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Leibniz-Zentrum für Informatik

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https://www.dagstuhl.de/21152

April 11 - 16, 2021, Dagstuhl Seminar 21152

Multi-Level Graph Representation for Big Data Arising in Science Mapping

Organizers

Katy Börner (Indiana University - Bloomington, US) Stephen G. Kobourov (University of Arizona – Tucson, US)

For support, please contact

Susanne Bach-Bernhard for administrative matters Shida Kunz for scientific matters

Documents

List of Participants

Shared Documents

Dagstuhl Seminar Wiki Dagstuhl Seminar Schedule (Upload here)

(Use personal credentials as created in DOOR to log in)

Documentation

In the series Dagstuhl Reports each Dagstuhl Seminar and Dagstuhl Perspectives Workshop is documented. The seminar organizers, in cooperation with the collector, prepare a report that includes contributions from the participants' talks together with a summary of the seminar.

Download d overview leaflet (PDF).

Publications

Furthermore, a comprehensive peerreviewed collection of research papers can be published in the series Dagstuhl Follow-Ups.

Dagstuhl's Impact

Please inform us when a publication was published as a result from your seminar. These publications are listed in the category Dagstuhl's Impact and are presented on a

On-site participants

- Katy Börner (Indiana University Bloomington, US) [dblp]
- Ingo Günther (Worldprocessor Studio New York, US)
- Francis Harvey (Leibniz Institut für Länderkunde Leipzig, DE) [dblp]
- Michael Kaufmann (Universität Tübingen, DE) [dblp]
- Alexander Wolff (Universität Würzburg, DE) [dblp]

Remote participants

- Patrizio Angelini (John Cabot University Rome, IT) [dblp]
- Michael A. Bekos (Universität Tübingen, DE) [dblp]
- Kevin Boyack (SciTech Strategies Inc. Albuquerque, US)
- David Chavalarias (CNRS Paris, FR)
- Giuseppe Di Battista (University of Rome III, IT) [dblp]
- Sara Irina Fabrikant (Universität Zürich, CH) [dblp]
- Jean-Daniel Fekete (INRIA Saclay Orsay, FR) [dblp]
- Lynda Hardman (CWI Amsterdam, NL) [dblp]
- Ben Jacobsen (University of Arizona Tucson, US)
- Philipp Kindermann (Universität Trier, DE) [dblp]
- Karsten Klein (Universität Konstanz, DE) [dblp]
- Stephen G. Kobourov (University of Arizona Tucson, US) [dblp]
- Thomas Köhler (TU Dresden, DE)
- Vincent Larivière (University of Montreal, CA)
- Tamara Mchedlidze (Utrecht University, NL) [dblp]
- Guy Melançon (University of Bordeaux, FR) [dblp]
- Staša Milojevic (Indiana University Bloomington, US)
- Filipi Nascimento Silva (Indiana University Bloomington, US)

- Martin Nöllenburg (TU Wien, AT) [dblp]
- Adam Ploszaj (University of Warsaw, PL)
- Sergey Pupyrev (Facebook Menlo Park, US) [dblp]
- Chrysanthi Raftopoulou (National Technical University of Athens, GR) [dblp]
- Andrea Scharnhorst (Royal Netherlands Academy of Arts and Sciences, NL) [dblp]
- André Skupin (San Diego State University, US) [dblp]
- Cassidy Rose Sugimoto (Indiana University Bloomington, US)
- Antonios Symvonis (National TU Athens, GR) [dblp]
- Markus Wallinger (TU Wien, AT)
- Angela Zoss (Duke University Durham, US)

Motivation

For centuries, cartographic maps have guided human exploration. While being rather imperfect initially, they helped explorers find promised lands and return home safely. Recent advances in data, algorithms, and computing infrastructures make it possible to map humankind's collective scholarly knowledge and technology expertise by using topic maps on which "continents" represent major areas of science (e.g., mathematics, physics, or medicine) and zooming reveals successively more detailed subareas. Basemaps of science and technology are generated by analyzing citations links between millions of publications and/or patents. "Data overlays" (e.g., showing all publications by one scholar, institution, or country or the career trajectory of a scholar as a pathway) are generated by science-locating relevant publication records based on topical similarity. Despite the demonstrated utility of such maps, current approaches do not scale to the hundreds of millions of data records now available. The main challenge is designing efficient and effective methods to visualize and interact with more than 100 million scholarly publications at multiple levels of resolution.

This Dagstuhl Seminar will bring together researchers in cartography, information visualization, science of science, and graph drawing to discuss novel graph mining and layout algorithms and their application to the development of science mapping standards and services. We will also organize an exhibition of art contributed by scientists and science maps contributed by artists, and use this to stimulate discussion.

This Dagstuhl Seminar will bring together researchers in cartography, information visualization, science of science, and graph drawing to discuss novel graph mining and layout algorithms and their application to the development of science mapping standards and services. We will also organize an exhibition of art contributed by scientists and science maps contributed by artists, and use this to stimulate discussion.

One of our main goals is to create a special journal issue on the topics related to the development of the next generation science map, SciMap2020. Among others, we will aim to answer:

- What data is most robust to design SciMap2020?
 What information should the nodes and link encode in SciMap2020?
- 3. What user experience metaphors, functionality, and interactive user interfaces are best?
- 4. What user studies should be run to compare options and study knowledge gains?

On the algorithmic front, specific research problems include:

- Construct a hierarchy of graphs, so that each represents the underlying large graph well
- Study the complexity of underlying problem: computing multi-level graph sketches
 Design efficient algorithms for computing multi-level graph sketches and clustering.
- 3. Design efficient algorithms for computing multi-level graph sketches and clustering4. Design graph layout algorithms, driven by multi-level sketches and clustering
- We look forward to a stimulating week that brings together world-leading experts to tackle these research challenges.

Monday

07:30-08:45 Breakfast

09:00-09:15 Welcome by Katy Börner

09:15-10:00 Brief Introductions / Research Overviews

- · Francis Harvey, University of Leipzig
- David Chavalarias, ISC-PIF
- Mohammad Khaledur Rahman, IU, "BatchLayout: A batch-parallel force-directed graph layout algorithm in shared memory"

10-10:30 Overview Talk

• Katy Börner, IU: "Big Data Arising in Science Mapping" (30mins)

10:30-11:00 Coffee Break

11:00-12:00 Brief Introductions / Research Overviews

- Thomas Koehler, TU Dresden
- Kilian Buehling, TU Dresden
- Andrea Scharnhorst, DANS, NL; https://pure.knaw.nl/portal/en/persons/andrea-scharnhorst
- Ingo Günther, https://ingogunther.com/worldprocessor

12:15-13:00 Lunch

Brief Introductions / Research Overviews

- Title slide with name, affiliation(s), picture
- Main research areas
- Research relevant for this Dagstuhl seminar
- Why did you decide to attend this seminar?
- What paper might you contribute to the July/Aug 2022 special issue in *IEEE Computer Graphics and Applications* on "Multi-Level Graph Representations for Big Data in Science"?

