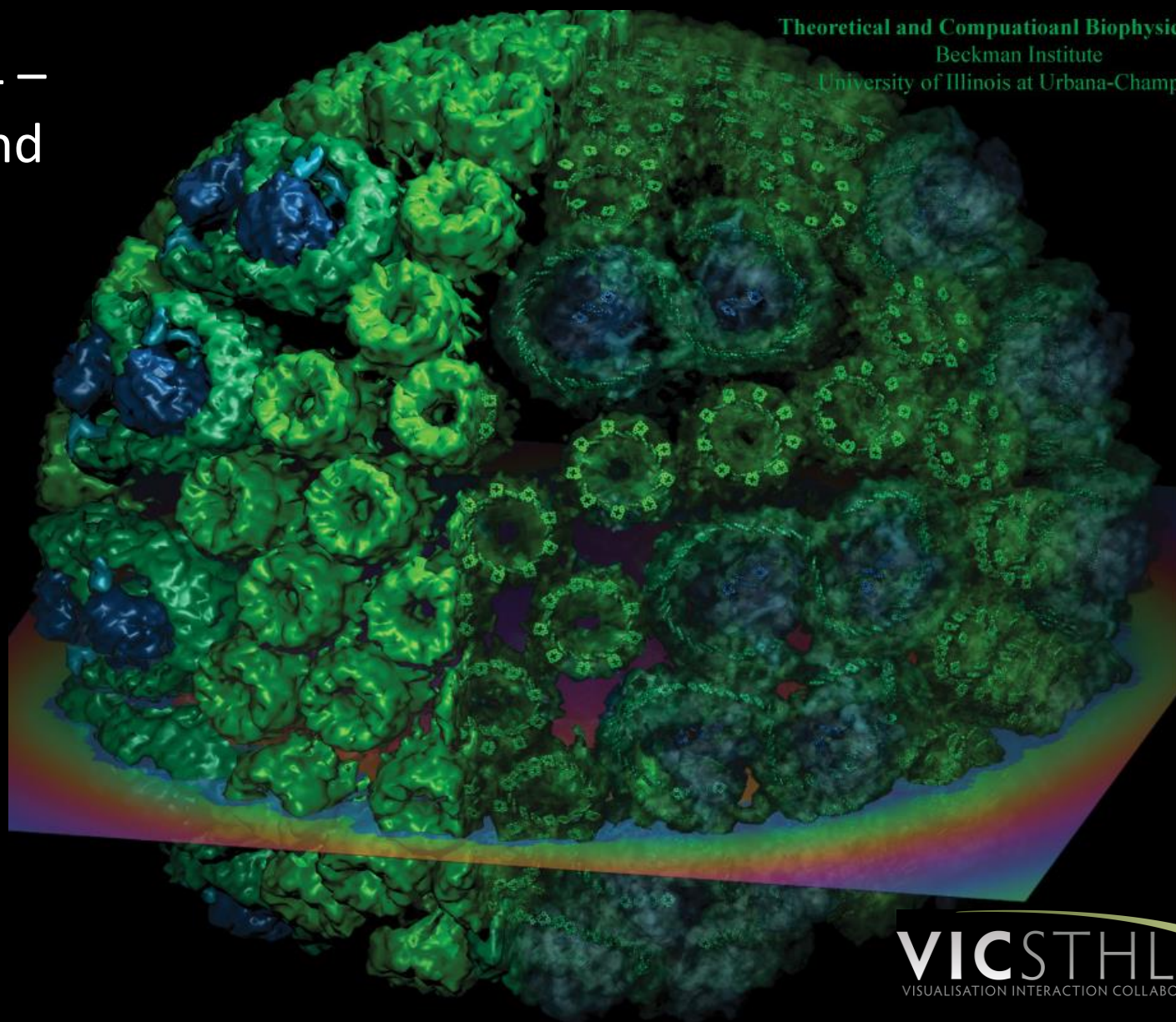


# Visualization 2014 – Lecture 4: VMD and Biomolecular Visualization

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2014/04/08



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# Prelude Videos



**TED**

Log in



Drew Berry:

## **Animations of unseeable biology**

TEDxSydney · 9:08 · Filmed May 2011

# Schedule

L1	Tue	25 mar	08:00-10:00	Introduction	
L2	Thu	27 mar	15:00-17:00	Why Visualization, Visualization Pipeline	
L3	Tue	1 apr	08:00-10:00	Visit Pipeline, Scientific Visual Storytelling	P1
<b>L4</b>	<b>Tue</b>	<b>8 apr</b>	<b>08:00-10:00</b>	<b>VMD Pipeline, Group formations</b>	<b>P2</b>
L5	Tue	15 apr	08:00-10:00	Volume Rendering	P3
L6	Tue	22 apr	08:00-10:00	Proposals	P4.1
L7	Tue	29 apr	15:00-17:00	“Hello World”	P4.2
L8	Tue	6 may	08:00-10:00	Update 1	P4.3
L9	Fri	9 may	15:00-17:00	Update 2	P4.3
L10	Tue	13 may	08:00-10:00	Update 3	P4.3
L11	Thu	15 may	15:00-17:00	Final Demo	P4.4
	Thu	22 may	23:59	Webpage Report	P4.5

# Outline

1. Subject Header: "VIS14"
2. Previously on VIS14
3. Next readings
4. Project 2 – VMD
  - a) Reading discussions
5. Project 3
6. Groups Project 4

# PREVIOUSLY ON IVIS14







# Discussion



CUBOID ( VOLUME, VOXELS, 3D ARRAY, SCALAR FIELD )

MORPHOLOGY

✓ THRESHOLD

OPEN CV

BINARY IMAGE (0,1)

✓ MARCHING CUBES

RESULT.

