Computational Sciences at Uni Computing

Visual Computing Forum
2012-04-13

Klaus Johannsen, Uni Computing, Director

uni Computing

Overview

- Introduction
- Activities
- Visualization
- Todo

Introduction

- Uni Computing is a department of Uni Research AS, the research company associated with the University of Bergen
- Uni Computing is organized in five groups with more than 60 staff.

- Our Vision

  Uni Computing carries out research and development in basic and applied areas with a focus on computational techniques.

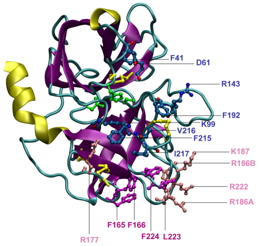
  We seek the comprehensive uptake of our results, methods, services and competences within science, industry and wider society.

Introduction (cont'd)

- Uni Computing is organized in five groups:
  - CBU: *Bio-informatics, research in molecular biology and genomics*
  - CEU: *Computational ecology, individual based population dynamics*
  - CLU: *Language technology, computational linguistics, Lexicography, computational media analysis*
  - EFG: *Oceanography, meso- and micro-climatology, CFD, wave-modeling, artificial intelligence*
  - Parallab: *High Performance Computing, e-Infra-structures, Programming*

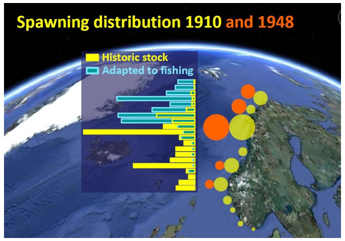
Introduction (cont'd)

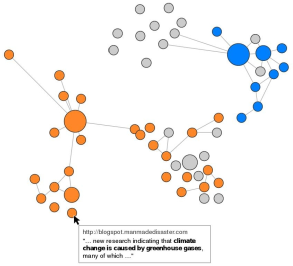
- Uni Computing research activities are pretty heterogeneous



Proteinase 3: Key amino acids for ligand recognition and membrane binding (Reuter et.al., CBU)

Cod: Spawning dristribution along the Norwegian coast, 1910 and 1948 (Jørgensen et.al., CEU, 2008)

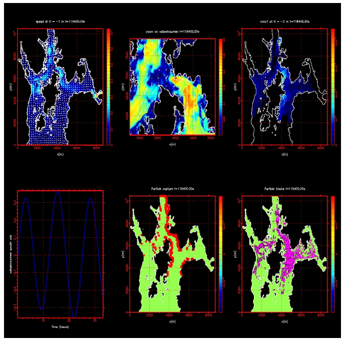



http://blogspot.manmadedisaster.com
"… new research indicating that climate change is caused by greenhouse gases, many of which …"

A graph displaying blog posts collected around the topic of climate change (Salway et. al., CLU, 2012)

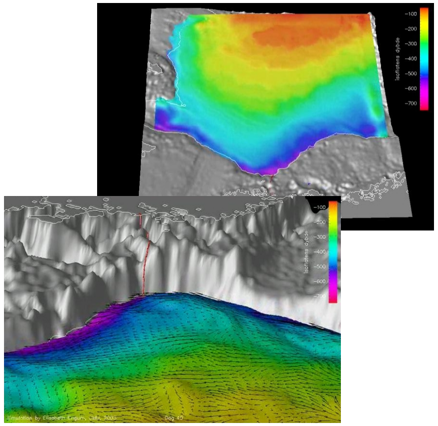
Introduction (cont'd)

- Uni Computing research ...



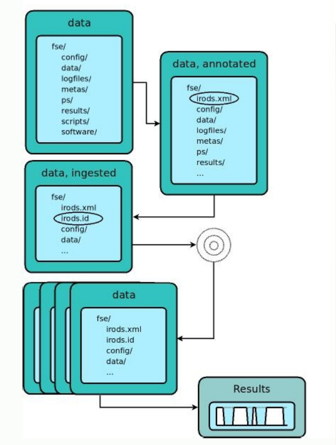
Simulation of oil spill, Rocknes accident at Vatlestraumen (Torsvik et.al., EFG, 2009)

Ormen Lange process studies (Avlesen et.al., EFG, 2005)



Hexagon: Supercomputer operated in collaboration with II/UiB (Parallab, 2012)

