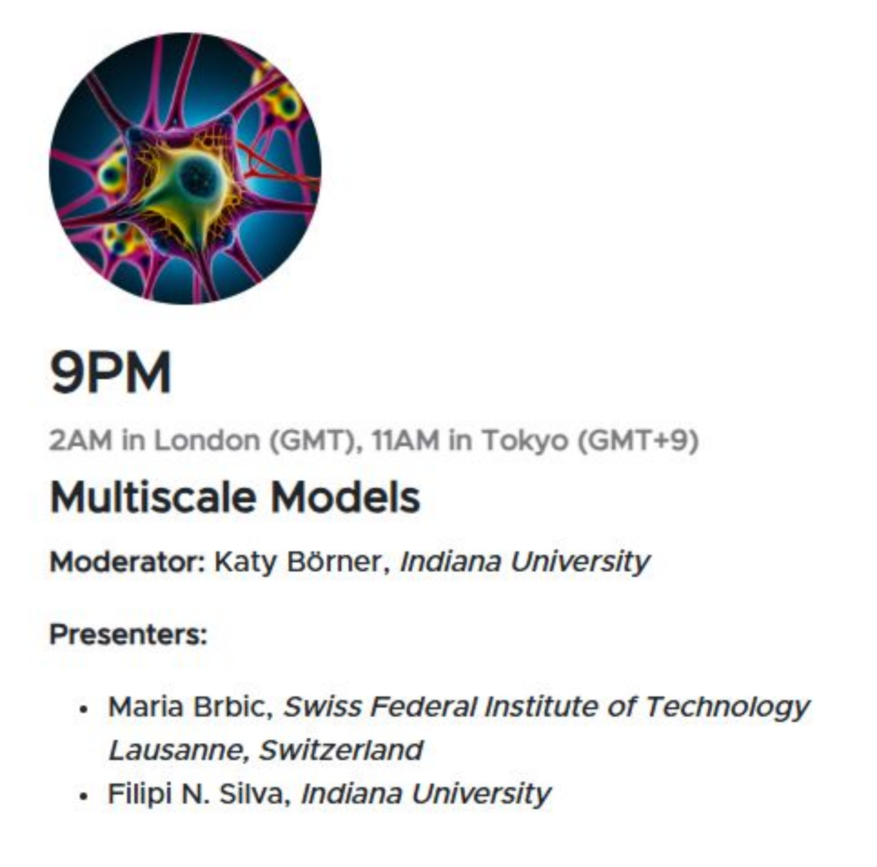


9PM

2AM in London (GMT), 11AM in Tokyo (GMT+9)

Multiscale Models

Moderator: Katy Börner, *Indiana University*

Presenters:

- Maria Brbic, *Swiss Federal Institute of Technology Lausanne, Switzerland*
- Filipi N. Silva, *Indiana University*

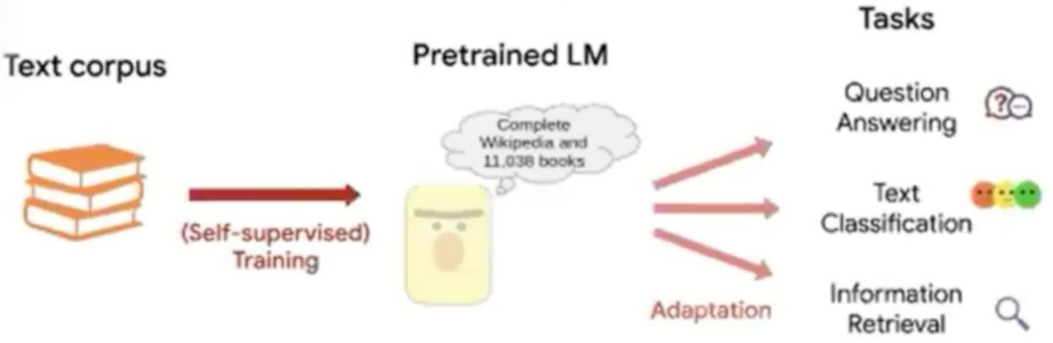
Maria Brbic, *Swiss Federal Institute of Technology Lausanne*

AI Revolution

Generative AI paradigm and the era of foundation models

Foundation Model

Model that has learnt features transferable to a wide range of downstream tasks



How can we leverage these AI advances in single cell biology?

What are their current limitations for biomedical applications?

Single-cell Data Is Challenging for Today's AI

1. Heterogenous experiments

2. Novel and unknown phenomena

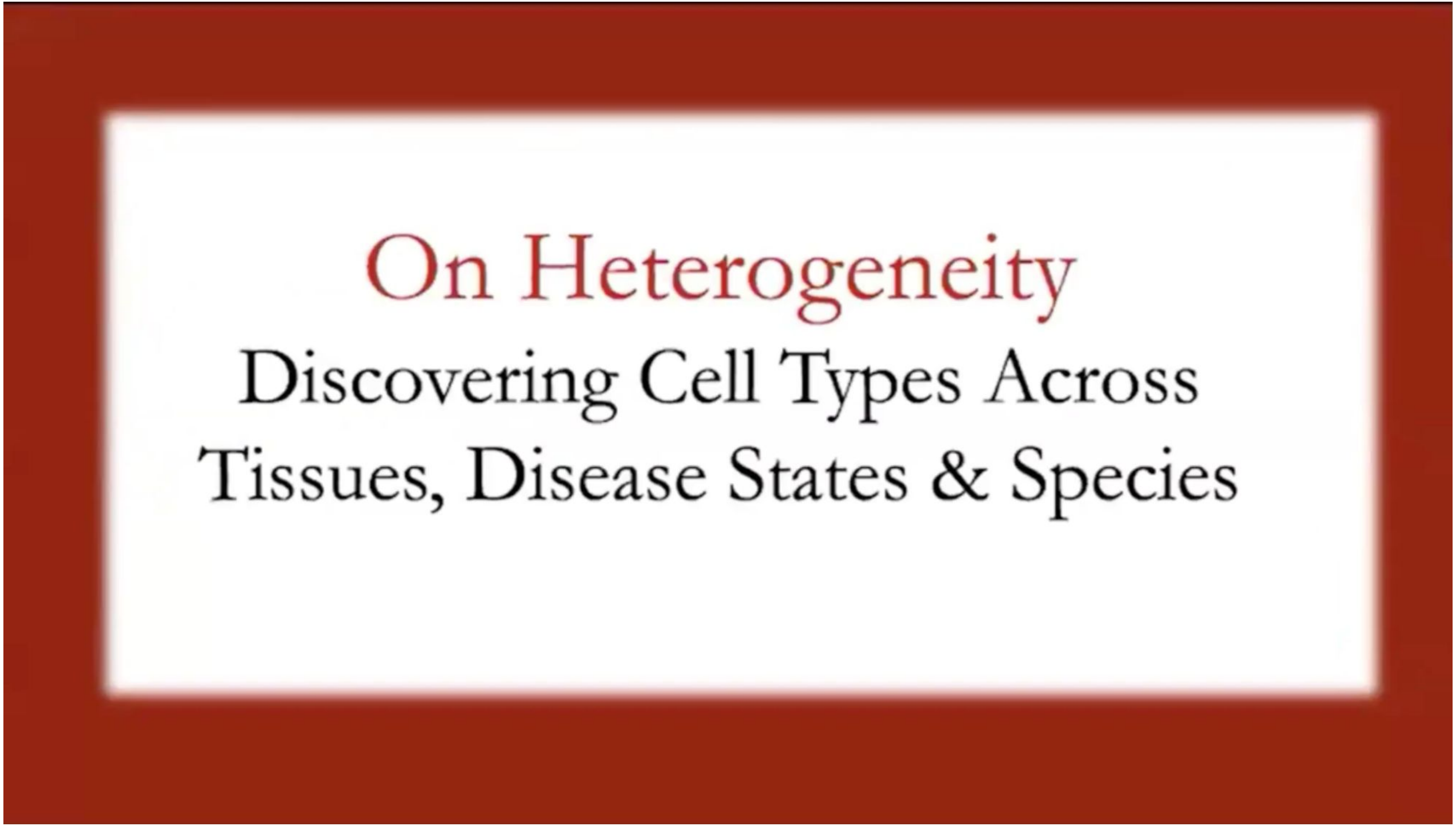
3. Different modalities with different challenges

1. Heterogenous experiments

2. Novel and unknown phenomena

3. Different modalities

Today’s talk: How to overcome some of these challenges

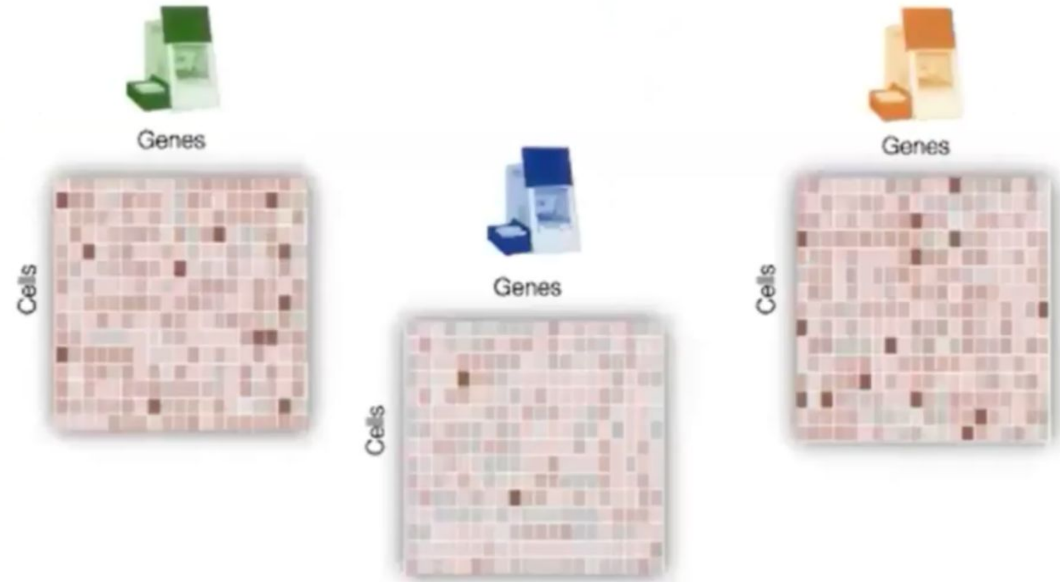


On Heterogeneity

Discovering Cell Types Across Tissues, Disease States & Species

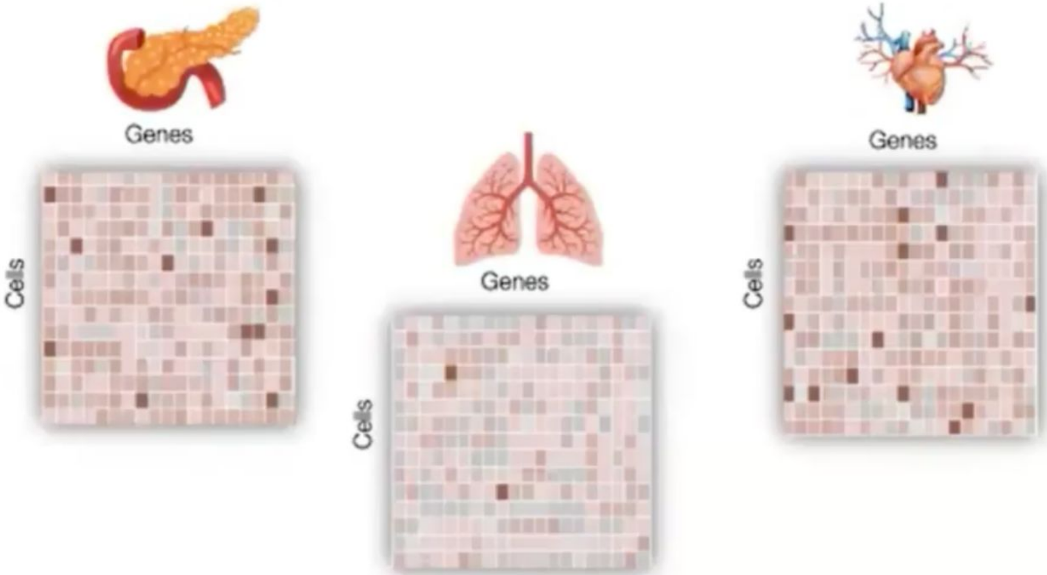
Data with Large Heterogeneity

different labs…



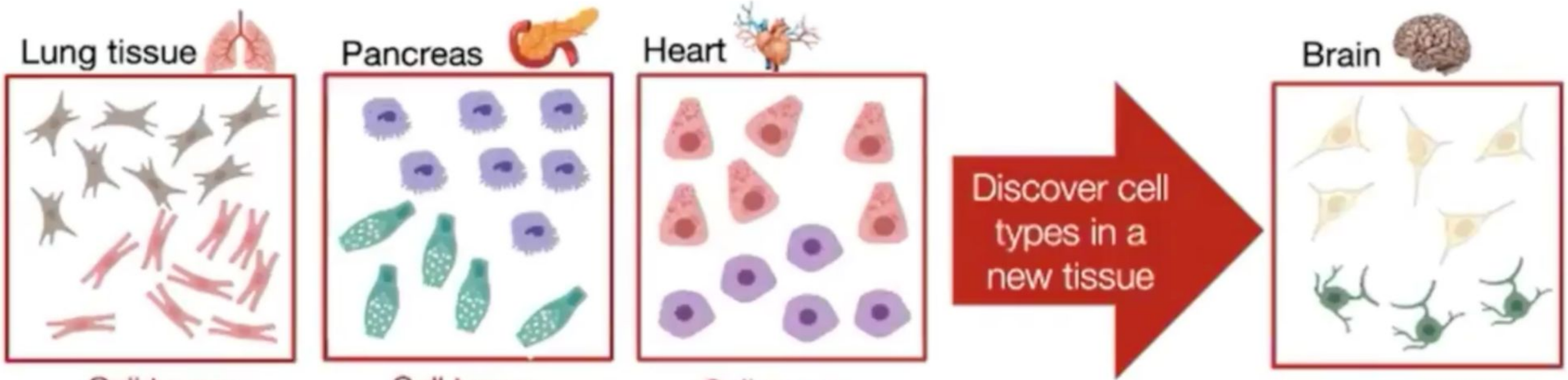
Data with Large Heterogeneity

different tissues…



How do we jointly analyze and gain new insights from these heterogenous datasets?

MARS: Learn Cell Embeddings to Discover Novel Cell Types



Lung tissue

Pancreas

Heart

Discover cell types in a new tissue

Brain

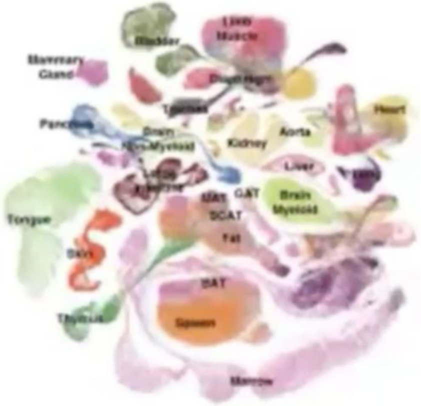
Cell types: fibroblasts, cardiomyocytes

Cell types: pneumocytes, goblet

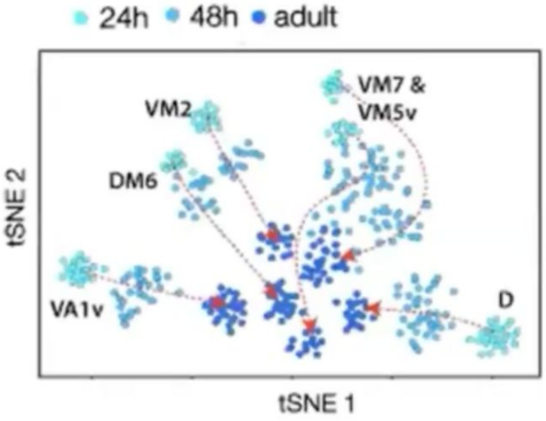
Cell types: alpha, beta

Brbic et al. *Nature Methods*' 20

Cell Type Discovery across Experiments



Across tissues of the
Mouse Cell Atlas

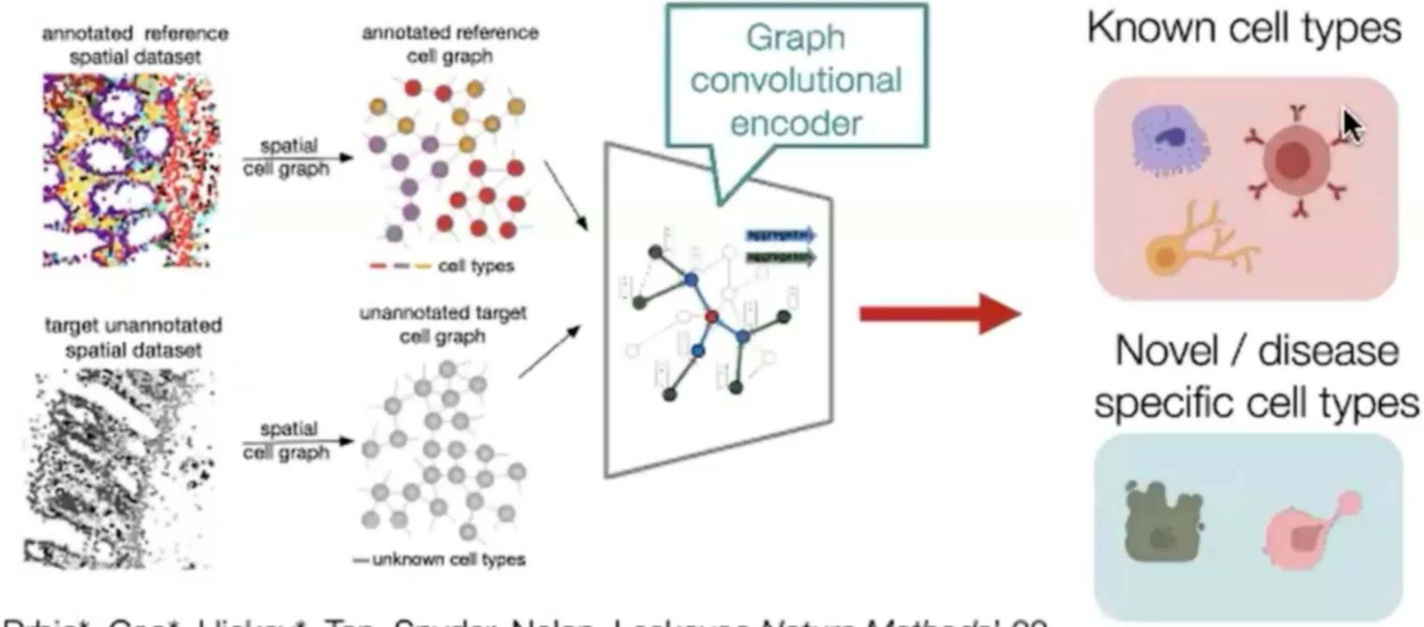


Xie*, Brbic* et al. *eLife* '21

Fly Cell Atlas

Li*, Janssens* et al. *Science* '22

STELLAR: Novel Cell Type Discovery Across Conditions



annotated reference spatial dataset

annotated reference cell graph

spatial cell graph

— — — cell types

target unannotated spatial dataset

unannotated target cell graph

spatial cell graph

— unknown cell types

Graph convolutional encoder

Known cell types

Novel / disease specific cell types

Brbic*, Cao*, Hickey*, Tan, Snyder, Nolan, Leskovec *Nature Methods*' 22

Towards Universal Cell Embeddings

Can we create cell embeddings for any species, any set of genes?

Tabula Muris
Nature '18, '20

Fly Cell Atlas
Science '22 '23

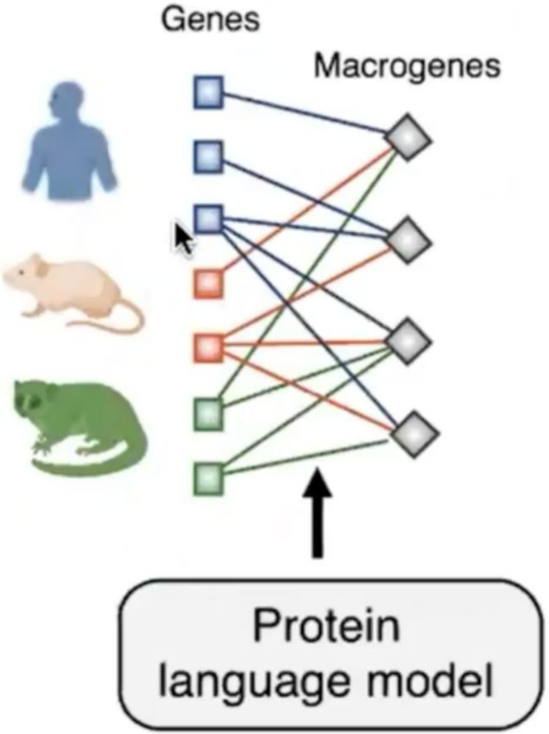
Tabula Sapiens
Science '22

Maria Brbic, EPFL

Our Approach: SATURN

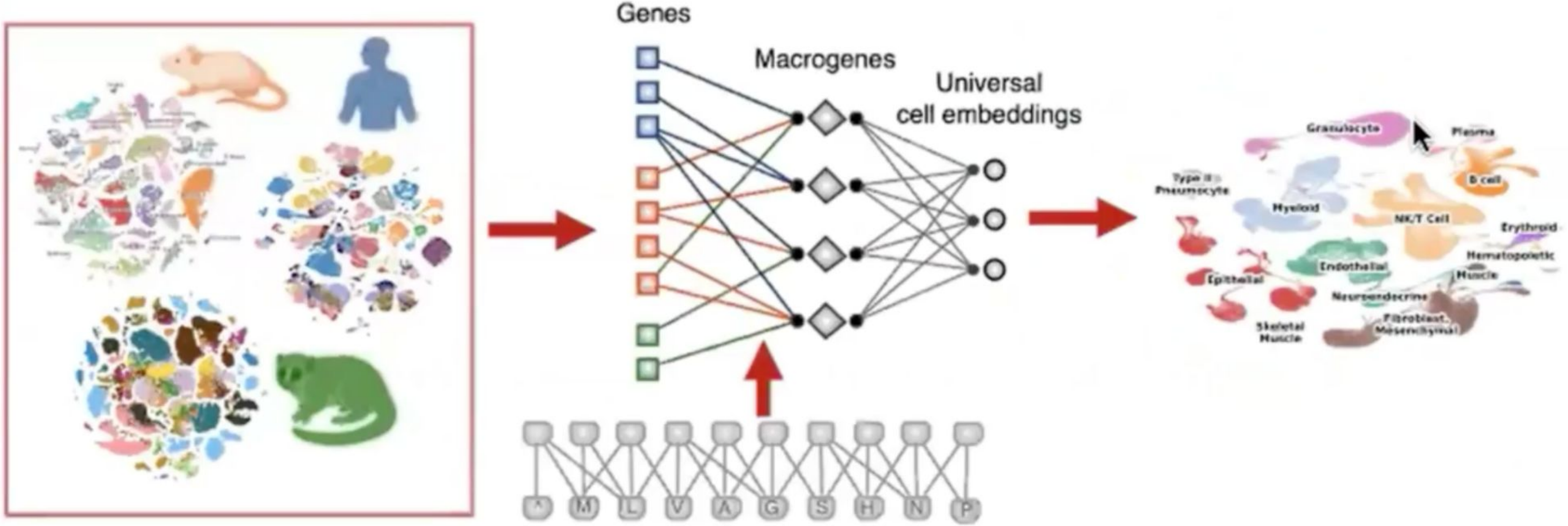
Key Idea: Map diverse sets of genes in the joint space of macrogenes

- Macrogenes: groups of functionally related genes
- Learn macrogene space using protein embeddings from language models

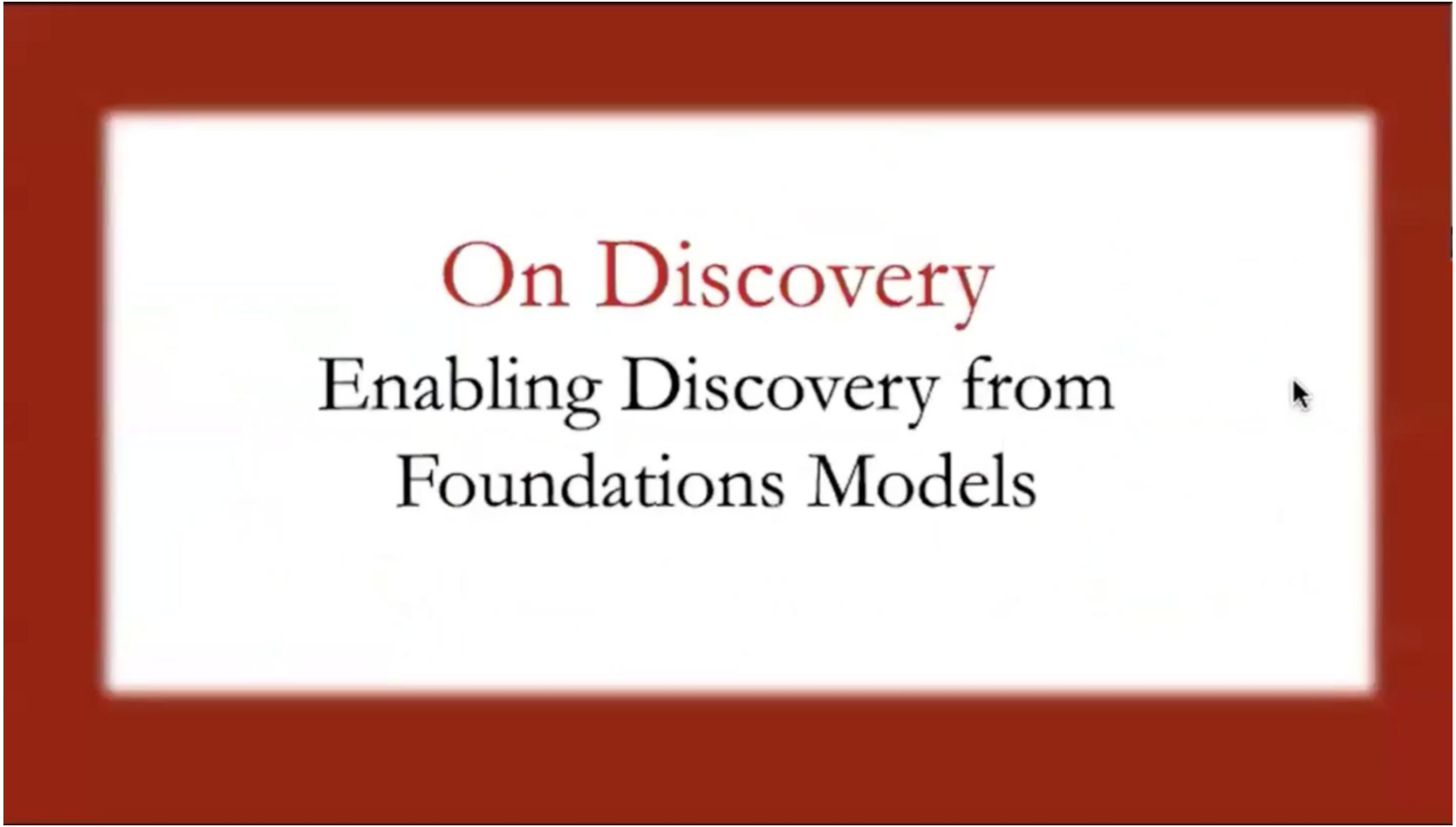


Rosen*, Brbic*, Roohani*, Swanson, Li, Leskovec. *Nature Methods* ‘24

SATURN: Integrating Datasets across Species



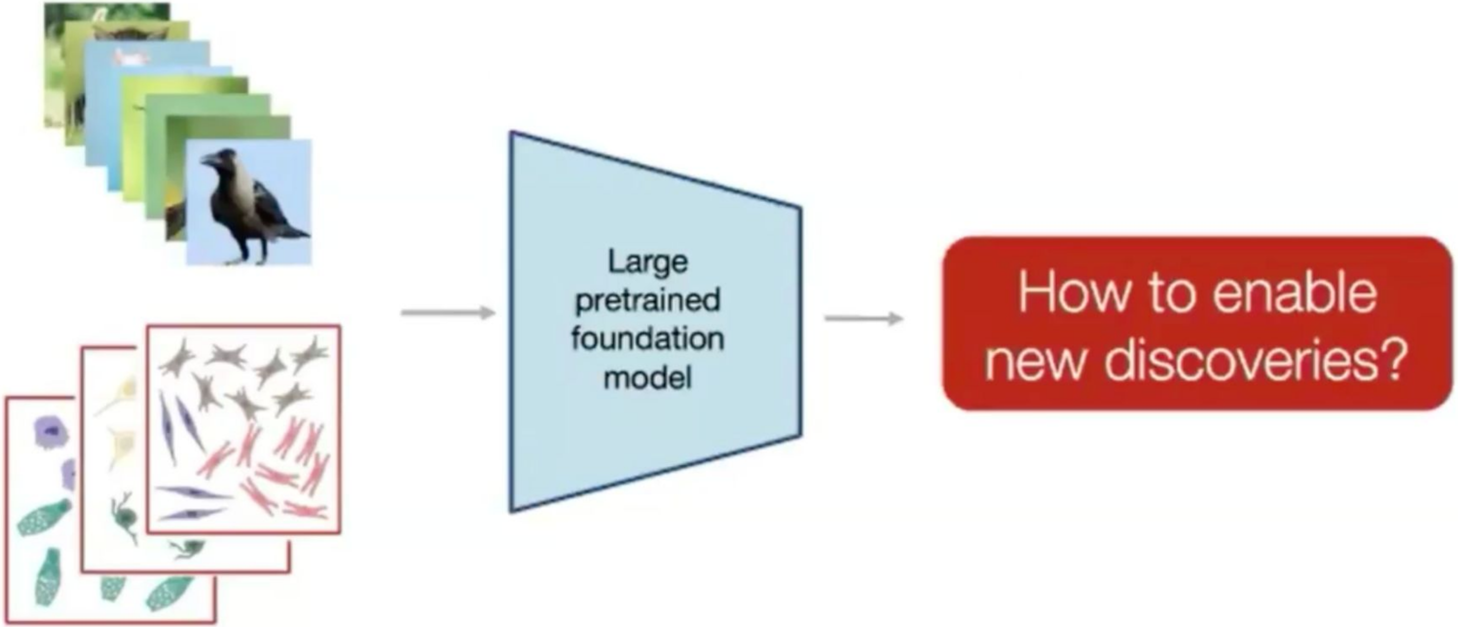
Rosen*, Brbic*, Roohani*, Swanson*, Li, Leskovec *Nature Methods*' 24



On Discovery

Enabling Discovery from Foundations Models

How To to Enable New Discoveries from Foundation Models?

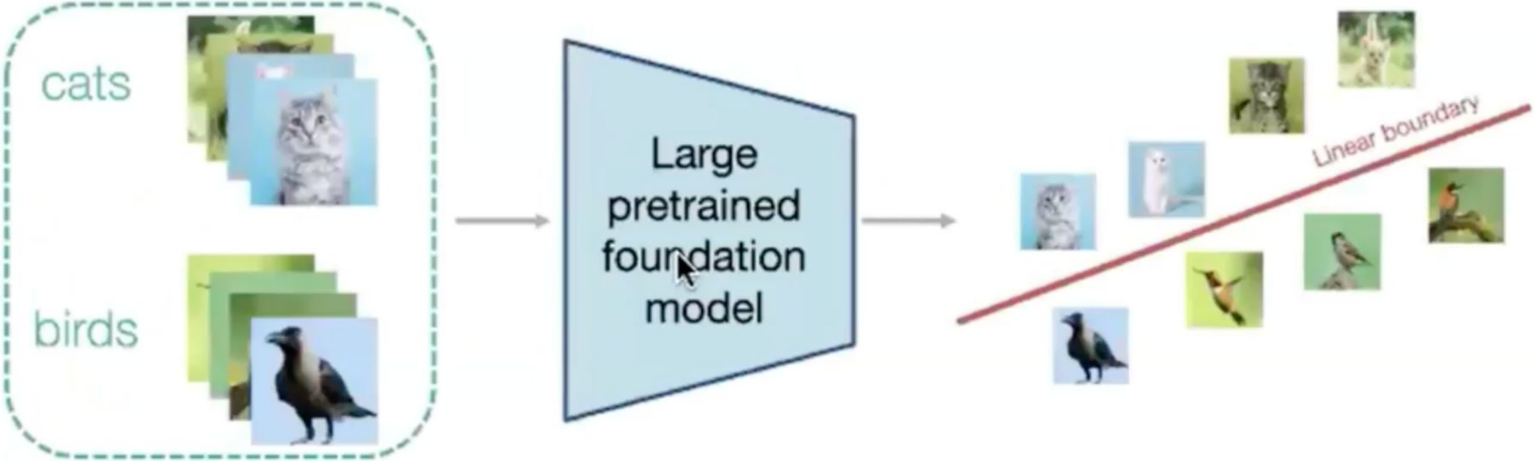


Large pretrained foundation model

How to enable new discoveries?

