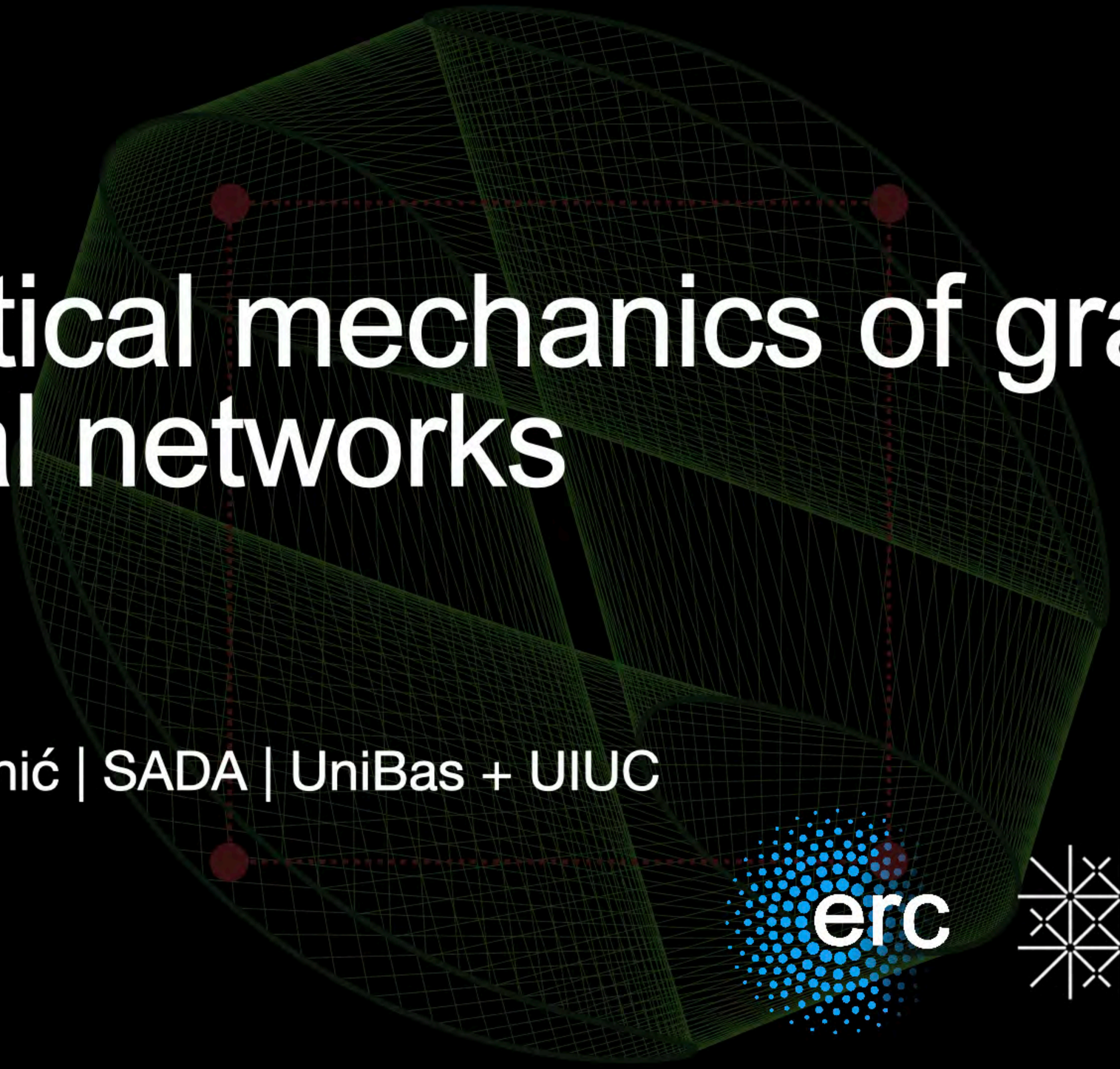


statistical mechanics of graph neural networks

math+x
ivan dokmanić | SADA | UniBas + UIUC

november 9, 2022

erc

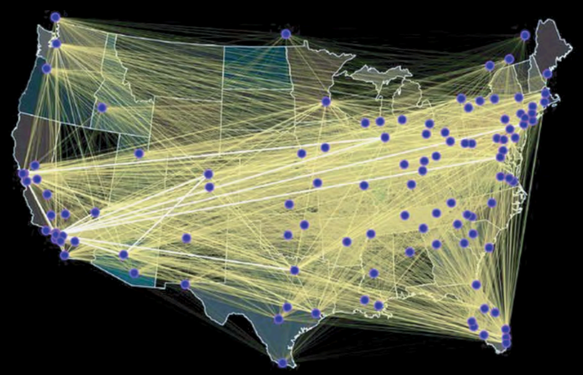
University of Basel

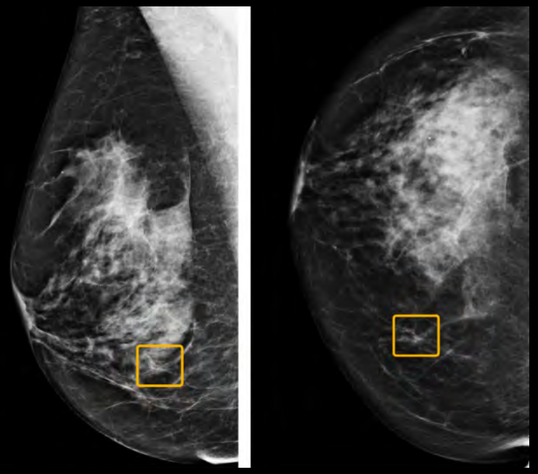
(we shrunk but we will regrow)

teaching

autumn	spring	occasionally
pattern recognition	a practical introduction to data science	computational sustainability
mathematics of data science	(ML on graphs)	AI 4 social good

research: tools and theory





ML + physics of complex networks

ML + dynamical systems

ML for imaging

ML for Earth and planetary science

$\mathcal{X}$ hypothesis $f \in \mathcal{F}$ $\mathcal{Y}$

unknown $p_{X,Y}$ $\underset{f \in \mathcal{F}}{\text{minimize}}\ \mathbb{P}\left[f(X) \neq Y\right]$



