

Visual Computing at the Electronic Visualization Laboratory

G. Elisabeta Marai

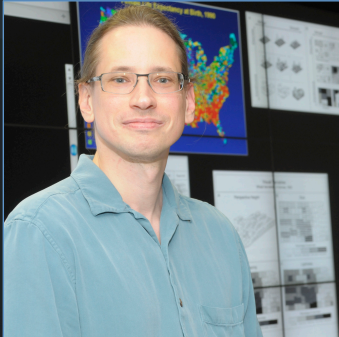
Electronic Visualization Lab
University of Illinois at Chicago

UIC Electronic Visualization Laboratory (EVL)

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EVL Director, CS



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Associate Professor, CS



Robert Kenyon,
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Research Professor, CS

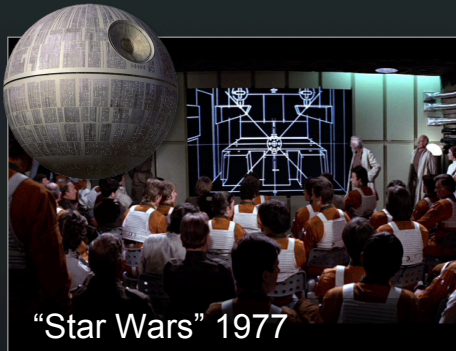
Funded through research
grants from:

NIH
NSF
DARPA
NASA
NIDRR
ANL

and partial support from:
UIC, State of IL

EVL's Visual Computing and Virtual Reality Hardware and Software Help Teams Manage “Big Data”

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“Star Wars” 1977



CAVE 1992



TacTile 2008



SAGE (2004-2014) and SAGE2 (2014-present)



CAVE2 2012

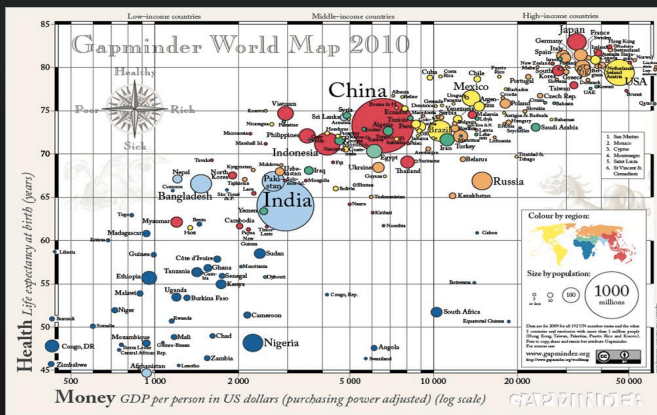
Rat fetus using SAGE2



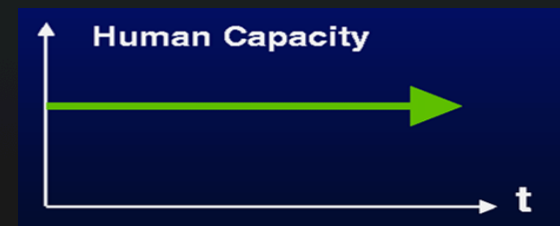
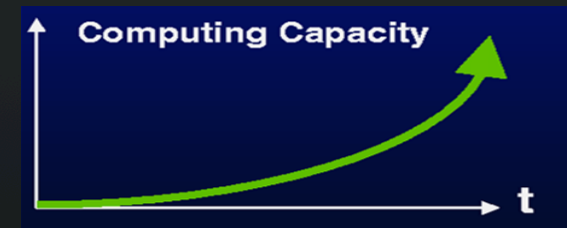
High-resolution optical scan of a near-mid-section of a rat fetus at 19 days, acquired by the Monash Histology Platform, Monash University. At low magnification, this 123K x 74K pixel image shows the entire organism and its central organs and anatomy, yet there is sufficient resolution sufficient to identify, at high magnification, the nuclei of red blood cells forming in the liver.

Visual Computing

- Computing over images and 3D models, including the processes at the interface between (visual) data and humans



visualization of human development
<http://tools.google.com/gapminder/>

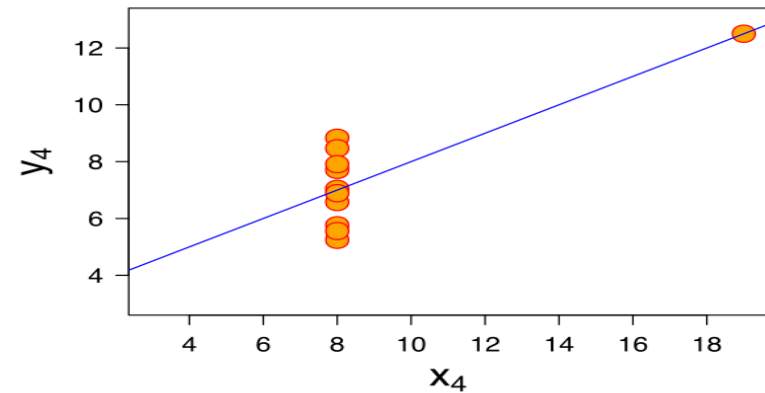
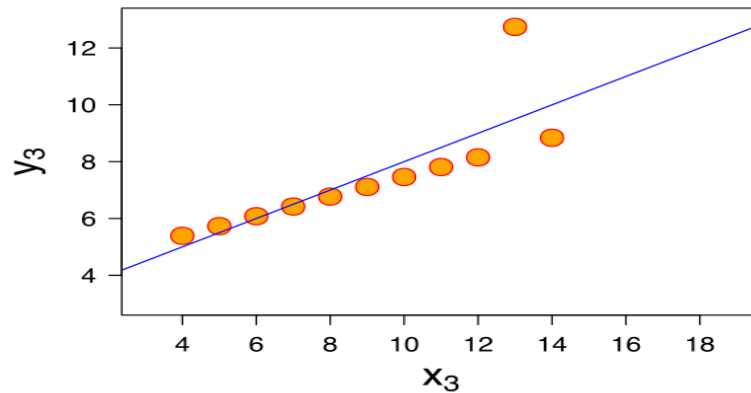
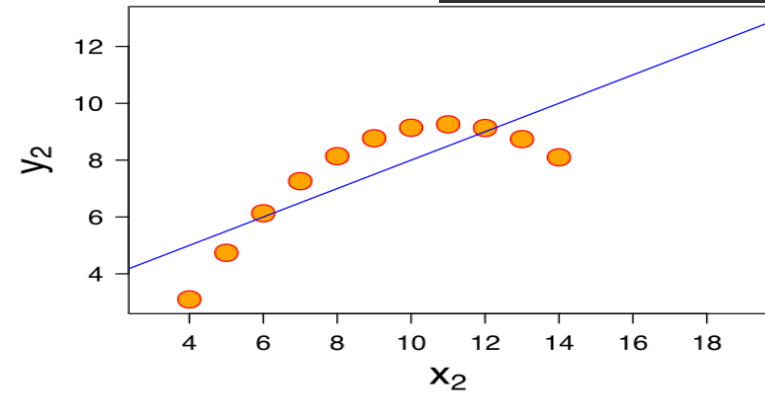
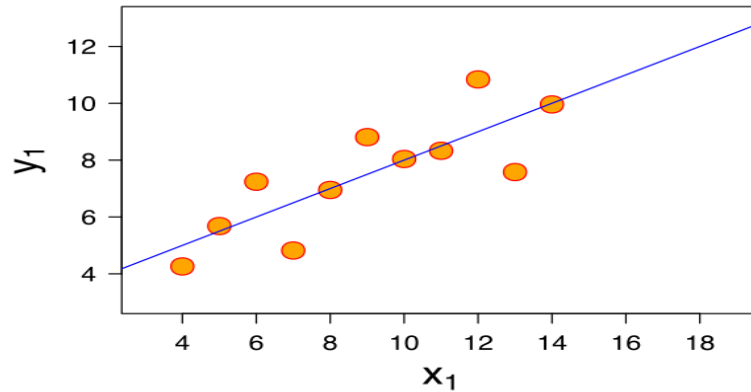


- Systems that provide *visual representations of datasets* designed to help people carry out tasks more effectively.

Anscombe's Quartet

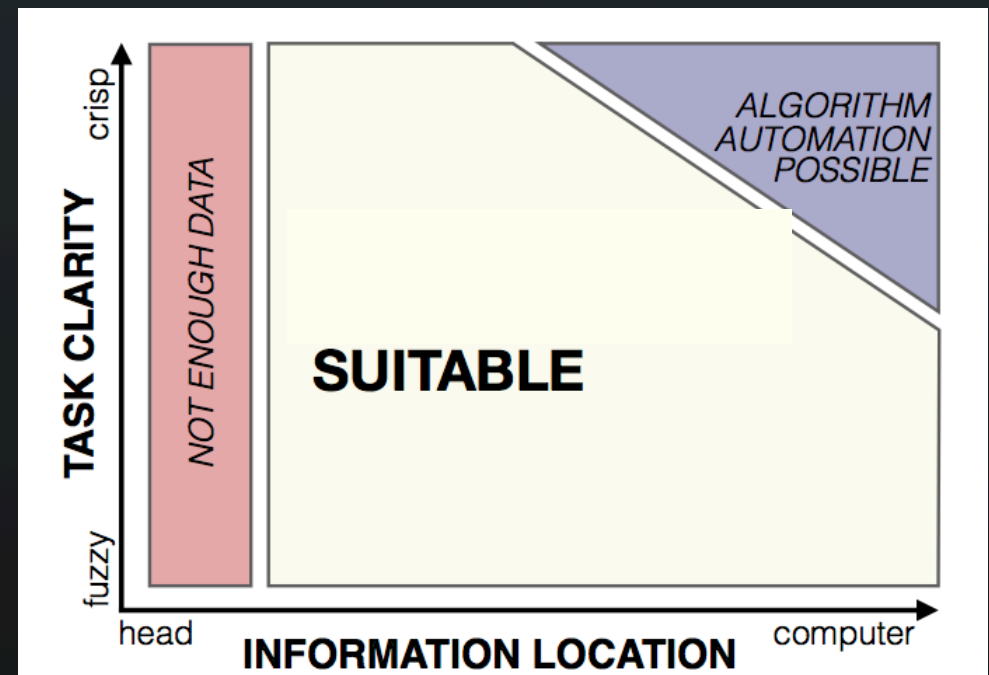
	I		II		III		IV	
	x	y	x	y	x	y	x	y
	10	8,04	10	9,14	10	7,46	8	6,58
	8	6,95	8	8,14	8	6,77	8	5,76
	13	7,58	13	8,74	13	12,74	8	7,71
	9	8,81	9	8,77	9	7,11	8	8,84
	11	8,33	11	9,26	11	7,81	8	8,47
	14	9,96	14	8,1	14	8,84	8	7,04
	6	7,24	6	6,13	6	6,08	8	5,25
	4	4,26	4	3,1	4	5,39	19	12,5
	12	10,84	12	9,13	12	8,15	8	5,56
	7	4,82	7	7,26	7	6,42	8	7,91
	5	5,68	5	4,74	5	5,73	8	6,89
SUM	99,00	82,51	99,00	82,51	99,00	82,50	99,00	82,51
AVG	9,00	7,50	9,00	7,50	9,00	7,50	9,00	7,50
STDEV	3,32	2,03	3,32	2,03	3,32	2,03	3,32	2,03

Visualizing Anscombe's Quartet



Visual representations (Visualization) also not always appropriate

- Use when there is a need to augment human capabilities rather than replace people with computational decision-making methods.

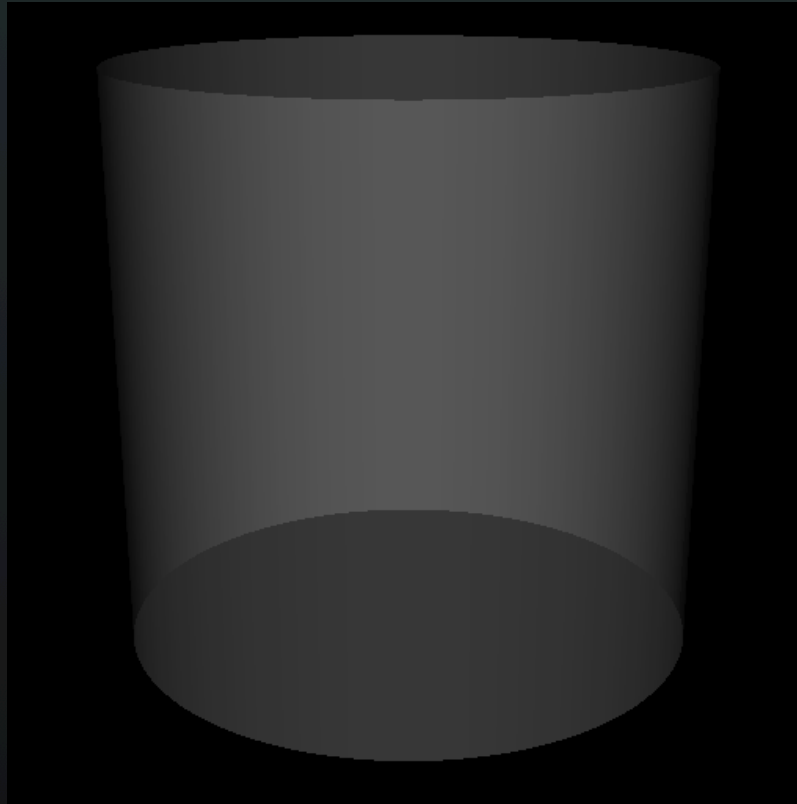


Roadmap

- EVL and Visual Computing
- **Beyond ParaView**
- Precision Medicine
- Bioinformatics

