GeWare 2.0 - On the way to a virtual repository

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What's GeWare

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♦ GeWare 2.0 Approach

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Kernel and

Module Concepts

Conclusion &
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Thesis Topics

- Platform for managing and analyzing large sets of experimental data generated by
 - high-thoughput expression experiments (Affymetrix)
 custom-made CGH arrays (platform extension)

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- Generic approach to manage experiment annotations and import clinical data using annotation templates and controlled vocabularies

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- Hybrid integration of web data using SRS

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- Generic approach to manage experiment annotations and import clinical data using annotation templates and controlled vocabularies
- Hybrid integration of web data using SRS
- Closed loop analysis workflow: Use of chip and gene/clone groups for easy and iterative analysis execution
- Data analysis by R BioCondutor (reuse of existing analysis software)

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New Requirements

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- Requirements born by upcoming very (!) large scale projects and clinical trials
- New experimental data types generated by new high-throughput array techniques, e.g., tiling , exon , snp arrays
- New chip producers, e.g., Illumina
- Integration of third party data management solutions, e.g. BC|SNPMax
- Generic exchange of clinical data, e.g., by using XML
- Need for a generic approach to store all types of object groups
- User-right-management: rights per <u>user</u> on data and function

New Requirements cont.

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- Flexible analysis integration (upload and execution of R analysis scripts)
- Move of (long running) analysis jobs to dedicated analysis servers
- Storage and return (on demand) of RData objects for every analysis
- Flexible analysis annotation (use of ontologies?)
- Versioned integration of web-data
- Web-GUI using Web 2.0 techniques
- Fat client on desktop (e.g., Rich Client)

GeWare 2.0

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Need for a redesign of GeWare (\leq 1.0) \rightarrow GeWare 2.0 **GeWare 2.0**: Mediator on warehouses

own warehouse (ext. DB schema of GeWare 1.0)

other sources of high-throughput data

GeWare 2.0

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- Need for a redesign of GeWare (\leq 1.0) \rightarrow GeWare 2.0 **GeWare 2.0**: Mediator on warehouses
 - own warehouse (ext. DB schema of GeWare 1.0)
 - other sources of high-throughput data
- Generic source access layer
 - independence of source-specific query syntax
 portability

GeWare 2.0

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 - own warehouse (ext. DB schema of GeWare 1.0)
 - other sources of high-throughput data
- Generic source access layer
 - independence of source-specific query syntax
 - portability
- Modularization: Kernel and task-specific modules
 - system vs. plug-in modules
 - flexible module development (integrate a new or replace an existing module) by using a defined abstract module interface

System Architecture



Generic Source Access Layer

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- Initialization by a set of data source connections Transparent data source access by kernel and modules Connection pooling for fast and parallel access
 - Problem: Which modules can store / retrieve data from which data source?
 - Solution: source-specific metadata

source-metadata(source id, module name, schema version)

- Mount (and unmount) data sources on system's runtime
- Further problems:
 - Uniqueness of object identifiers
 - Selection of insert source

Uniqueness of Object Identifiers

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Problem: No unique object identifiers when multiple sources are used for same type of data

 Solution: Encoding and decoding of source-specific object identifiers

 $f: \mathbb{N} \times \mathbb{N} \to \mathbb{N}$ $f(id_{Src\;k-Obj}, k) = id_{Sys-Obj} = id_{Src\;k-Obj} * c + k$

 $k \in \mathbb{N} :=$ unique source identifier $c = 10^e, e \in \mathbb{N}, e > 0(e.g., c = 1000)$

 $f_{Src}^{-1}(id_{Sys-Obj}) = k = id_{Sys-Obj} \mod c$ $f_{Obj}^{-1}(id_{Sys-Obj}, k) = id_{Src\ k-Obj} = (id_{Sys-Obj} - k)/c$

Project Manager

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Project

- typically, singular (planned) process for a specified time
- in GeWare: Container for storing every type of data; project semantics keeps in user's responsibility
- Problem: Selection of an insert source Solution:
 - Association of each project and module with a singluar data source as selection for insert operation
 - read, update and delete for all other data sources



