

# Visualization For the Physical Sciences: Part II

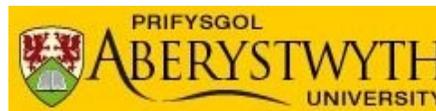
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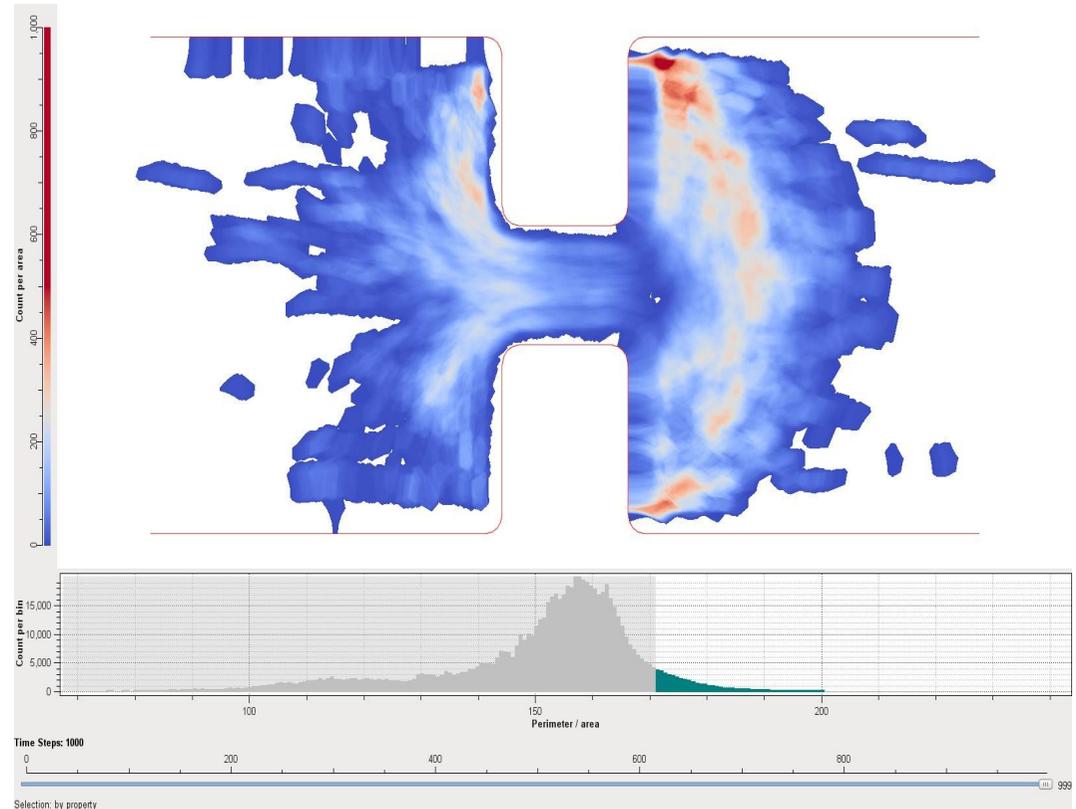


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# Overview

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  - Introduction, Challenges
  - Classification, Overview
  - Astronomy
- Part 2: Robert S. Laramee
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    - Organic Chemistry
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- Part 3: Richard Walker
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    - Gravitation
    - Mechanics
    - Optics
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# Chemistry

- **Chemistry:** concerned with properties and structure of substances, transformations they undergo and energy exchanged during those processes [QEE\*05].
- (Physics studies structure and behavior of individual atoms while chemistry studies properties and reactions of molecules [bri10b])

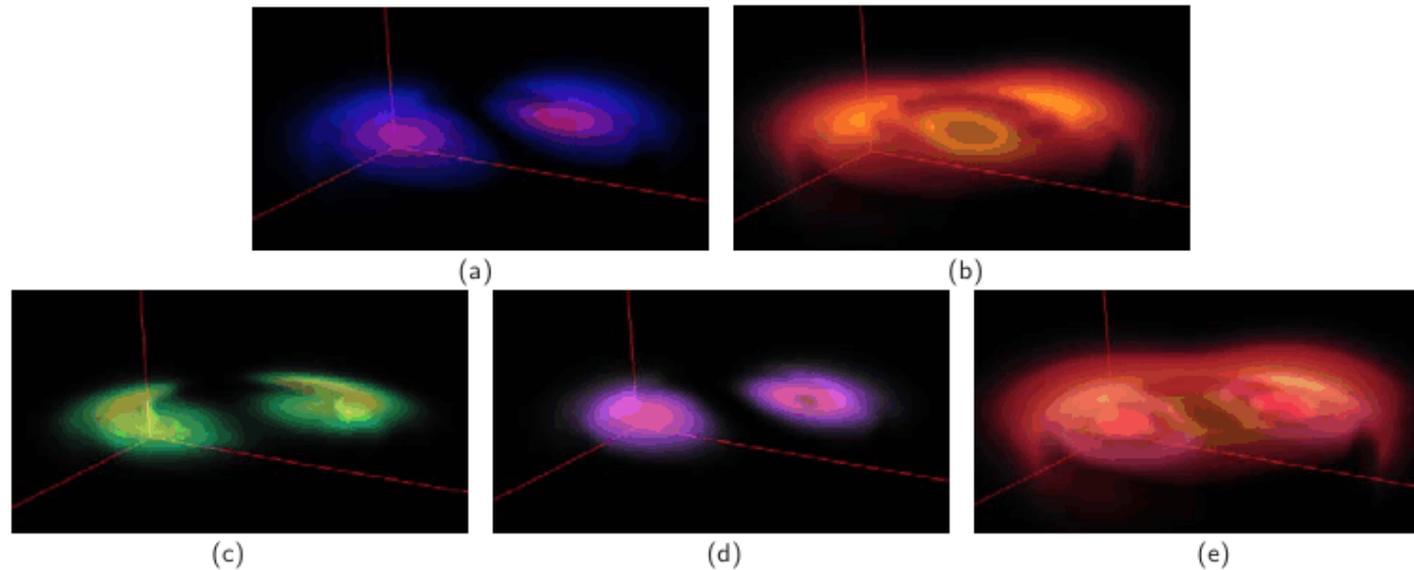


Figure 11: The electron orbitals of a 21 million atom InAs QD device in the first excited state: (a), (b), (c) and (d) are up and down spins combined s, p, d and s\* orbitals, respectively, and (e) is the overall electron cloud.

# Chemistry: Nanotechnology

- **Nanotechnology:** manipulation of atoms, molecules and materials to form structures at nano-meter scales.
- Structures typically have new properties than building blocks due to quantum mechanics.
- Nanotechnology is interdisciplinary: involving physics, chemistry, biology, material science and engineering.
- “Nanotechnology” refers to both science and engineering of field [bri10e].
- Included in our survey are contributions that visualize formation of nanoparticles in turbulent flows [SIG05], and present a web based nanotechnology visualization tool [QMK\* 06].

