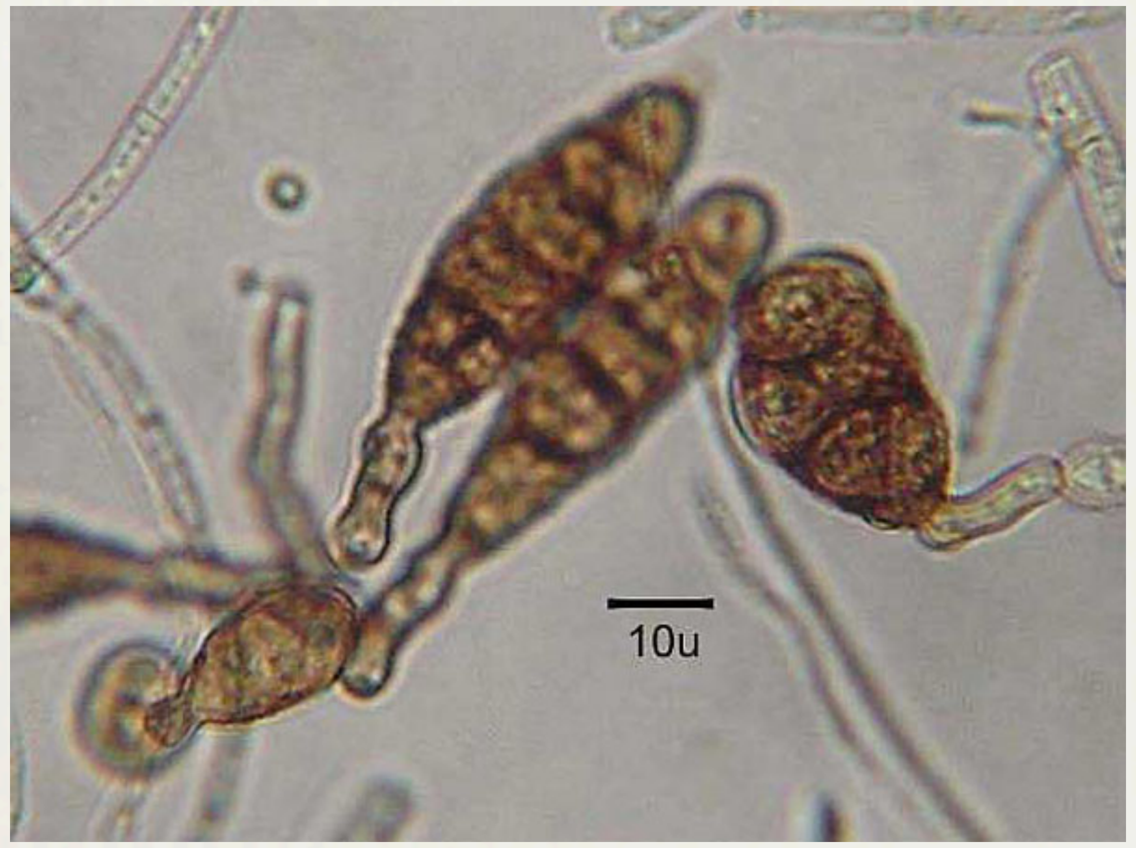
bacteria

1 μm

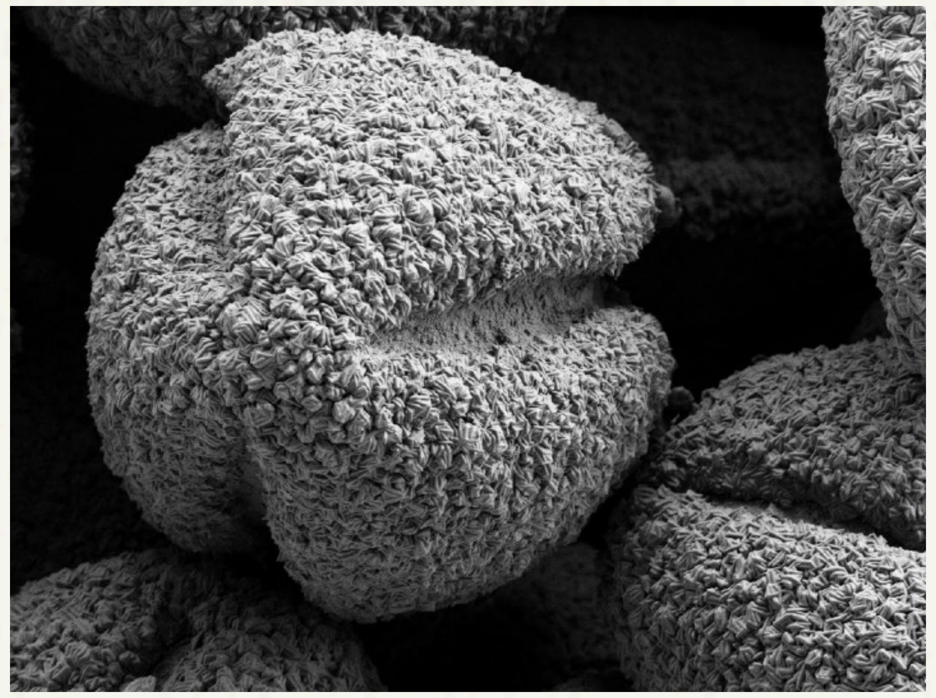
<



Fungal spores



Pollen



Introduction: transported components

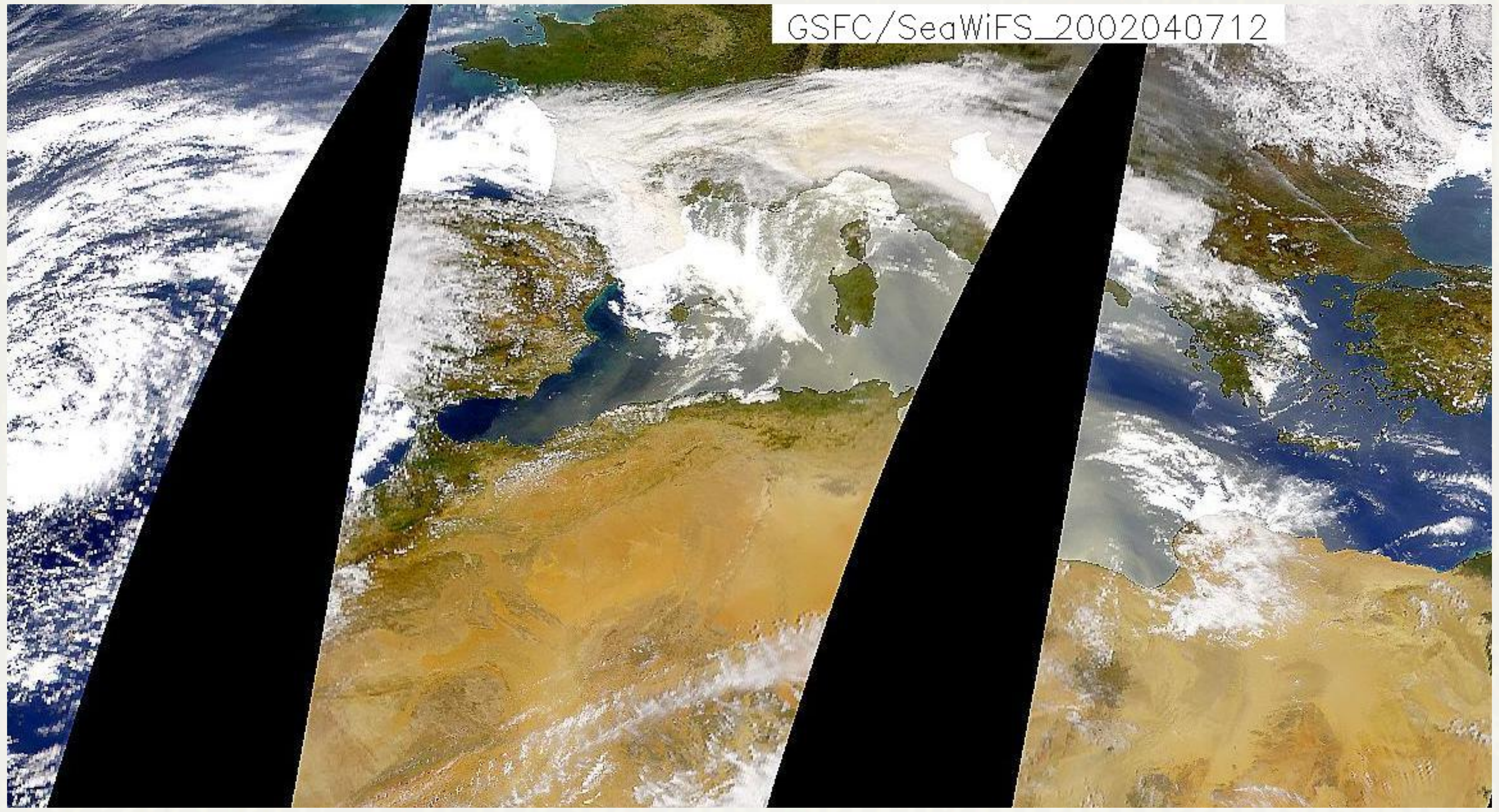
- Contaminants (organic and inorganic)

- Chemicals (gases)