12:15-13:00 Lunch

- 14:00 Introduction of Medina who will serve as the VCA Monday-Thursday 14:00-20:00.
- 14:10-15:00 Overview Talks (30mins each)
- Stephen Kobourov, UA: Welcome by Stephen & Multi-Level Graph Representations
- Sara Fabrikant, Department of Geography, University of Zürich: Cognitive research on landmarks, color, uncertainty & <u>The Future of Geographic Information Displays</u>
 Maybe better for this late in the evening: <u>Susceptibility of domain experts to color manipulation indicate a need for design principles</u> in data visualization
- 15:00-15:30 Coffee Break / Katy welcomes all to Amatria's Virtual Birthday Party
- 15:30-16:30 Brief Introductions / Research Overviews (10mins each)
- Andreas Bueckle, IU: Science Map Metaphors: A Comparison of Network Versus Hexmap-Based Visualizations
- Angela Zoss, Duke U: XXX
- Pino di Battista: Schematic Representation of Large Biconnected Graphs
- Alexander Wolff, U Würzburg: Using the Metro Map Metaphor for Drawing Hypergraphs
- Guy Melançon, Vice President of Digital Transformation, Université de Bordeaux*
- Adam Ploszaj, University of Warsaw
- 16:30-18:00 Challenges & Opportunities and Discussion of Topics for Special Issue in IEEE Computer Graphics and Applications (Katy and Stephen)
- 18:00-19:00 Dinner
- 19:00-20:00 WEBINAR Special Event: Dagstuhl Exhibit Debut with Francis Harvey & Katy Börner

The July/Aug 2022 special issue in *IEEE Computer Graphics and Applications* on "Multi-Level Graph Representations for Big Data in Science"

Articles due for review: December 29, 2021

Guest editors:

- Katy Börner, Indiana University, Bloomington, US
- Stephen G. Kobourov, University of Arizona, Tucson, US

https://www.computer.org/digitallibrary/magazines/cg/call-for-papersspecial-issue-on-multi-level-graphrepresentations-for-big-data-in-science

Call for Papers: Special Issue on Multi-level Graph Representations for Big Data in Science

CG&A seeks submissions for this upcoming special issue.

For centuries, cartographic maps have guided human exploration. While being rather imperfect initially, they helped explorers find promised lands and return home safely. Recent advances in data, algorithms, and computing infrastructures make it possible to map humankind's collective scholarly knowledge and technology expertise by using topic maps on which "continents" represent major areas of science (e.g., mathematics, physics, or medicine) and zooming reveals successively more detailed subareas. Basemaps of science and technology are generated by analyzing citations links between millions of publications and/or patents. "Data overlays" (e.g., showing all publications by one scholar, institution, or country or the career trajectory of a scholar as a pathway) are generated by science-locating relevant publication records based on topical similarity. Despite the demonstrated utility of such maps, current approaches do not scale to the hundreds of millions of data records now available. The main challenge is designing efficient and effective methods to visualize and interact with more than 100 million scholarly publications at multiple levels of resolution.

This special issue invites researchers in cartography, data visualization, science of science, graph drawing, and other domains to submit novel and promising new research on graph mining and layout algorithms and their application to the development of science mapping standards and services. Topics of interest include:

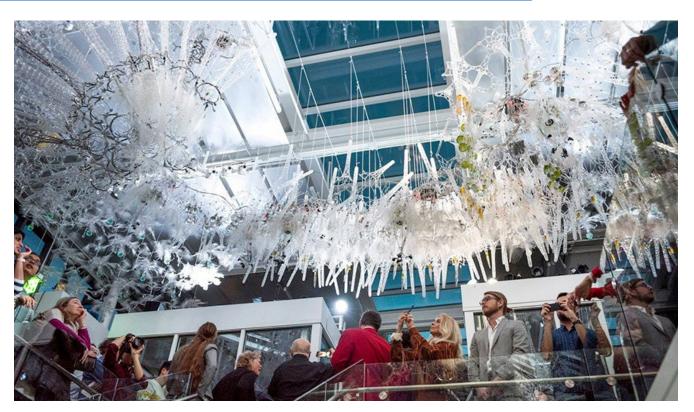
- · Science of science user needs and applications
- · Efficient multi-level graph algorithms
- Network visualizations
- · Effective user interfaces to large-scale data visualizations

Deadlines

Submissions due: 29 December 2021 Preliminary notification: 2 March 2022

Revisions due: 6 April 2022
Final notification: 11 May 2022
Final version due: 25 May 2022
Publication: July/August 2022

15:00-15:30 Coffee Break / Katy welcomes all to <u>Amatria's Virtual Birthday Party</u>







Mapping Science Exhibit http://scimaps.org



101st Annual Meeting of the Association of American Geographers, Denver, CO. April 5th - 9th, 2005 (First showing of Places & Spaces)



University of Miami, Miami, FL. September 4 - December 11, 2014.



Duke University, Durham, NC. January 12 - April 10, 2015



http://scimaps.org





The David J. Sencer CDC Museum, Atlanta, GA. January 25 - June 17, 2016.

Places & Spaces: Mapping Science Exhibit

1st Decade (2005-2014)

Maps



2nd Decade (2015-2024)

Macroscopes









100

MAPS

in large format, full color, and high resolution.

248



MAPMAKERS

from fields as disparate as art, urban planning, engineering, and the history of science.

43



MACROSCOPE MAKERS including one whose job title is "Truth and Beauty Operator."

20

MACROSCOPES

for touching all kinds of data.

382

DISPLAY VENUES

from the Cannes Film Festival to the World Economic Forum.