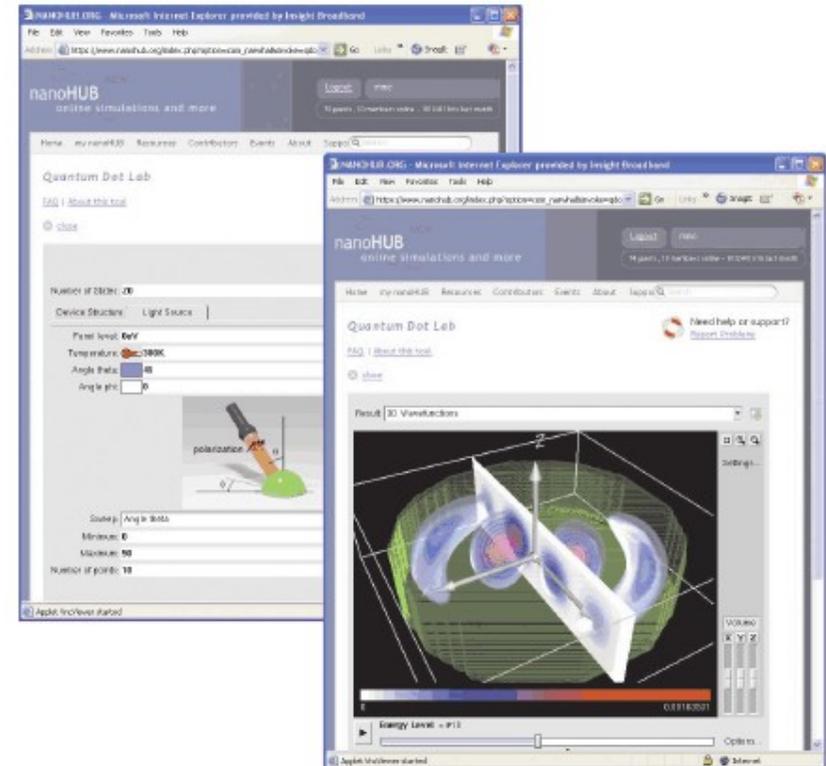
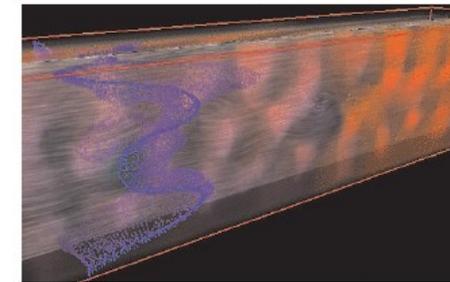
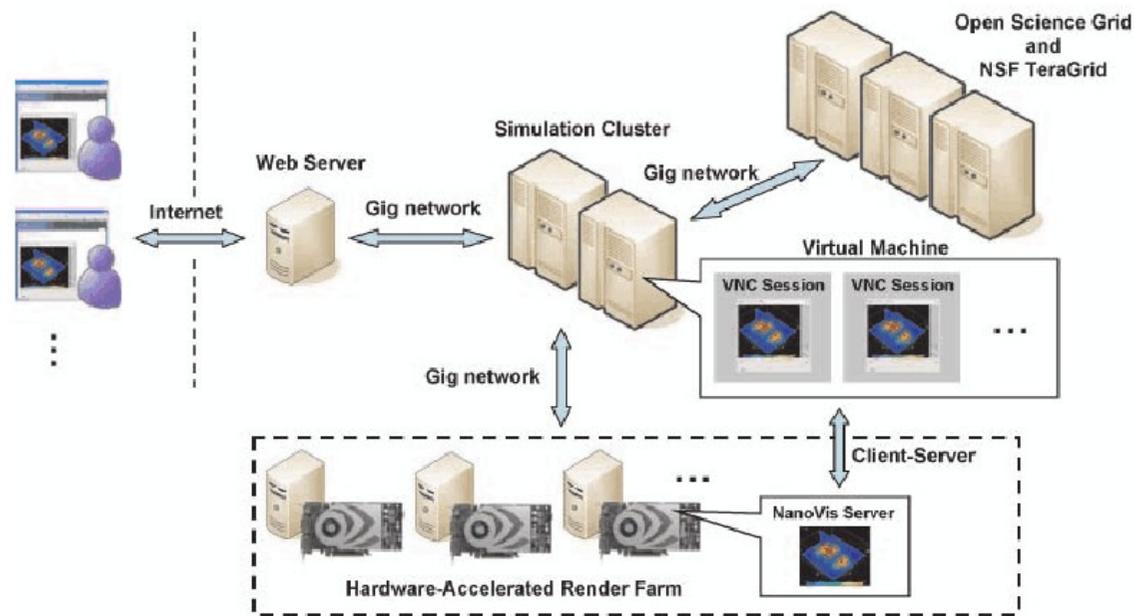


Fig. 2. nanoHUB web-based interface: simulation (back) and visualization (front).

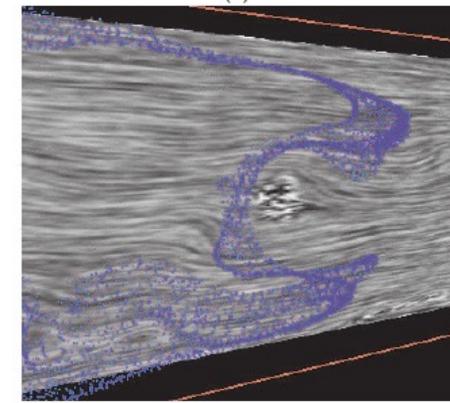
# Chemistry: Nanotechnology

## Hub-based Simulation and Graphics Hardware Accelerated Visualization for Nanotechnology Applications by Qiao et al [QMK\* 06]

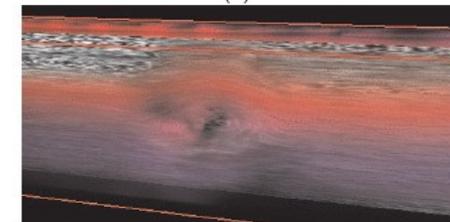
- web based application that gives many users access to powerful simulation and visualization resources.



(a)



(b)



(c)

Fig. 6. Electron gas simulation: (a) hybrid electron flow and potential visualization, (b) impurity causing electrons to swirl around, (c) sharp drop of electron potential surrounding the impurity.

# Physical Chemistry

- **Physical chemistry:** measures, correlates and explains quantitative aspects of chemical processes (as opposed to focussing on classes of materials that share common structural and chemical features).
- Modern physical chemistry uses quantum mechanical model of atomic and molecular structure [bri10b].
- This section presents visualizations of quantum chemistry simulations [QEE\*05, JV09].

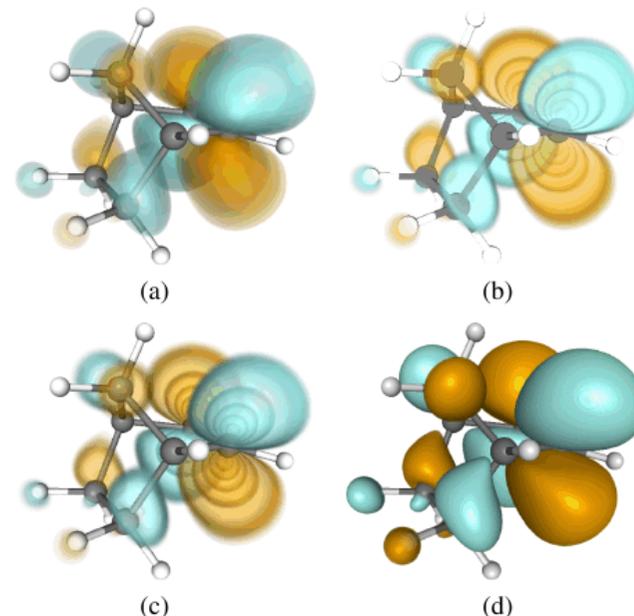


Fig. 6. Volume rendering of the molecular orbital for  $C_4H_2CH_2CH_2CH_4$ . Warm color represents positive values and cool color represents negative values. (a) is a conventional volume rendering with local illumination and (b) is a volume rendering with the edge coloring using the sinusoidal TF without illumination. (c) shows a boundary enhanced contour volume rendering with the sinusoidal TFs and (d) presents an isosurface rendering with local illumination.

# Physical Chemistry

**VolQD: Direct Volume Rendering of Multi-million Atom Quantum Dot Simulations by Qiao et al [QEE\*05].** -hardware-accelerated direct volume rendering system for visualizing multivariate wave functions in semi-conducting quantum dot (QD) simulations

- Contains probability density values of multiple electron orbitals for up to tens of millions of atoms

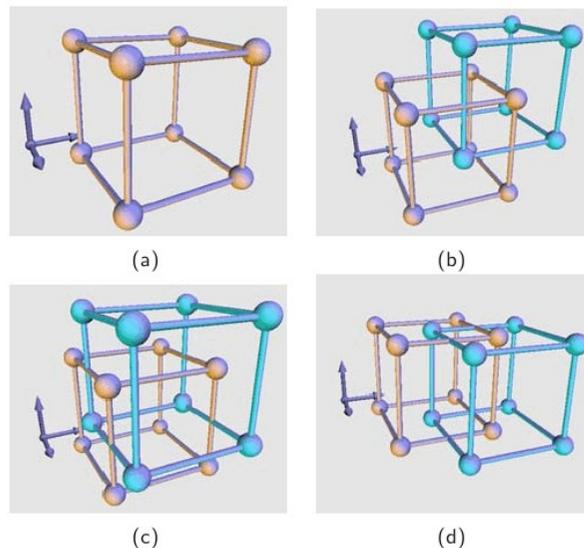


Figure 3: Decomposition of a FCC lattice: (a) is the base cubic cell composed of corners; (b), (c) and (d) are cubic cells composed of opposing face centers shown in relation to the base cell.