Viscous finger evolution

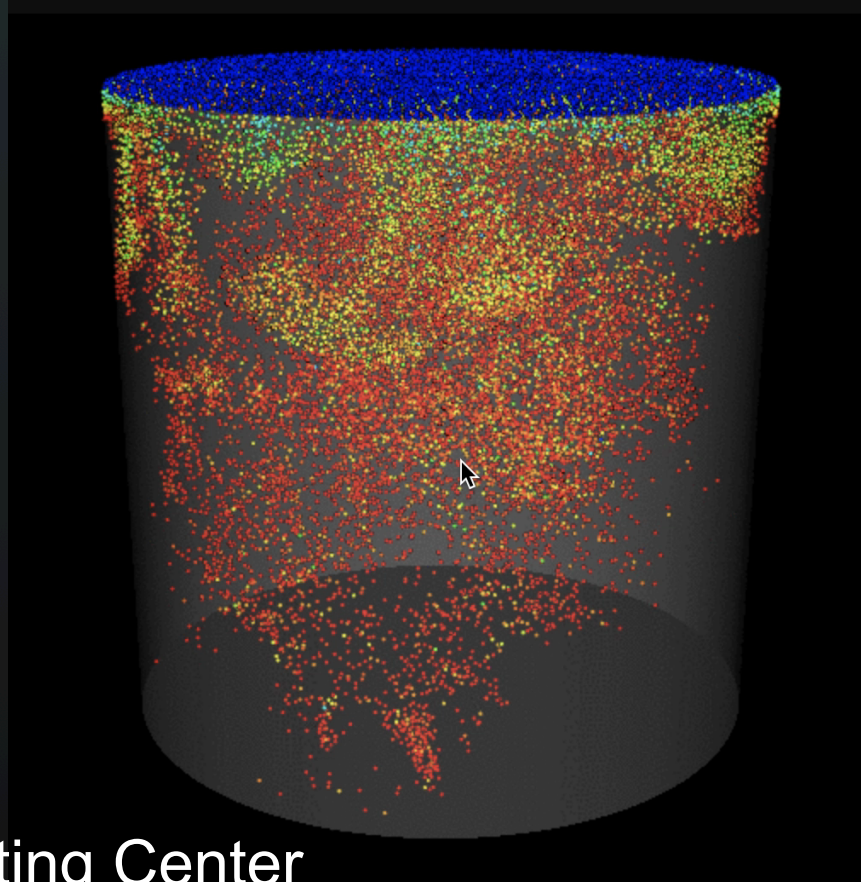
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SciVis Contest 2016
San Diego SuperComputing Center

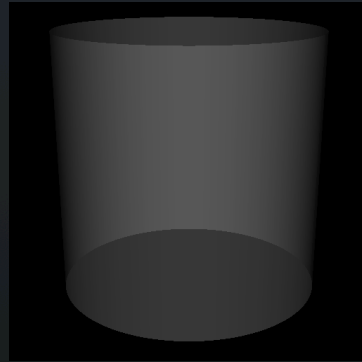
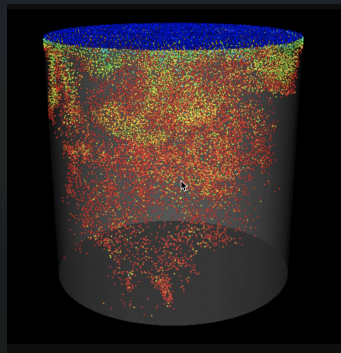
Viscous finger evolution

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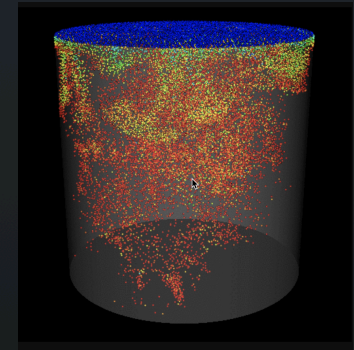


SciVis Contest 2016
San Diego SuperComputing Center

Many stochastic simulations



...



- Results in a simulation ensemble, to be analyzed

CFD in general: two processes

Process 1

- Identify somehow features of interest
 - “[The feature] is hard to define, but when you see it, you recognize it immediately”
- Summarize the features somehow (e.g., mean and stddev)

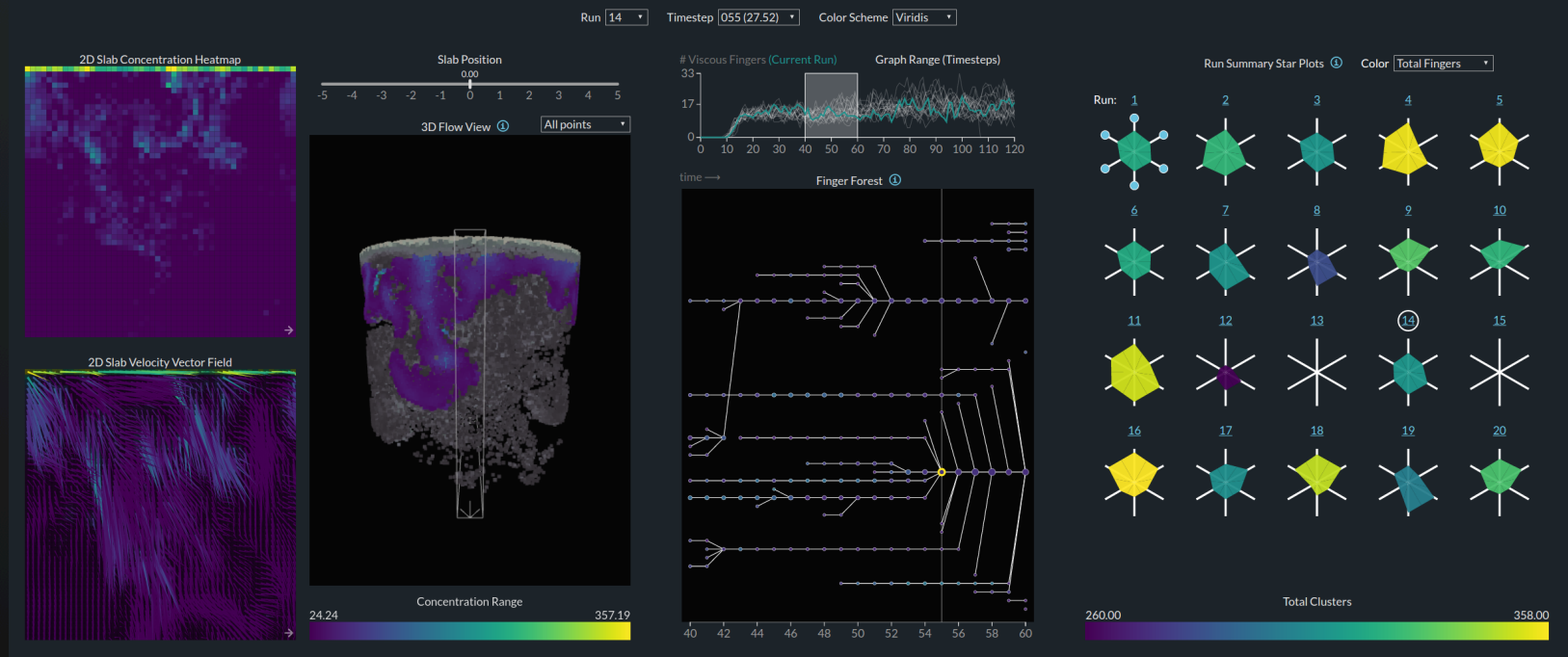
Process 2

- Explore summarization looking for unusual patterns

Unified process using D3 and other web technologies

FingerFinder

Scientific Visualization Contest 2016



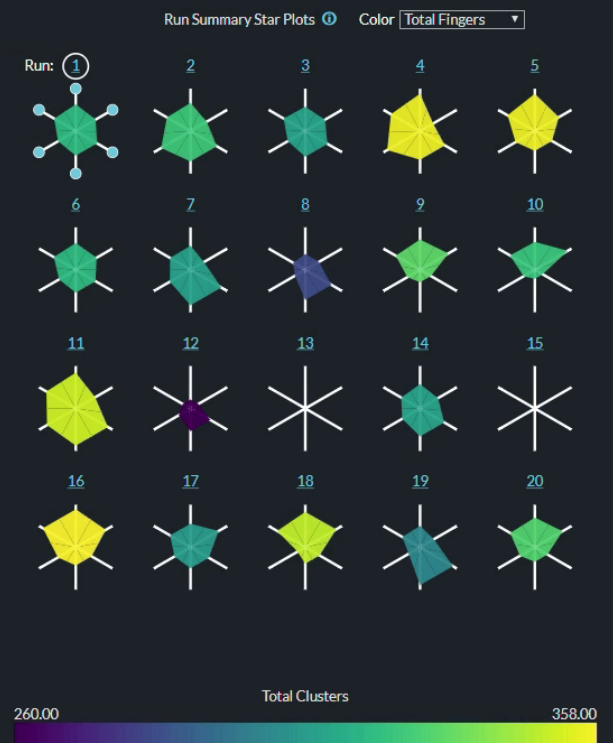
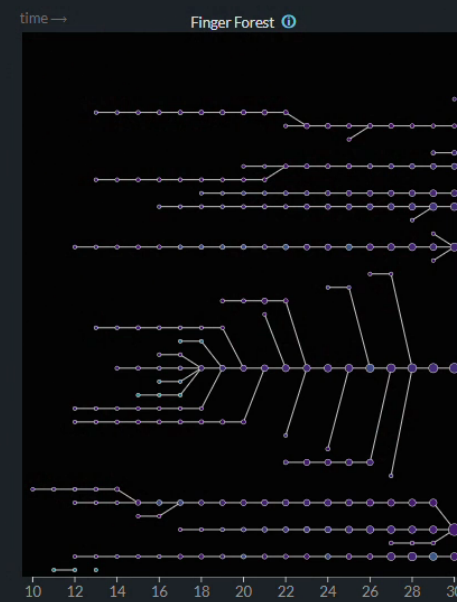
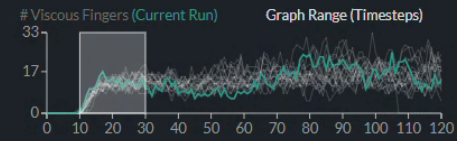
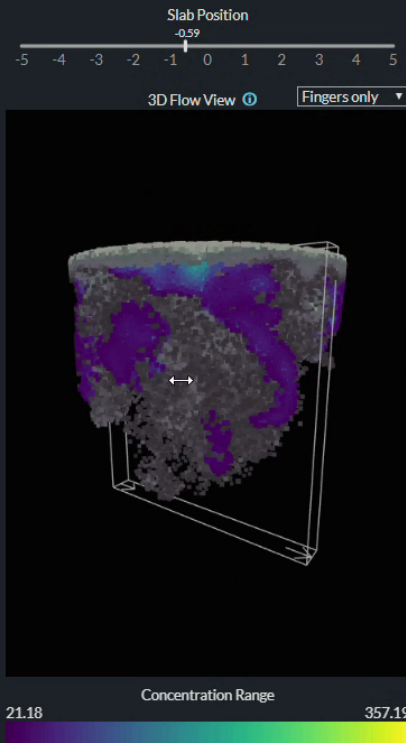
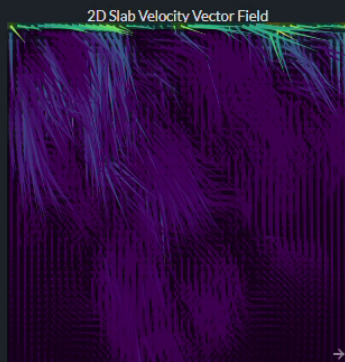
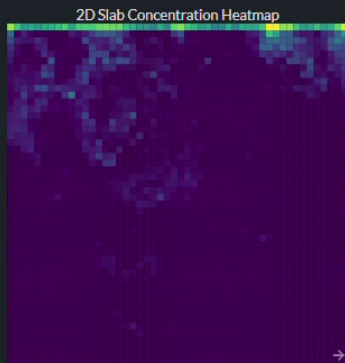
FingerFinder

Scientific Visualization Contest 2016

Run **01**

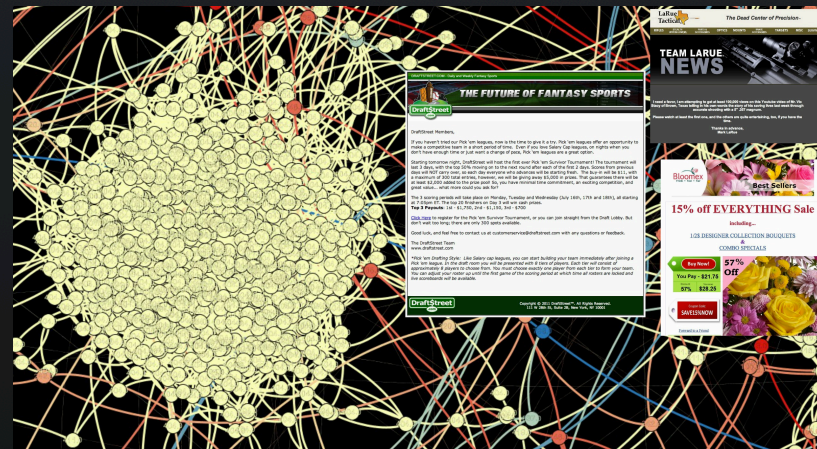
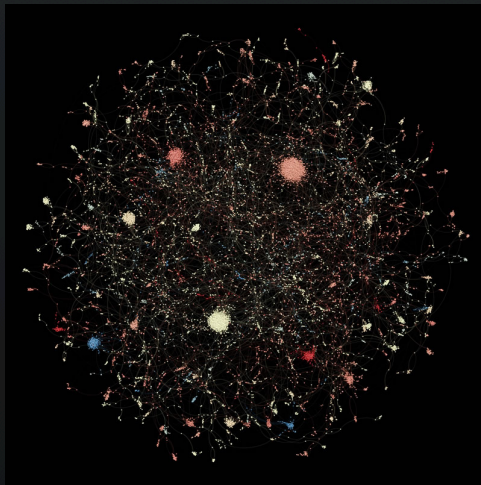
Timestep **044 (22.00)**

Color Scheme **Viridis**



At the human-data interface

- The Shneiderman (or Visual Info Seeking) Mantra:
“Overview first, Zoom in and Filter, then Details on demand”

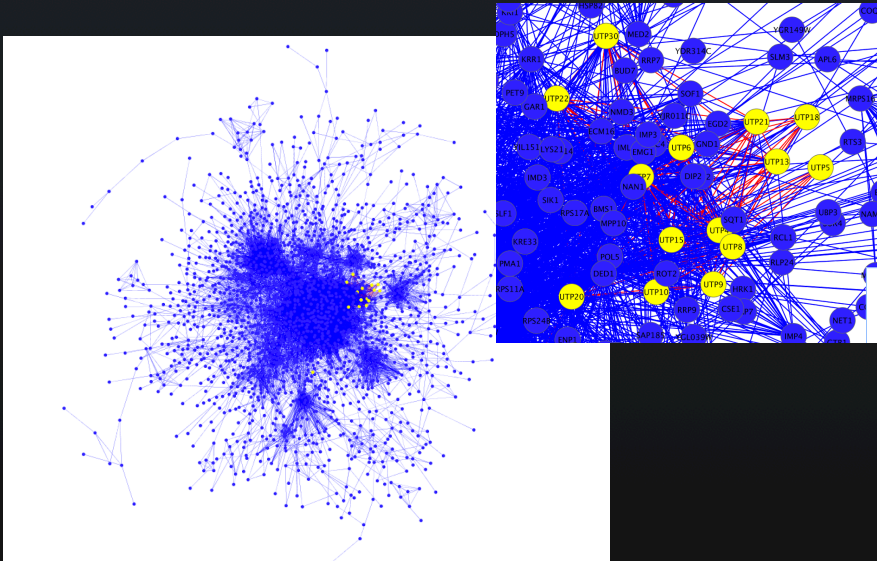


Shneiderman, Ben. "The eyes have it: A task by data type taxonomy for information visualizations." Visual Languages, 1996. Proceedings., IEEE Symposium on. IEEE, 1996.

