Slide 1

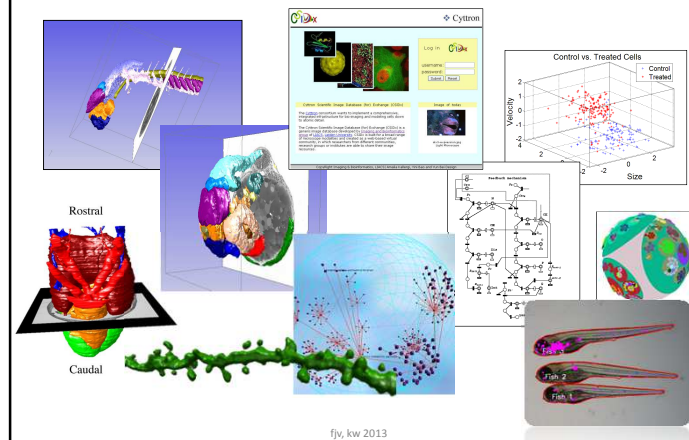# Imaging & BioInformatics

FJ. Verbeek, K. Wolstencroft

A. Gultyaev, J Slob, R Carvalho, L. Cao,
C. Fuyu, E Larios, M. Tleis, Z. Xiong

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Slide 2

Imaging & BioInformatics @ LIACS

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Slide 3

WEBSERVICES & WORKFLOWS

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Slide 4

Web Services and Workflows for Scientific Reproducibility

- Investigate the use of web services and workflows for improving scientific reproducibility, using case studies from LIACS research.
- Design new interactive user interfaces for a collection of web services and workflows for text mining tools developed at the LUMC

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The Data Deluge

21st C = century of information
Open access to distributed data
Open access to analysis tools and algorithms

- World bank/financial
- Climate change data
- Large scale physics
  - Large Hadron collider
  - Astronomy
- Life Sciences
  - 'Omics data
  - Next Gen Sequencing
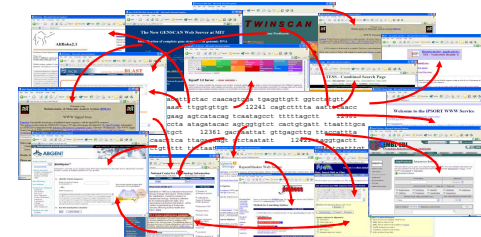- Personalised medicine
- eGovernment

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Exploiting Data Resources and Tools

- Sequential use of distributed tools
- Analysing large data sets and iterating over lots of data
- Repeating the same analyses
- Incompatible input and output formats
- Difficult to record parameter selections

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Web Services

- Machine-to-machine interaction over the network
- Users can access and run analyses and algorithms (services) at distributed locations
- Services are hosted and maintained by their creators – no installation, no maintenance

  – WSDL (SOAP) – Web Services Description Language
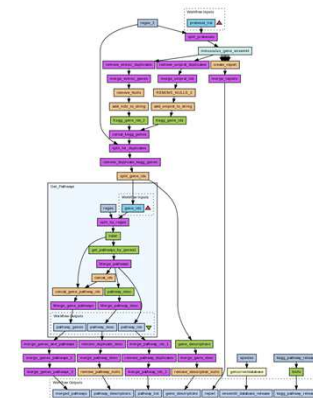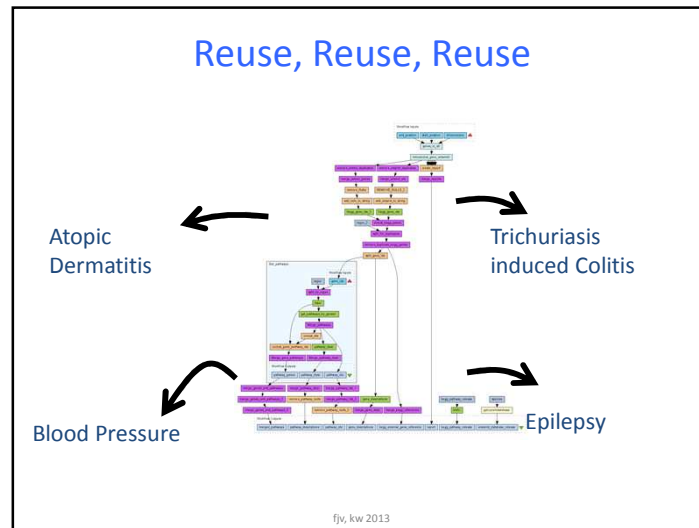 – REST – REpresentational State Transfer