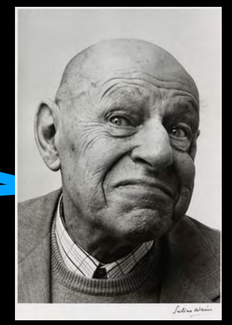




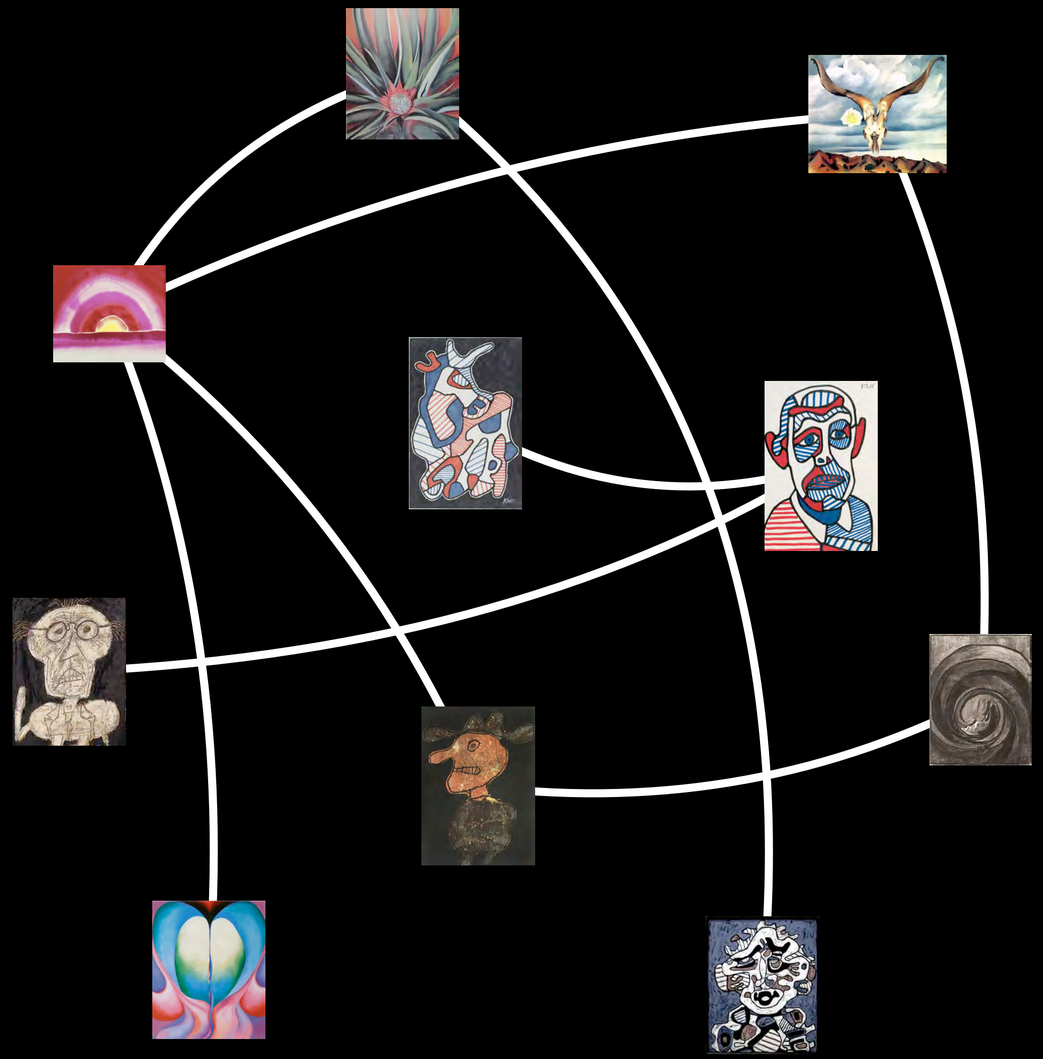


"training set"

$$\mathcal{T} = \{(x_n, y_n)\}_{n=1}^{N} \overset{\text{iid}}{\sim} p_{X,Y}$$



$$\underset{f \in \mathcal{F}}{\text{minimize}}\ \frac{1}{N} \sum_{n=1}^{N} \mathbf{1}\left[f(x_n) \neq y_n\right]$$



a combinatorial graph

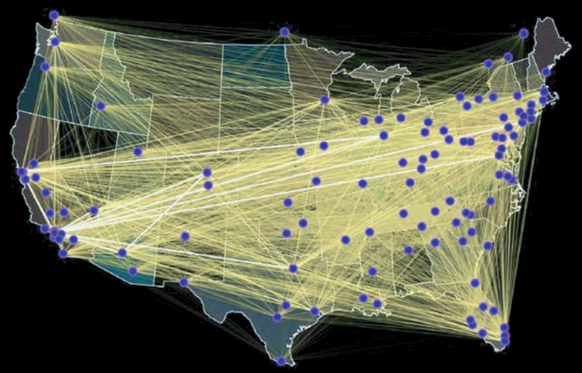
$$G = (V, E) \qquad E \subseteq \binom{V}{2}$$

an adjacency matrix

$$A = (a_{ij})$$

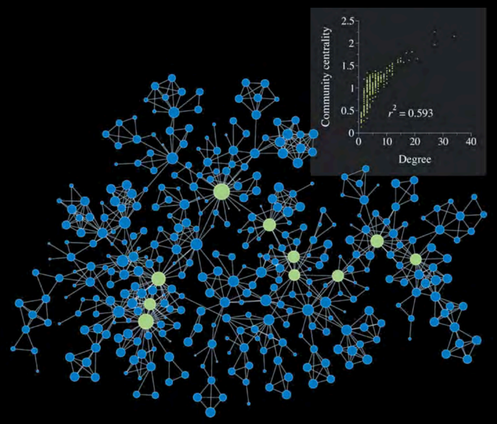
$$a_{ij} = \begin{cases} 1 & (i,j) \in E \\ 0 & (i,j) \notin E \end{cases}$$

