ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Introduction to scientific visualization

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SC-EPFL Data Visualization course (COM-480)
4 December 2018

Visualization | Overview

Global goal

To provide an introduction to scientific visualization, the techniques employed, and how it can assist scientific discovery and communication.

Specific topics :

- What is scientific visualization?
- Why it is not data visualization
- What is visual communication ?

} general definitions

- Techniques for scientific visualization
- Visualization tools
- Some illustrative examples

} visual concepts, techniques & applications

- Where to now ?

} future directions

CS – indicates that computer scientists can help in an activity

Visualization | Overview

My current professional activities at EPFL

- Computational Granular Dynamics (CGD) group leader
  - research & teaching in CGD, CFD and particle-based numerical simulation methods
  - participated in high-visibility projects (e.g. Hydroptère, Alinghi, Formula 1, Hermes)

- Coordinator of Computational Engineering (CE)
  - ACCES network promotes CE within School of Engineering
  - established recently the Collaborative Visualization (CoViz1) facility
  - facilitator and user of scientific visualization – not a visualization developer or expert !

- Lecturer in Mechanical Engineering (SGM)
  - Numerical Flow Simulation (MA course, 60 students)
  - Particle-based Methods (MA course, 20 students)

The present talk will combine contributions from each of these activities.

Visualization | What is visualization ?

What is “Data Visualization” ?

Data Visualization . . .

- . . . is the study of (interactive) visual representations of abstract data to reinforce human cognition.

- . . . helps users analyze and reason about data and evidence. It makes complex data more accessible, understandable and usable.

- . . . may be employed for processing, analyzing and communicating “big data”, i.e. the increased amount of data created by Internet activity and an expanding number of sensors in the environment.

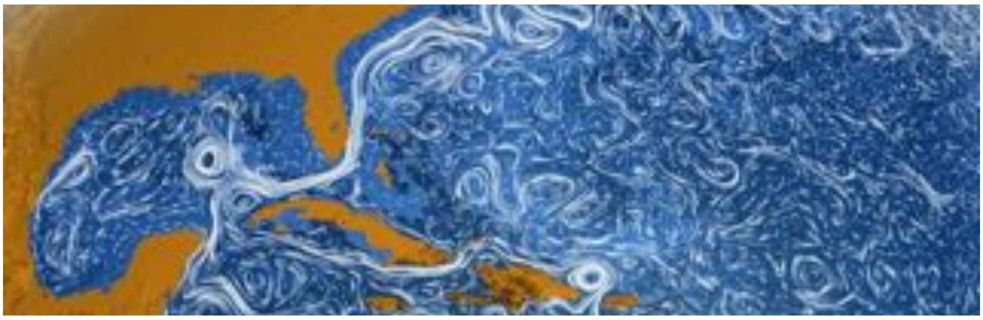
What is "Scientific Visualization" ?

Scientific Visualization . . .

- . . . is the graphical illustration of scientific data that enable scientists to understand, illustrate and glean insight from their data (i.e. scientific discovery).
- . . . is the qualitative post-processing of the results of numerical simulations of real phenomena based on simplified physical models.
- . . . is primarily concerned with visual representations of 3D phenomena (e.g. architectural, meteorological, medical, biological), where the emphasis is on realistic renderings of volumes, surfaces, etc. possibly with a dynamic (time) component.

How are Scientific Visualization & Data Visualization similar ?

- The purpose of visualization is insight, not pictures.
- Visualization provides a means to present a complex collection of numbers by a simple, global visual representation (e.g. image, animation, interactive graphics).
- Visualization provides a means to communicate a message to diverse audiences ("Visual Communication")

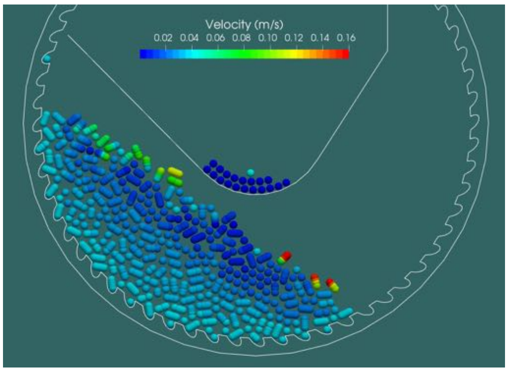


Ocean currents off US coast (NASA Perpetual Ocean)

Visualization — What is visualization ?

How do Scientific Visualization & Data Visualization differ?

- Scientific visualization => spatial representation is **given**
- Data visualization => spatial representation is **chosen**



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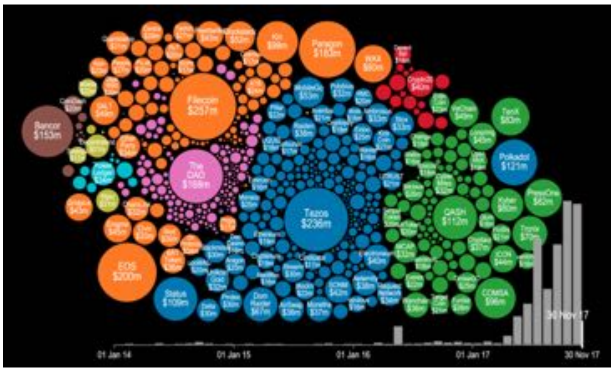


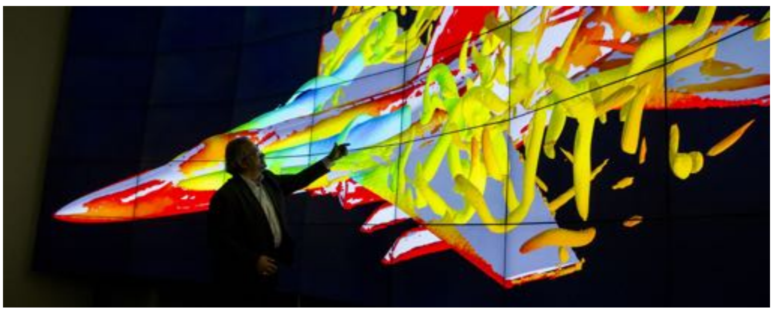
ICO explosion (Elementus)

Visualization — Scientific Visualization

Why use Scientific Visualization ?

- Visual presentation of scientific data (e.g. research results) with the goal to:
  - enhance scientific discovery (i.e. provide insights, trends)
  - solution steering of large-scale computations
  - communicate scientific results to peers (e.g. researchers, funding bodies)
  - improve student comprehension (i.e. pedagogical)
  - outreach (e.g. general public)

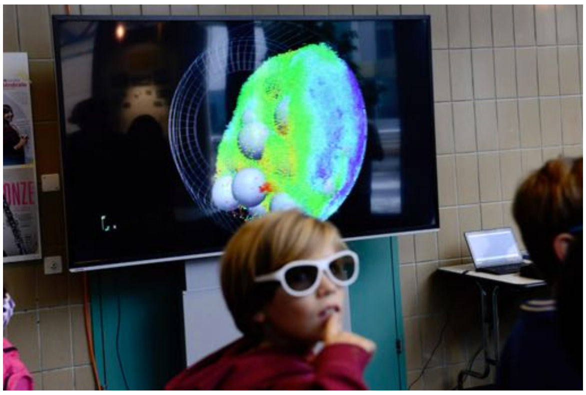
The first two goals: scientific visualization. The last three goals: visual communication.



flow over an aircraft (Stanford Uni.)