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Scientific Workflows (Taverna)

- Sophisticated analysis pipelines
- A set of services to analyse or manage data (either local or remote)
- Automation of data flow
- Iteration over data sets
- Control of service invocation
- Provenance collection
- Experimental protocol

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Reuse, Reuse, Reuse

Atopic Dermatitis

Trichuriasis induced Colitis

Blood Pressure

Epilepsy

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Web Services and Workflows for Scientific Reproducibility

- Develop web service interfaces for tools and algorithms produced @ LIACS
- Integrate these tools into workflows with existing tools and resources
- Investigate the implications of providing a web service interfaces on:
  - Scientific reproducibility
  - Providing and maintaining the service

- Requirements: Java, XML

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Alternative Interfaces for the Anni Text Mining Suite

- Anni http://biosemantics.org/index.php?page=anni-2-0
- Anni already has web services and a series of workflows (developed @ LUMC)
  - Create new user interfaces that use the web services and workflows
  - Transform user requirements into technical specifications
  - Explore new ways of interacting with the services
    - E.g. Plugins to other environments, Android apps etc

- Requirements: Java, XML

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Slide 13

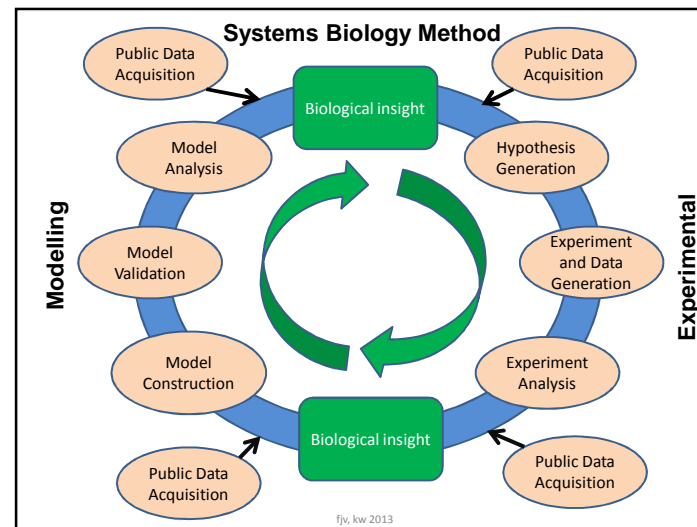**VISUALIZATION**

Slide 14

LIACS BigEye VideoWall

With Kinect or Wii-Mote

Slide 15
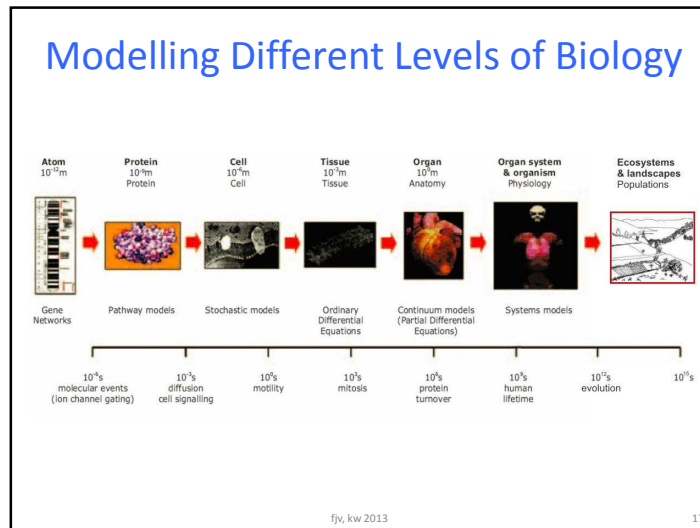
Visualising and Exploring Systems Biology Models