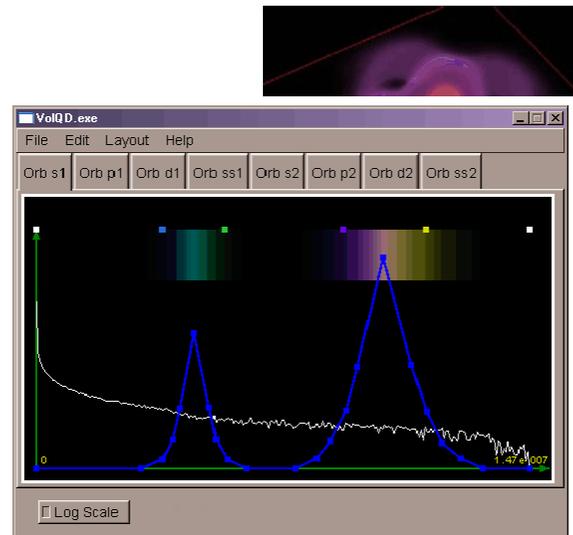


Figure 7: Multi-channel transfer function editor interface: channels are organized in a tabbed format.

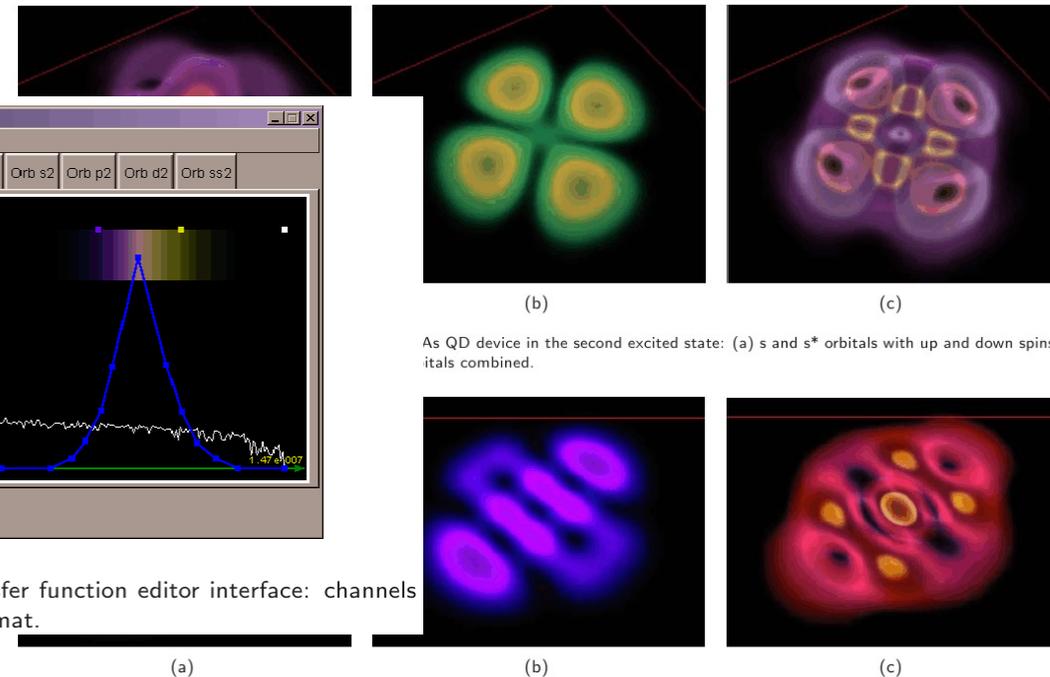


Figure 9: The electron orbitals of a two million atom InAs QD device in the third excited state: (a) s and s\* orbitals with up and down spins, (b) p and d orbitals with up and down spins, (c) all orbitals combined.

# Physical Chemistry

**Interactive Volume Rendering of Functional Representations in Quantum Chemistry (Jang and Varetto) [JV09] -evaluate and visualize molecular orbital data on GPU without re-sampling.**

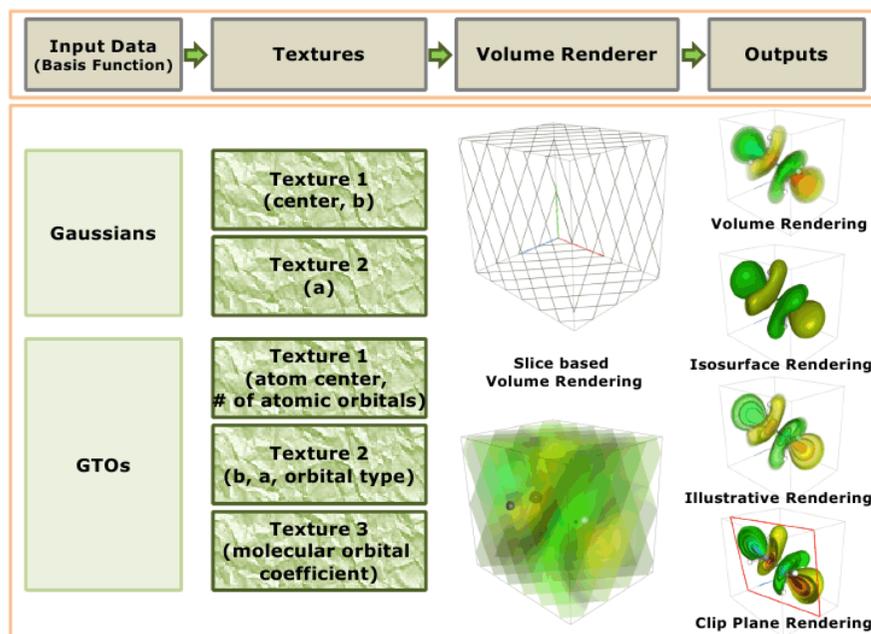


Fig. 1. Overview of our interactive visualization system. Two types of data are stored in textures and evaluated and visualized on our volume rendering. Different rendering results, such as volume rendering, isosurface rendering, illustrative rendering, and volume clipping rendering, are produced using our system.

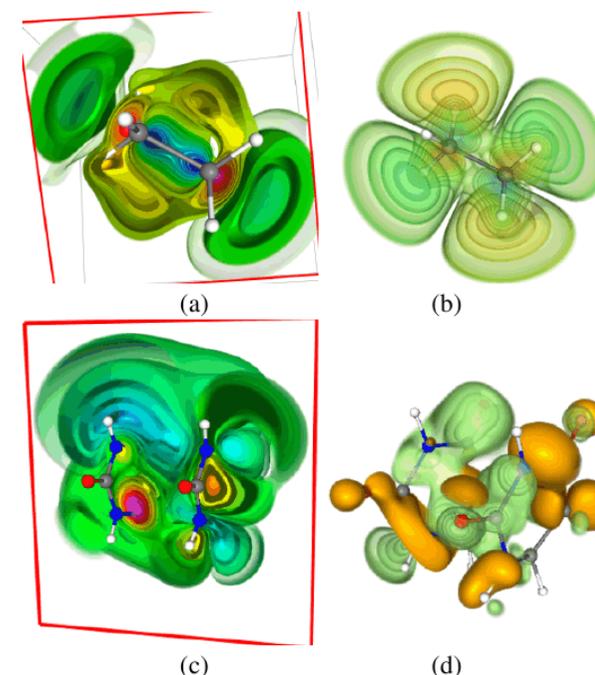
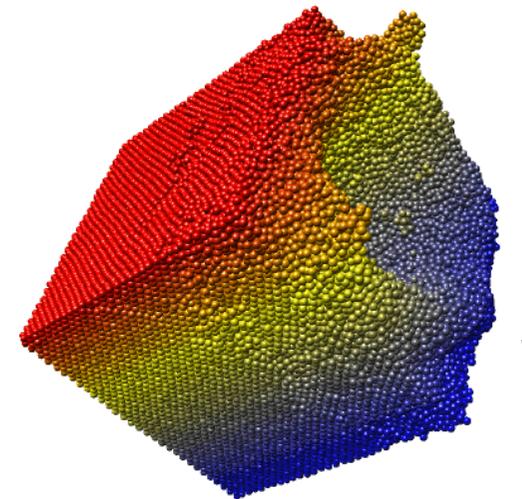


Fig. 12. More rendering results of  $C_2H_6$  (a, b) and  $N_2C_4O_2H_4N_2C_4O_2H_4$  (c, d). (a) and (b) are the 17<sup>th</sup> and 20<sup>th</sup> molecular orbitals with the boundary enhanced contour volume. (c) shows the isosurface rendering of the 27<sup>th</sup> molecular orbital with multiple isosurfaces and the volume clipping. (d) presents both isosurfaces (orange) and volume contours with the sinusoidal TF (green) of the 30<sup>th</sup> molecular orbital.