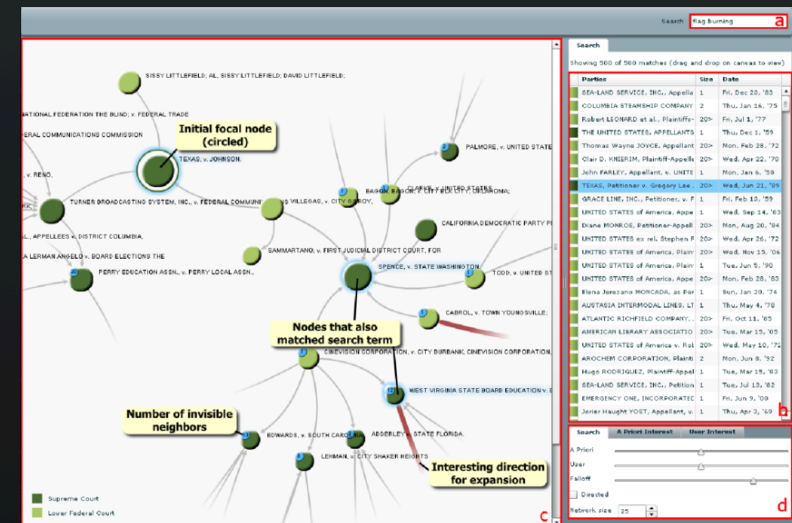
<https://www.recordedfuture.com/information-seeking-mantra/>

At the human-data interface

- The van Ham and Perer Mantra:
“Search first, Show Context, Expand on demand”
aka NOT THIS



BUT
THIS



Van Ham, Frank, and Adam Perer. ““Search, show context, expand on demand”: Supporting large graph exploration with degree-of-interest.” IEEE Transactions on Visualization and Computer Graphics 15.6 (2009).

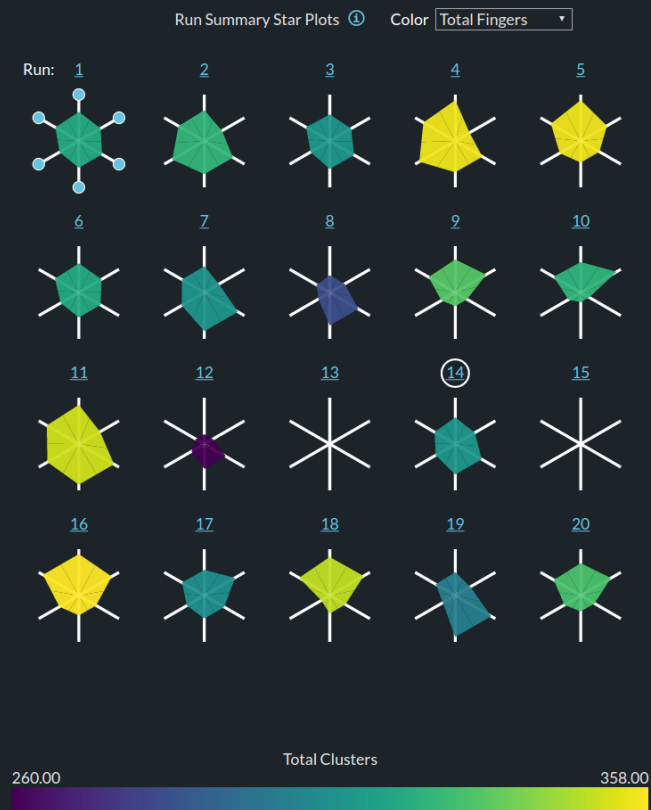
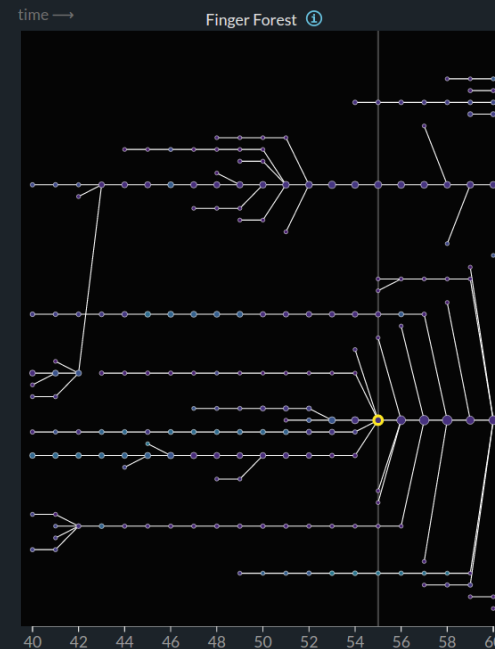
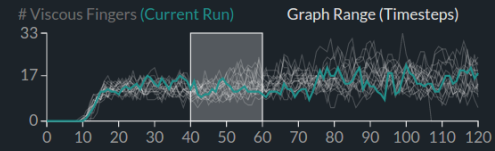
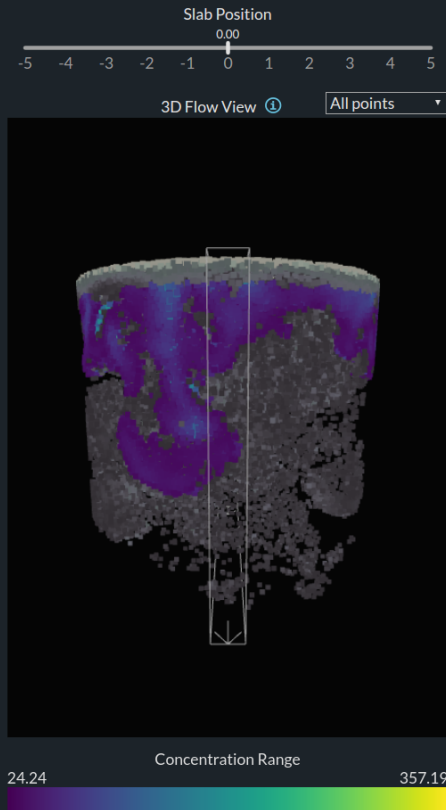
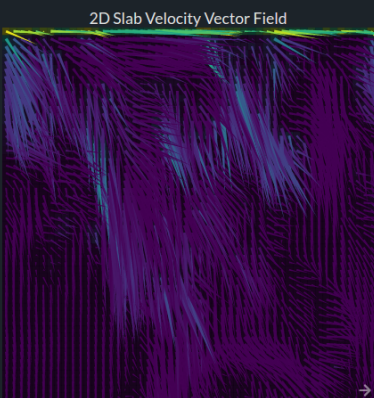
FingerFinder

Scientific Visualization Contest 2016

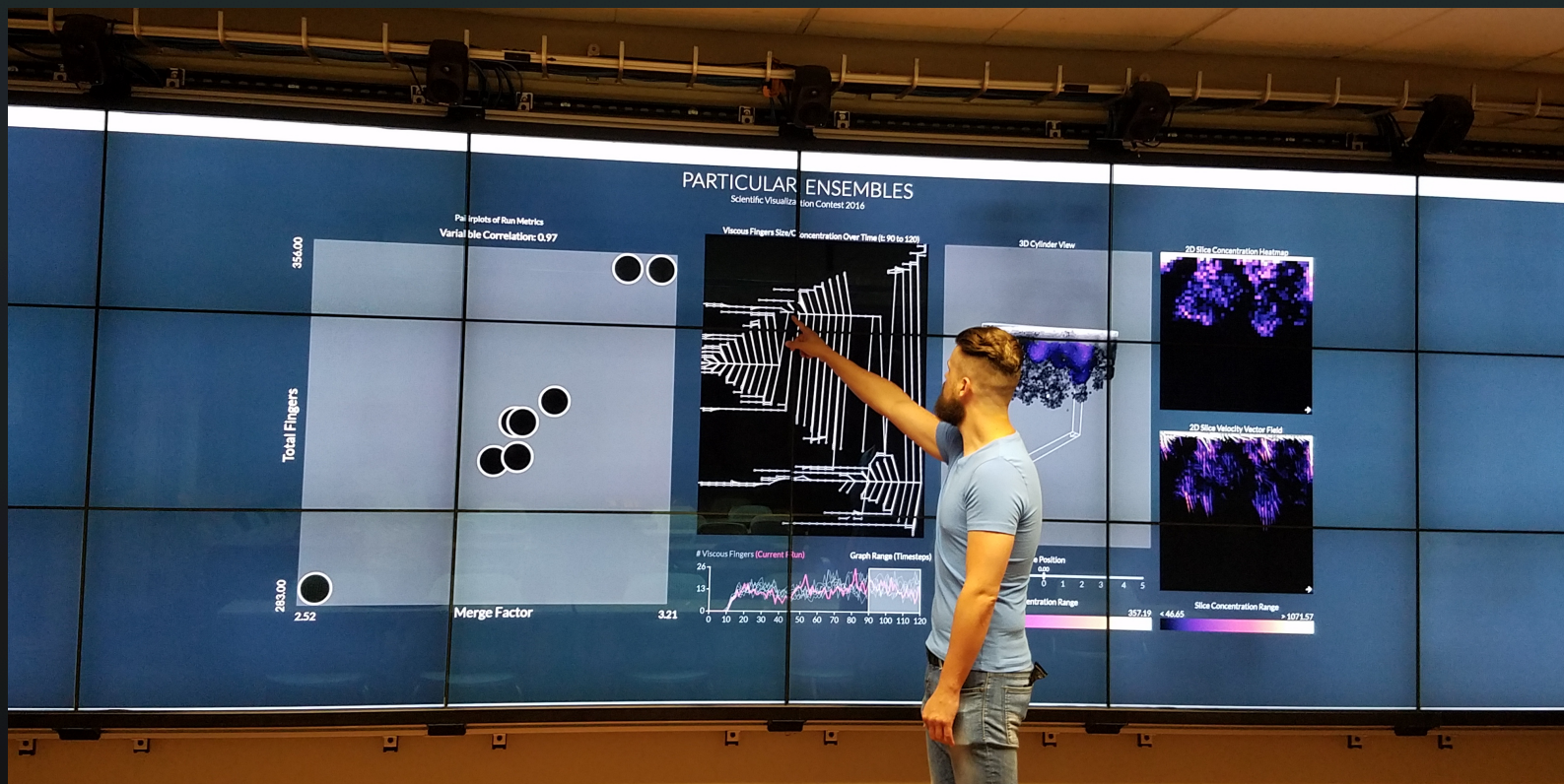
Run **14**

Timestep **055 (27.52)**

Color Scheme **Viridis**



Wall displays



Scientific Workflow theory

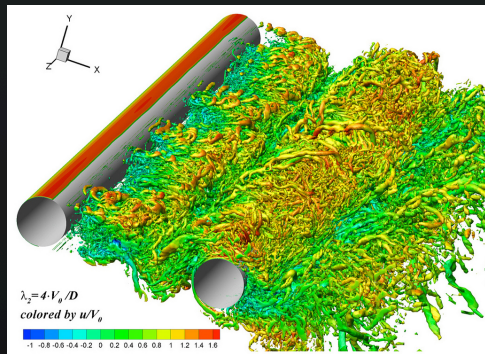
Interface Concept	Data	Control	Resource
Overview	Ensemble \mathbf{E}	Let $\mathbf{E} = \{S_1, S_2, \dots, S_N\}$	
Context	\ni Simulations \mathcal{S} \supset Pointsets \mathbf{P} \supset Finger Subsets \mathbf{F}	Foreach S_j in \mathbf{E} Simulate S_j as $\mathbf{S}_j = \{\mathbf{P}_1, \dots, \mathbf{P}_M\}$ Foreach \mathbf{P}_i in \mathbf{S}_j Calculate $\mathbf{F}_{i,j}$ Analyze $\mathbf{F}_{i,j}$ Track \mathbf{F}_j Analyze \mathbf{F} Summarize \mathbf{F} Analyze $\mathcal{S}(\mathbf{F})$ Summarize $\mathcal{S}(\mathbf{F})$ Analyze $\mathbf{E} \ni \mathcal{S}(\mathbf{F})$	human human human human

$N = \#$ of simulations
 $M = \#$ of timesteps

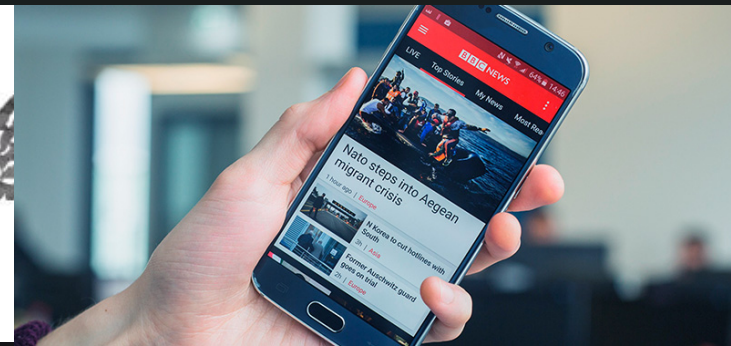
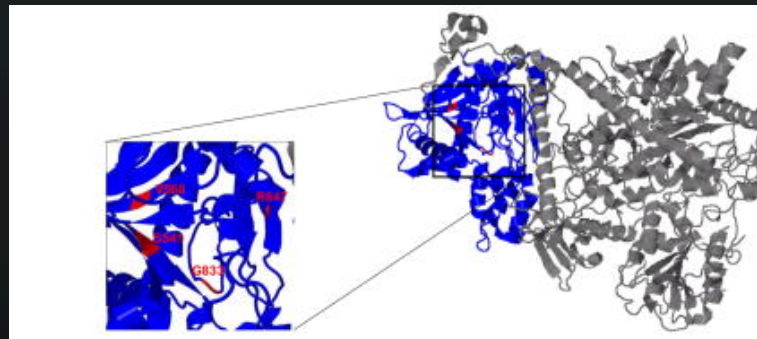
A third theoretical guideline

Luciani, Burks, Sugiyama, Komperda, Marai

- “Details first, Show context, Overview last”
IEEE VIS’18, TVCG 2018
- Details-first in the wild: eng, bio, journalism