Scales

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

Saharan dust event

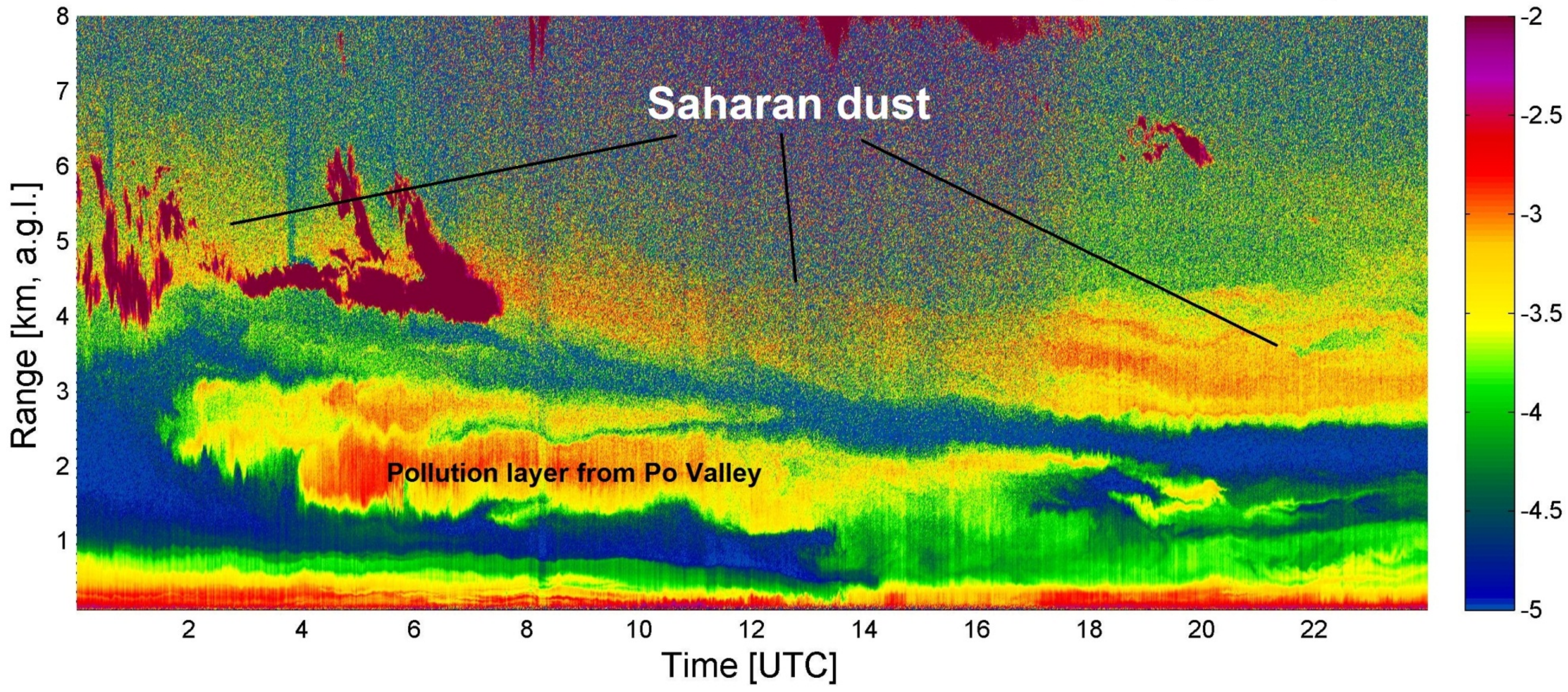


vs

Tracer diffusion

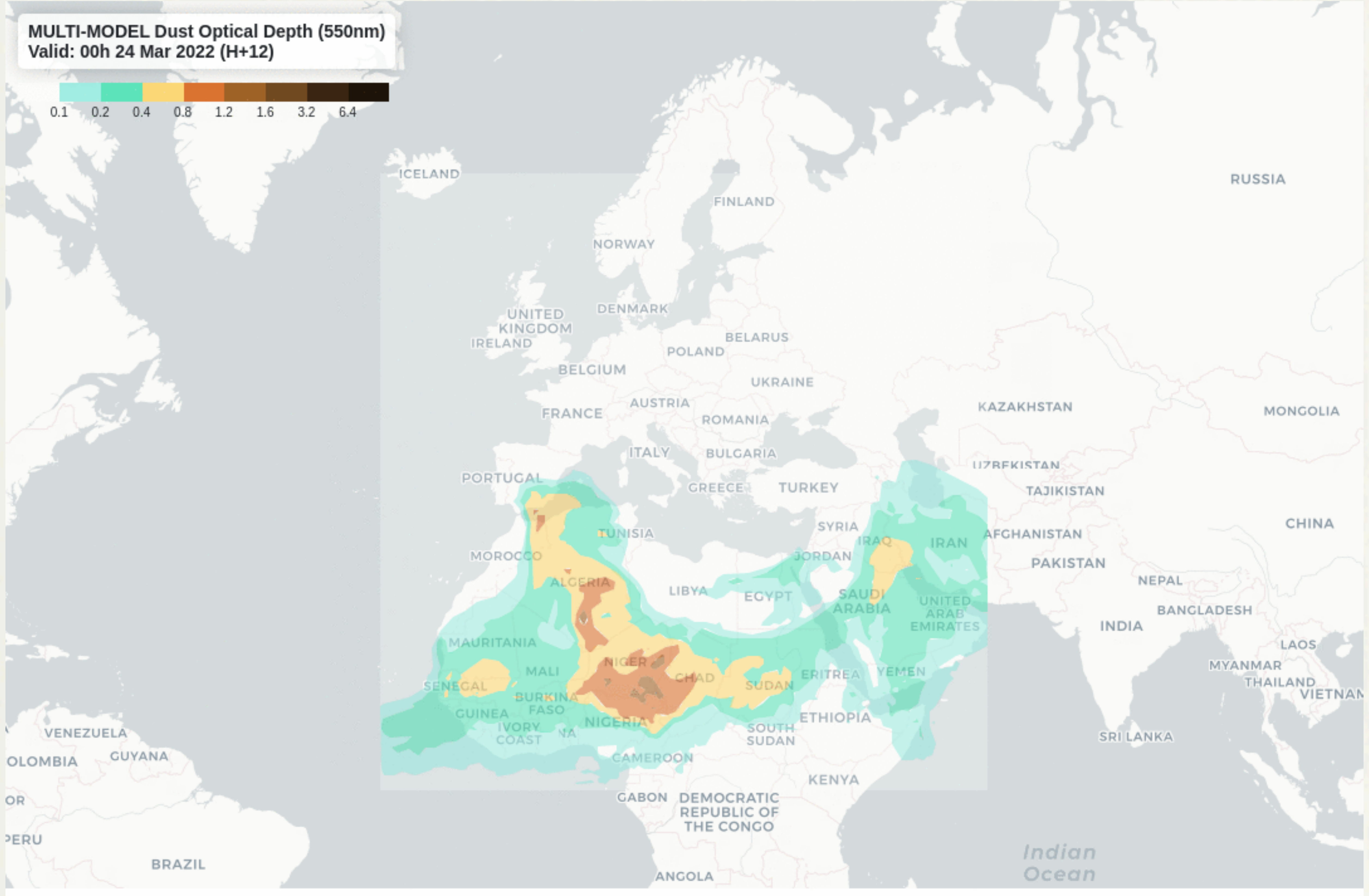
Scales

Transport of Saharan dust: LIDAR measurement in Payerne



Scales

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



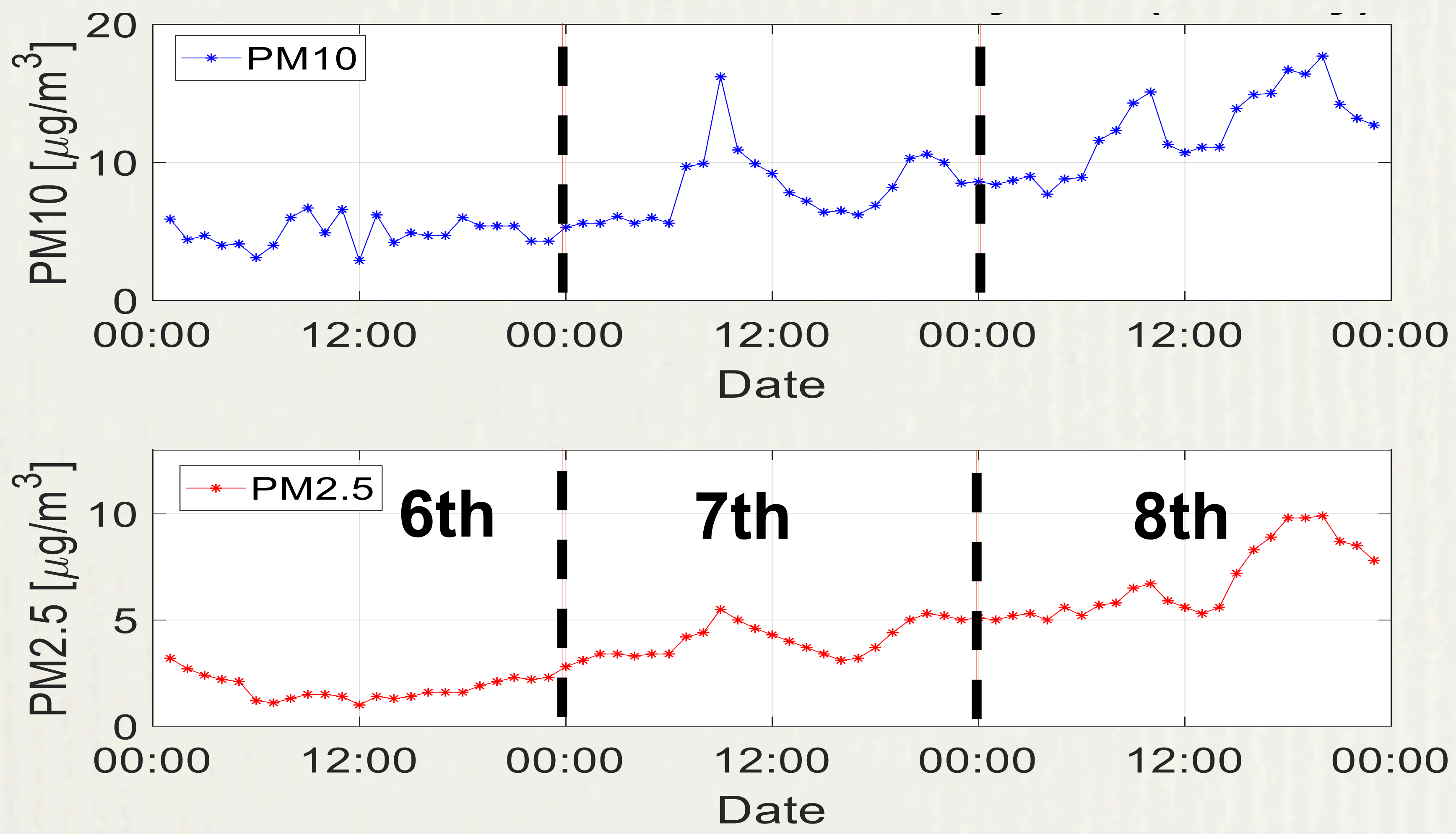
https://atmosphere.copernicus.eu/global-forecast-plots

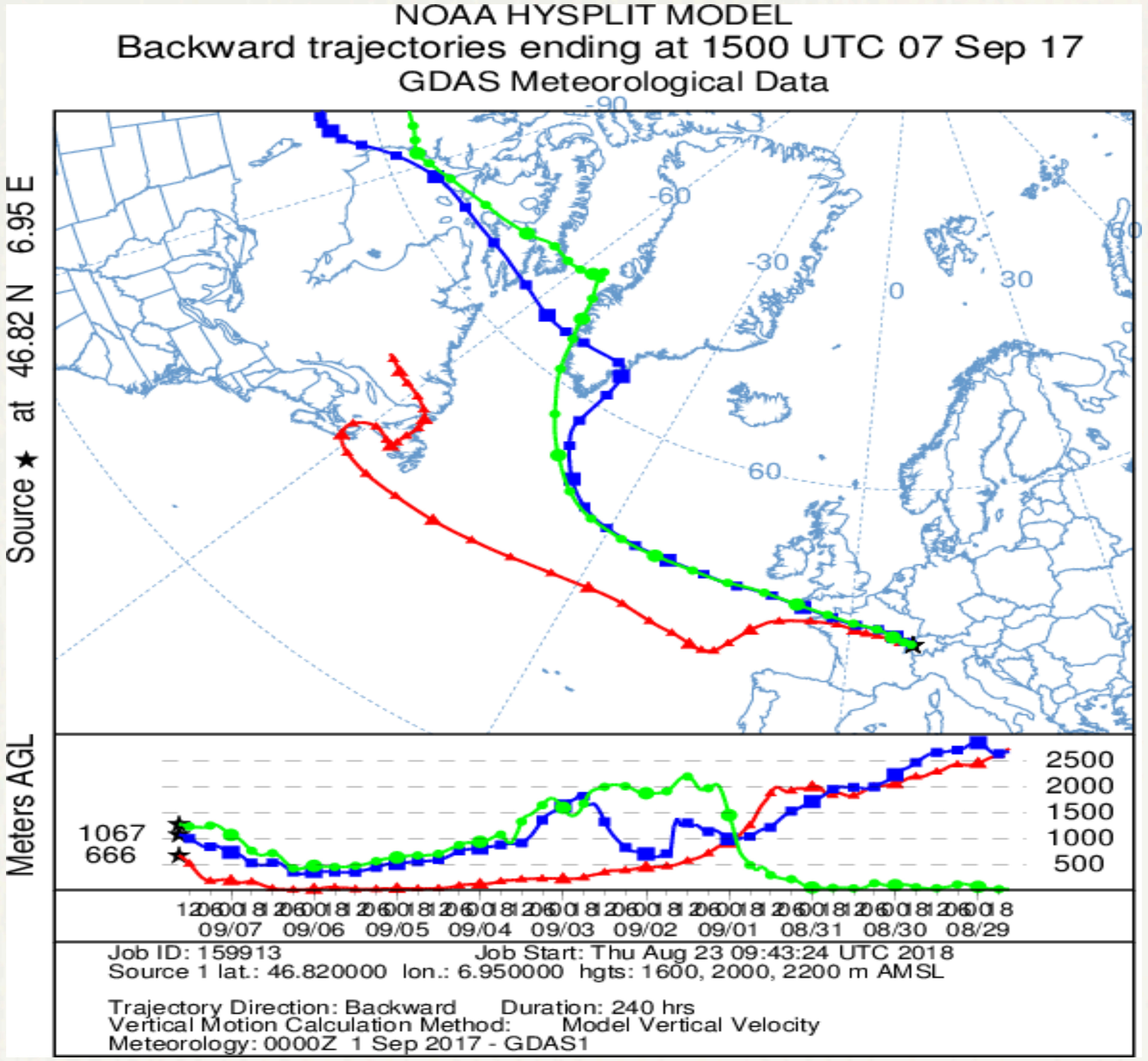
https://atmosphere.copernicus.eu/charts/packages/cams/products/fire-activity?base_time=202309270000&projection=classical_global