# Organic Chemistry

- **Organic Chemistry:** studies correlation between physical and chemical properties of substances with their structural features.
- Applicability to design and synthesis of novel molecules with some desired properties. Most visualization for organic chemistry show the 3D structure of molecules [bri10b].
- We survey papers that: visualize molecules [BDST04, TCM06] and molecular surfaces [LBPH10, KBE09],
- Generate triangulations of molecular surfaces [CS04, CS05],
- Visualize solvent pathlines near protein cavities [BGB\* 08],
- Detect anomalous structures in molecular dynamics simulation data [MHM\* 04],
- Visualize large molecular dynamics simulations [RE05, GRDE10]

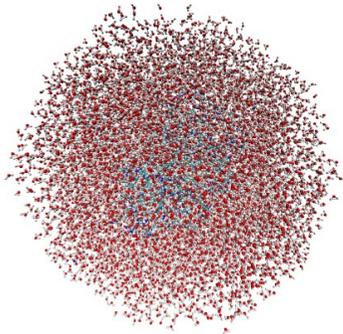


**Figure 2:** Data set D1 obtained from a small laser ablation simulation (107,391 atoms). Although the number of atoms is small, a brute-force raycasting of the atoms as spheres results in low performance (27 fps) due to the large number of depth replacements caused by the highly overlapping glyphs.

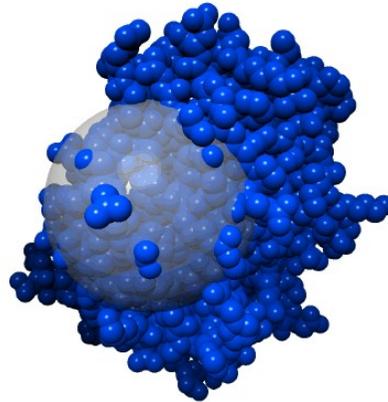
# Organic Chemistry

## Visual Abstractions of Solvent Pathlines near Protein Cavities by Bidmon et al [BGB\*08]

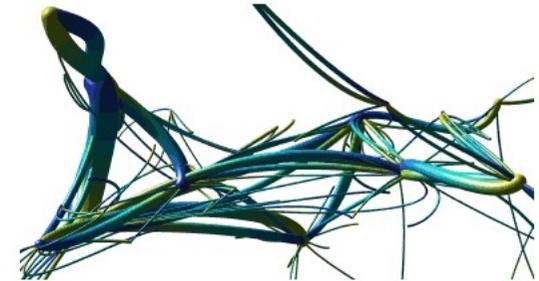
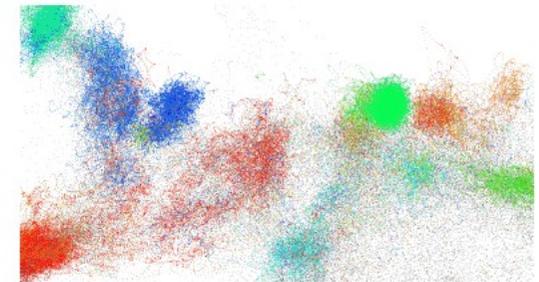
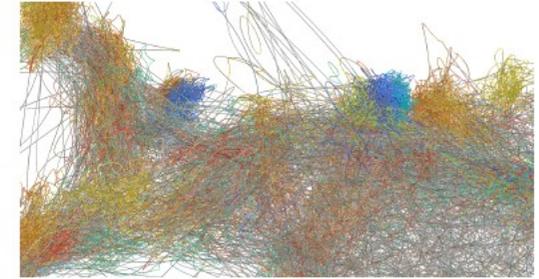
- focuses on visualising solvent paths entering and leaving cavities of protein
- enables study route and dynamics of exchange of tightly bound internal water molecules with bulk solvent.



**Figure 1:** A protein-solvent system represented without any filtering of the solvent molecules.



**Figure 2:** The protein in spacefill representation. The grey sphere marks the region of interest enclosing the cavity. Solvent molecules outside are neglected in further processing.

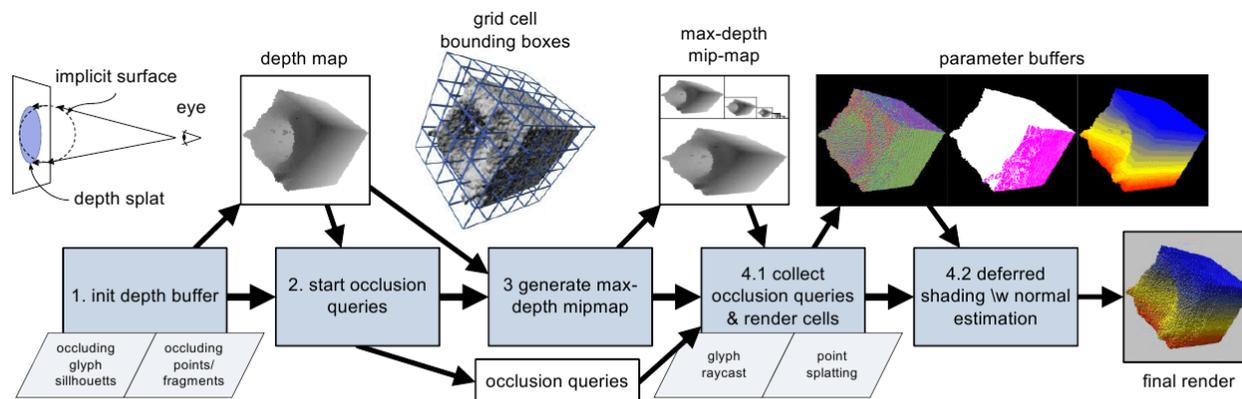


**Figure 7:** Abstraction of the pathlines. The upper figure shows all pathlines. The middle figure shows the vertices of all pathlines, coloured based on the detected clusters of slower motion. Positions of conserved water correspond to the larger clusters. The lower figure shows the extracted principal paths.

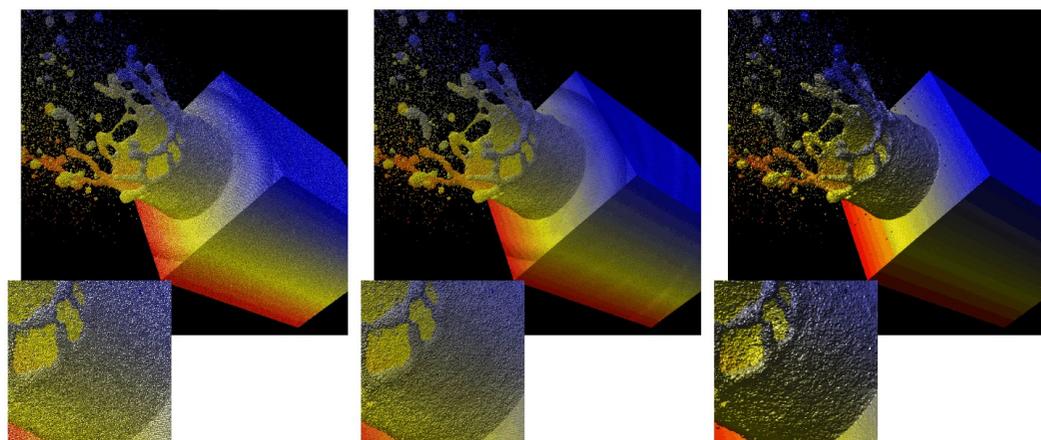
# Organic Chemistry

## Coherent Culling and Shading for Large Molecular Dynamics Visualization, Grottel et al [GRDE10]

- Collection of software and hardware strategies for maximum performance based on rendering only visible objects.



