

COMPUTE kick-off
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Computational Methods in Biological Physics

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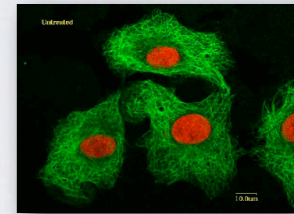
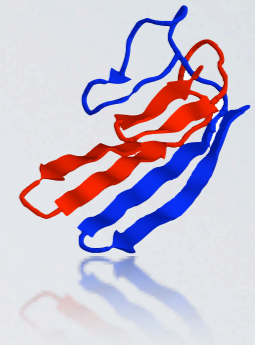
Henrik Jönsson
Mattias Ohlsson
Carsten Peterson

Bo Söderberg
Carl Troein
Stefan Wallin

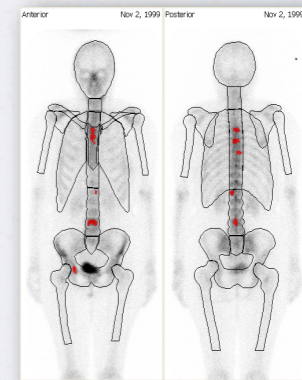
Research overview

- Proteins: folding, aggregation and binding
- Bio-nano physics
- Systems biology: stem cell differentiation, plant growth, circadian clocks
- Decision support systems in medicine (Mattias Ohlsson)

nanometer



meter



Physics, biology, chemistry and medicine..

Proteins

Protein modeling - overview

- Protein folding
- Protein aggregation
 - Alzheimer
 - ALS
 - Parkinson
- Protein-peptide binding