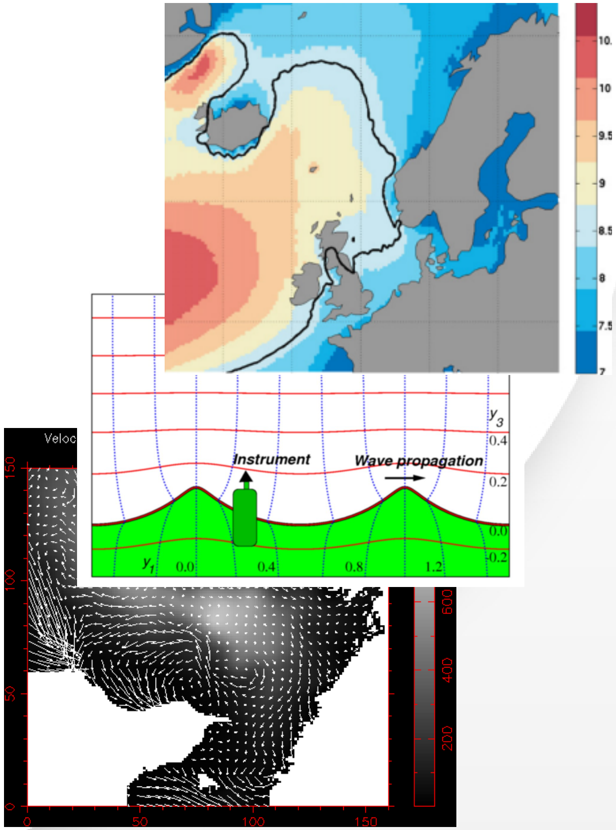
HPC-Europa2: Usage pattern of a postprocessing e-infrastructure (Anderlik et.al., Parallab, 2011)



Activities: The WWW-Column (EFG)

- Focusing on what makes sense (in Norway). Integrating
  - Wind, waves & currents in fjords
  - Atmospheric & marine dispersion
  - Marine physics & ecology

- With application to
  - Offshore wind: resource assessment & forecasting
  - Env. management of aquaculture
  - Marine oil spills & releases
  - Subsea CO_2 storage: hazards & impact assessment

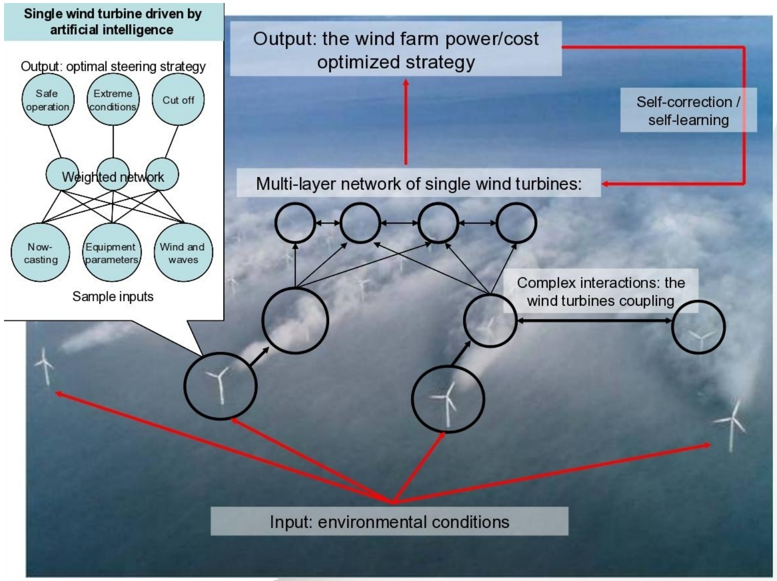


Activities: NORCOWE (EFG)

- WP1 - Wind and ocean conditions (Uni lead)
  - Climatology of met / ocean conditions
  - Modelling of the atmospheric boundary layer over sea
- WP2 - Offshore wind technology & innovative concepts
- WP3 - Offshore deployment & operation
- WP4 - Wind farm optimisation
- WP5 - Common themes
  - Education
  - Impact assessment
  - Infrastructure
  - Data storage & management

Activities: AI & Floating Wind Farms (EFG)

- A network of *Artificial Neural Networks* to describe floating wind farms using
  - Simplified wind turbine models
  - Empirical models for turbine-turbine/wake-wake and other complex interactions
- With applications to
  - Short term power forecast
  - Optimal operational strategies



Single wind turbine driven by artificial intelligence

Output: optimal steering strategy

Safe operation

Extreme conditions

Cut off

Weighted network

Now-casting

Equipment parameters

Wind and waves

Sample inputs

Output: the wind farm power/cost optimized strategy

Self-correction / self-learning

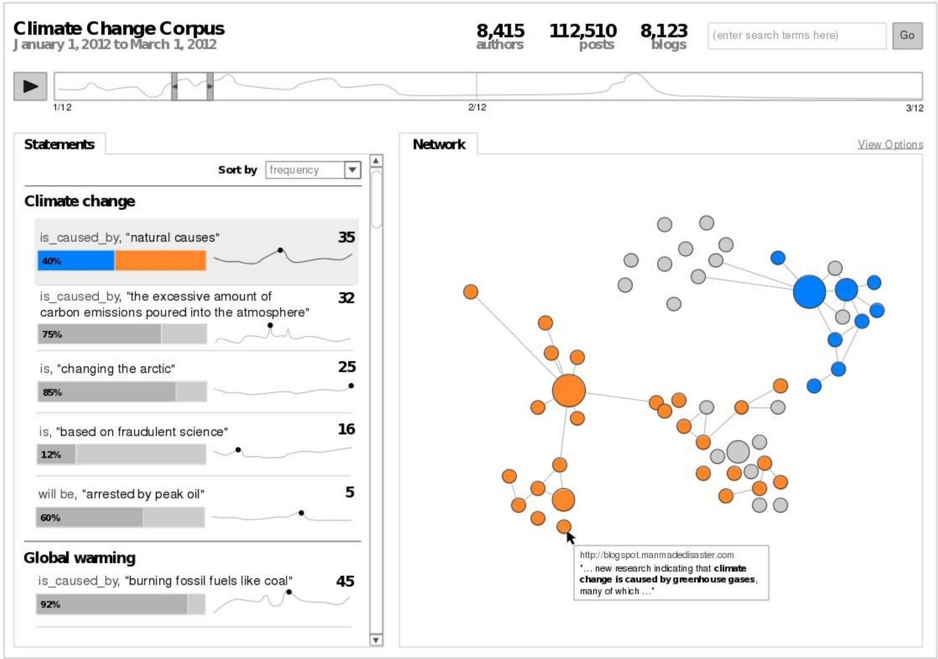
Multi-layer network of single wind turbines:

Complex interactions: the wind turbines coupling

Input: environmental conditions

Activities: New Tools for Soc Scie (CLU)

- Using/enhancing our knowledge about text-processing to form semantic units (e.g. *key-statements)*
- Relate units to form a knowledge-base to be analysed by
  - Social science researchers
  - Media monitoring companies
- Interactive visualization to understand the dynamics of human society



Climate Change Corpus
January 1, 2012 to March 1, 2012

8,415 authors 112,510 posts 8,123 blogs

Climate change

is_caused_by, "natural causes" 35 40%

is_caused_by, "the excessive amount of carbon emissions poured into the atmosphere" 32 75%

is, "changing the arctic" 25 85%

is, "based on fraudulent science" 16 12%

will be, "arrested by peak oil" 5 60%

Global warming

is_caused_by, "burning fossil fuels like coal" 45 92%

http://blogspot.manmadedisaster.com
'... new research indicating that **climate change is caused by greenhouse gases**, many of which ...'

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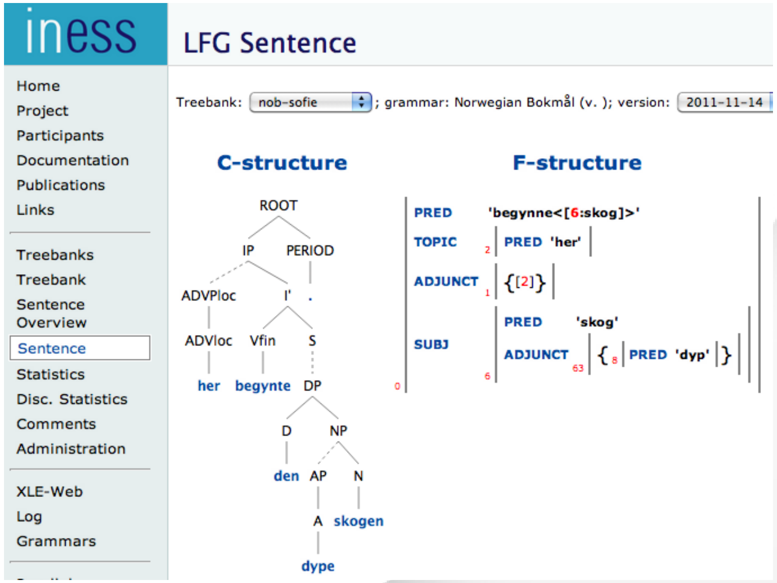
Activities: INESS (CLU)

- Norwegian Infrastructure to Explore of Syntax and Semantics
- Interactive, language independent system for hosting, building, accessing and exploiting treebanks

- Build a 50 million sentence treebank of Norwegian
- Step towards developing the next generation of language technology applications