Current Paradigms Still Require Supervision

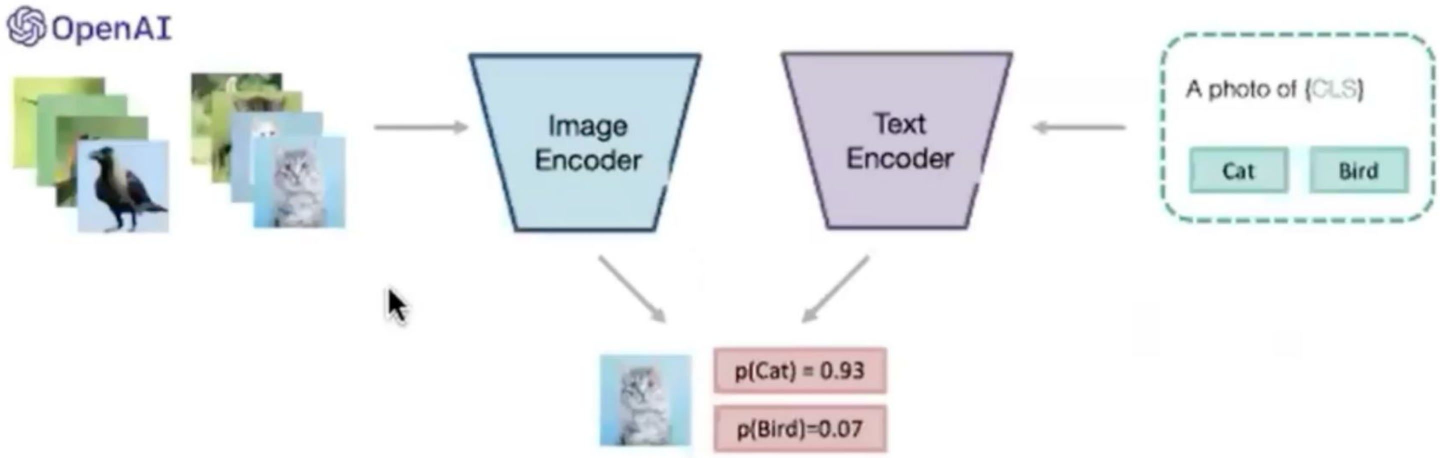
- Current paradigms:
  1. Fine-tune on the task of interest using labeled data



Current Paradigms Still Require Supervision

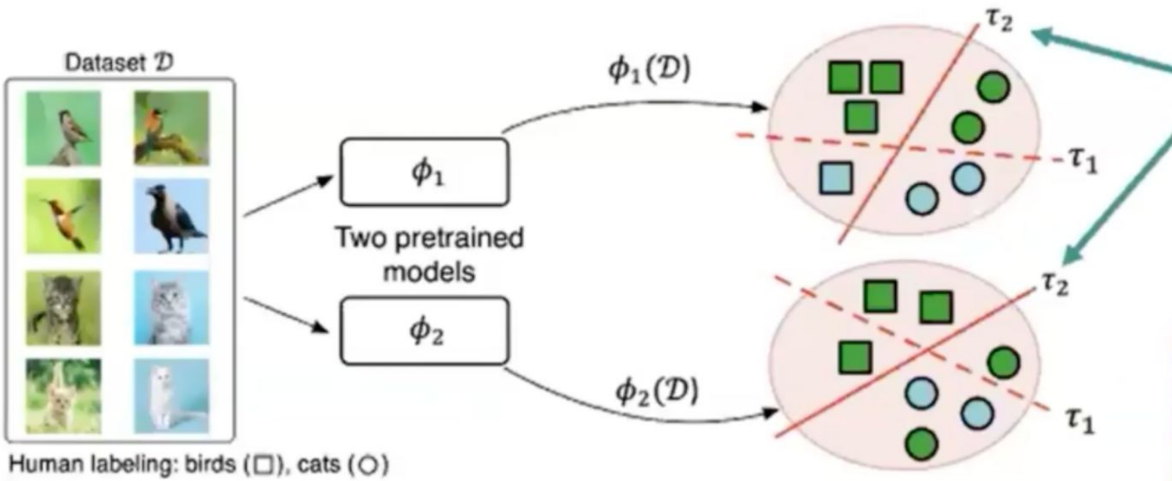
- Current paradigms:

  2. Zero-shot transfer on the task of interest using instructions



How to Infer Labeling without Any Supervision?

Key idea: Search for a labeling such that linear models will generalize well in different representation spaces



Human labeling: birds (□), cats (○)

Labeling with a lower generalization error

Artyom Gadetsky

Yulun Jiang

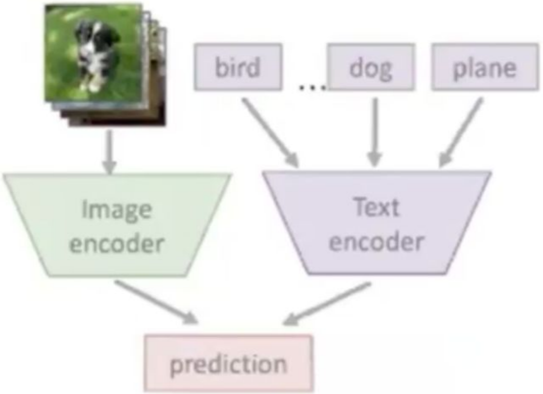
Gadetsky, Brbić. *NeurIPS* ‘23 (spotlight)
Gadetsky*, Jiang*, Brbić. *ICML* ‘24

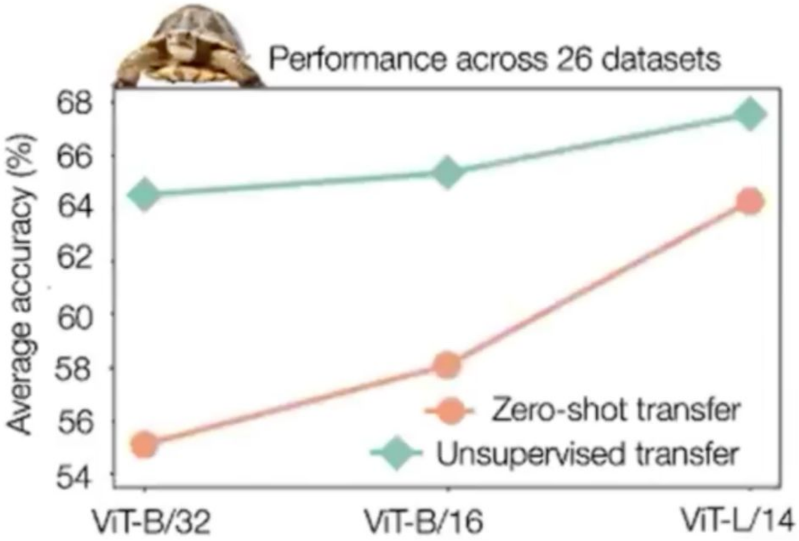
Unsupervised Transfer Outperforms Zero-Shot

SOTA unsupervised performance

- 26 datasets benchmark from CLIP

OpenAI Zero-Shot CLIP Model

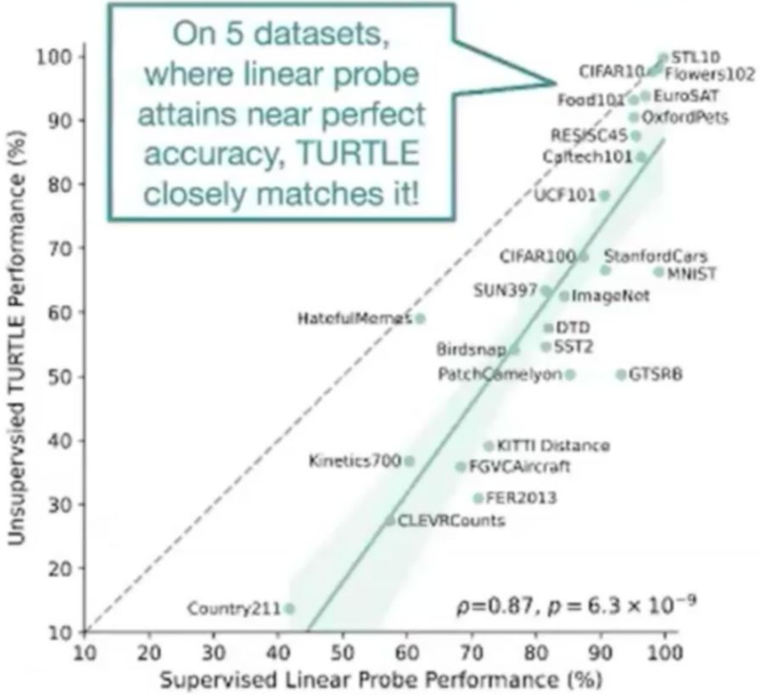



Performance across 26 datasets

TURTLE is fully unsupervised!

Gadetsky*, Jiang*, Brbić. *ICML '24*

TURTLE's Performance Is Correlated to Linear Probe

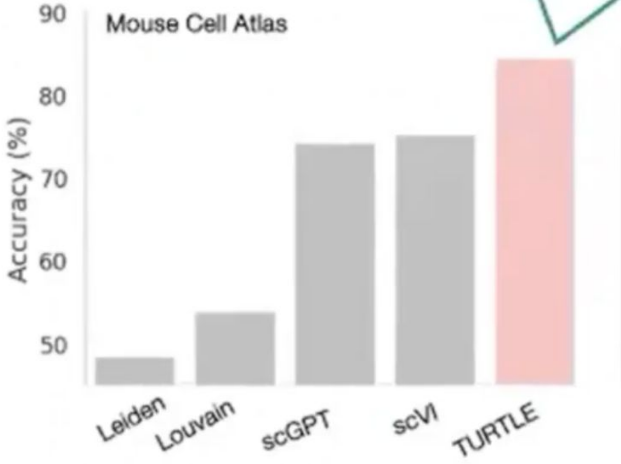


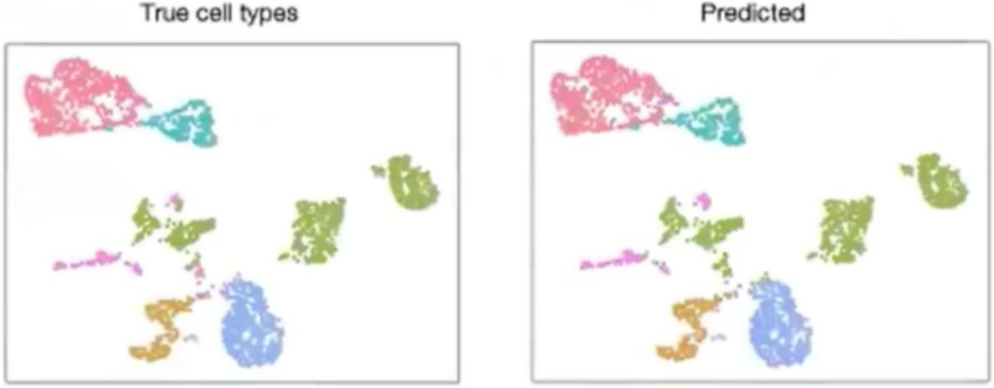
On 5 datasets, where linear probe attains near perfect accuracy, TURTLE closely matches it!

TURTLE can infer "optimal" classifier without supervision given high-quality representations

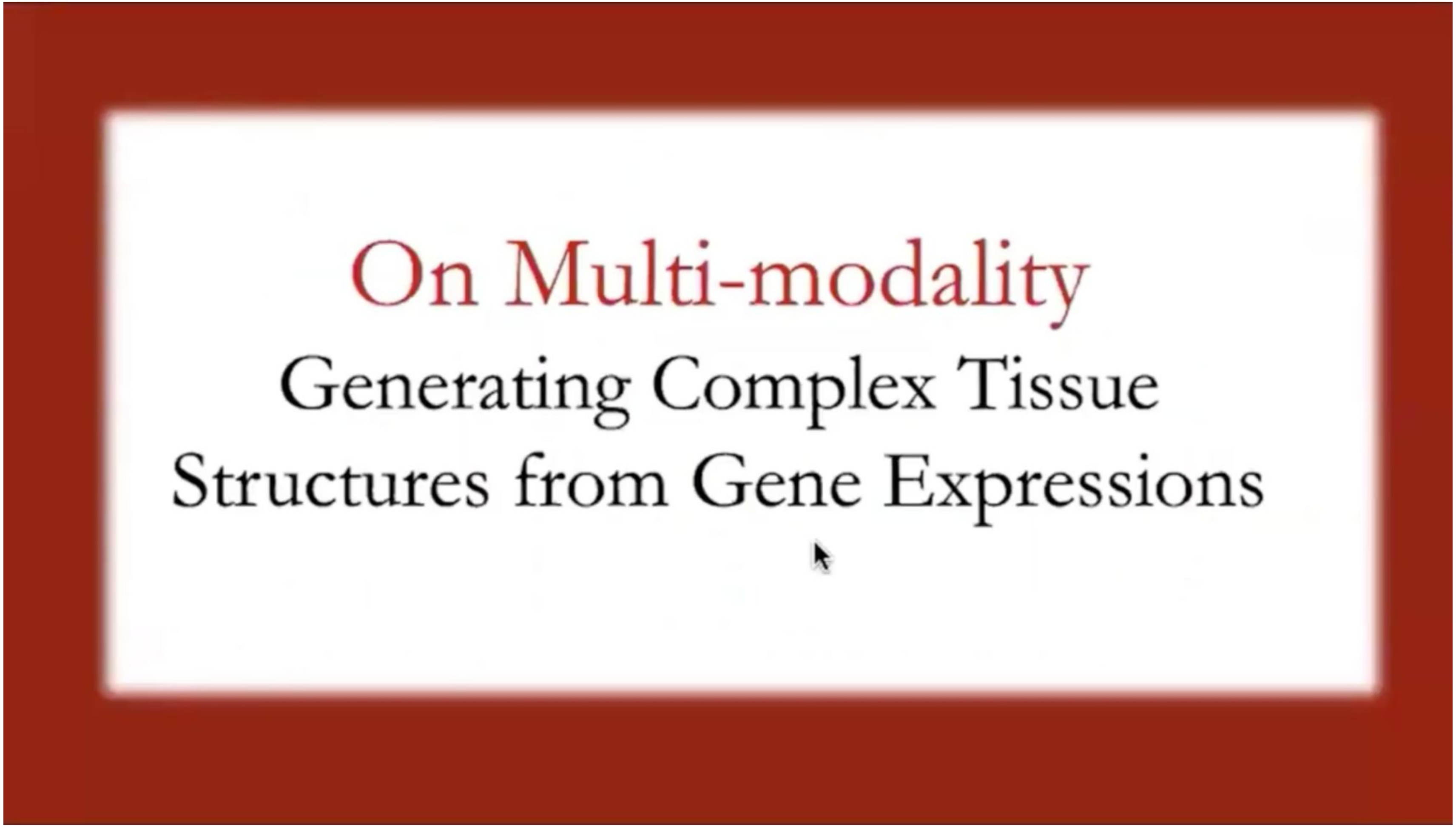
Application to Single-Cell Data

Unsupervised transfer on top of scGPT and scVI spaces





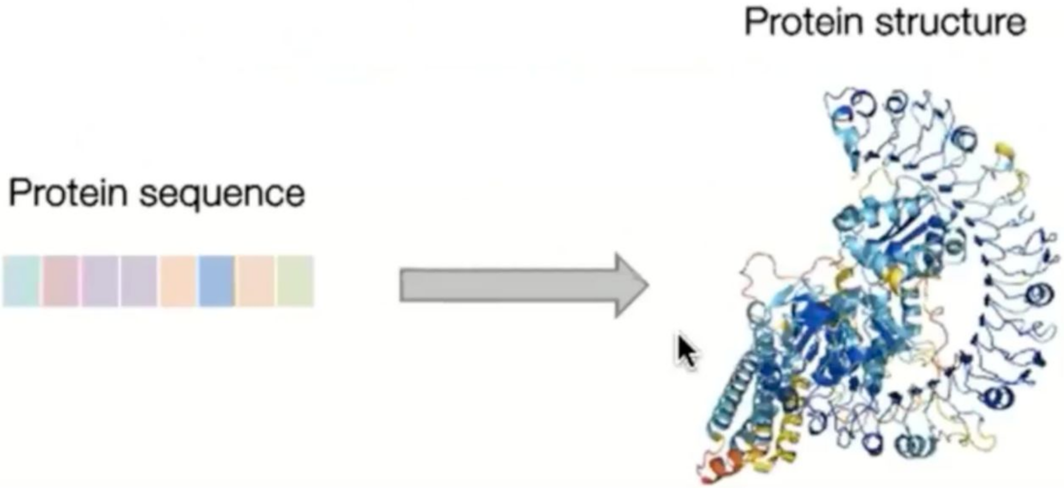
Example: Brown adipose tissue (BAT)



On Multi-modality

Generating Complex Tissue Structures from Gene Expressions

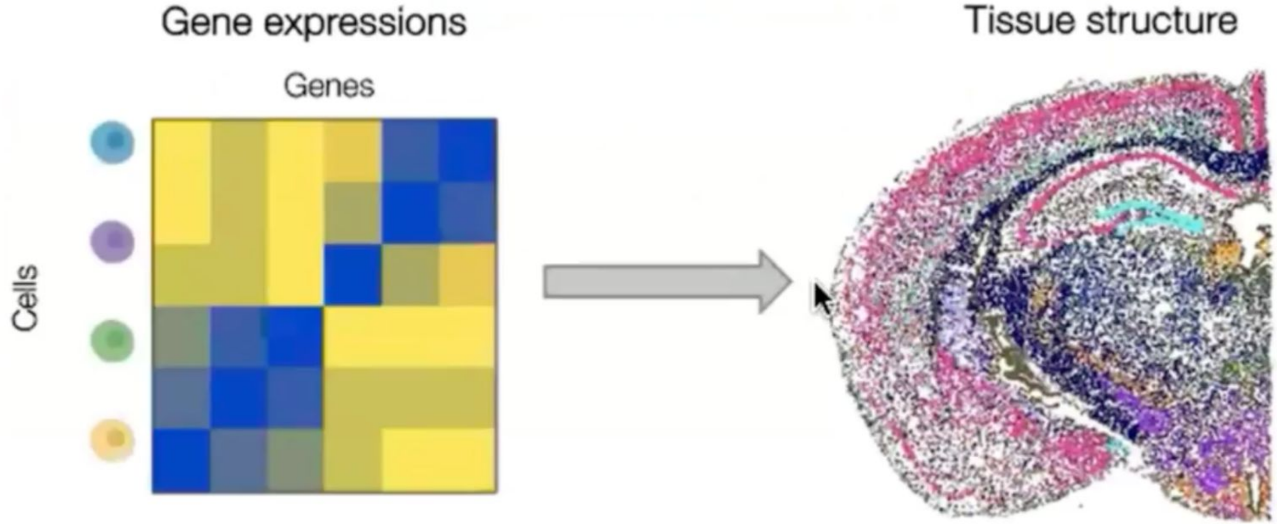
AlphaFold For Cells



Protein sequence

Protein structure

AlphaFold For Cells

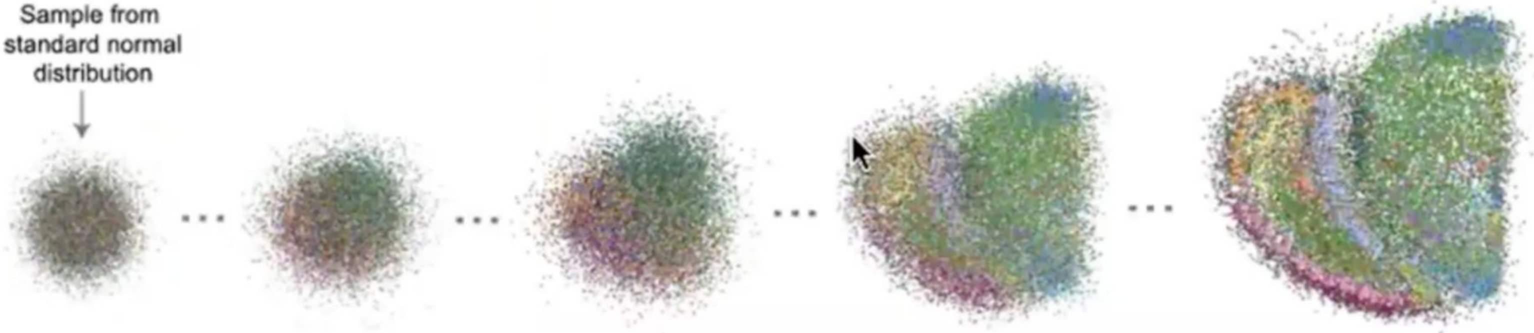


LUNA: From Cells to Locations

A generative model for mapping cells to their locations and generating tissue structures

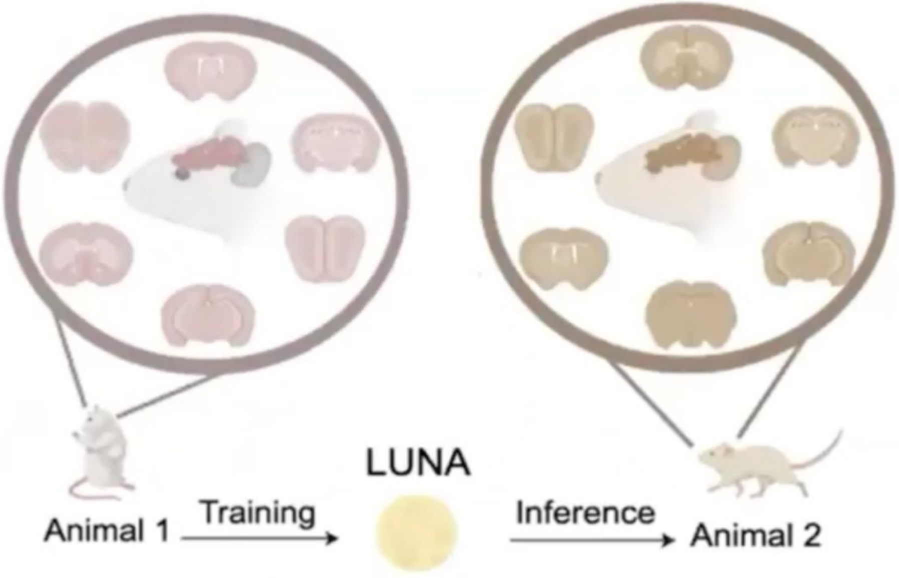
Yist Yu

Chanakya Ekbote



Unpublished work

Reconstruction of Whole Mouse Brain MERFISH Atlas



Unpublished work

Dataset:

- MERFISH Mouse Brain Atlas with over 4 million cells

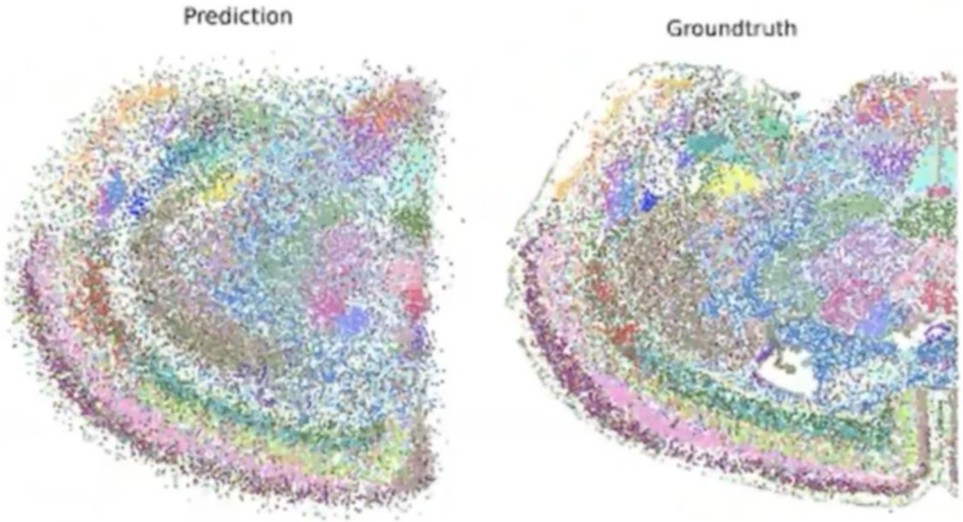
Training dataset:

- 2.85 million cells across 147 slices from one mouse

Target unlabeled dataset:

- 1.23 million cells across 66 slices from another mouse

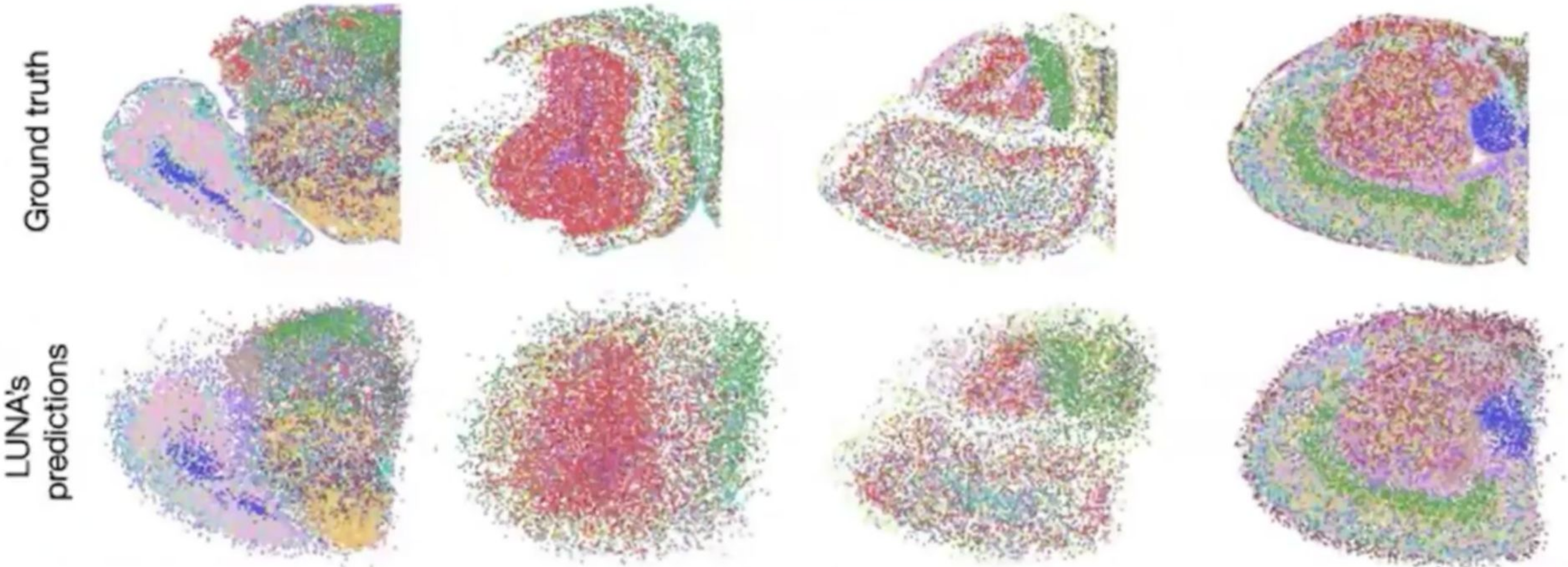
Reconstruction of Whole Mouse Brain MERFISH Atlas



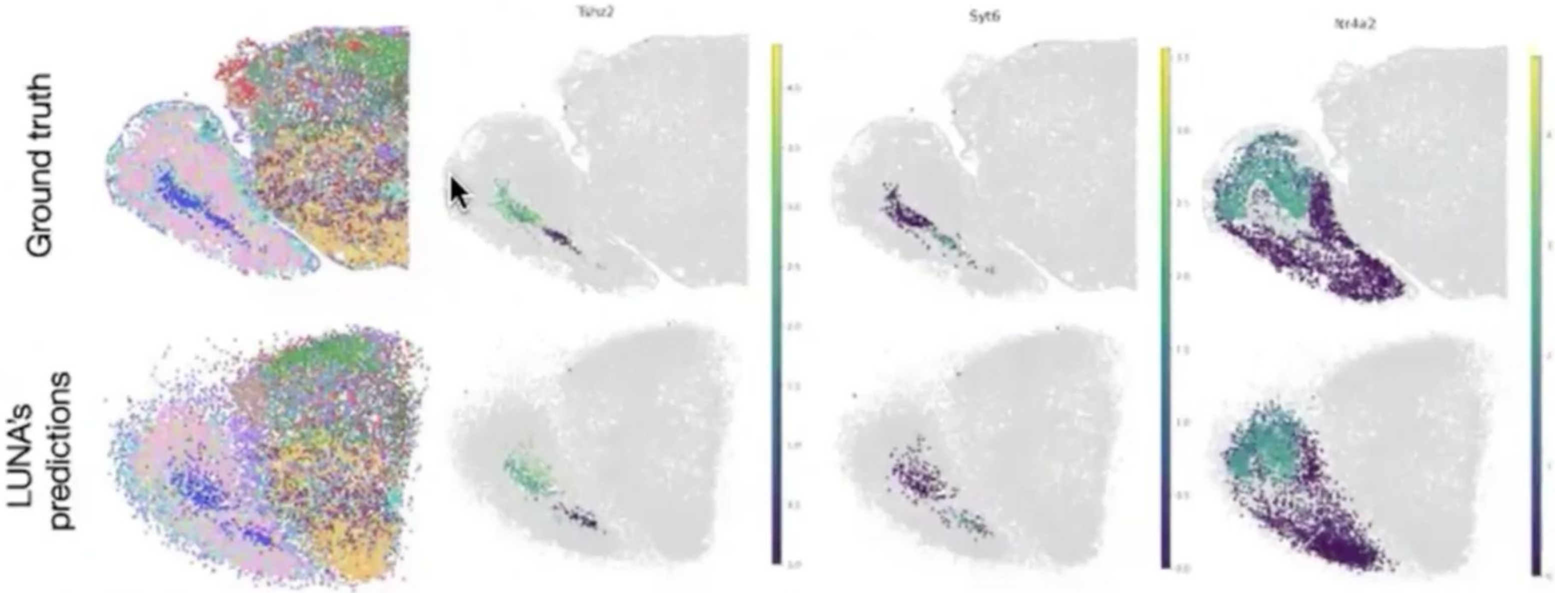
Unpublished work

Reconstruction of Whole Mouse Brain MERFISH Atlas

338 different subclasses!