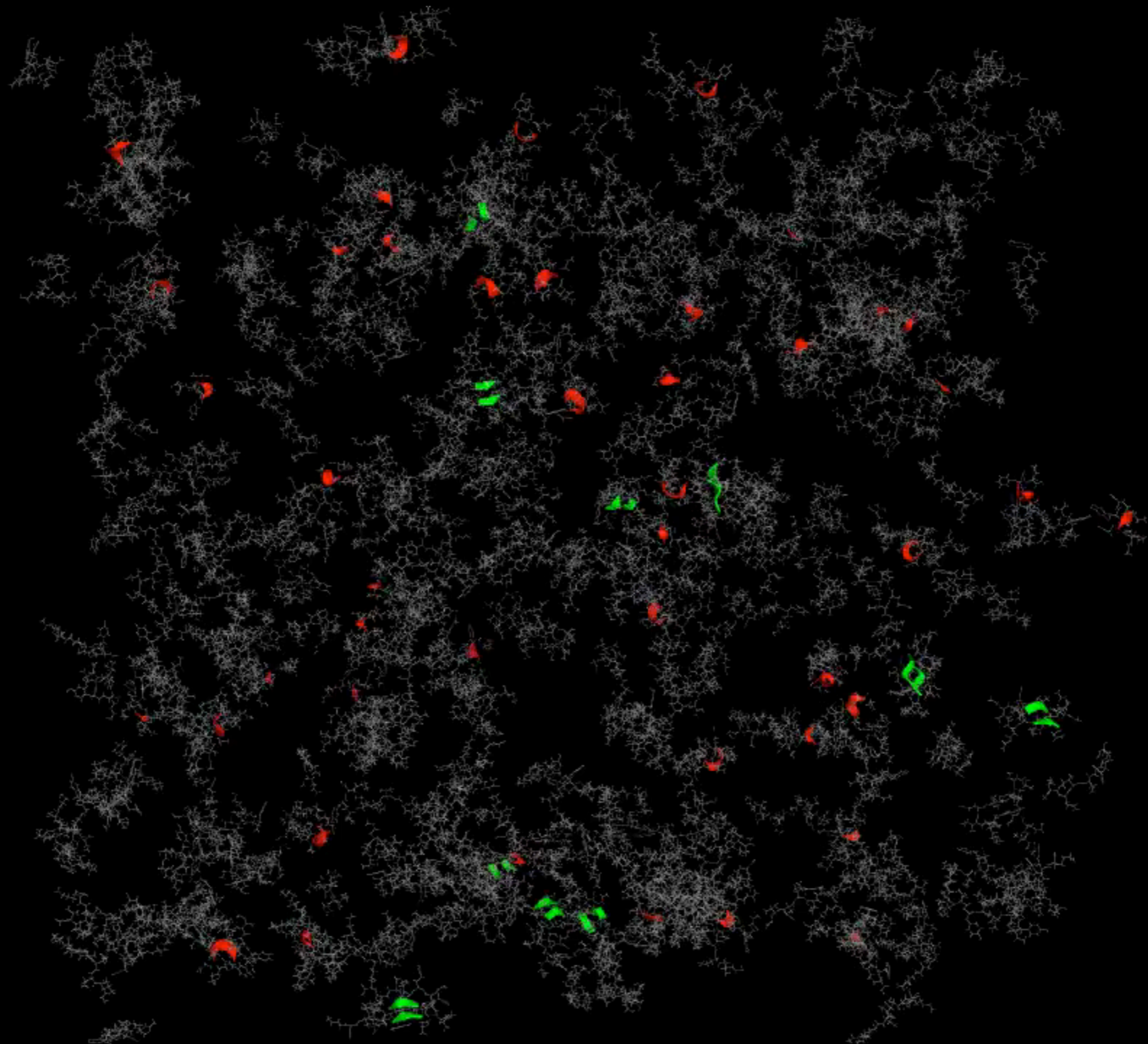
Computational methods

- Monte Carlo
- Exact enumeration schemes

Anders Irbäck, Stefan Wallin

Monte Carlo simulation

protein aggregation

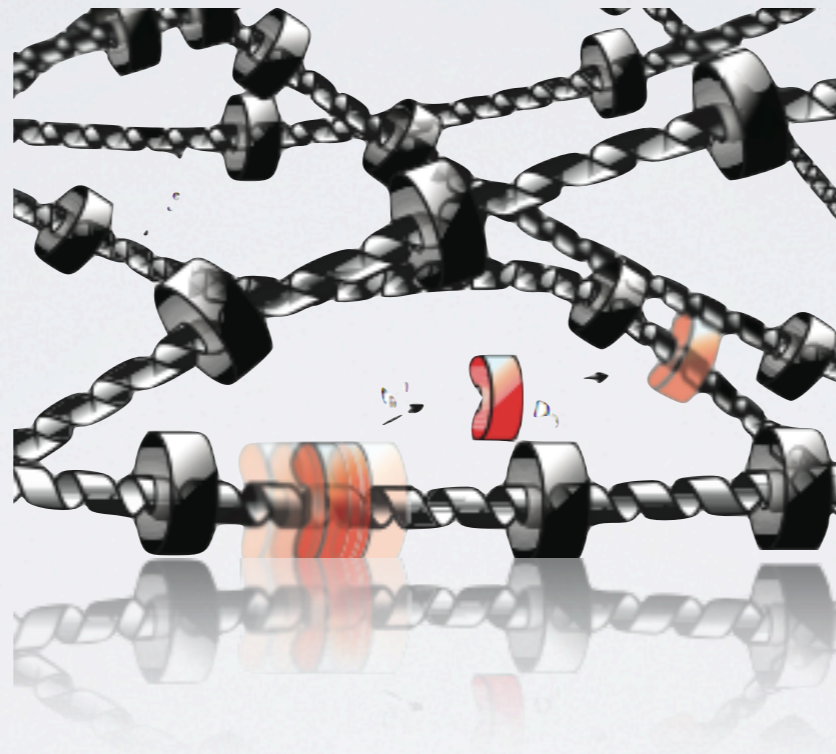


PROFASI,
Jülich
Super-
computing
Facility

Bio-nano physics

Bio-nano physics - overview

- DNA-melting in nanochannels
- Diffusion in crowded systems
- Using nanoparticles for biosensing

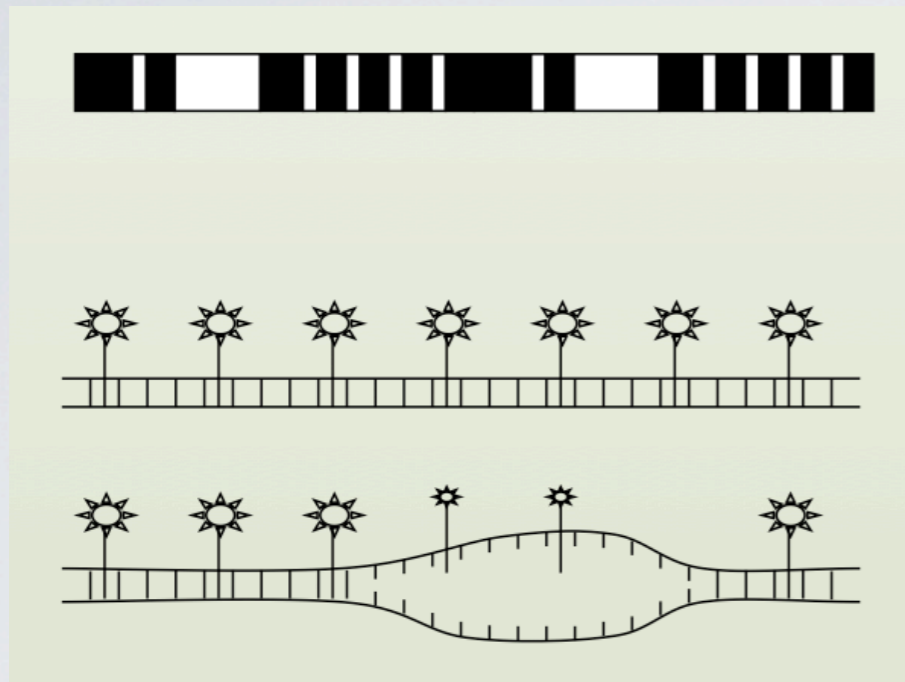


Computational methods

- Recursive relations for partition function
- Gillespie algorithm
- Solving Laplace equation

