

# HOBIT at the BiBiServ

Jan Krüger    Henning Mersch

Bielefeld Bioinformatics Service  
Institute of Bioinformatics  
CeBiTec Bielefeld University

[jkrueger@TechFak.Uni-Bielefeld.DE](mailto:jkrueger@TechFak.Uni-Bielefeld.DE)  
[hmersch@TechFak.Uni-Bielefeld.DE](mailto:hmersch@TechFak.Uni-Bielefeld.DE)

Cologne, March 2005



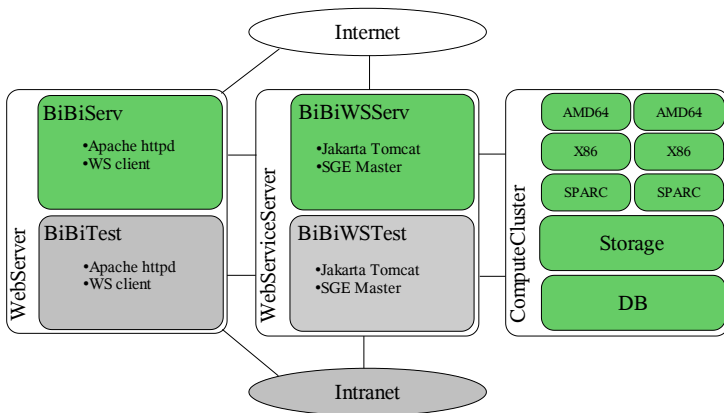
# Overview

<http://bibiserv.techfak.uni-bielefeld.de/hobit/>

- 1 Overview
- 2 General Work
  - Security
  - BiBiWS
- 3 WebServices
  - Oligo Design
  - Alignments
  - Genome Comparison
  - Evolutionary Relationship
  - Other WebServices
- 4 Requests to HOBIT



# BiBiServ Environment



# Solaris 10: Zones

- new feature of Solaris 10 release
- virtualize OS services
- a global zone (GZ) serves up to 8192 non-global zones (NGZ)
- communication between NGZ only via network
- GZ can restrict resources of NGZ  
(CPU-time, memory usage, network,IO ...)



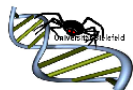
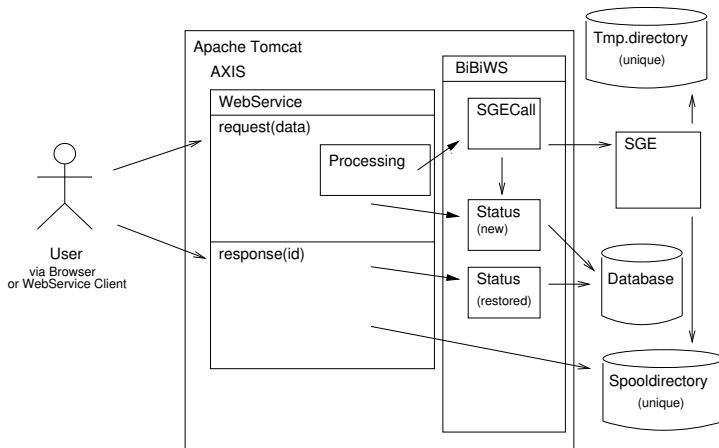
# Tomcat / Java

- allows to define very fine granulated access policies to Java sandbox behaviour
- available since Java 1.2
- configuration via policy file
  - hard to read for human eyes :-)
  - awful GUI : Policy Configuration Tool (part of J2SDK)
- not very well documented



# Architecture

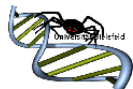
<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>



# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

- returns XML-DOM-Document



# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

- returns XML-DOM-Document
- Tmp. dir (auto flush)





# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

- returns XML-DOM-Document
- Tmp. dir (auto flush)
- Spooldir: delete (3 days) / clean (30 days)



# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

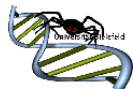
- returns XML-DOM-Document
- Tmp. dir (auto flush)
- Spooldir: delete (3 days) / clean (30 days)
- Webservice - documentation site



# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

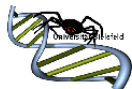
- returns XML-DOM-Document
- Tmp. dir (auto flush)
- Spooldir: delete (3 days) / clean (30 days)
- Webservice - documentation site
- Perl SOAP::Lite Patch



# BiBiWS - Update

<http://bibiserv.techfak.uni-bielefeld.de/bibiws/>

- returns XML-DOM-Document
- Tmp. dir (auto flush)
- Spooldir: delete (3 days) / clean (30 days)
- Webservice - documentation site
- Perl SOAP::Lite Patch
- DRMAA (not yet)