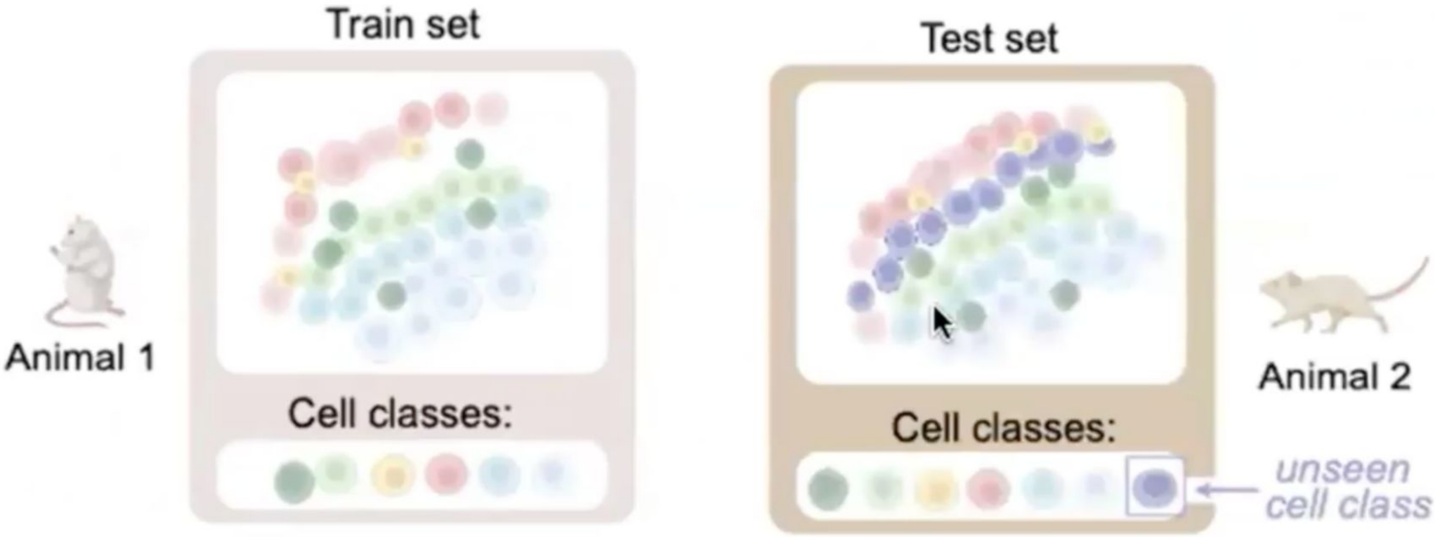


Reconstruction of Whole Mouse Brain MERFISH Atlas



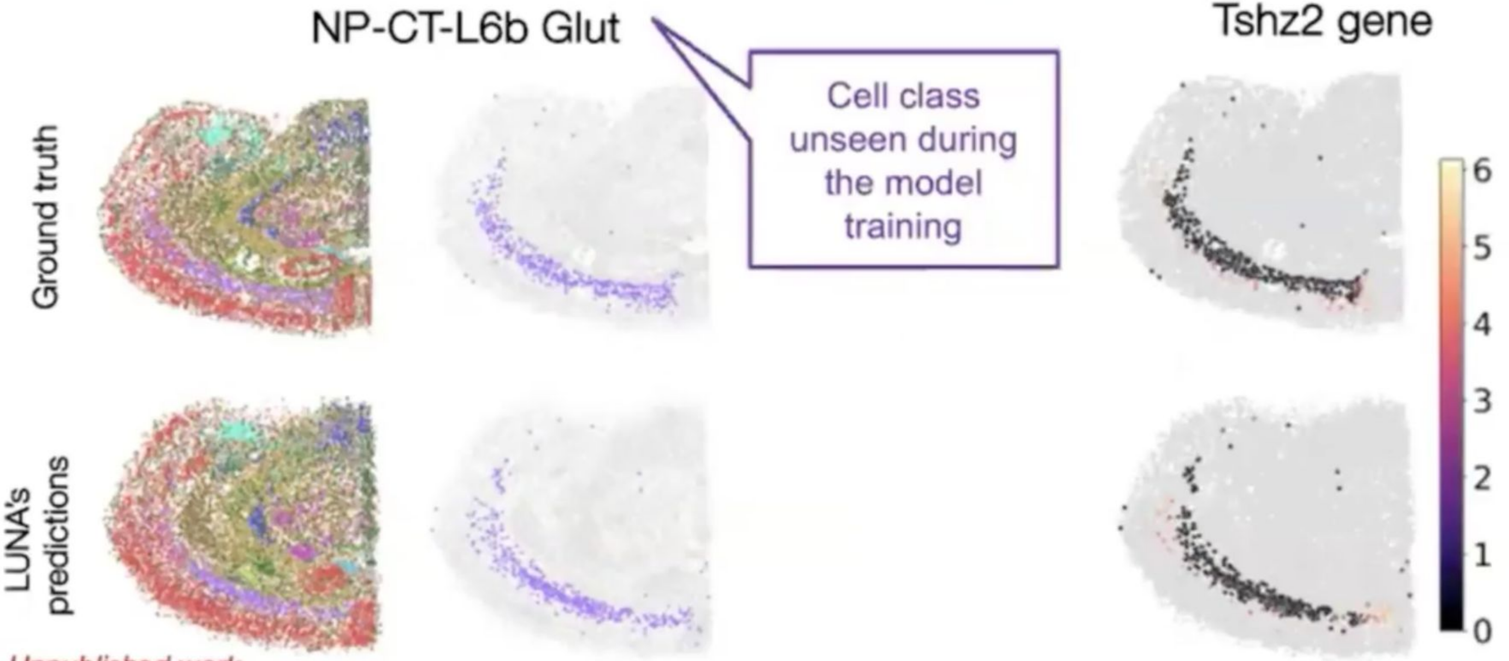
Maria Brbić, EPFL

LUNA: Zero-Shot Setting



Unpublished work

Zero-Shot Generalization to Unseen Cell Types



NP-CT-L6b Glut

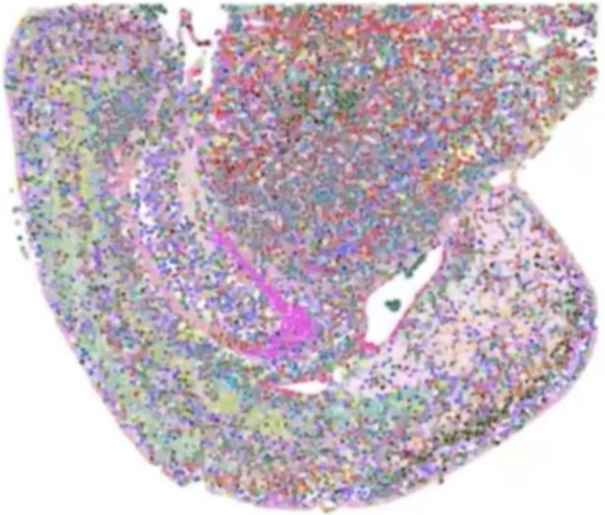
Tshz2 gene

Cell class unseen during the model training

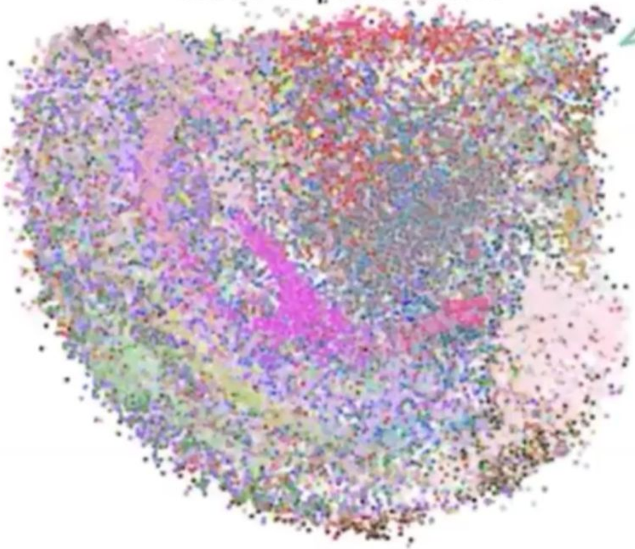
Unpublished work

De Novo Reconstruction of CNS ScRNA-seq Atlas

Estimated ground truth



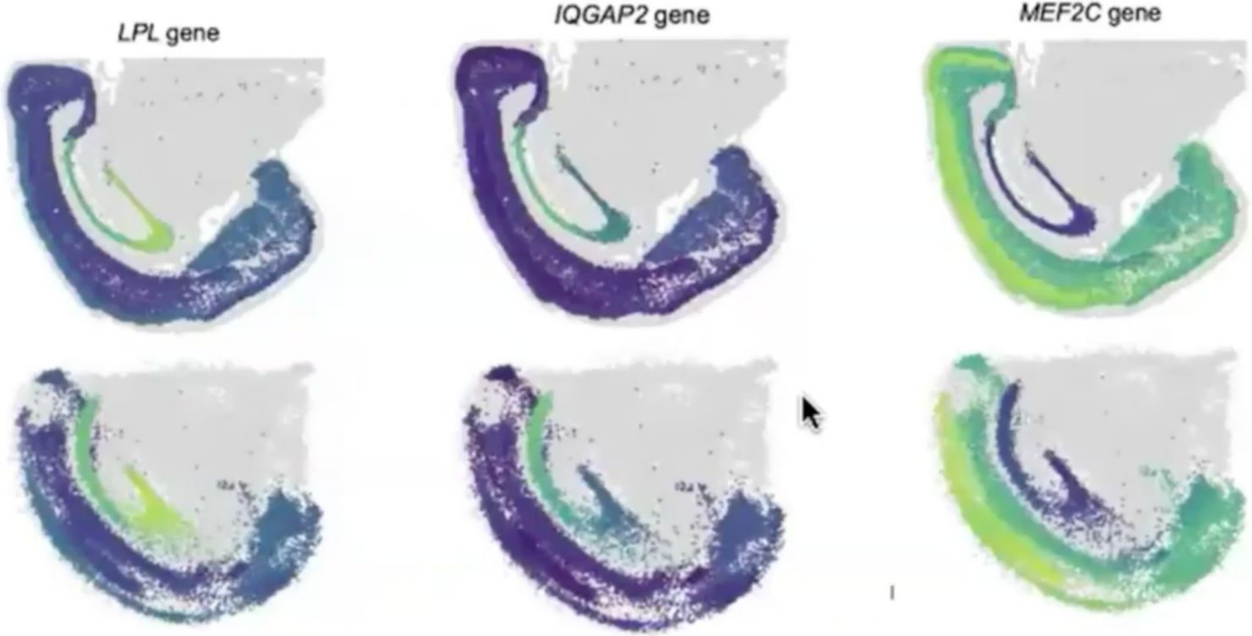
LUNA's predictions



216 cell classes

Unpublished work

De Novo Reconstruction of CNS ScRNA-seq Atlas



LPL gene

IQGAP2 gene

MEF2C gene

Unpublished work

Acknowledgements

Machine Learning

MLBio lab@EPFL

Biomedicine

PhD students

Artyom Gadetsky

Shuo Wen

Tingyang Yu

Yulun Jiang

Siba Panigrahi

Postdocs:

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Myeongho Jeon

Research engineers

Jeremy Goumaz

Assistant:

Marie Künzle

Collaborators:

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Yanay Rosen, Stanford

Yusuf Roohani, Stanford

Kaidi Cao, Stanford

John Hickey, Duke

Hongjie Li, Baylor College of Medicine

Yuqi Tan, Stanford

Liqun Luo, Stanford

Michael Snyder, Stanford

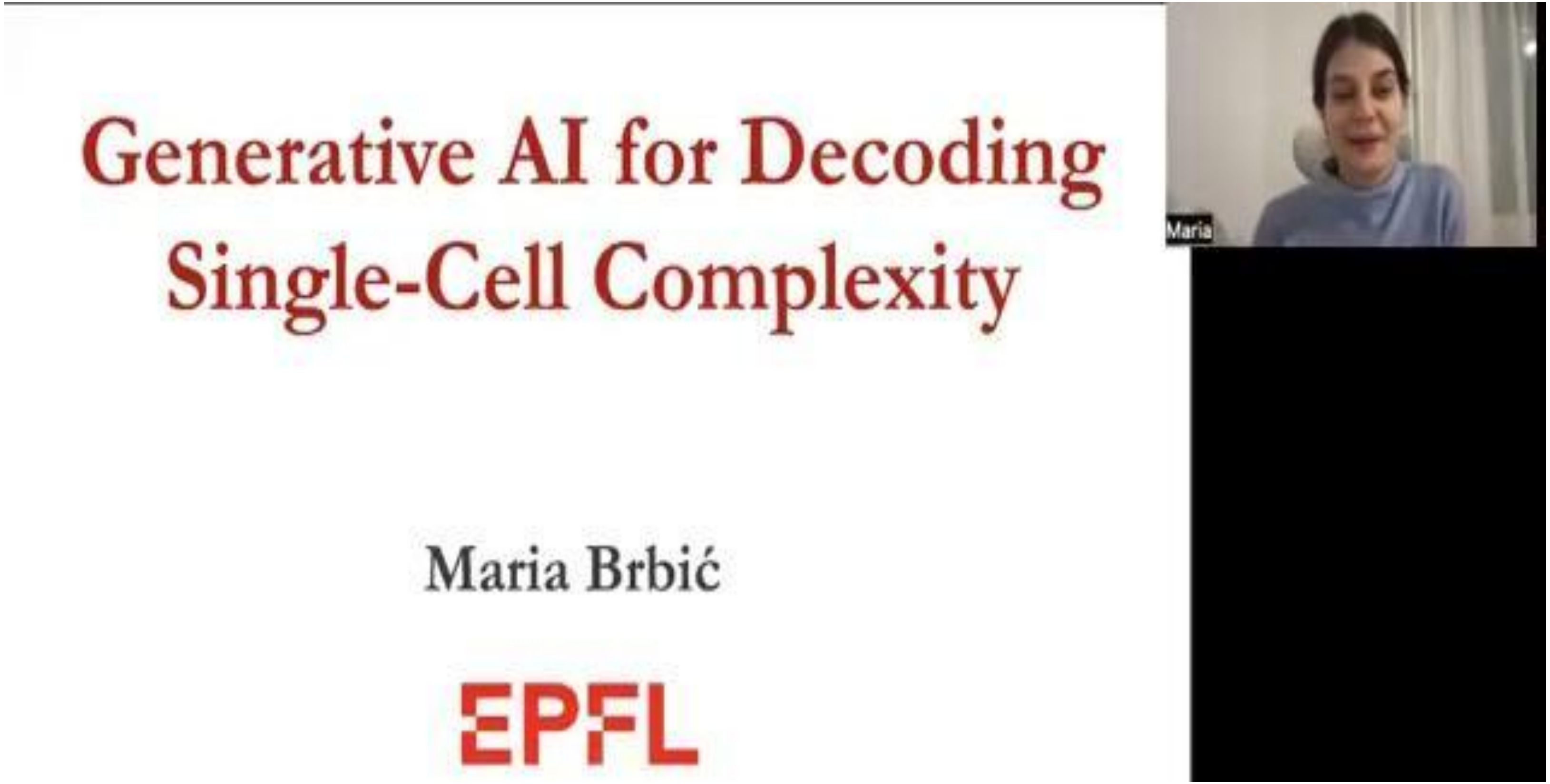
Garry Nolan, Stanford

Pascal Frossard, EPFL

Chanakya Ekbote, MIT

Swiss National
Science Foundation

NIH ImmGen



Generative AI for Decoding Single-Cell Complexity

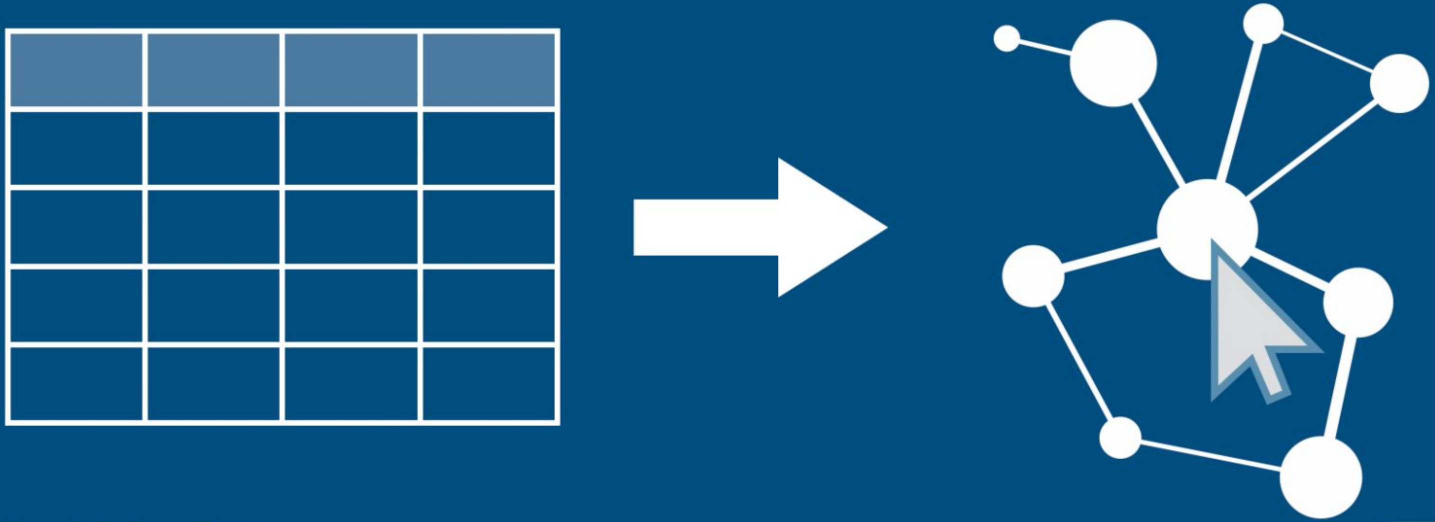
Maria Brbić

EPFL

Filipi Silva, *Indiana University*

Charting Complexity: Interactive real-time visualizations of large-scale networks and embeddings with Helios-Web

https://www.icloud.com/keynote/018HYK4JjBOCRA8N5NGjU7dVg#Embeddings_Visualization_reduced

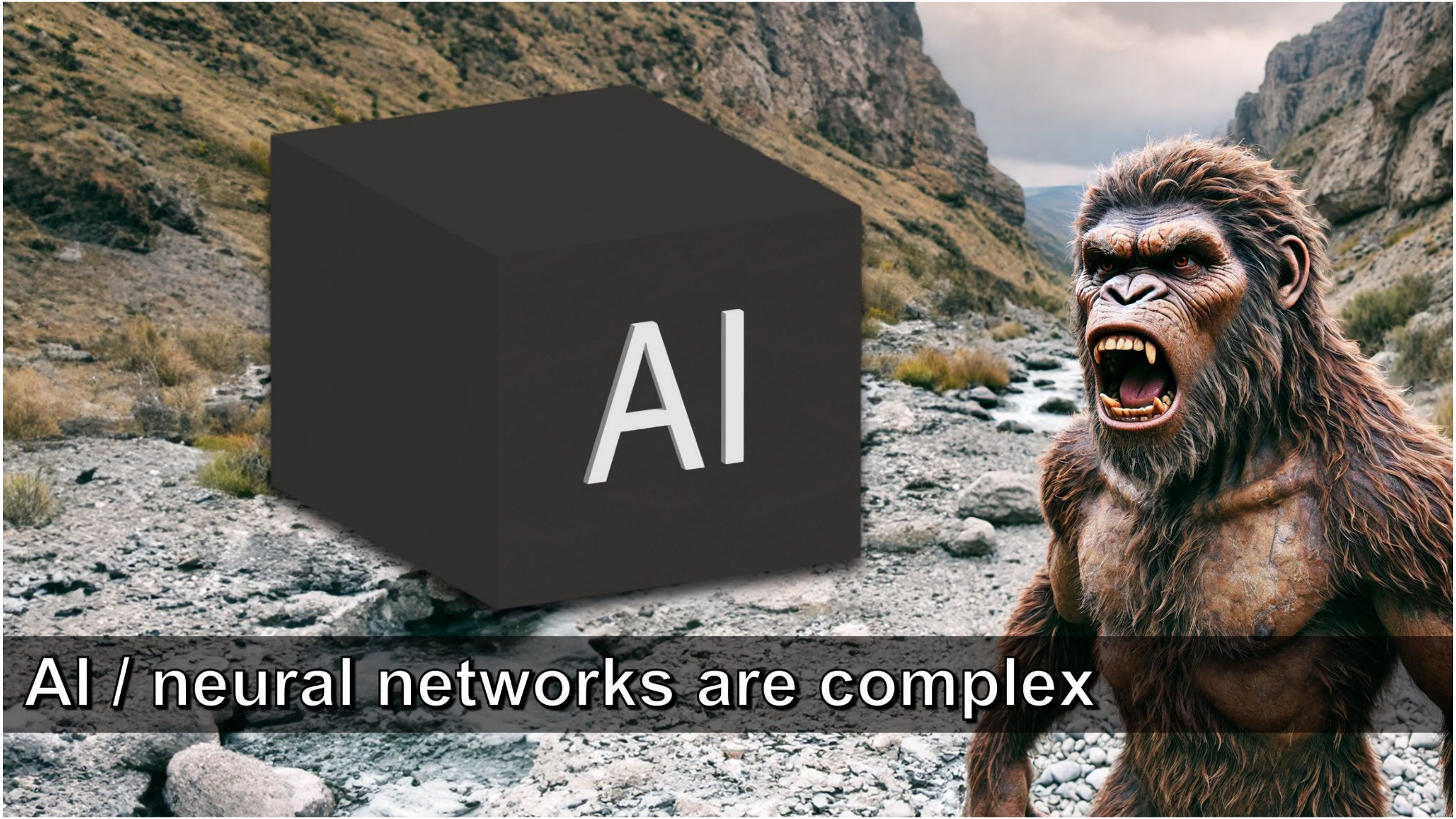


Filipi N. Silva

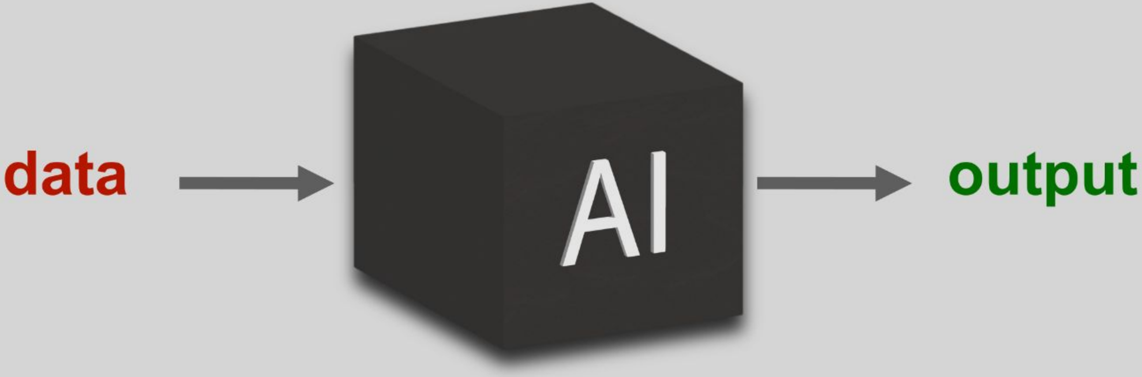
research scientist - Indiana University

filipinascimento.github.io • filsilva@iu.edu

heliosweb.io



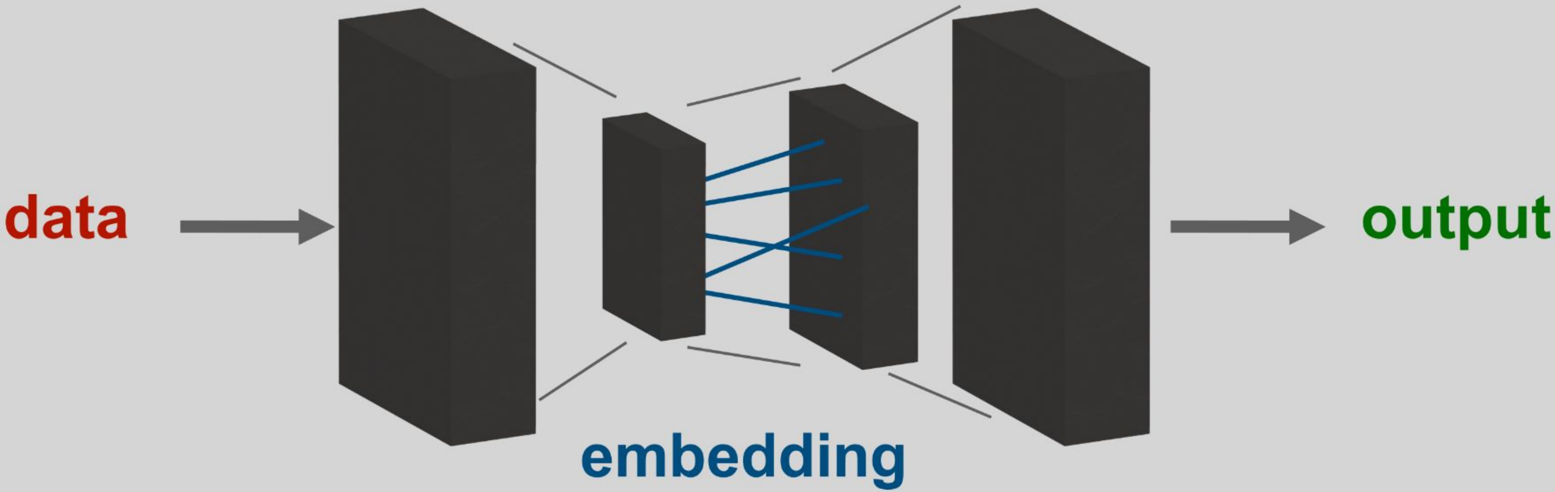
AI / neural networks are complex

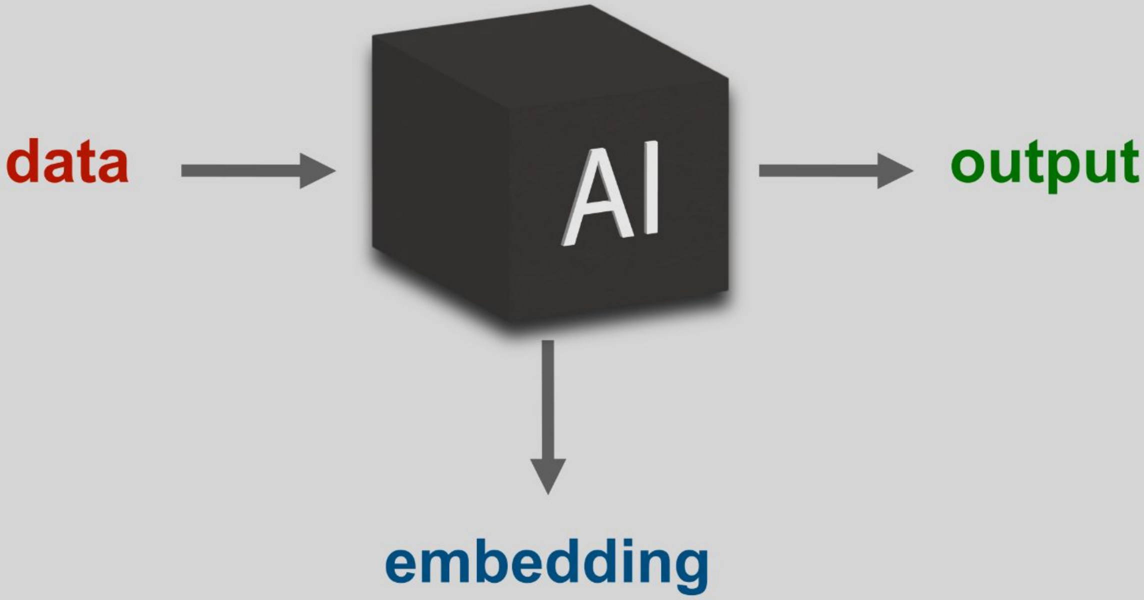


data

AI

output

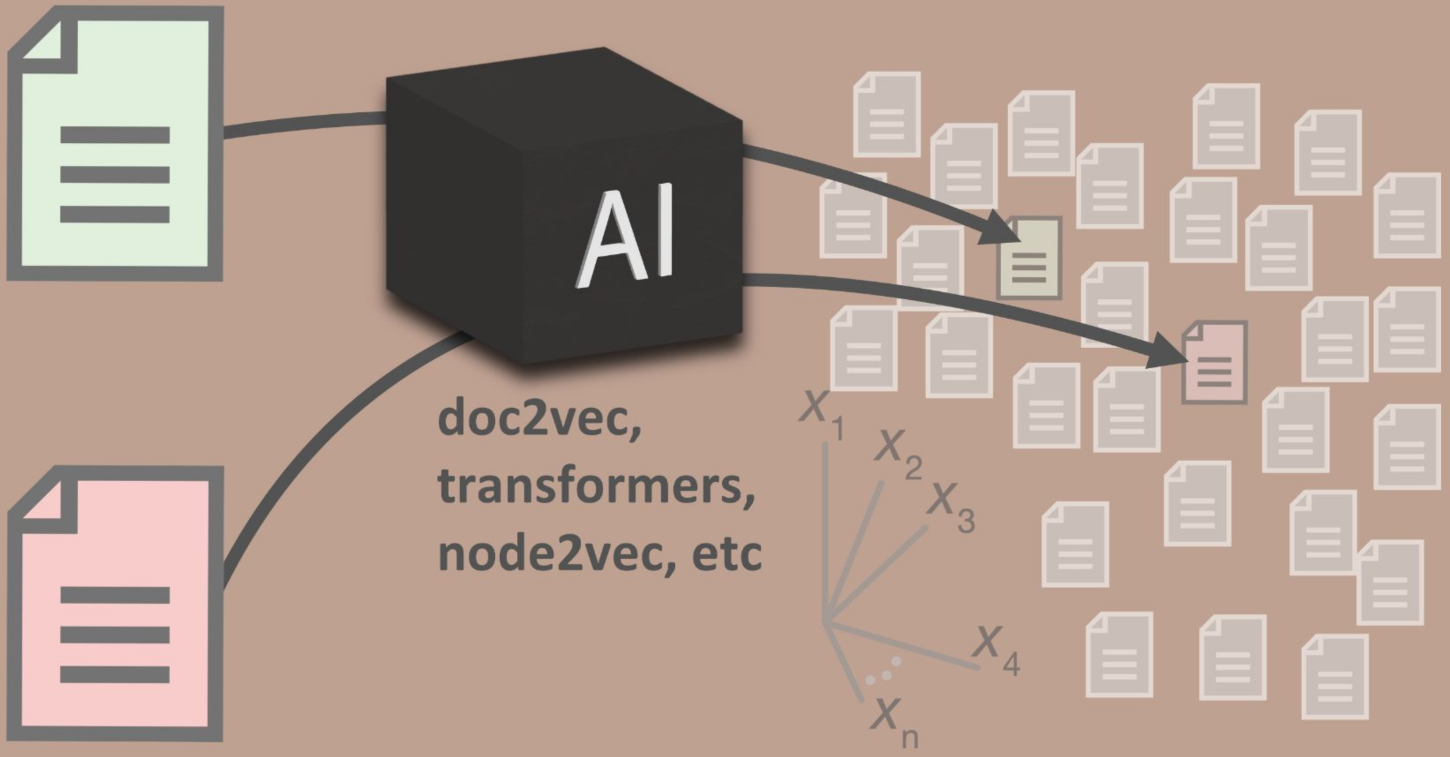

data
embedding
output



data

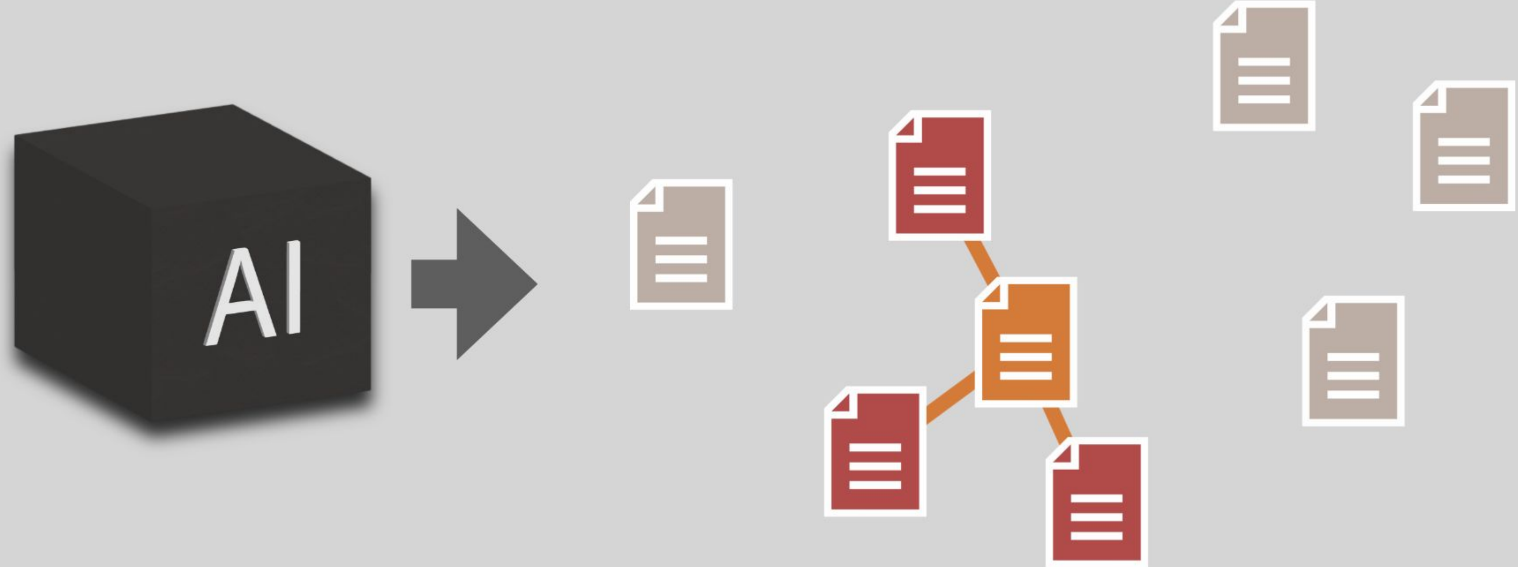
output

embedding



doc2vec,
transformers,
node2vec, etc

Embeddings



Recommendation systems

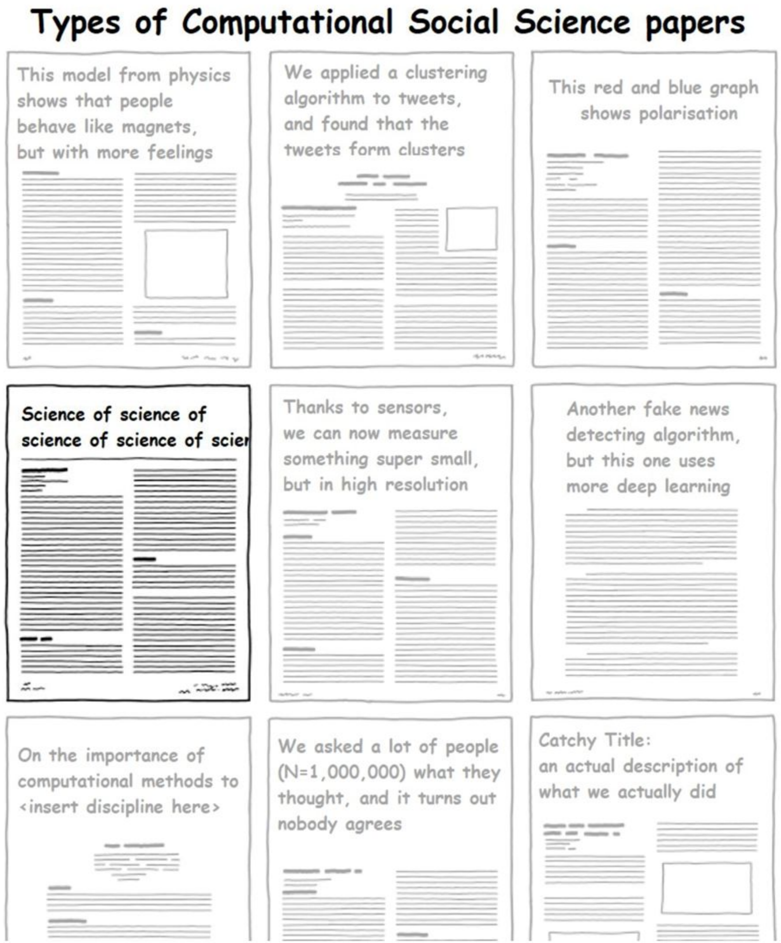
Databases/Search engine

Retrieval-Augmented Generation (RAG)

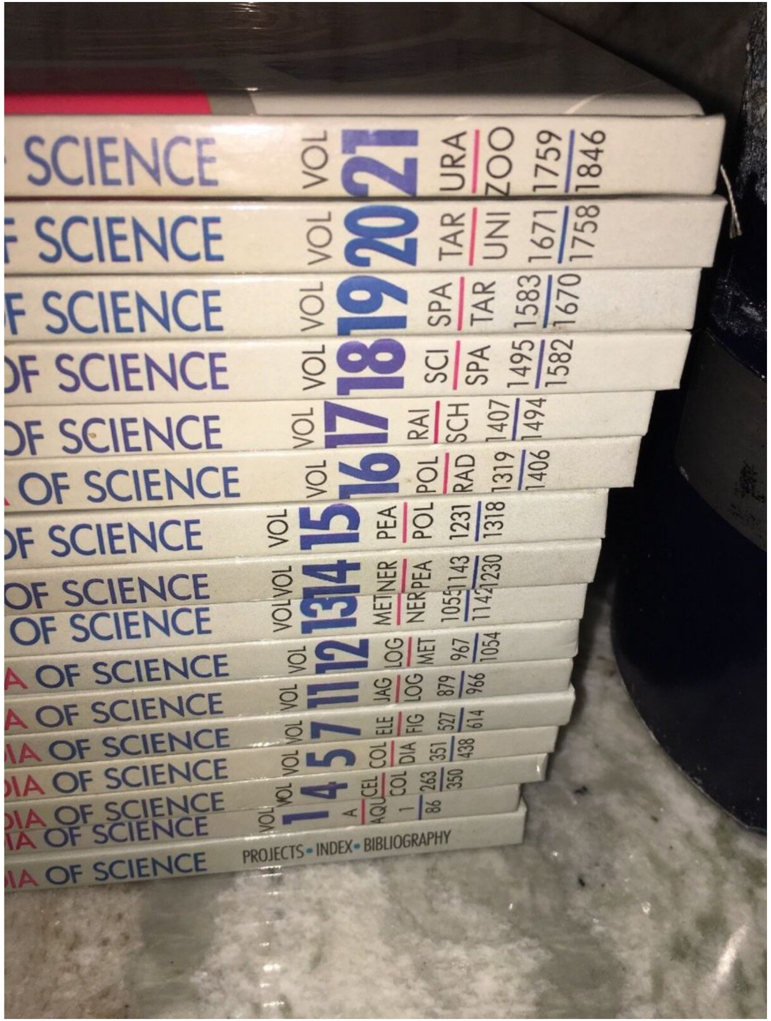
Anomaly Detection

...