Scales

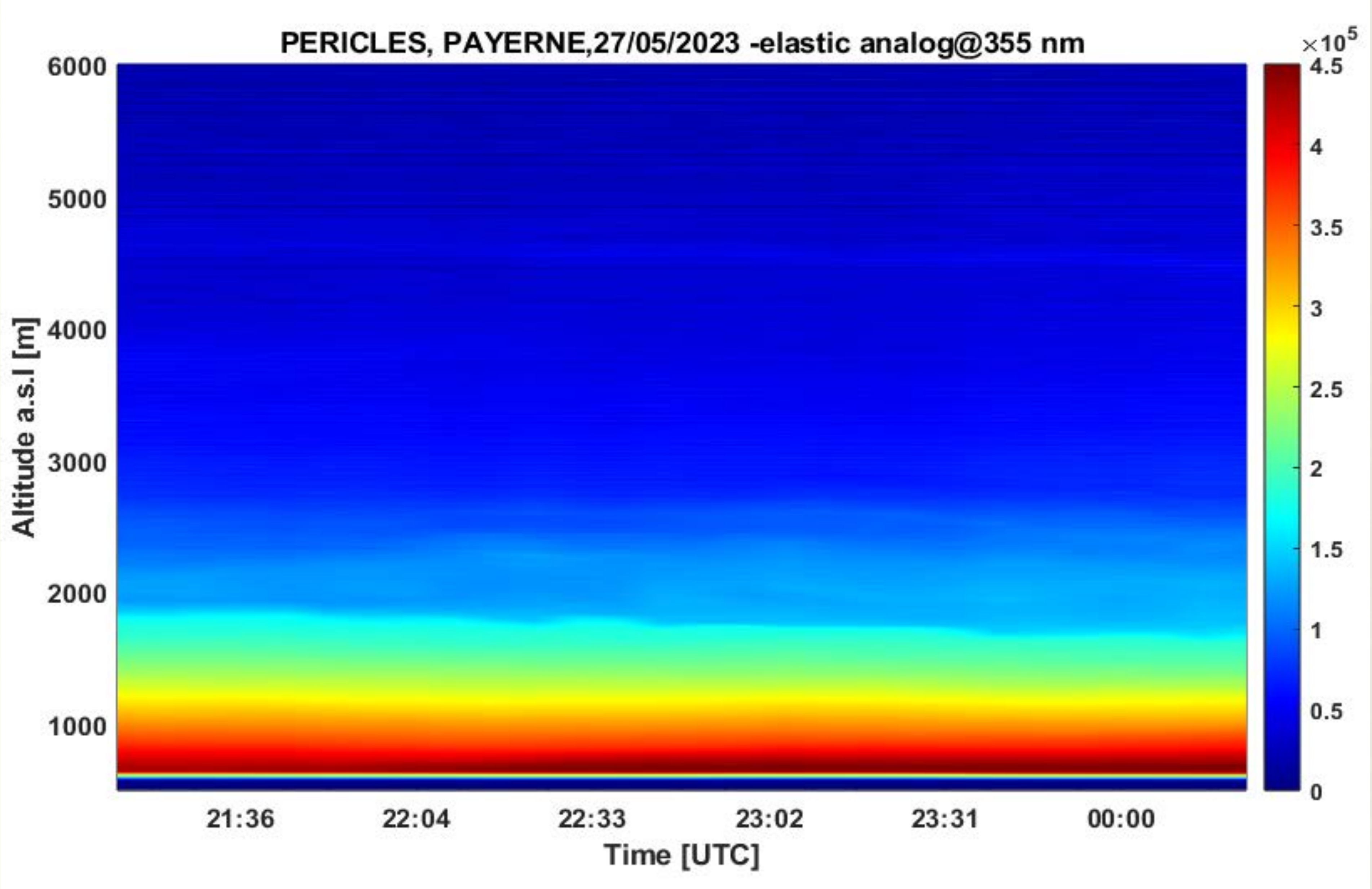
2017 north America fires

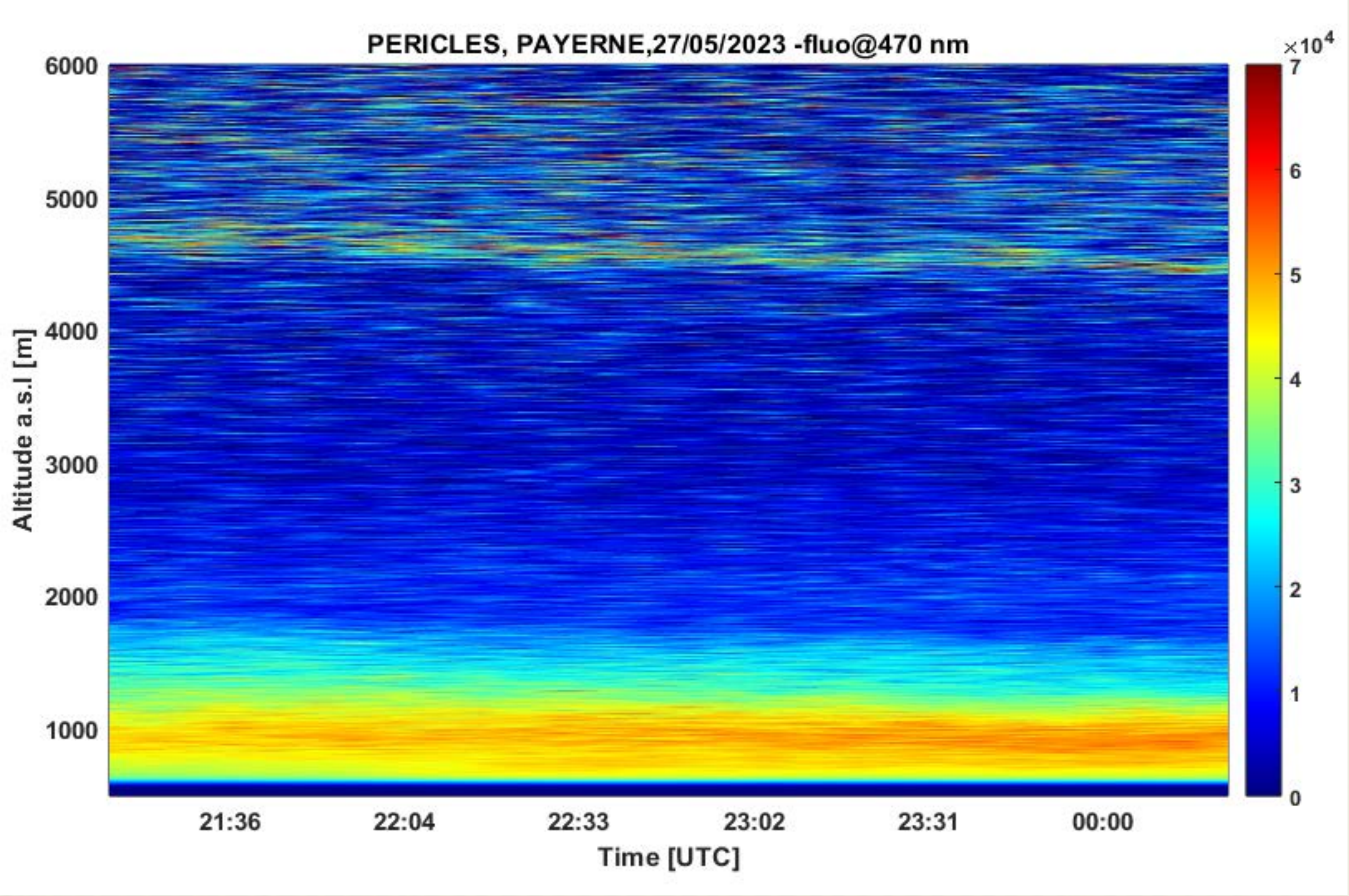
Surface PM concentration (Payerne, CH)