Garbaruk et al 2010

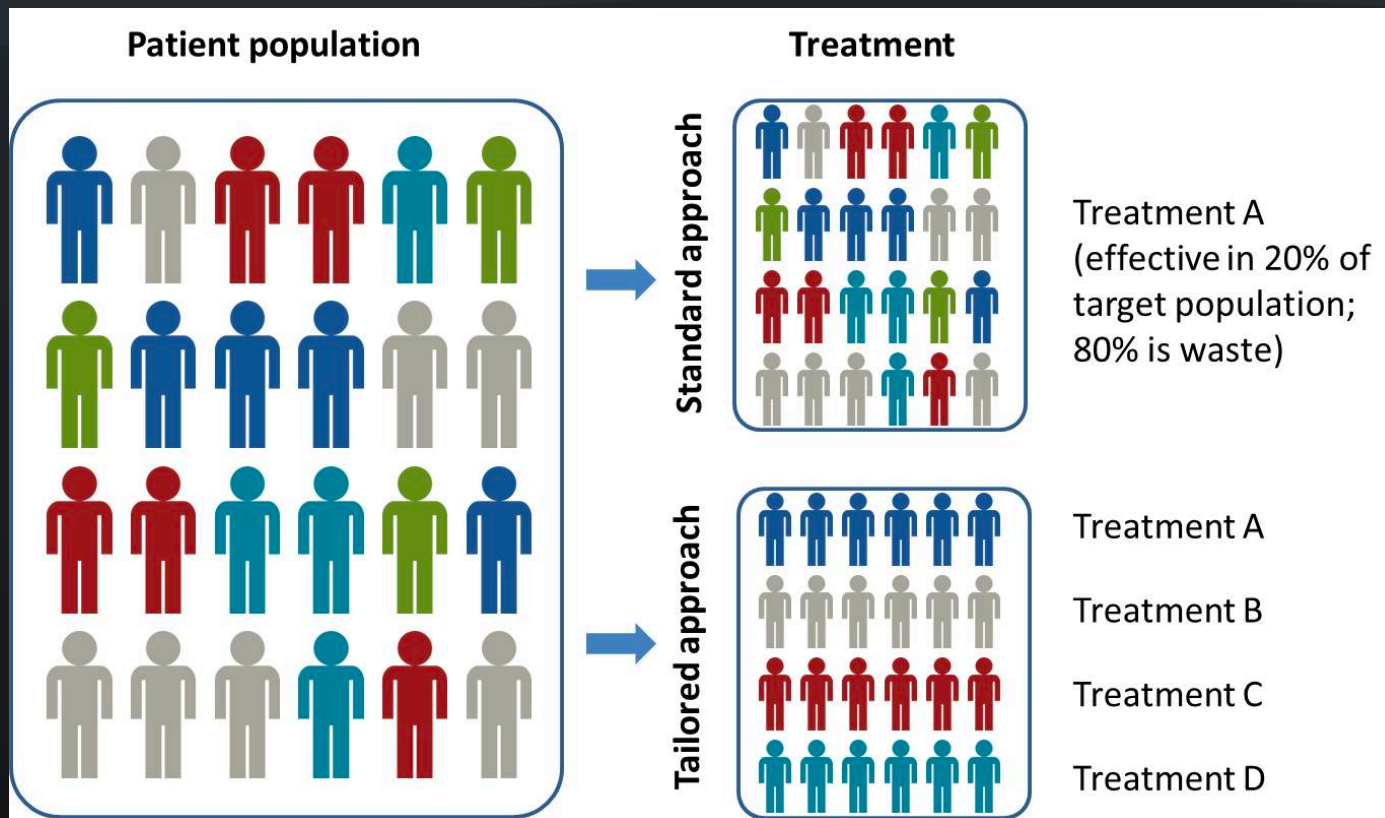


Theory of VIS

- Not a general critique of Shneiderman mantra, but of its sometimes inappropriate application, w/out due consideration to the user workflows, interests, and data flow
- How do we figure out what the domain expert needs?
 - “Activity-Centered Domain Characterization”, Marai, TVCG 2018

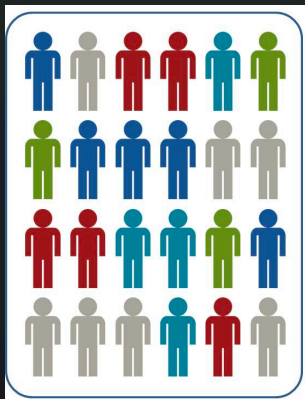
Visual Computing in Precision Medicine

Precision Medicine



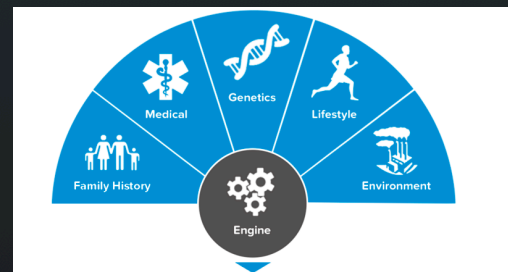
[<http://www.questdiagnostics.com/>]

Data science in medicine



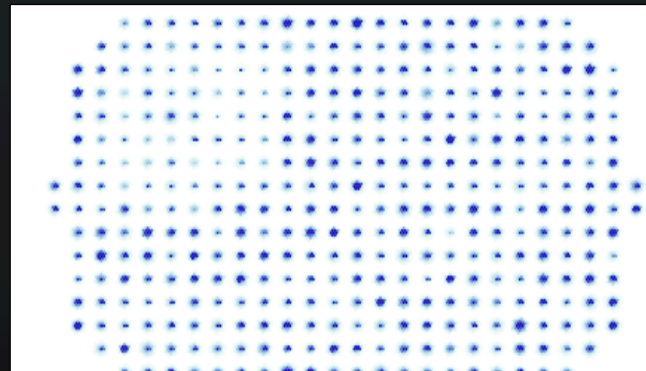
High-dimensional data

+

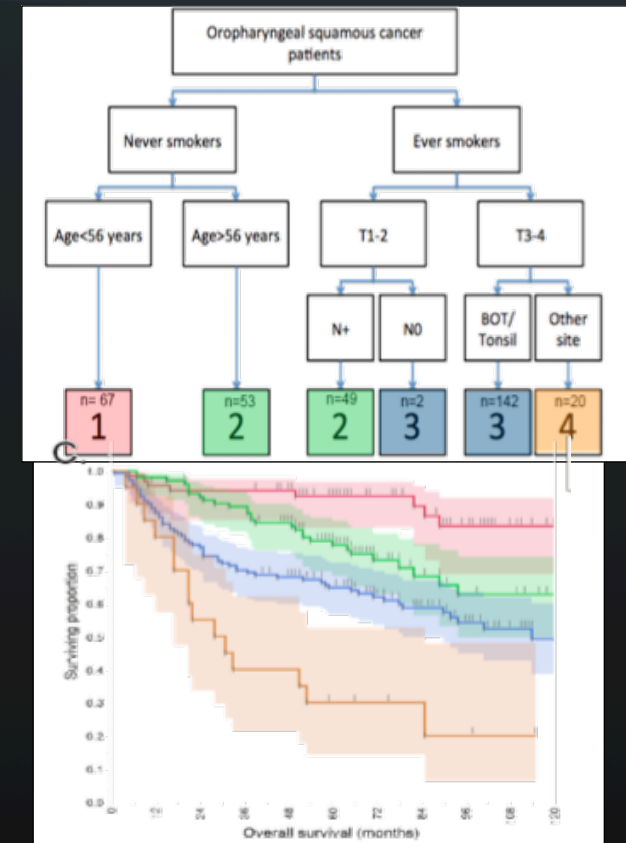


Heterogeneous data

+



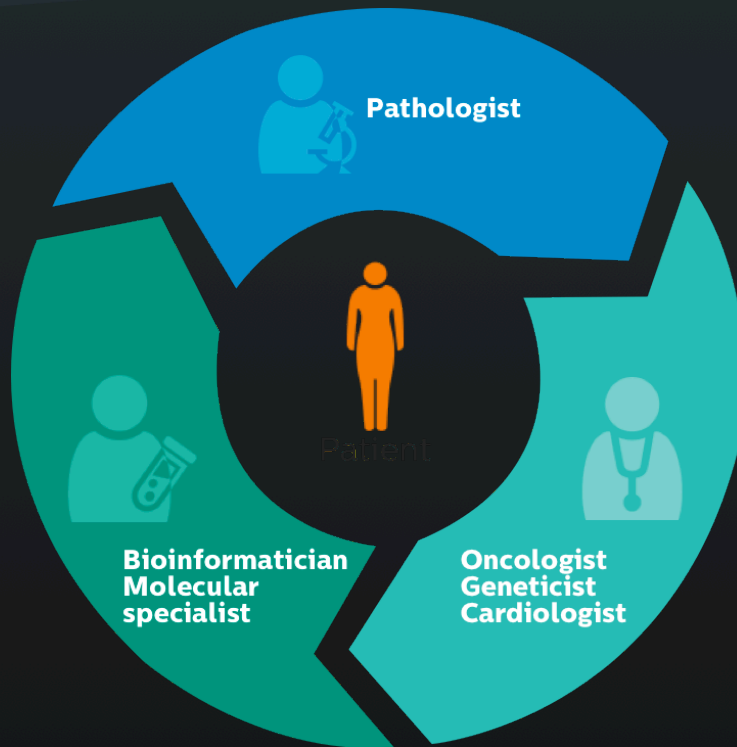
Locally-sparse data



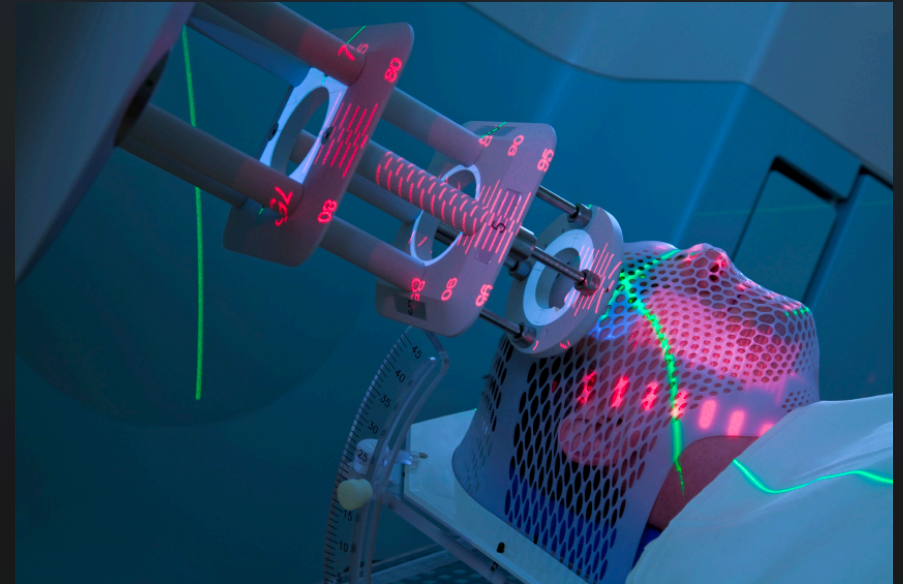
Dynamic data

Head & Neck Oncology

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[<http://hitconsultant.net/>]

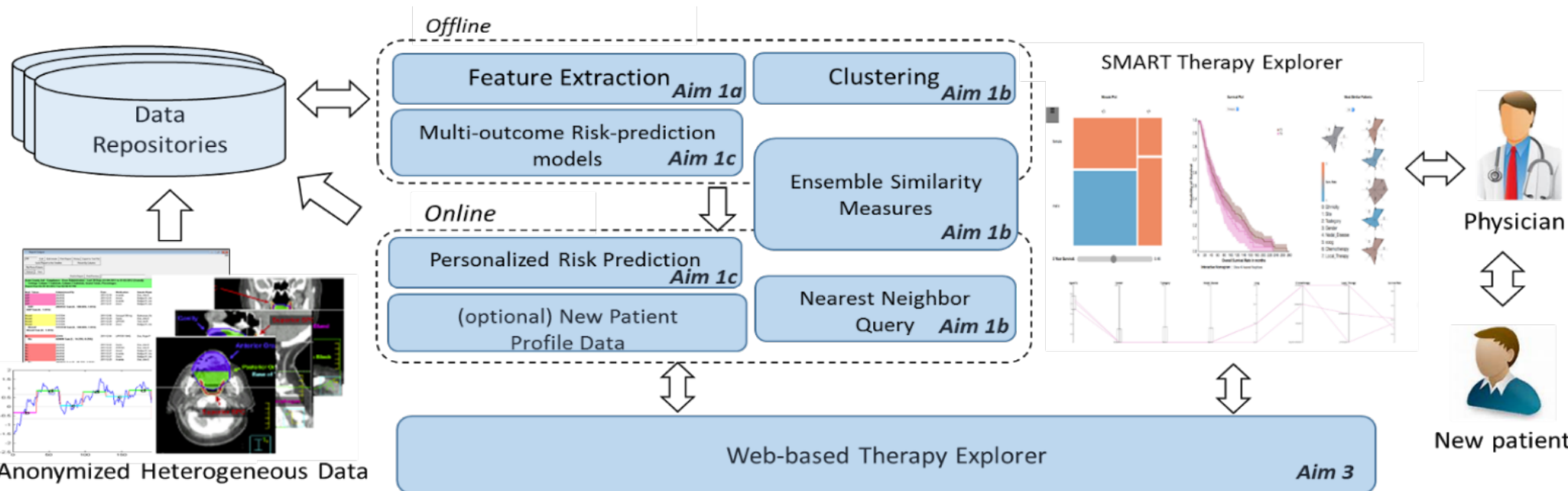


[headandneckcancerguide.org]

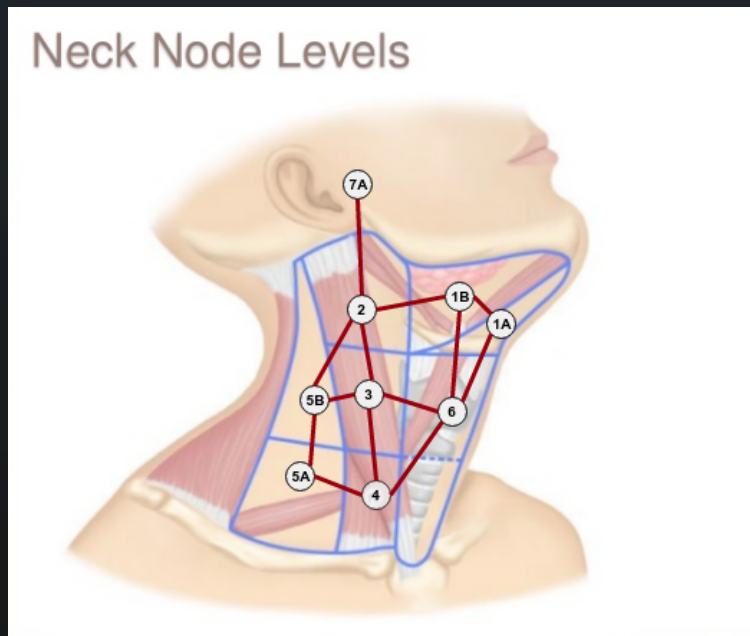
SMART-ACT

(G.E. Marai, G. Canahuate, C.D. Fuller, D. Vock)