Benson et al. 2016



air transport network in the US

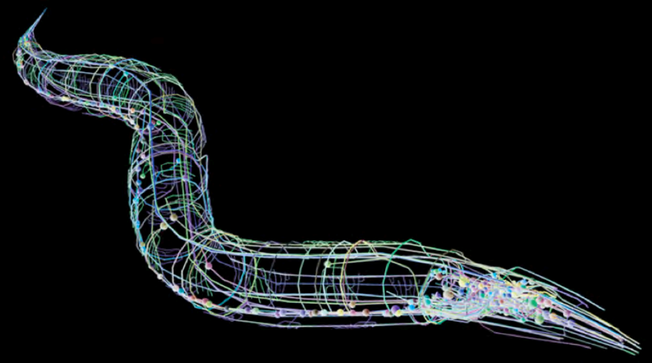
Newman 2006



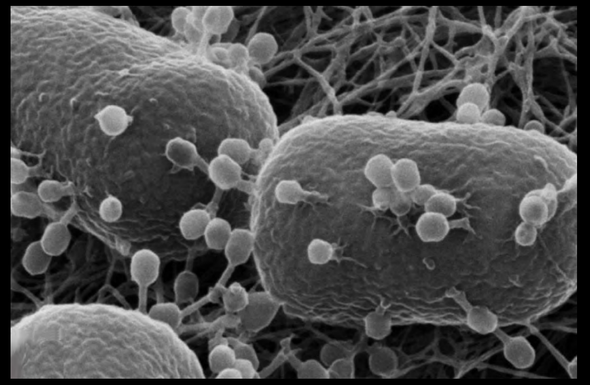
collaboration network of network scientists