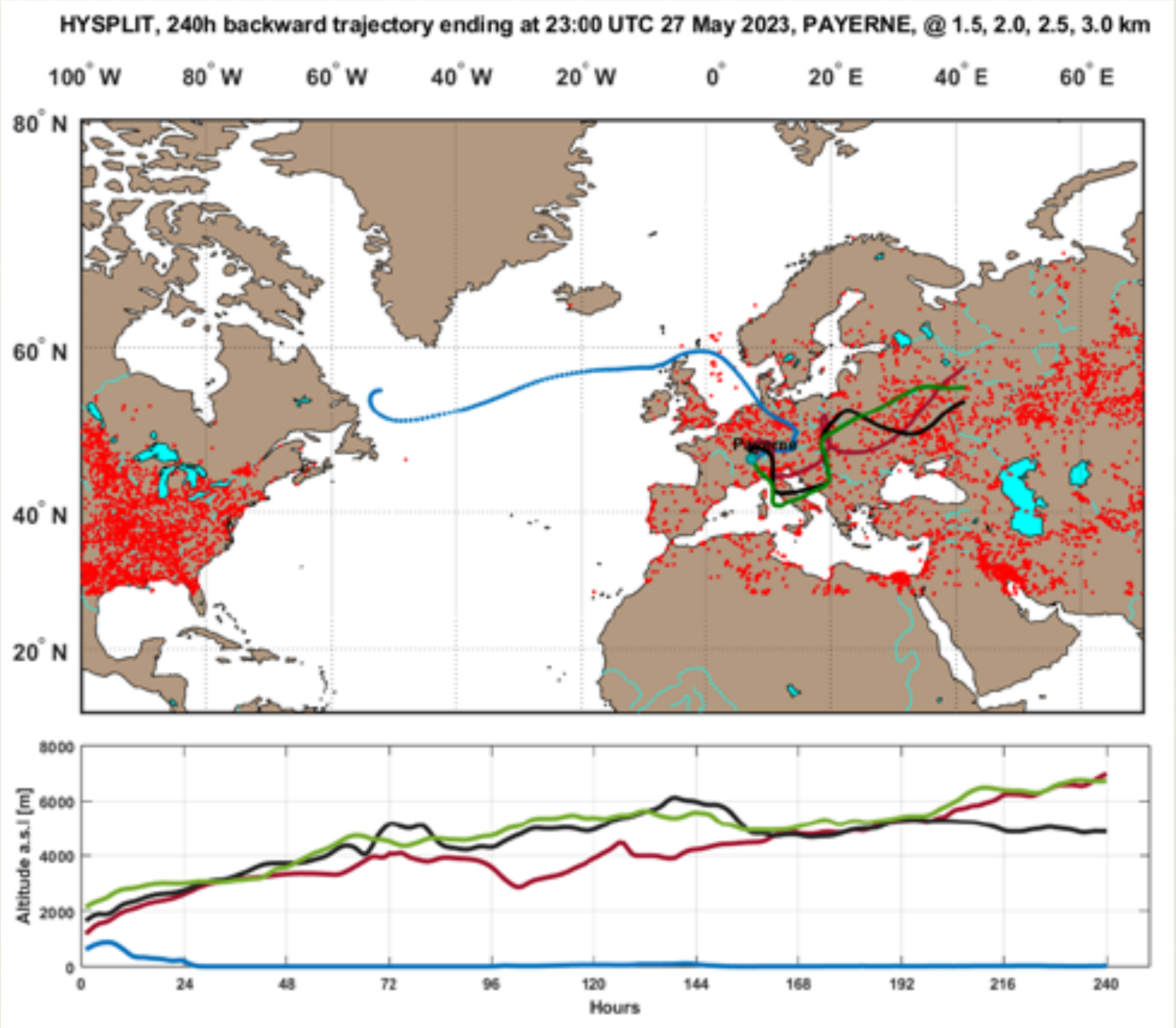


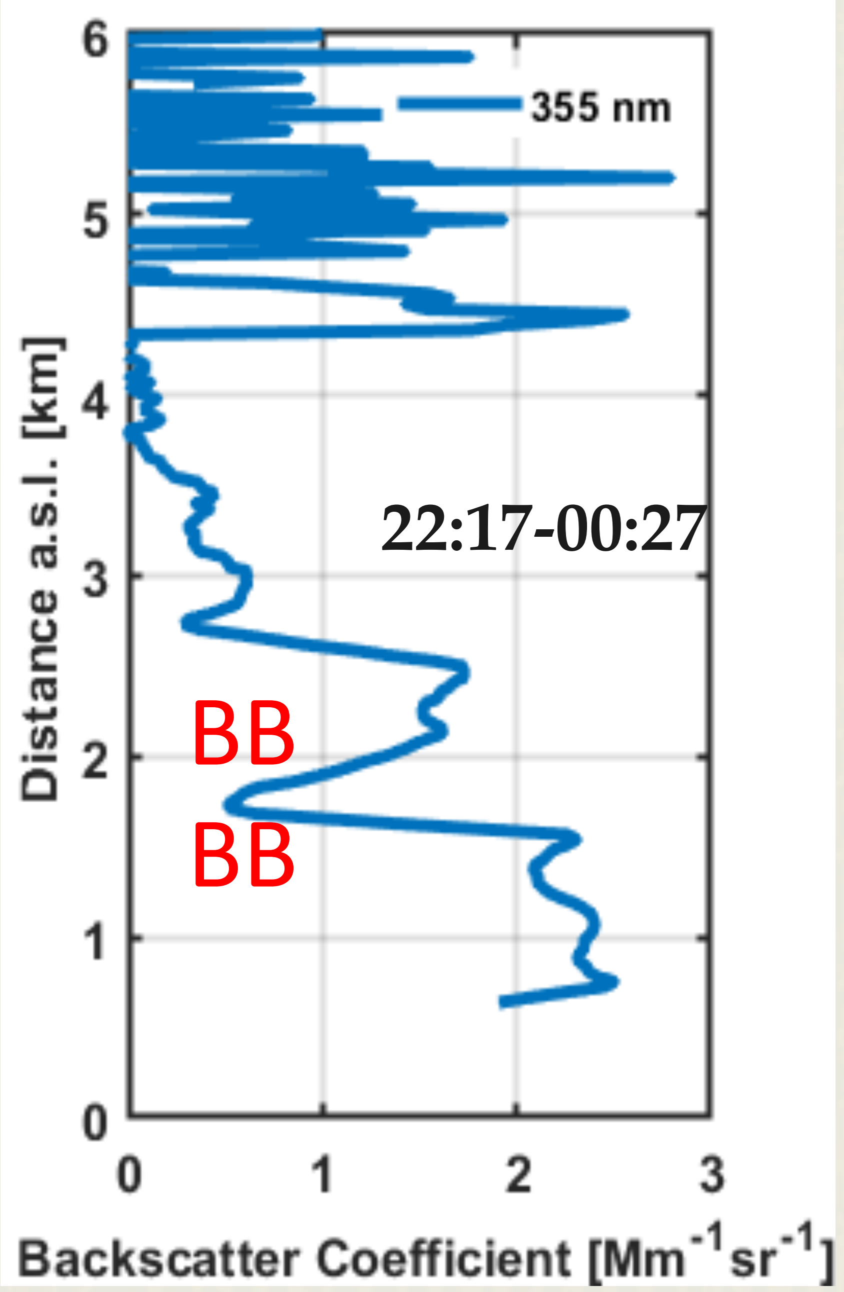


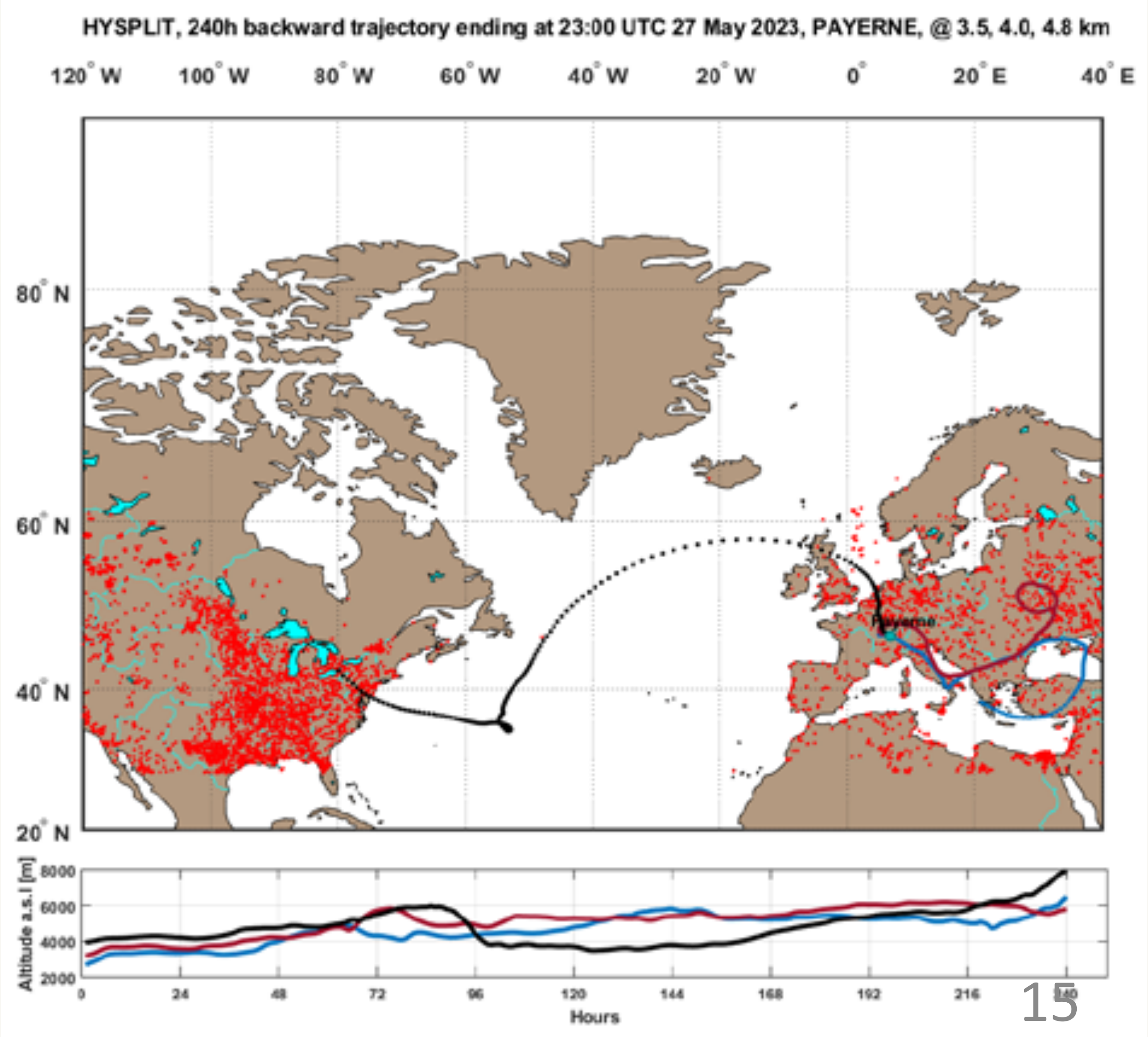
Scales: 2023 Canada fires











Methods

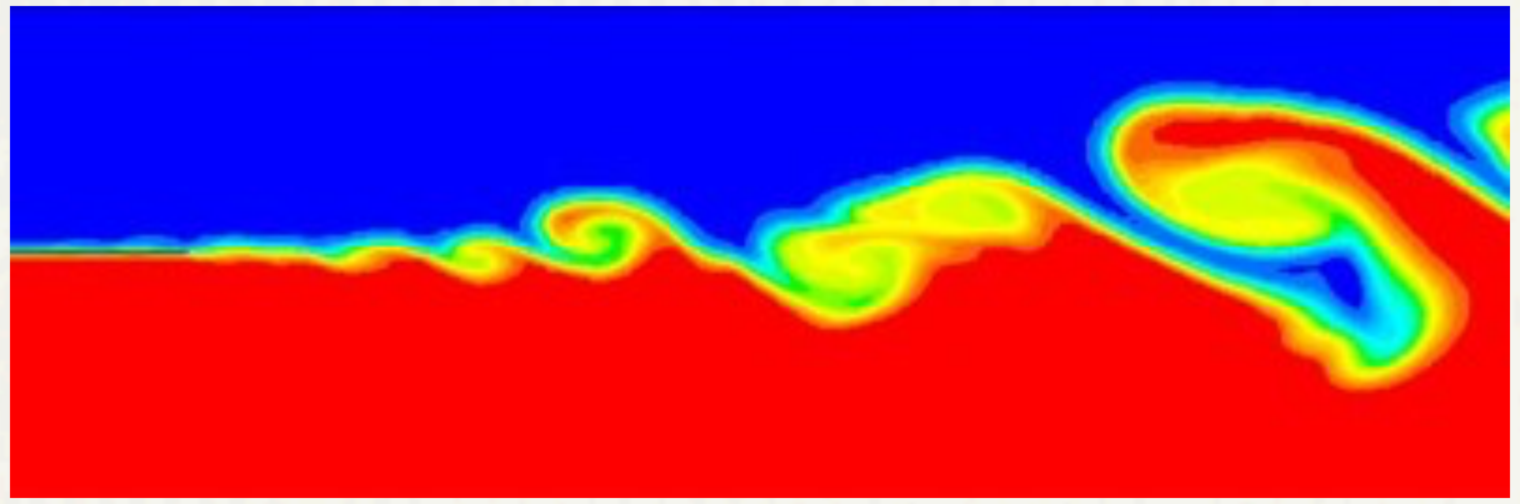
Depending on the scale and on the substance, various approaches are applied

- **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)

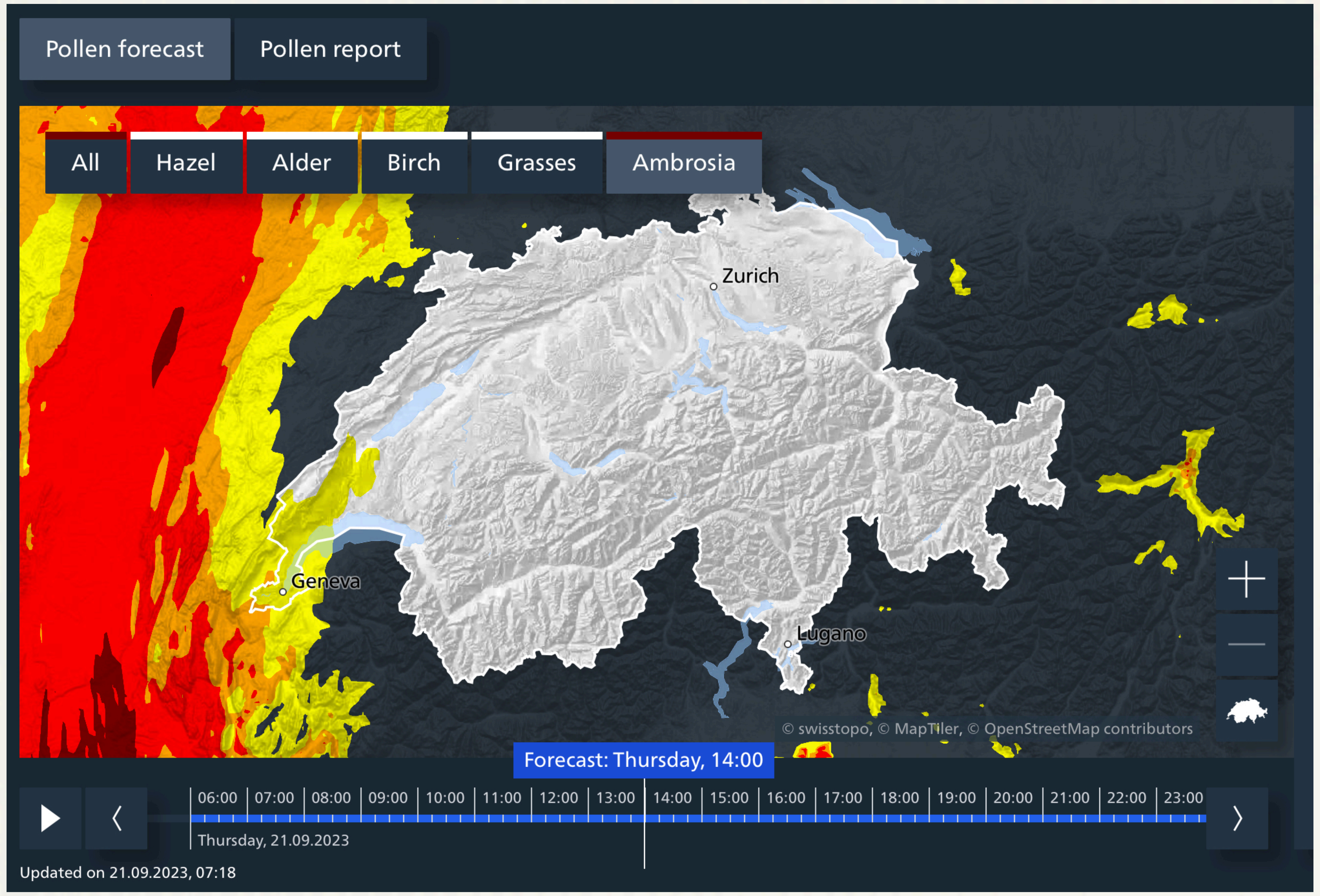
- Simplified **physical models**



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

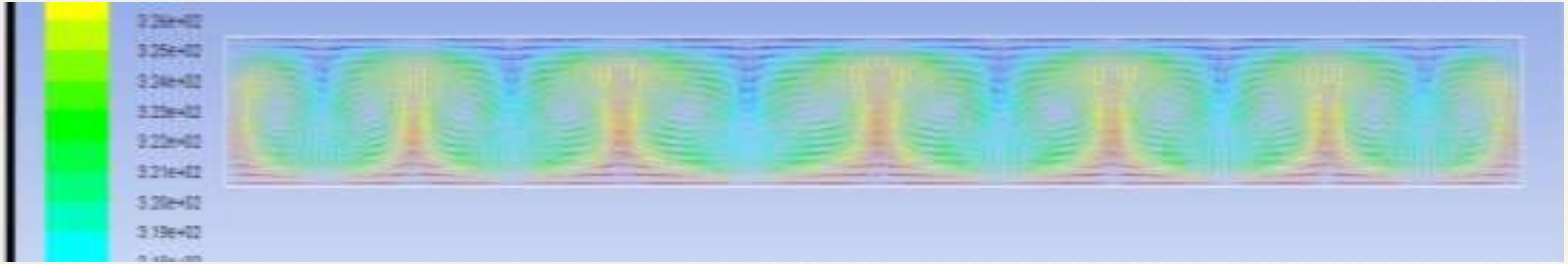
If we have only transport by advection

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

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

What are the relevant transport processes ?