Scientific Visualization – Example

- Scientastic Open Day – numerical simulation for the general public
  - illustration of MARVEL / ACCES activities using stereoscopic movies



https://acces.epfl.ch/outreach

Photography © 2015 www.sandipde.com

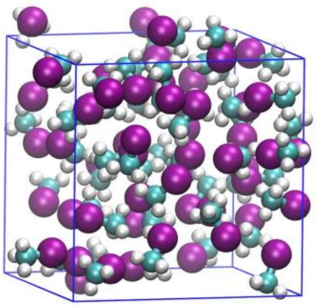
Classification – Representation

- Scientific representation
  - a realistic rendition of scientific reality and/or data
  - generally used for visualizing macroscopic systems
  - often used for engineering systems

- Artistic representation
  - an artistic rendition of scientific reality and/or data
  - generally used for visualizing microscopic systems
  - often used for biological systems

These two representations are not entirely independent

Pelton turbine / Ch. Vessaz, EPFL

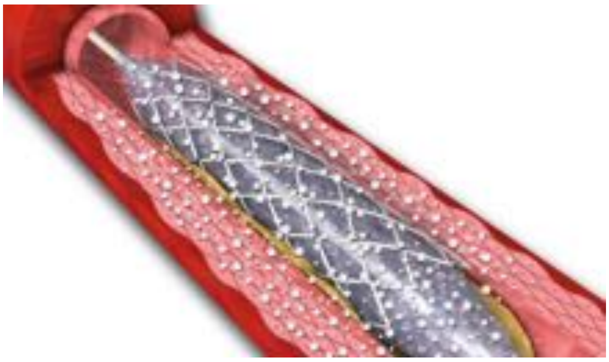


Visualization | Scientific Visualization

Classification – Representation

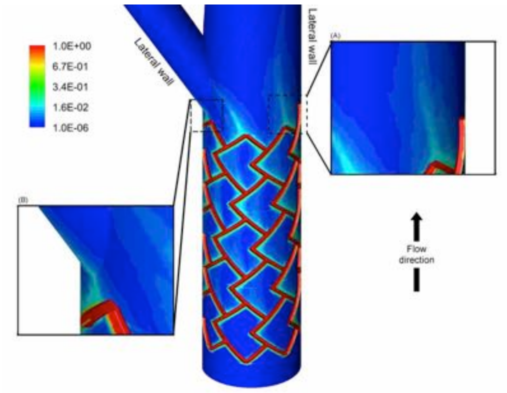
Example : Operation of a drug-eluding stent in an artery

artistic representation



Drug release from a drug-eluding coronary artery stent (Cardionovum AG)

scientific representation



Concentration of drug released from a stent in a bifurcating artery (E. Edelman & V.B. Kolachalama, MIT)

Visualization | Visual Communication

Classification – Utilisation

- Visual Communication

In the context of this lecture …

Visual communication involves the use of scientific visualization
(e.g. images, animations, interactive graphics) for the purpose of communication

"Advanced" visual communication involves the use of novel scientific visualization
… that are NOT employed by your colleagues … for the purpose of communication.

Visualization | Visual Communication

What are appropriate design criteria ?

- Visual communication should be based on pre-defined design criteria, not on the user's visualization capabilities (i.e. "visual objects designed for communication")

- Scientific paper (e.g. publication, poster, event)
  - publication in a top journal (e.g. Nature, Science) is not sufficient – aim also for the cover !
  - goal is for cover image / poster to have both scientific content and aesthetic appeal
  - cover image should be "**striking**" and attract attention to your paper

- Scientific presentation (e.g. live or recorded seminar, MOOC)
  - use images & animations as a communication support
  - goal is for visual objects to highlight your presentation
  - visual objects should be "**memorable**" and enable presentation to be remembered

Visualization | Visual Communication

What are appropriate design criteria ?

- A "striking" visual object is
  - *attracting attention by reason of being unusual, extreme or prominent* *
  - *dramatically good-looking or beautiful* *

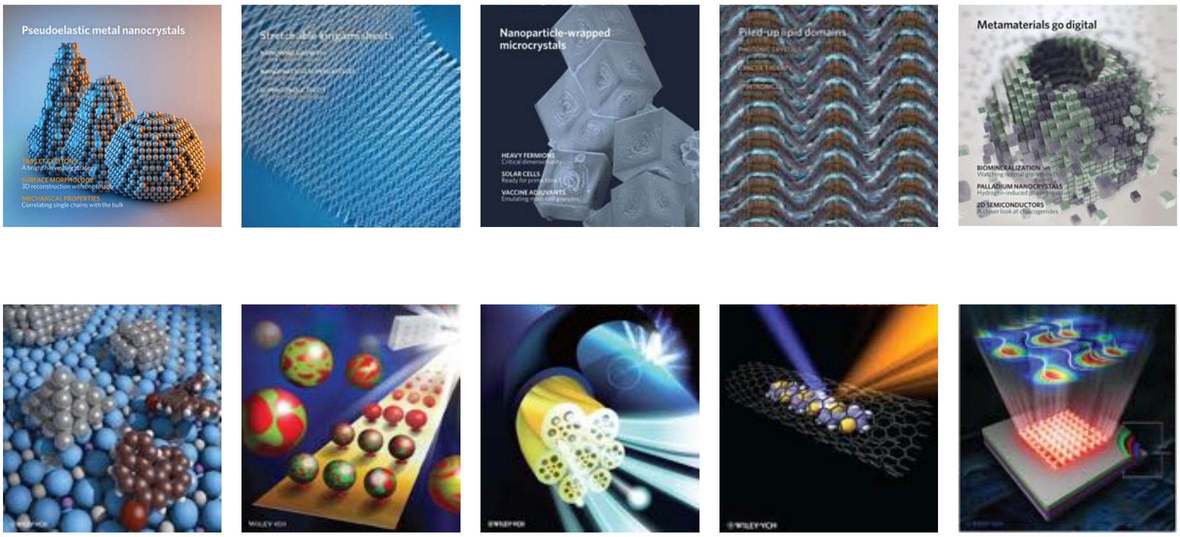
- A "memorable" visual object is
  - *worth remembering or easily remembered, especially because of being special or unusual* *

For effective visual communication (that requires either striking or memorable content), "standard" visual objects should be replaced by "unusual" visual objects

* *Oxford dictionary*

Visualization | Visual Communication

Materials journals' covers – are they "striking" ?



Visualization | Visual Communication

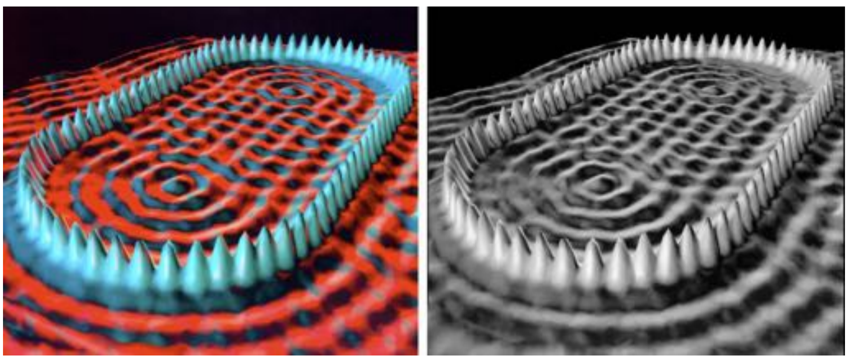
What are appropriate design criteria ?