Treebank: nob-sofie; grammar: Norwegian Bokmål (v.); version: 2011-11-14

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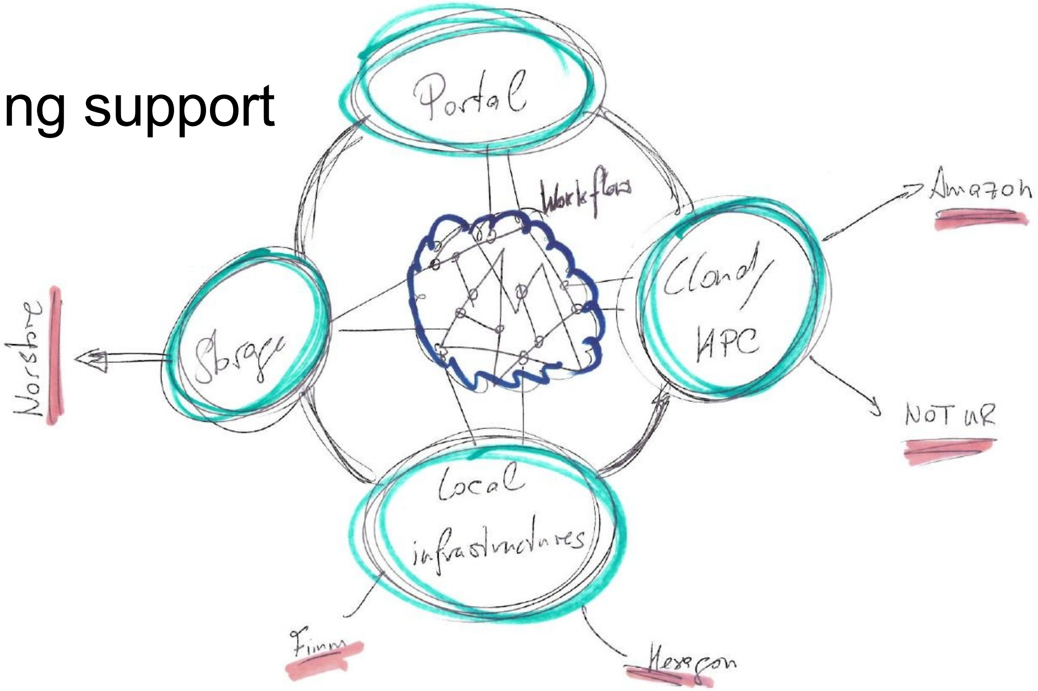
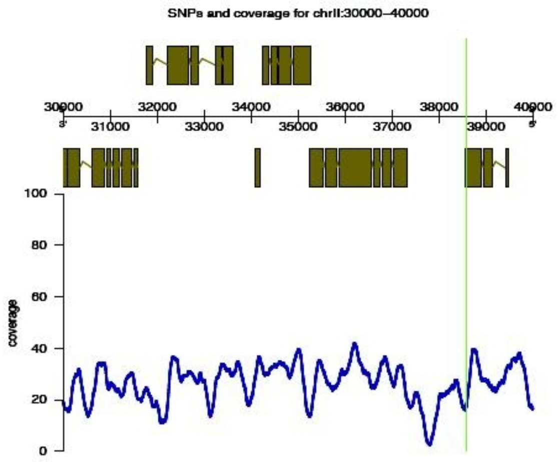
Activities: New Services (Parallab)

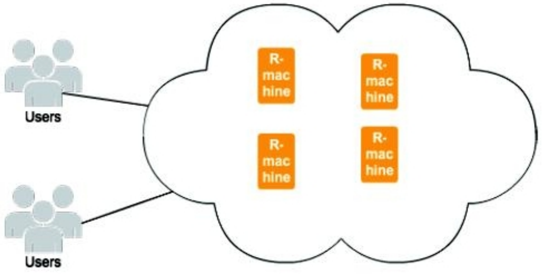
- Anticipating the future to be ready when people (scientists and others?) need us
  - Intelligent vertical e-infrastructures (interactive end-points)
  - GPU-programming support
  - Cloud services



Activities: Cloud Computing (Parallab)

- Use cloud computing/virtual machines for scaling up scientific applications
- Access to on-demand computing ready to use. Highly configurable with respect to operation system, memory and processor(s)
- Pilot project: use Amazon Cloud to run R(r-project.org) based scripts for statistical analysis. Used e.g. in eSysBio

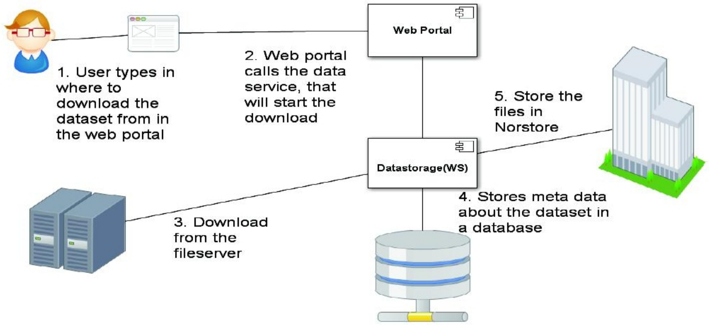




Activities: StoreBioinfo (CBU)

- StoreBioinfo has two aims
  - Together with NorStore develop data storage policies and govern a large block allocation of storage dedicated to Life Sciences
  - Establish e-services providing Life Science users integrated access to storage and computational resources from NorStore/Notur

- E-services used to integrate Genomic HyperBrowser for analysis on data stored in StoreBioinfo


Web Portal
1. User types in where to download the dataset from in the web portal
2. Web portal calls the data service, that will start the download
5. Store the files in Norstore
Datastorage(WS)
4. Stores meta data about the dataset in a database
3. Download from the fileserver

- Portal in production (storebioinfo.norstore.no)

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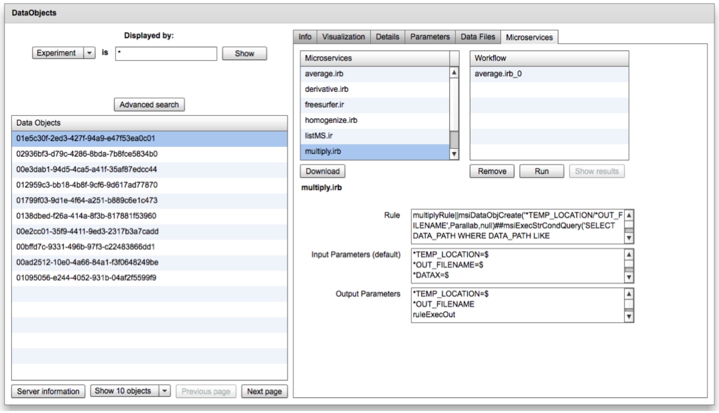
Activities: HPC-Europa2 (Parallab)