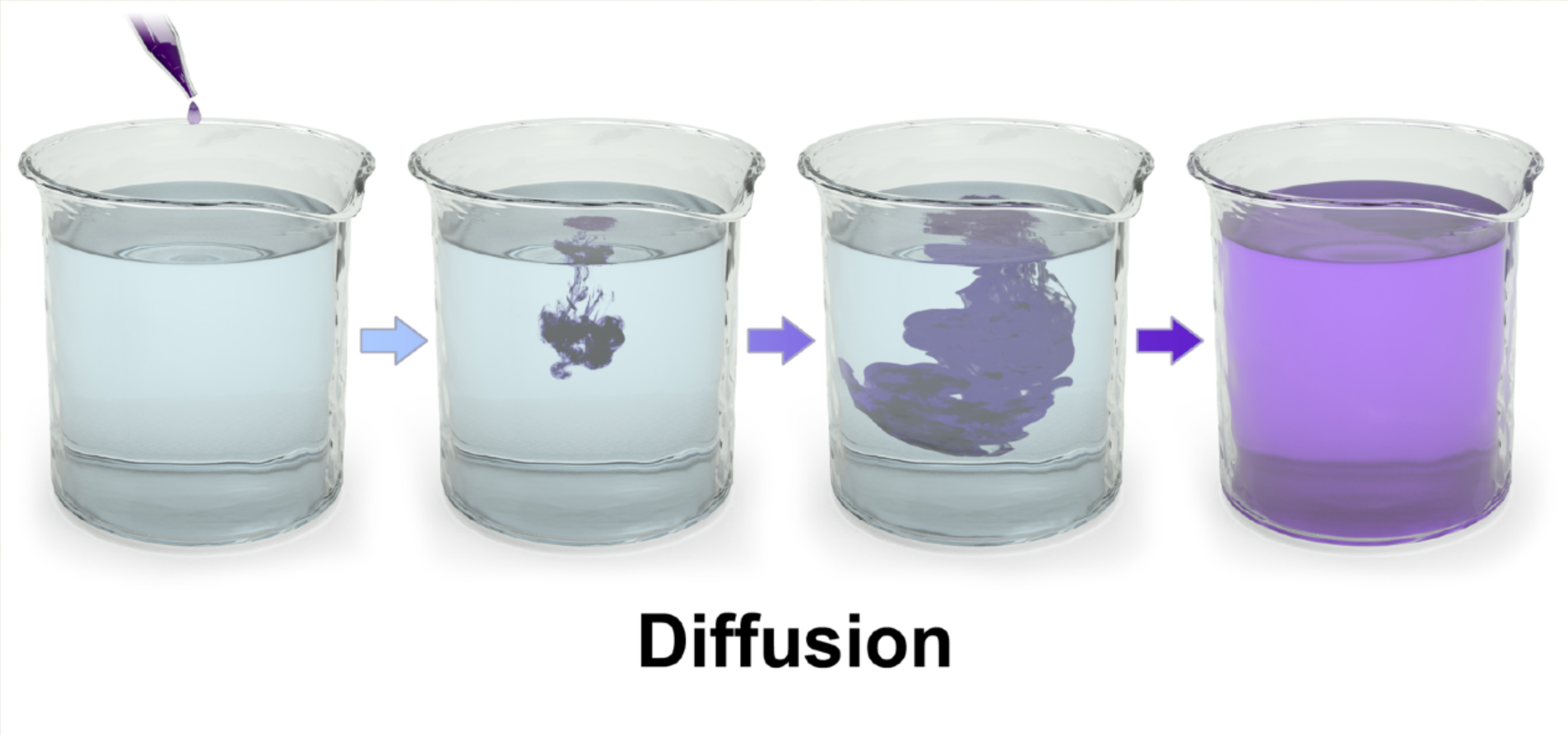
- **Convection**: buoyancy-driven motion. Not directly treated in this lecture,

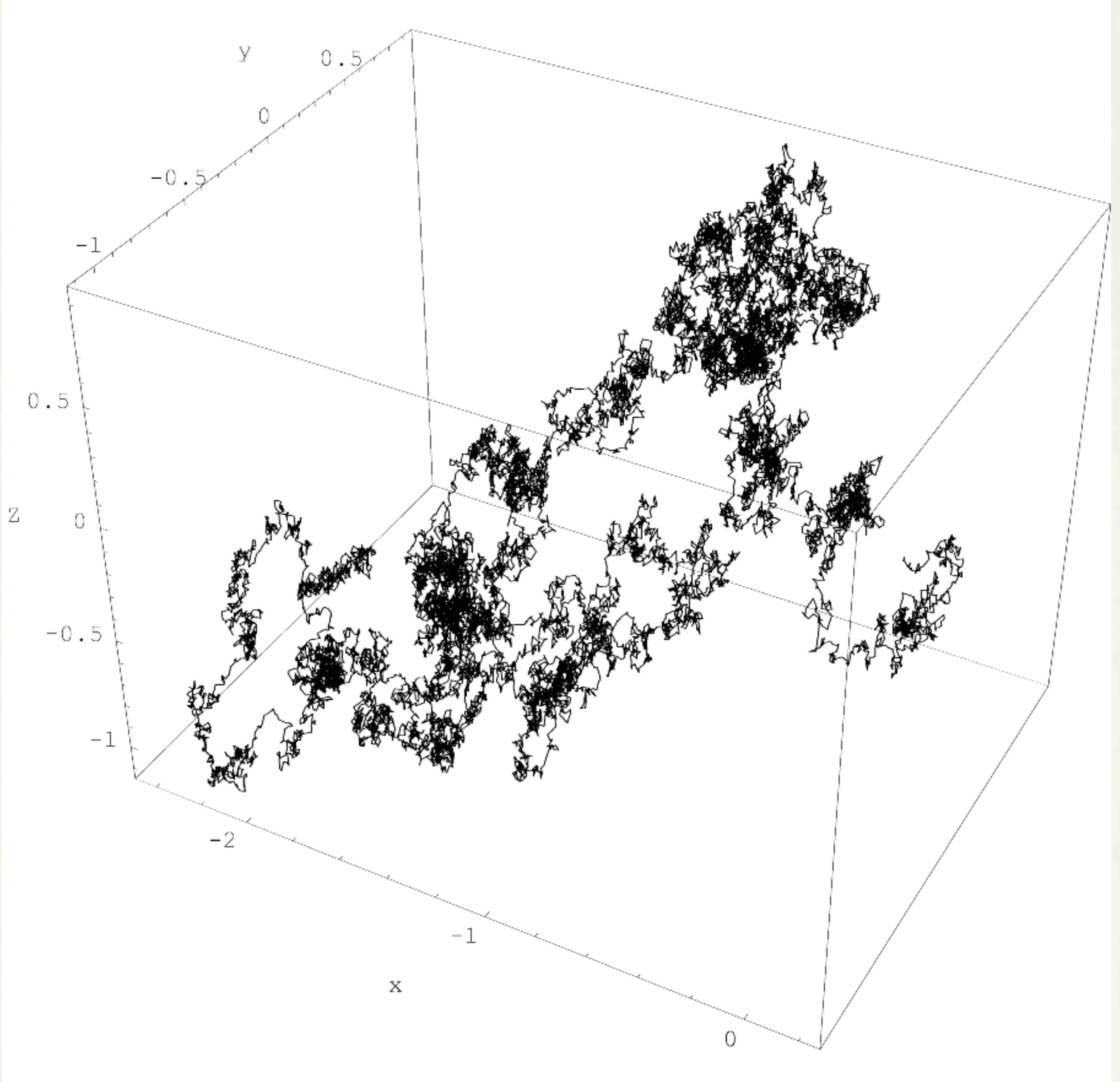


Rayleigh-Bénard instability

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.