- Less is better … sometimes simplicity is preferable
- for example, eliminating colours can improve comprehension

Standing wave patterns of electron density in a quantum corral

in "Visual Strategies: a practical guide to graphics for scientists & engineers"

F.C. Frankel & A.H. DePace (2012)



youtu.be/fAFjfacIvfU

Visualization | Visual Communication

What are appropriate design criteria ?

- Less is better … when hyper-realism is excessive !

- “Call of Duty” (2003) – sales of more than $10 billion in ~ 10 years
  [cf. James Bond series : $7 billion in ~ 50 years]

Visualization | Visual Communication

What are appropriate design criteria ?

- Less is better … sometimes simplicity is preferable

```
YOU ARE STANDING AT THE END OF A ROAD BEFORE A SMALL BRICK BUILDING.
AROUND YOU IS A FOREST.  A SMALL STREAM FLOWS OUT OF THE BUILDING AND
DOWN A GULLY.

> enter

YOU ARE INSIDE A BUILDING, A WELL HOUSE FOR A LARGE SPRING.
THERE ARE SOME KEYS ON THE GROUND HERE.
THERE IS A SHINY BRASS LAMP NEARBY.
THERE IS TASTY FOOD HERE.
THERE IS A BOTTLE OF WATER HERE.
```

- “Colossal Cave Adventure” (1976) : first interactive computer game (free distribution)

http://rickadams.org/adventure

What are appropriate design criteria ?

- In designing a visual object, consider the following aspects
  - Who is the audience (e.g. level of scientific knowledge) ?
  - How will it be used (e.g. paper, talk, poster) ?
  - What is the goal of the visual object (i.e. the message to convey) ?
  - What is the challenge (i.e. what difficulties exist to convey message) ?

What is needed for effective Visual Communication?

- The following basic elements are generally required
  - numerical / application data (the basis of the model)
  - visualization software, techniques and expertise CS
  - display hardware and competence CS
  - basic design concepts (e.g. use of colour, forms, arrangement, media) CS
  - imagination, experience and creativity

Effective visual communication requires adequate knowledge & investment

“Soft skills” are an important aspect of visual communication

Visualization	Visual Communication

Is Visual Communication globally employed ?

- General observations
  - visual communication is performed “if I have some spare time” *(low priority)*
  - minimal / no investment in specialized visualization infrastructure *(under invested)*
  - wide range of different visualization software available *(confusing)*
  - designing visualization for communication poorly understood *(complicated)*
  - “There’s no science, just nice pictures” ! *(counter-productive)*

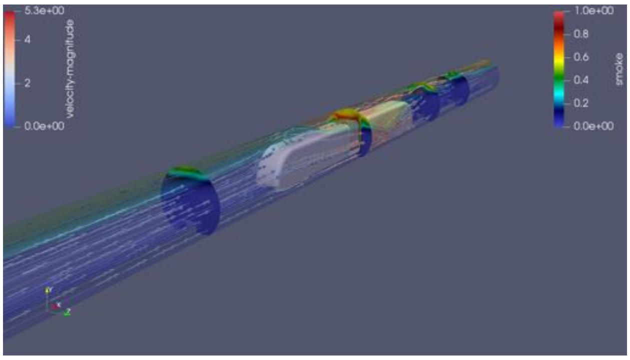
Scientific visualization (for communication) is not exploited to its maximum capacity CS

Visualization	Visual Communication

Comparison of Scientific Visualization & Visual Communication

Representation of a train on fire in a tunnel

Scientific Visualization



ParaView

Visual Communication

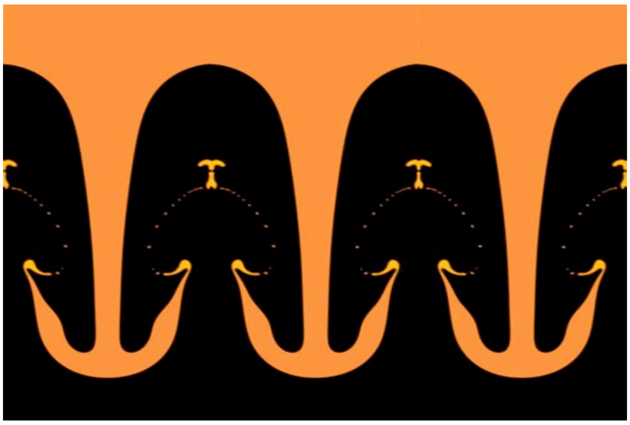
Blender

Visualization | Visual Communication

Comparison of Scientific Visualization & Visual Communication

Representation of the Rayleigh-Taylor instability

Scientific Visualization



ParaView

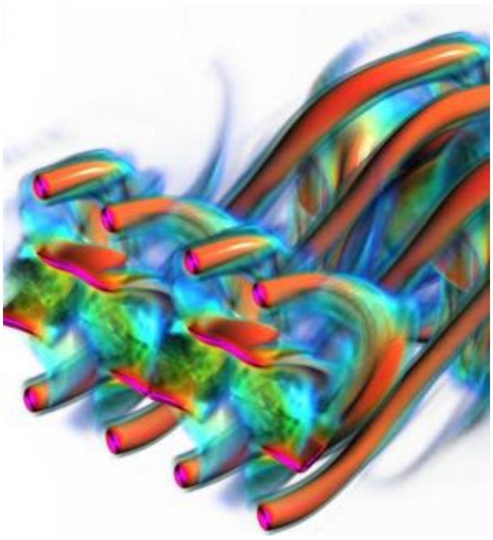
Visual Communication

SketchUp & Maxwell Render

Visualization | Specific techniques

Classification – Techniques

- Scientific visualization is a combination of :
  - plotting techniques for 2D data
  - iso-surfaces and volume rendering for 3D data
  - CS — data mining & pattern discovery (coherent structures)
  - CS — rendering techniques
  - animation techniques
  - stereoscopy (depth information)
  - CS — photorealism (ray tracing & texturing)
  - CS — colour and human perception
  - aesthetics (artistic aspects)
  - CS — software implementation
  - CS — hardware implementation
  - …



Advanced scientific visualization

- Novel techniques assist visualizations to be more effective.
- These techniques exist for a long time, but are still not integrated into standard engineering practice.
- Computer scientists have strongly contributed to generating tools, but less to their application.