**Figure 3:** The stages of our method: 1. initialization of the depth buffer with known occluders in  $O_{i-1}$ , 2. start of occlusion queries for all grid cells by testing against the bounding boxes, 3. generation of maximum-depth mipmap, 4.1. collection of occlusion queries, updating of list  $O_i$  of visible cells, and rendering of remaining visible glyphs. Stages 1 and 4.1 can output raycast glyphs, or points if the glyphs become too small in image-space, 4.2. deferred shading: image-space calculation of normals and phong lighting. Note that the rendering in stage 1 initializes the depth buffer with a conservative depth splat for the maximum-depth mipmap, as well as for subsequent render passes.



**Figure 6:** Comparison between standard and deferred shading (please zoom the electronic version). Left: standard, naïve raycasting of spheres. Middle:  $8 \times 8$  super-sampling of raycast spheres. Right: deferred shading with artificial normals.

# Earth Sciences

- **Earth sciences** study solid earth (geologic sciences), its waters (hydrologic sciences), the air around it (atmospheric sciences) and their evolution in time [bri10d].
- Consists of many disciplines which include study of water on and within ground, glaciers and ice caps, oceans, atmosphere and its phenomena, world's climate, physical and chemical makeup of solid earth, study of land formation and geologic history of Earth.



# Earth Sciences: Atmospheric

- **Atmospheric sciences:** deal with properties, structure and composition of atmosphere, understanding atmospheric phenomena such as clouds, fog and dew, understanding weather changes and ability to accurately forecast weather.
- Survey presents papers that visualize cloud scale weather data [REHL03], visualize warm rain formation, compare weather models with radar observation [SYS\* 06] and analyze air pollution [QCX\* 07].



Fig. 1. Hong Kong's air pollution problem. The spectacular harbor view has been increasingly crippled by a massive haze [1, 3, 4].

# Earth Sciences: Atmospheric

An Atmospheric Visual Analysis and Exploration System by Song et al. [SYS\* 06]  
 -focuses on (1) understanding warm rain formation and (2) comparison of weather prediction models vs radar observations.

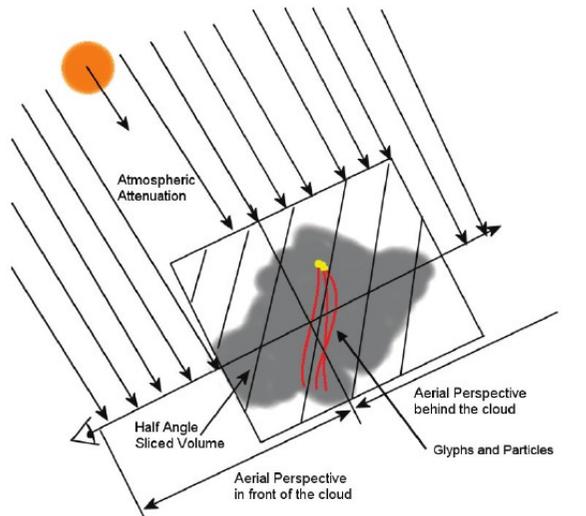


Fig. 1. Our volume rendering engine incorporates half-angle slicing technique for multi-field, multi-scattering, physics-based atmospheric rendering as well as particle trace and glyph rendering.

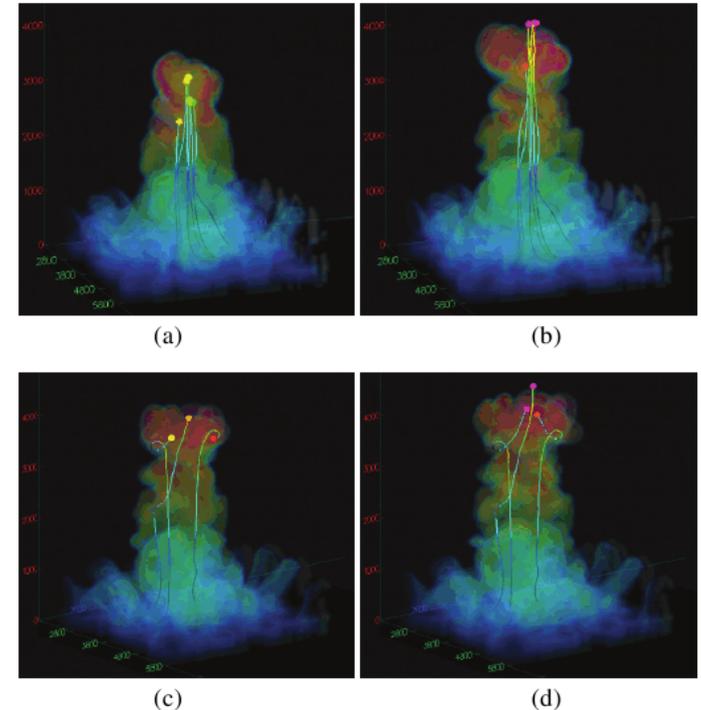
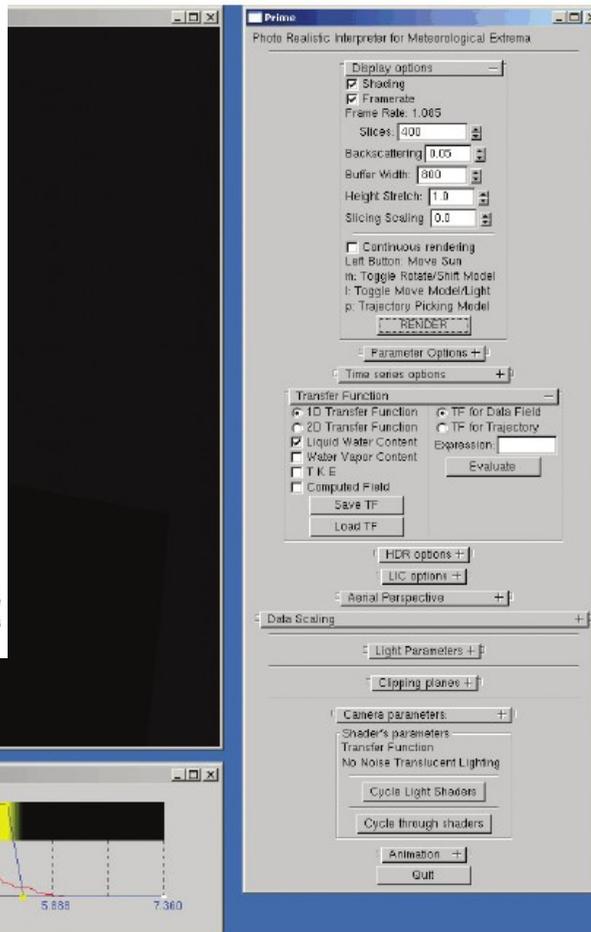
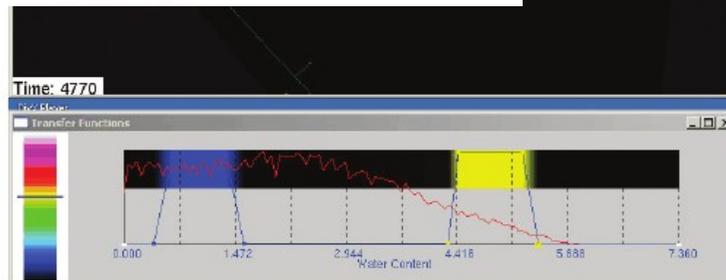


Fig. 5. Droplet trajectories plotted upon field of calculated eddy dissipation rate (which includes regions below the actual base of the cloud, near the earth's surface), for trajectories ascending straight up the core of the cloud at (a) 4590 and (b) 4680 s, and for trajectories caught in eddies at the cloud edge at (c) 4680 and (d) 4740 s. Eddy dissipation rate color scale ranges from less than  $100 \text{ cm}^2 \text{ s}^{-3}$  (blue, green),  $100$  to  $400 \text{ cm}^2 \text{ s}^{-3}$  (yellow, orange) to greater than  $400 \text{ cm}^2 \text{ s}^{-3}$  (red, pink), and is also used for sphere color. Color of trajectories varies from cool colors, indicating that it occupies a region of the cloud with less cloud water, to warm colors, indicating regions of greater cloud water.