# WSDL-Repository

<http://bibiserv.techfak.uni-bielefeld.de/wSDL/>



## BiBiServ

Bielefeld University Bioinformatics Server

Tools

Education

Administration

News

Links

### Tools

#### Genome Comparison

AGenDa  
REPuter  
...more

#### Alignments

e2g  
PoSuSearch  
...more

#### Primer Design

GeneFisher

#### RNA Studio

RNAshapes  
RNAhybrid  
...more

#### Evolutionary Relationship

RCS-E  
SplitsTree  
...more

#### Others

PREditor  
GenDB  
...more

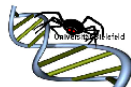
### WebService Overview

#### Tools, which are currently offered as a webservice

Name	WSDL	Description
<a href="#">bibws</a>	<a href="#">link</a>	Demonstration Webservice for BIBIWS Lib
<a href="#">e2g</a>	<a href="#">link</a>	e2g is a web-based tool which aligns genomic sequence to cDNA and EST data sets. The server hosts huge EST databases of a few gigabases in size in indexed data structures. This allows users to rapidly (i) detect new genes, (ii) verify the exon-intron structure of predicted genes, and (iii) determine splice variants in the uploaded genomic region of interest. The Web interface provides a graphical overview of the results. Alignments can be visualized and matching sequences downloaded for further processing.
<a href="#">REPuter</a>	<a href="#">link</a>	REPuter computes all maximal duplications and reverse, complemented and reverse complemented repeats in a DNA input sequence.
<a href="#">SplitsTree</a>	<a href="#">link</a>	SplitsTree uses the split decomposition method to analyse and visualize distance data, e.g. data derived from biosequences. See also the original side of splitstree at the University of Tuebingen.

#### Tools, which are currently offline (due to maintance)

Name	Description
<a href="#">BLAST</a>	A sample webservice using NCBI blast for aligning two sequences that was developed during a HOBIT workshop in Bielefeld, 6/7th October 2004.
<a href="#">DIALIGN</a>	DIALIGN is a novel alignment program based on segment-to-segment comparison. It is especially suited to detect local similarities among distantly related sequences.



# WSDL-Repository

<http://bibiserv.techfak.uni-bielefeld.de/wsdl/>

## WebService Overview

### Tools, which are currently offered as a webservice

Name	WSDL	Description
<a href="#">bibisws</a>	<a href="#">link</a>	Demonstration Webservice for BiBiWS Lib
<a href="#">e2g</a>	<a href="#">link</a>	e2g is a web-based tool which aligns genomic sequence to cDNA and EST data sets. The server hosts huge EST databases of a few gigabases in size in indexed data structures. This allows users to rapidly (i) detect new genes, (ii) verify the exon-intron structure of predicted genes, and (iii) determine splice variants in the uploaded genomic region of interest. The Web interface provides a graphical overview of the results. Alignments can be visualized and matching sequences downloaded for further processing.
<a href="#">REPuter</a>	<a href="#">link</a>	REPuter computes all maximal duplications and reverse, complemented and reverse complemented repeats in a DNA input sequence.
<a href="#">SplitsTree</a>	<a href="#">link</a>	SplitsTree uses the split decomposition method to analyse and

# WSDL-Repository

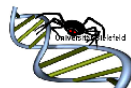
<http://bibiserv.techfak.uni-bielefeld.de/wsd/>

[SplitsTree](#) [link](#)

SplitsTree uses the split decomposition method to analyse and visualize distance data, e.g. data derived from biosequences. See also the original side of splitstree at the University of Tuebingen.

## Tools, which are currently offline (due to maintainece)

Name	Description
<a href="#">BLAST</a>	A sample webservice using NCBI blast for aligning two sequences that was developed during a HOBIT workshop in Bielefeld, 6/7th October 2004.
<a href="#">DIALIGN</a>	DIALIGN is a novel alignment program based on segment-to-segment comparison. It is especially suited to detect local similarities among distantly related sequences.



# Promide

<http://bibiserv.techfak.uni-bielefeld.de/promide/>

- design of oligo sequences for microarrays

S. Rahmann

**Fast large scale oligonucleotide selection using the longest common factor approach**

Journal of Bioinformatics and Computational Biology, 1(2):343-361, 2003





# Promide

<http://bibiserv.techfak.uni-bielefeld.de/promide/>

- design of oligo sequences for microarrays
- input: string containing target and background sequences (FASTA), parameter array (key → value)

S. Rahmann

**Fast large scale oligonucleotide selection using the longest common factor approach**  
Journal of Bioinformatics and Computational Biology, 1(2):343-361, 2003



# Promide

<http://bibiserv.techfak.uni-bielefeld.de/promide/>

- design of oligo sequences for microarrays
- input: string containing target and background sequences (FASTA), parameter array (key → value)
- output: Oligo/Target matrix (new XSD)

S. Rahmann

**Fast large scale oligonucleotide selection using the longest common factor approach**

Journal of Bioinformatics and Computational Biology, 1(2):343-361, 2003



# Promide

<http://bibiserv.techfak.uni-bielefeld.de/promide/>

- design of oligo sequences for microarrays
- input: string containing target and background sequences (FASTA), parameter array (key → value)
- uses *OligoSelection* (FU-Berlin) for non-unique design
- output: Oligo/Target matrix (new XSD)

