Illustrative Molecular Visualization with Continuous Abstraction

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Molecular Visualization

Crystal structure of a molybdenum oxide nanowheel. Science 327(1), January 2010

Ribbon diagram of the EspG structure. Biochemistry 50(21)
Molecular Visualization - Structure

Space-fill
Molecular Visualization - Structure

Balls-and-sticks
Molecular Visualization - Structure

Licorice
Molecular Visualization - Structure

Backbone
Molecular Visualization - Structure

Ribbon
Molecular Visualization

Goodsell, 2005
Molecular Visualization

Goodsell, 2003
Structural abstraction

Lampe et al., 2007
Support of spatial perception

Tarini et al., 2006
Illustrative rendering

Weber, 2009
Challenges

- *Continuous* transition from volumetric primitives to line primitives
- Choice and order of depth cueing techniques
- Large datasets ($\geq 10^4$ atoms)
Abstraction Space
Abstraction Space

- Structural abstraction
- Abstraction through the visual style
  - Support of spatial perception
  - Illustrativeness
Continuous Abstraction Space
Structural abstraction
Structural Abstraction

• Transition from Space-fill to balls-and-sticks
  – Reduce atom radii
Structural Abstraction

- Transition from balls-and-sticks to licorice
  - Reduce atom radii to zero and remove atoms
Structural Abstraction

- Transition from licorice to backbone
  - Remove bonds which are not part of the backbone
  - Start with bonds which are furthest away
  - Shorten bonds and remove when length is zero
Atom rank

\[
\text{rank}(a) = \begin{cases} 
0 & \text{if } a \in \text{backbone} \\
1 + \min_{b \in \text{conn}(a)} \{\text{rank}(b)\} & \text{else}
\end{cases}
\]

\text{conn}(a) \text{ are all the atoms which are connected to atom } a
• **Transition from backbone to ribbons**
  – Interpolate between (linear) bond position and smooth ribbons
  – Also modify orientation for helices
Structural Abstraction
Support of spatial perception
Ambient Occlusion

Following Tarini et al., 2006
Object attenuation / Dolly zoom

Following Everts et al., 2009
Halos

Following Tarini et al., 2006 and Everts et al., 2009
Ordering of effects

• Apply halos last, because of blocking effect
• Combine ambient occlusion and object attenuation/dolly zoom to avoid gaps in the abstraction space
Support of spatial perception
‘Illustrativeness’
Photorealistic

• Realistic shading
• Colors indicate atom type
• “Normal” visualization
Cartoon

- Cel shading
- Pastel colors based on the photorealistic colors
- Colors indicate atom types
- Shows less details
- Flattens the image, shows overall shape of molecule
Black-and-white

- Flat shading
- Hatching patterns indicate atom types
- For black-and-white printing
- Black-and-white and intermediate stages for visual de-emphasis
Visual Style - Illustrativeness
Beyond global abstraction
Local structural abstraction
Local ‘illustrativeness’
Focus and context
Feedback

• Combining styles preferred over blending
• Continuity is useful for teaching
• Intermediate stages might provide new insight
• Easier than PyMol
Contributions

• Abstraction space for molecular visualization

• Seamless transformation of
  – Structural abstraction
  – Support of spatial perception
  – ‘Illustrativeness’

• GPU shader implementation of transitions

• Dedicated interactive control of abstraction in illustrative visualization
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