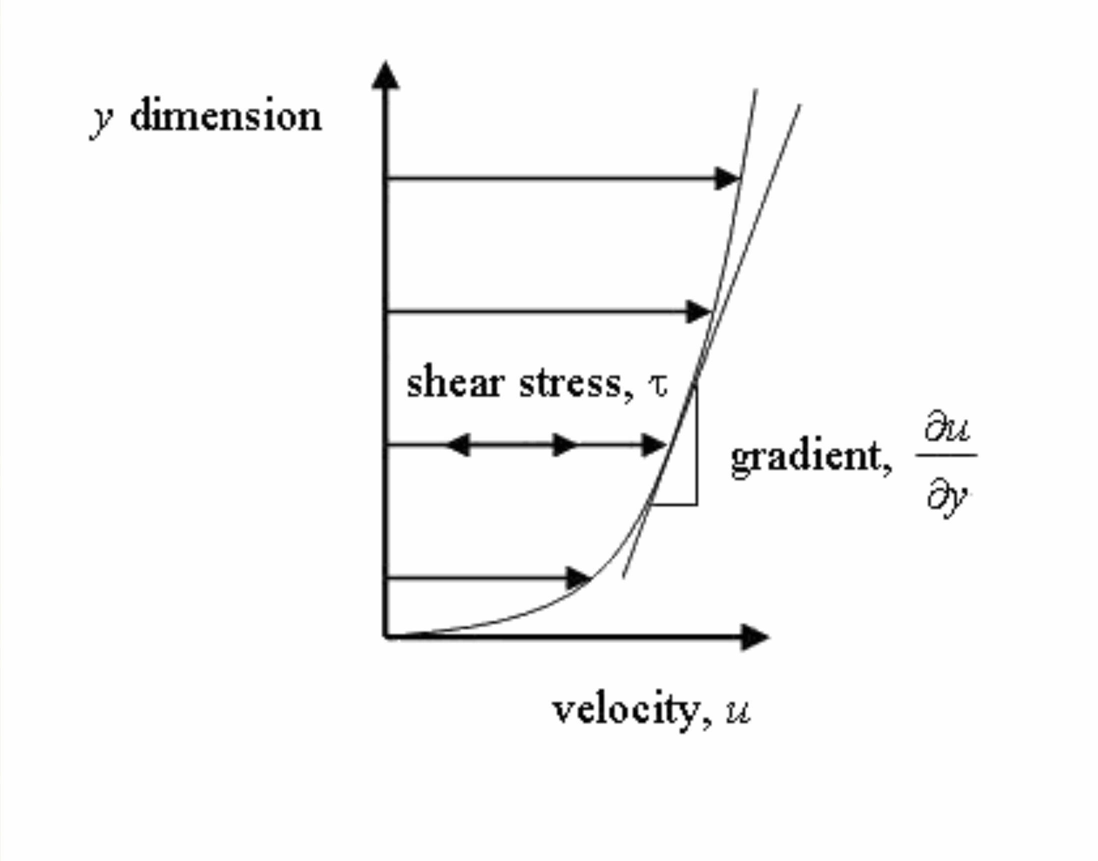




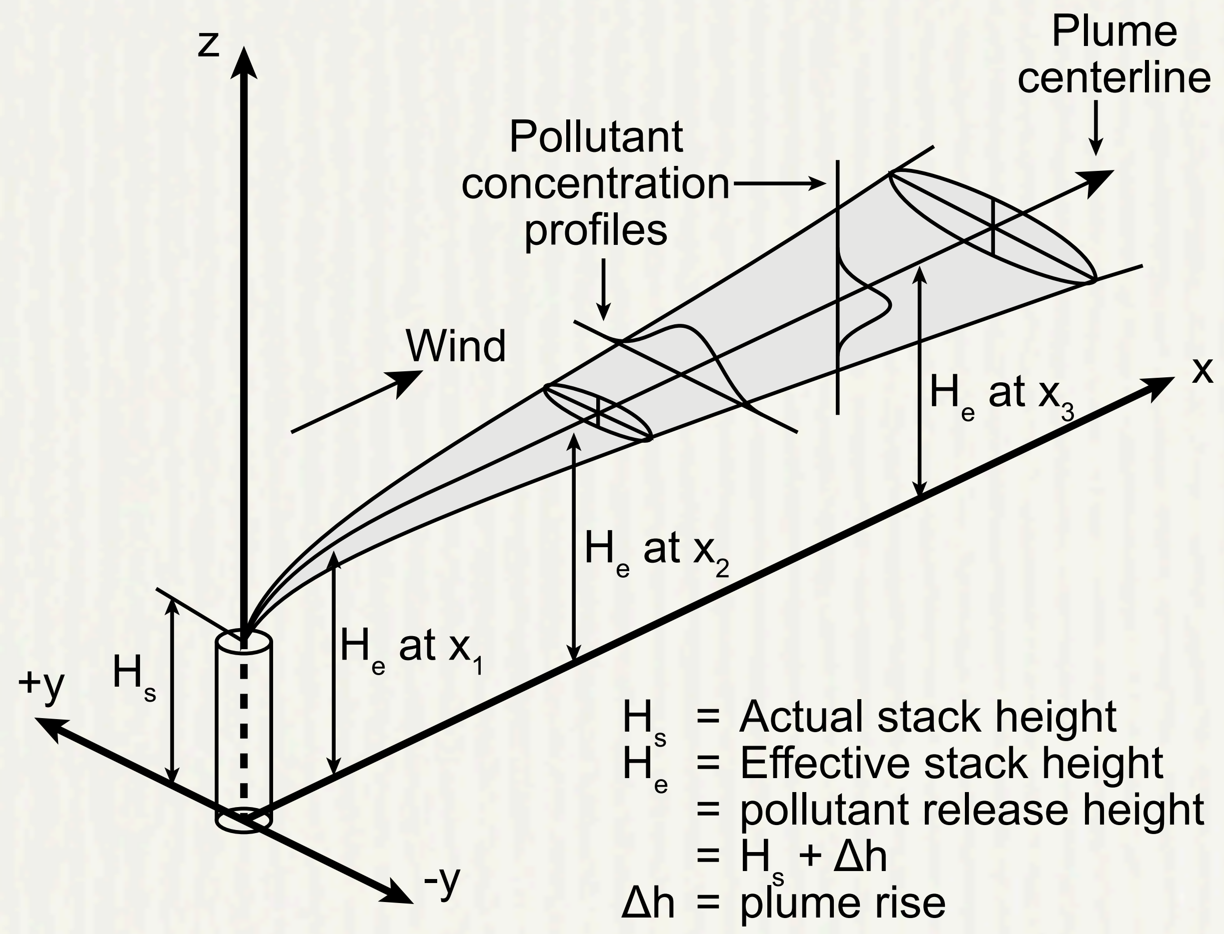
- **Turbulent** diffusion: similar to molecular diffusion but occurs in a turbulent flow. Similar mathematical description, but diffusion coefficient typically orders of magnitude larger.

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)

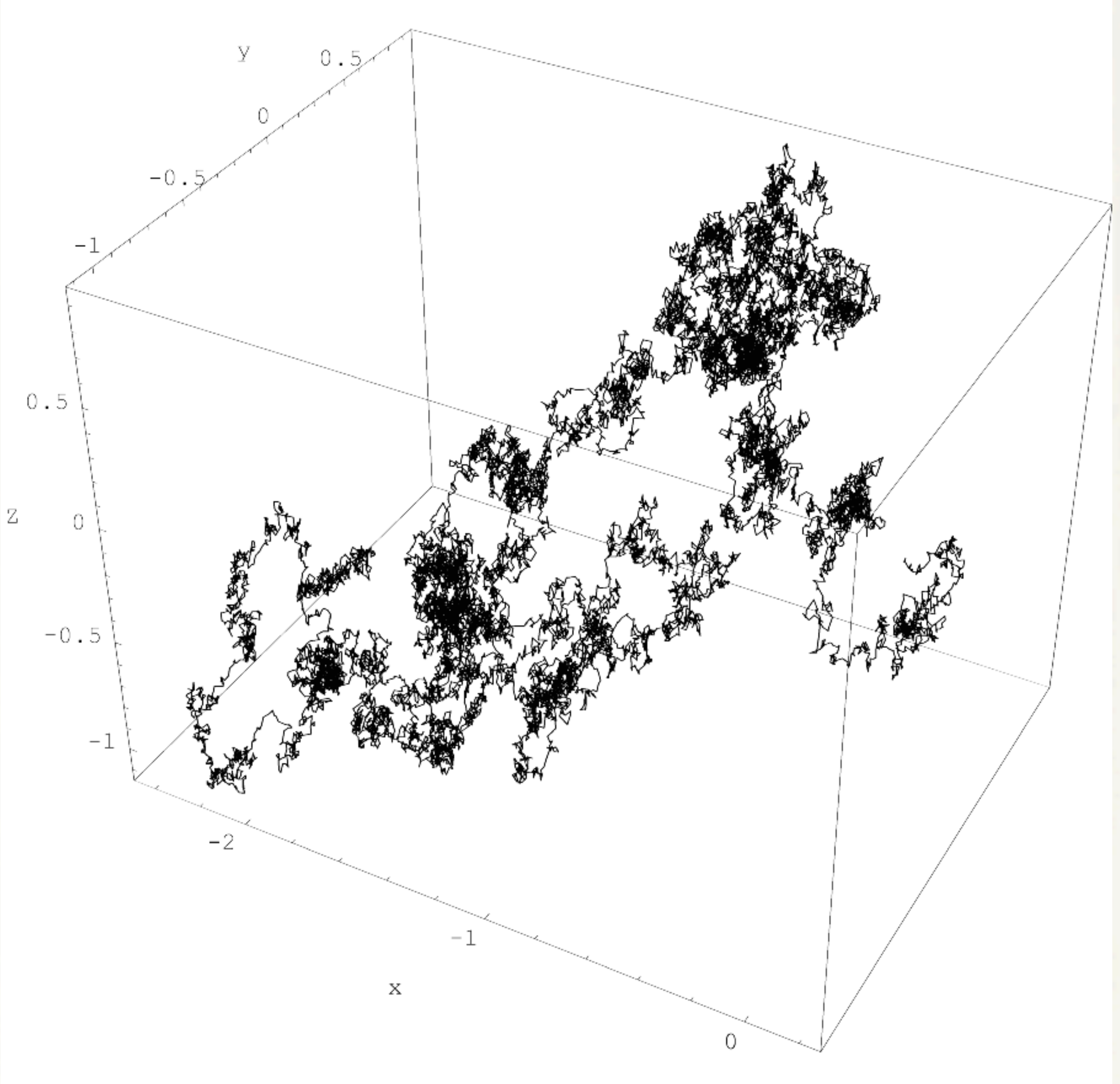
Kinetic energy (average !): $\langle \frac{1}{2} m v_x^2 \rangle = \frac{1}{2} k_B T$

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**.



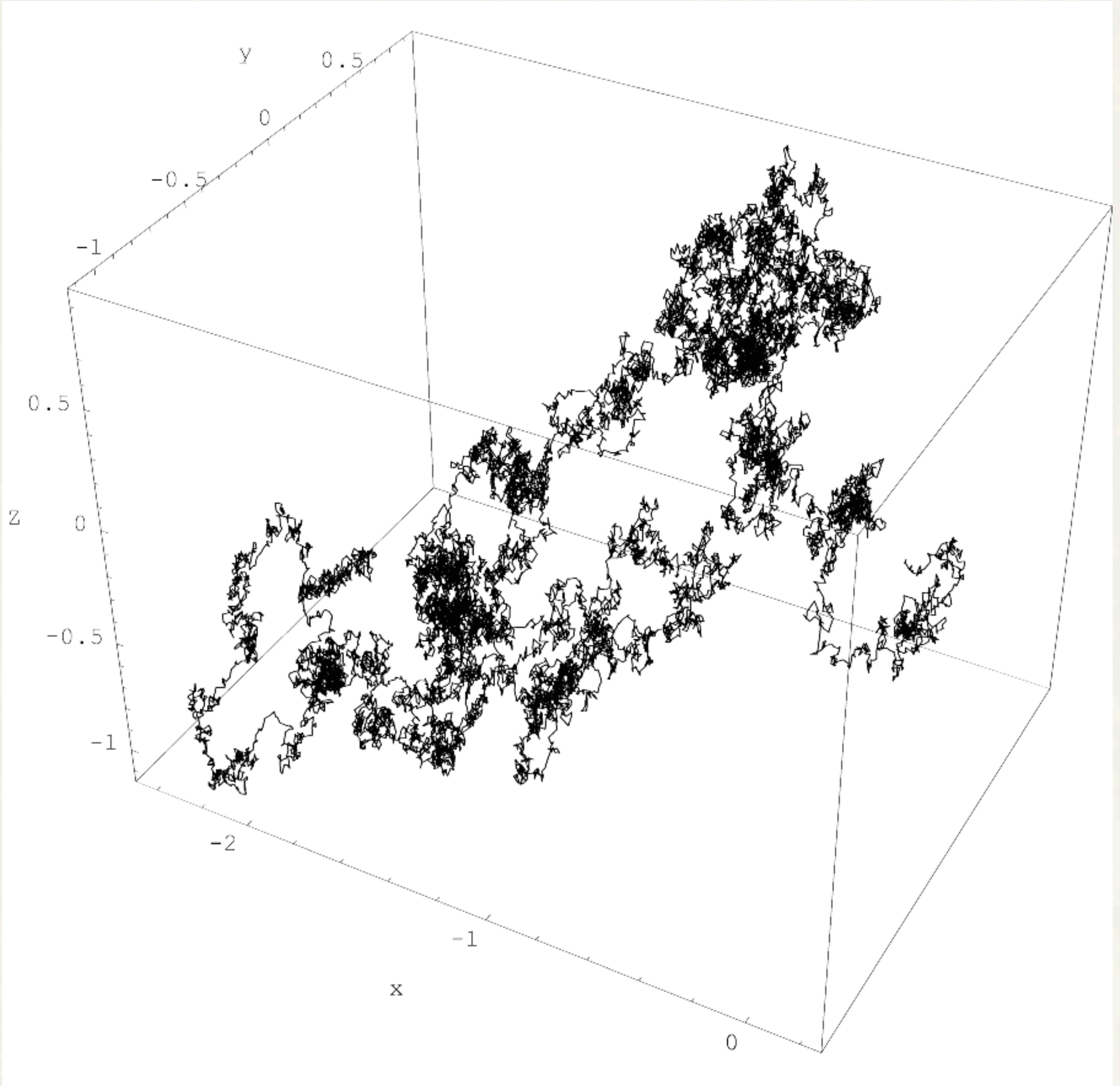
Average velocity of N_2 molecules at room temperature: 464 m/s !

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).

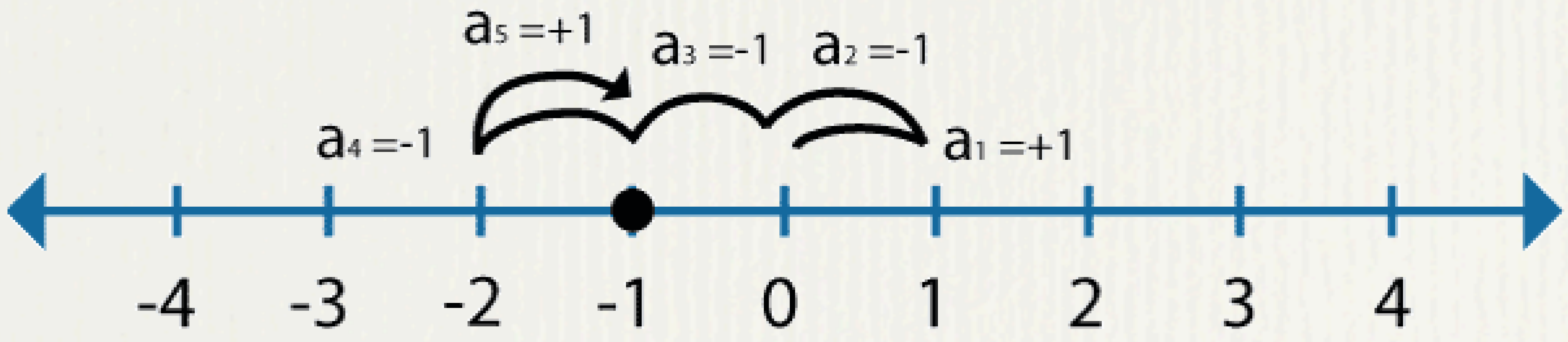
Many particles (N): probability density p(x,y,z,t) proportional to concentration.