"Advanced" techniques

- High resolution (e.g. on 4K / UHD displays)
- High-fidelity rendering (e.g. photorealism using ray tracing)
- Panoramic images
- Stereoscopy (i.e. 3D)
- Immersion (i.e. virtual reality) CS

Rendering – traditional rasterization

- Scientific visualization software has traditionally used rasterization techniques to map visual objects onto a 2D screen
- In a traditional 3D graphics pipeline contains the following (simplified) steps:
  - read input dataset
  - create collection of geometric primitive objects (generally, triangles)
  - transform local coordinates to world system oriented according to camera viewpoint
  - Illuminate scene according to prescribed lighting
  - transform 3D coordinates into 2D view plane
  - rasterize the scene, converting objects into pixels that can be displayed on a 2D monitor screen
- Rasterization is extremely fast, but limited in producing realistic details

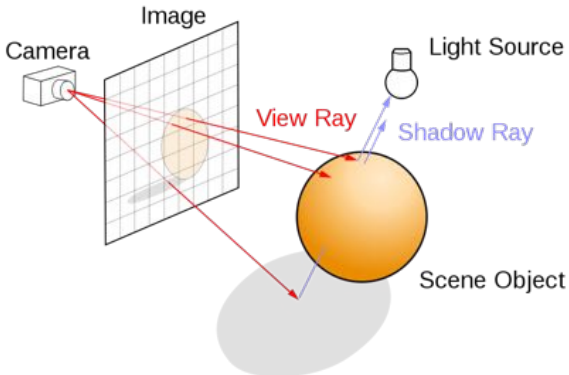
High-fidelity rendering

- Augments the quality of a visual object
  - include optical effects to render the image "photorealistic"
- Uses ray-based techniques, e.g. :
  - ray tracing
  - path tracing
- Employed extensively in :
  - architecture
  - animation cinema

Blender (cycles renderer), Jay-Artist

High-fidelity rendering – ray tracing

- Generate image by tracing the path of light from the viewpoint through the pixels in an image plane, and simulating the effects of its interaction with virtual objects
  - high degree of realism
  - capable of simulating wide variety of optical effects:
    - reflection
    - refraction
    - scattering
    - chromatic aberration
  - computationally expensive
  - best for off-line rendering, not real-time visualization



High-fidelity rendering – ray tracing

- A diverse set of optical effects are possible, depending on material properties :

Luo Zhen – semester project

Panoramic images

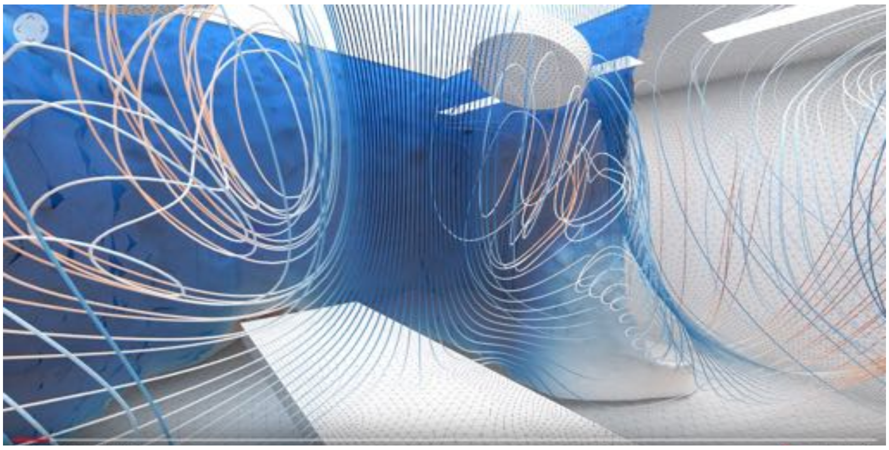
- Provides a 360º view of image space ; view only a 90º segment at a time
- Single panoramic image with ratio 2:1 (equirectangular format)
- Basic tools:
  - development : Blender
  - display : Kolor / GoPro VR Player
    Memento360

360º equirectangular view of chessboard

Visualization | Specific techniques

Panoramic images – Example

- Numerical study of ventilation in a hospital operating theatre



Actiflow – youtu.be/By3L6SeSnJ0

Visualization | Specific techniques

Stereoscopy – visualize data in 3D ?

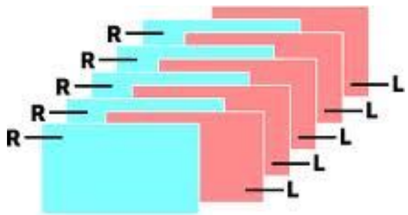
- Numerical simulation data is often 3D, but essentially all derived visual objects are 2D
- The human brain is only capable of partially reconstructing a 2D representation of a 3D object
- 3D imagery has existed since 1830s; recently there was a short-lived interest in 3D TVs
- Three main categories of stereoscopic techniques :
  - active
  - passive
  - autostereoscopy

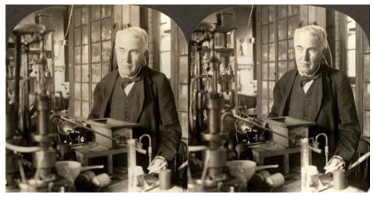
  These provide a means to send different images to the left and right eyes.

Visualization | Specific techniques

Stereoscopy – visualize data in 3D ?

- Left / right eye channels can be separated by :
  - time (shuttering)
  - space (side-by-side, top-bottom)
  - colour (anaglyph)
  - polarization (circular / linear)



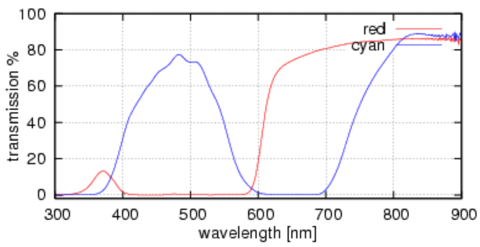


Visualization | Specific techniques

Passive stereoscopy

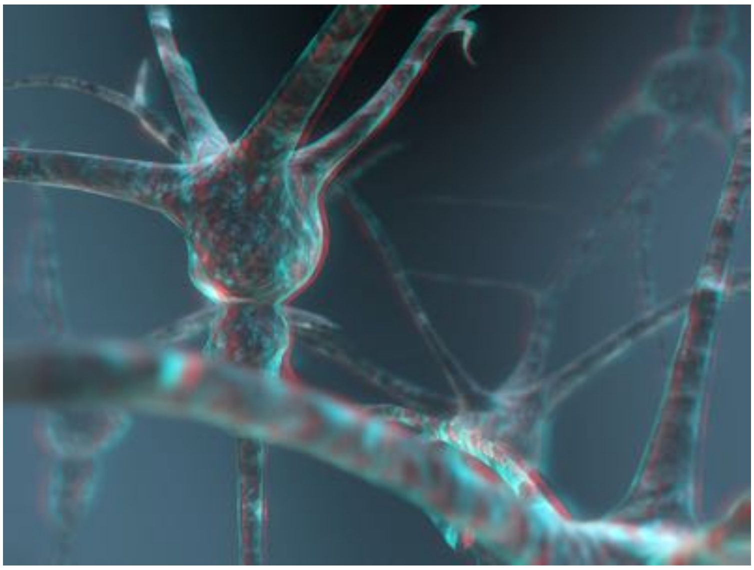
- Anaglyphs: a universal (low-quality) technique
  - incorporated into many scientific visualization software
- Equipment required
  - no special display required, only very cheap glasses