# Earth Sciences: Atmospheric

## Visual Analysis of the Air Pollution Problem in Hong Kong by Qu et al [QCX\* 07] -information visualization centered system for weather data visualization

Table 1. Data Attributes Collected at Different Monitoring Stations.

| Name                                    | Unit  |
|---|---|
| Precipitation                           | mm  |
| Wind Direction                          | bearing   |
| Air Temperature                         | Degree Celsius  |
| Wind Speed                              | m/s   |
| Dew Point                               | Degree Celsius  |
| Relative Humidity                       | %   |
| Sea Level Pressure                      | hPa   |
| Respirable suspended particulates (RSP) | ug/m3   |
| Nitrogen dioxide (NO <sub>2</sub> )     | ppb   |
| Sulphur dioxide (SO <sub>2</sub> )      | ppb   |
| Ozone (O <sub>3</sub> )                 | ppb   |
| Carbon monoxide (CO)                    | ppb   |
| Solar Radiation                         | mw/cm2  |
| Air Pollution Index (API)               | scale 100   |
| Contributed Pollutant to API            | RSP, O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> or CO |

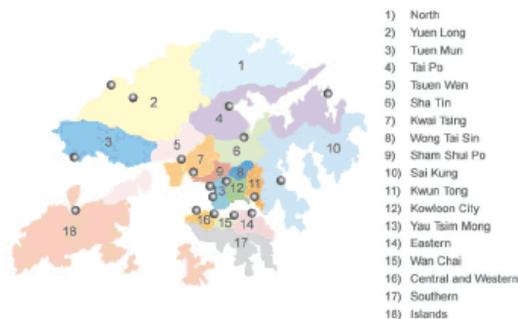


Fig. 2. Locations of different air quality monitoring stations shown as dots in 18 districts of Hong Kong.

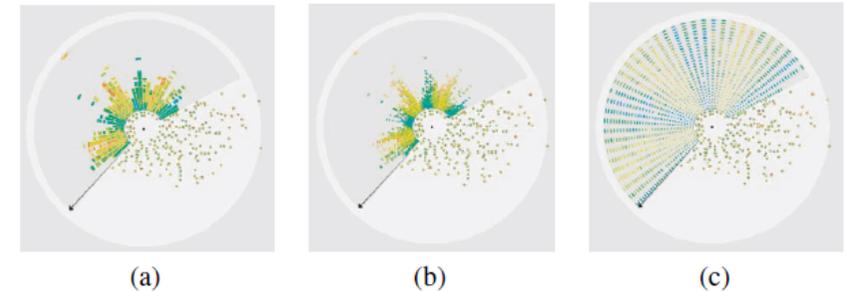


Fig. 6. Polar system with time information: (a) x-position, y-position, and color of the sector indicate the month of observation, amount of SO<sub>2</sub>, and temperature, respectively; (b) the x-position now represents the day in which the entry was recorded; (c) the y-position now encodes the day and the x-position encodes the month.

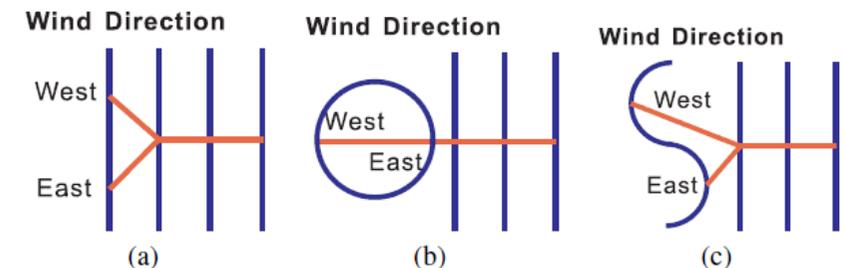


Fig. 7. Different layouts of parallel coordinates: (a) Traditional layout; (b) Circular layout; (c) S-style layout.

# Earth Sciences: Climatology

- **Climatology:** [bri10c] concerned with climate differences between different regions and climate changes over long periods.
- Climatology seeks to identify slow acting influences on climate and identify consequences of climate change.
- We review papers that visualize climate variability changes [JBMS09], identify regions in atmosphere acting as indicators for climate change [KLM\* 08] and describe visualization for public-resource climate modeling [SFW04].

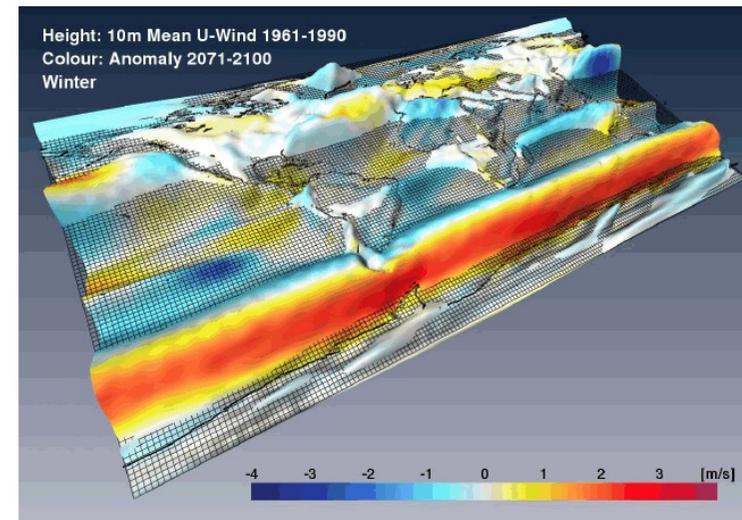


Fig. 14. Visualization of global changes for U10M (DJF): height encodes the mean U10M of the years 1961 – 1990, color encodes the projected change for the U10M wind for 2071 – 2100 relative to the same period.

# Earth Sciences: Climatology

**Hypothesis Generation in Climate Research with Interactive Visual Data Exploration** by Kehrer et al [KLM\*08] -aims to identify regions in atmosphere (e.g., certain height layers) which can act as sensitive and robust indicators for climate change.

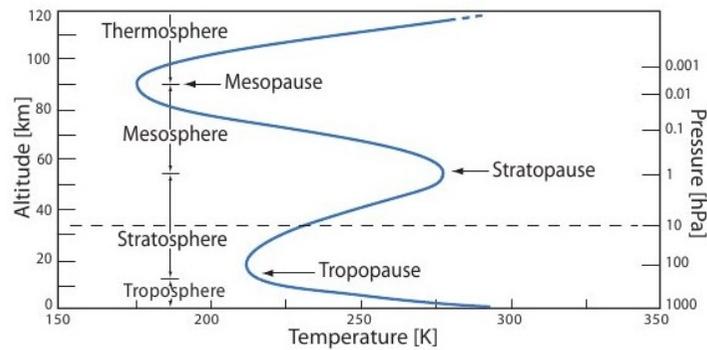


Fig. 1. Illustration of the vertical thermal structure of the atmosphere, reflecting a balance between radiative, convective and dynamical heating and cooling processes of the surface-atmosphere system. Different layers of the standard atmosphere are shown (illustration adapted from Melbourne et al. [13]). Changes in the upper troposphere-lower stratosphere region have strong impact on the Earth's climate system [27].