von Mering 2002

protein–protein interaction graph in yeast

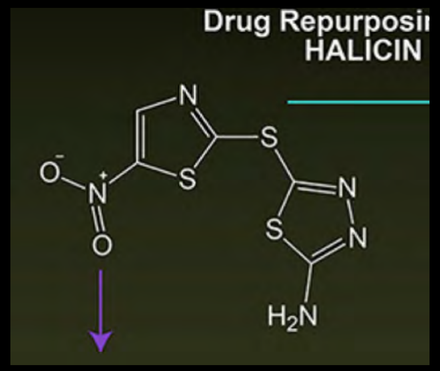


neural network of c. elegans

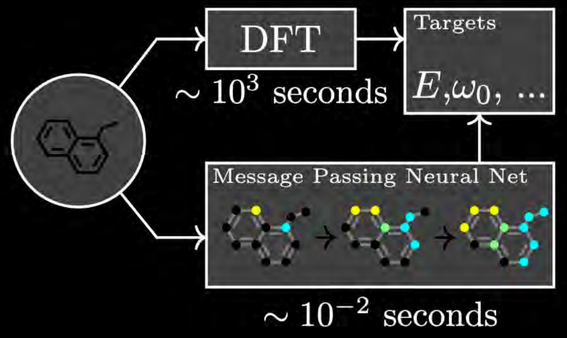


reactions between metabolites in e. coli

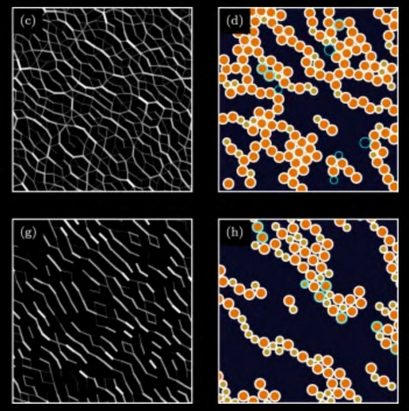
killer applications



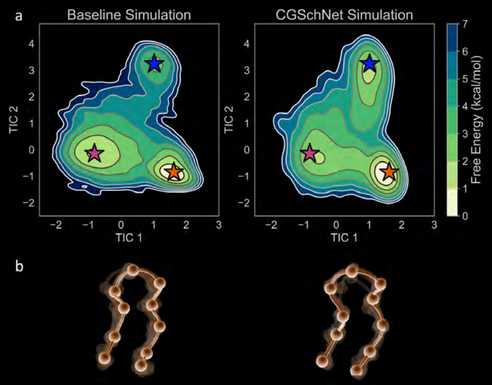
molecule design
Stokes et al. 2020



quantum chemistry
Gilmer et al. 2017



force chains in jammed solids
Mandal, Caser, Sollich 2022



fast molecular dynamics
Husic et al. 2020

$$-(\Delta - \eta)u = f \quad (\eta > 0) \qquad -(\Delta + k^2)u = f$$

Ernst, Gander, 2012. **Why is it difficult to solve Helmholtz problems with classical iterative methods?**