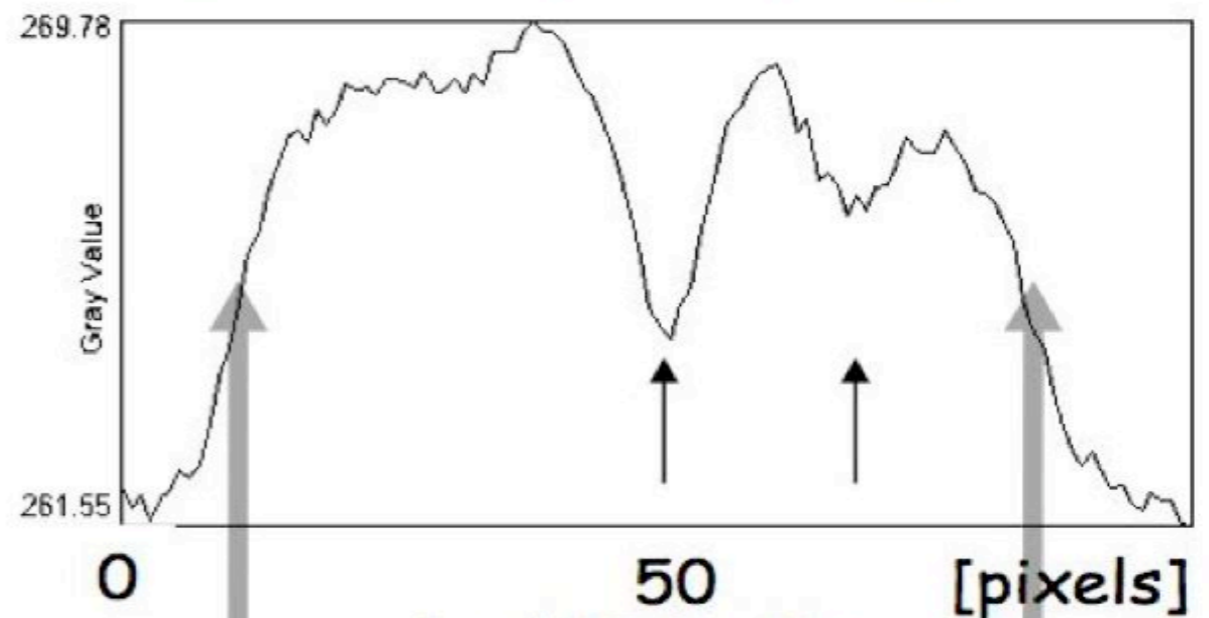
Tobias Ambjörnsson, Bo Söderberg

DNA melting in nanochannels

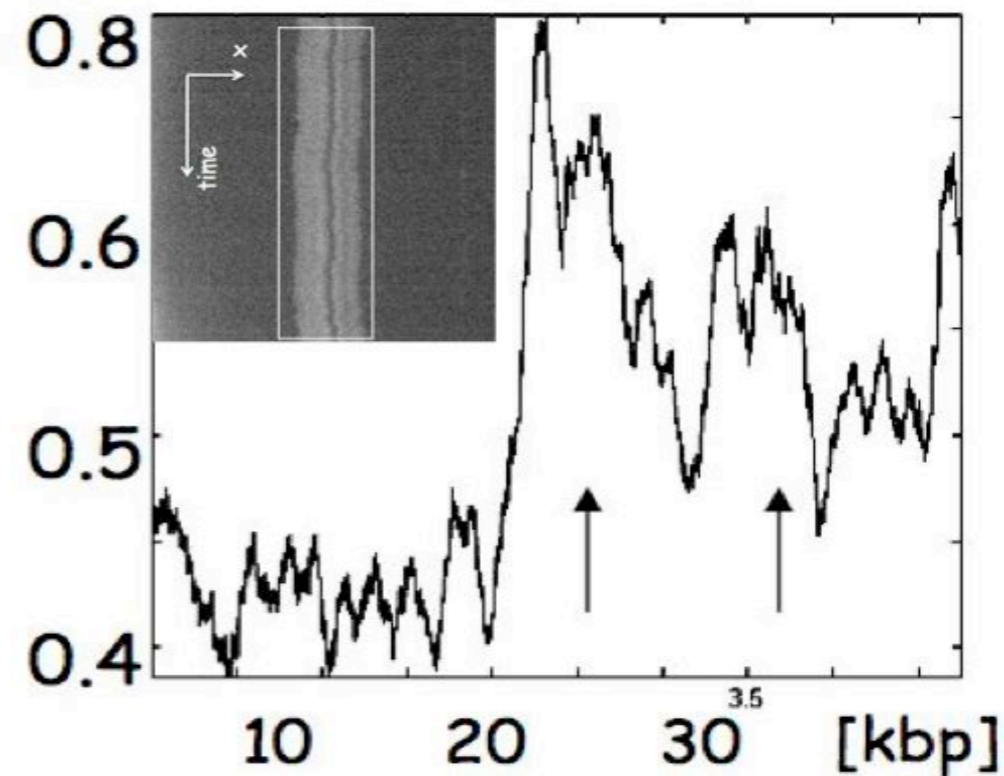


Jonas Tegenfeldt's lab,
Göteborg University

Intensity scan along molecule (averaged over box)