- Common requirements for many scientific applications: large datasets, many files, need for metadata, and post-processing



Experiment is *

Data Objects
01e5c30f-2ed3-427f-94a9-e47f53ea0c01
02936bf3-d79c-4286-8bda-7b8fce5834b0
00e3dab1-94d5-4ca5-a41f-35af87edcc44
012959c3-bb18-4b8f-9cf6-9d617ad77870
01799f03-9d1e-4f64-a251-b889c6e1c473
0138dbed-f26a-414a-8f3b-817881f53960
00e2cc01-35f9-4411-9ed3-2317b3a7cadd
00bffd7c-9331-496b-97f3-c22483866dd1
00ad2512-10e0-4a66-84a1-f3f0648249be
01095056-e244-4052-931b-04af2f5599f9

Microservices
average.irb
derivative.irb
freesurfer.ir
homogenize.irb
listMS.ir
multiply.irb

Workflow
average.irb_0

multiply.irb

Rule

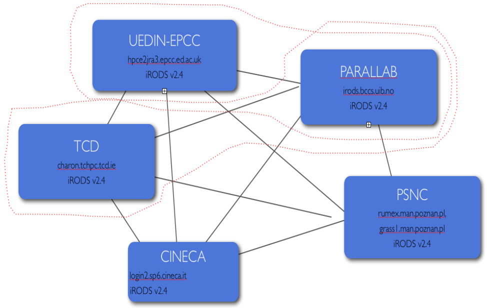
```
multiplyRule||msiDataObjCreate('*TEMP_LOCATION/*OUT_F
ILENAME',Parallab,null)##msiExecStrCondQuery('SELECT
DATA_PATH WHERE DATA_PATH LIKE
```

Input Parameters (default)

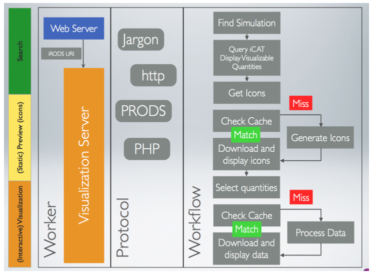
```
*TEMP_LOCATION=$
*OUT_FILENAME=$
*DATAX=$
```

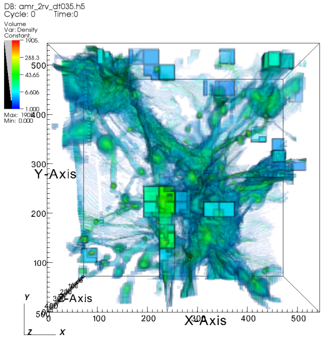
Output Parameters

```
*TEMP_LOCATION=$
*OUT_FILENAME
ruleExecOut
```



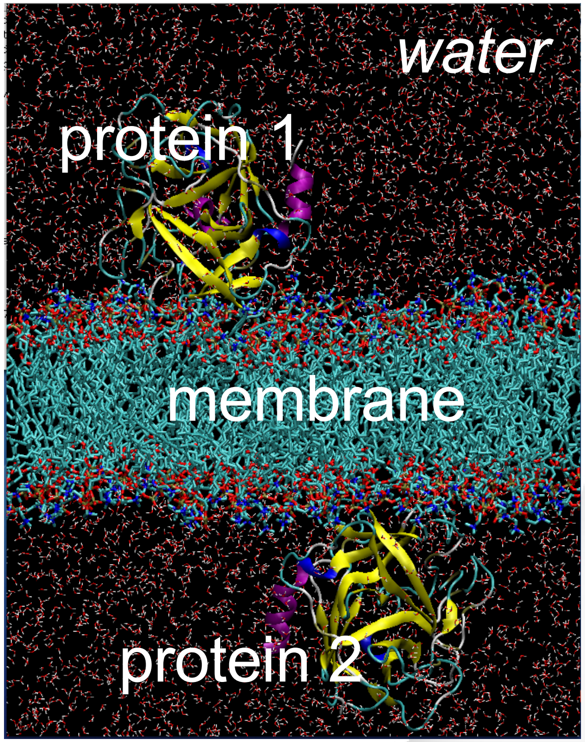
- Established distributed storage infrastructure (iRODS)
- Developed advanced clients featuring: data and metadata management, search, filtering, post-processing and visualization of the data

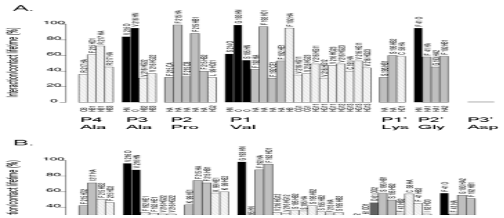




Activities: Protein Dynamics (CBU)