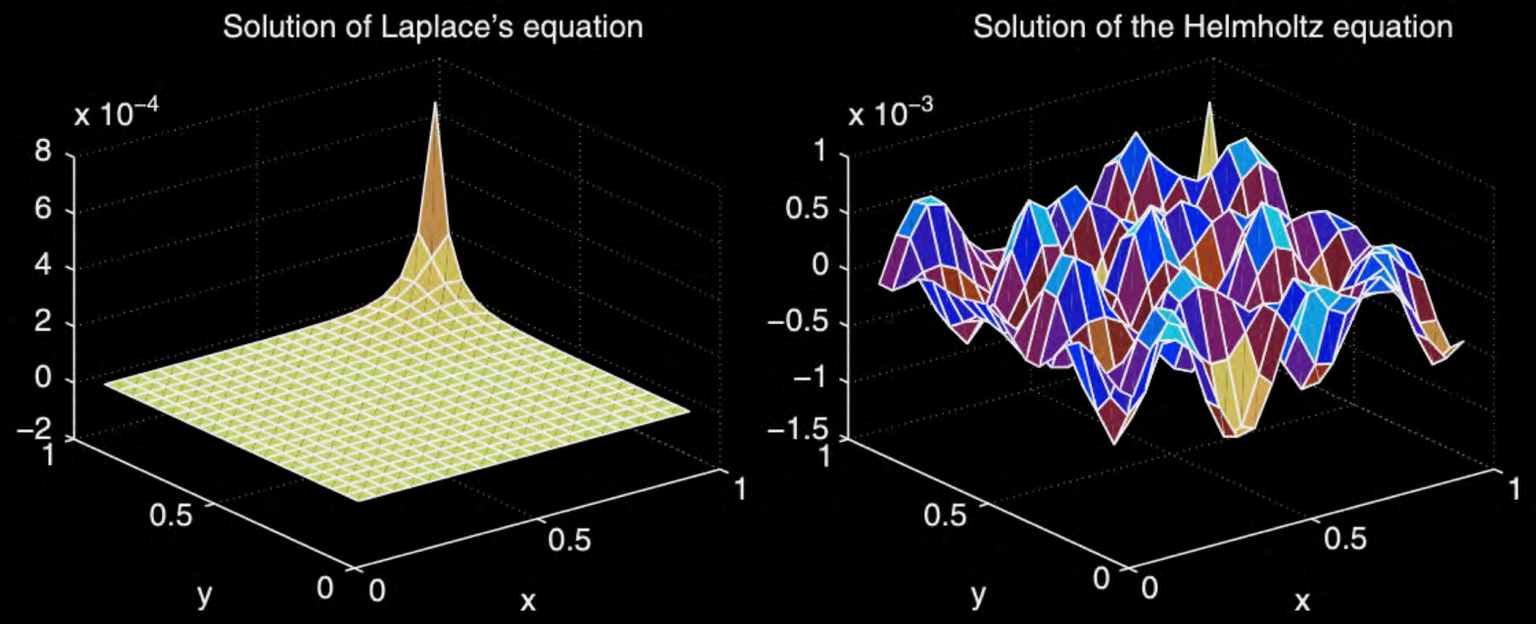
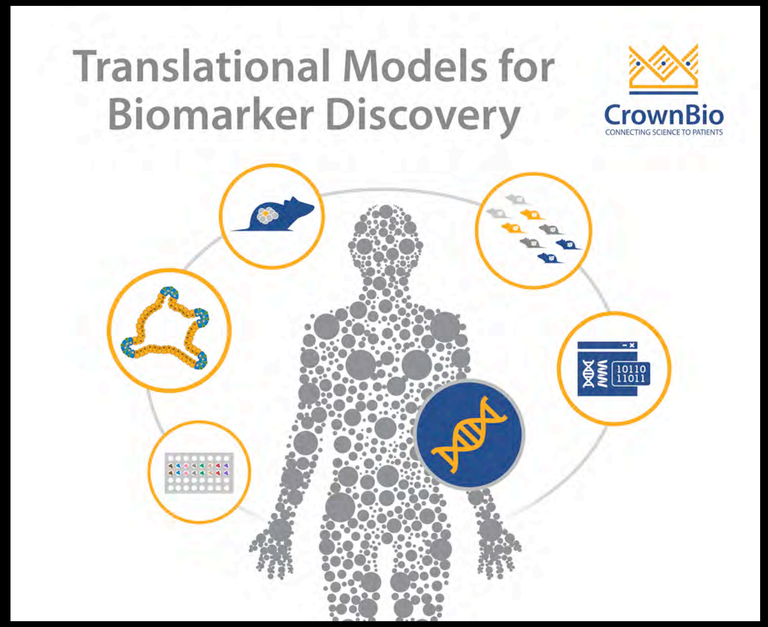