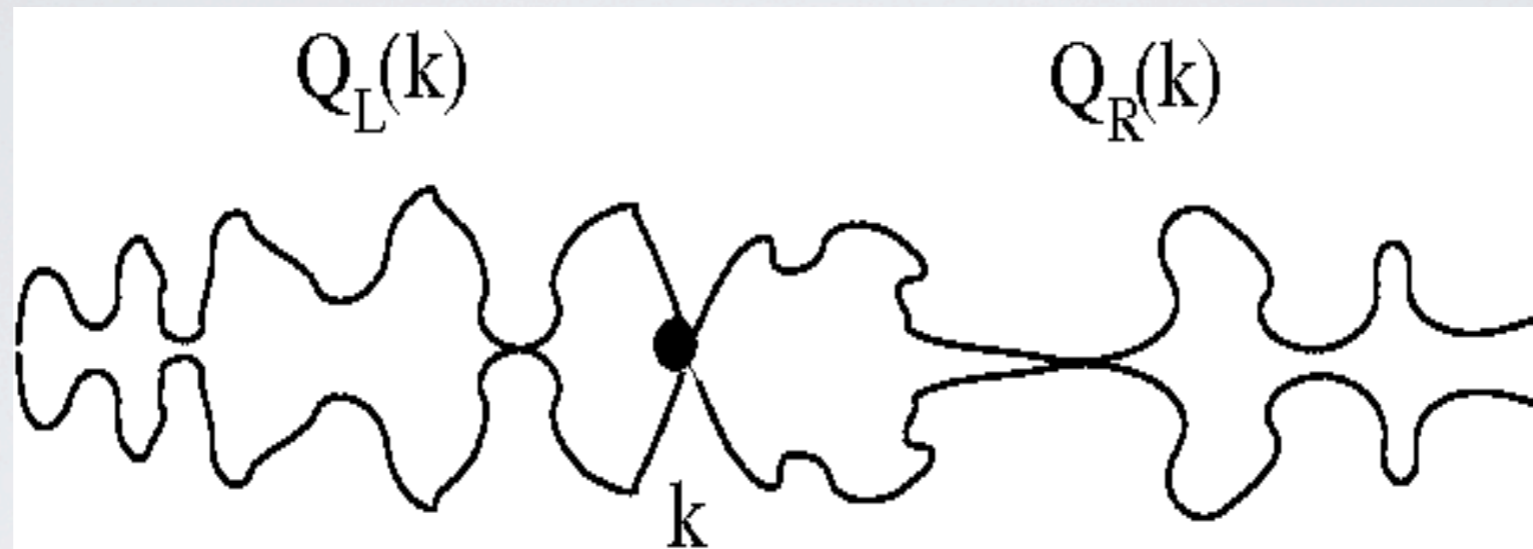


0 50 [pixels]



0.4 0.5 0.6 0.8 10 20 30 35 [kbp]

Poland-Scheraga model & algorithms



instead of
Monte
Carlo

$$Q_L(k) = Q_L(k-1) + \xi u_{k-1,k}^{st} \sum_{j=0}^{k-1} \gamma_{k,j}^L Q_L(k-j-2) g(j+1)$$

D. Poland, Biopolymers 13, 1859 (1974),

T. Garel and H. Orland, Biopolymers 75, 453 (2004)

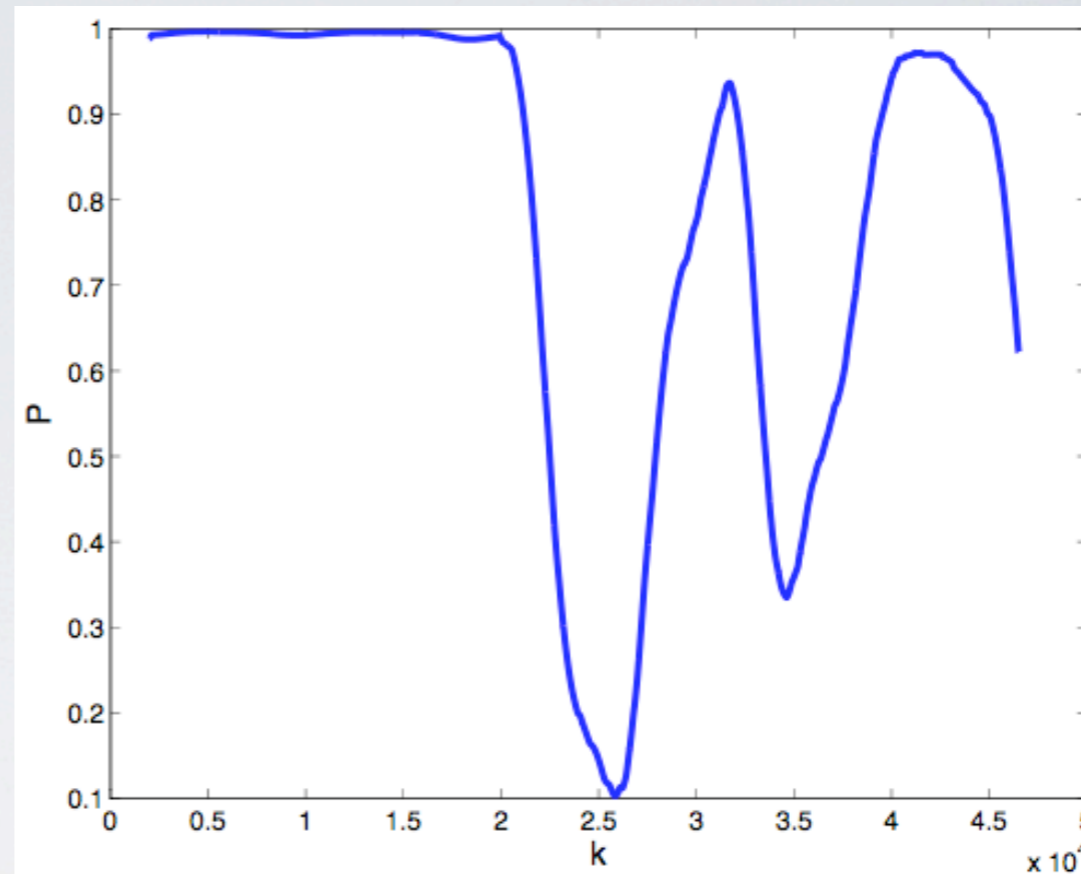
Poland algorithm: N^2 -scaling.