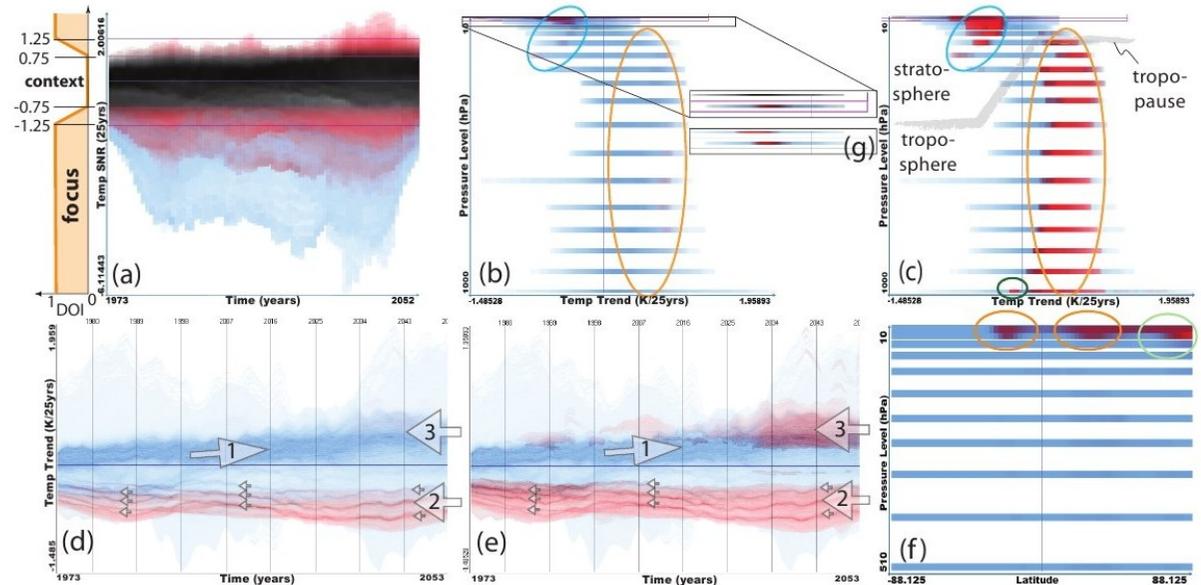


Fig. 3. Hypothesis generation using interactive visual exploration of derived temperature parameters in the ECHAM5 climate model. Features selected in multiple linked view are highlighted in red (focus), features only selected in the current view (2<sup>nd</sup> level focus) depicted in blue, and context information in black (more details in the text).

# Earth Sciences: Hydrology

- **Hydrology:** studies waters of Earth, their distribution, circulation as well as their chemical and physical properties.
- Included is study that describes visualization tools for an environmental observation and forecasting system for Columbia River [**JCSB03**].

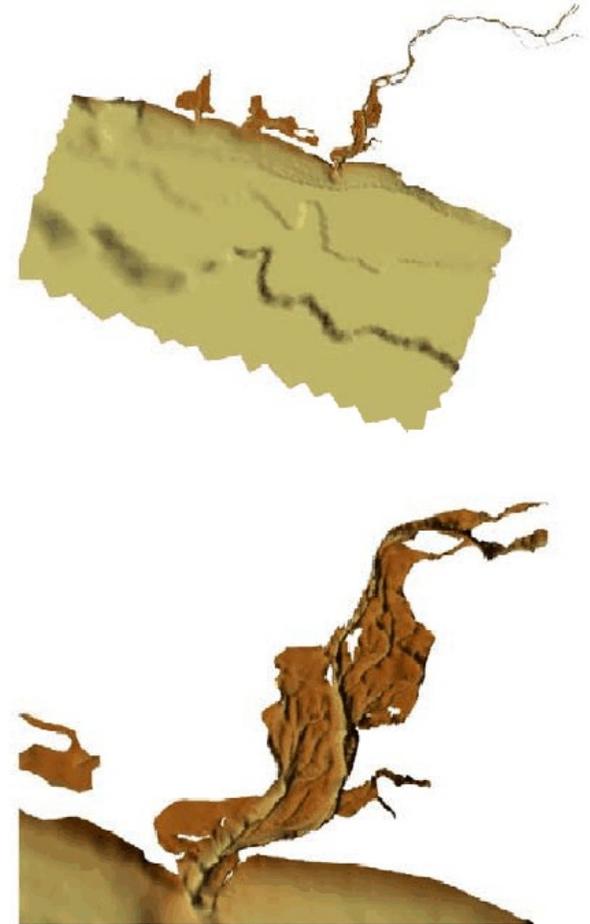


Figure 6: Columbia River topology and bathymetry (bottom) and insertion of the estuary in the continental shelf (top).

# Earth Sciences: Hydrology

**Visualizing Spatial and Temporal Variability in Coastal Observatories** by Jimenez et al [JCSB03] -system for modeling and evaluating effects of natural resource management decisions. CORIE (a coastal observatory) was designed as scalable, multi-use, real-time environmental and observational forecasting system (EOFS).

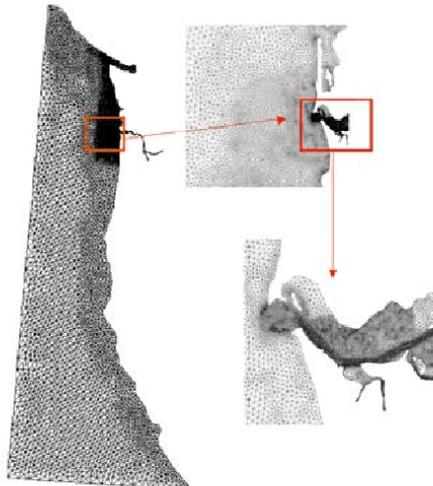


Figure 2: The CORIE computational domain extends along the continental shelf from British Columbia to California. An horizontally unstructured grid enables enhanced refinement in areas of primary interest, including the near-field plume, the estuary entrance and the navigation channel.

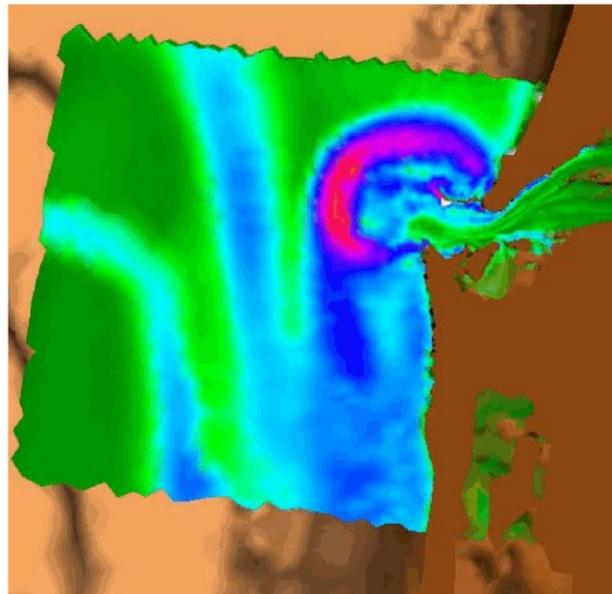


Figure 9: Maximum gradients of salinity reveal potential locations of ecologically significant fronts in the Columbia River plume.

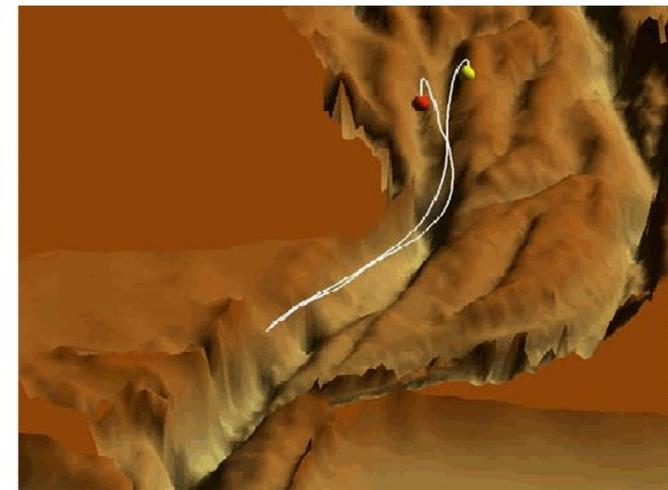


Figure 11: Observed and simulated trajectories of a Lagrangian drifter released near the mouth of the estuary at the beginning of a flood tide. The red sphere represents the real drifter, and the yellow the simulated drifter.