Data is also complex


Types of Computational Social Science papers
This model from physics shows that people behave like magnets, but with more feelings
We applied a clustering algorithm to tweets, and found that the tweets form clusters
This red and blue graph shows polarisation
Science of science of science of science of scier
Thanks to sensors, we can now measure something super small, but in high resolution
Another fake news detecting algorithm, but this one uses more deep learning
On the importance of computational methods to <insert discipline here>
We asked a lot of people (N=1,000,000) what they thought, and it turns out nobody agrees
Catchy Title: an actual description of what we actually did

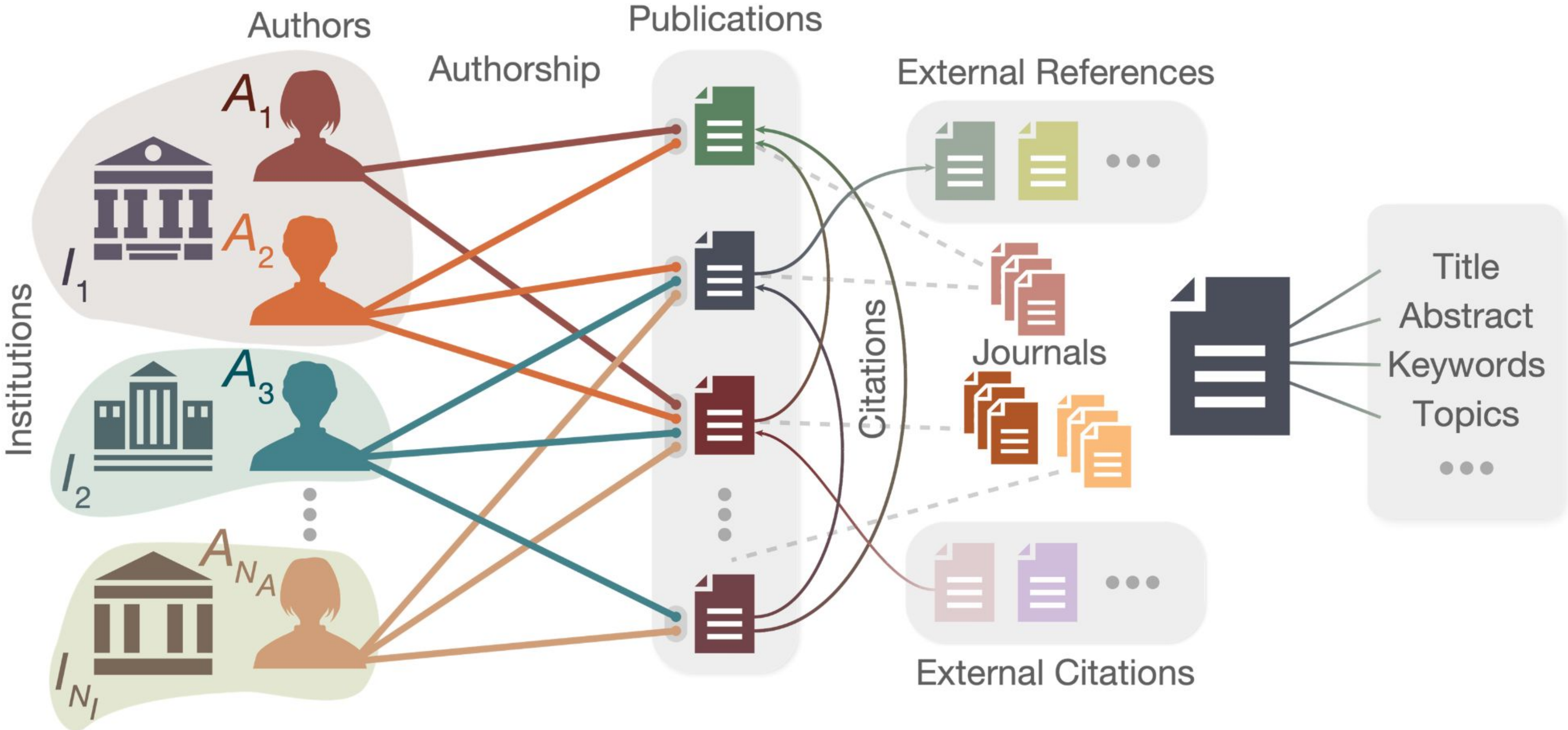
by Chico Camargo (Twitter)
https://twitter.com/evoluchico/status/1388137531552718860



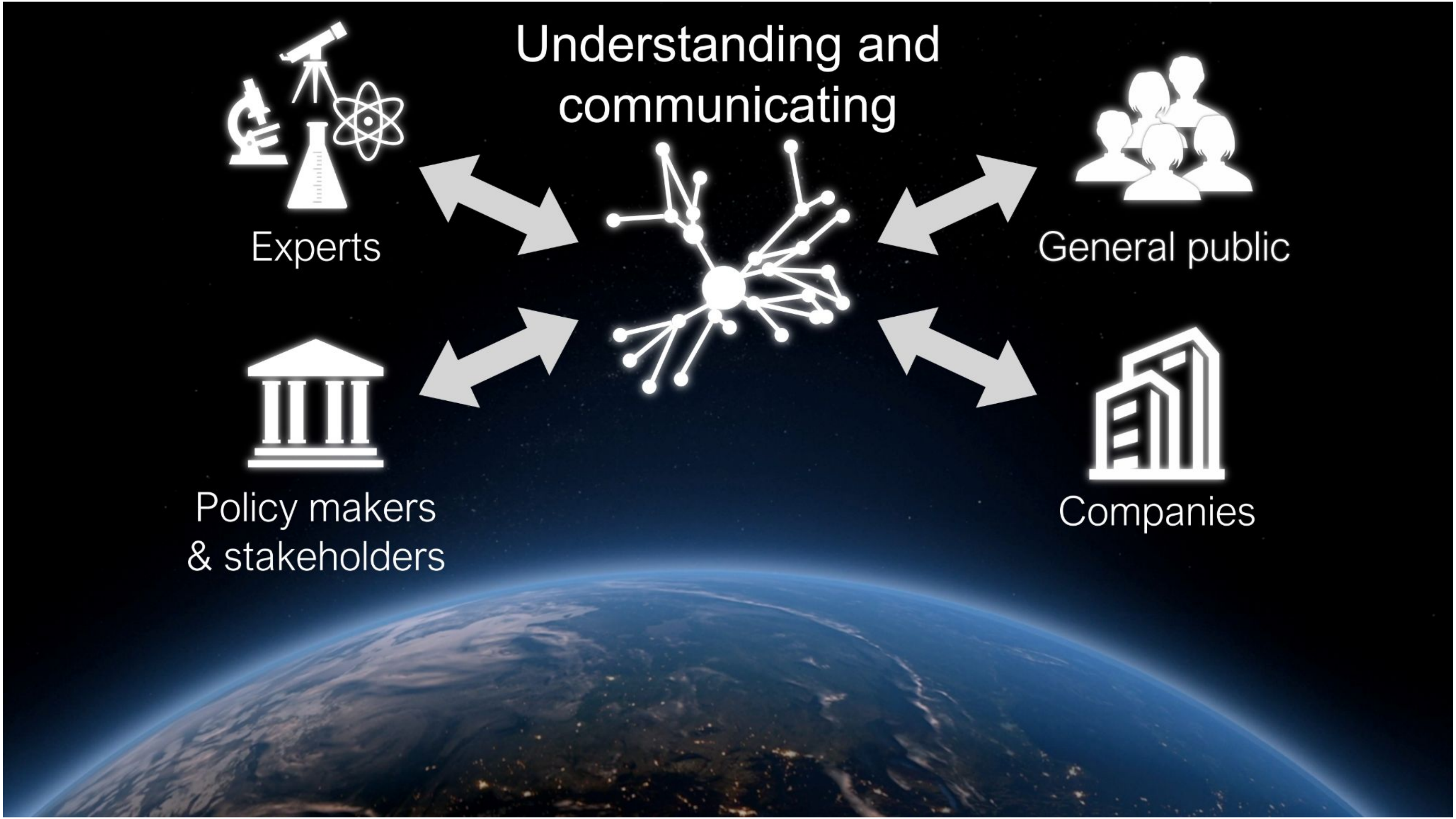
Science of Science

- How science is evolving?
- How researcher teams are formed?
- Is science becoming more interdisciplinary?
- Can we predict success in science?
- How to properly evaluate researchers? journals? papers?
- Can tools/approaches accelerate the scientific development?
- Can we predict the benefits of implementing a policy?
- ...

Publications


Authors
Authorship
Publications
External References
A_1
A_2
A_3
A_{N_A}
I_1
I_2
I_{N_I}
Institutions
Citations
Journals
External Citations
Title
Abstract
Keywords
Topics

Understanding and communicating



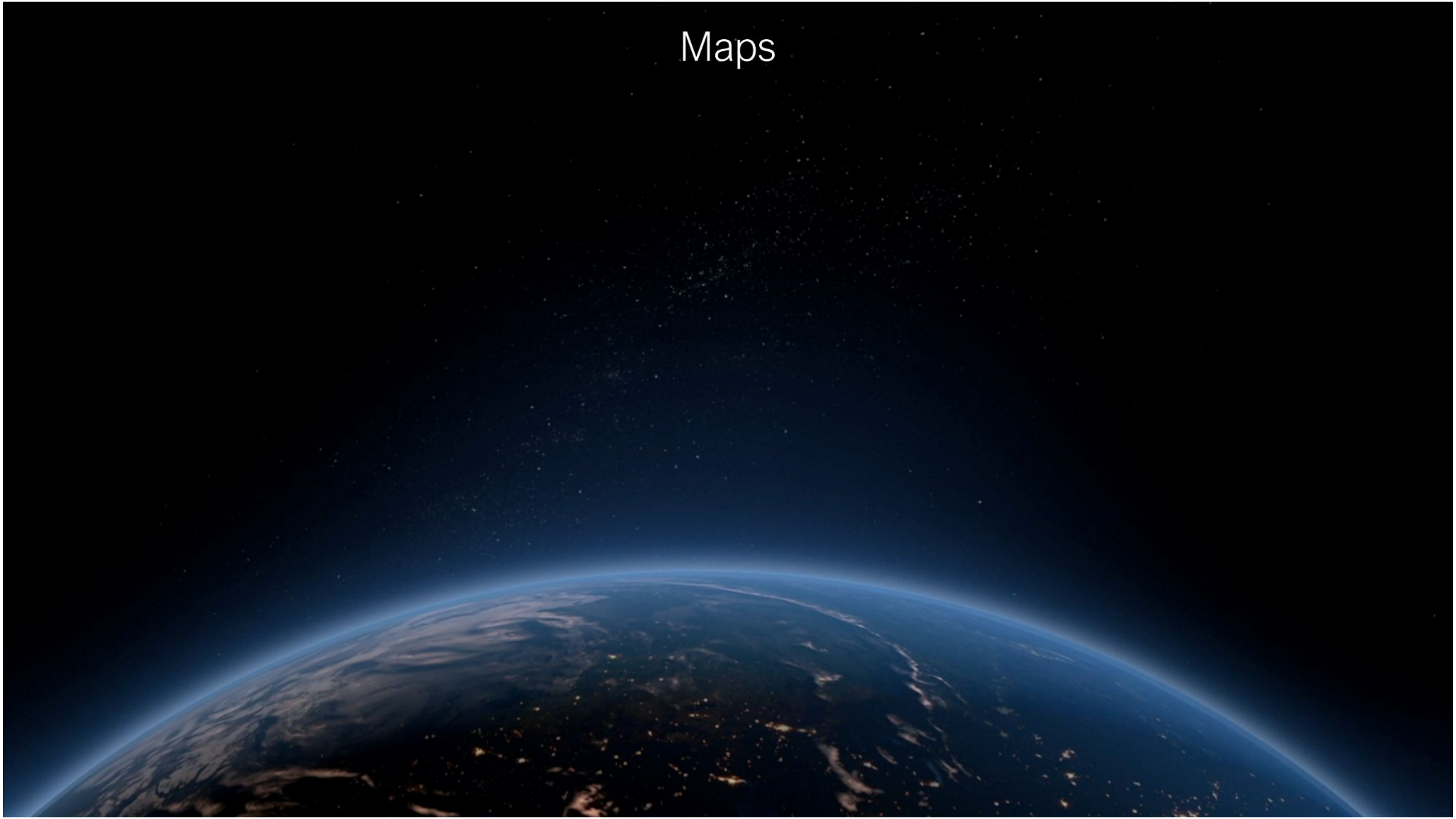
Experts

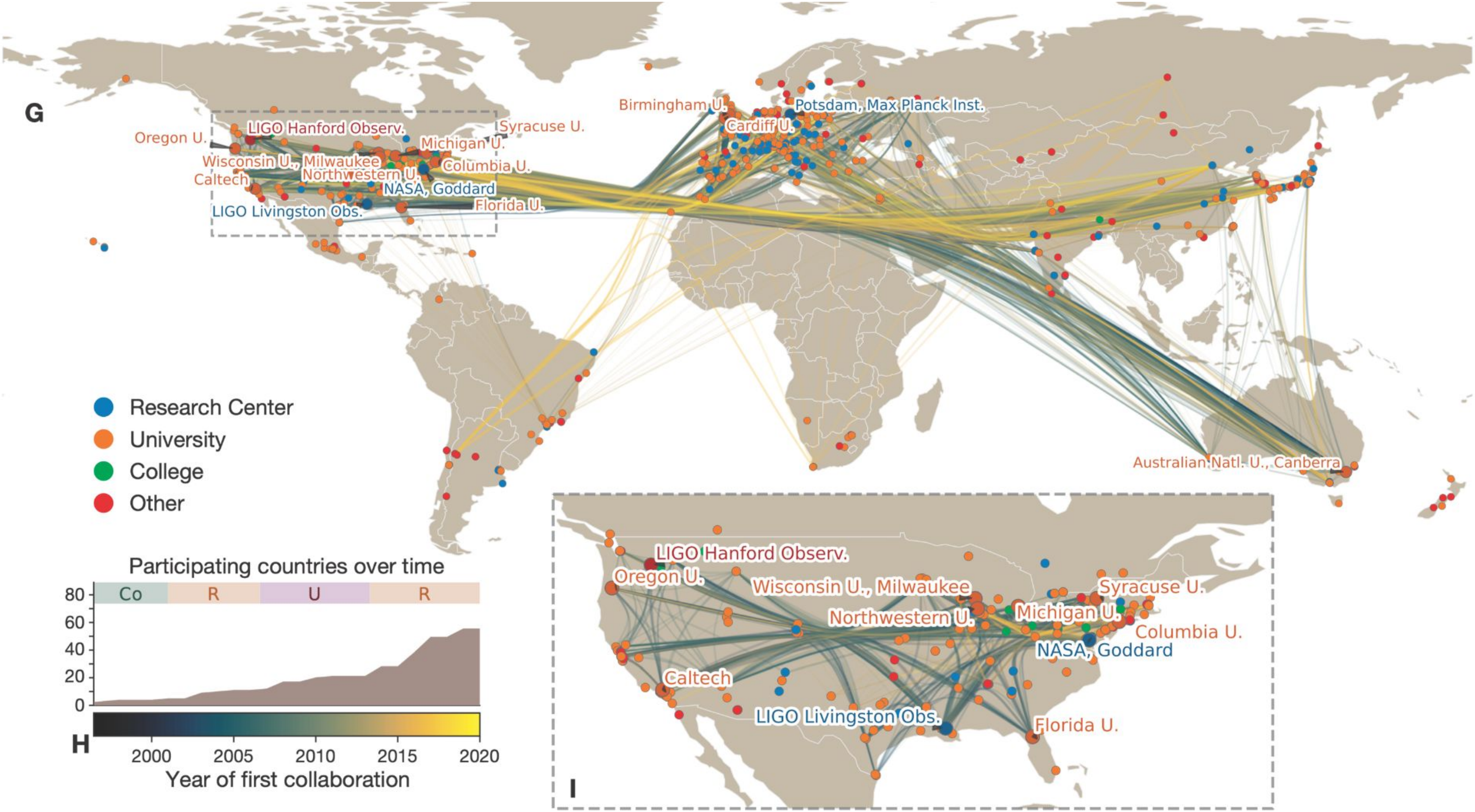
General public

Policy makers & stakeholders

Companies

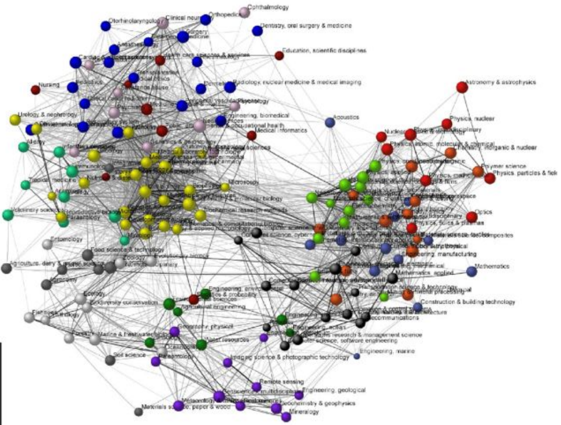
Maps



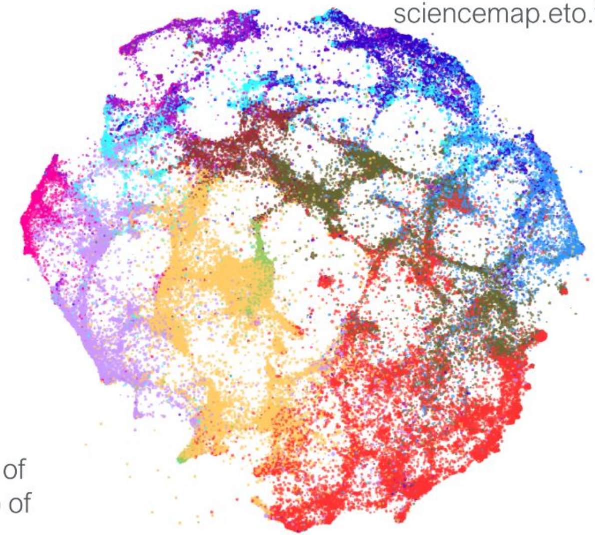


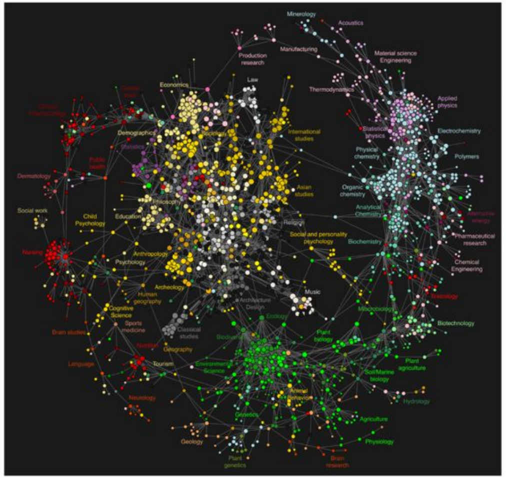
Börner, K., Silva, F. N., & Milojević, S. (2021).
Visualizing big science projects. Nature Reviews Physics, 3(11), 753-761.

Leydesdorff, Loet, and Ismael Rafols. "A global map of science based on the ISI subject categories." Journal of the American Society for Information Science and Technology 60.2 (2009): 348-362.


Ophthalmology
Dentistry, oral surgery & medicine
Education, scientific disciplines
Astronomy & astrophysics
Physics, nuclear
Acoustics
Polymer science
Physics, particles & fields
Optics
Mathematics
Construction & building technology
Engineering, marine
Engineering, geological
Geochemistry & geophysics
Mineralogy
Remote sensing
Imaging science & photographic technology
Nursing
Entomology
Food science & technology
Biodiversity conservation
Soil science
Materials science, paper & wood

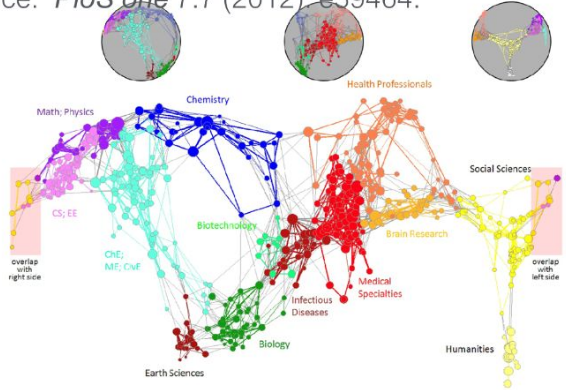
ETO Map of Science
sciencemap.eto.tech

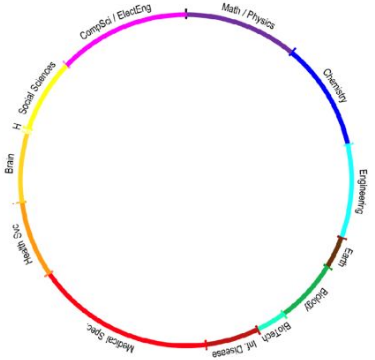


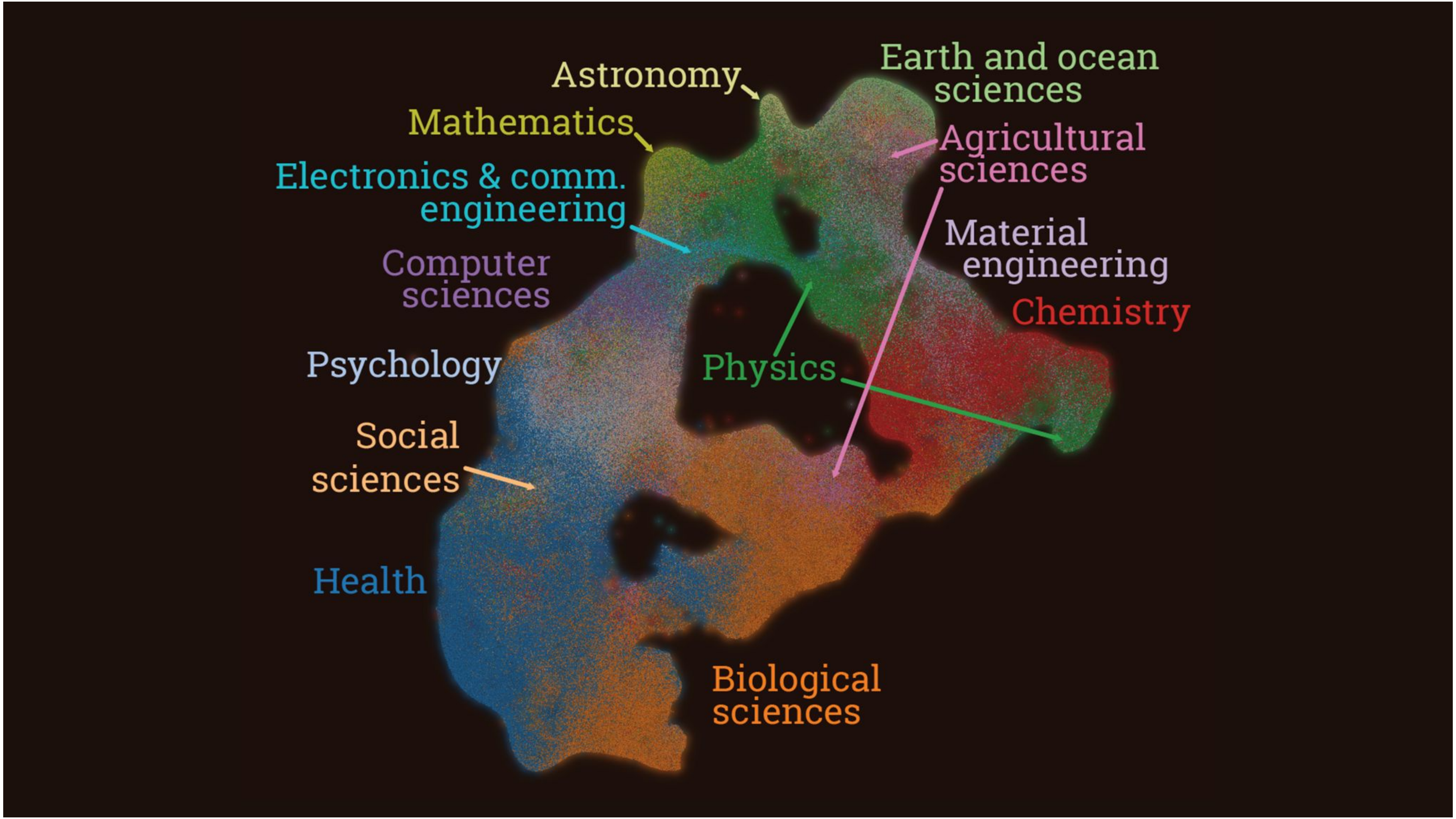


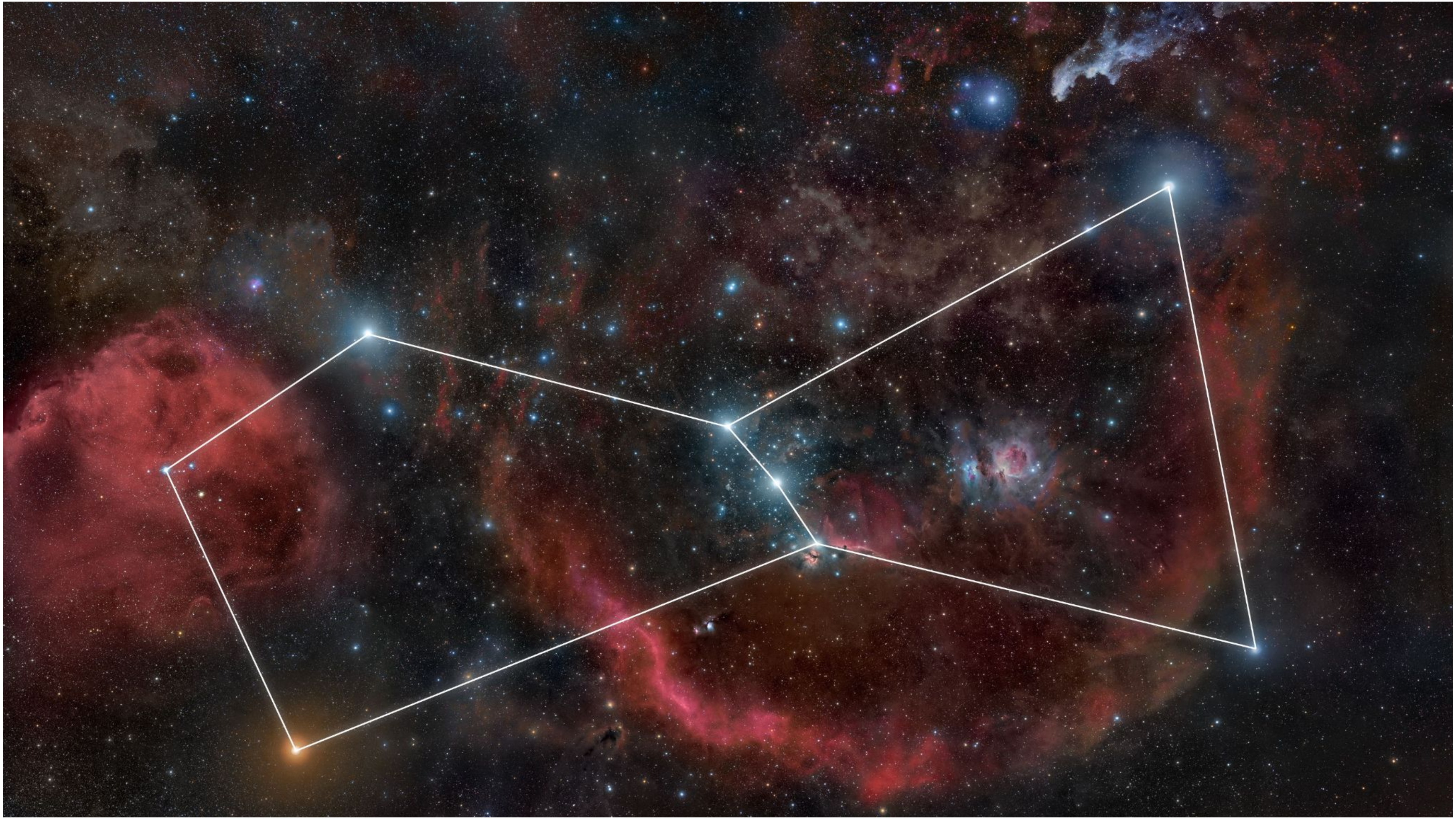
Bollen, Johan, et al. "Clickstream data yields high-resolution maps of science." PloS one 4.3 (2009): e4803.

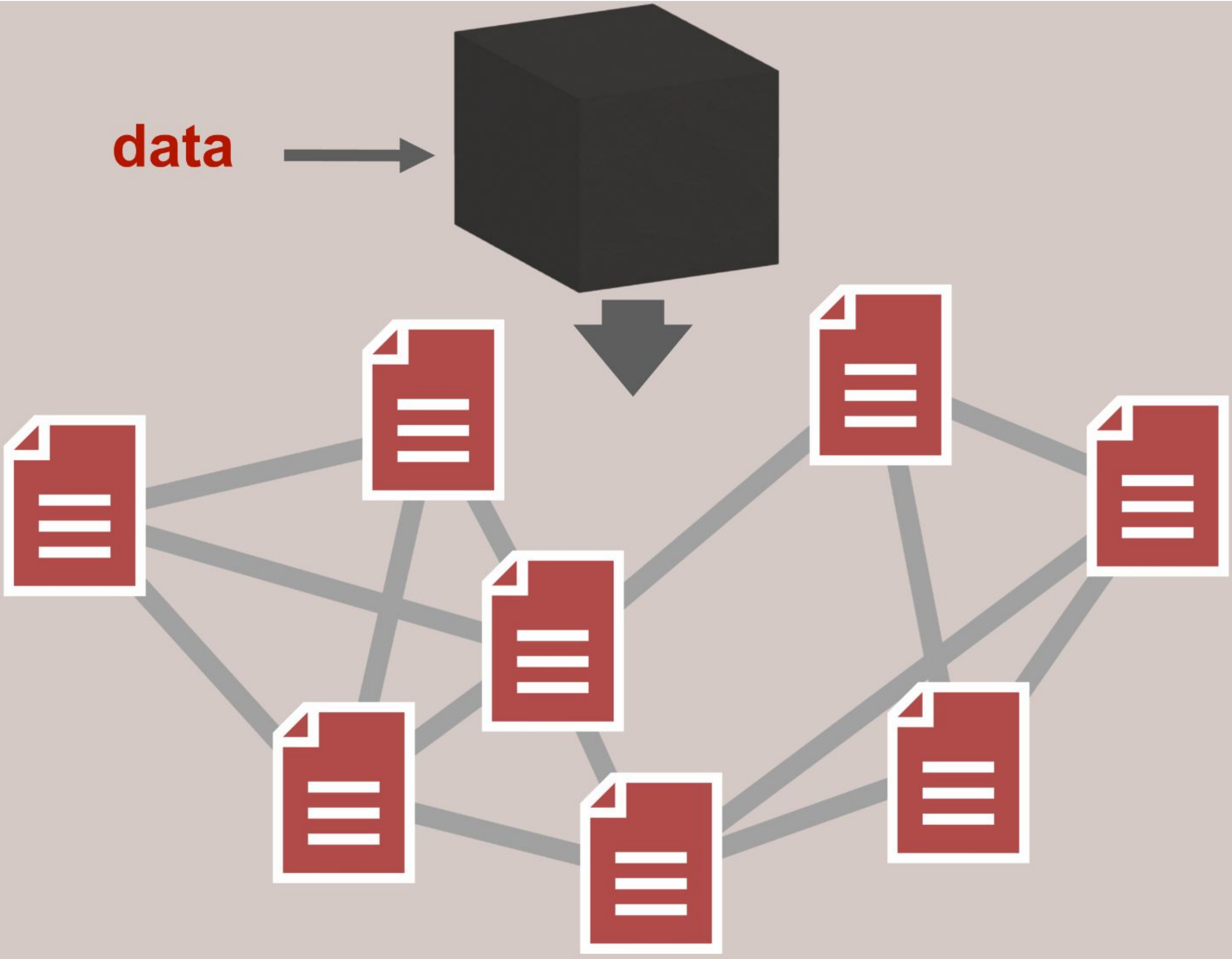
Börner, Katy, et al. "Design and update of a classification system: The UCSD map of science." *PloS one* 7.7 (2012): e39464.

