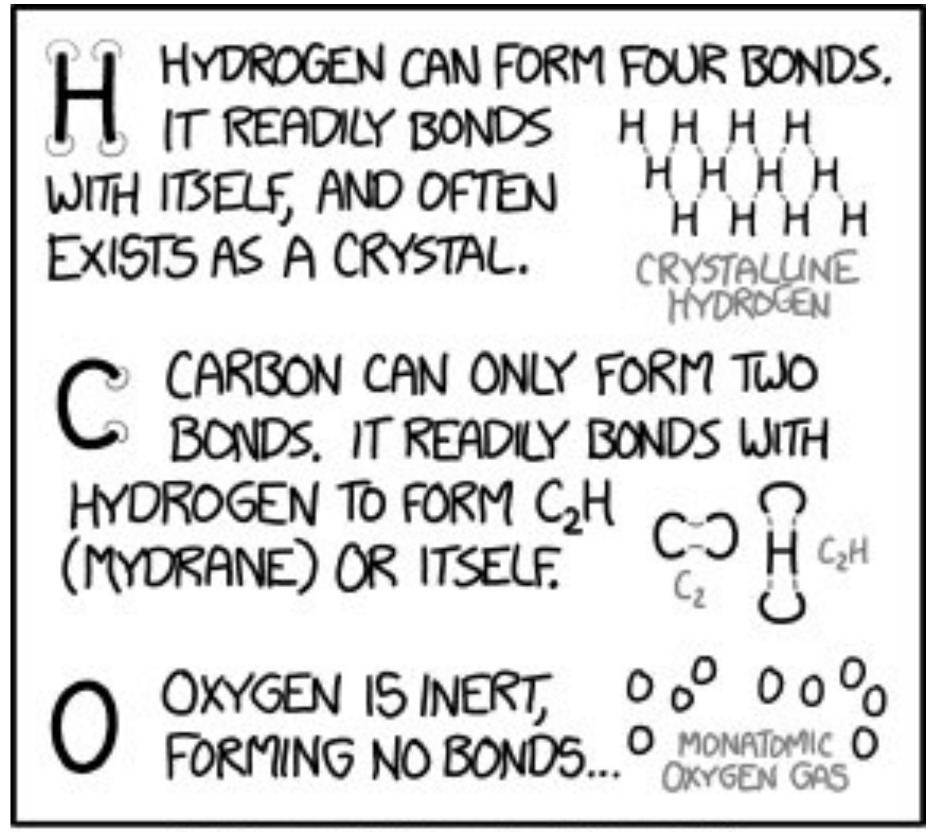
- **Theme Music:**
  Willie Nelson
  The Gambler
- **Cartoon:**
  Randall Munroe
  xkcd