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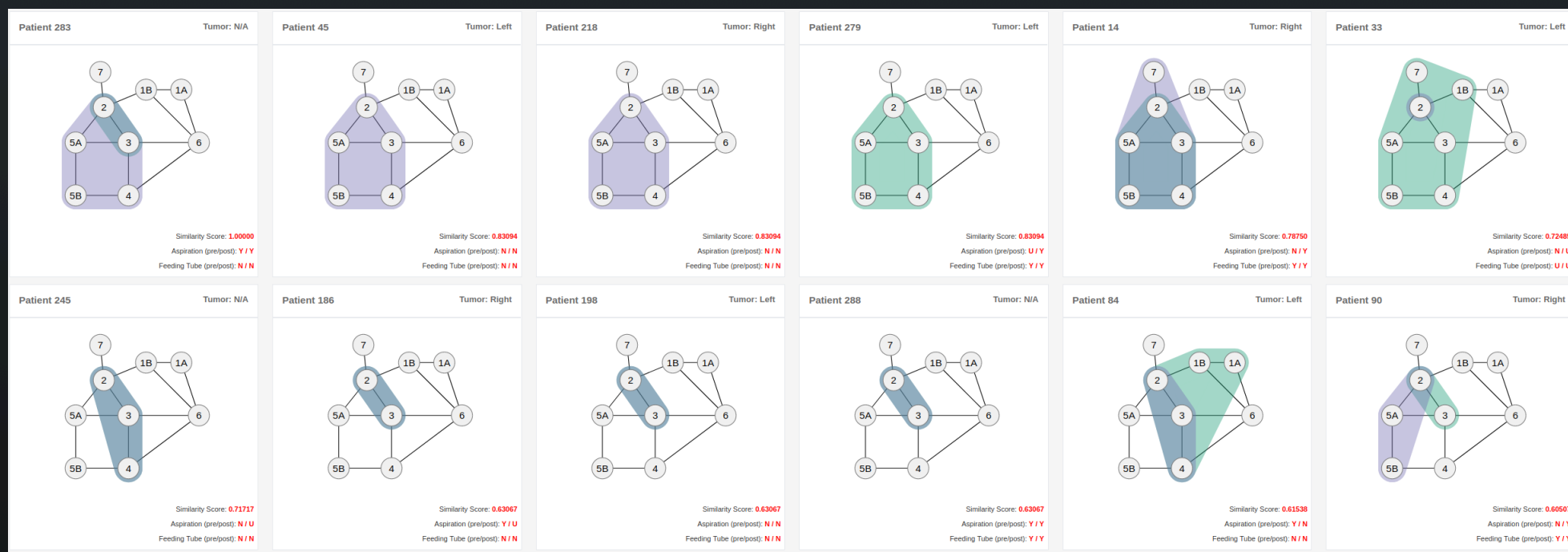


Lymph-node similarity



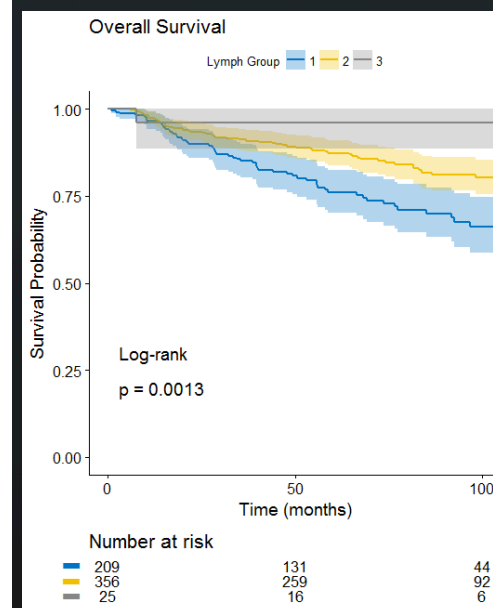
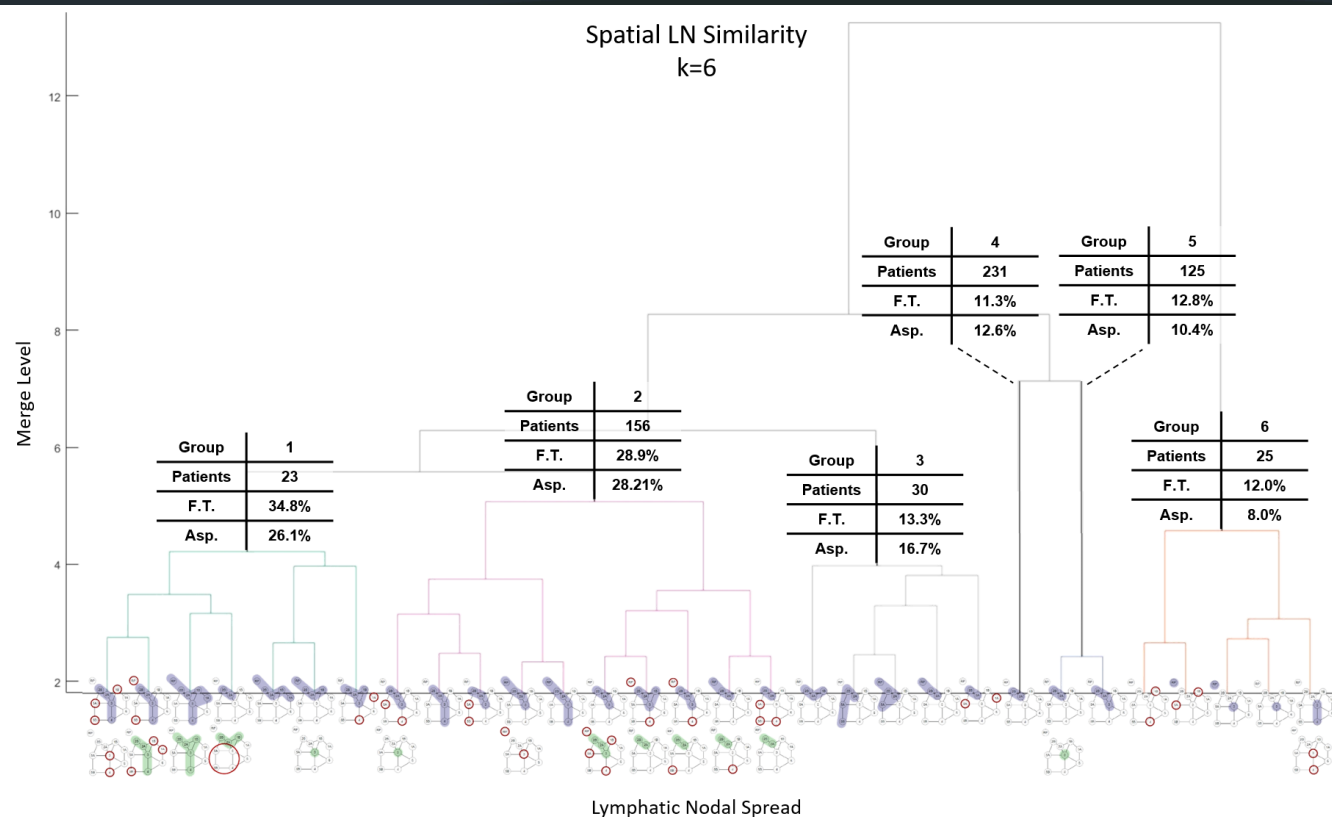
NCI-R01: SMART-ACT Spatial Methodological Approaches for Risk Assessment and Therapeutic Adaptation in Cancer Treatment
(Lead PI on multi-site project: UIC, MDACC, U Iowa, UMN)

Lymph-node similarity



w/ T.Luciani

Correlates w/ toxicity

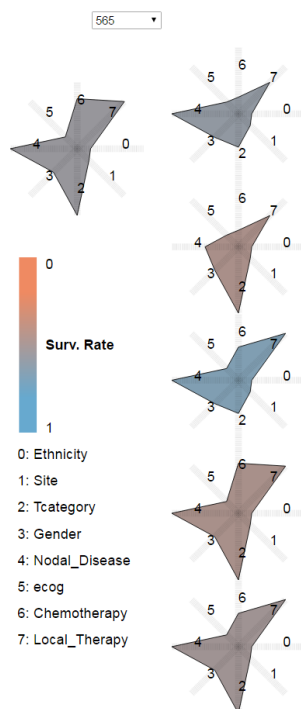


Sharing the results

SMART Therapy Explorer



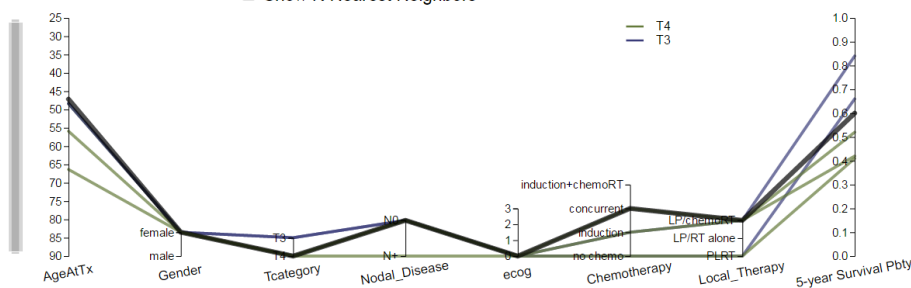
Most Similar Patients ?



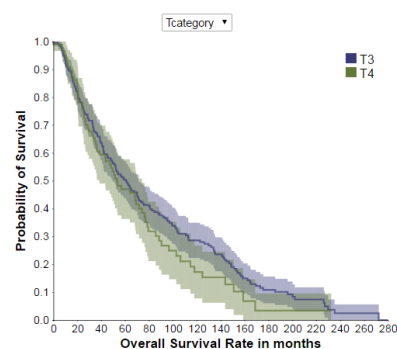
- ☒ AgeAtTx
 - ☒ Gender
 - ☒ Ethnicity
 - ☒ Tcategory
 - ☒ Site
 - ☒ Nodal_Disease
 - ☒ ecog
 - ☒ Chemotherapy
 - ☒ Local_Therapy
 - ☒ 5-year Survival Pbty
- Update Reset
- ☐ Filtered KNN Search
- ☒ Therapy Search

Nomogram Risk Prediction ?

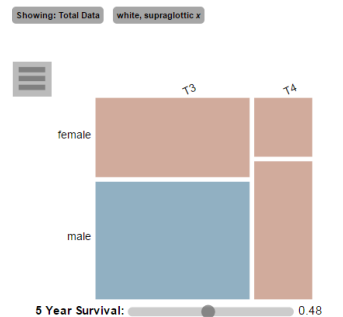
☒ Show K-Nearest Neighbors



Survival Over Time ?



Mosaic Context ?