354

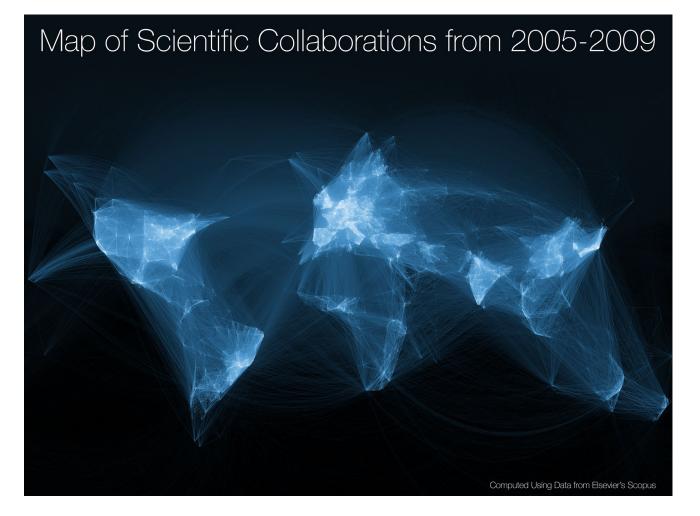


PRESS ITEMS

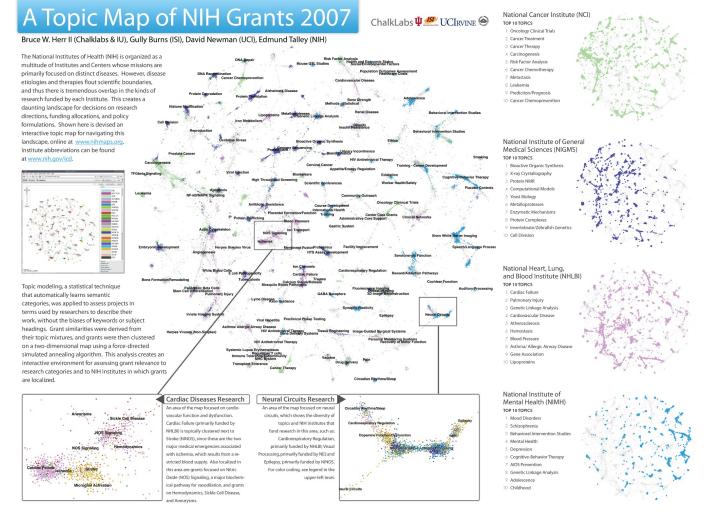
including articles in *Nature*, Science, USA Today, and Wired.

http://scimaps.org

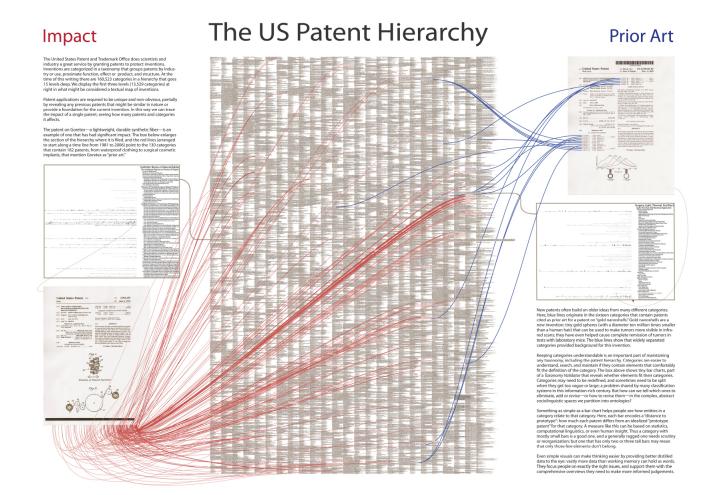


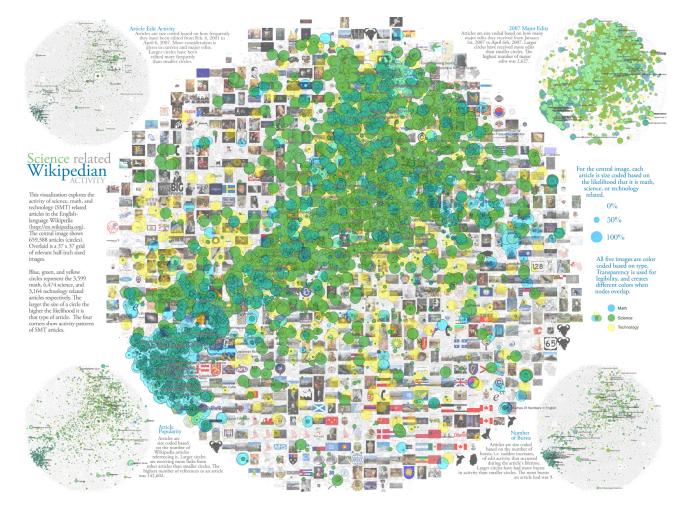


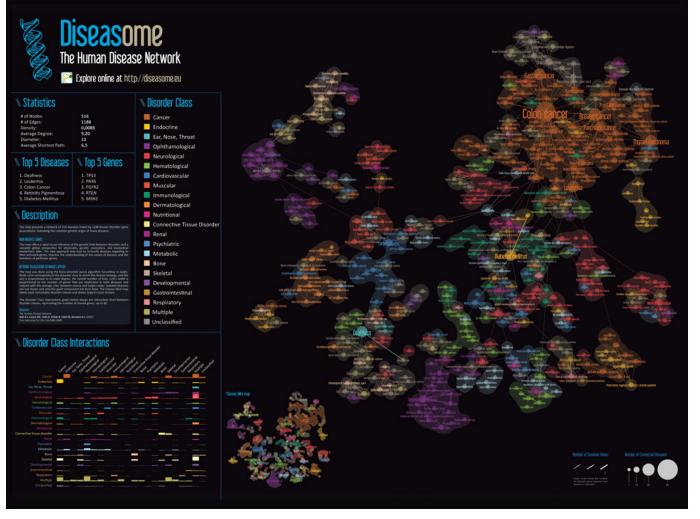
VII.6 Stream of Scientific Collaborations Between World Cities - Olivier H. Beauchesne - 2012