Fixman-Freire approximation: N -scaling!

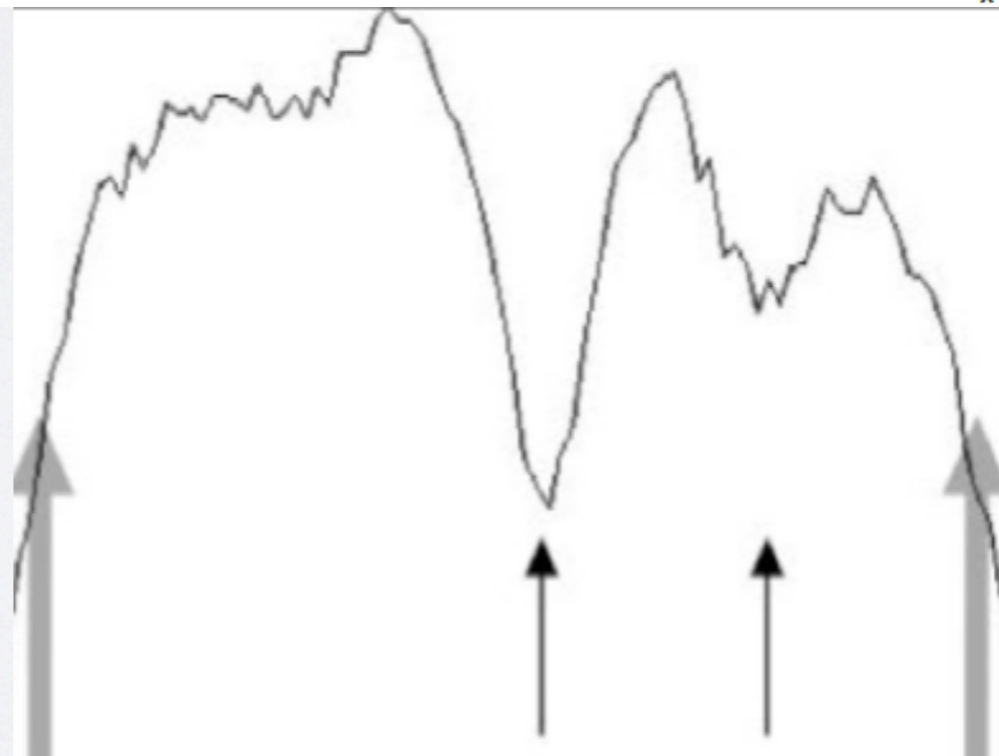
M. Fixman & J.J. Freire, Biopolymers 16, 2693 (1977).