# Earth Sciences: Geology

- **Geology:** scientific study of Earth, its composition, structure and physical properties.
- Included in survey are contributions that visualize hot fluids discharges from sea floor vents [SBS\* 04] and produce illustrative rendering of geologic layers [PGTG07], [PGT\*08].

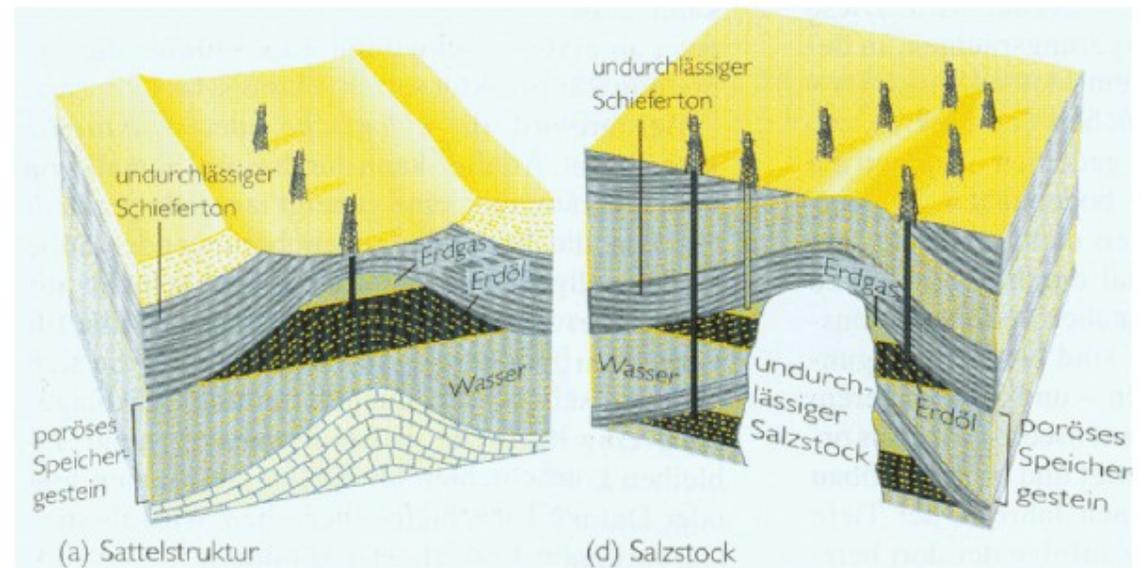


Fig. 1. Hand crafted illustrations of an oilfield. Left: Notice how the brick texture in the lowest layer and the stippled lines in the oil area are bending along the strata. Pictures are taken from Grotzinger et al. [8]

# Earth Sciences: Geology

The Seismic Analyzer: Interpreting and Illustrating 2D Seismic Data, Patel et al, [PGT\*08] -replace manual hand-drawn diagrams with automated visualization techniques

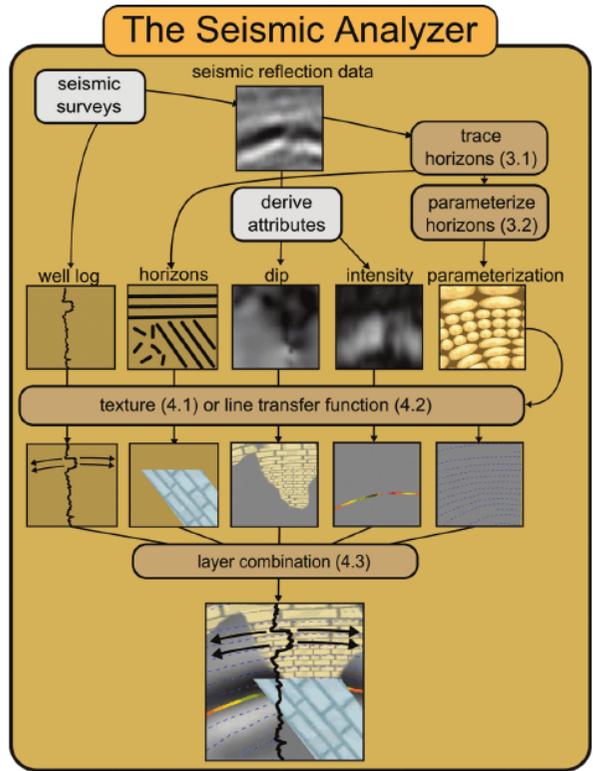


Fig. 4. The seismic analyzer. The brown rounded rectangles represent our algorithms and refer to the sections describing them. The 'seismic surveys' rectangle represents the process of obtaining the seismic data. The 'derive attributes' rectangle represents the process of deriving attributes using external software.

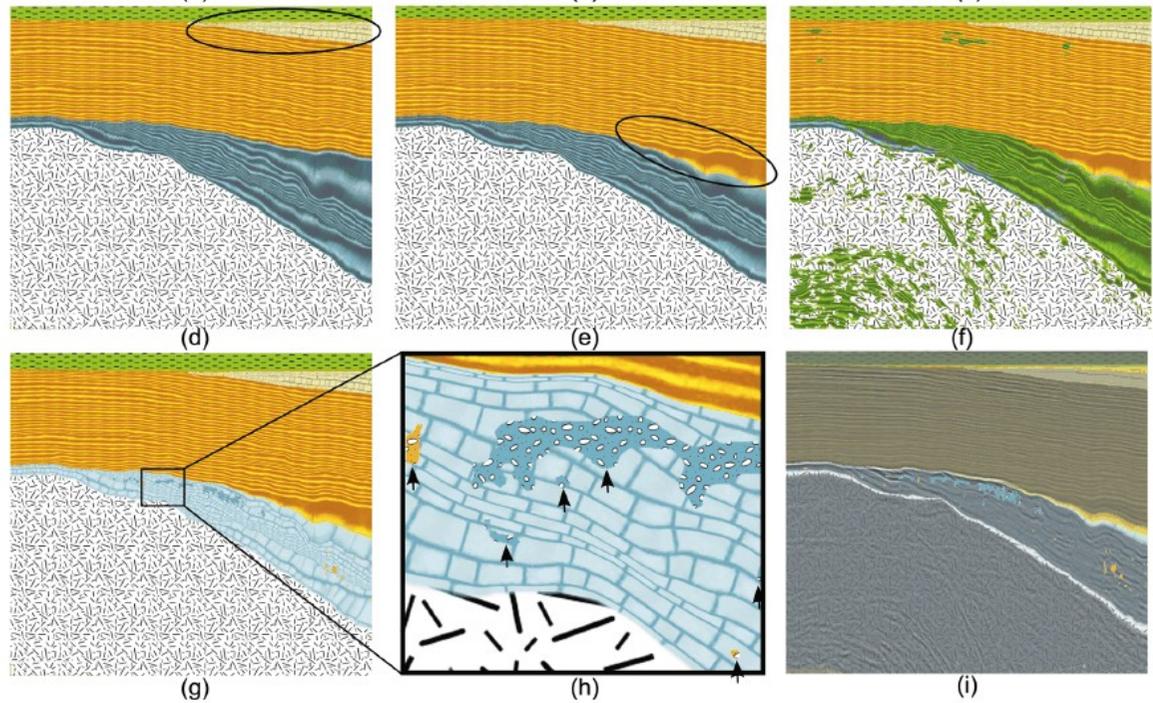


Fig. 13. Images created during an interpretation. Figure a) shows manually drawn yellow lines for separating strata. Figures b)-i) are rendered with our system. They are discussed in Section 5.2. Ellipses in (d) and (e) pinpoint the difference from the previous image. Arrows in (h) point out areas of medium (orange) and high (blue) mound characteristics.



# End of Part II

- Thank you for your attention! Any questions?

We would like to thank the following:

- M. Chen and all authors featured in the survey
- The **R**esearch **I**nstitute for **V**isual and **I**nteractive **C**omputing (RIVIC)
- PDF version of STAR available at:

<http://cs.swan.ac.uk/~csbob>

- Next up: Rick Walker and Part III