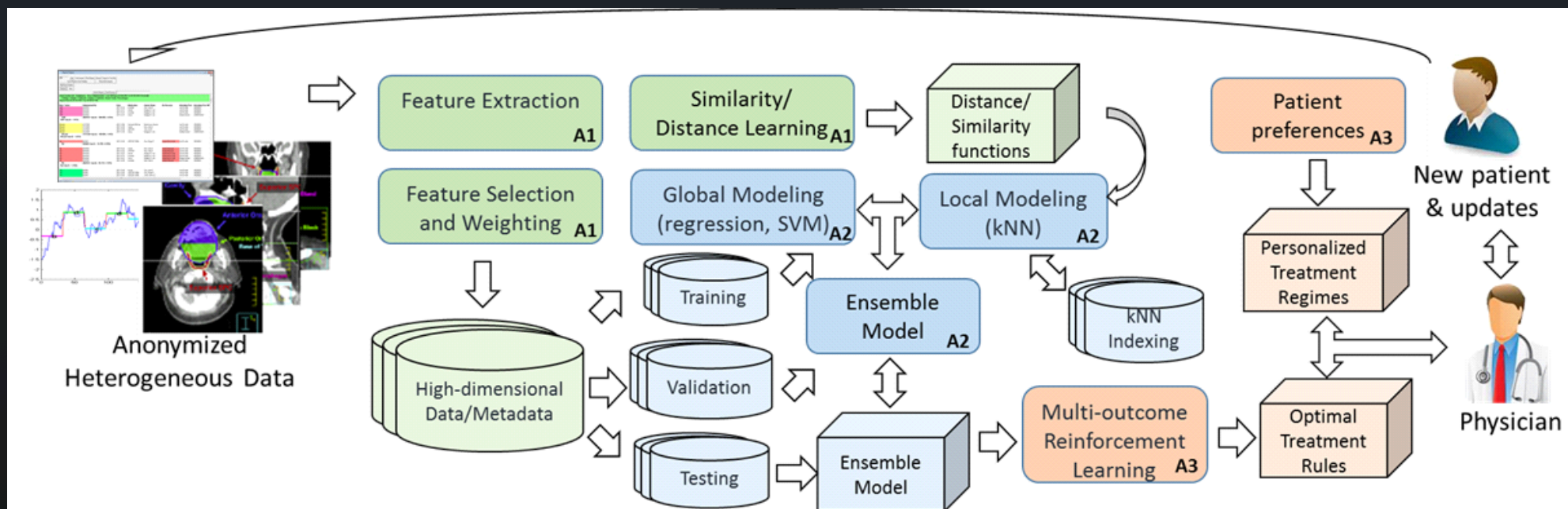


TVCG 2018, Precision Risk Analysis, Marai et al

w/ C.Ma, A. Burks, F.Pellolio, ASR Mohamed,
G. Canahuate, CD Fuller, D. Vock

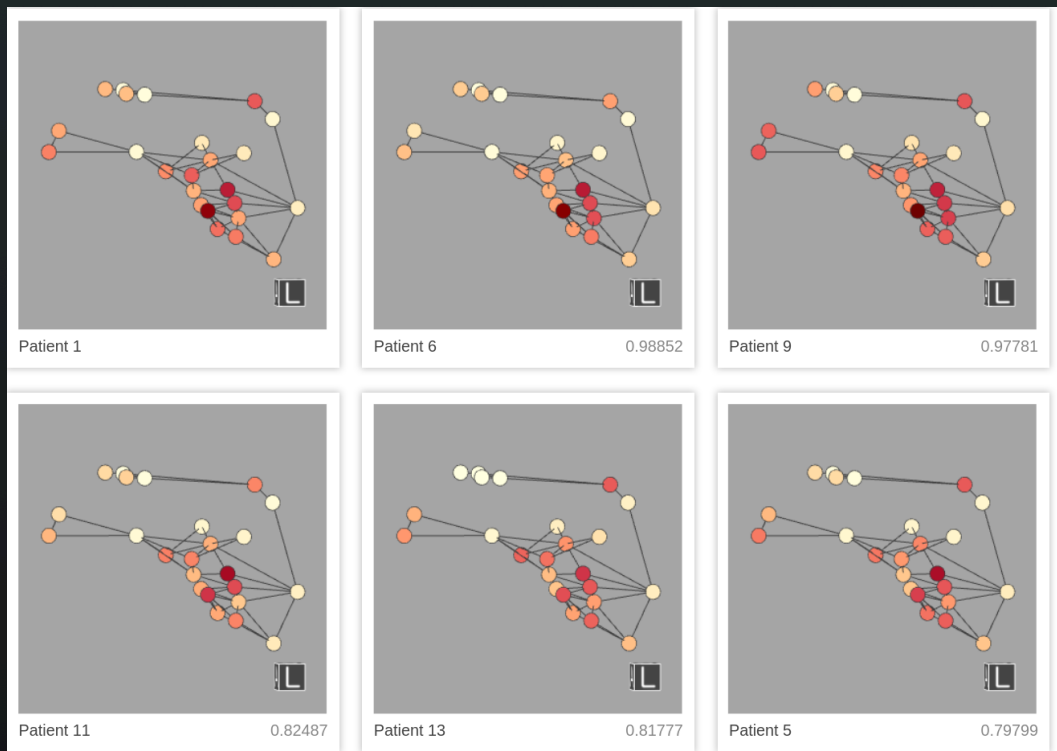
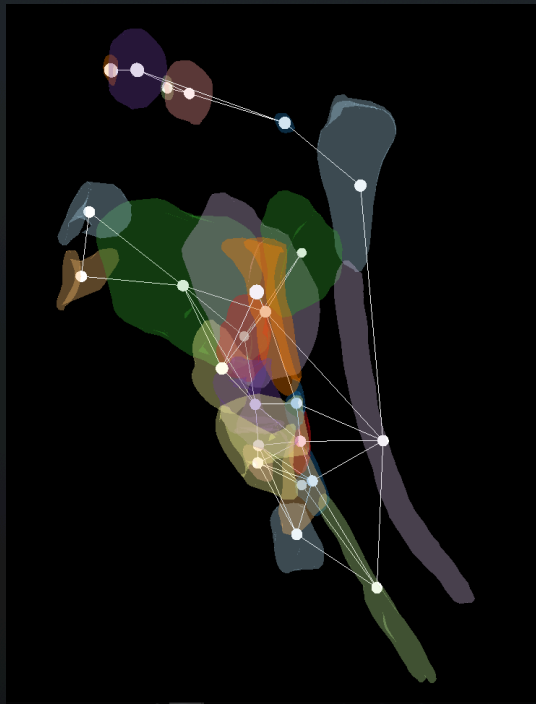
E-Radiomics

(Marai, G. Canahuate, C.D. Fuller, D. Vock)



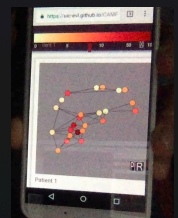
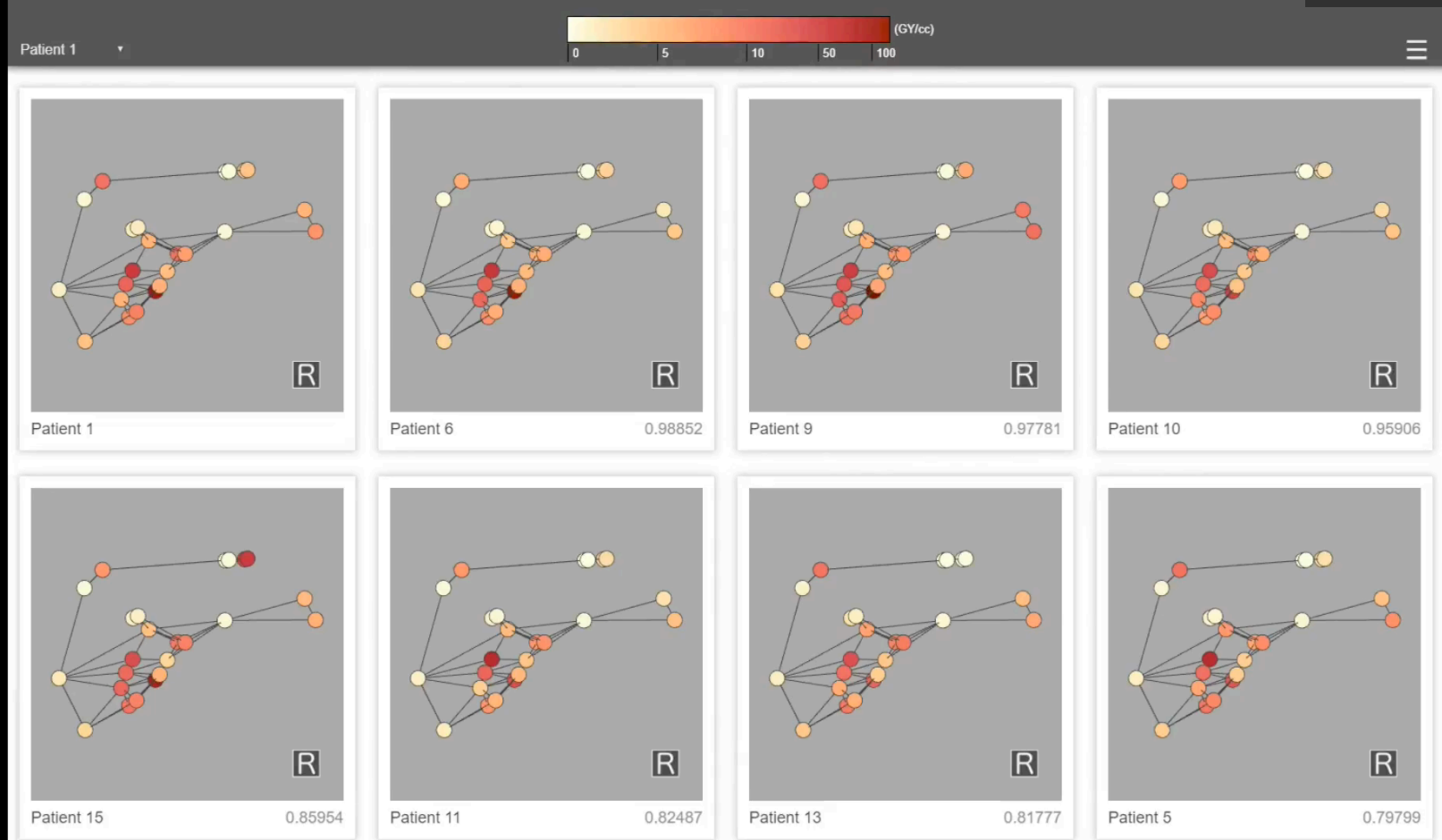
NCI-R01: QuBBD Precision E –Radiomics for Dynamic Big Head & Neck Cancer Data
(Lead PI on multi-site project: UIC, MDACC, U Iowa, UMN)

Radiation Therapy



w/ T. Luciani, P. Hanula, B. Elgohari, ASR. Mohamed, CD. Fulle

RT plan similarity



Visual Computing in Bioinformatics

RuleBender: scientific software with thousands of users

[Vis BioVis 2011] Best Paper Award

[BMC J Bioinformatics 2012]

[J Bioinformatics 2011] w/ J.Faeder, A.Smith, W.Xu

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The screenshot displays the RuleBender software interface, which is divided into two main panels: the Model Editor on the left and the Visualization Viewer on the right.

Model Editor: The top menu bar includes File, Edit, Format, View, Actions, Help, and Options. Below the menu is a toolbar with icons for various actions. The main text area shows a BBNGL script for a model named 'fceri_ji.bngl'. The script includes several reaction rules for the phosphorylation and dephosphorylation of Syk and Rec proteins. The bottom console shows the following messages:

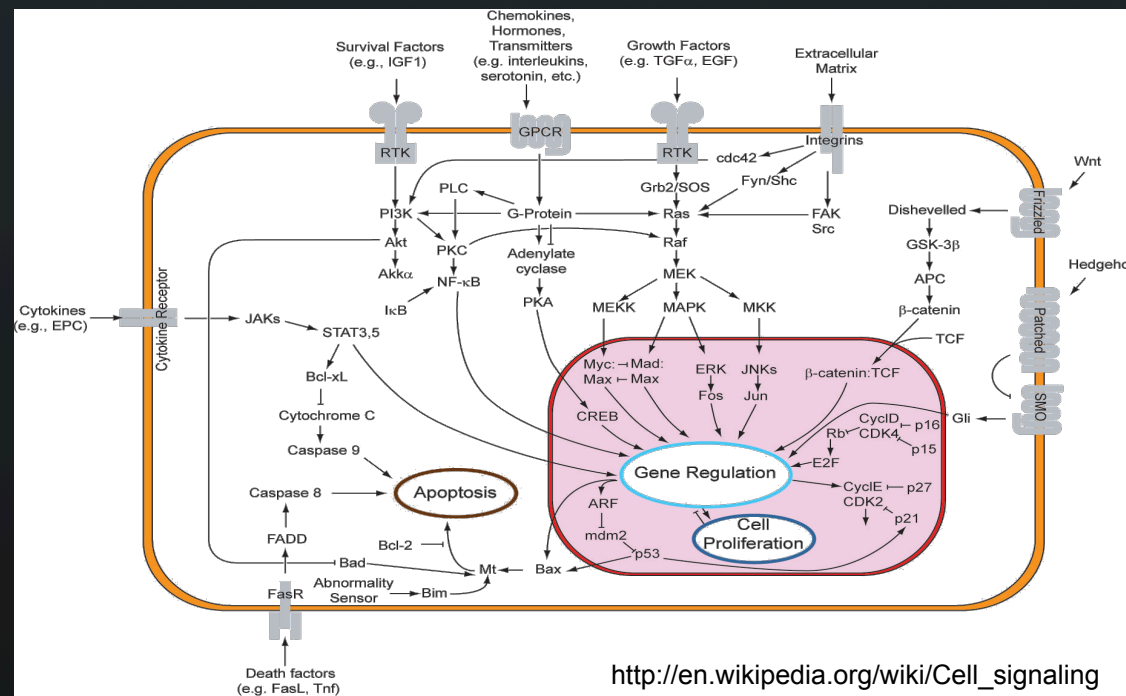
```
Workspace set to /Users/mr_smith22586/Documents/workspace/BNGModels
Parsing Contact Map model...
Contact Map model finished parsing.
Parsing file for Influence Graph...
Influence Graph model finished parsing.
```

Visualization Viewer: The top menu bar includes Model Visualization and Species Browser. The main area shows a network diagram with nodes representing proteins (Syk, Rec, Lig, Lyn) and their interactions. The nodes are color-coded and labeled with their respective states (e.g., Syk, Rec, Lig, Lyn). The bottom area shows a network diagram with nodes representing rules (Rule2, Rule4, Rule5, Rule7, Rule8, Rule10) and their interactions.

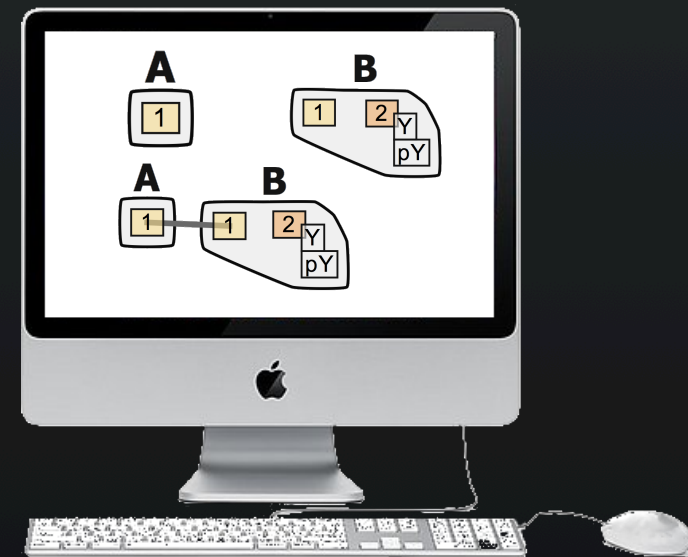
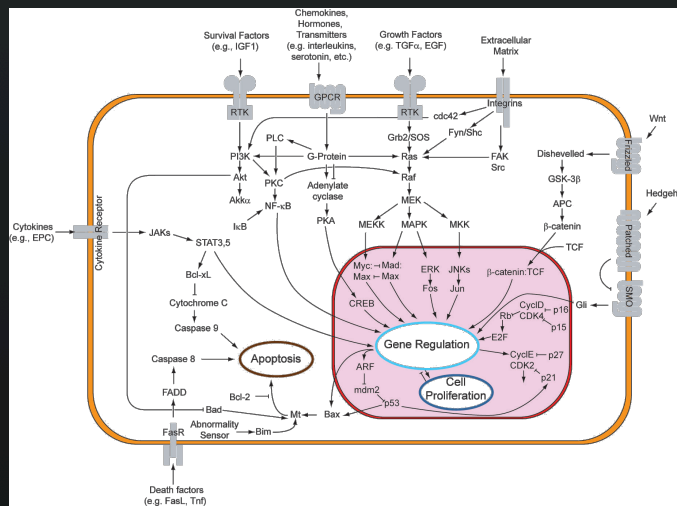
Species Browser: A table on the right side of the Visualization Viewer lists various attributes and their values for the selected species (Syk).