Case study: λ -phage

Theory



Experiments



≈ 50000 basepairs

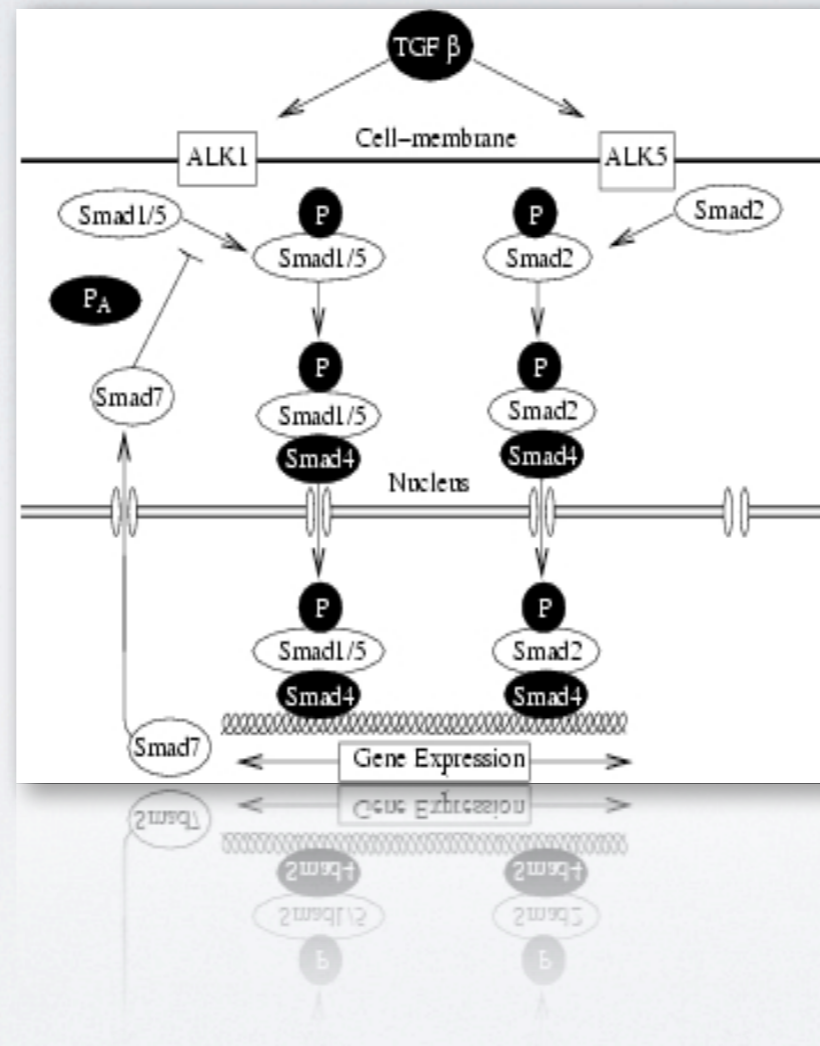
$T=85$ °C

100 mM NaCl

Systems biology

Systems biology - overview

- Cell signaling
- Stem cell differentiation
- Plant growth
- Neurosphere formation

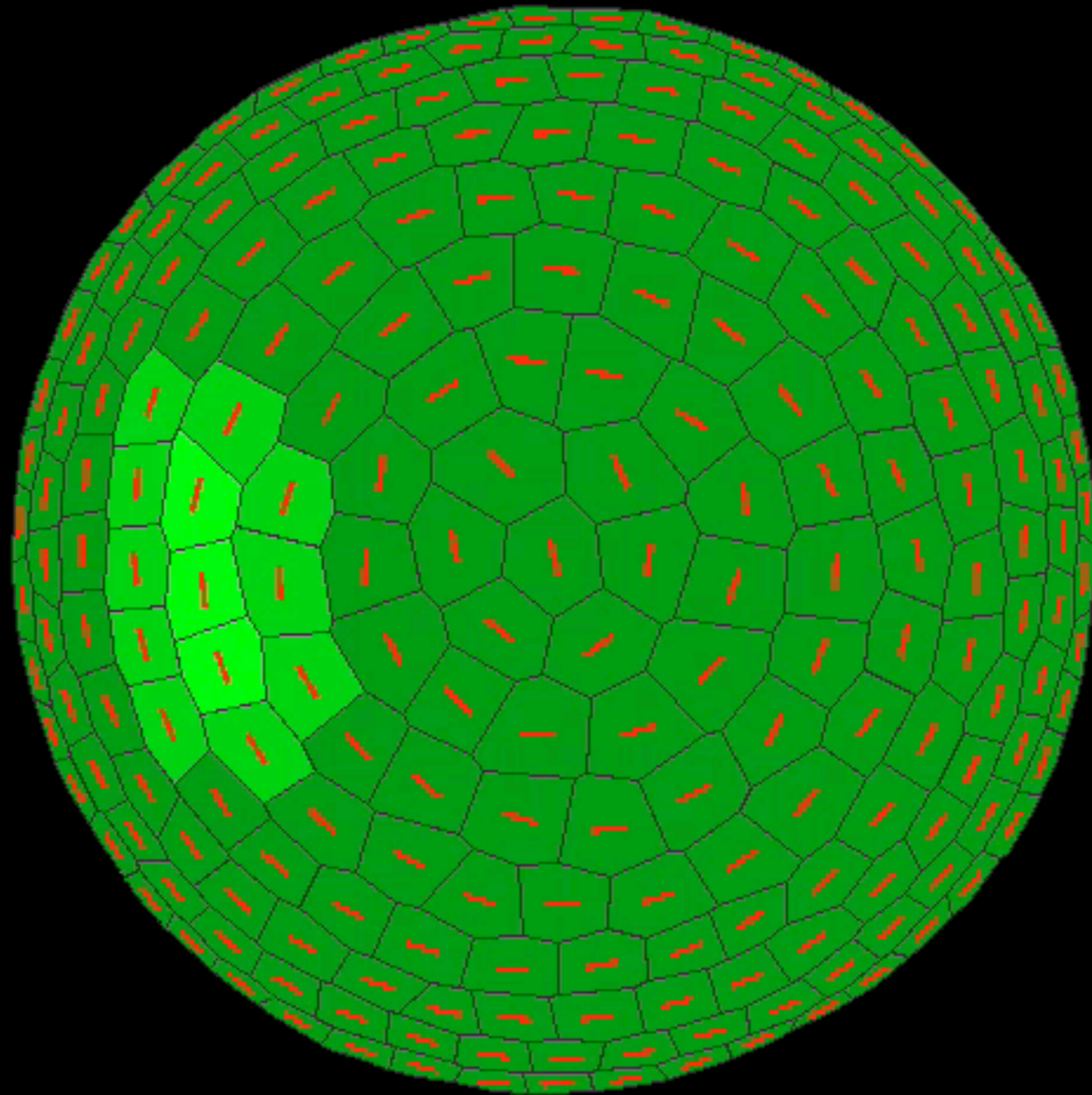


Computational methods

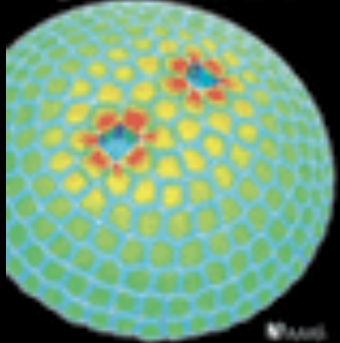
- Solving large systems of ODEs
- Optimization
- Gillespie algorithm