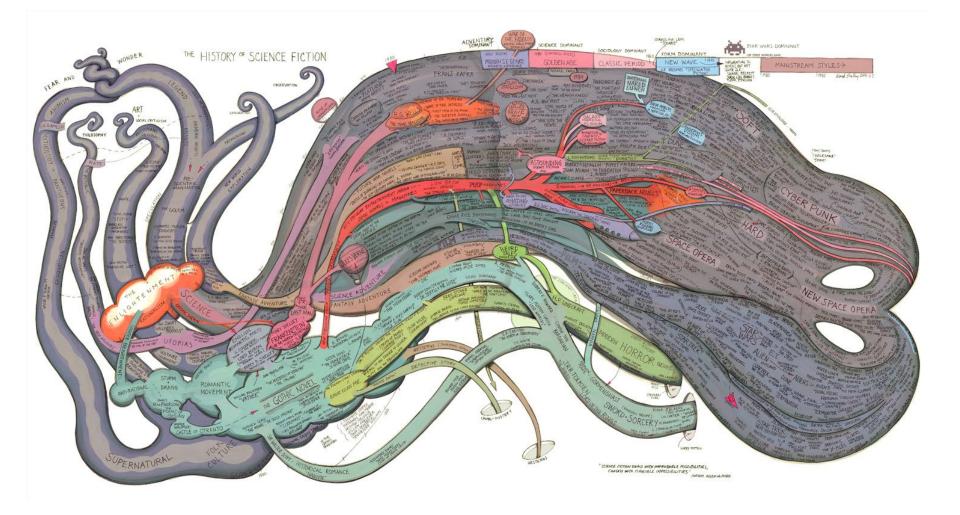


The Structure of Science We are all familiar with traditional maps that show the relationships between countries, provinces, states, and cities. Similar relationships exist between the various disciplines and research topics in science. This allows us to map the structure of science. One of the first maps of science was developed at the Institute for Scientific Information over 30 years ago. It identified 41 areas of science from the citation patterns in 17,000 scientific papers. That early map was intriguing, but it didn't cover enough of science to accurately define its structure. The Social Sciences are the smallest and is our starting point, the purest of all sciences. It lies at the outer edge of the map. most diffuse of all the sciences. Psychology Computer Science, Electrical Engineering, and Optics are applied sciences that draw upon knowledge in Mathematics and Physics. These three disciplines provide a good example of a Things are different today. We have enormous computing power and advanced visualization serves as the link between Medical Sciences software that make mapping of the structure of science possible. This galaxy-like map of science (Psychiatry) and the Social Sciences. Statistics linear progression from one pure science (Mathematics) to another (Physics) through multiple (left) was generated at Sandia National Laboratories using an advanced graph layout routine (VxOrd) serves as the link with Computer Science disciplines. Although applied, these disciplines are highly concentrated with distinct bands of from the citation patterns in 800,000 scientific papers published in 2002. Each dot in the galaxy and Mathematics. research communities that link them. Bands indicate interdisciplinary research. represents one of the 96,000 research communities active in science in 2002. A research community is a group of papers (9 on average) that are written on the same research topic in a given year. Over time, communities can be born, continue, split, merge, or die. Research is highly concentrated in Phys These disciplines have few, but very The map of science can be used as a tool for science strategy. This is the terrain in which distinct, bands of research communities that link organizations and institutions locate their scientific capabilities. Additional information about the them. The thickness of these bands indicates an scientific and economic impact of each research community allows policy makers to decide which extensive amount of interdisciplinary research, areas to explore, exploit, abandon, or ignore. which suggests that the boundaries between Physics and Chemistry are not as distinct as one We also envision the map as an educational tool. For children, the theoretical relationship between areas of science can be replaced with a concrete map showing how math, physics, chemistry, biology and social studies interact. For advanced students, areas of interest can be located and neighboring areas can be explored. Nanotechnology Most research communities in nanotechnology are concentrated in However, many disciplines in the Life and Medical Sciences also have nanotechnology applications. Research communities in proteomics are centered in Biochemistry. In addition, there is a heavy focus in the tools section of chemistry, such as The balance of the proteomics communities are widely dispersed among the Life and Medical Sciences. The Life Sciences, including Biology and **Pharmacogenomics** Biochemistry, are less concentrated than Chemistry or Physics. Bands of linking Pharmacogenomics is a relatively new research can be seen between the larger field with most of its activity in Medicine. areas in the Life Sciences; for instance It also has many communities in The Medical Sciences include broad therapeutic studies and targeted areas of Treatment (e.g. central between Biology and Microbiology, and Biochemistry and two communities in between Biology and Environmental Science the Social Sciences. nervous system, cardiology, gastroenterology, etc.) Biochemistry is very interesting in that it is a large discipline that has visible links Unlike Physics and Chemistry, the medical disciplines are more spread out, suggesting a more multito disciplines in many areas of the map, disciplinary approach to research. The transition into including Biology, Chemistry, Neuroscience, Life Sciences (via Animal Science and Biochemistry) and General Medicine. It is perhaps the most interdisciplinary of the sciences.

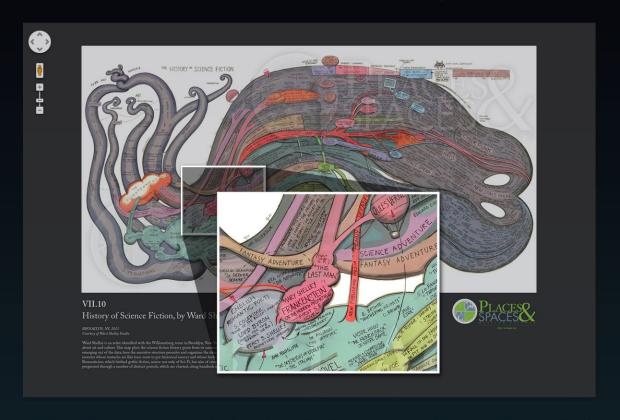








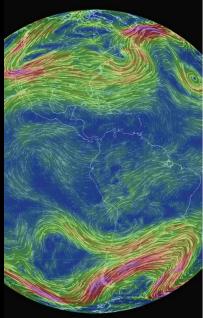
Check out our Zoom Maps online!



Visit scimaps.org and check out all our maps in stunning detail!

(i) MACROSCOPES FOR INTERACTING WITH SCIENCE











Earth

Weather on a worldwide scale

AcademyScope

Exploring the scientific landscape

Mapping Global Society

Local news from a global perspective

Charting Culture

2,600 years of human history in 5 minutes

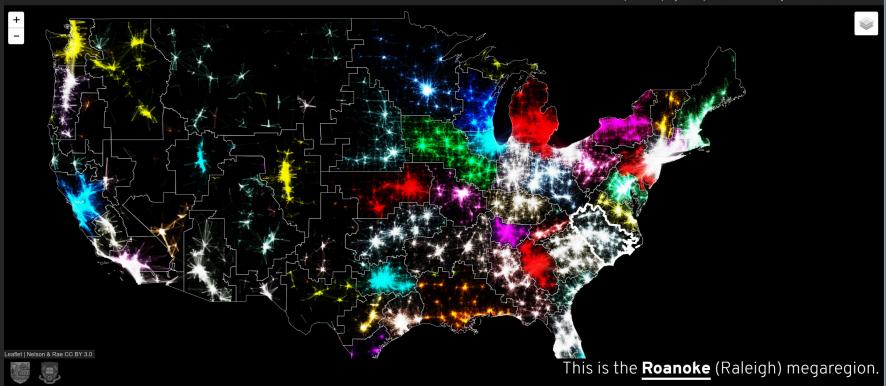




THE MEGAREGIONS OF THE US

Explore the new geography of commuter connections in the US.