Attribute	Value
Compartment	Y,a~Y~pY
Estimates of constants	
UniProt	
PathwayCommons	
HPRD	
Reactome	
UCSD-Nature	
InterPro	
PROSITE	
KEGG	
ChEBI	
PubChem	

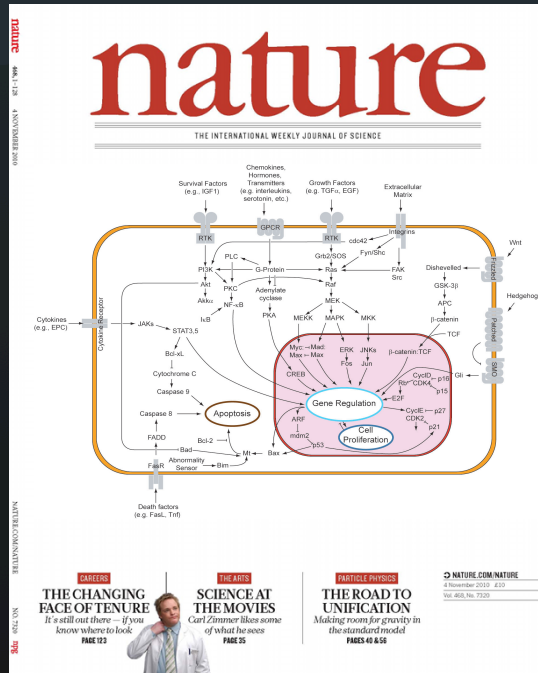
Cell Signaling



Cells as electric circuits



Modeling workflow



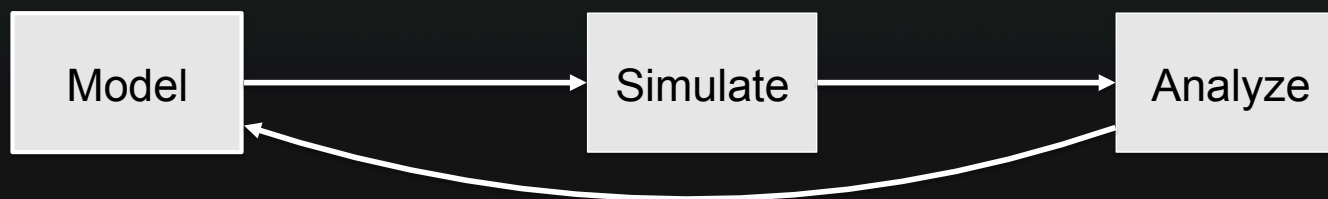
```
File Edit Tools Help
...
begin species
# Set to zero for equilibration
L(r) 0
# r binds to l of R

R(l,r,a) R_tot
# l binds to r of L
# r binds to r of R

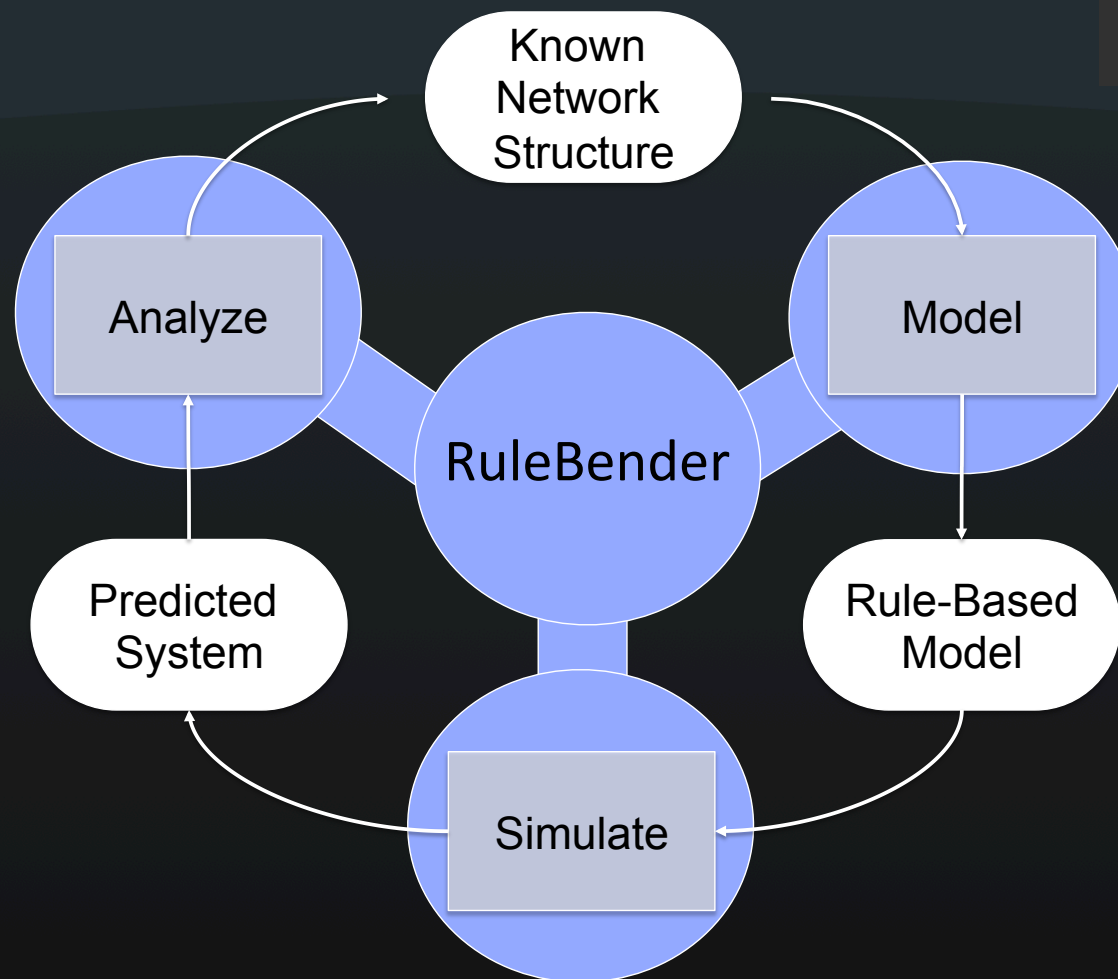
A(r,k) A_tot
# r binds to a of R
# k binds to a of K
...

begin reaction rules
# Ligand binding (L+R)
L(r) + R(l,r) <-> L(r!1).R(l!1,r) kpL,
kmL

#Receptor binding to adaptor (R+A)
A(r) + R(a) <-> A(r!1).R(a!1) kpA,kmA
```



[Vis BioVis 2011] **Best Paper Award**
[BMC J Bioinformatics 2012]
[J Bioinformatics 2011]
w/ J.Faeder, A.Smith, W.Xu



RuleBender: scientific software with thousands of users

[Vis BioVis 2011] Best Paper Award

[BMC J Bioinformatics 2012]

[J Bioinformatics 2011] w/ J.Faeder, A.Smith, W.Xu

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The screenshot displays the RuleBender software interface, which is divided into two main panels: the Model Editor on the left and the Visualization Viewer on the right.

Model Editor: The top section shows a menu bar (File, Edit, Format, View, Actions, Help, Options) and a toolbar. Below this is a text area containing a list of reaction rules for a biological model. The rules are numbered and include comments describing the processes, such as "Transphosphorylation of Syk by SH2-bound Lyn" and "Dephosphorylation of Rec beta". The bottom section of the Model Editor is a console window showing the status of the workspace and the parsing of the model.

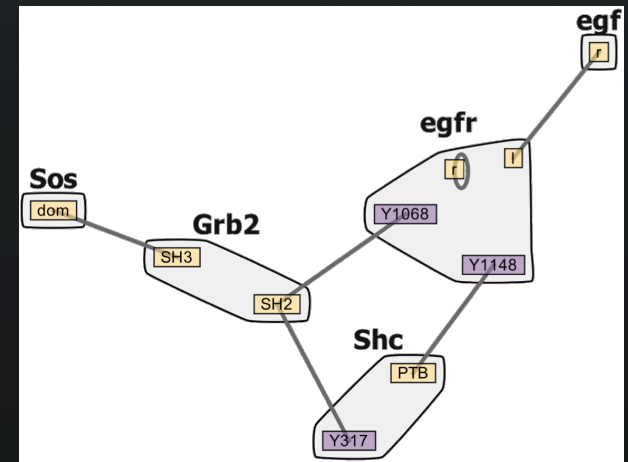
Visualization Viewer: The top section shows a menu bar (Model Visualization, Species Browser) and a toolbar. Below this is a large area for visualizing the model. The main visualization shows a network of nodes (Syk, Rec, Lig, Lyn) and edges representing interactions. The nodes are represented by colored shapes with labels indicating their state (e.g., Syk, Rec, Lig, Lyn). The edges are represented by colored lines with labels indicating the reaction rules (e.g., Rule2, Rule4, Rule5, Rule7, Rule8, Rule10). The bottom section of the Visualization Viewer shows a smaller, more detailed view of the network.

Species Browser: A table on the right side of the Visualization Viewer lists various attributes and their values for the species. The table has two columns: Attribute and Value.

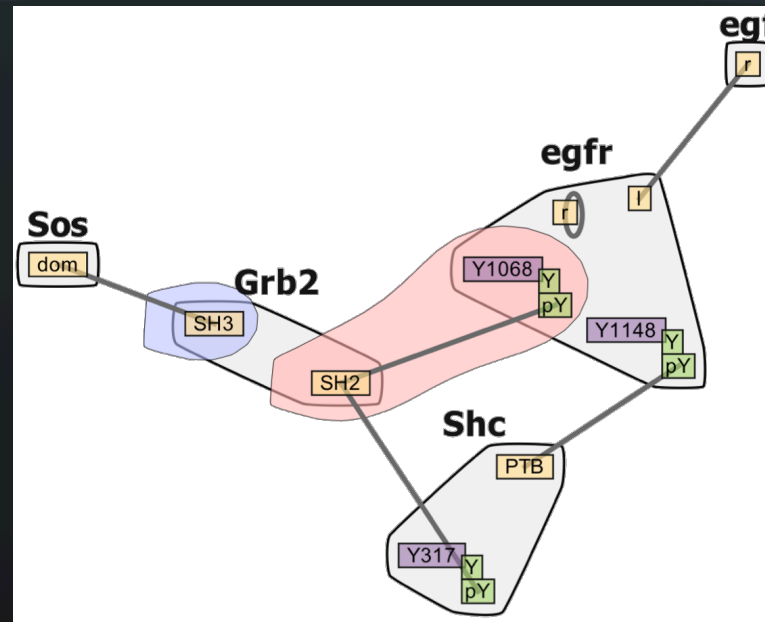
Attribute	Value
Compartment	Y,a~Y~pY
Estimates of constants	
UniProt	
Pathway Commons	
HPRD	
Reactome	
UCSD-Nature	
InterPro	
PROSITE	
KEGG	
ChEBI	
PubChem	

Contact map

- Concise, scalable, graph representation
 - Example: 6 molecules, 37 interactions
 - (generated 365 molecules, more than 3000 interactions)
- Provides global view of a model
- Molecules, internal domains, and states
- Rules:
 - Bond creation/destruction
 - State change

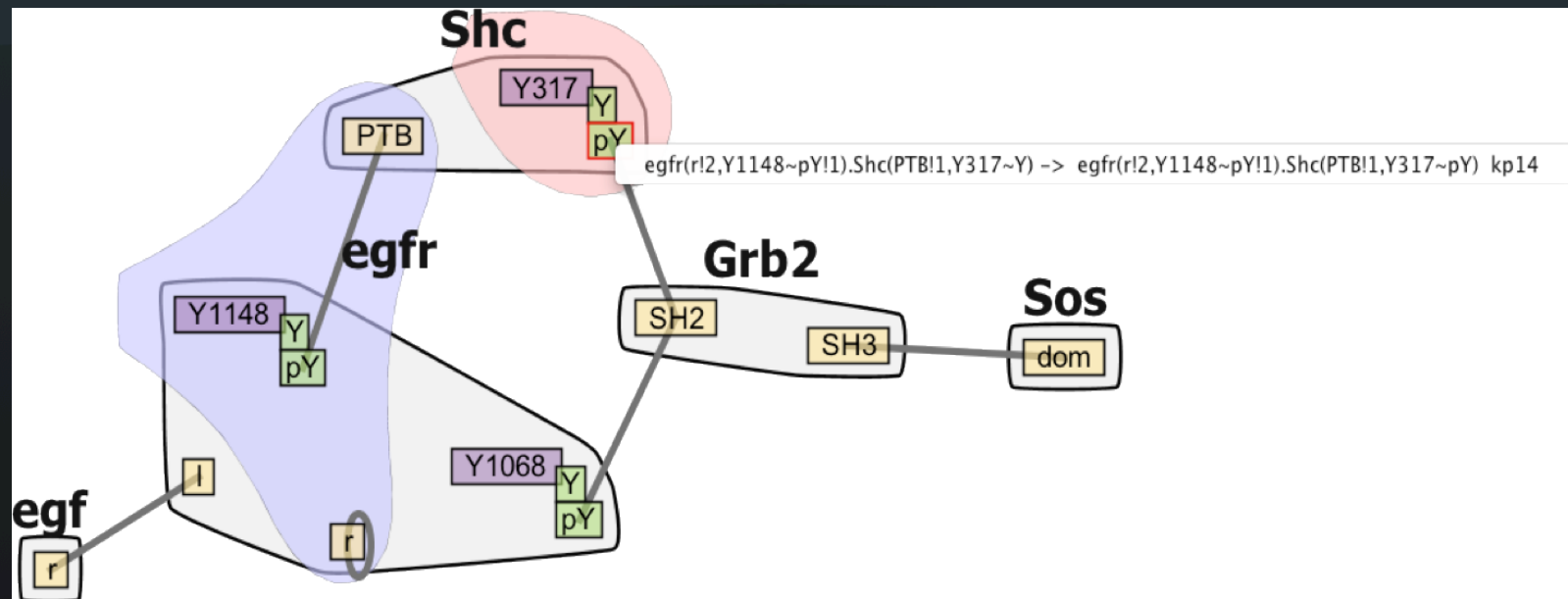


Bubble Sets, Filtering and Data on Demand



$\text{egfr}(\text{Y1068} \sim \text{pY}) + \text{Grb2}(\text{SH2}, \text{SH3}) \leftrightarrow \text{egfr}(\text{Y1068} \sim \text{pY!1}).\text{Grb2}(\text{SH2!1}, \text{SH3})$

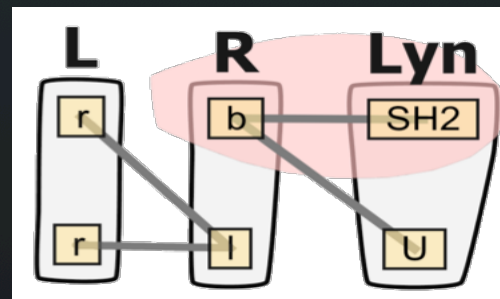
Case Study: EGFR: 6 molecules and 37 rules



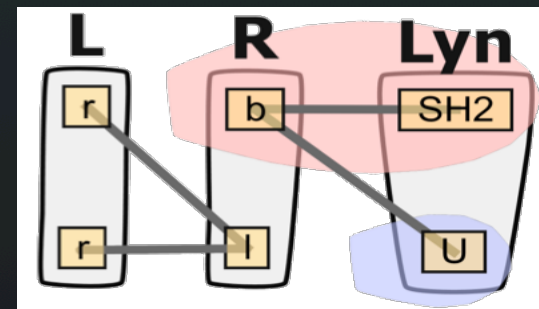
- Contact Map shows two paths for Sos binding
- Bubble Sets shows that egfr dimerization is a necessary condition for the recruitment to take place.