Experiment Manager

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- **Experiment** = Collection of
 - metadata (name, type, etc.) about high-throughput arrays, e.g., expression, exon, ... arrays
 array-based experiment annotation

Experiment Manager

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- **Experiment** = Collection of
 - metadata (name, type, etc.) about high-throughput arrays, e.g., expression, exon, ... arrays
 - array-based experiment annotation
- Experiment annotation on basis of annotation templates
 - set of hierarchically organized categories for which values can be captured
 - can be organized on pages

Experiment Manager

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- Experiment annotation on basis of annotation templates
 - set of hierarchically organized categories for which values can be captured
 - can be organized on pages
- Input values
 - manual input
 - selected ontology concepts (no flat vocabularies)

Experiment Manager cont.



Feature Set Manager

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Feature = **generic object** representing an object of interest, such as genes, proteins but also chips

analysis result

user-specified

Feature Set Manager

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- Feature = **generic object** representing an object of interest, such as genes, proteins but also chips
 - analysis result
 - user-specified
- Feature Set = user-specified / pre-specified set of features
- Capture
 - semantics by using a meaningful object type and
 - data lineage given by a physical source

Feature Set Manager

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- Capture
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- Methods for
 - retrieval and im-/export
 - set manipulation, e.g., union, intersect, diff, majority

Feature Set Manager cont.



Annotation View Manager

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- Annotation = Description, explaination of specific object by using an attribute set
- Annotation view = defined set of attributes and corresponding values describing a primary (biological) object

Annotation View Manager

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Primary object

Annotation (set of describing attributes)

Probe Set ID	Gene Title	Gene Symbol	go biological process term	go molecular function term	go cellular component term	Pathway
1000_at	mitogen- activated protein kinase 3	MAPK3	protein amino acid phosphorylation protein amino acid phosphorylation cell cycle	nucleotide binding protein kinase activity protein serine/threonine kinase activity MAP kinase activity MAP kinase activity protein binding ATP binding		MAPK_Cascade S1P_Signaling TGF_Beta_Signaling_Pathway

Annotation View Manager

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Annotation View Manager cont.



Web-Source Integration Manager

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- Current idea: Use of BioFuice to integrate data from different source
- Implementation of integration workflows (iFuice scripts)

Web-Source Integration Manager

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- Current idea: Use of BioFuice to integrate data from different source
- Implementation of integration workflows (iFuice scripts)
- Problems:
 - versioning of physical and logical sources
 - generation of annotation views

Web-Source Integration Manager

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- Current idea: Use of BioFuice to integrate data from different source
- Implementation of integration workflows (iFuice scripts)
- Problems:
 - versioning of physical and logical sources
 - generation of annotation views
- Solution (First Approach)
 - versioning: physical source name = source name + version
 - view generation: new method genView() in BioFuice

 $view = genView(M_1, \ldots, M_n, A_{s_i})$

where it exists a compositional path from mapping M_1 to M_n and set of attributes A_{s_i} from sources $s_i \in (domain(M_j) \in \{M_1, \ldots, M_n\} | range(M_j) \in \{M_1, \ldots, M_n\})$

Conclusion & Future Work

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Need for a redesign of GeWare based on new requirements

• GeWare 2.0: Mediator of warehouses

Modularization: Kernel and task-specific modules

Current state: Concept and implementation of system architecture, kernel and most modules

Conclusion & Future Work

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- Need for a redesign of GeWare based on new requirements
- GeWare 2.0: Mediator of warehouses
- Modularization: Kernel and task-specific modules
 - Current state: Concept and implementation of system architecture, kernel and most modules
 - Future work
 - Need to implement: Experiment & Web-Source Integration Manager
 - Need a detailed concept for analysis handling, monitoring, distribution (e.g., by using available Grid infrastructure), and annotation

Topics for Diploma/Master/Bachelor Thesis

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- Web-GUI (re-)design
- Rich client application
- Application allowing to configure the clinical data exchange
 - Analysis management and distribution

GeWare-Coders-Club

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"Gehirnsturm am Freitagabend"