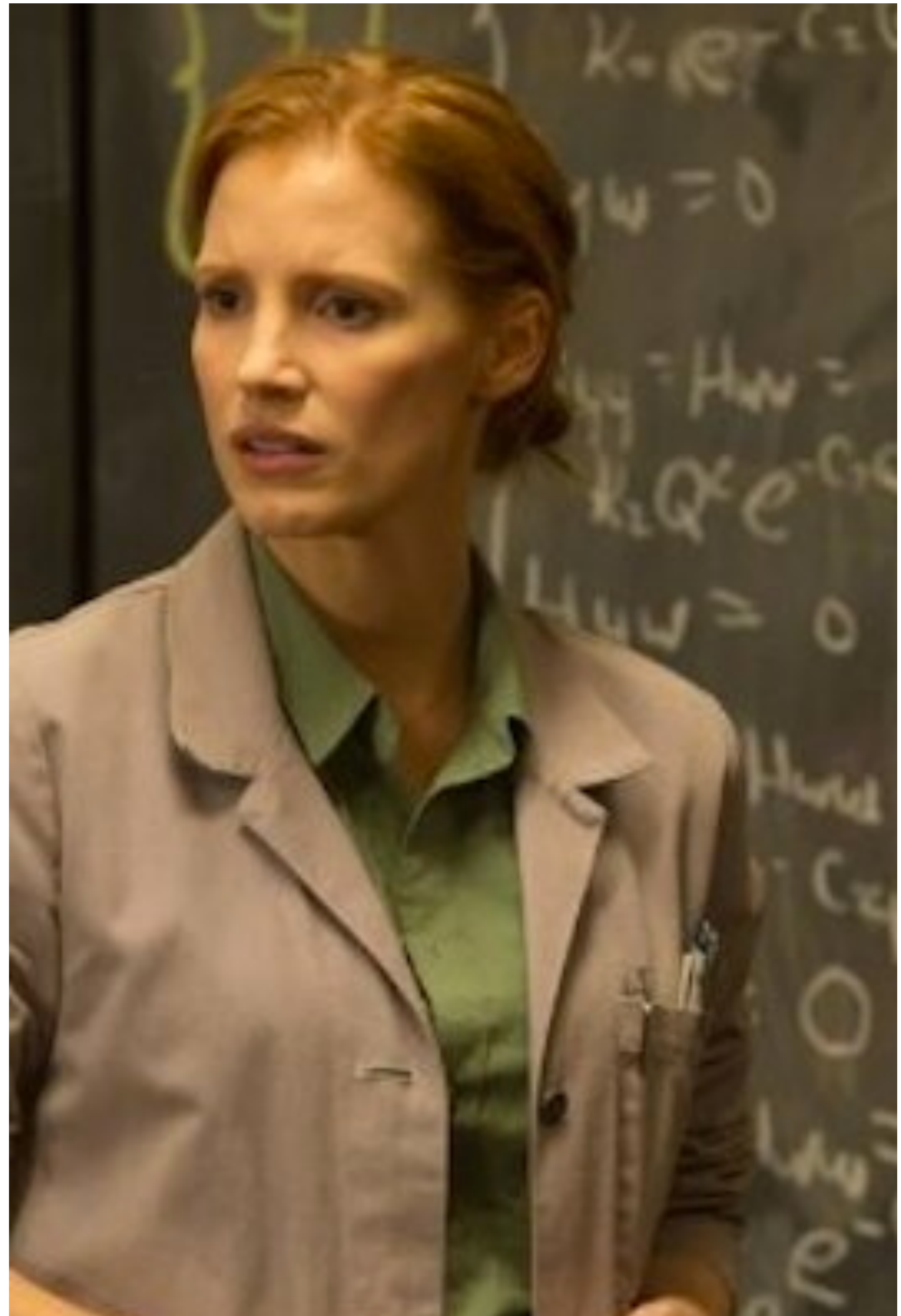
TYPOGRAPHIC CHEMISTRY

The Equation of the Day

Fick's Laws

$$\left\langle (\Delta x)^2 \right\rangle = 2D(\Delta t)$$

$$J = -D\frac{dn}{dx}$$



Foothold principles: Randomness

- Matter is made of of molecules in constant motion and interaction. This motion moves stuff around.
- If the distribution of a chemical is non-uniform, the randomness of molecular motion will tend to result in molecules moving from more dense regions to less.
- This is **not** directed but is an emergent phenomenon arising from the combination of random motion and non-uniform concentration.

A new start

- Our mathematical model based on identifying position, velocity, and all the forces on an object and then calculating the motion using Newton's second law is too hard for a small particle being hit by many molecules.
- An alternative starting point is to describe the result of all the forces acting on a small object as random motion.
- Average phenomena that emerge from the randomness can still be reliable even though the motion at any given instant can't be predicted.

Foothold principles: Fick's first Law

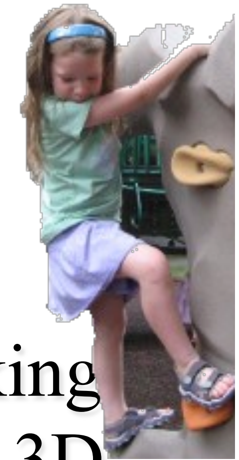
- If a set of molecules is not distributed uniformly in 1D (there is a concentration gradient) there will be an effective flow of those molecules according to

$$J = -D\frac{dn}{dx}$$

(or in 3D) $\vec{J} = -D\vec{\nabla}n$

- In a gas, the diffusion constant D is given by $\frac{1}{2\sqrt{3}}\lambda\bar{v}$
- In a liquid, the diffusion constant is given by $D = \frac{k_B T}{6\pi\mu R}$