1950's entertainment



Visualization | Specific techniques

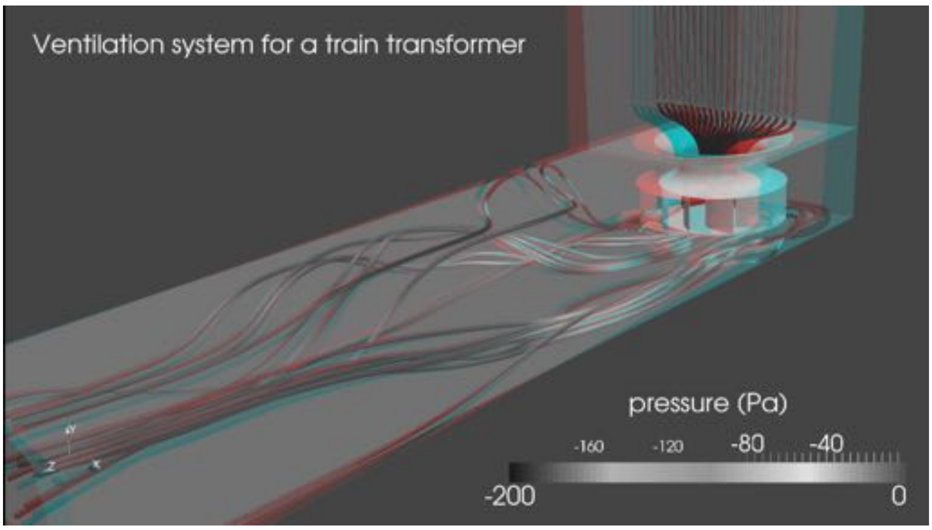
Passive stereoscopy – Anaglyph example



neuron anaglyph
M. Ramsey – abduzeedo.com

Visualization | Specific techniques

Passive stereoscopy – Anaglyph example



Streamlines in 3D flow

Visualization | Specific techniques

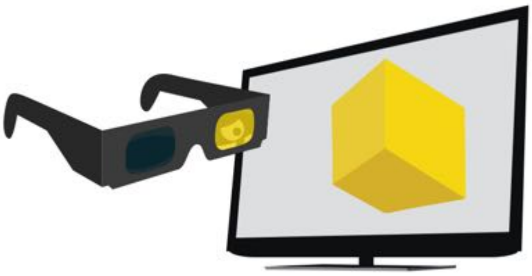
Passive stereoscopy

- Polarization: a high-quality cost-effective technique
  - left and right images in alternate lines of the display
  - excellent quality
  - reduced spatial resolution (in vertical direction)
- Equipment required
  - polarized display (e.g. certain TVs)
  - inexpensive (circularly) polarized glasses

Visualization | Specific techniques

Active stereoscopy

- A high-quality technique
  - left and right images switched alternatively
  - excellent quality (maybe flickering)
  - full spatial resolution
- Equipment required
  - synchronized display (e.g. certain TVs)
  - more expensive shutter glasses (heavier, battery, synchronized)



Visualization | Specific techniques

Auto-stereoscopy

- A technique under development
  - various approaches to this “holy grail of 3D”
- Equipment required
  - display depends on technique
  - glasses-free
- Techniques employed:
  - Wiggle stereo
  - Toshiba 55ZL2 TV

static image

wiggle stereogram

Visualization | Specific techniques

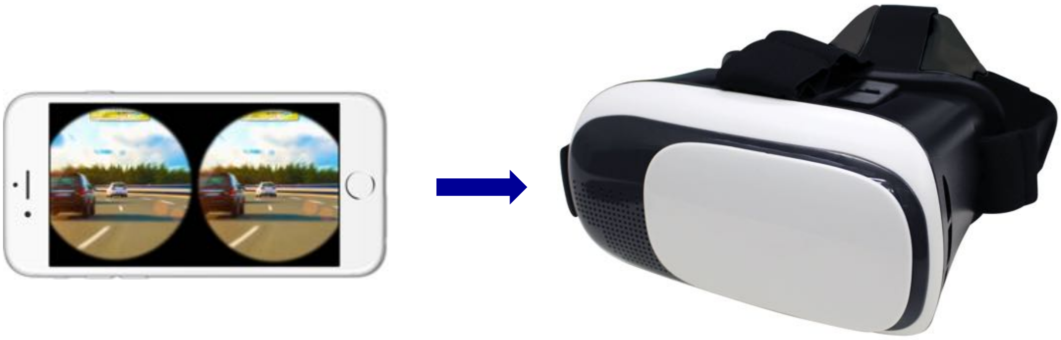
Immersion – Virtual Reality

- 360^{o} + stereoscopy => virtual reality
- Immerse viewer within the data field to enhance perceptive experience
- Two basic approaches
  - multiple side projection room (CAVE) CS
    - more than one viewer simultaneously
    - very expensive
  - headset (Oculus Rift, Google Cardboard, etc.) CS
    - generally a single viewer
    - inexpensive => expensive (depending on functionality)

Visualization | Specific techniques

Immersion – Virtual Reality

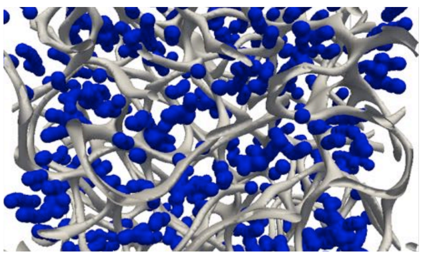
- Inexpensive entry-level VR experience
  - passive headset (inexpensive)
  - smartphone (with gyroscope)
  - VR app / website

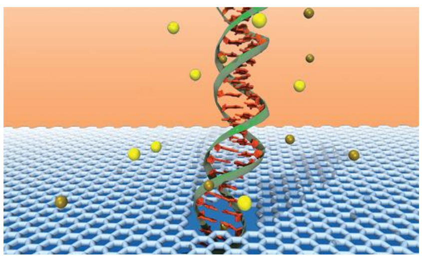


Visualization | Software

Scientific visualization software used by EPFL Engineering

- ParaView
  - high-end general-purpose 3D scientific software
  - modular structure using filters to extend functionality
  - high-performance treatment for very large datasets
- VMD (Visual Molecular Dynamics)
  - high-end 3D visualization of MD simulations
  - modular structure using plug-ins to extend functionality
  - capable of treating large bio-molecular datasets





Many other software are used for scientific visualization.

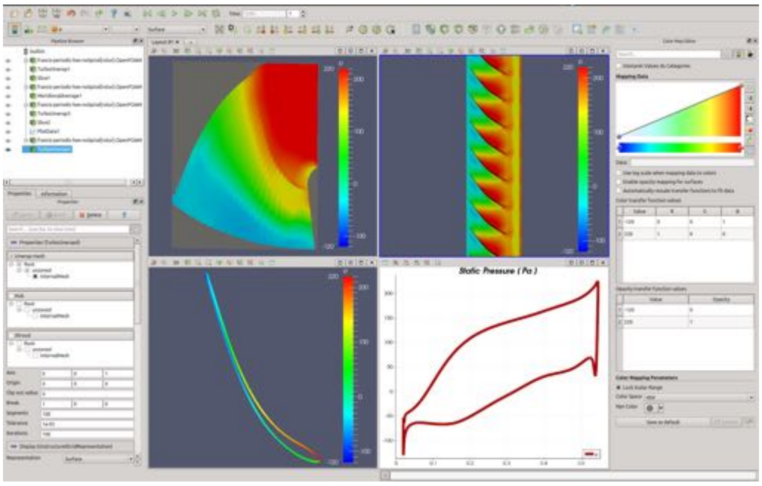
Visualization | Software

Example – ParaView

ParaView is a general-purpose software package for interactive data visualization and analysis. It is based on the graphics library VTK, and is open source and supported by Kitware Inc.