Tap to identify regions. Tap and hold to see a single location's commuteshed.



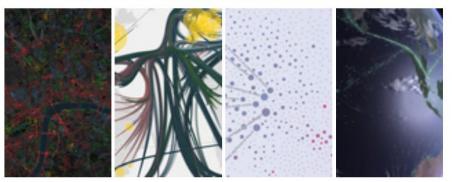






Iteration XII (2016)

Macroscopes for Making Sense of Science



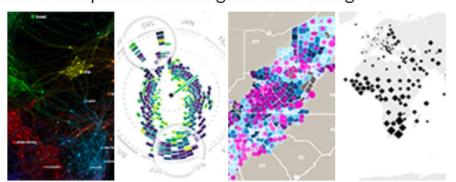
Iteration XIII (2017)

Macroscopes for Playing with Scale



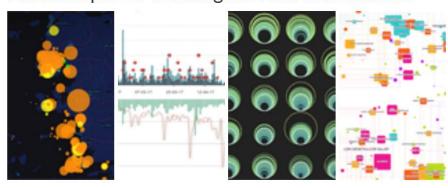
Iteration XIV (2018)

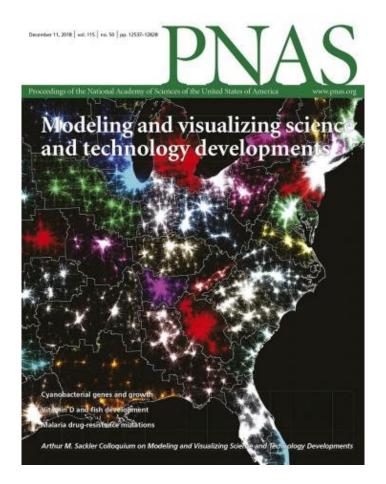
Macroscopes for Ensuring our Well-being

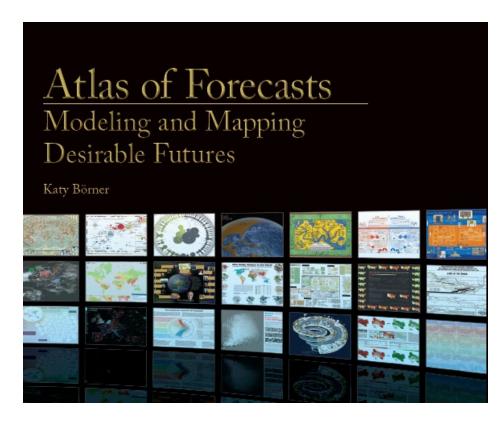


Iteration XV (2019)

Macroscopes for Tracking the Flow of Resources







Acknowledgments

Exhibit Curators



The exhibit team: Lisel Record, Katy Börner, and Todd Theriault.

http://scimaps.org

Plus, we thank the more than 250 authors of the 100 maps and 16 interactive macroscopes.

Exhibit Advisory Board



Gary Berg-Cross Cognitive psychologist (PhD, SUNY-Stony Brook). Potomac, MD, USA



André Skupin Associate Professor of Geography at San Diego State University, California



Donna J. Cox, MFA, Ph.D.
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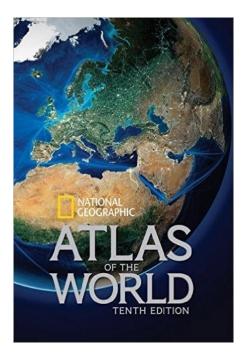


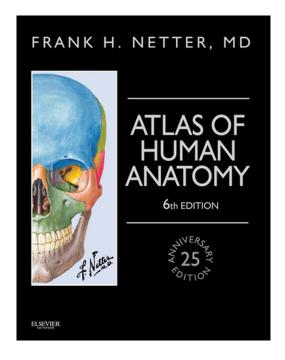
Lev Manovich
Professor, The Graduate Center, City
University of New York; Director, Software
Studies Initiative (big data, digital
humanities, visualization)

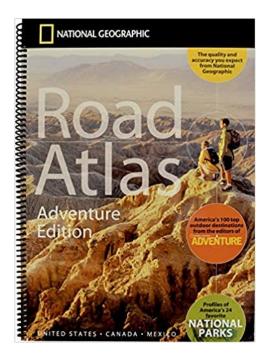


HuBMAP Reference Atlas: Toward a human [reference] map

An **atlas** is an oversized, bound book of maps. It has descriptive text, an index, possibly other data visualizations.







An human cell **atlas** might show a landscape of all cells, or

Maps of cells per tissue type/anatomical structure.

Article | Published: 25 March 2020

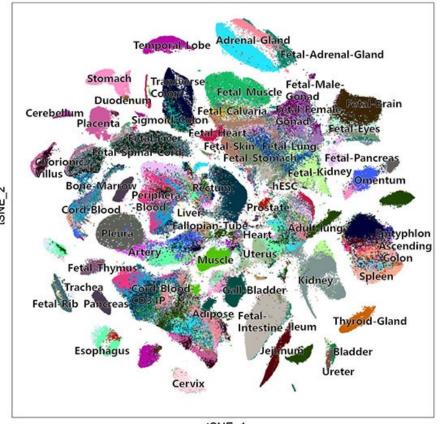
Construction of a human cell landscape at single-cell level

Xiaoping Han $\stackrel{\textstyle ullet}{}$, Ziming Zhou, [...] Guoji Guo $\stackrel{\textstyle ullet}{}$