- Systems Biologists use mathematical models to represent complicated dynamic relationships in living systems
- Models need to be visualised and integrated to interpret biological functions
- Exploring new ways of interactively visualising and navigating Systems Biology models by creating mash-ups of existing tools and resources
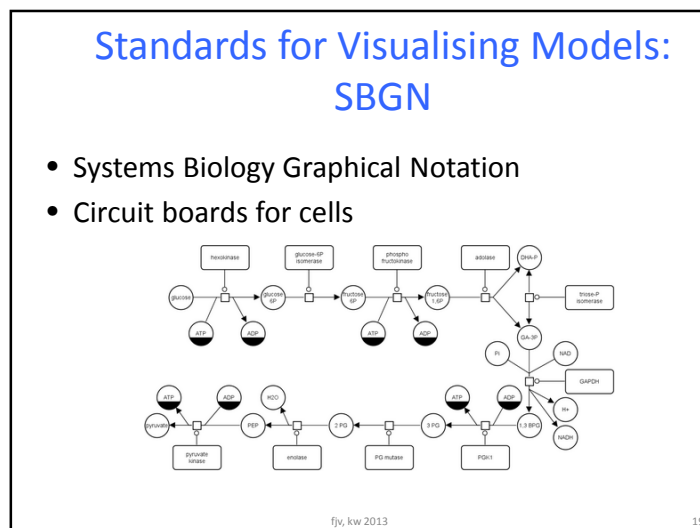
Slide 16

Systems Biology Method

Modelling — Experimental

- Public Data Acquisition
- Biological insight
- Public Data Acquisition
- Model Analysis
- Hypothesis Generation
- Model Validation
- Experiment and Data Generation
- Model Construction
- Experiment Analysis
- Public Data Acquisition
- Biological insight
- Public Data Acquisition

Modelling Different Levels of Biology

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Tools for Visualising Biological Networks: Cytoscape
(http://www.cytoscape.org)

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Standards for Visualising Models: SBGN

- Systems Biology Graphical Notation
- Circuit boards for cells

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Project Summary

- Develop new approaches to visualising and navigating through and between Systems Biology models using Cytoscape (or other visualisation tools) and SBGN.
- Zooming in/out, linking, integrating external data
  - Mash-ups of existing tools
  - Visualisation techniques
  - Integration of distributed data

- Requirements: Java and XML

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COMPUTATION

Cluster

Scientific Cluster

- 48 Dell 2u 8x cores
- Cluster
  - Head Node
  - Main Node
  - Worker Nodes
- Map computational intensive programs to Cluster
  - image processing/analysis
  - pattern recognition
  - bioinformatics jobs from workflows
- RESEARCH
  - Develop strategy/template for web-services
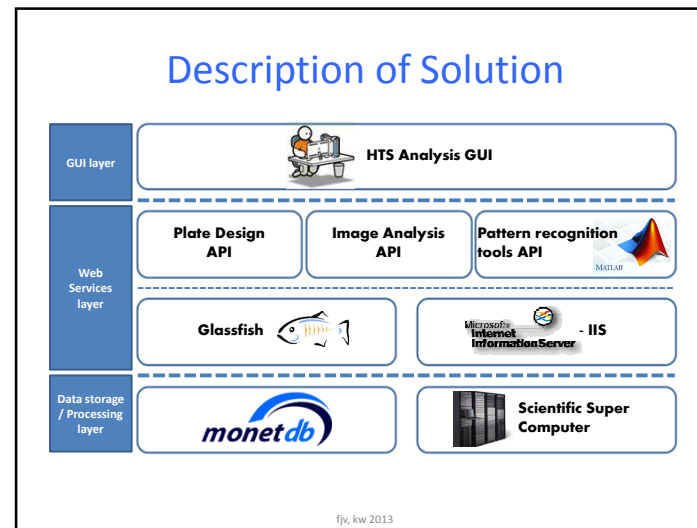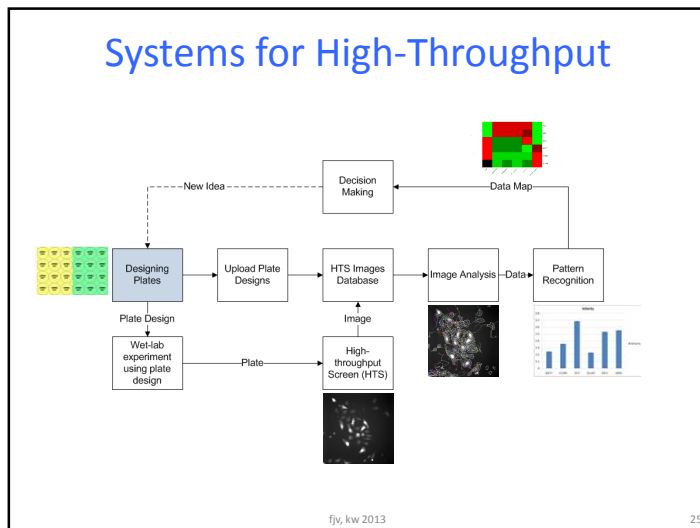 - Develop strategy for Parallelization