Henrik Jönsson, Carl Troein, Patrik Edén, Carsten Peterson

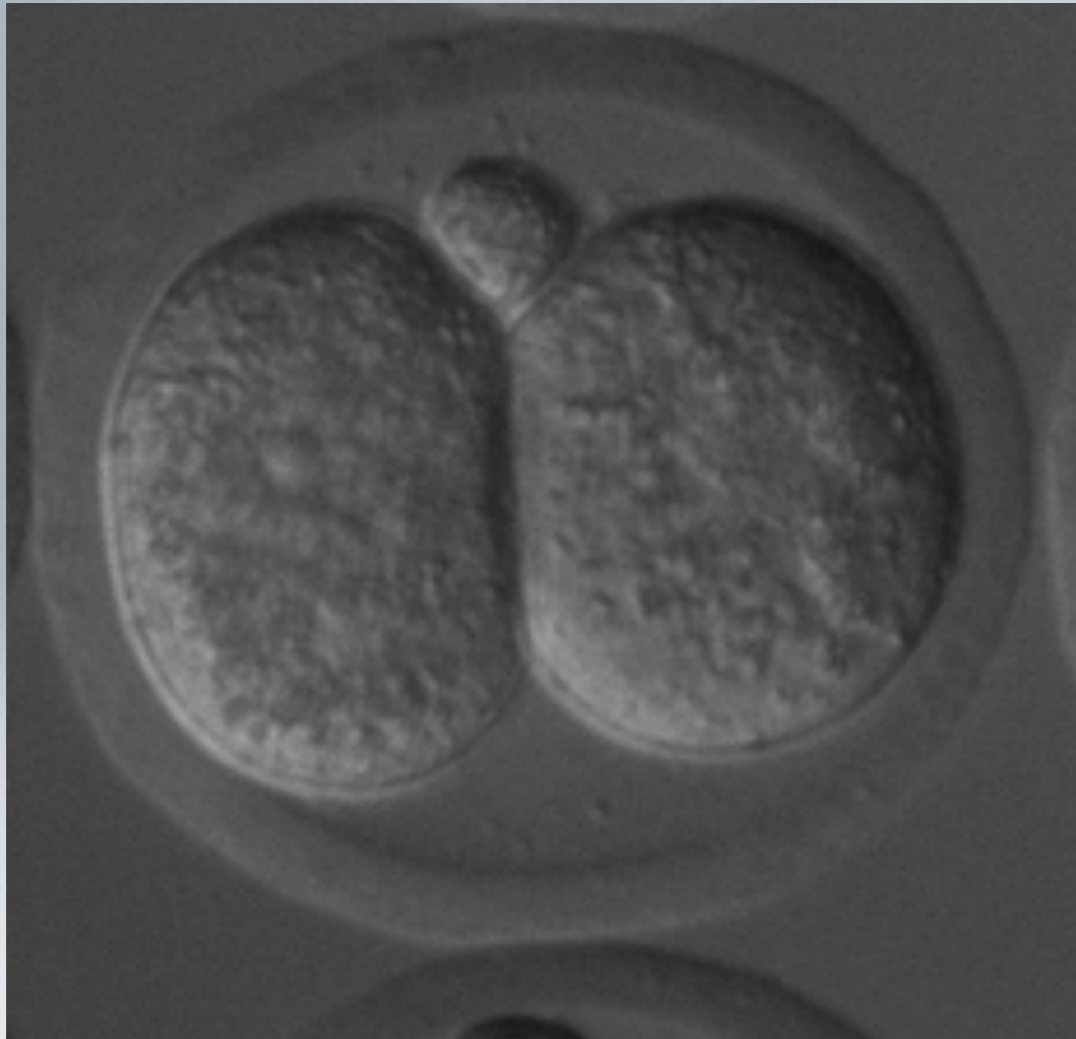
Shoot development in plants



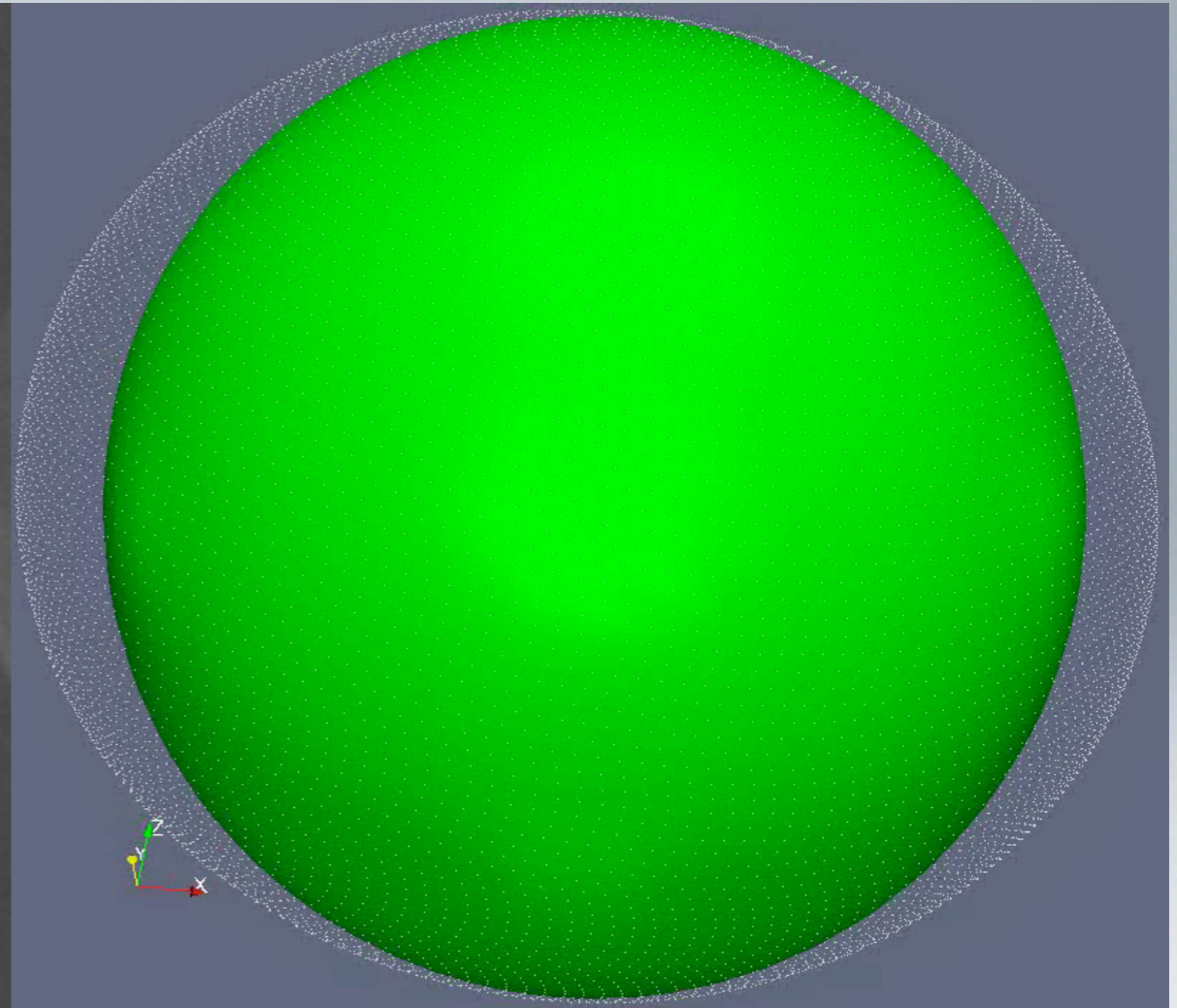
Science



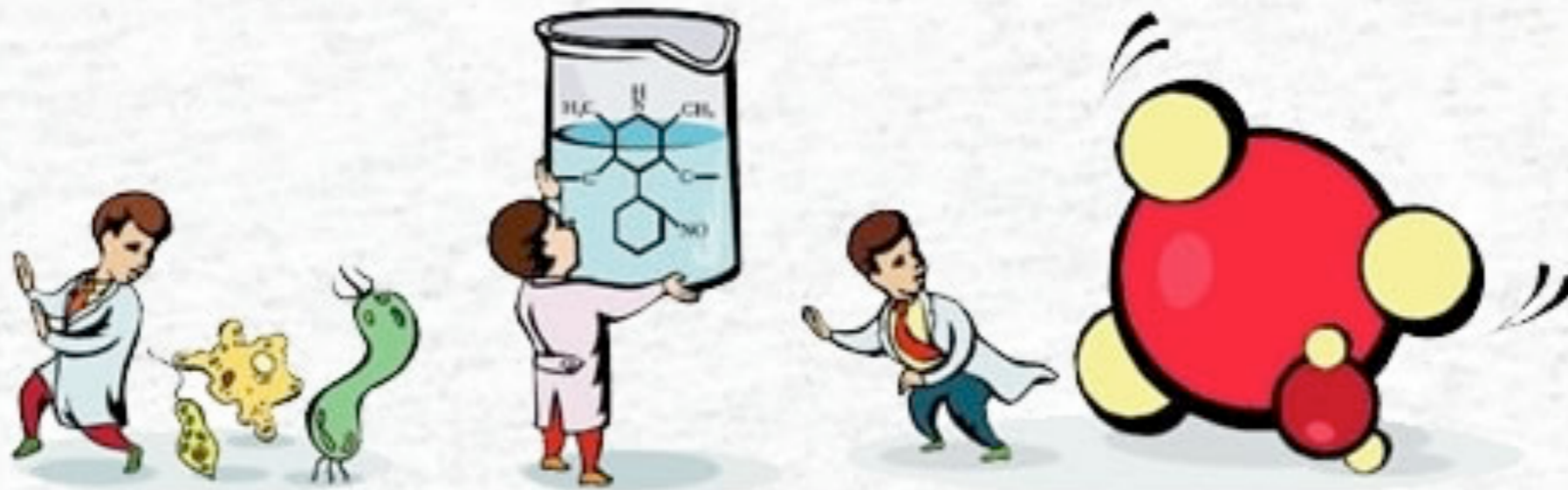
Embryonic development



Motosugi et al (2005)



Pawel Krupinski
Carsten Peterson



**If it's green or wriggles, it's biology.
If it stinks, it's chemistry.
If it doesn't work, it's physics!**

In **CBBP** we combine it
all..!