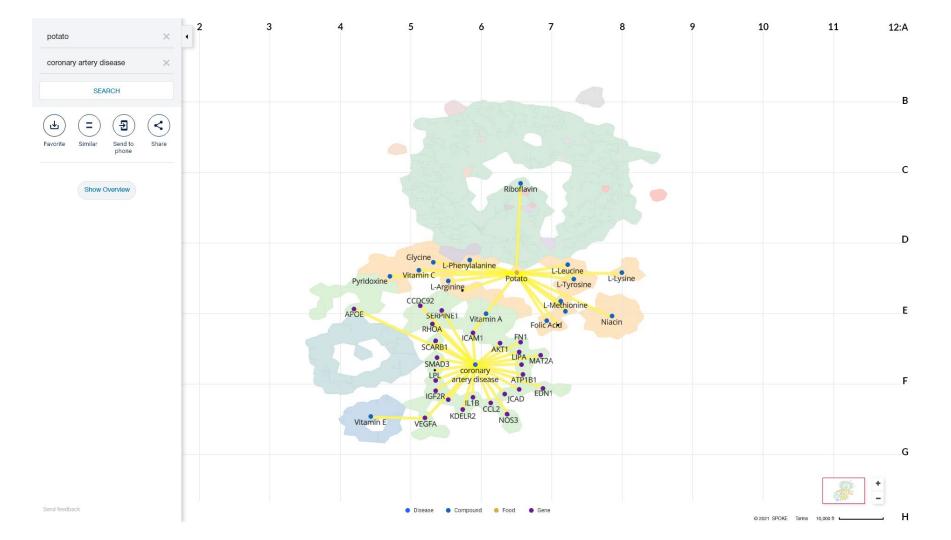
Nature **581**, 303–309(2020) | Cite this article

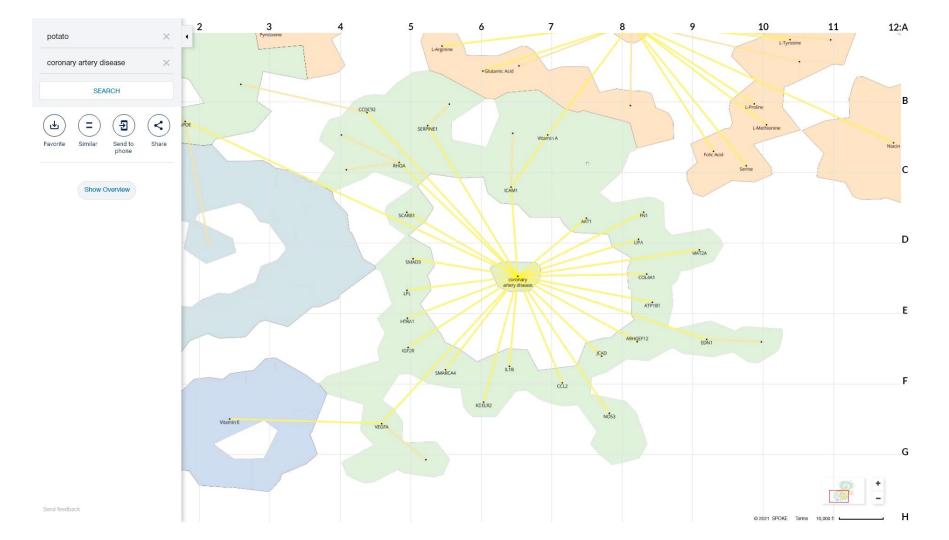
55k Accesses | 32 Citations | 409 Altmetric | Metrics

Tissue



tSNE_1



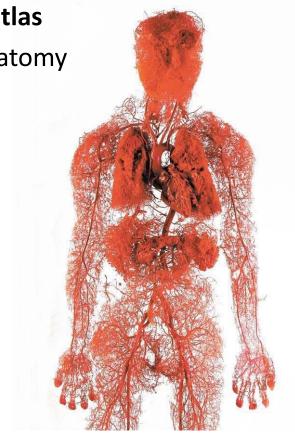


A human reference atlas

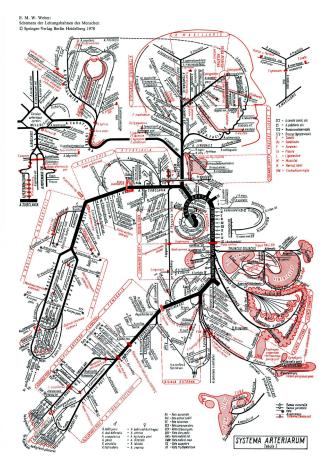
might use human anatomy

as a 'basemap,' or

an abstract space.



https://bodyworlds.com



Weber, 1978

The Human Body at Cellular Resolution: The NIH Human Biomolecular Atlas Program. Snyder et al. *Nature*. 574, p. 187-192.

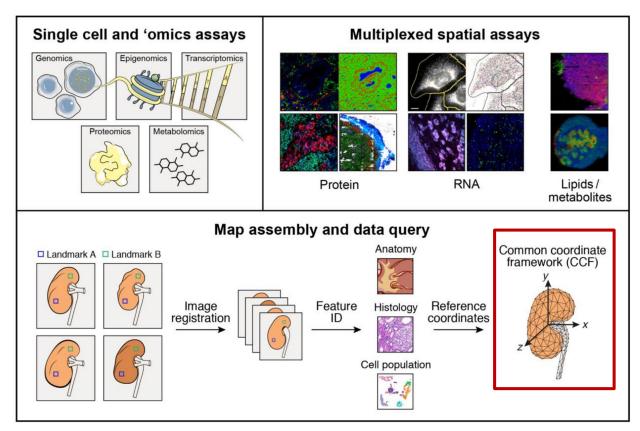


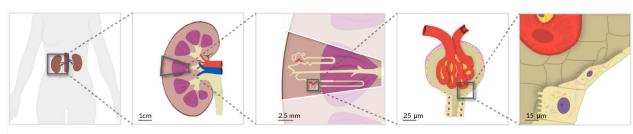
Fig. 3 | Map generation and assembly across cellular and spatial scales. HuBMAP aims to produce an atlas in which users can refer to a histological slide from a specific part of an organ and, in any given cell, understand its contents on multiple 'omic levels—genomic, epigenomic, transcriptomic, proteomic, and/or metabolomic. To achieve these ends, centres will apply a combination of imaging, 'omics and mass spectrometry

techniques to specimens collected in a reproducible manner from specific sites in the body. These data will be then be integrated to arrive at a high-resolution, high-content three-dimensional map for any given tissue. To ensure inter-individual differences will not be confounded with collection heterogeneity, a robust CCF will be developed.

CCF Requirements

The CCF must capture major **anatomical structures**, **cell types**, **and biomarkers** and their interrelations across **multiple levels of resolution**.

It should be **semantically explicit** (using existing ontologies, e.g., Uberon, CL) and **spatially explicit** (e.g., using 3D reference organs for registration and exploration).