ParaView features include:

- uses a series of pipelined data-processing operations (filters)
- filters can be pre-defined, or user-programmed
- handles a wide range of data types (structured / unstructured mesh, point)
- hardware rendering (using OpenGL)
- parallel computation on distributed-memory systems (using MPI)
- open source, with commercial support
- Linux, Windows, MacOS X



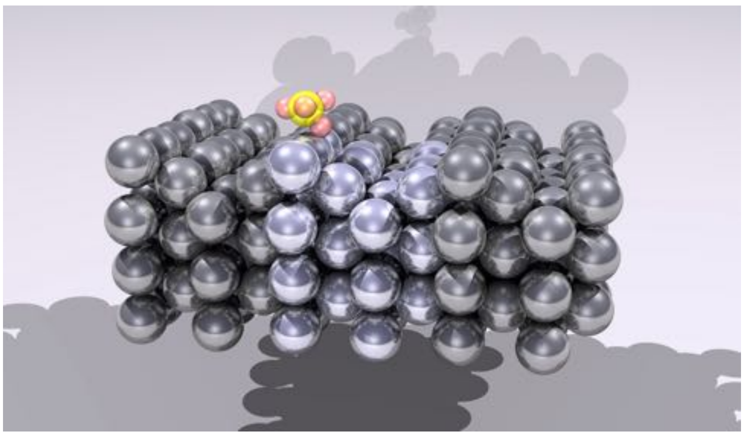
EPFL

Visualization | Software

High-fidelity rendering – ray tracing

- Many software packages using ray tracing are available :
  - Open source
    - Blender (www.blender.org)
    - POV-ray (www.povray.org)
    - Mitsuba (www.mitsuba-renderer.org)
  - Commercial
    - Maya
    - Maxwell Renderer

    \+ many others
- Steep learning curve CS



Tachyon ray-tracer, Nicola Marzari (EPFL)

EPFL

Visualization | Software

Example – Blender

Blender is a professional, free and open-source 3D computer graphics software product used for creating animated films, visual effects, art, 3D printed models, interactive 3D applications and video games. It further features an integrated game engine.

Blender features include:

- 3D modeling
- texturing
- raster graphics editing
- fluid and smoke simulation
- particle simulation
- soft body simulation
- sculpting
- animating
- camera tracking
- rendering
- video editing
- compositing
- . . .

Visualization | Software

Require combination of Science & Art – but I'm not an artist !

- Convert (automatically) your scientific images on-line into artwork
  - Deep-Art uses a neural network algorithm based on the 19-layer model of Simonyan & Zisserman

CS

http://deepart.io

Visualization | Display hardware

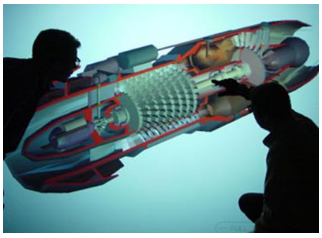
What display hardware is suitable

- Personal
  - computer monitor
  - laptop
  - smartphone / tablet
  - wearable display
  - virtual reality headset (e.g. Oculus Rift)
- Collaborative
  - (tiled) display wall
  - (immersive) CAVE
  - remote sites (videoconferencing)
- Concurrent
  - runtime visualization

CS
CS

CS

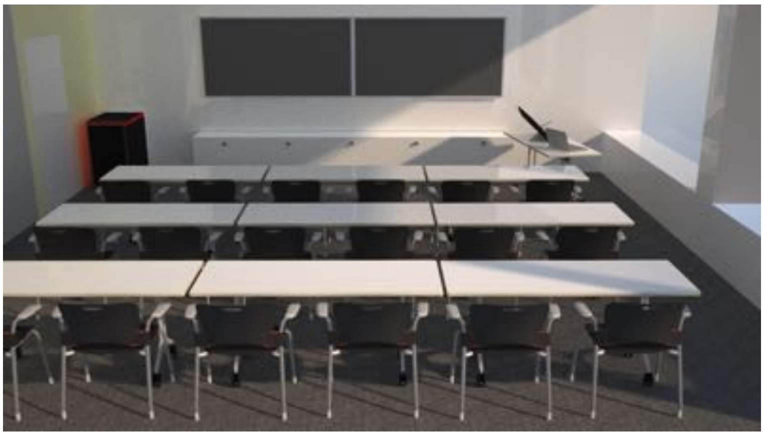
CS



Visualization | Display hardware

ACCES Collaborative Visualization (CoViz1) facility

- Shared facility for two engineering schools (STI & ENAC) at EPFL
  - two 84” UHD/4K stereoscopic screens
  - dual 4-core server (Intel Xeon E5-2660, 128 GB RAM)
  - 2 nVidia Quadro K5000 cards
  - Wacom 22” pen touch display
  - Cisco SX80 videoconf. codec
  - free of charge!



Maxwell render, acces.epfl.ch/coviz1

Visualization | Display hardware

Proposed communication wall

- Shared facility to be installed in MED building (next to Rolex)
  - 8 m x 1.8 m display (11520 x 2160 pixels)
  - 3 ceiling-mounted 4K laser projectors

Communication wall mock-up

Visualization | Concurrent Visualization

Runtime visualization

- Computational engineering
  - numerical study of complex engineering systems
  - use model to define governing equations (3D nonlinear partial differential equations)
  - develop numerical methods to solve these equations (computation phase)
  - visualization is generally a post-processing task

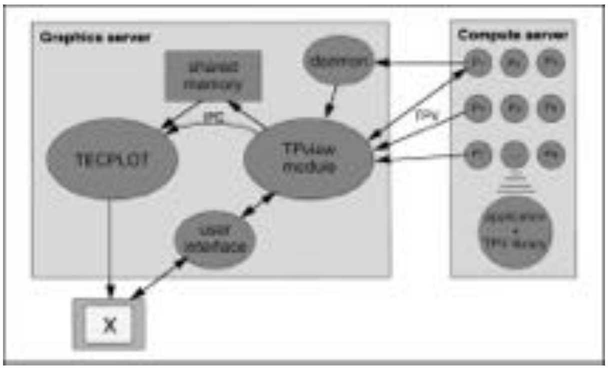
- Runtime visualization
  - provides insights into numerical problems
  - provides solution examination before end of computation phase
  - enables interactive solution steering

Runtime visualization enables concurrent computation and visualization

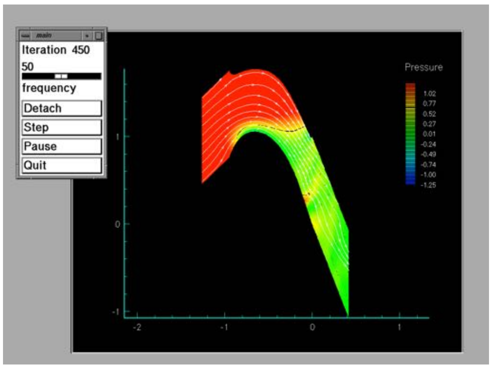
Visualization | Concurrent Visualization

Solution steering – Example

Example : TPview – Runtime visualization & solution steering



Schematic diagram of distributed setup



Solution visualization during computation phase

(Williams et al., EPFL)