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

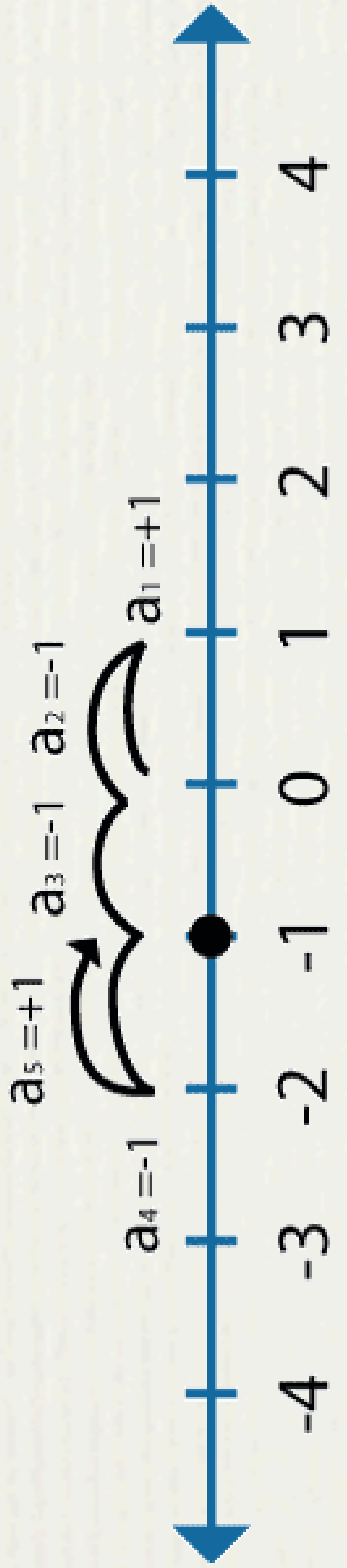
1D random walk

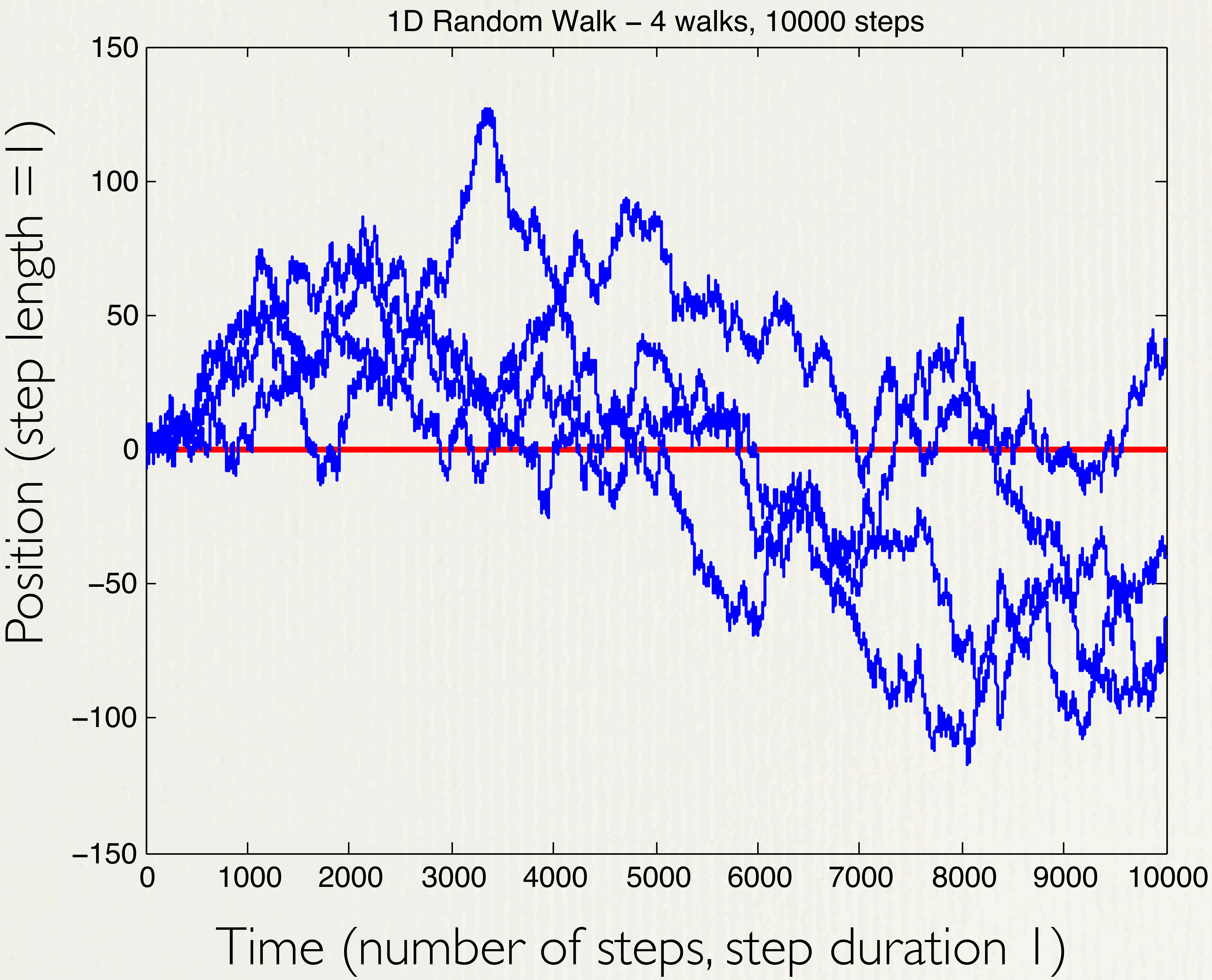
Simple **model** for diffusion: the 1D random walk (example diffusion of tracer molecules in a narrow pipe).