Body

- Body
- · Kidney (Left, Right)
- Aorta
- Renal artery
- Renal vein
- Ureter

Organ

- Renal capsule
- Renal pyramid
- Renal cortex
- Renal medulla
- Renal calyx
- Renal pelvis

Functional Tissue Unit

- Nephron
- Renal corpuscle
- Proximal convoluted tubule
- Loop of Henle
- Distal convoluted tubule
- Connecting tubule
- Collecting duct

FTU Sub-structure(s) Cellular

- Bowman's capsule
- Glomerulus
- Efferent arteriole
- Afferent arteriole
- Parietal epithelial cell
- Capillary endothelial cell
- Mesangial cell
- Podocyte

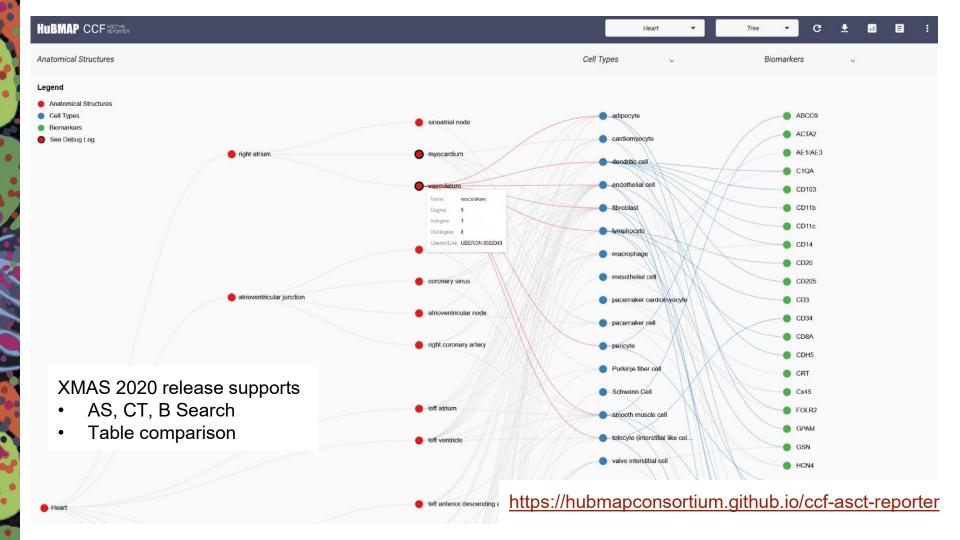
ASCT+B Tables

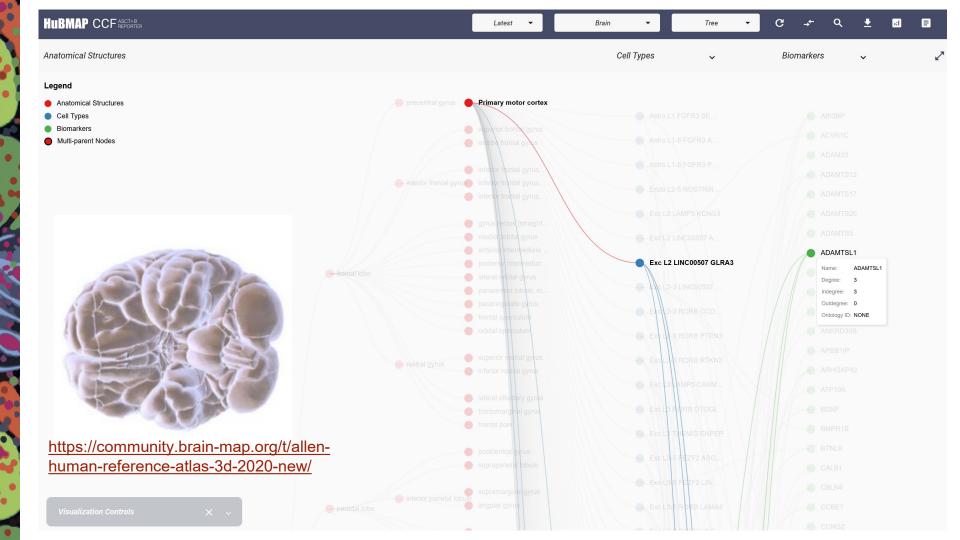
Anatomical Structures, Cell Types, and Biomarkers (ASCT+B) tables aim to capture the partonomy of anatomical structures, cell types, and major biomarkers (e.g., gene, protein, lipid or metabolic markers).

Structure/Re	Substructure/Sub	Cell Type	Subset of Marker Genes	
gion	region			
Renal	Bowman's Capsule	Parietal epithelial cell	CRB2*, CLDN1*	
Corpuscle	Glomerulus	Podocyte	NPHS2*, PODXL*, NPHS1*	
		Capillary Endothelial Cell	EHD3*, EMCN*, HECW2*,	
			FLT1*, AQP1*	
		Mesangial Cell	POSTN*, PIEZO2*, ROBO1*,	
			ITGA8*	

Partial ASCT+B Table from

• El-Achkar et al. A Multimodal and Integrated Approach to Interrogate Human Kidney Biopsies with Rigor and Reproducibility: The Kidney Precision Medicine Project. bioRxiv. 2019, Updated Aug 2020. doi:10.1101/828665





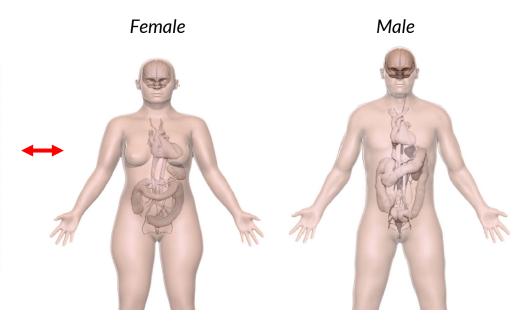
ASCT+B Tables vs. 3D Reference Organs

ASCT+B for 10 organs on 11/30/2020, 5:37pm ET:

Organ	#AS	#CT	#B	#AS-CT	#СТ-В
Brain	184	127	254	127	346
Heart	23	16	35	73	42
Kidney	39	53	83	63	131
Large Intestine	22	33	45	306	72
Liver	16	27	34	29	35
Lung	18	62	103	110	128
Lymph nodes	34	30	50	63	110
Skin	14	32	57	37	99
Small Intestine	20	32	48	195	55
Spleen	33	26	46	48	72