Visualization | Examples

ACCES Visualization Contest *

2015 Contest – two categories : image, animation

2017 Contest – three categories : static, dynamic, interactive

Participants

- entries from Master students, PhD students, postdocs in engineering CS
- all entries are available online (http://acces.epfl.ch/contest)

Judging criteria

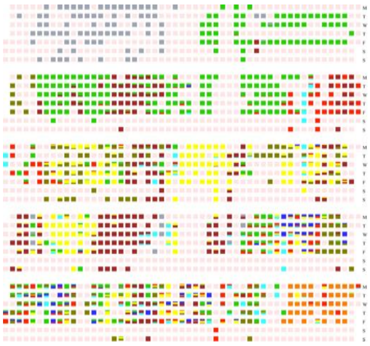
- innovative visualization approaches to communicate scientific / engineering content
- the creative use of the visual medium to reveal a remarkable aspect of engineering

** Sponsored by MARVEL NCCR*

Visualization | Examples

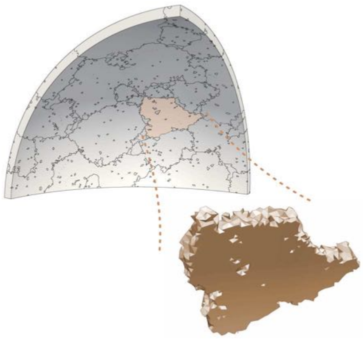
2015 ACCES Visualization Contest

- 3 of top entries in the Image category



Andrius Merkys (THEOS / STI)

Antonin Danalet (TRANSP-OR / ENAC)

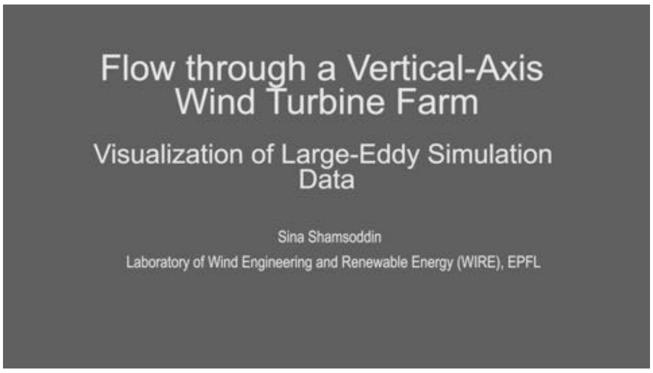


Marco Vocialta (LSMS / ENAC)

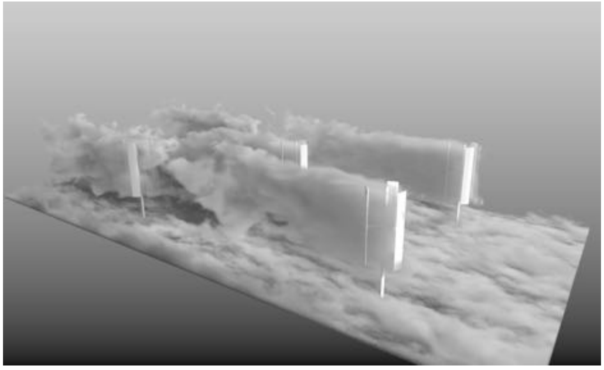
Visualization | Examples

2017 ACCES Visualization Contest

- Dynamic category (first prize)



mono animation



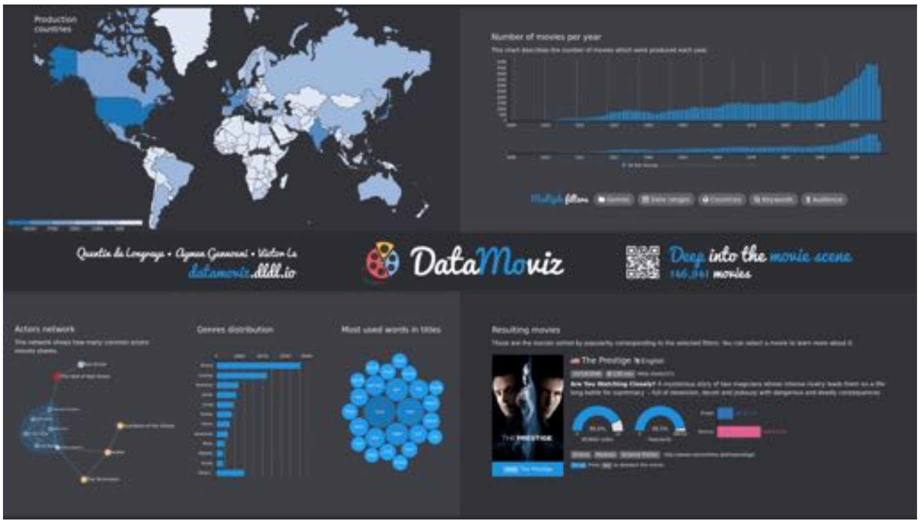
mono image

S. Shamsoddin, WIRE–ENAC–EPFL

Visualization | Examples

2017 ACCES Visualization Contest

- Interactive category (second prize) CS

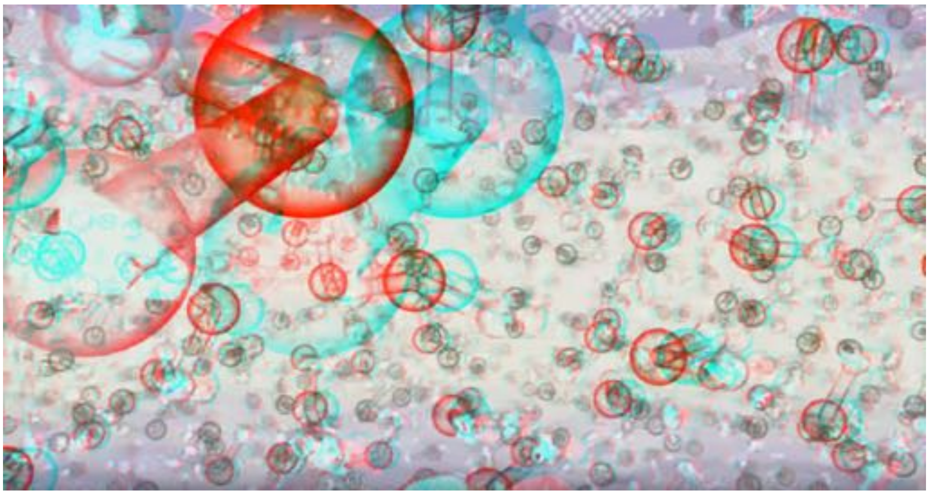


De Longraye, Le & Aymen, SSC-IC–EPFL

Visualization | Examples

Scientastic Open Day (Piero Gasparotto – COSMO-EPFL)

- Movement of water molecules
  - stereoscopic view



youtu.be/CPMFZq3VF2s

Visualization | Examples

Environmental impact (Jamani Caillet – SGC-EPFL)