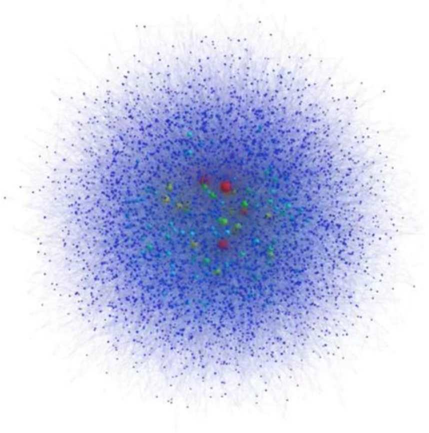
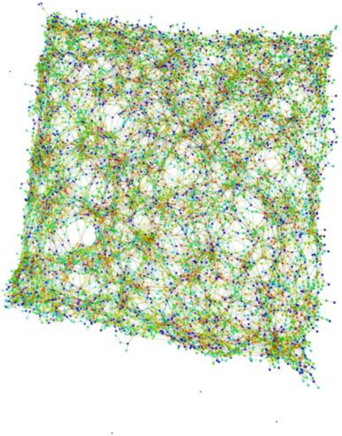
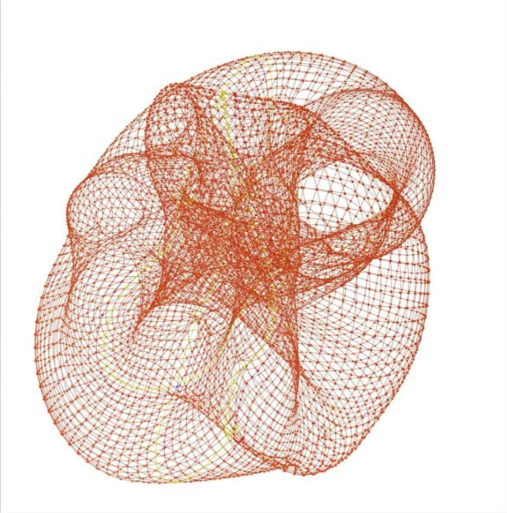
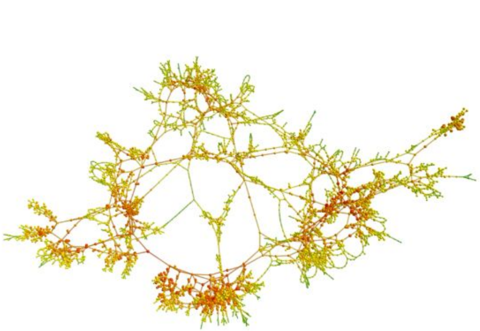
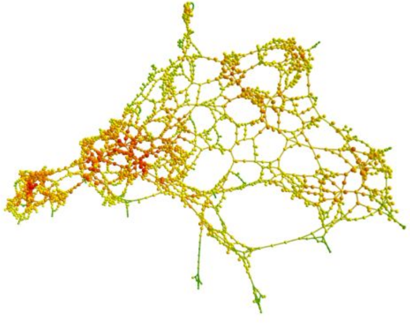
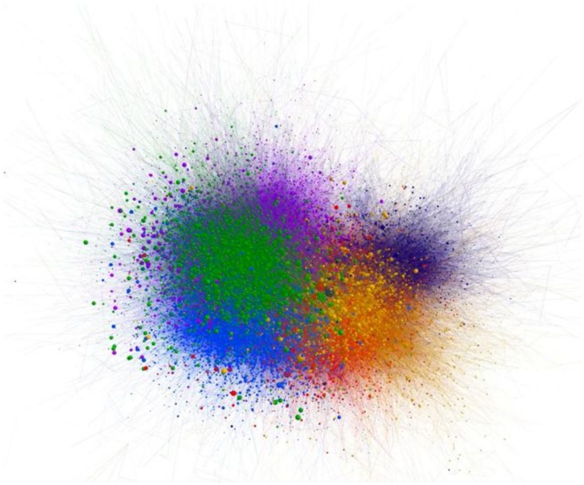


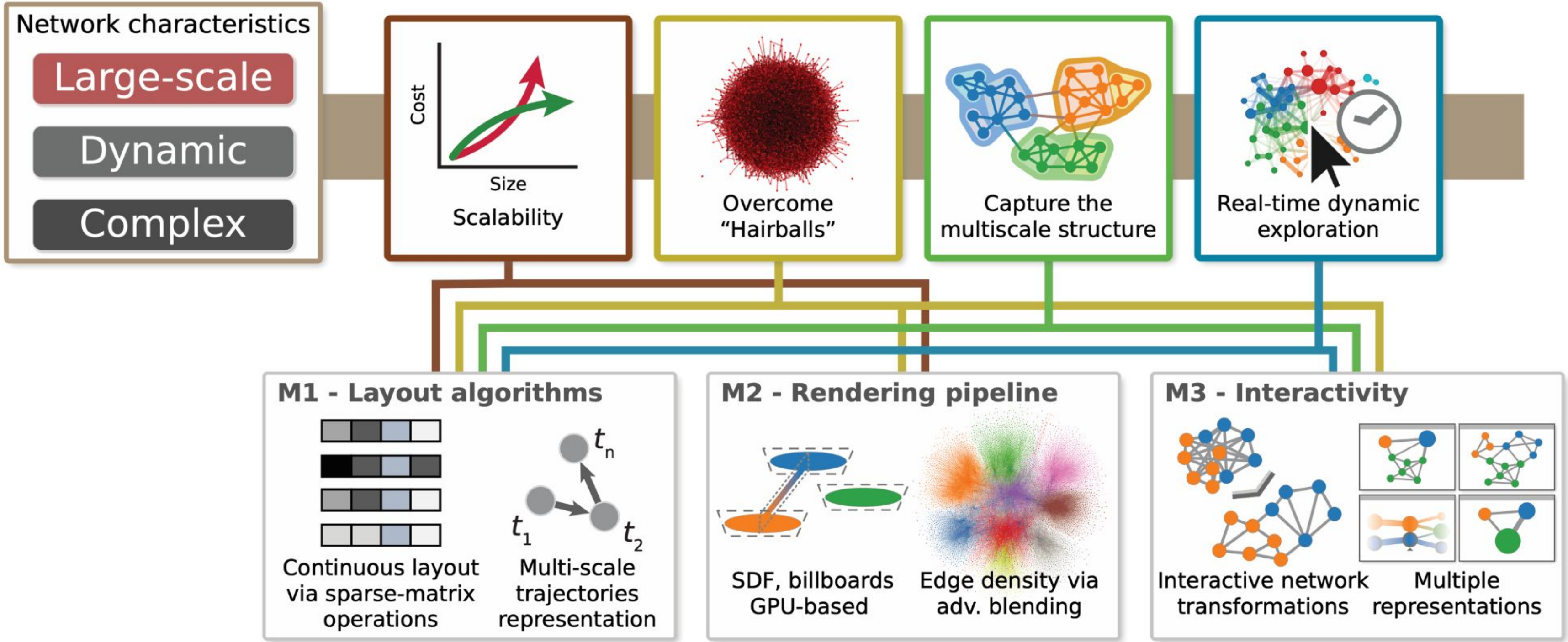



Astronomy
Earth and ocean sciences
Mathematics
Agricultural sciences
Electronics & comm. engineering
Material engineering
Computer sciences
Chemistry
Psychology
Physics
Social sciences
Health
Biological sciences




data



Network characteristics

Large-scale

Dynamic

Complex

Scalability

Overcome “Hairballs”

Capture the multiscale structure

Real-time dynamic exploration

M1 - Layout algorithms

Continuous layout via sparse-matrix operations

Multi-scale trajectories representation

M2 - Rendering pipeline

SDF, billboards GPU-based

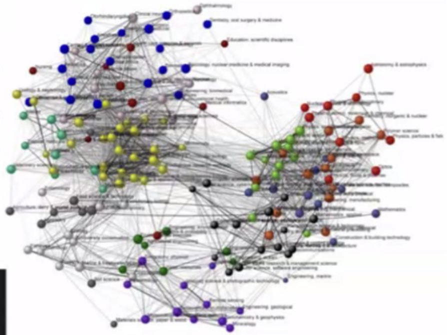
Edge density via adv. blending

M3 - Interactivity

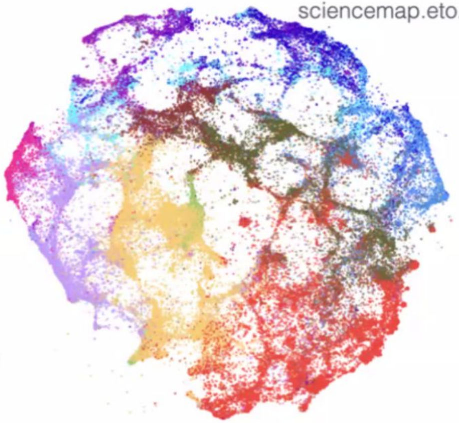
Interactive network transformations

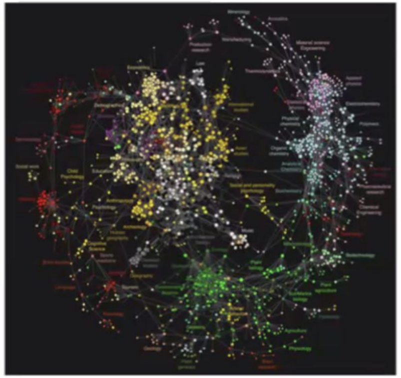
Multiple representations

Leydesdorff, Loet, and Ismael Rafols. "A global map of science based on the ISI subject categories." Journal of the American Society for Information Science and Technology 60.2 (2009): 348-362.



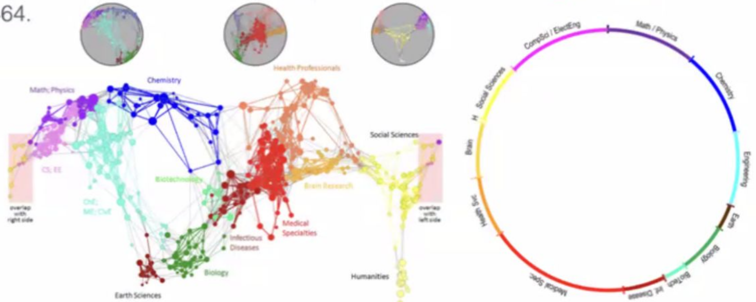
ETO Map of Science
sciencemap.eto.tech

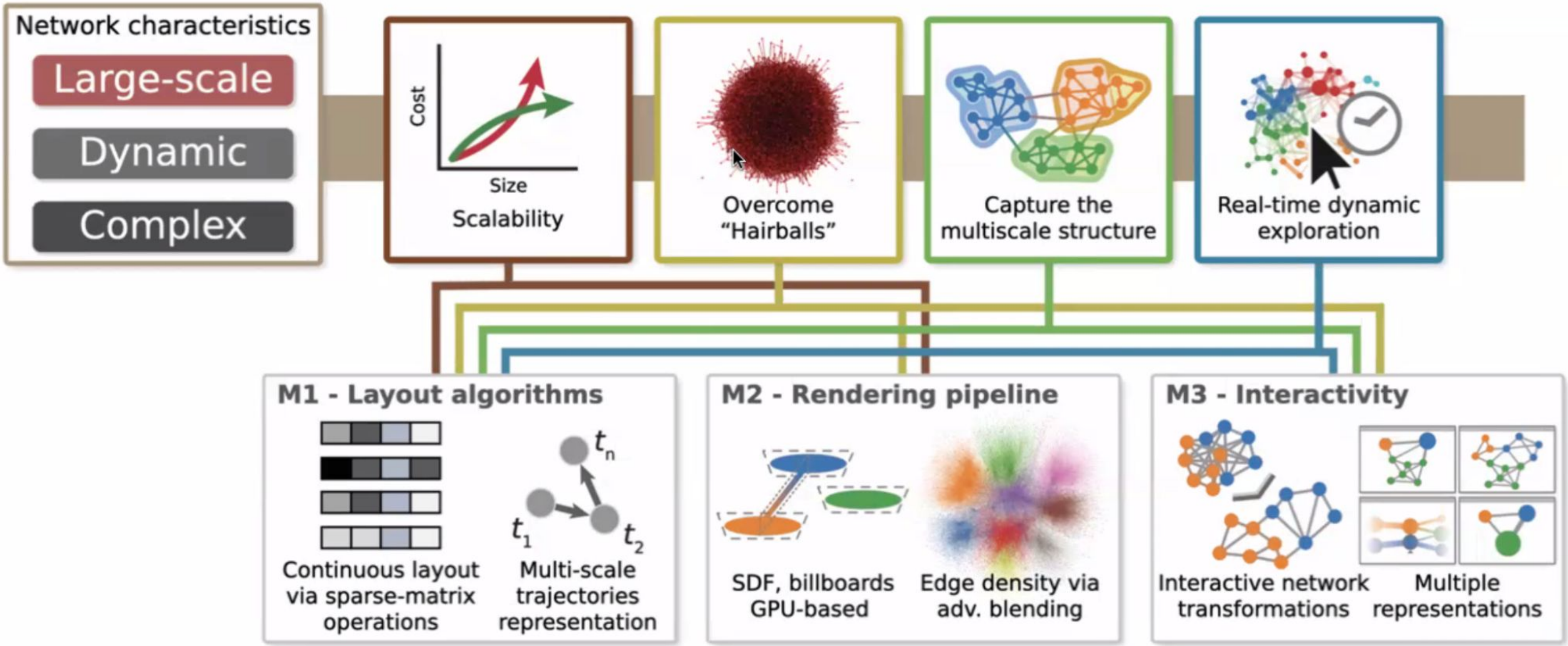




Bollen, Johan, et al. "Clickstream data yields high-resolution maps of science." PloS one 4.3 (2009): e4803.

Börner, Katy, et al. "Design and update of a classification system: The UCSD map of science." *PloS one* 7.7 (2012): e39464.





Network characteristics

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Multiple representations

Helios web

An open-source visualization library for the web

heliosweb.io

web Helios

Open-source web framework

can be integrated in websites, portals, dashboards ...

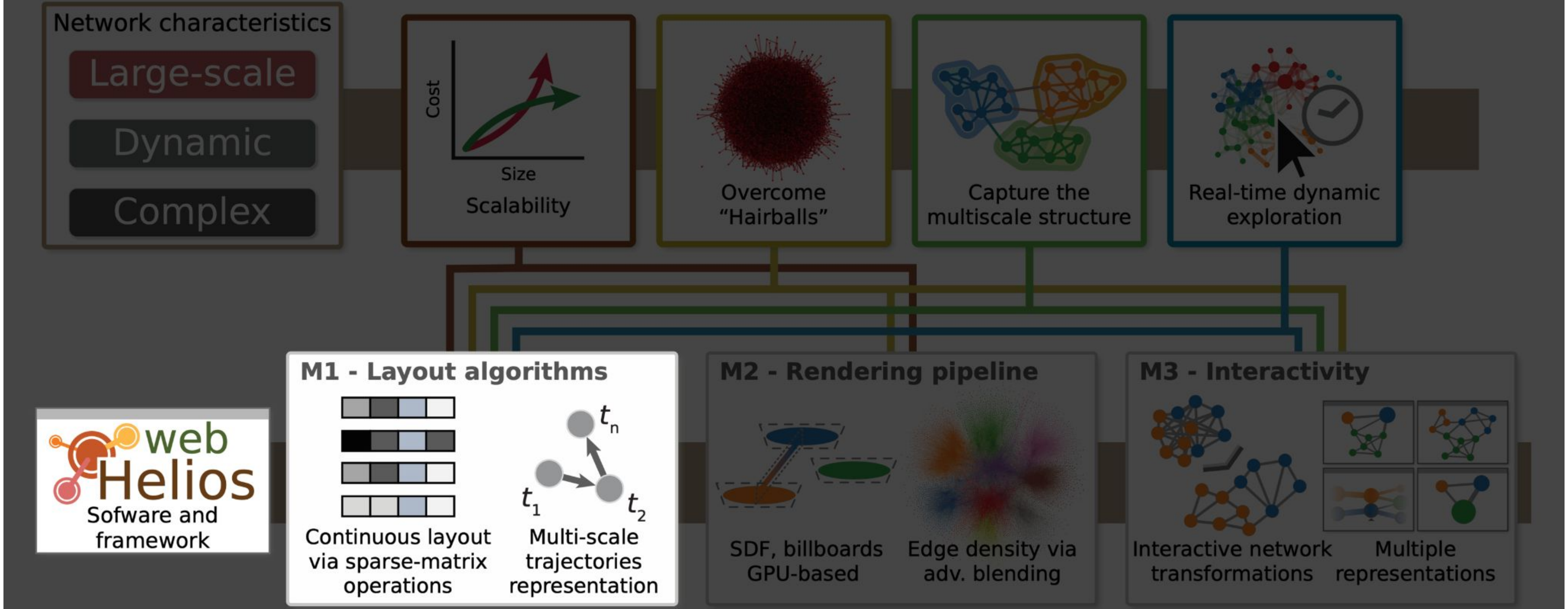
Optimized rendering and layouts

can visualize large networks, high-quality rendering ...

Interactivity*

allows picking, filtering, navigation, multi-representations ...

*in development



Network characteristics

Large-scale

Dynamic

Complex

Scalability

Overcome “Hairballs”

Capture the multiscale structure

Real-time dynamic exploration

web Helios

Sofware and framework

M1 - Layout algorithms

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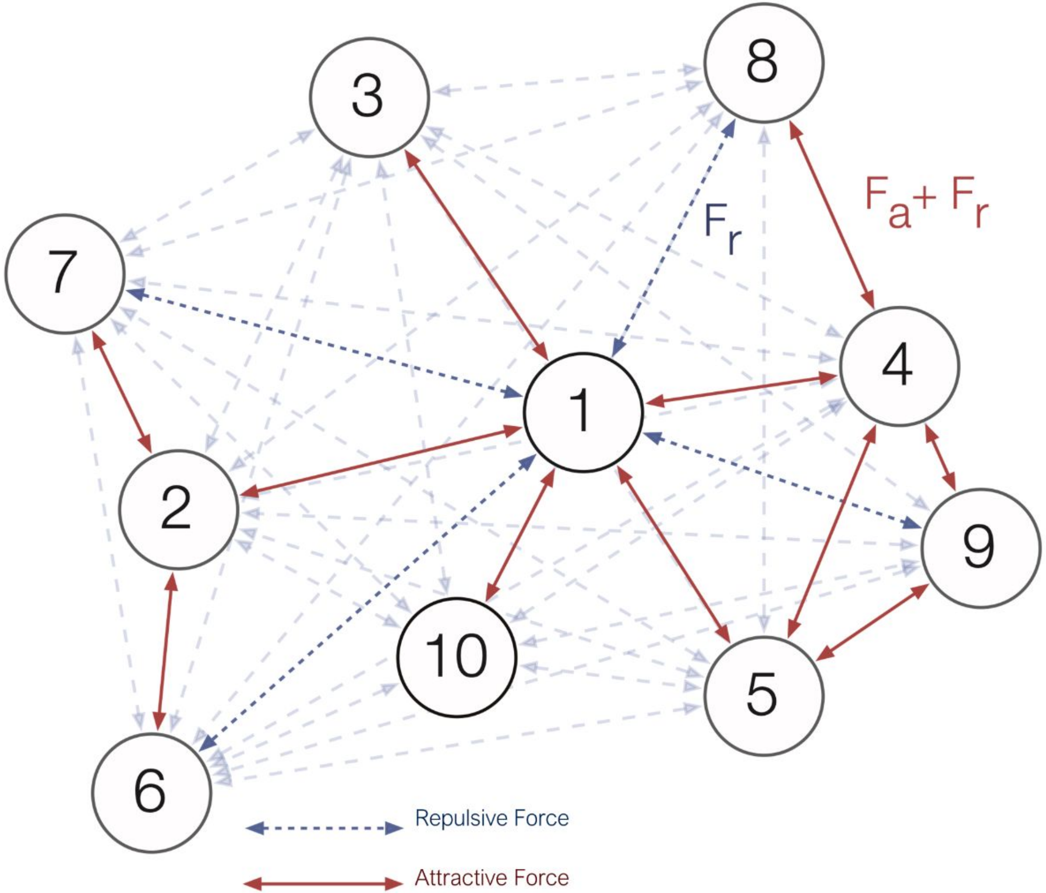
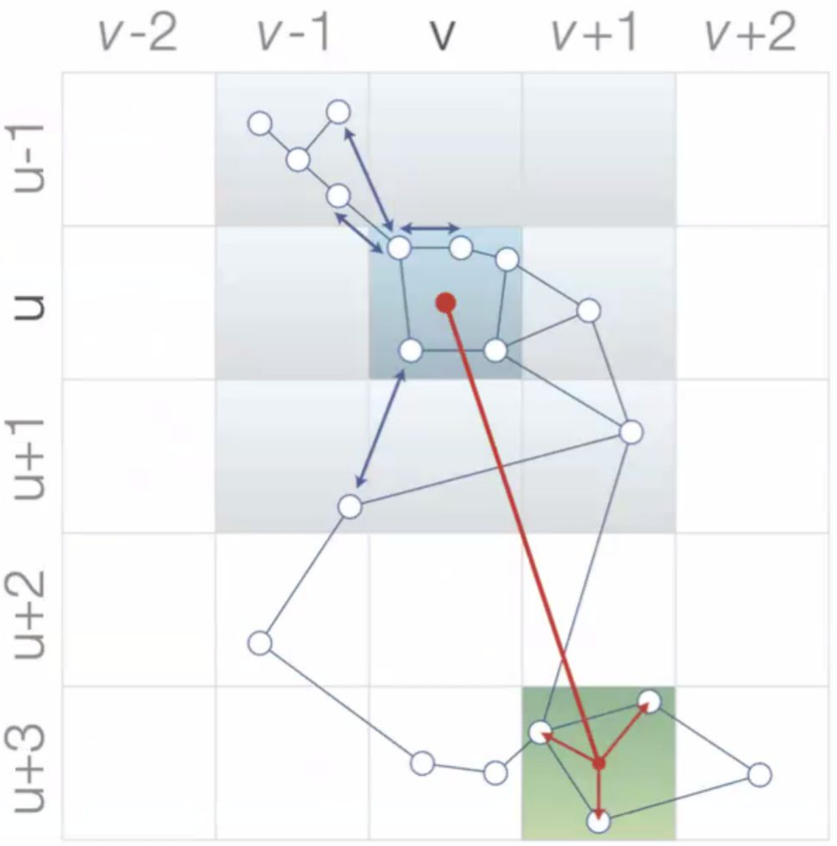
Multiple representations


3
8
Fr
Fa+ Fr
7
1
4
2
9
10
5
6
Repulsive Force
Attractive Force

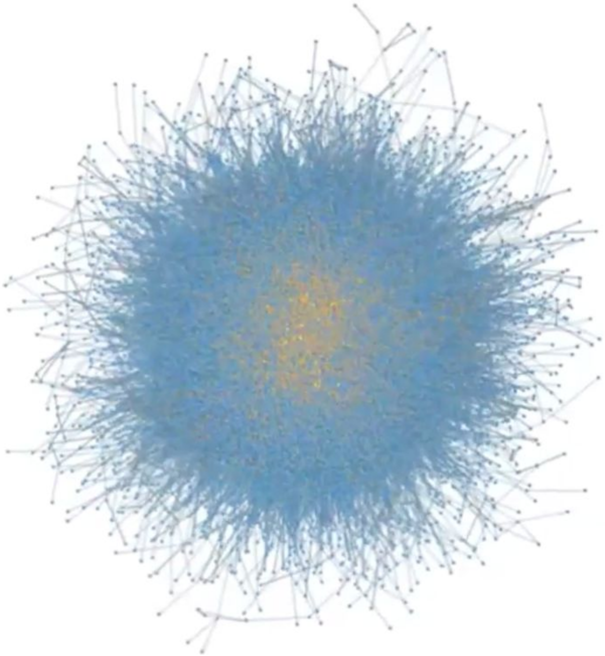
Layout optimizations

- Molecular dynamics simulation is O(N²) .
- We can use multipole expansion (FM3):
- Segment the space
- Real-time continuous layout

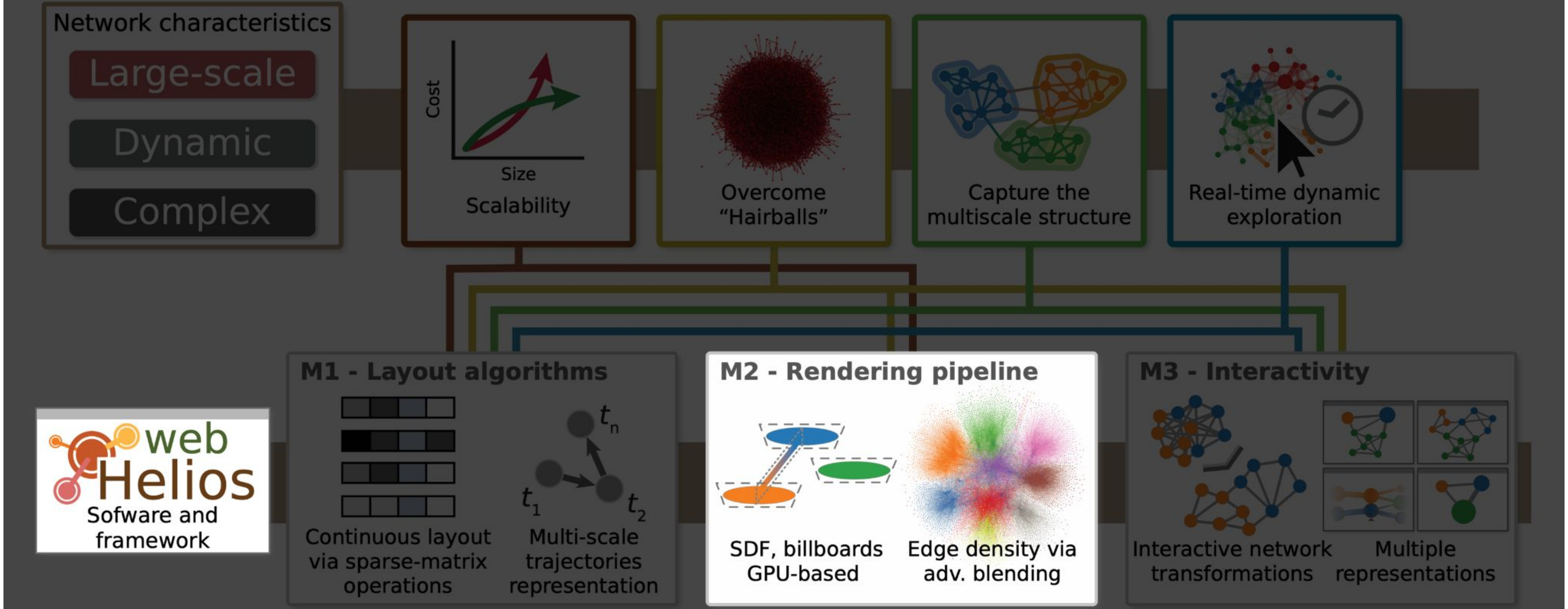


* S. Hachuland M. Jünger. Drawing large graphs with a potential-field-based multilevel algorithm. In International Symposium on Graph Drawing, pp. 285–295. Springer, 2004. doi: 10.1007/978-3-540-31843-9_29

Wiki Medicine and Mathematics

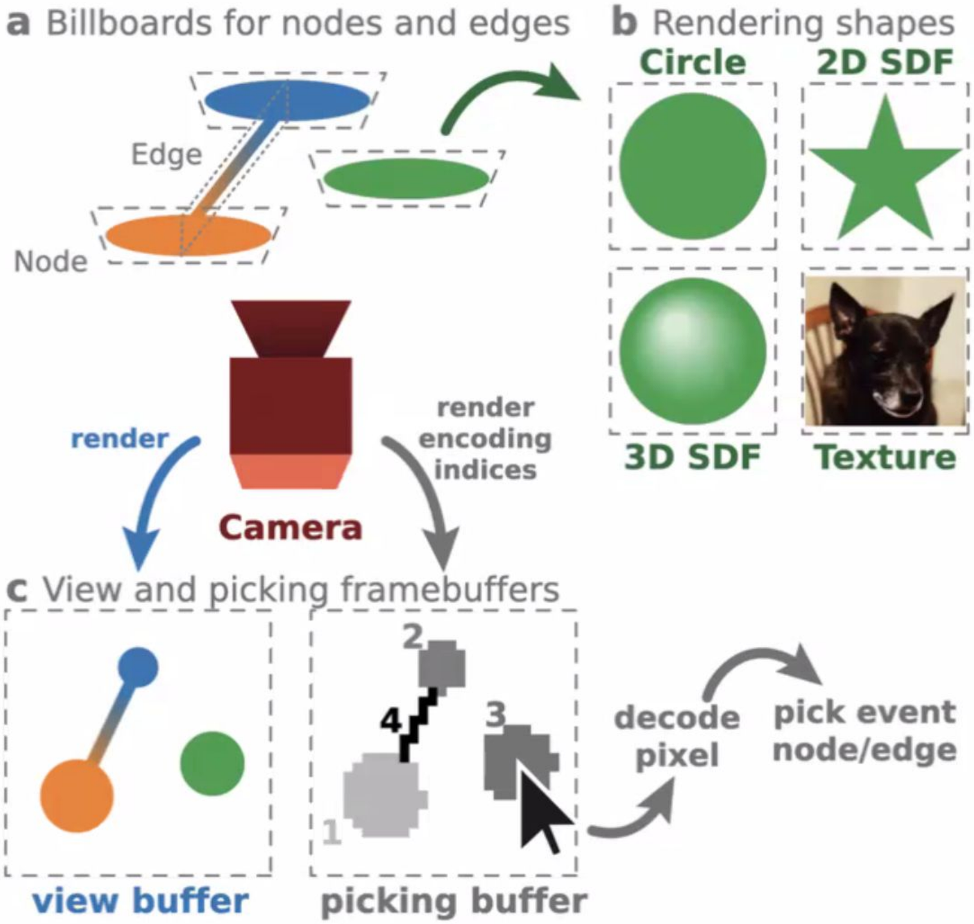


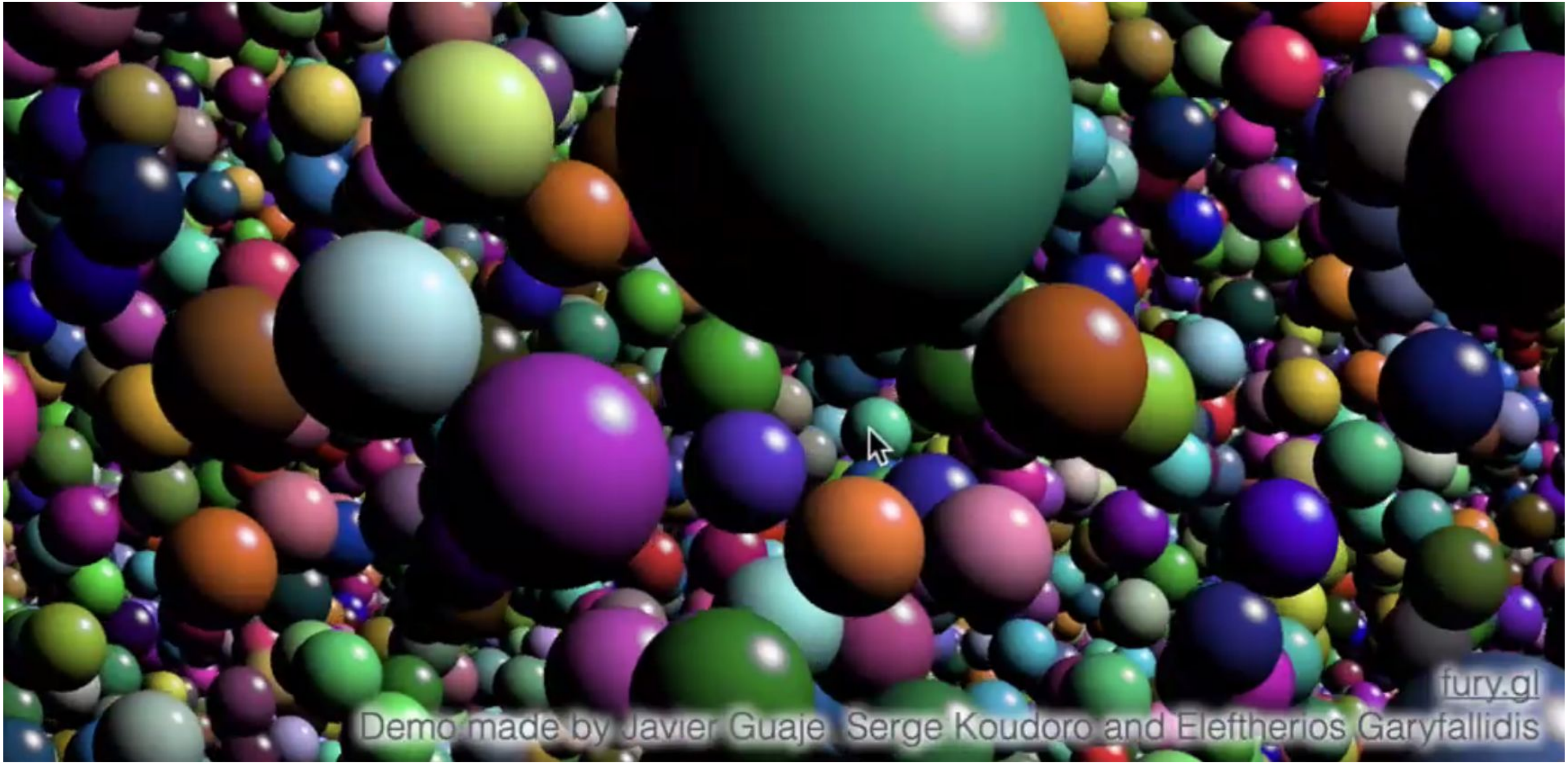
Visualizing Complex Networks (CDT-5)
Silva, F. N. and Costa, L. da F.
http://dx.doi.org/10.13140/RG.2.2.21310.74567/1