S. Rahmann

**Fast large scale oligonucleotide selection using the longest common factor approach**

Journal of Bioinformatics and Computational Biology, 1(2):343-361, 2003



# Promide

<http://bibiserv.techfak.uni-bielefeld.de/promide/>

- design of oligo sequences for microarrays
- input: string containing target and background sequences (FASTA), parameter array (key → value)
- uses *OligoSelection* (FU-Berlin) for non-unique design
- output: Oligo/Target matrix (new XSD)
- under development

S. Rahmann

**Fast large scale oligonucleotide selection using the longest common factor approach**  
Journal of Bioinformatics and Computational Biology, 1(2):343-361, 2003



## e2g

<http://bibiserv.techfak.uni-bielefeld.de/e2g/>

- e2g WebService efficiently maps large EST/cDNA data sets to genomic using VMatch
- input: parameter array (key → value), string containing a single sequence (FASTA)
- output: EBI - Application Alignment format
- XML-based input format, Java based GUI client (under development)

J. Krüger, A. Sczyrba, S. Kurtz, R. Giegerich

e2g - An Interactive Web-Based Server for Efficiently Mapping large EST and cDNA sets to Genomic Sequences  
Nucleic Acids Research, 2004



# REPuter

<http://bibiserv.techfak.uni-bielefeld.de/reputer/>

- REPuter Webservice allows fast computation of degenerate repeats in complete genomes, based on VMatch.
- input: string containing one or more sequences in FASTA, parameter array (key → value)
- output: EBI - Application Alignment format
- XML-based input format, Java based graphically client (under development)

S. Kurtz, J. V. Choudhuri, E. Ohlebusch, C. Schleiermacher, J. Stoye, R. Giegerich  
**REPuter: The Manifold Applications of Repeat Analysis on a Genomic Scale.**  
Nucleic Acids Res. 2001



# SplitsTree

<http://bibiserv.techfak.uni-bielefeld.de/splits/>

- SplitsTree WebService uses the split decomposition method to analyze and visualize distance data
- input: string containing distance data in NEXUS format
- output: string containing visualized data in PostScript format
- under development: XML-based input and output format (SVG instead of PostScript)

D.H. Huson

**SplitsTree: Analyzing and visualizing evolutionary data**

Bioinformatics, 14(1):68-73 (1998)



# Other WebServices

currently in development

- **dialign** constructs pairwise and multiple sequence alignments by comparing whole segments of the sequences

B. Morgenstern

**DIALIGN 2: improvement of the segment-to-segment approach to multiple sequence alignment**  
Bioinformatics 15, 211 - 218

A.W.M. Dress, G.Füllen, S.W. Perrey

**A Divide and Conquer Approach to Multiple Alignment**  
AAAI Press, Menlo Park, CA, USA, 107-113, 1995

J. Stoye, D. Evers, F. Meyer

**Generating Benchmarks for Multiple Sequence Alignments and Phylogenetic Reconstructions**  
Proceedings of the Fifth International Conference on Intelligent Systems for Molecular Biology, AAAI Press





# Other WebServices

currently in development

- **dialign** constructs pairwise and multiple sequence alignments by comparing whole segments of the sequences
- **dca** produces fast, high quality simultaneous multiple sequence alignments of amino acid, RNA, or DNA sequences

B. Morgenstern

**DIALIGN 2: improvement of the segment-to-segment approach to multiple sequence alignment**  
Bioinformatics 15, 211 - 218

A.W.M. Dress, G.Füllen, S.W. Perrey

**A Divide and Conquer Approach to Multiple Alignment**  
AAAI Press, Menlo Park, CA, USA, 107-113, 1995

J. Stoye, D. Evers, F. Meyer

**Generating Benchmarks for Multiple Sequence Alignments and Phylogenetic Reconstructions**  
Proceedings of the Fifth International Conference on Intelligent Systems for Molecular Biology, AAAI Press



# Other WebServices

currently in development

- **dialign** constructs pairwise and multiple sequence alignments by comparing whole segments of the sequences
- **dca** produces fast, high quality simultaneous multiple sequence alignments of amino acid, RNA, or DNA sequences
- **Rose** implements a probabilistic model of the evolution of RNA-, DNA-, or protein-like sequences.

B. Morgenstern

**DIALIGN 2: improvement of the segment-to-segment approach to multiple sequence alignment**  
Bioinformatics 15, 211 - 218

A.W.M. Dress, G.Füllen, S.W. Perrey

**A Divide and Conquer Approach to Multiple Alignment**  
AAAI Press, Menlo Park, CA, USA, 107-113, 1995

J. Stoye, D. Evers, F. Meyer

**Generating Benchmarks for Multiple Sequence Alignments and Phylogenetic Reconstructions**  
Proceedings of the Fifth International Conference on Intelligent Systems for Molecular Biology, AAAI Press



# Requests to HOBIT

- MSA Grammar (*BSML* ?)



# Requests to HOBIT

- MSA Grammar (*BSML* ?)
- *Hobit Statuscode* discussion



# Requests to HOBIT

- MSA Grammar (*BSML* ?)
- *Hobit Statuscode* discussion
- WebService Repository



# Requests to HOBIT

- MSA Grammar (*BSML* ?)
- *Hobit Statuscode* discussion
- WebService Repository
- Reliability of WebServices