- Aim: Drug discovery
- Simulations are based Newton's mechanics: Atoms in force-fields, formally ODEs.
- Simulations calculate the trajectories of all atoms. Typically
  - 100k atoms
  - T=200ns (10days · 500 cores)
  - Output: 5GB





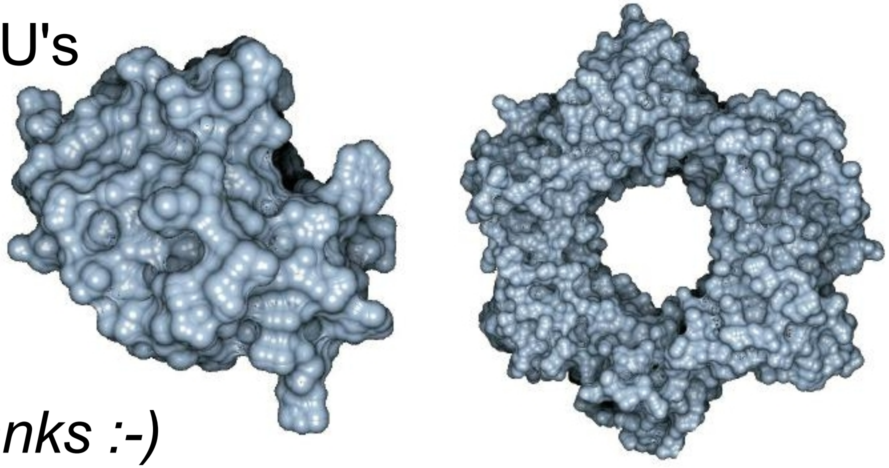
- From output calculate molecular properties

Activities: Fruitful Collaborations (CBU)

- We highly appreciate fruitful collaborations like the one *Július Parulek – Natalie Reuter:*

  Implicit Representation of Molecular Surfaces, Július Parulek et.al.

- The tool enables much faster scientific progress on CBU's side



(-: BTW: Natalie says thanks :-)

Activities: Time Scales (Sci Comp)

- Scientific Computing approach to quantify uncertainties in unstable dynamics

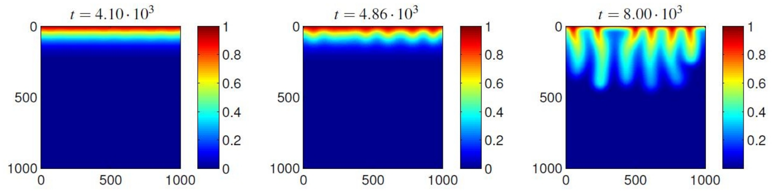


Fig. 4 Concentration of solute in the domain at three times. The first visible signs of instability appear around $t = 4.1 \cdot 10^3$. At the nonlinear onset time (center figure), 6 fingers are clearly visible. The wavelengths are therefore approximately $1000/6 = 170$.

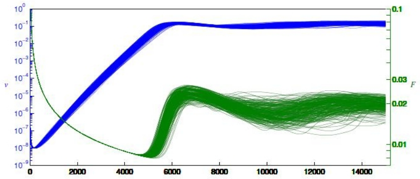


Fig. 1 Values of the dissolution rate (green) and finger-velocity (blue).

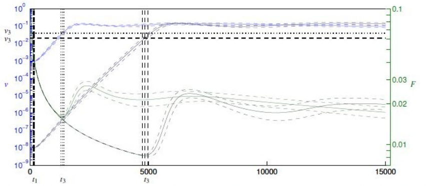


Fig. 2 Statistical parameters of the dissolution rate (green) and finger-velocity (blue) with $v_1 = 10^{-8}$ (dark green and dark blue) and $v_1 = 9.4 \cdot 10^{-4}$ (lighter green and blue). We also show the time- and velocity-scales t_1, t_3 and v_3 with average values and standard deviations for $v_1 = 10^{-8}$ (dashed lines) and $v_1 = 9.4 \cdot 10^{-4}$ (dotted lines).

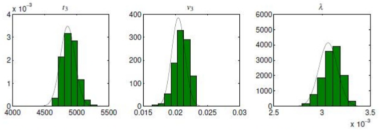


Fig. 3 Probability density distributions for selected parameters together with the corresponding normal distributions.

- Statistics over large ensembles of parallel computations
- Post-processing using a vertical-e-infrastructure
- The basis for homogenization?