Network characteristics
Large-scale
Dynamic
Complex
Cost
Size
Scalability
Overcome "Hairballs"
Capture the multiscale structure
Real-time dynamic exploration
webHelios
Sofware and framework
M1 - Layout algorithms
Continuous layout via sparse-matrix operations
t_n
t_1
t_2
Multi-scale trajectories representation
M2 - Rendering pipeline
SDF, billboards GPU-based
Edge density via adv. blending
M3 - Interactivity
Interactive network transformations
Multiple representations

Rendering in the GPU

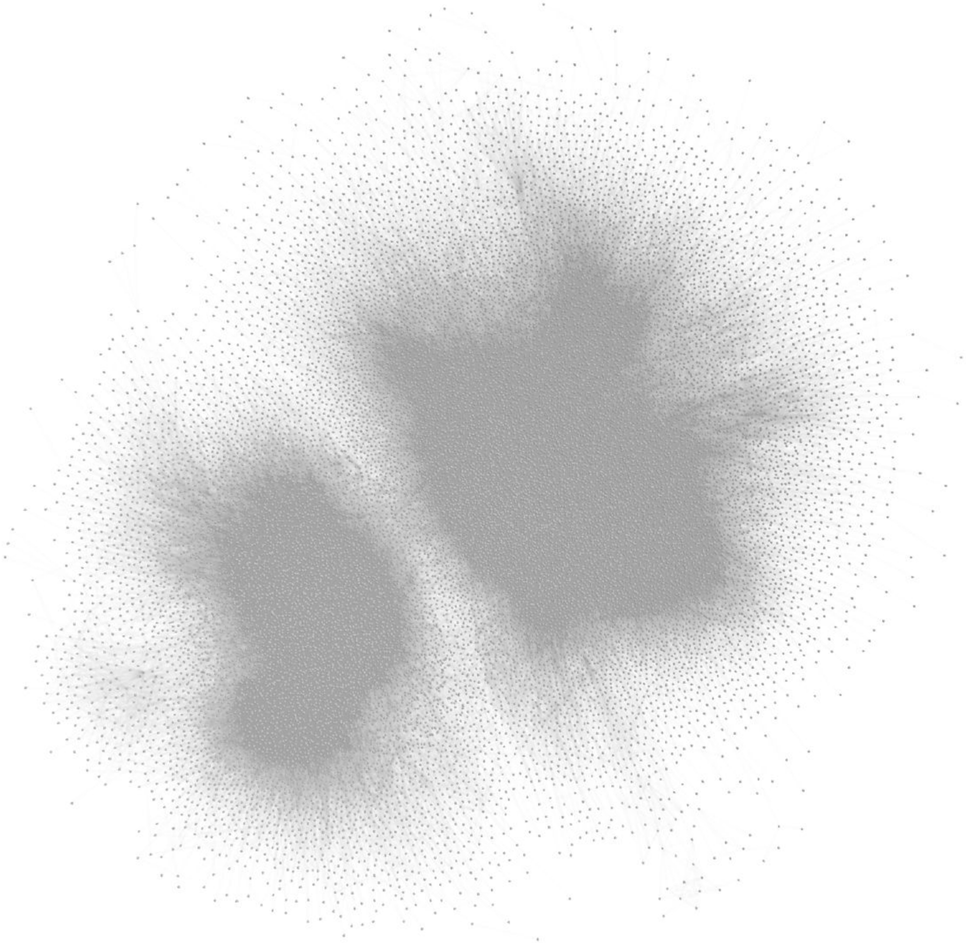




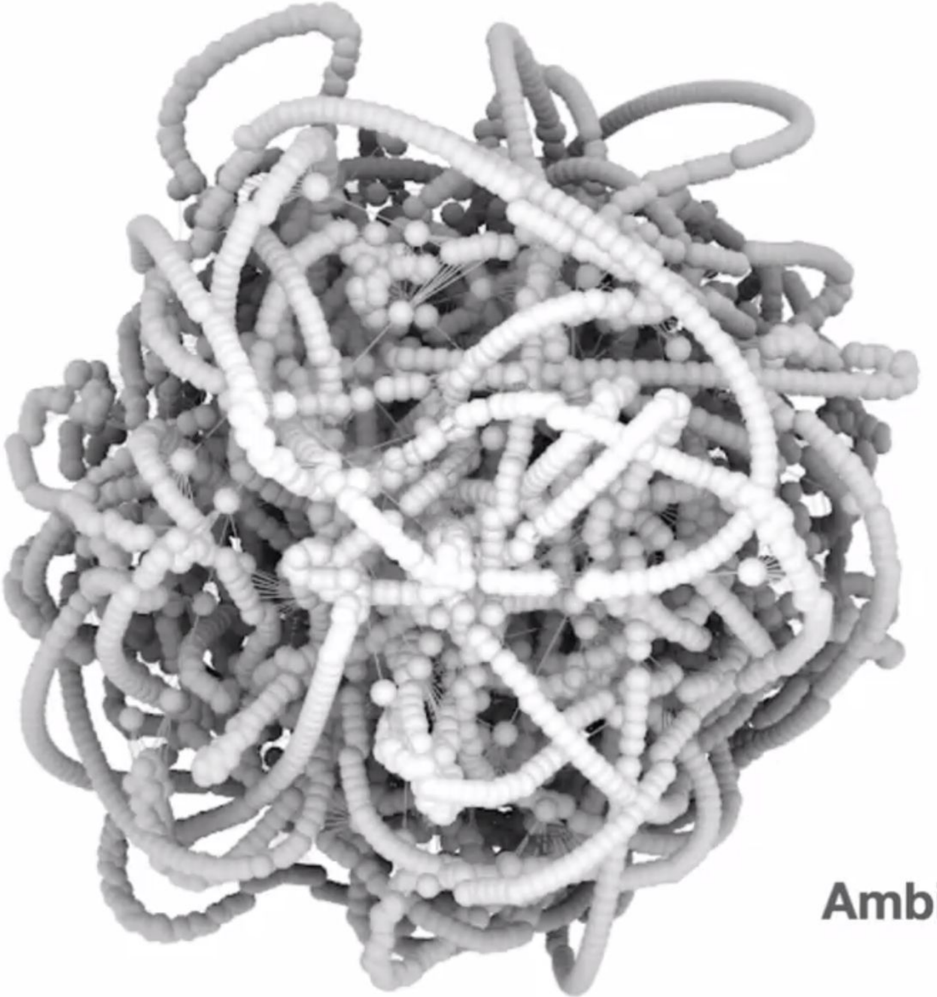
fury.gl

Demo made by Javier Guaje, Serge Koudoro and Eleftherios Garyfallidis

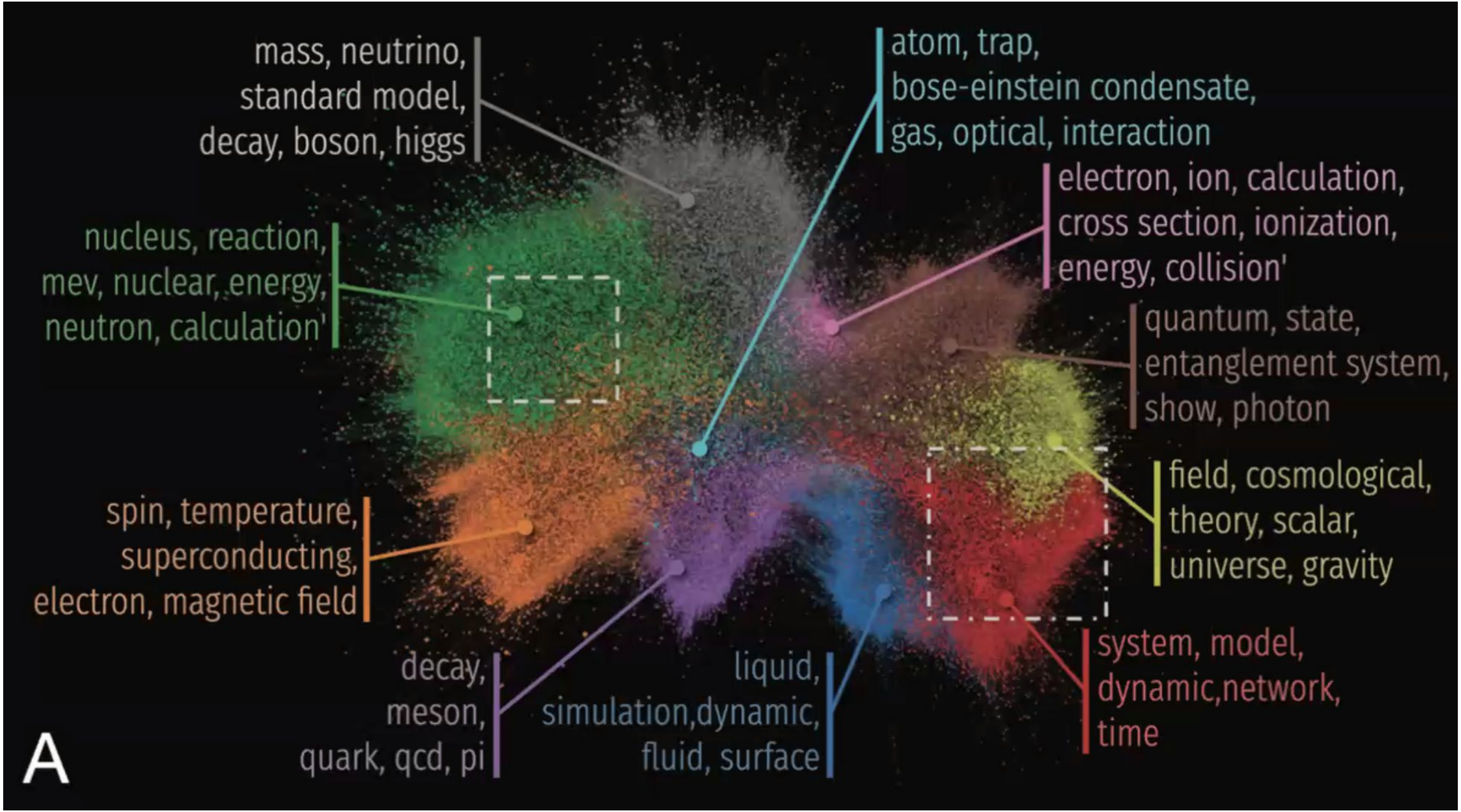
Rendering

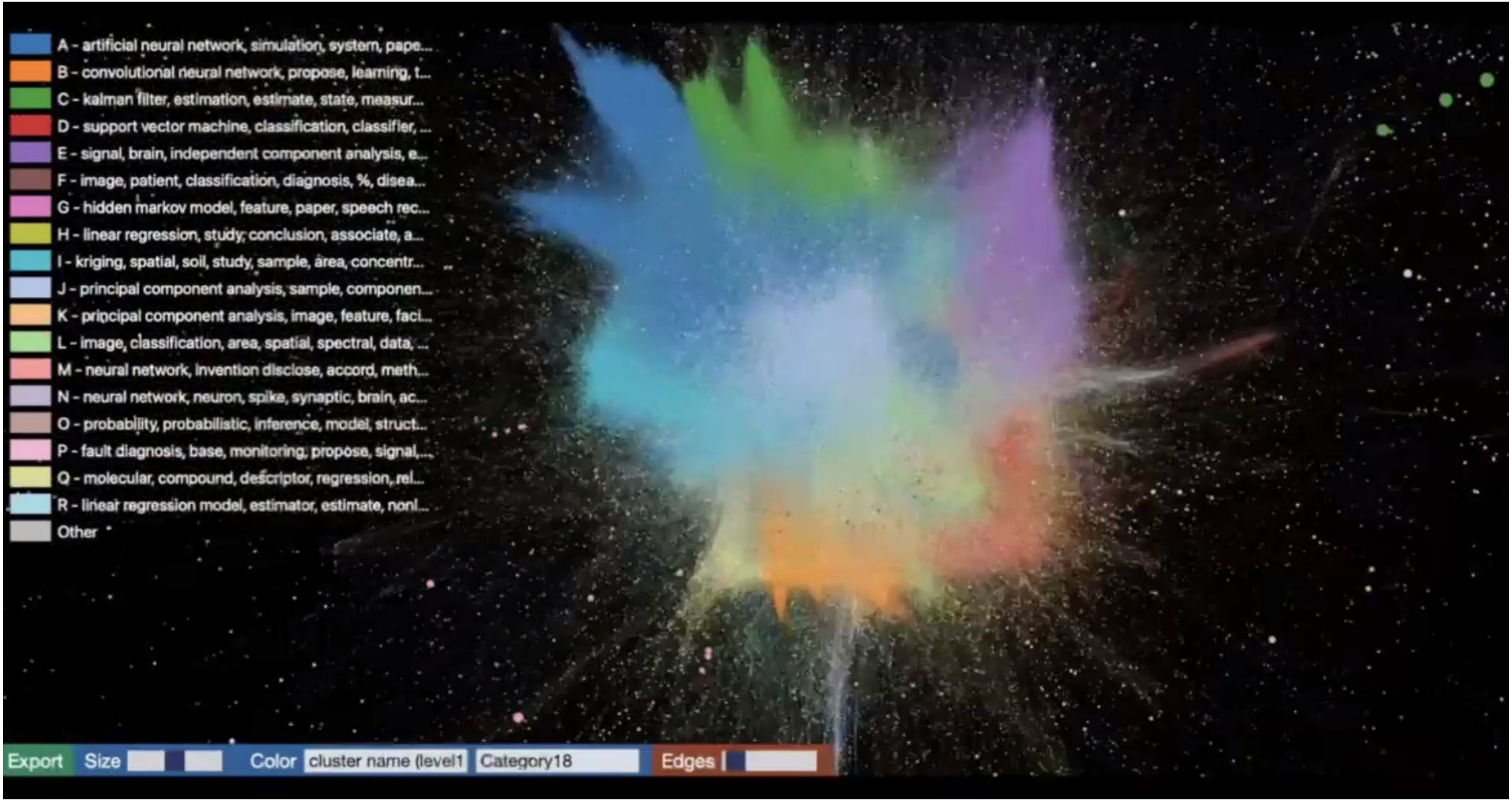


Edge density

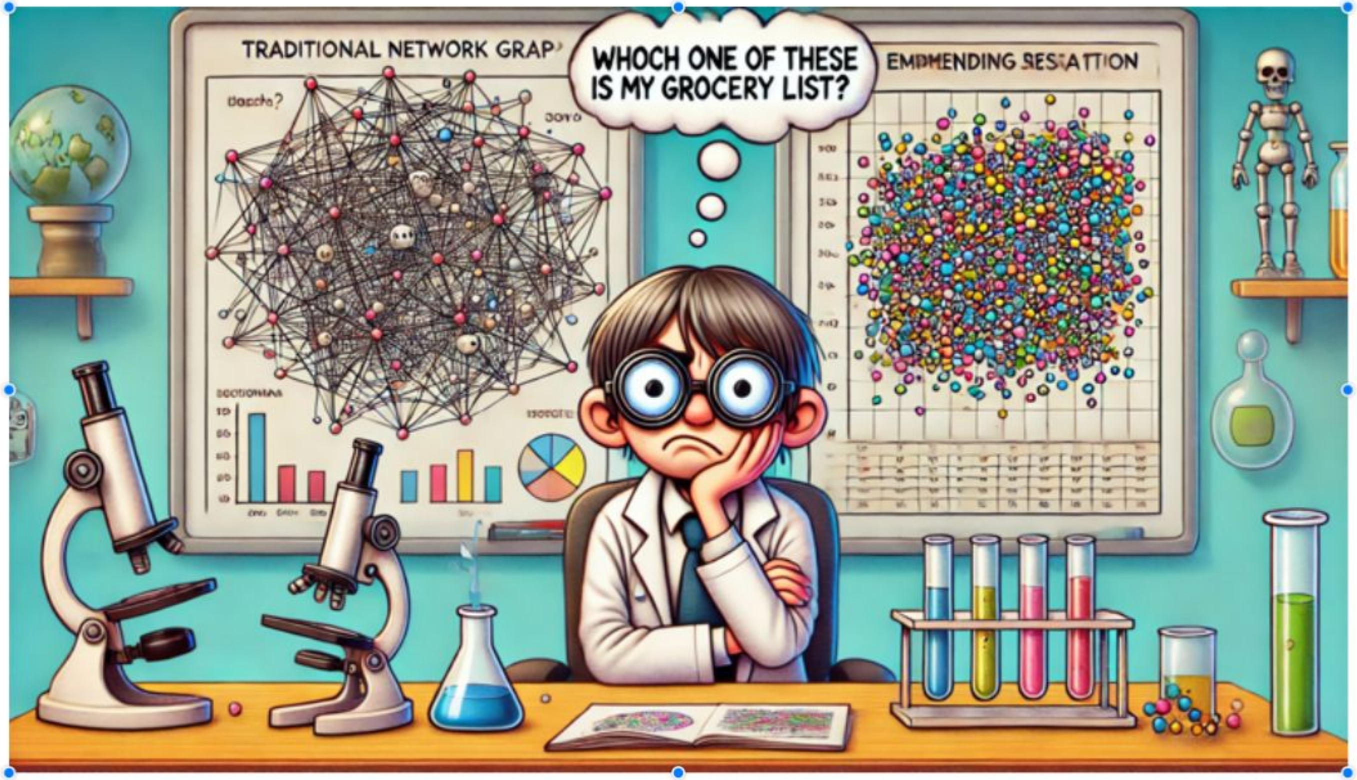


Ambience Occlusion


mass, neutrino, standard model, decay, boson, higgs
atom, trap, bose-einstein condensate, gas, optical, interaction
electron, ion, calculation, cross section, ionization, energy, collision'
nucleus, reaction, mev, nuclear, energy, neutron, calculation'
quantum, state, entanglement system, show, photon
field, cosmological, theory, scalar, universe, gravity
spin, temperature, superconducting, electron, magnetic field
system, model, dynamic,network, time
decay, meson, quark, qcd, pi
liquid, simulation,dynamic, fluid, surface
A

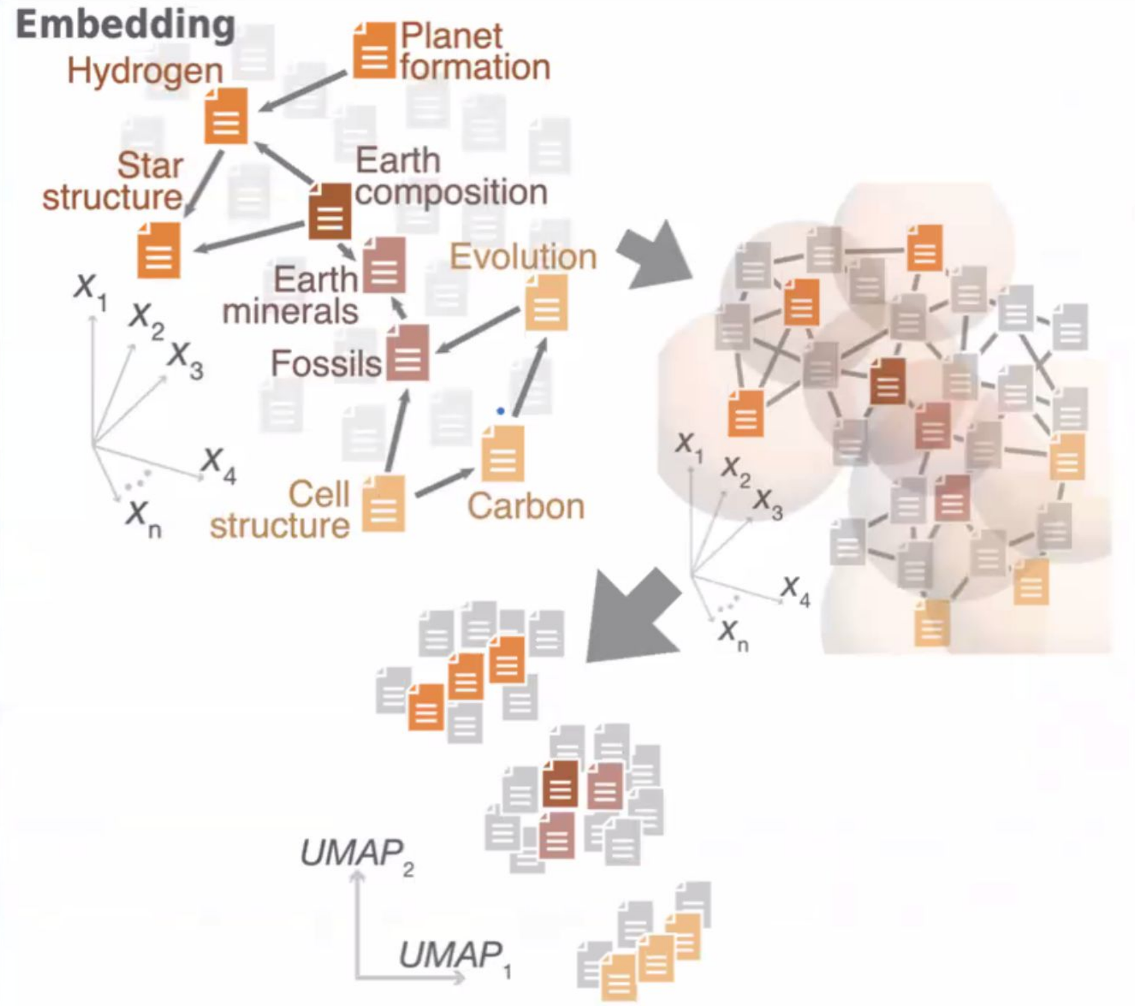

A - artificial neural network, simulation, system, pape...
B - convolutional neural network, propose, learning, t...
C - kalman filter, estimation, estimate, state, measur...
D - support vector machine, classification, classifier, ...
E - signal, brain, independent component analysis, e...
F - image, patient, classification, diagnosis, %, disea...
G - hidden markov model, feature, paper, speech rec...
H - linear regression, study, conclusion, associate, a...
I - kriging, spatial, soil, study, sample, area, concentr...
J - principal component analysis, sample, componen...
K - principal component analysis, image, feature, faci...
L - image, classification, area, spatial, spectral, data, ...
M - neural network, invention disclose, accord, meth...
N - neural network, neuron, spike, synaptic, brain, ac...
O - probability, probabilistic, inference, model, struct...
P - fault diagnosis, base, monitoring, propose, signal,...
Q - molecular, compound, descriptor, regression, rel...
R - linear regression model, estimator, estimate, nonl...
Other
Export
Size
Edges

Color cluster name (level1 Category18



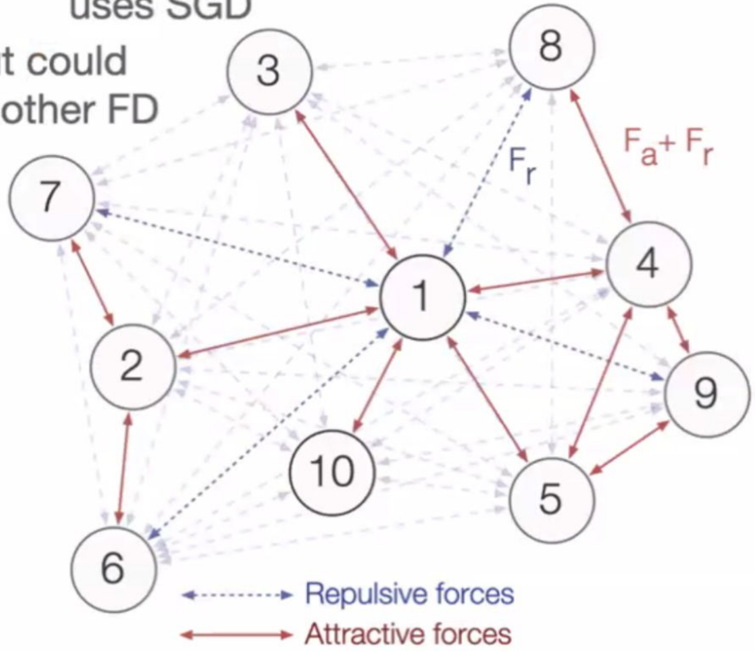
Ok, but what about embeddings?

UMAP


Embedding
Hydrogen
Planet formation
Star structure
Earth composition
Earth minerals
Evolution
Fossils
Cell structure
Carbon
X_1
X_2
X_3
X_4
X_n
X_1
X_2
X_3
X_4
X_n
$UMAP_2$
$UMAP_1$

UMAP uses SGD

but could use other FD



For large embeddings: >10M points

Negative samples rate : Number of repulsive interactions to update for each positive.

increased to 10 (default = 5)

Epochs: Number of iterations

increased to 200000 (default = 200) !!!

Number of neighbors: Number of neighbors in the NN graph

increased to 30 (default = 15) !!!

umap-learn.readthedocs.io

attractive repulsive

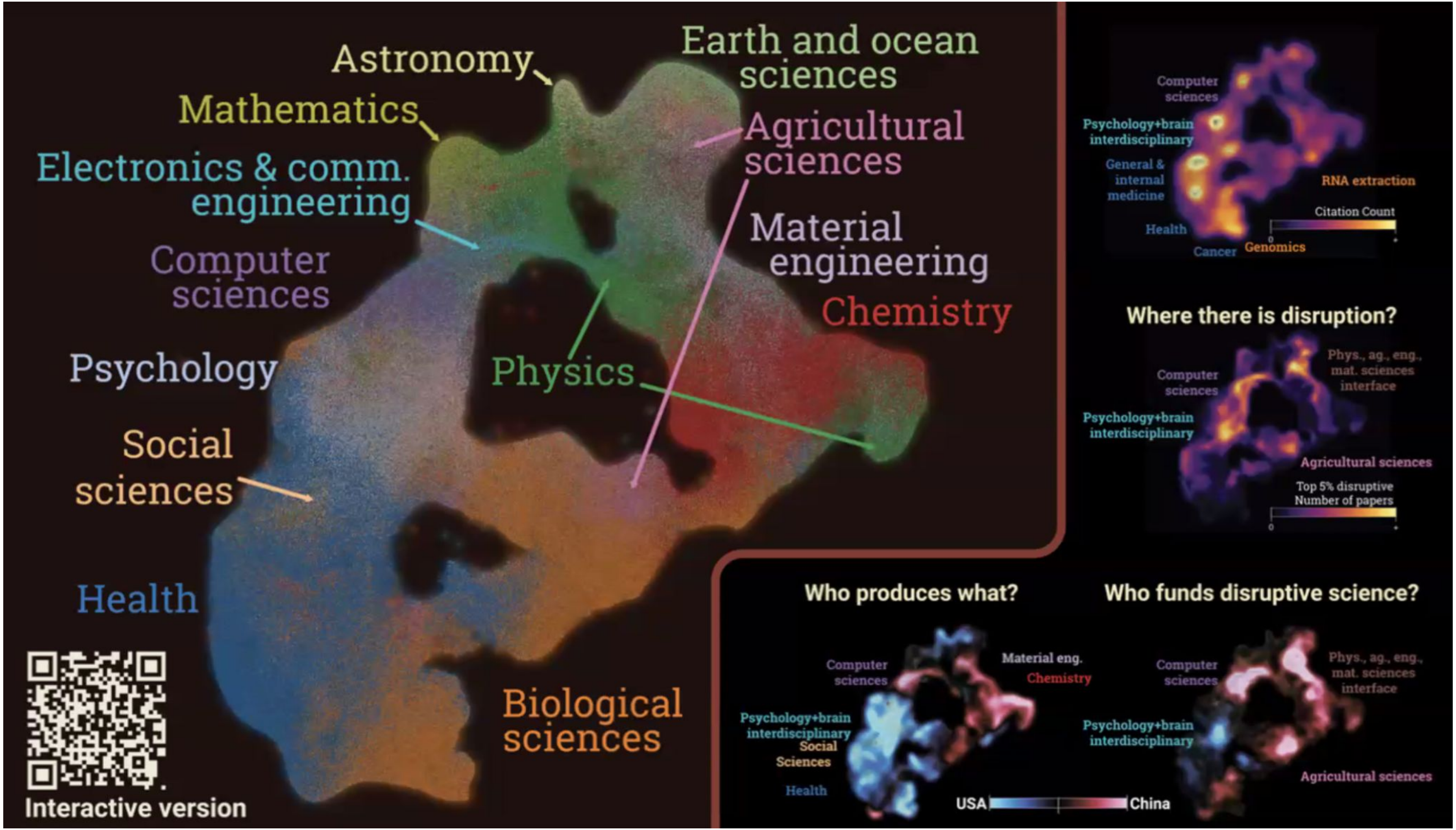
$$\frac{\partial \mathcal{L}_{\mathrm{UMAP}}(\gamma)}{\partial \mathbf{y}_i} \sim \sum_j v_{ij} w_{ij} (\mathbf{y}_i - \mathbf{y}_j) - \gamma \sum_j \frac{1}{d_{ij}^2 + \epsilon} w_{ij} (\mathbf{y}_i - \mathbf{y}_j).$$

GPU version (much faster!)

beware: it has bugs that lead to bad projections

https://docs.rapids.ai/api/cuml/stable/api/#umap

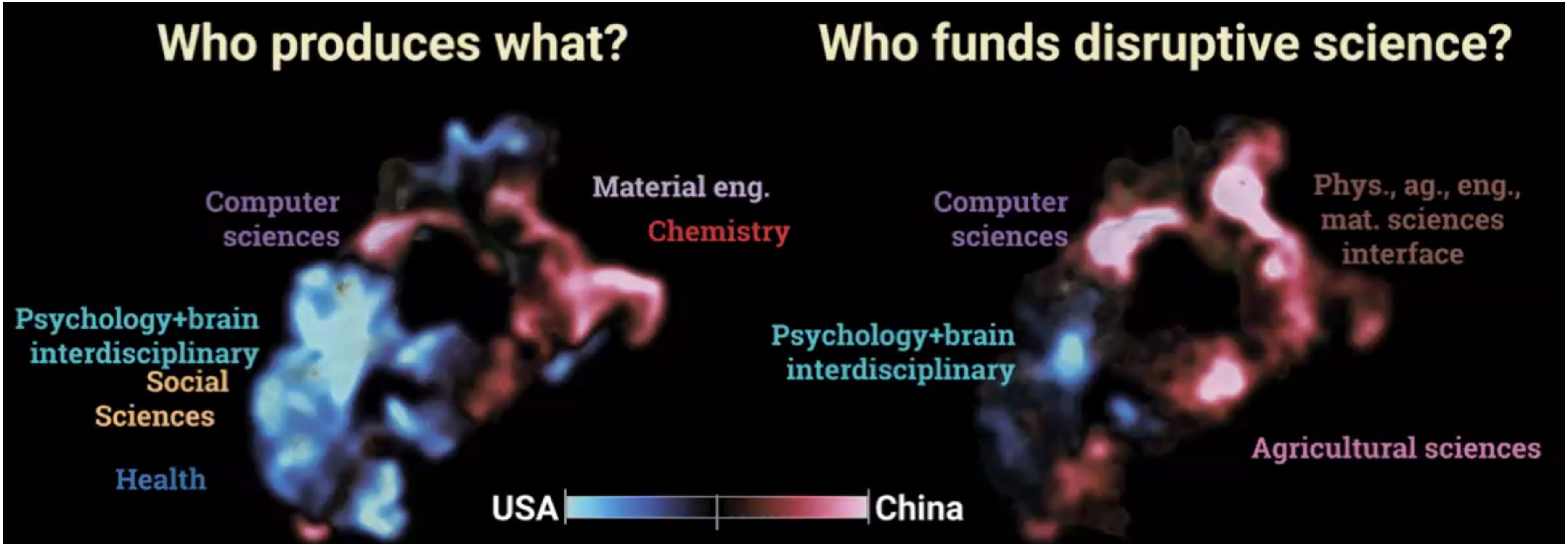
Böhm, J. N., Berens, P., & Kobak, D. (2022). Attraction-repulsion spectrum in neighbor embeddings. The Journal of Machine Learning Research, 23(1), 4118-4149.