Foothold principles: Fick's second Law

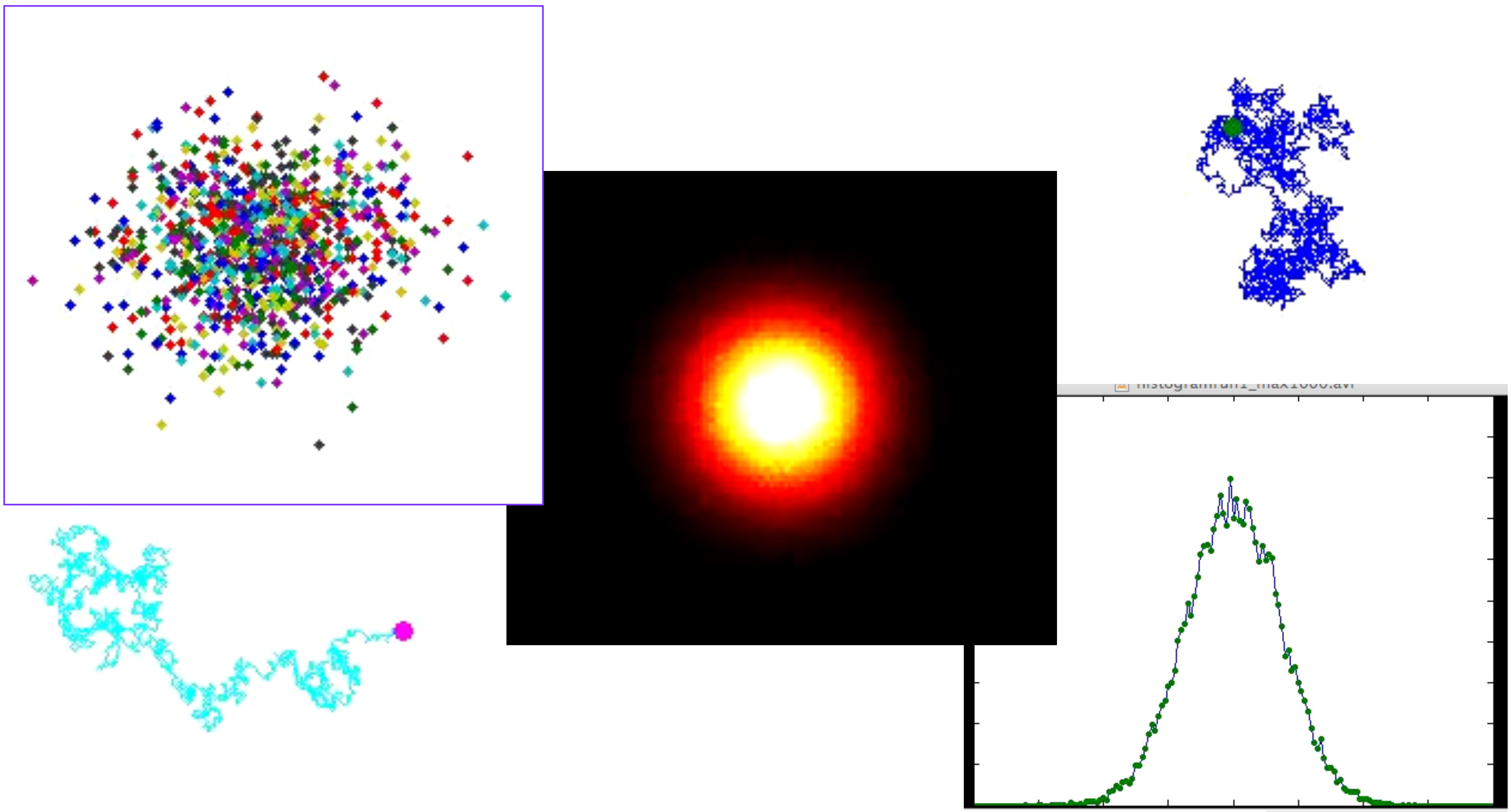


- The average square displacement of a random walking molecule in a thermal bath after a time *t* is given in 3D by Fick's second law:

$$\left\langle \Delta r^2 \right\rangle = \left\langle \Delta x^2 \right\rangle + \left\langle \Delta y^2 \right\rangle + \left\langle \Delta z^2 \right\rangle = 6D\Delta t$$

- The radius of a small blob of chemical in a liquid will grow at this rate.
- The displacement, $\Delta r = \sqrt{\left\langle \Delta r^2 \right\rangle}$, only grows like $\sqrt{\Delta t}$ For larger organisms, this is too slow and is the reason transport systems for air and blood have evolved.

2D Simulations: Multiple representations



Simulations by Alex Morozov & Kerstin Nordstrom

2D Simulations: Multiple representations

1. Watch all the particles.
2. Look at the density of the particles
   – What do the colors represent?
3. Look at a plot of the density along a slice through the middle.
   – What it will look like and what it will do.
4. Look at the motion of individual particles.