- 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

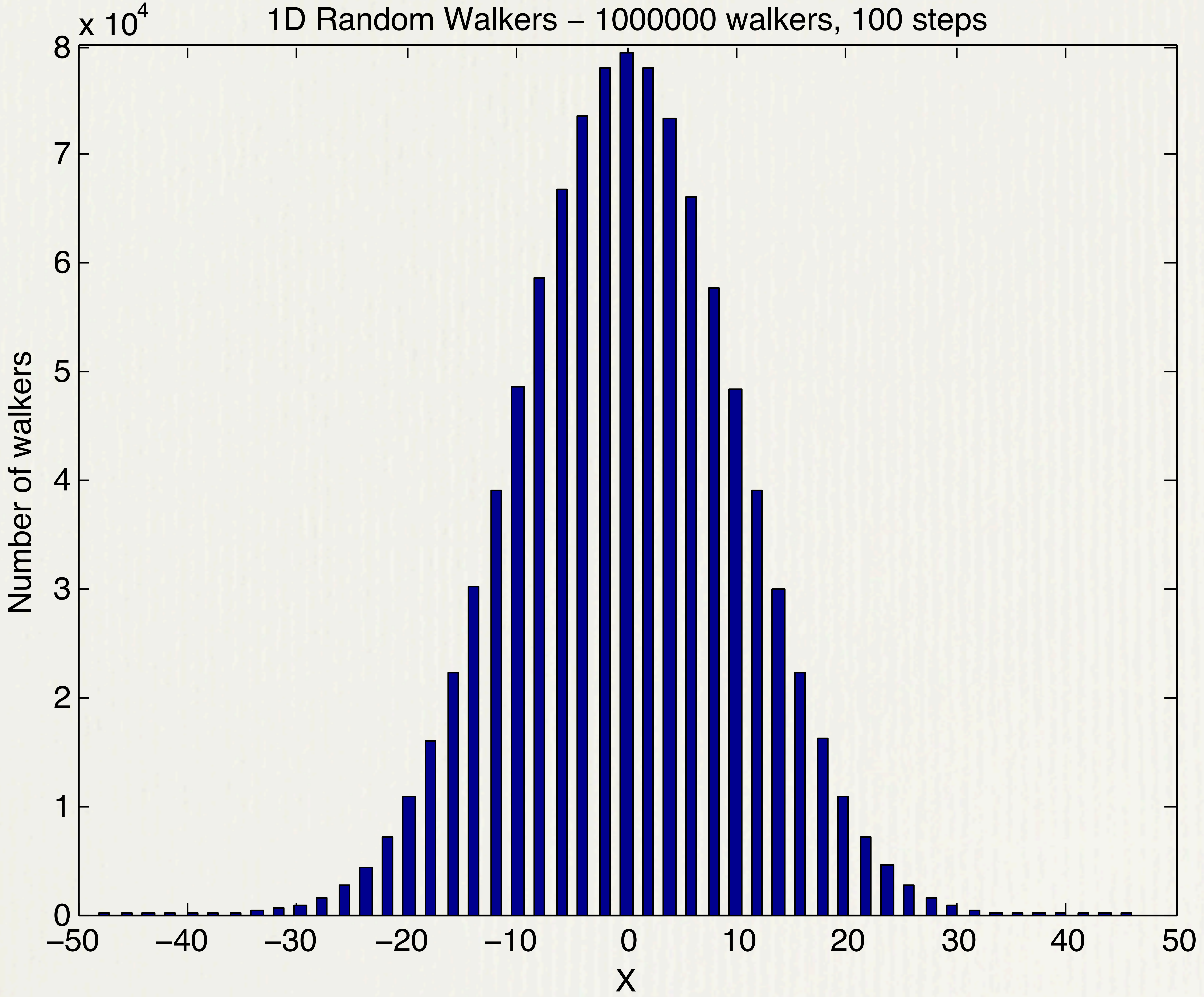


1D random walk: example trajectories

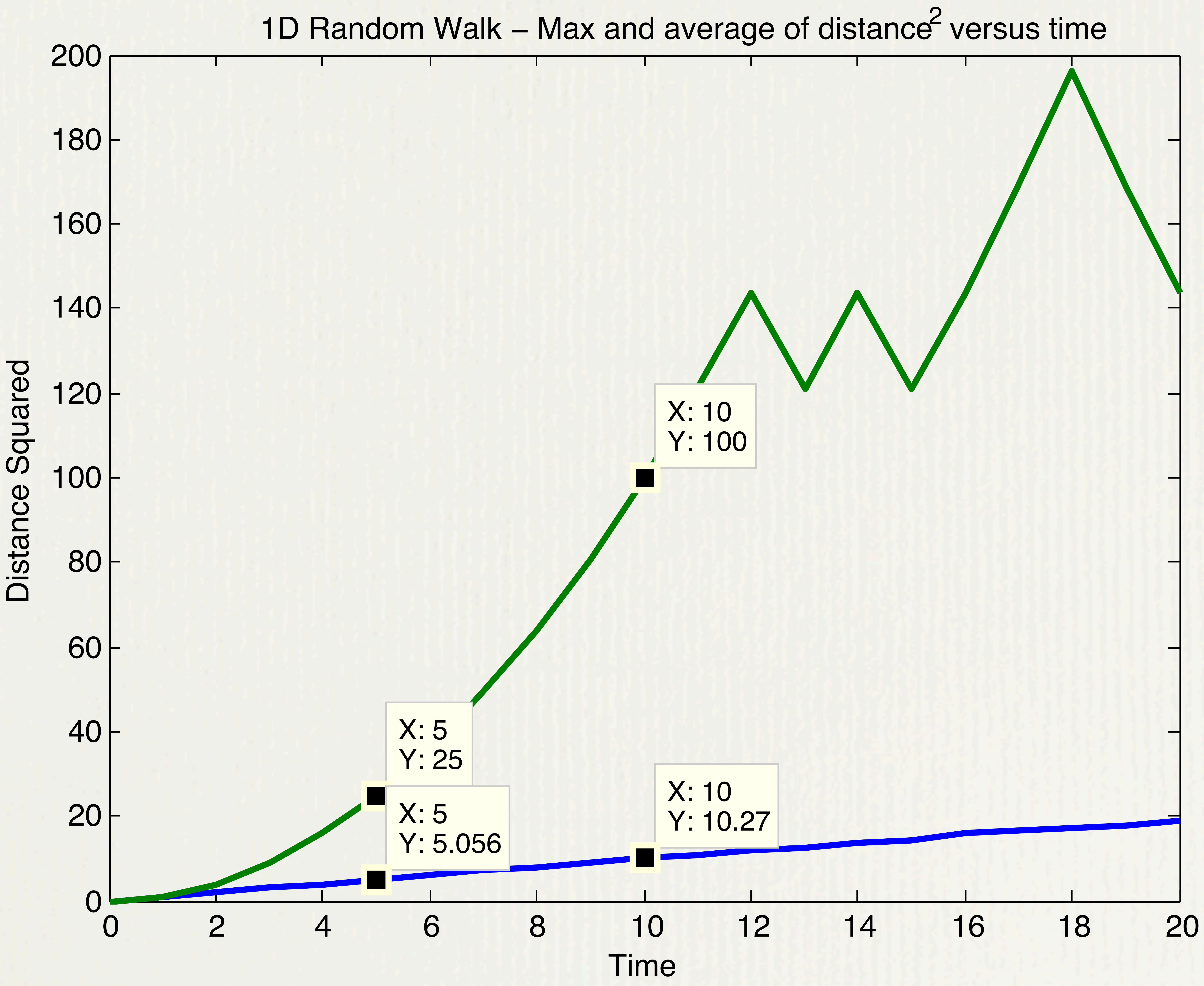




1D random walk: histograms of positions

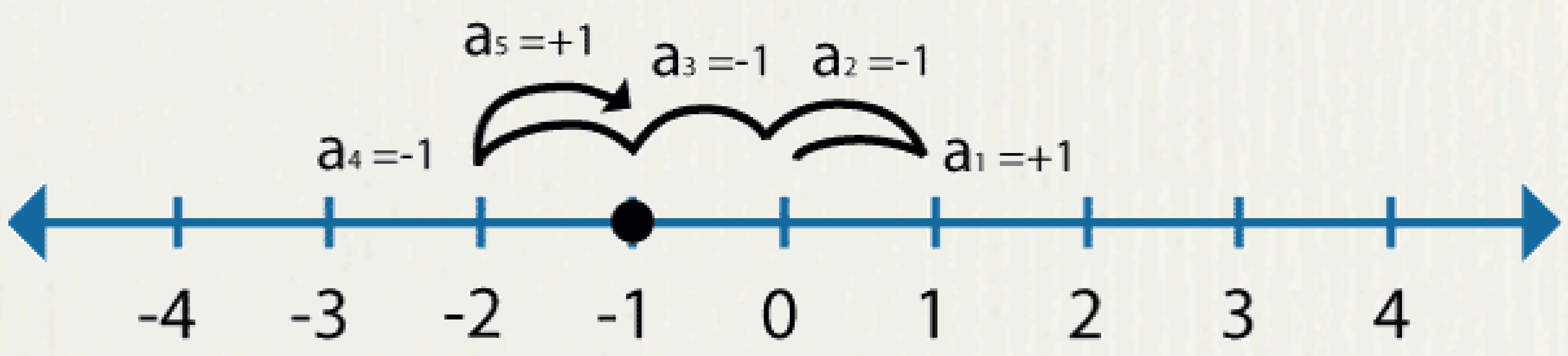


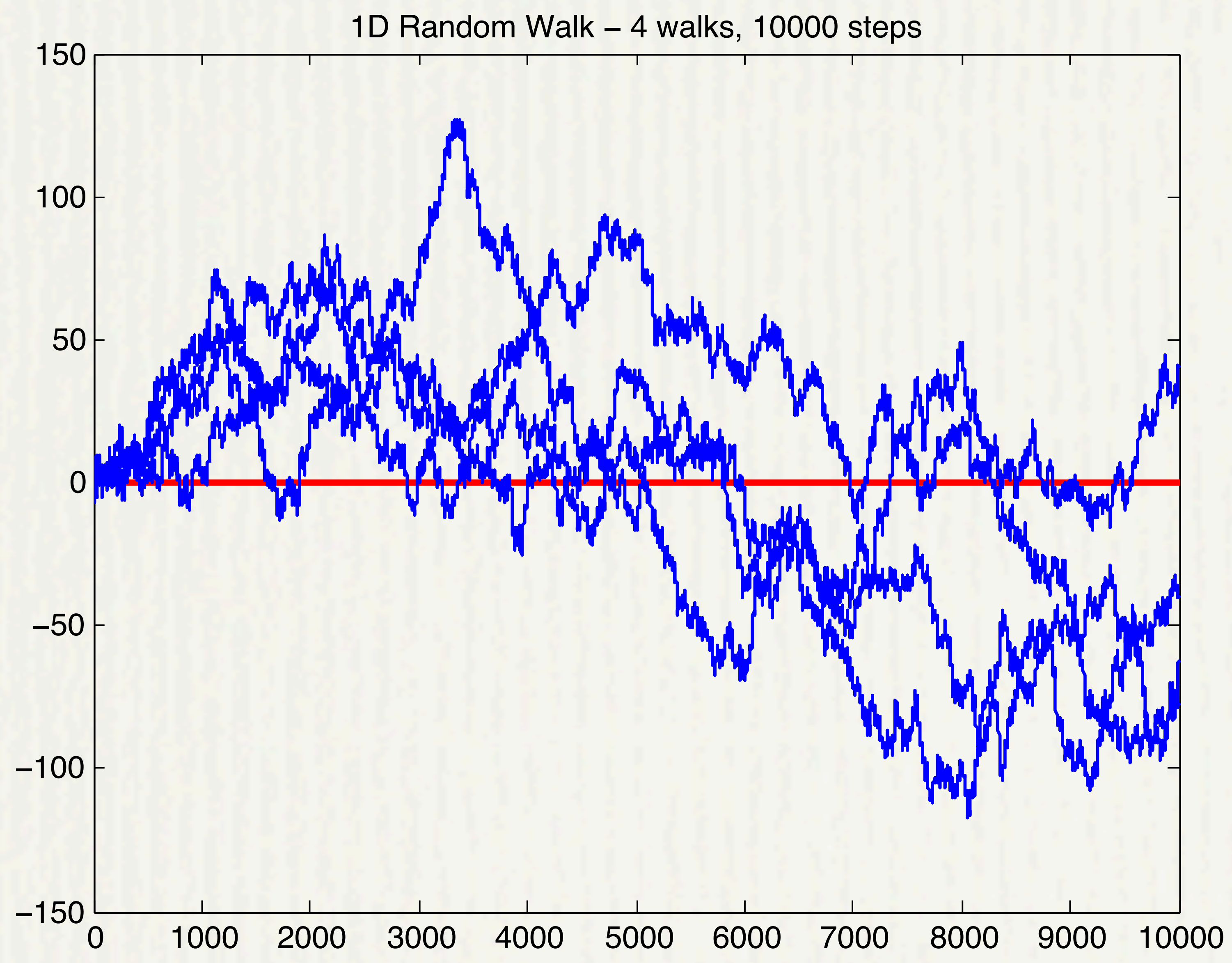
1D random walk: average and max distance^2



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.

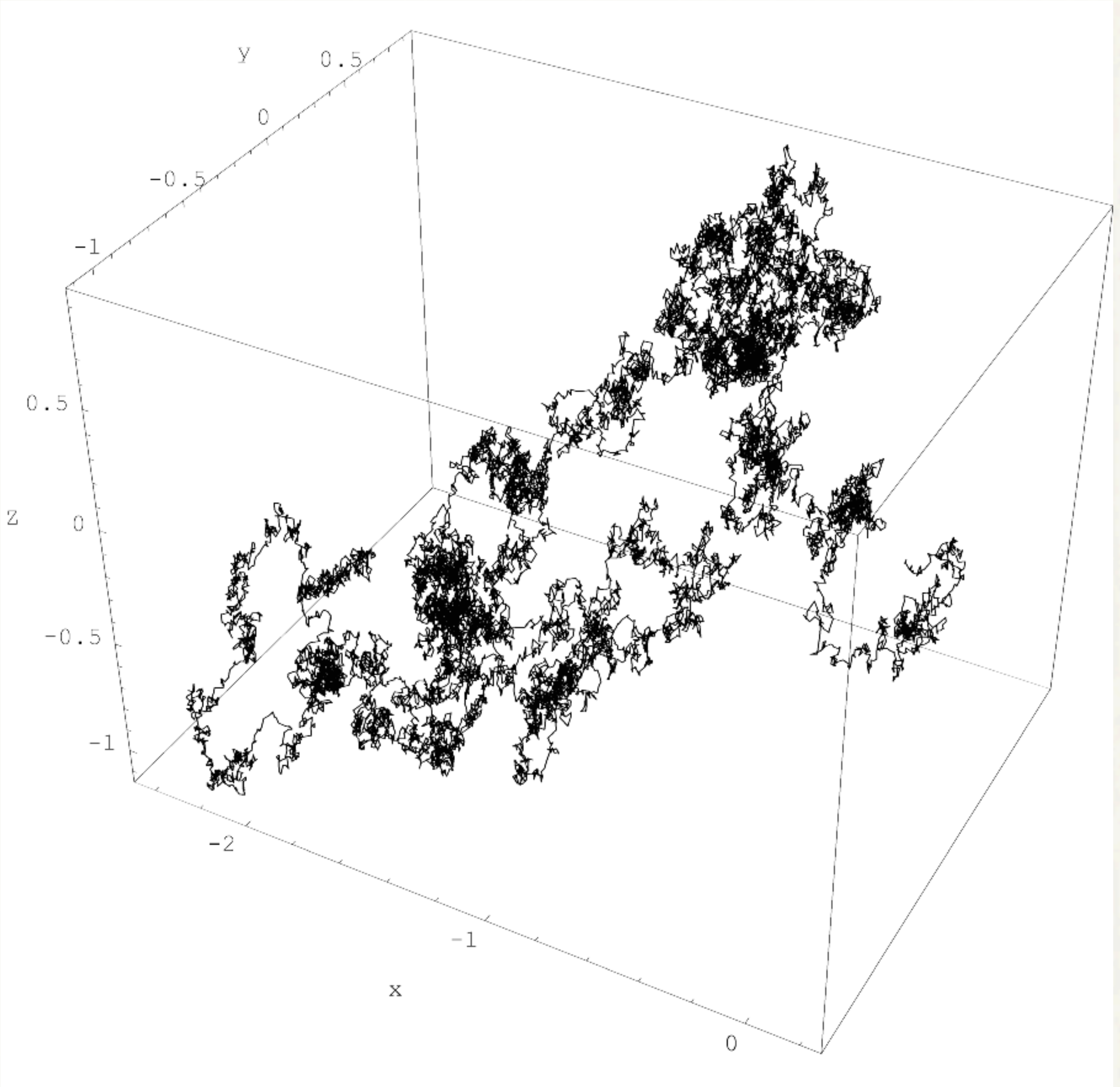
- **Turbulence** results in a diffusion coefficient orders of magnitude larger.

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.

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

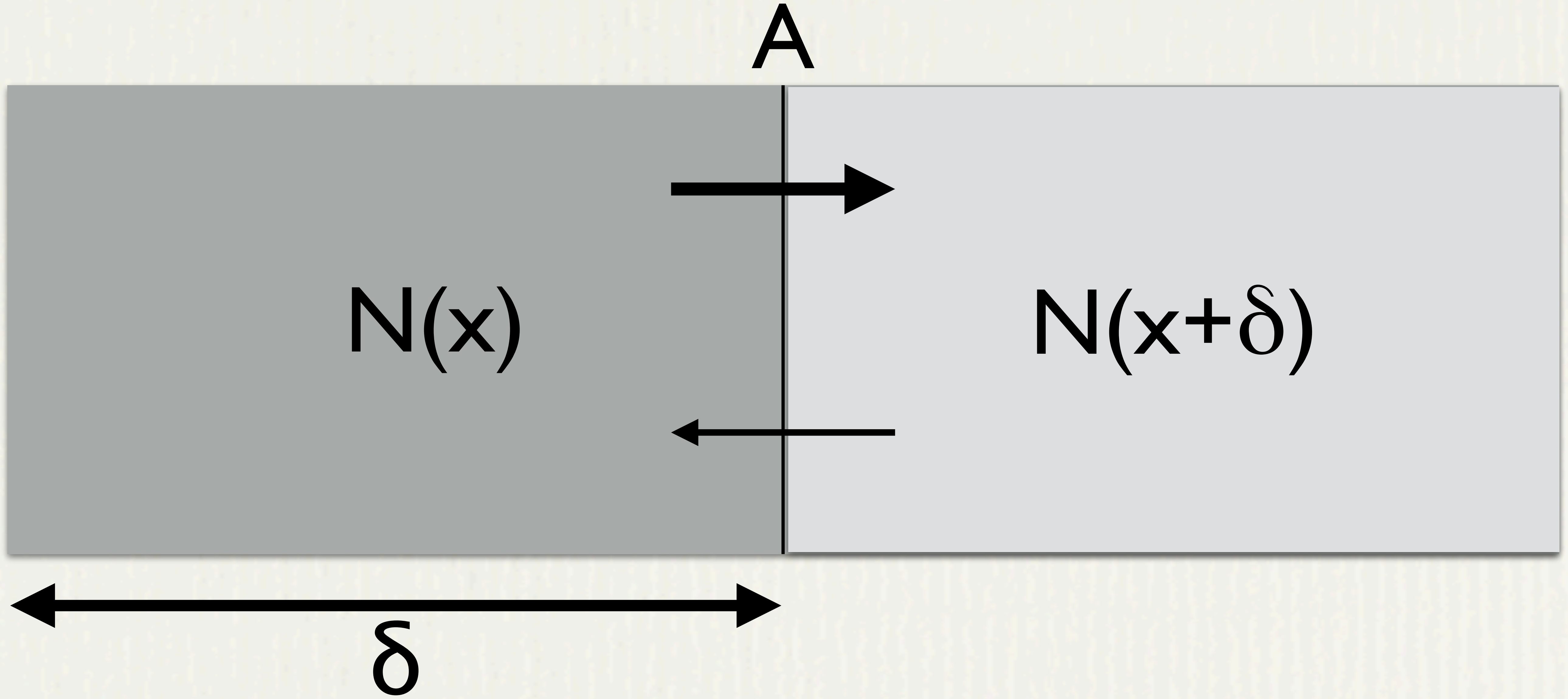


- Non-trivial effect: probability never to return at origin is 0 in 1D and 2D. However, a drunk bird only has a 34% chance to return home (3D diffusion).

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

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

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

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

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