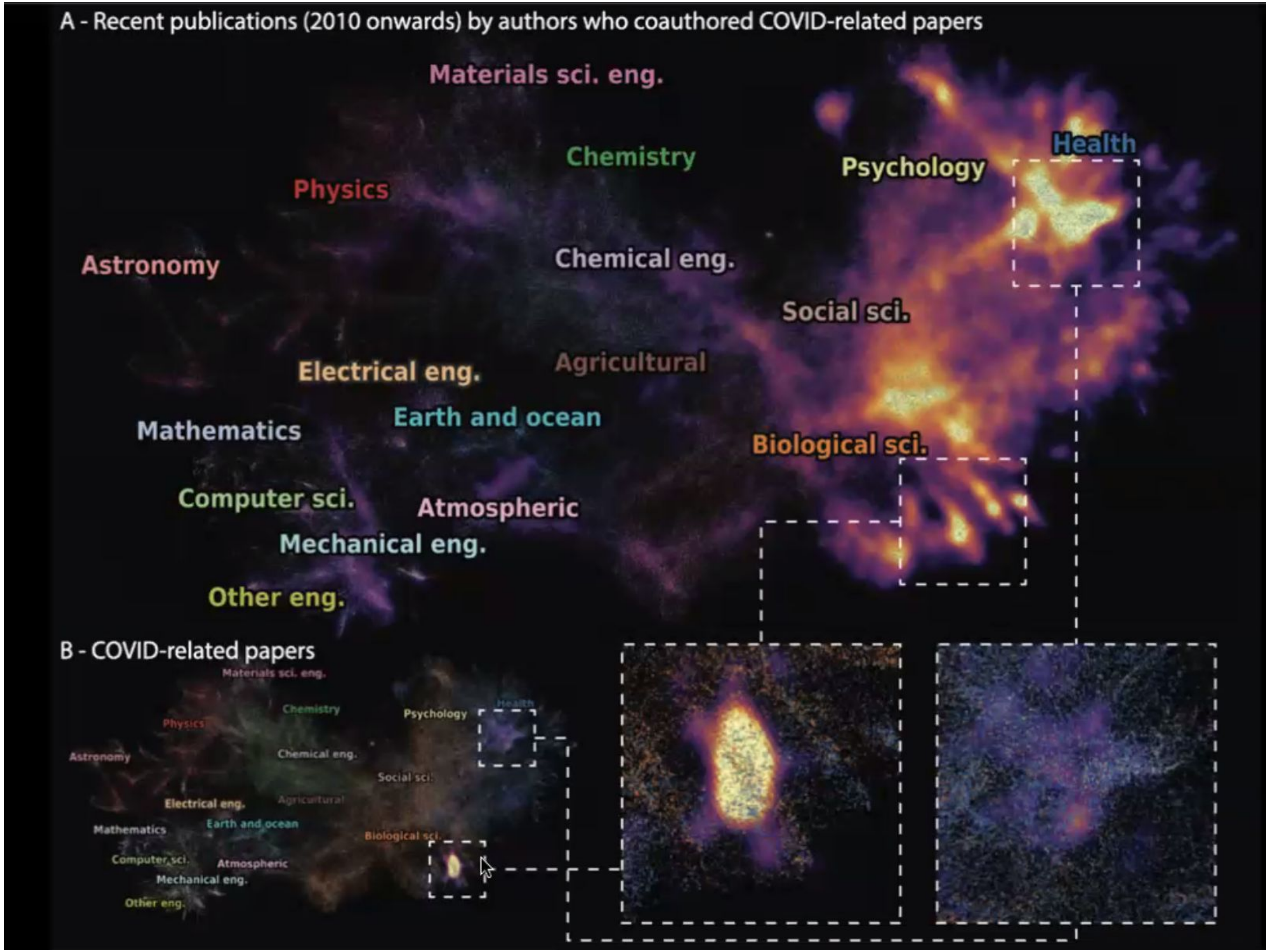


Where there is disruption?

Who produces what?

Who funds disruptive science?

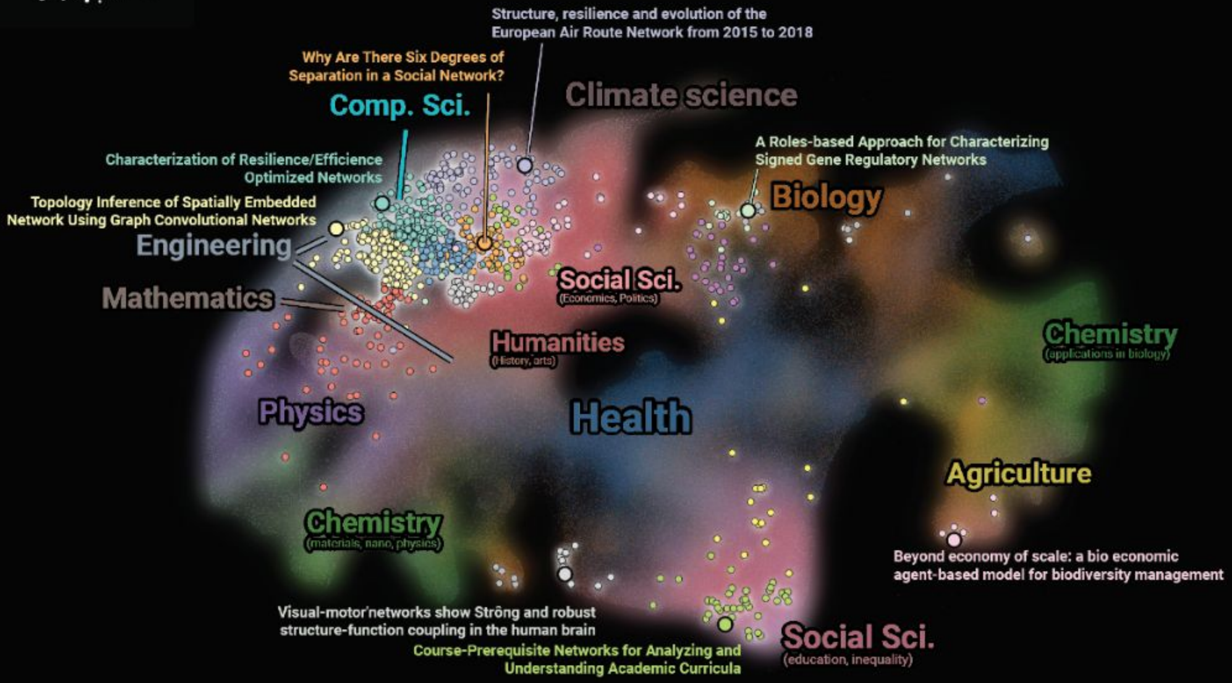

Who produces what?
Who funds disruptive science?
Computer sciences
Material eng.
Chemistry
Psychology+brain interdisciplinary
Social Sciences
Health
USA
China
Computer sciences
Phys., ag., eng., mat. sciences interface
Psychology+brain interdisciplinary
Agricultural sciences



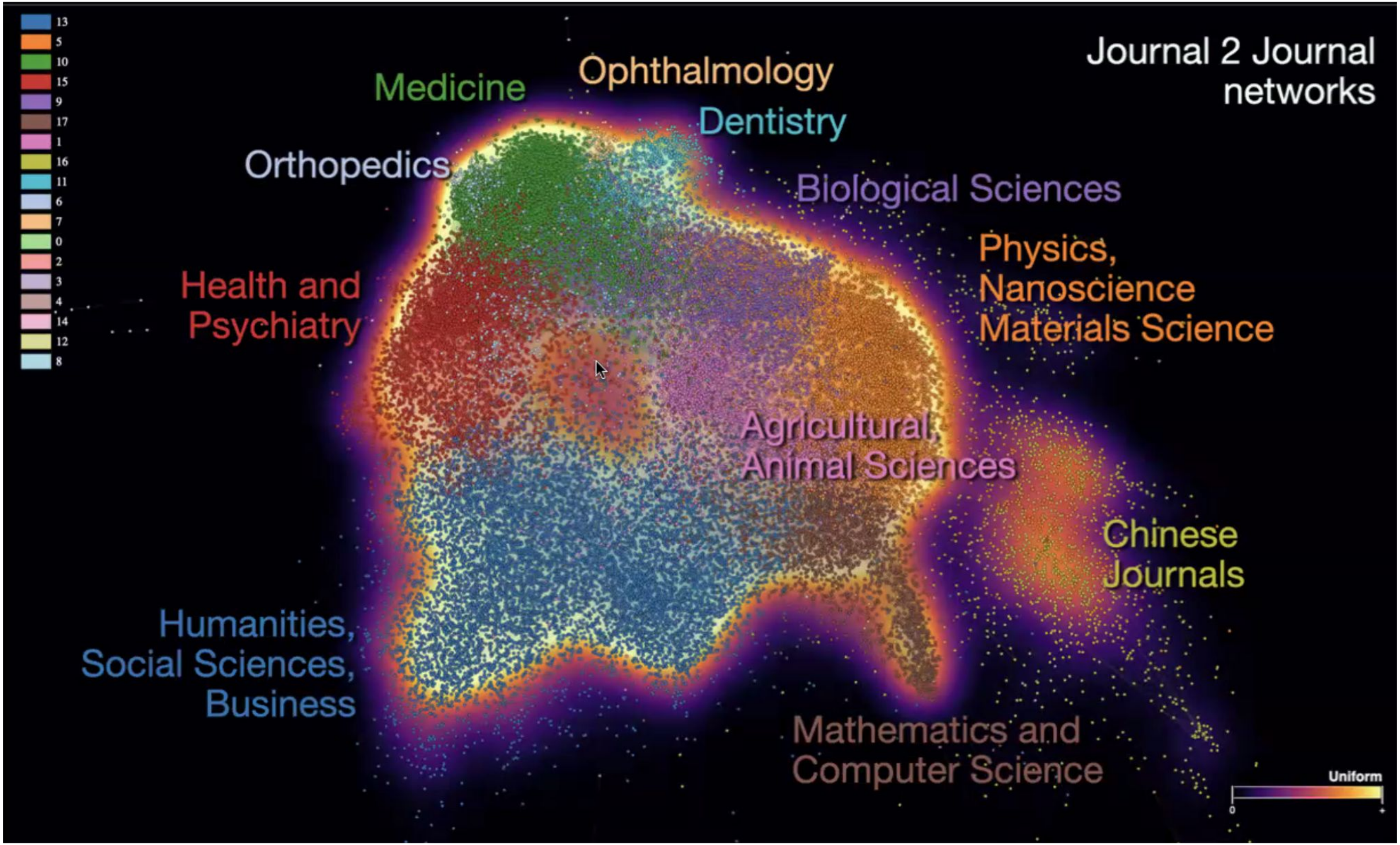
A - Recent publications (2010 onwards) by authors who coauthored COVID-related papers

B - COVID-related papers

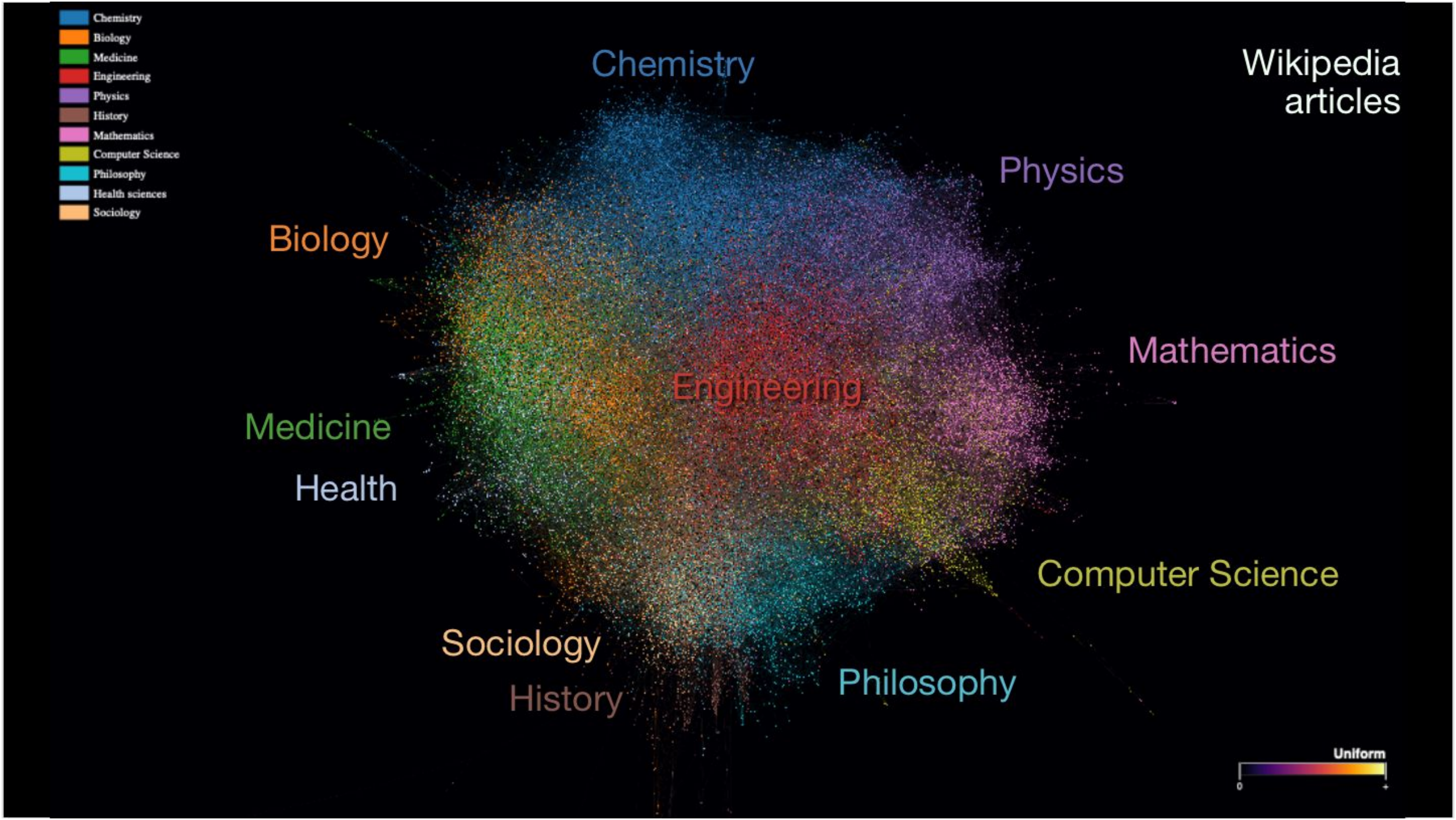
Where in the world of knowledge is NetSci?


Structure, resilience and evolution of the European Air Route Network from 2015 to 2018
Why Are There Six Degrees of Separation in a Social Network?
Comp. Sci.
Climate science
A Roles-based Approach for Characterizing Signed Gene Regulatory Networks
Characterization of Resilience/Efficience Optimized Networks
Biology
Topology Inference of Spatially Embedded Network Using Graph Convolutional Networks
Engineering
Social Sci.
(Economics, Politics)
Mathematics
Humanities
(History, arts)
Chemistry
(applications in biology)
Physics
Health
Agriculture
Chemistry
(materials, nano, physics)
Beyond economy of scale: a bio economic agent-based model for biodiversity management
Visual-motor'networks show Strông and robust structure-function coupling in the human brain
Course-Prerequisite Networks for Analyzing and Understanding Academic Curricula
Social Sci.
(education, inequality)

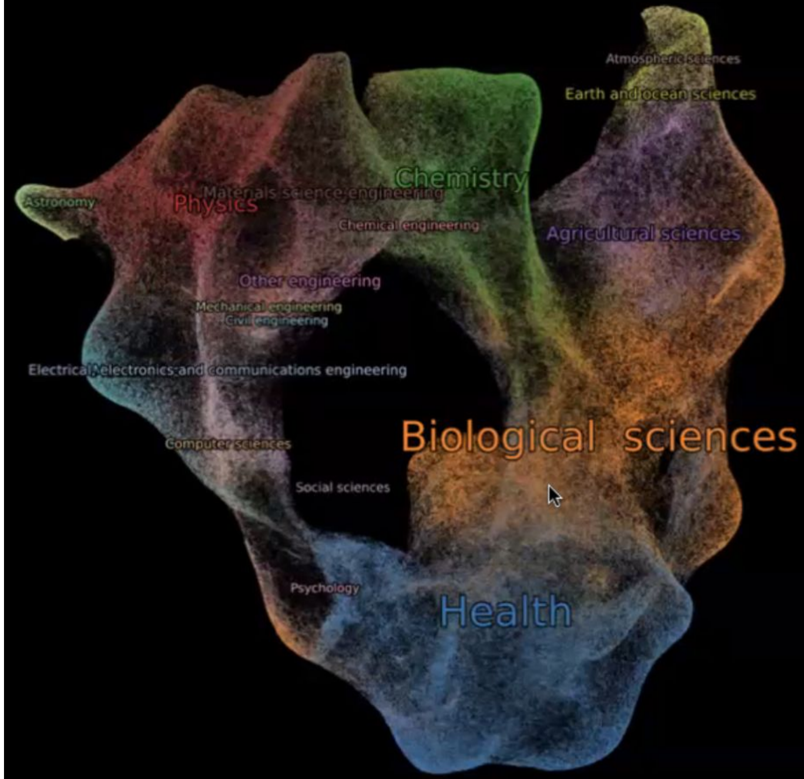
A science map constructed from the titles and abstracts of publications in the Web of Science. On top of that, we project NetSci contributions from 2023 and 2024.



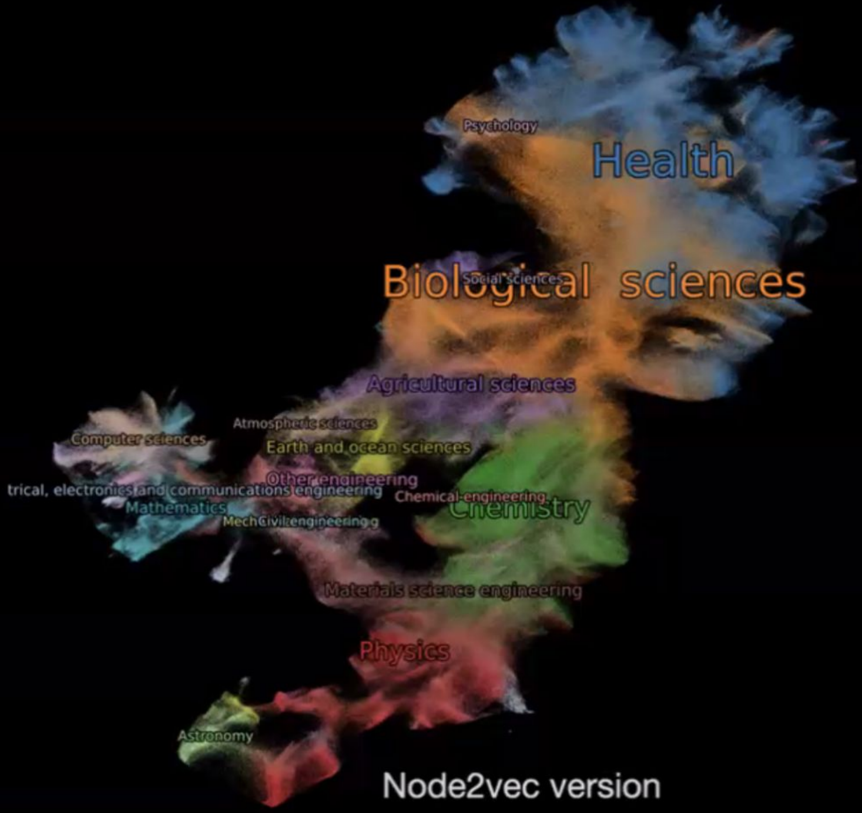
Journal 2 Journal networks



Wikipedia articles

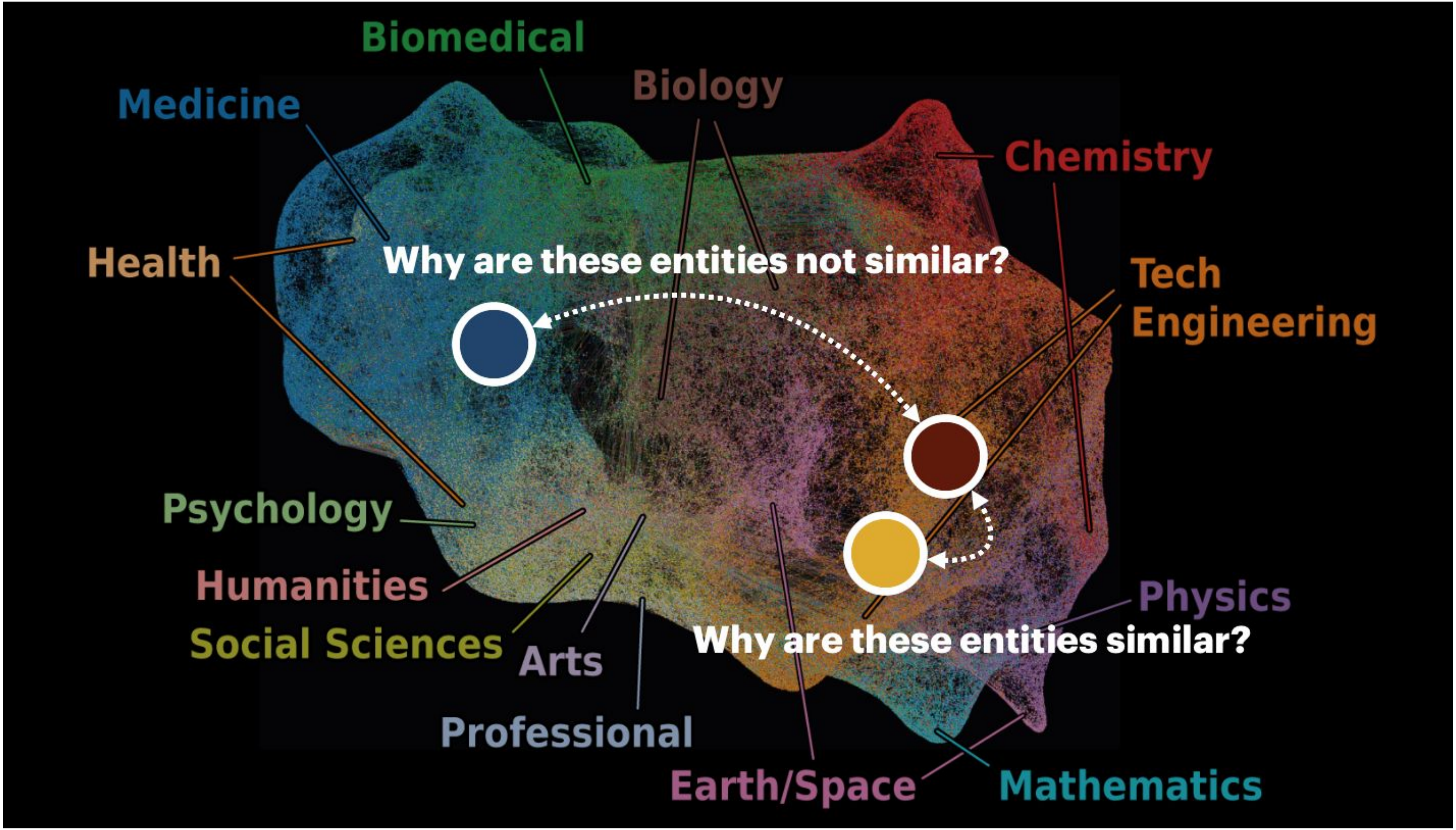


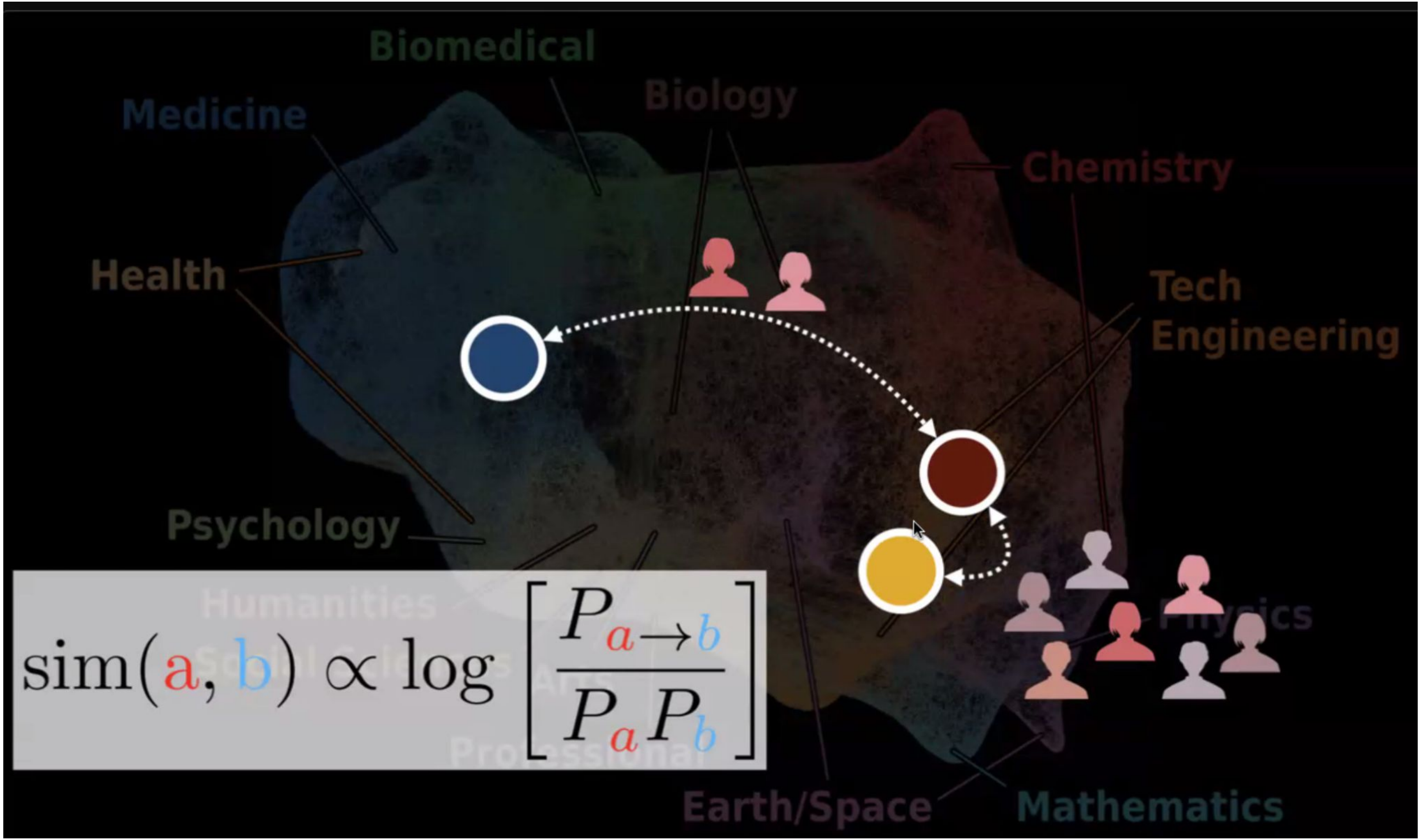
SPECTER (titles + fine tuning via citation network)
embedding of the whole science
Microsoft Academic Graph (more than 200M works)



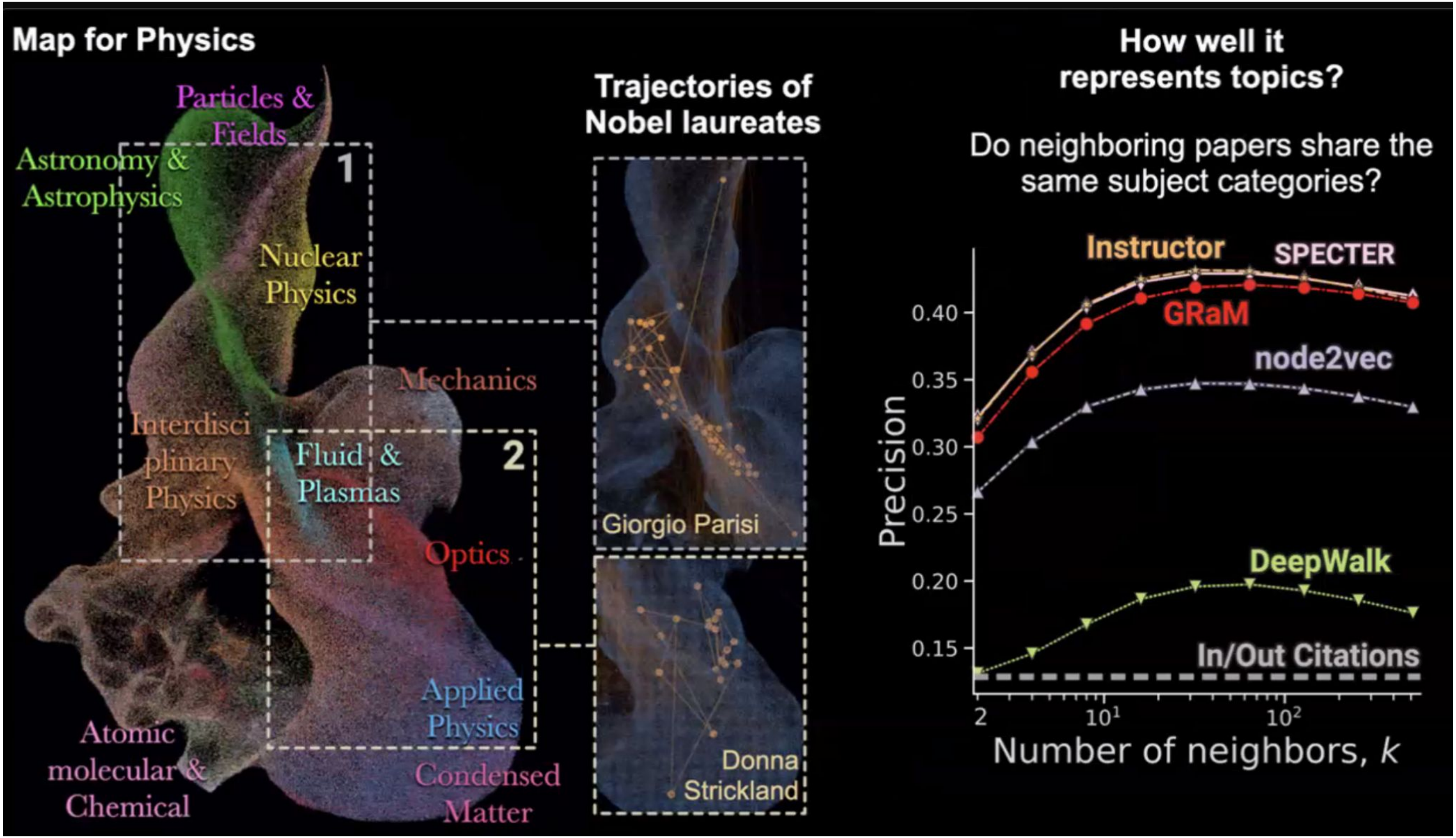
Node2vec version

Ongoing project with YY Ahn, Sadamori Kojaku and others


Biomedical
Medicine
Biology
Chemistry
Health
Why are these entities not similar?
Tech
Engineering
Psychology
Humanities
Social Sciences
Arts
Professional
Physics
Why are these entities similar?
Earth/Space
Mathematics