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Visualization

- What does mean visualization to us?
- For us, non visualization-people, visualization
  a) Is interesting science (which we don't do)
  b) Provides SW that enables new developments in our field
  c) Provides SW that helps us with presentations, easing our life
- So essentially, when we use it, it is a SW
  - Vertical, as it is specific
  - Similar to MW and e-IS
- Hence, when the SW becomes mature it is difficult to finance

Visualization (cont'd)

- To complete the picture, let's plot science vs. services (for Uni Computing)

	Bioinformatics	Env. Flow	Ecology	Language
IT (hor)	T	T	T	T
SW (ver)	D,S	D,S	D,S	D,S
MW/e-IS (ver)	D,S			
Viz (ver)	S	T	S	S

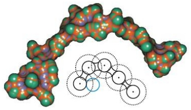
T – Tool
D – Development
S – Science-enabling

Green – ongoing
Red – potentially

Visualization (cont'd)

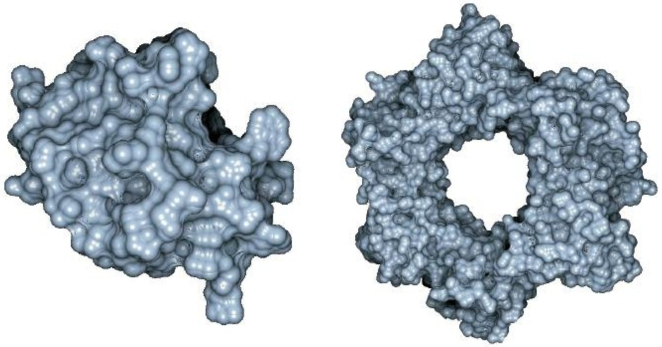
- Uni Computing has a big need for visualization
  - Bioinformatics: *Has shown already in (at least) two collaborations with Viz/II its potential*
  - Env. Flow: *Has a need for visualization tools (maybe not research for Viz/II here?). More the standard (CFD, …)*
  - Ecology: *Needs visualization, which likely will enable new ecology-type research*
  - Language: *Needs visualization, which likely will enable new research*
- Let's have a look to some details

Visualization: Bioinformatics

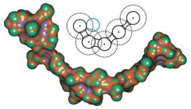


- *Július Parulek/Viz* has developed an *Implicit Representation of Molecular Surfaces* to visualize the surface of proteins

- The method allows for fast rendering of surfaces and allows the researcher to identify important geometric properties

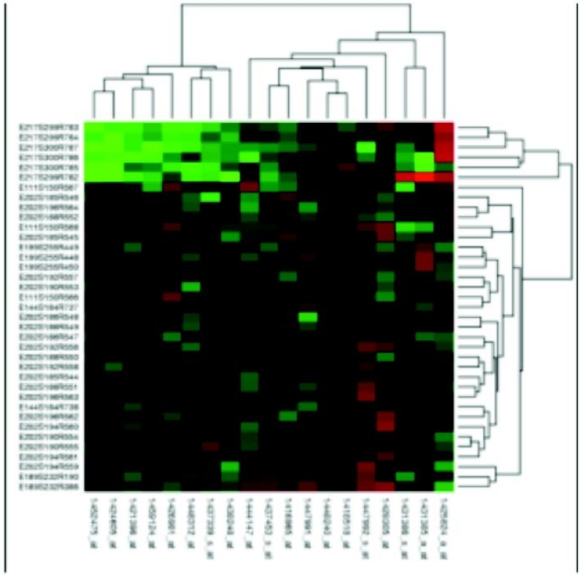


- A production-type software-tool with these features would be of very high value to Bioinformatics/II and to the community
- A linux port would be desirable



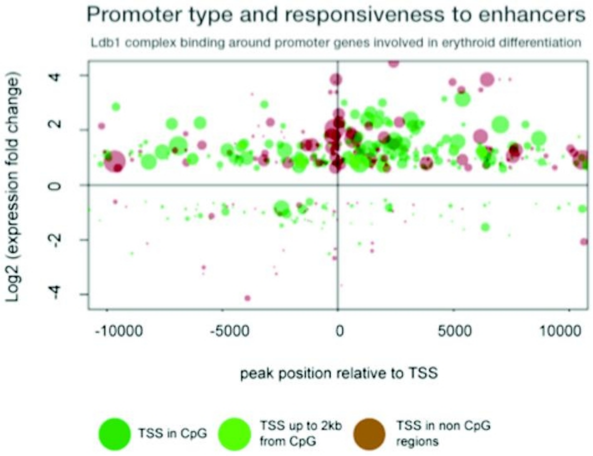
Visualization: Bioinformatics II

- To help data interpretation



Heatmap – gene expression profiles (genes – rows; samples columns – clustered two-ways; red: over-expression; green: under-expression)

Eisen et al 1998

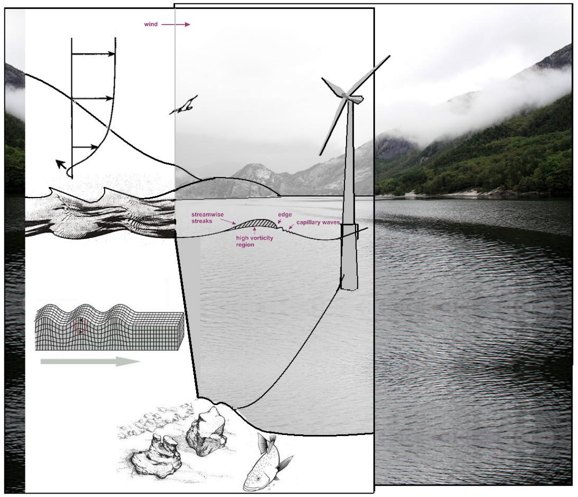


Promoter-enhancer interactions – plot showing expression change (vertical) and binding of regulatory proteins (x-axis) – size of circle – amount of binding

Lenhard.