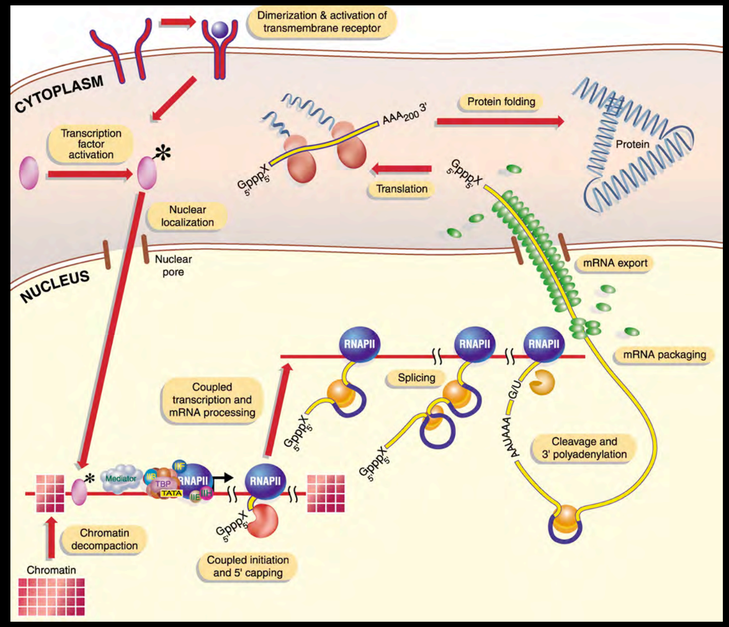