$$\mathrm{sim}(a, b) \propto \log\left[\frac{P_{a\to b}}{P_a P_b}\right]$$



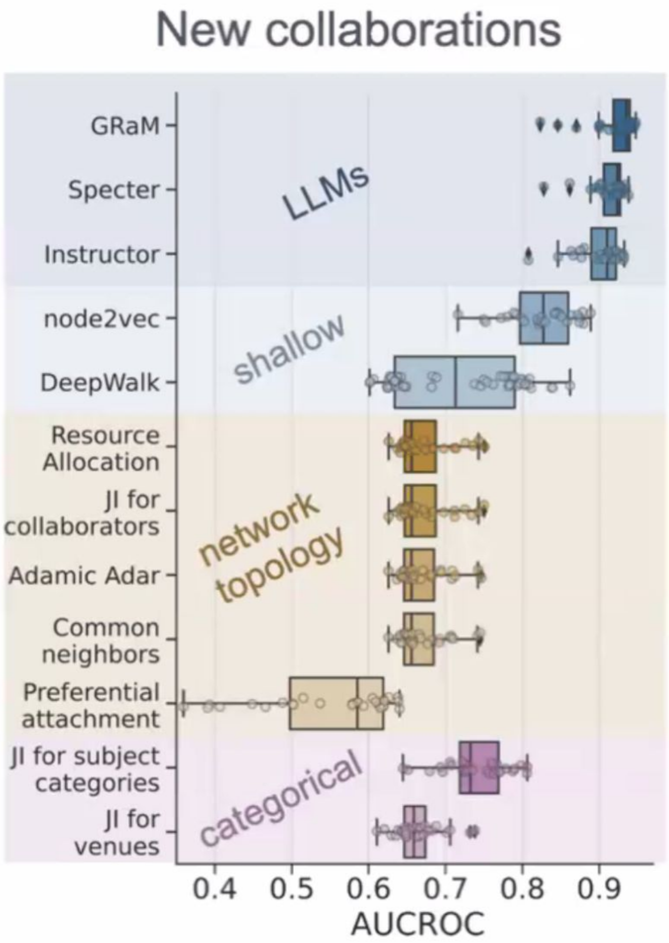
Map for Physics

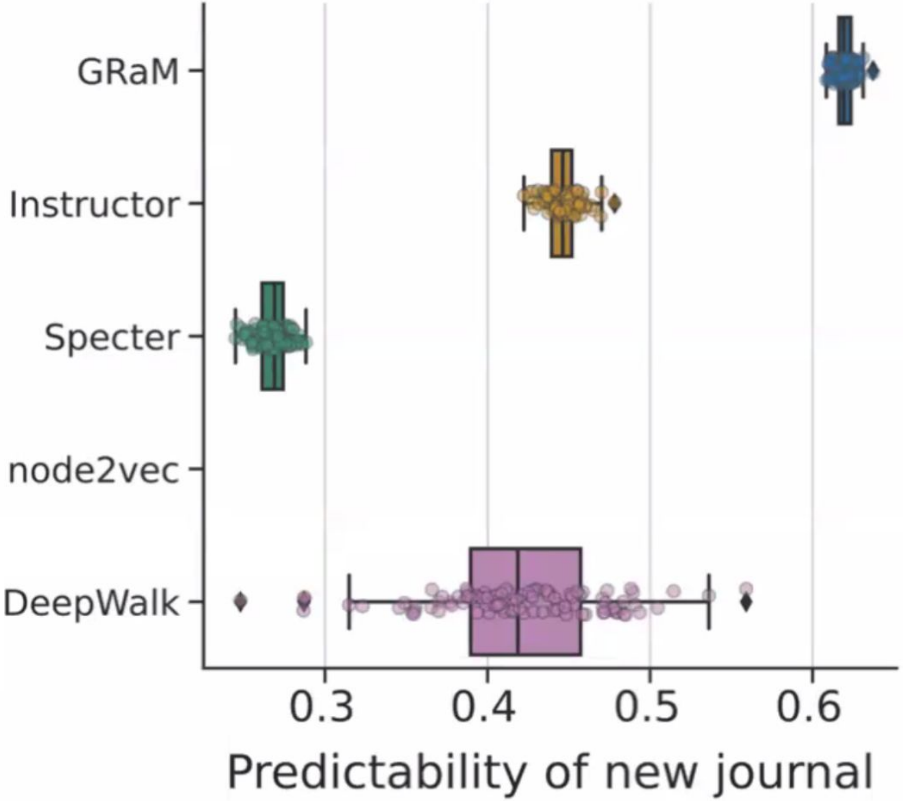
Trajectories of Nobel laureates

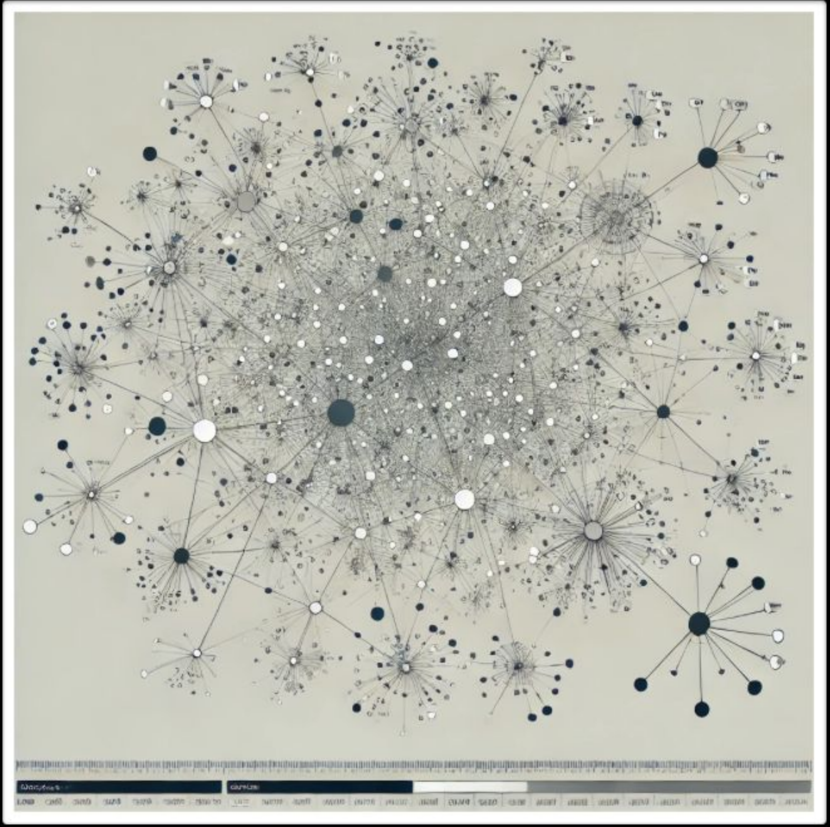
How well it represents topics?

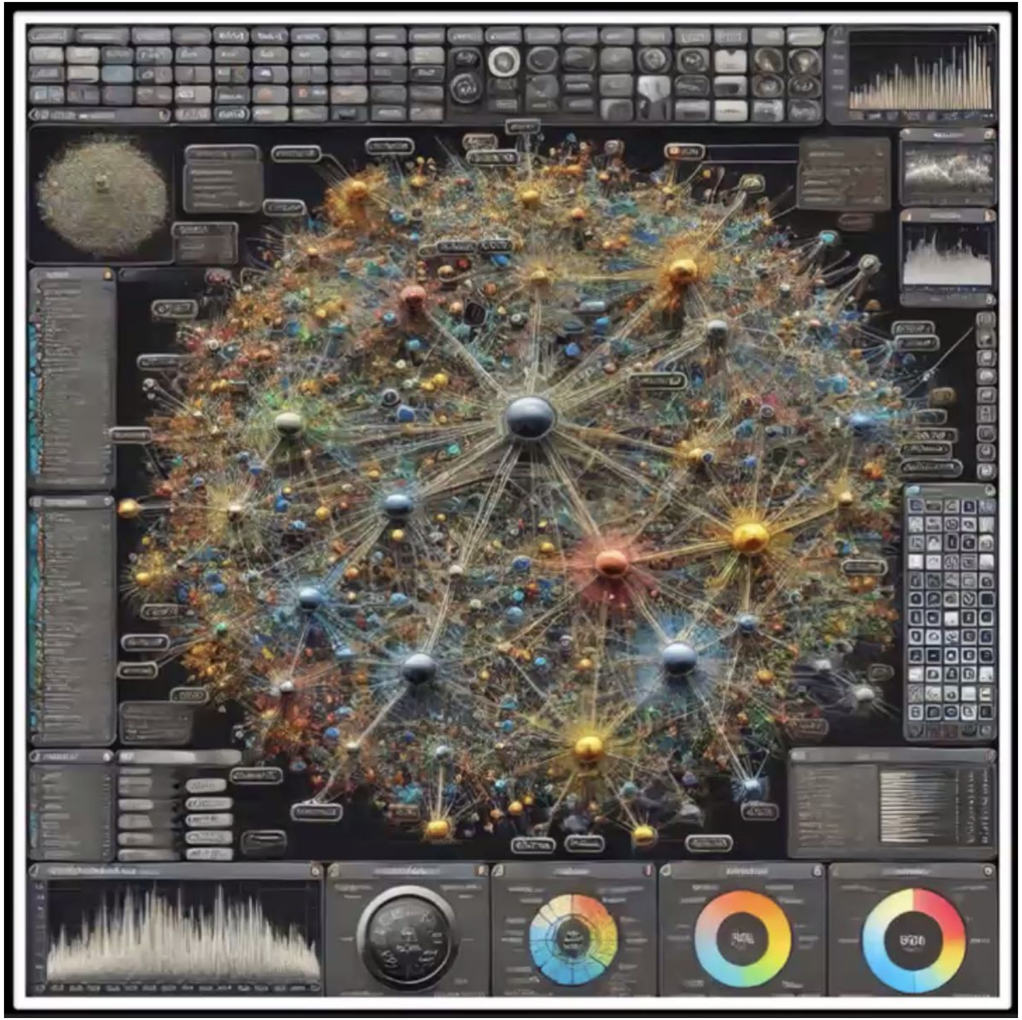
Do neighboring papers share the same subject categories?

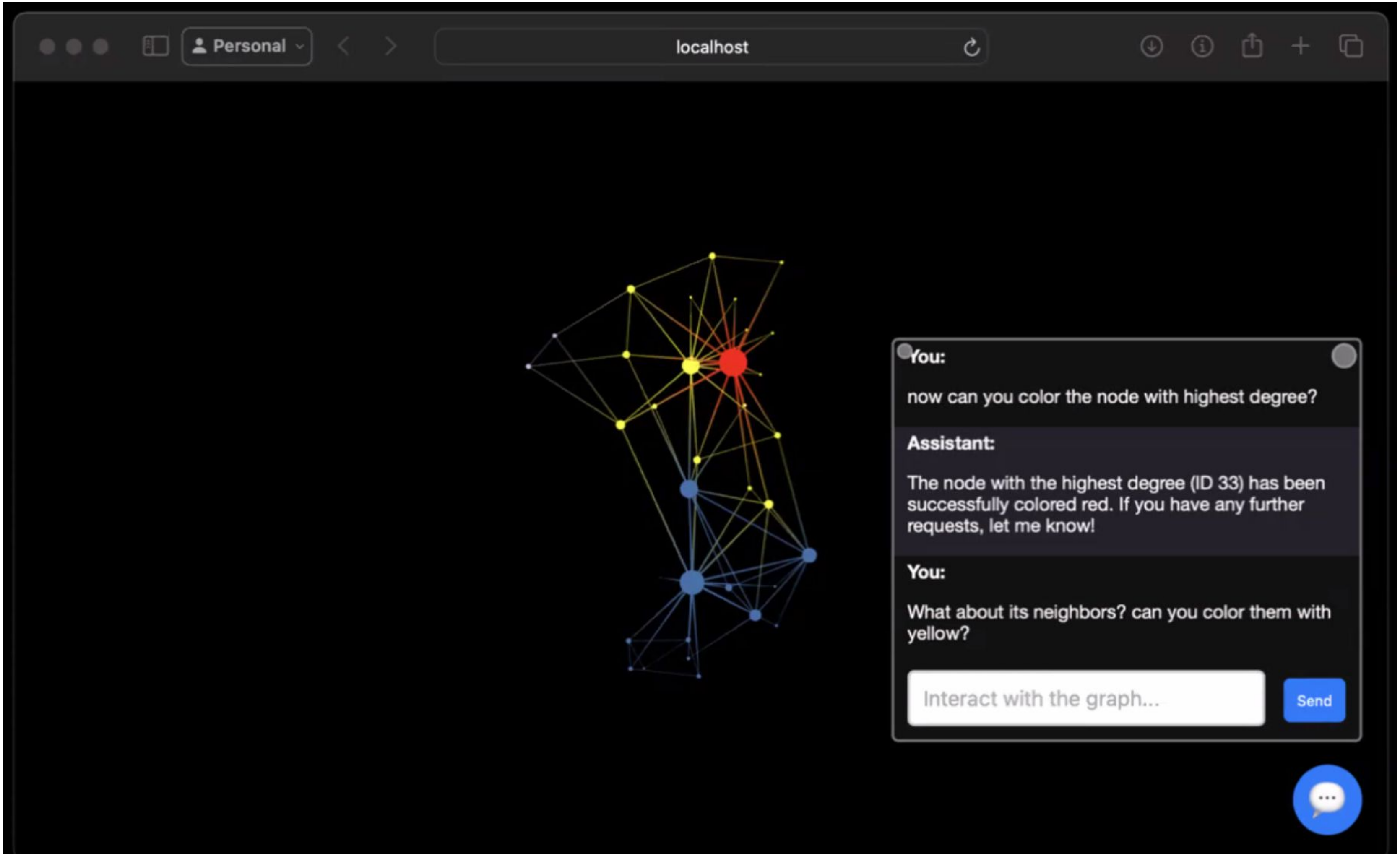
Predictive power of the GRaM











You:

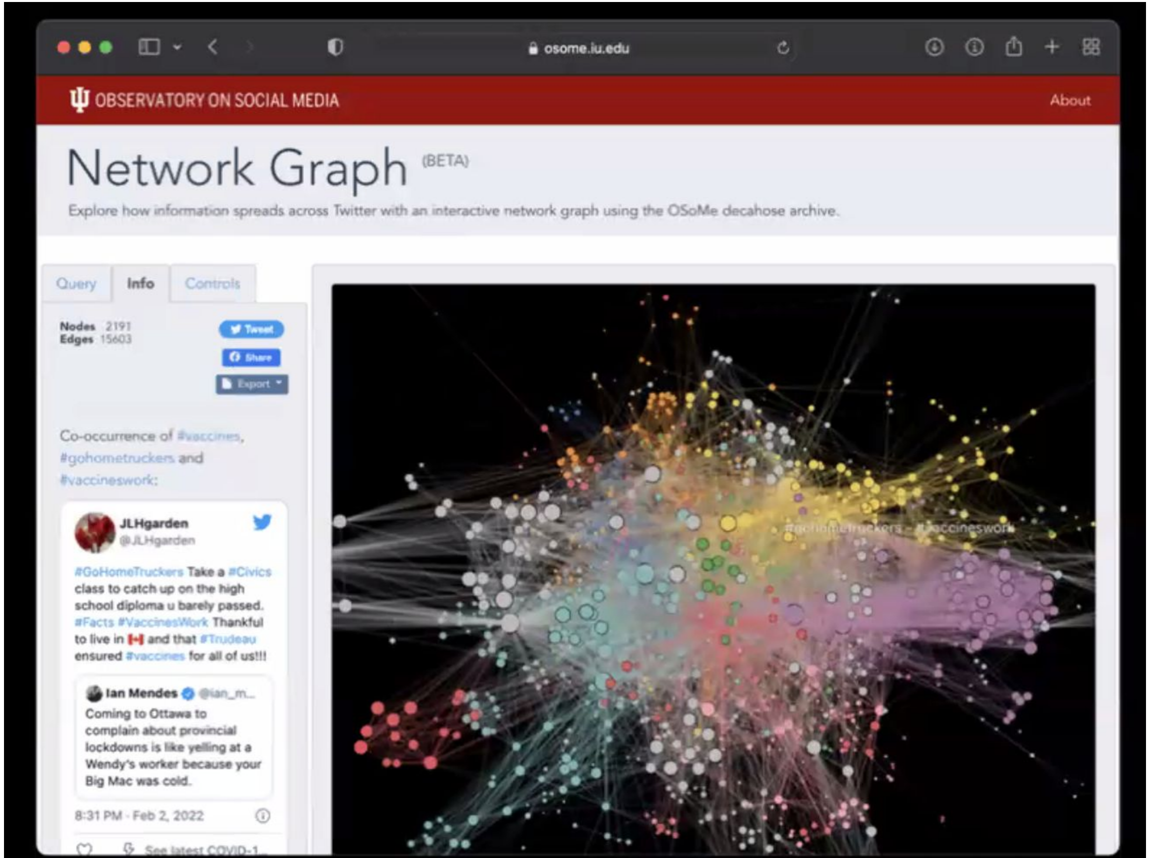
now can you color the node with highest degree?

Assistant:

The node with the highest degree (ID 33) has been successfully colored red. If you have any further requests, let me know!

You:

What about its neighbors? can you color them with yellow?



Network Graph (BETA)

Explore how information spreads across Twitter with an interactive network graph using the OSoMe decahose archive.

Nodes 2191
Edges 15603

Co-occurrence of #vaccines, #gohometruckers and #vaccineswork:

JLHgarden
@JLHgarden

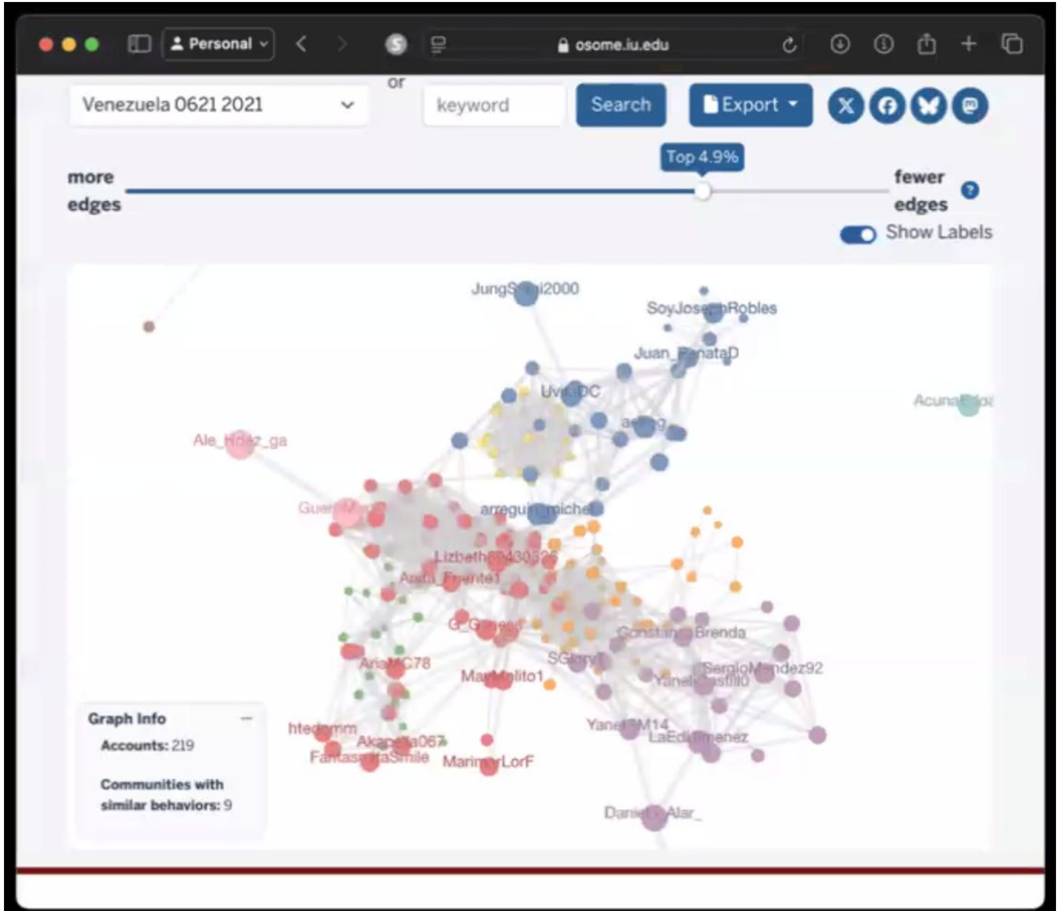
#GoHomeTruckers Take a #Civics class to catch up on the high school diploma u barely passed. #Facts #VaccinesWork Thankful to live in 🇨🇦 and that #Trudeau ensured #vaccines for all of us!!!

Ian Mendes @ian_m...
Coming to Ottawa to complain about provincial lockdowns is like yelling at a Wendy's worker because your Big Mac was cold.

8:31 PM · Feb 2, 2022

See latest COVID-1...

http://osome.iu.edu/tools/networks



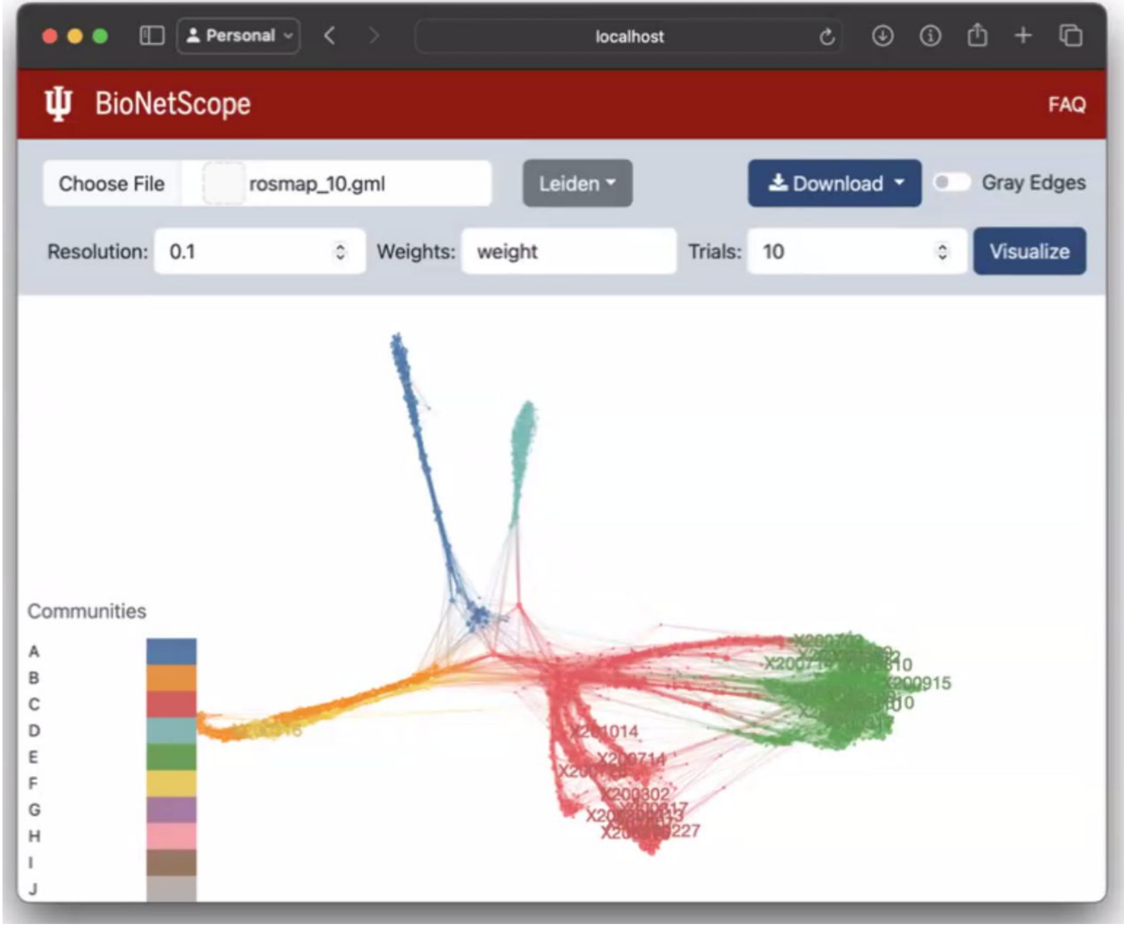
Graph Info

Accounts: 219

Communities with similar behaviors: 9

https://osome.iu.edu/tools/coordiscope

Adapting these models and tools for biomedical research



Choose File: rosmap_10.gml

Leiden

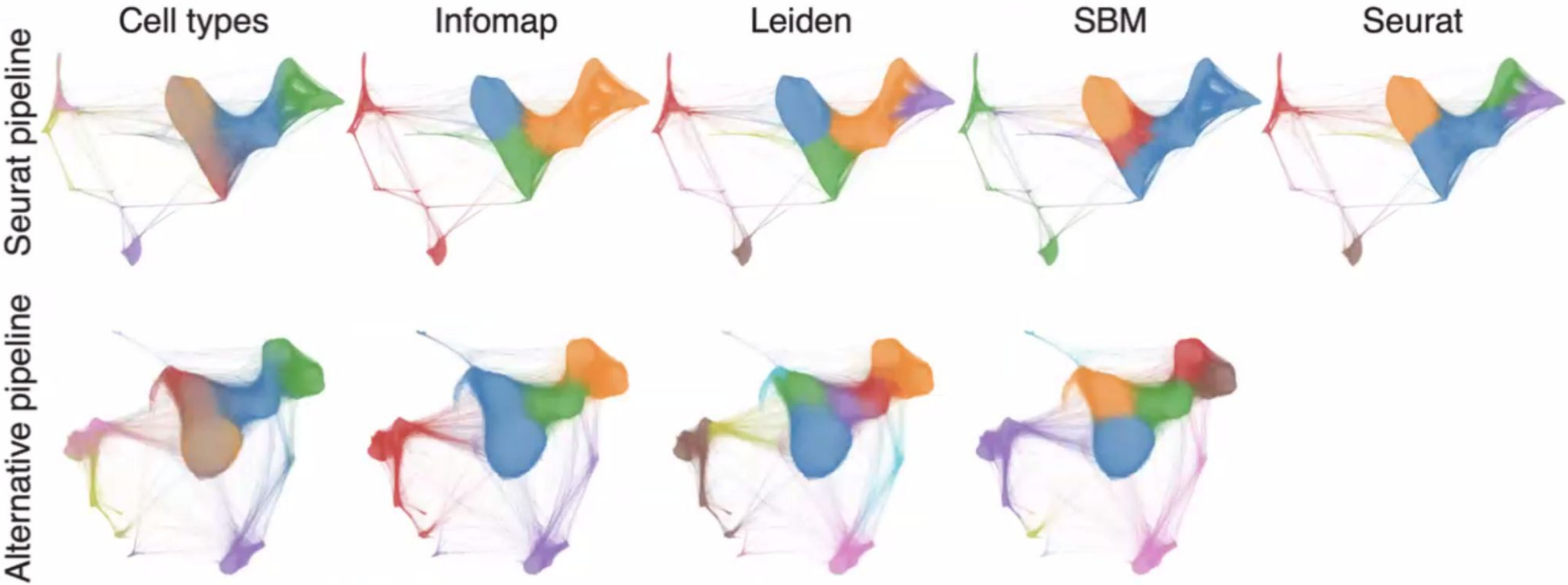
Resolution: 0.1

Weights: weight

Trials: 10

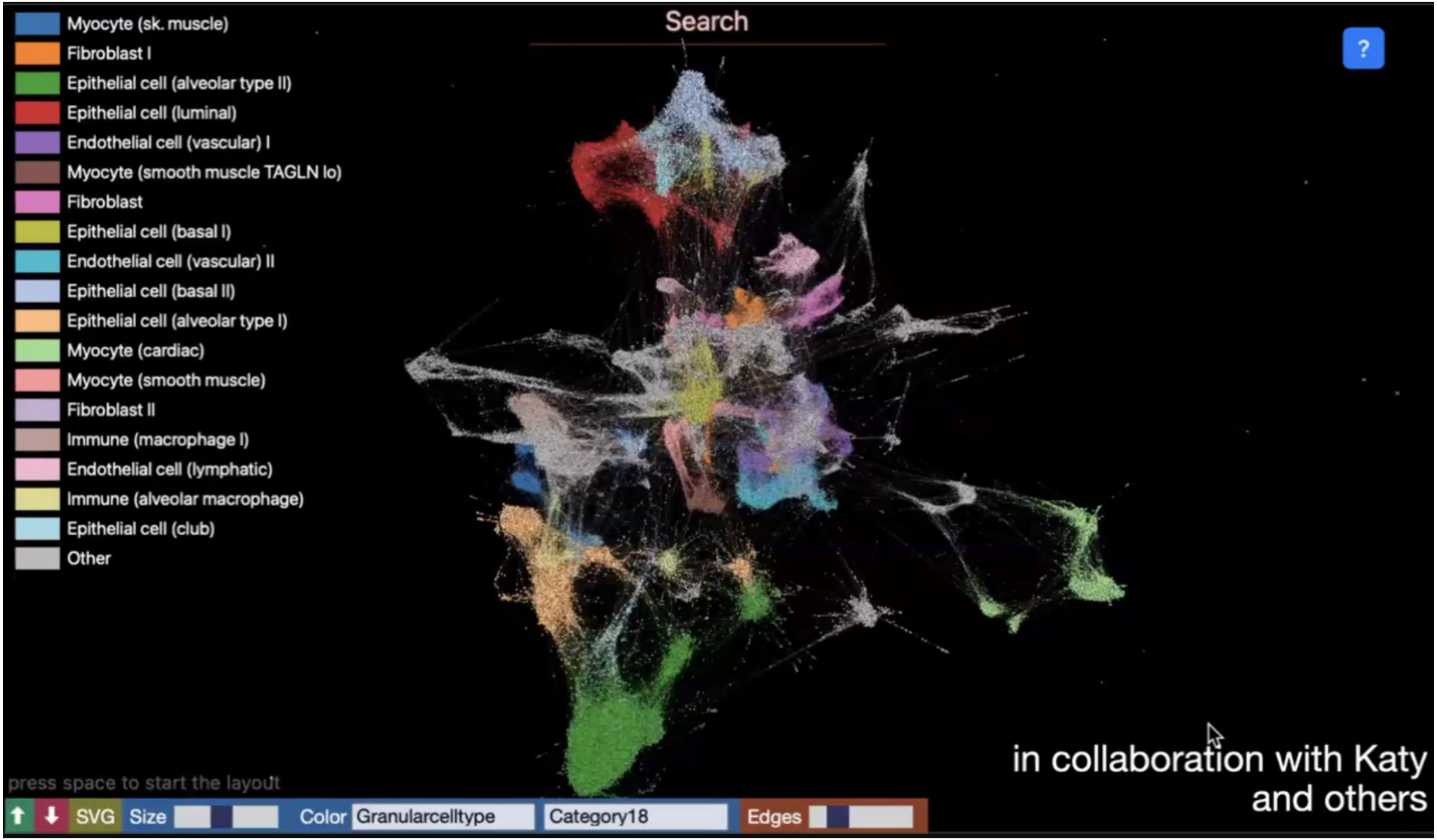
- Single cell RNA-seq data
- Microbiome associations with tissue gene expression
- Brain networks across age
- Metabolomics

Cell Type Differentiation Using Community Detection



68k human Peripheral Blood Mononuclear Cells (PBMCs) scRNA-seq dataset

Fatemi Nasrollahi, F. S., Silva, F. N., Liu, S., Chaudhuri, S., Yu, M., Wang, J., ... & Fortunato, S. (2024). Cell Type Differentiation Using Network Clustering Algorithms. bioRxiv, 2024-12.


Myocyte (sk. muscle)
Fibroblast I
Epithelial cell (alveolar type II)
Epithelial cell (luminal)
Endothelial cell (vascular) I
Myocyte (smooth muscle TAGLN lo)
Fibroblast
Epithelial cell (basal I)
Endothelial cell (vascular) II
Epithelial cell (basal II)
Epithelial cell (alveolar type I)
Myocyte (cardiac)
Myocyte (smooth muscle)
Fibroblast II
Immune (macrophage I)
Endothelial cell (lymphatic)
Immune (alveolar macrophage)
Epithelial cell (club)
Other
Search
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press space to start the layout
SVG
Size
Edges

Color Granularcelltype

Category18

in collaboration with Katy and others

Thanks

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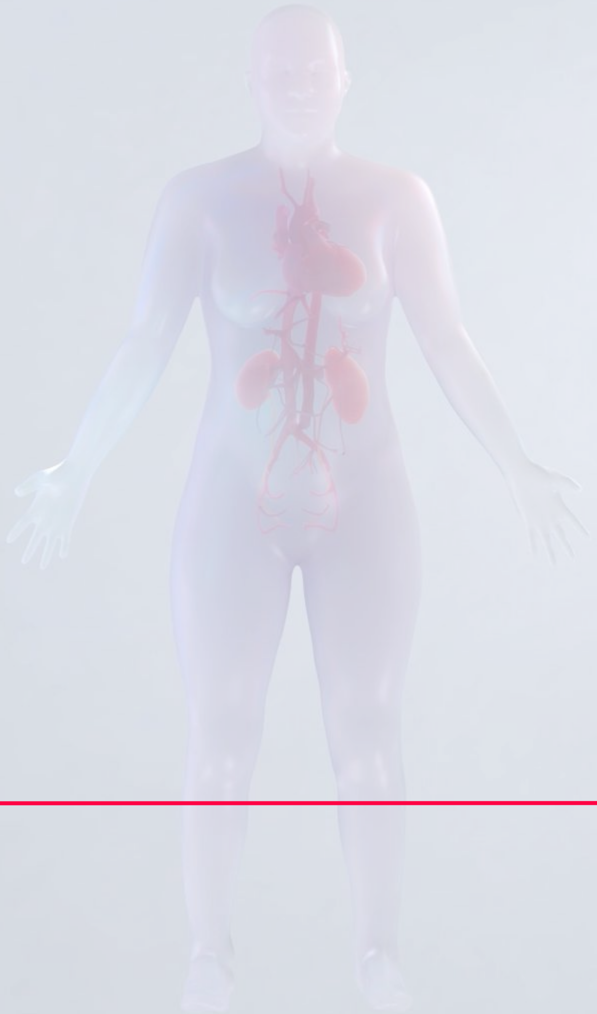
Q&A



https://humanatlas.io/events/2024-24h

Questions

How do we define a Multiscale Human?

How do we map a Multiscale Human?

How do we model a Multiscale Human?

How can LLMs or RAGs be used to advance science and clinical practice?

Thank you