Visualization: Environmental Flow

- The Env Flow Group is working towards a integrated *Wind-Water-Wave* model to simulate dispersion,marine physics and ecology.

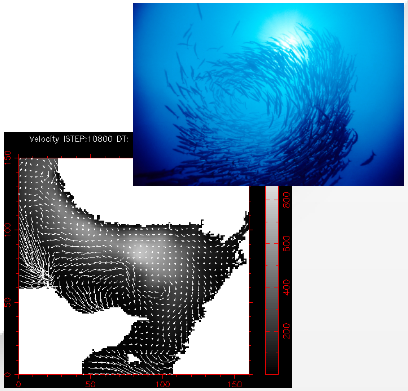


- Integrated visualization of wind, currents and waves together with the distribution of e.g. pollutants would be highly desirable
- Desirable features
  - Automatic image- and movie generation
  - Client-server implementation
  - Possible integration/visualization of external data

Visualization: Evolutionary Ecology

- *Individual-based evolutionary ecology* derives the dynamics of a population from the individual level
- The population of e.g. fish is described by a dynamical system of 50-100k individuals described by a set of continuous (age, weight, location, ...) and discrete (gender, …) parameters subject to a set of environmental conditions
- To gain further insight into the dynamics, we need a data analysis tool able to visualize
  - Env conditions (temp, salinity, flow, nutrition, …)
  - Swarm properties (age, weight, ...)

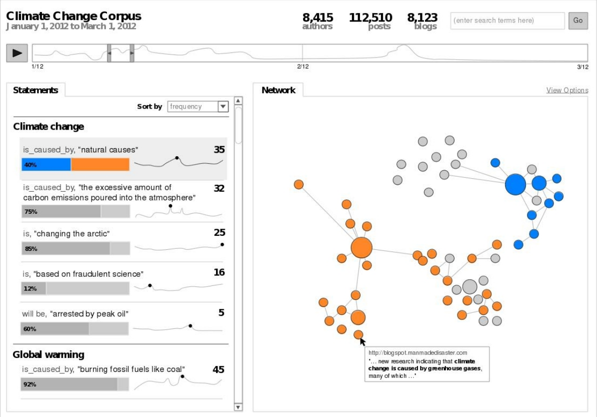
  simultaneously in space and time.
- To analyze effiently an emsemble populations



Visualization: Analyzing the Blogosphere

- Visualize the distribution, flow and development of knowledge and opinions across online social networks

- The example on the right shows the mockup of a SW displaying 56 blogs about *Climate Change* and their inter-relation (over time)
- A realistic corpus of blogs will have 1-10M blogs, to be analyzed



Climate Change Corpus
January 1, 2012 to March 1, 2012

8,415 authors · 112,510 posts · 8,123 blogs

Statements

Sort by: frequency

Climate change

is_caused_by, "natural causes" — 35 — 40%

is_caused_by, "the excessive amount of carbon emissions poured into the atmosphere" — 32 — 75%

is, "changing the arctic" — 25 — 85%

is, "based on fraudulent science" — 16 — 12%

will be, "arrested by peak oil" — 5 — 60%

Global warming

is_caused_by, "burning fossil fuels like coal" — 45 — 92%

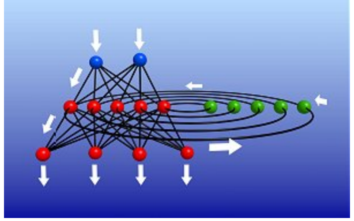
Network

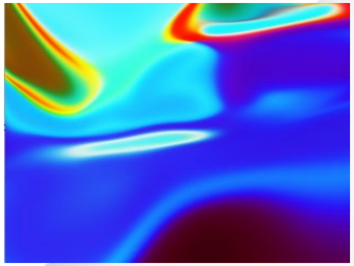
http://blogspot.manmadedisaster.com
"... new research indicating that **climate change is caused by greenhouse gases**, many of which ..."

- We need a visualization able to handle and analyze large graphs interactively

Visualization: ANN Learning Process

- We need to understand Artificial Neural Network learning processes
  - Understand the dynamics of the learning process
  - Show under- and overfitting effects
  - Compare quality of different networks' architectures
  - Identify input space regions whith potential problems
  - Visually compare various optimization procedures
  - Investigate stability of network classification
  - Estimate confidence in classification





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Todo

- There is something to do

  For the scientists on both sides: Identify areas of collaboration. Then to write research applications … That's the easy part ;-)

But there are some problems

- Uni C needs probably research on the Viz-side of things. But sure, we need mature SW as well. May or may not be the interest of Viz.
- Uni C would probably be interested to develop SW … with some help.

  We shall both think if we have common ground. And then, in case, think how to realize that.

Thank you

for your attention

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