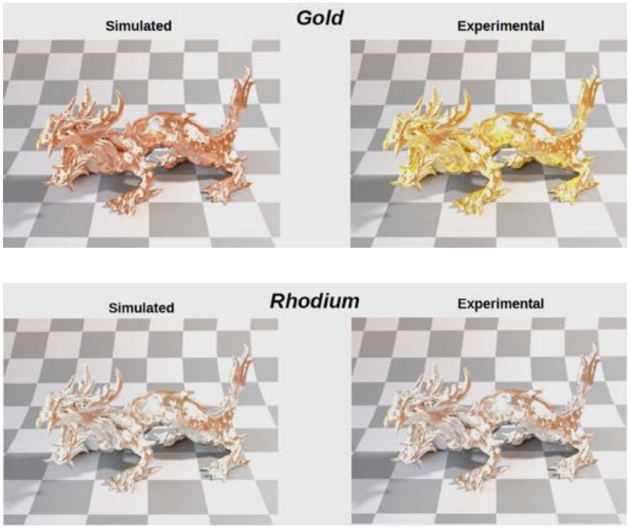
- Design of an artificial port on Lac Leman
  - Master project in Civil Engineering
  - structural feasibility
  - environmental impact
- Visual integration of the port design into the local environment using high-fidelity rendering

Blender, youtu.be/7Y9-vU1G50U

Visualization | Examples

High-fidelity rendering of metallic surfaces (Gianluca Prandini – THEOS-EPFL)

- Colour selection aided by first-principle simulations
  - Colour of gold and copper alloys is changed by varying the alloy additions
  - Spectral reflectivity curve determined from first-principle IP-RPA approach
  - Establish a database for different metallic materials (numerical ⟺ experimental)
  - Use Mitsuba renderer (W. Jakob, EPFL) to visualize surface appearance



Mitsuba, http://theos.epfl.ch

Visualization | Examples

Security analysis of N_2 transport in laboratory (Albert Taureg – SGM-EPFL)

- Computed evolution of N_2 level in room following a simulated accident

360º animation

Visualization | Examples

Photorealistic rendering for industry

- Incorporated in geometry design (CAD), numerical simulation & scientific visualization software
- Realistic material properties with low learning curve

SpaceClaim & Keyshot

Visualization | Where to now ?

Beyond the basics – using all your senses (i.e. "sensual communication")

- Vision CS
  - colour (e.g. optimal selection, adjusting for colour-blindness)
  - lighting (e.g. for photo-realism)
  - depth of field (e.g. 3D effects)
- Audio CS
  - frequency (pitch)
  - timbre (instrument)
- Touch CS
  - coordinated movement
  - dynamic cinema
- Smell & Taste CS

Montreux Jazz Heritage Lab (EPFL+ECAL)

Visualization | Where to now ?

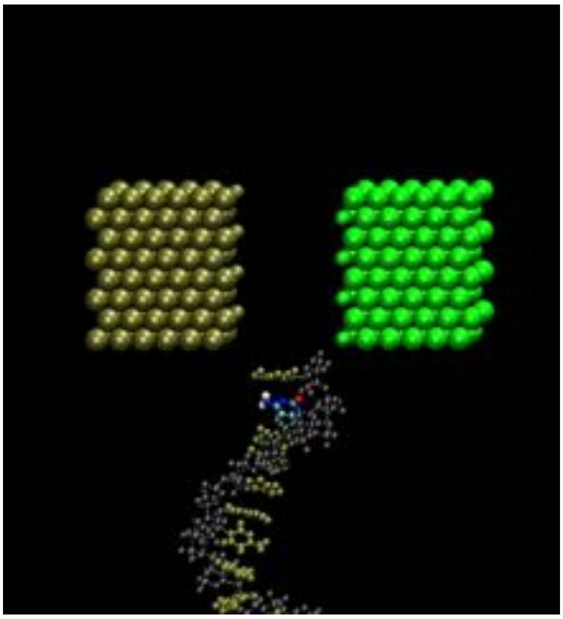
Beyond the basics – Auralization

Molecular dynamics simulation of single-stranded DNA passing through a nano-gap.

The audio represents the angle of each base in red, white and blue relative to the DNA backbone. Each base is represented by a different instrument whose volume is scaled by the distance between the base and nano-gap.

Note the tilting of each base as it passes through the nano-gap.

For more details, see:
A.P. Jallouk & P.T. Cummings, *Audibilization: Data analysis by ear*, J. Chem. Theory Comp. 10, 1387 (2014)



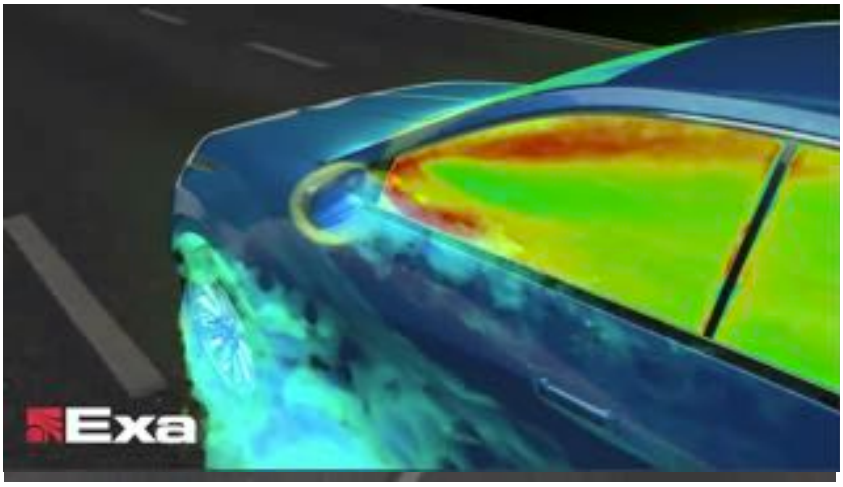
youtu.be/m0EWKDDkwuc

Visualization | Where to now ?

Auralization – Example

Aero-acoustic noise generated by a car side window

Simulate how the side mirror design modification changes the noise sources on the glass panels and reduces the noise heard by the driver.



Exa Corp. – youtu.be/zMvovjqqcVA

Contributions by Computer Scientists

Partial list of developments (related to CS activities) CS

- physically based renderer (Mitsuba)
- data visualization
- CAVE installation and development
- tools for interaction with visual display
- parallel visualization for numerical simulation
- transform automatically engineers into artists
- . . .

Novel visual methodologies can be validated and valorised by applying to engineering applications, via collaborations e.g. with computational scientist / engineers. CS

Visualization | Today's message

Regarding Scientific Visualization :

- Use visualization to **discover** new scientific insights and **communicate** a message to diverse audiences.
- **Invest** adequate time to perform effective visual communication :
  you will be rewarded if your visual objects are "**striking**" and/or "**memorable**" (i.e. "unusual").
- Ensure that your visual objects retain **scientific content** :
  otherwise scientists will consider that they are "just nice pictures".
- For your papers, posters and presentations, show artistic **creativity** wherever useful
  distinguish your contribution from those of colleagues and "competitors".
- Computer scientists can aid in development and application of novel visual methodologies
  contact engineers to form collaborations – **validate & valorise** your activities.

EPFL

Visualization | References

Further reading :

- F.C. Frankel & A.H. DePace, *Visual Strategies: a practical guide to graphics for scientists & engineers* (Yale, 2012)
- M. Rolandi, K. Cheng & S. Pérez-Kriz, *A brief guide to designing effective figures for the scientific paper* (2011), http://onlinelibrary.wiley.com/doi/10.1002/adma.201102518/full

\+ many other books and scientific articles

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