Case Study: Lyn Binding

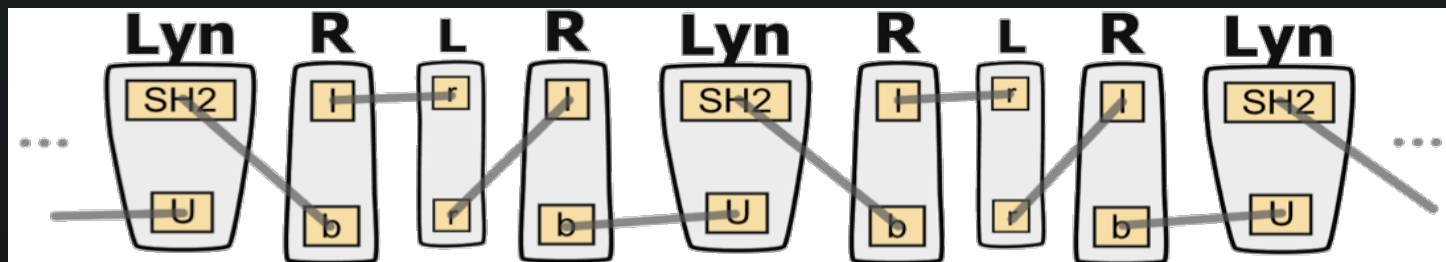
Contact Map:



Incorrect



Correct



Infinite Species

BioVis: 700 *E. Coli* genomes in comparative genomics



w/ J. Aurisano et al, "BactoGeNie", BMC Bioinformatics 2015

Images courtesy of the UIC Electronic Visualization Laboratory (Photos: Lance Long, UIC).

Roadmap

- EVL and Visual Computing
- **Beyond ParaView**
- Precision Medicine
- Bioinformatics

Visual computing can impact significantly scientific research

- Visual Computing: both applications and theory, algos, encodings
- In **engineering**: facilitate analysis of complex datasets and make insights possible
- In **precision medicine**: enable novel calculations over images and 3D models
- In **bioinformatics**: bridge wet-lab with in silico experimentation; enable analysis of large, heterogeneous datasets
- Create shared cognitive spaces; Facilitate communication of results

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- Collaborators and students
- Electronic Visualization Laboratory

Contact

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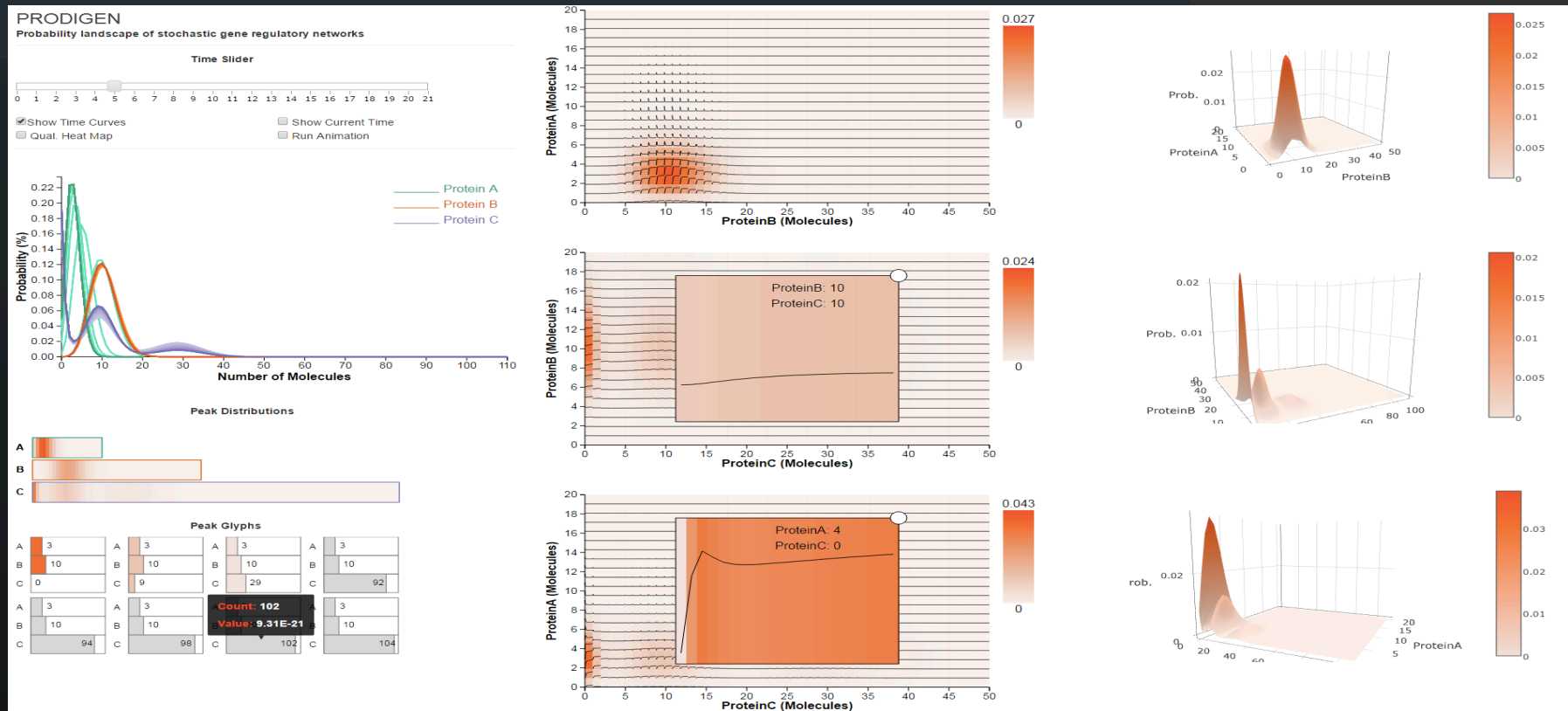


Liz Marai

Electronic Visualization Laboratory, Chicago IL, USA www.evl.uic.edu

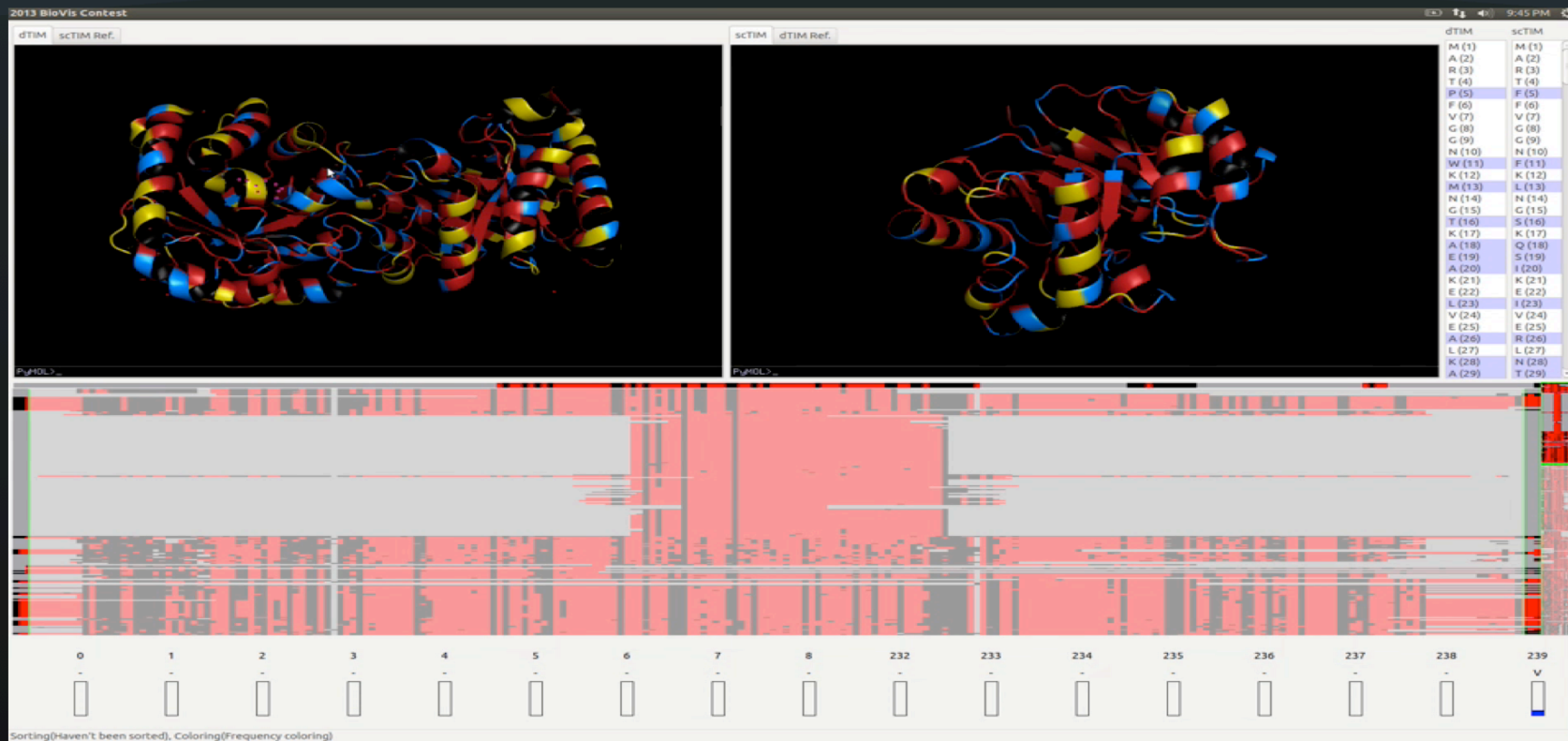
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Prodigen: exploring stochastic cell signaling networks



[Ma et al, BMC Bioinformatics'17] w/ C. Ma, J. Linag, A. Terebus

FixingTIM: identify which mutations are responsible for loss of functionality



[Luciani et al, BMC'13] BioVis Contest Award
w/ T. Luciani, J. Wenksovitch, K. Chen

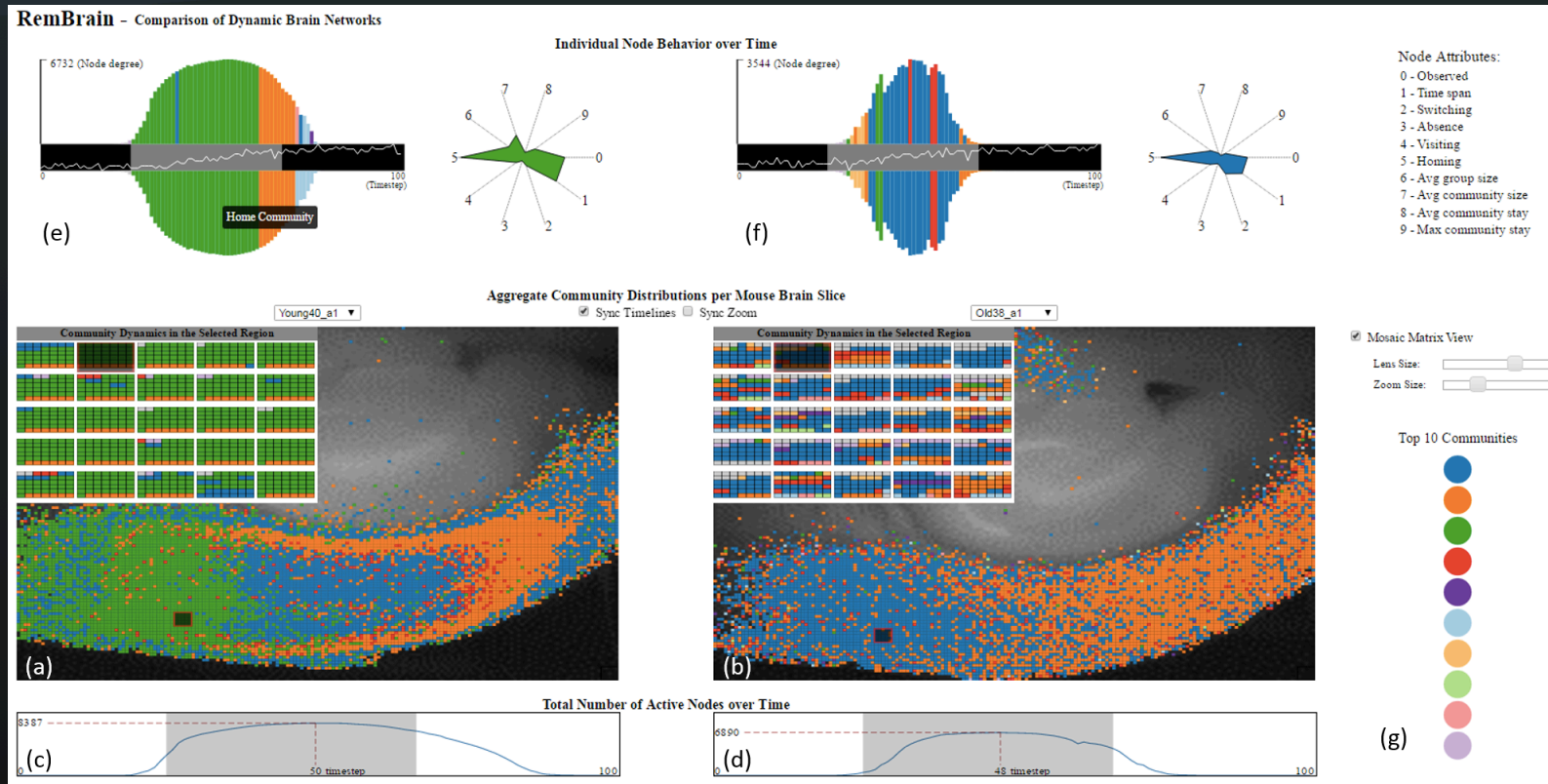
ECHO: effective care hand-offs in ICUs

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[VHAC'17] w/ M.Thomas, T.Kannampallil, J.Abraham

RemBrain: exploring dynamic networks in mouse brains



w/ C. Ma, R. Kenyon, D. Llano, T. Berger-Wolf