Vasculature 751

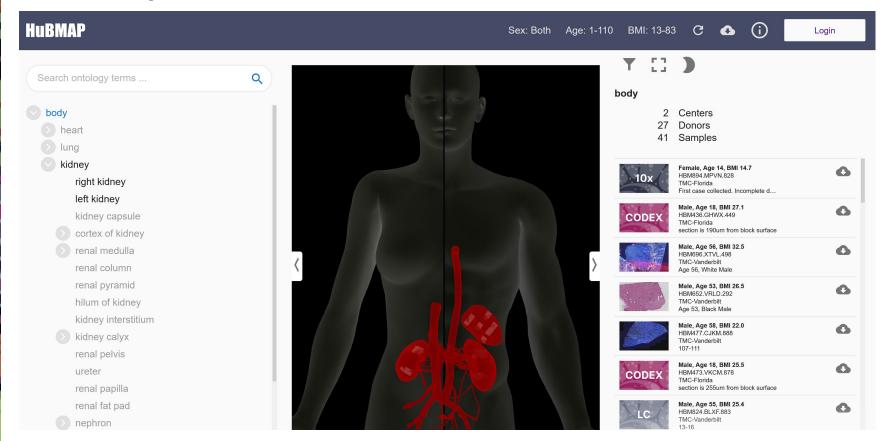
https://hubmapconsortium.github.io/ccf/pages/ccf-anatomical-structures.html



https://hubmapconsortium.github.io/ccf/pages/ccf-3d-reference-library.html (NLM VH organs) https://community.brain-map.org/t/allen-human-reference-atlas-3d-2020-new/ (brain)

https://www3.cs.stonybrook.edu/~ari/ (male colon)

CCF Exploration User Interface (EUI)



https://portal.hubmapconsortium.org/ccf-eui

HuBMAP Sex: Both Age: 1-110 BMI: 13-83 **C (4)** Logout

Q Search ontology terms ...





lung

kidney

right kidney

left kidney

kidney capsule

cortex of kidney

renal medulla renal column renal pyramid hilum of kidney kidney interstitium

kidney calyx major calyx minor calyx renal pelvis ureter

renal papilla renal fat pad

nephron

spleen

colon





body

1 Centers

9 Donors

40 Samples



Male, Age 55, BMI 25.4 HBM695.RTLJ.484

TMC-Vanderbilt



Male, Age 21, BMI 21.8

HBM634.MMGK.572 TMC-Vanderbilt Age 21, White Male, Trauma Patient



Female, Age 44, BMI 28.0 HBM457.NNQN.252

TMC-Vanderbilt Age 44, white female.



Female, Age 44, BMI 28.0 HBM465.VKHL.532 TMC-Vanderbilt Age 44, white female.



Male, Age 21, BMI 21.8 HBM693 HFFJ 752

TMC-Vanderbilt Age 21, White Male, Trauma Patient



Female, Age 58, BMI 23.0 HBM536.LDTZ.757

TMC-Vanderbilt Age 58, White Female



Male, Age 48, BMI 35.3 HBM334.GCCX.874 TMC-Vanderbilt

Age 48, White Male Male, Age 31, BMI 32.6

HBM776.PKJF.786 TMC-Vanderbilt Age 21, White Male

Female, Age 66, BMI 31.3 HBM284.TRCV.726

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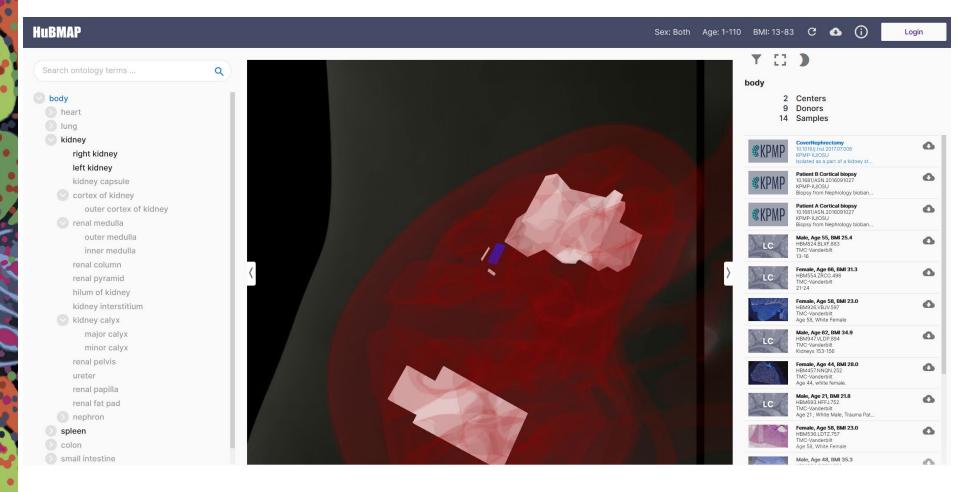
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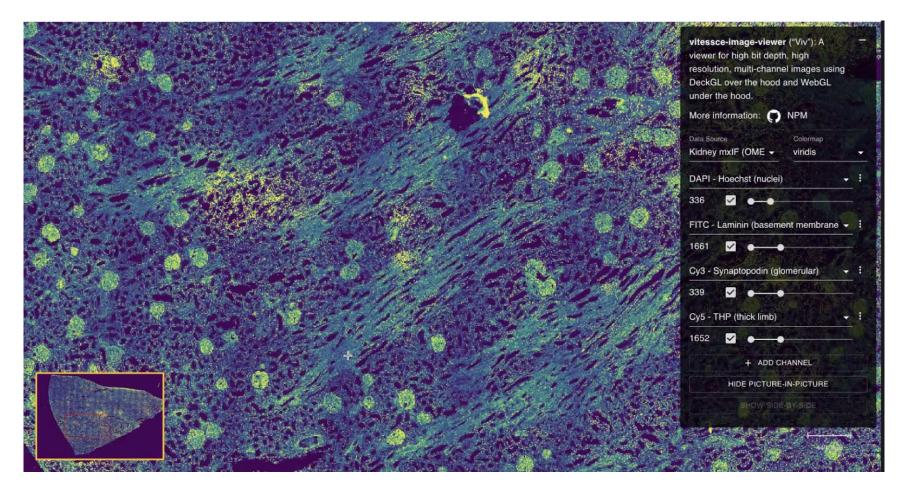
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Register your data via https://hubmap-ccf-ui.netlify.app/rui/ so it can be spatially/semantically explored in EUI.



http://gehlenborglab.org/research/projects/vitessce/

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TMCs



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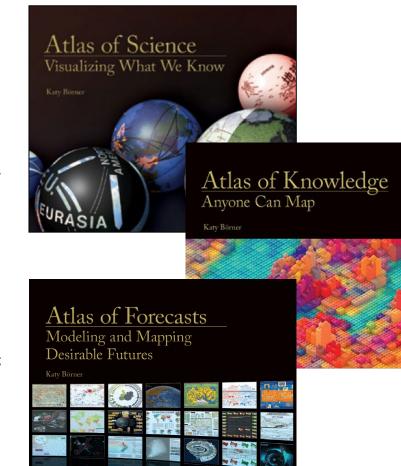
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Q&A