Fig. 1 Solution of Laplace's equation on the left, with a point source on the boundary, and on the right the solution of the Helmholtz equation, with the same boundary conditions

link prediction in complex networks

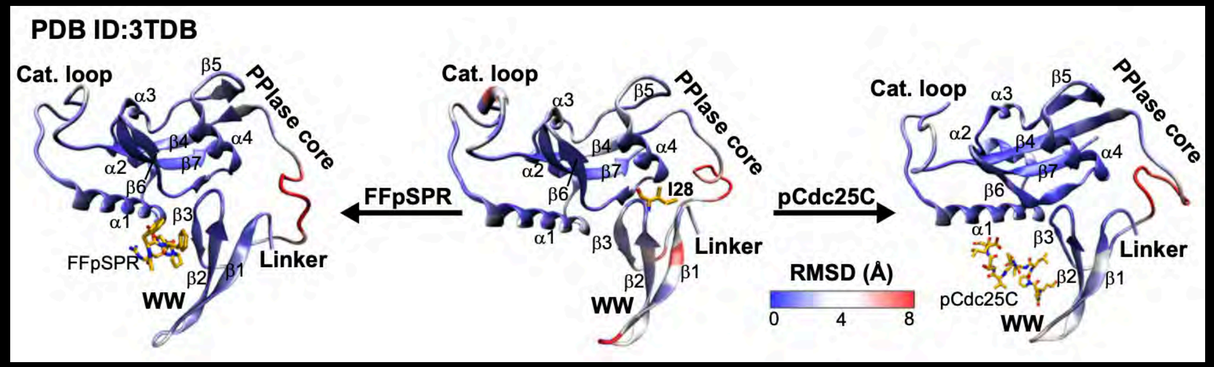
applications of walkpooling we're hearing about



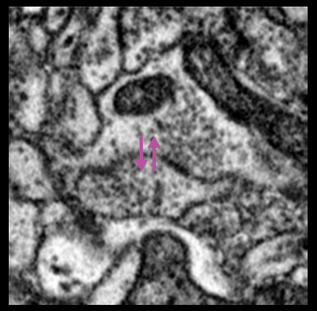


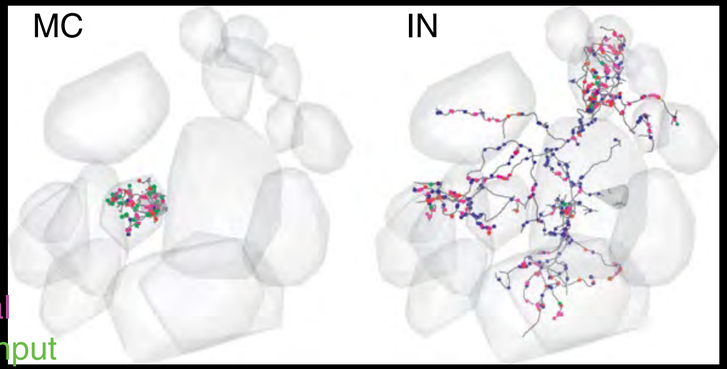
learning dynamical systems on networks

dynamics of proteins



dynamics of biological neural networks





Input
Output
Reciprocal
Sensory input


A medieval cemetery sheds light on Jewish history p. 940
The reasons why Siberia is catching fire pp. 944 & 1005
Harmonize copyright to facilitate research p. 951
Science
$15
2 DECEMBER 2022
science.org
AAAS
DEEP HEAT
Imaging the magma under the Yellowstone supervolcano
pp. 945 & 1001


Bilinear Interpolation
FunkNN
Ground truth
256×256 (×2)
512×512 (×4)
1024×1024 (×8)

a few possible theses

modeling earthquake dynamics along the San Jacinto fault by neural point processes & reinforcement learning

applying FunkNN to model continuously deforming protein surfaces

using graph neural networks to model dynamics of granular material

applying transformers or diffusion models to ultrasound breast tomography

machine learning for exoplanet detection

theory for any of the above

---

https://sada.dmi.unibas.ch/en/student-projects

Be cautious

Machine learning is a **hot** topic

Many are interested in machine learning

Machine learning requires math

Not everyone is familiar with math

Make sure you are familiar with math

(credit Alex Schwing / UIUC)