Cluster Computation

- NeCEN
  - Netherlands Centre for Electron Nanoscopy

- Cell Observatory
  - Collaboration within Faculty of Science
  - IBL, LIC, LION, LIACS

- High-Throughput imaging
  - 3D zebrafish imaging
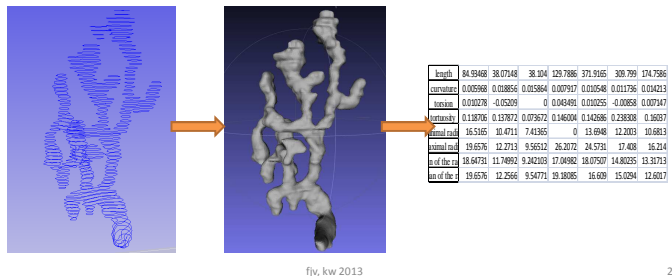
Systems for High-Throughput

Description of Solution

Project Summary

- Analyze software to be ported to the Cluster
- Develop mapping to the cluster architecture
- Apply the results to a dataset
- Generalize

  – NeCEN: C, Python, Java
  – Cell Observatory: Java
  – High Troughput: Java

ANALYSIS & VISUALIZATION
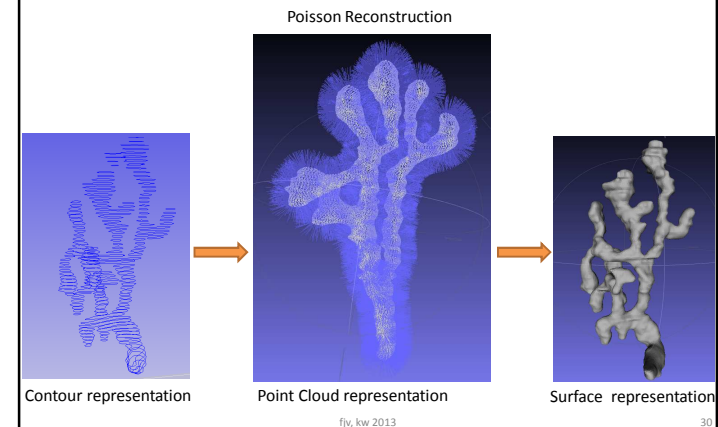
3D Model optimization

- We start from 3D models obtained from various sources
- Measurement

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Surface Reconstruction

Poisson Reconstruction

Contour representation   Point Cloud representation   Surface representation

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Connecting Components

- Read files
- Reconstruction & Optimization
  - Poisson reconstruction
  - Fourier based reconstruction
  - (L.Cao & FJ Verbeek, Electronic Imaging 2013)
- Visualization
  - VTK (visualization toolkit)
  - Geometrical data-structures
- GUI components

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Project Summary

- Analyze components
- Develop infrastructure that fits workflow for 3D modelling
- Develop interface
- Connect components

- C, C++, QT, VTK

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  URL

  http://bio-imaging.liacs.nl/projects

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