Visual Computing at the Electronic Visualization Laboratory

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Electronic Visualization Lab
University of Illinois at Chicago
UIC Electronic Visualization Laboratory (EVL)

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

<table>
<thead>
<tr>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
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<td>4.26</td>
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<td>4.74</td>
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<td>STDEV</td>
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</tr>
</tbody>
</table>

Marai: Intro to Bio Vis
Visualizing Anscombe’s Quartet

Marai: Intro to Bio Vis
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

SciVis Contest 2016
San Diego SuperComputing Center
Viscous finger evolution

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
At the human-data interface

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

At the human-data interface

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

BUT THIS

Wall displays
### Scientific Workflow theory

<table>
<thead>
<tr>
<th>Interface Concept</th>
<th>Data</th>
<th>Control</th>
<th>Resource</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overview</td>
<td>Ensemble $E$</td>
<td>Let $E = {S_1, S_2, \ldots, S_N}$</td>
<td></td>
</tr>
<tr>
<td>Context</td>
<td>Simulations $S_j$</td>
<td>Foreach $S_j$ in $E$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pointsets $P_i$</td>
<td>Simulate $S_j$ as $S_j = {P_1, \ldots, P_M}$</td>
<td></td>
</tr>
<tr>
<td>Details</td>
<td>Finger Subsets $F$</td>
<td>Foreach $P_i$ in $S_j$</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Calculate $F_{ij}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Analyze $F_{ij}$</td>
<td>Human</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Track $F_j$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Analyze $F$</td>
<td>Human</td>
</tr>
<tr>
<td>$N = #$ of simulations</td>
<td>Summarize $F$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M = #$ of timesteps</td>
<td>Analyze $S(F)$</td>
<td></td>
<td>Human</td>
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<tr>
<td></td>
<td>Summarize $S(F)$</td>
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<tr>
<td></td>
<td>Analyze $E \ni S(F)$</td>
<td></td>
<td>Human</td>
</tr>
</tbody>
</table>
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

Chapman et al 2011

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

Patient population

Treatment

Standard approach

- Treatment A (effective in 20% of target population; 80% is waste)

Tailored approach

- Treatment A
- Treatment B
- Treatment C
- Treatment D

[http://www.questdiagnostics.com/]
Data science in medicine

- High-dimensional data
- Heterogeneous data
- Locally-sparse data
- Dynamic data
Head & Neck Oncology

[http://hitconsultant.net/]

[headandneckcancerguide.org]
SMART-ACT
(G.E. Marai, G. Canahuate, C.D. Fuller, D. Vock)
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

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. Fuller
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
Cells as electric circuits
Modeling workflow

Modeling workflow

Model

Simulate

Analyze

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,k) + R(a) <-> A(r!1).R(a!1) kpA, kmA
RuleBender

- Known Network Structure
- Model
- Rule-Based Model
- Simulate
- Analyze
- Predicted System

[Vis BioVis 2011] Best Paper Award
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RuleBender: scientific software with thousands of users

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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

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

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- Electronic Visualization Laboratory
Contact

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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

[ 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