OBJECTIVE FILES .OBJ

✓ VISIT

✓ GEOMETRY

VIEW MODEL

VOLUME PRT  
TRANSFER FUNCTION

PARALLEL COORDINATE SYSTEM

→ "WENT TO RAW DATA" (!!)

OCCCLUDING DATA

ANALYTICAL TRAIL

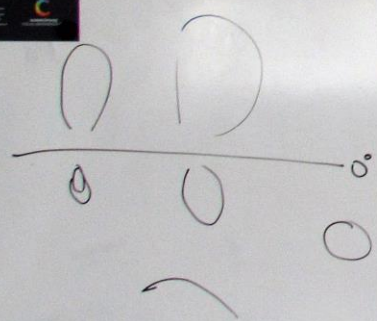
RAW DATA

DATA TRANSFORMATION

VIEW TRANSFORMATIONS (ROTATIONS)

THRESHOLDING

$$|V(x,y,z) \geq \theta|$$



# Readings for next class (L5)

- **Introduction to Scientific Visualization, Chapter 6, Visualizing Scalars**
  - Helen Wright
  - [LINK](#)
  - Write 100-word reflection on how you can use chapter 6 for your project 3.
- Drebin, Robert A., Loren Carpenter, and Pat Hanrahan. "Volume rendering." *ACM Siggraph Computer Graphics*. Vol. 22. No. 4. ACM, 1988.
  - [LINK](#)
  - Write 100-word reflection on how you will use this reading in project 3.
- **Send a PDF with both reflections to [marior@kth.se](mailto:marior@kth.se) by next Monday 15/4 at 23:59. Use "VIS14 – Reading L5" on the headline of the subject.**



# Project 3

- At the end today.

# Teach me VMD

1. Show me your projects
2. What did you learn?
3. What would you like to continue learning?
4. How do you use the readings to inform your project?
5. Let's teach!

# Whiteboard discussion

VMD VIS14-P2

VISUALIZATION MOLECULES

ATOMS  
POSITIONS  
BONDS  
ORIENTATION

→ DEFINE ROLE

.PDB: BASIC FILE

FIELDS | DIMENSIONS | VIEWS  
COLUMNS (TABLE: ROWS ARE ENTRIES)

CAMERA

YAW  
PITCH  
ROLL

MODEL: ROTATIONS

CONSTRUCTIVE CRITICISM

- MACRO WILL SELECT APPROPRIATE FEATURES BUT IF NOT IN MODEL SHOULD BE "GRAINED OUT"
- MULTI-WINDOW INTERFACE GETS IN THE WAY
- "WOULDN'T IT BE GREAT IF YOU COULD JUST CLICK ON IT."

WOULDER.

- MOLECULE
- EXTRACTING INSULIN
- RENDERING
- PROPER ZENDERING?
- RAY TRACING?

Focus & CONTEXT



# Project 3

Joel Hurlburt

Ferran Bertomeu

2014-04-08

# Speaking Volumes:

developing a method for the visualization  
and materialization of negative spaces  
defined through depth-sensor data

# Speaking Volumes:

developing a method for the visualization  
and **materialization** of negative spaces  
defined through depth-sensor data



# Materialization: Something from nothing



# Speaking Volumes:

developing a method for the visualization  
and materialization of **negative spaces**  
defined through depth-sensor data

# Negative Space





# Negative Space



The image displays the FedEx logo in a bold, sans-serif font. The word "Fed" is rendered in purple, and "Ex" is rendered in orange. A key design element is the negative space between the 'e' and the 'x', which forms a white arrow pointing to the right. This arrow is a classic symbol for FedEx, representing speed and delivery.

# Negative Space: Anish Kapoor



# Negative Space: Anish Kapoor



# Negative Space: Bruce Nauman



# Negative Space: Dance





# Speaking Volumes:

developing a method for the visualization  
and materialization of negative spaces  
defined through depth-sensor data

# Group Formation

- For next class, form groups.
- Think about who you want to collaborate with.
- Think about interests and skills.
- Use this file to help you.
- Use the visualizations from the previous course to help you.

# IVIS14 Project 1

- [http://www.aw-jansen.nl/IVIS14\\_1/](http://www.aw-jansen.nl/IVIS14_1/)
- <http://project1.net46.net/Project1.html>
- <http://www.csc.kth.se/~lgraf/ivis/project1/>
- <http://henrilouis.com/ivis/teams/>
- <http://www.nada.kth.se/~dmol/plugg/ivis14/project1/>
- <http://www.csc.kth.se/~dmans/ivis14/p1/tool.html>
- You could use the file and the visualizations above to create groups.
- You can group with people you know and work well with.

Thank you!

marior@kth.se