# Bioinformatics Ontology: Towards the Automatics Generation of Bioinformatics Workflow for Web Services

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# Introduction of Ontology

# Tacit and Explicit Knowledge

We should start from the fact that
*'we can know more than we can tell*'.

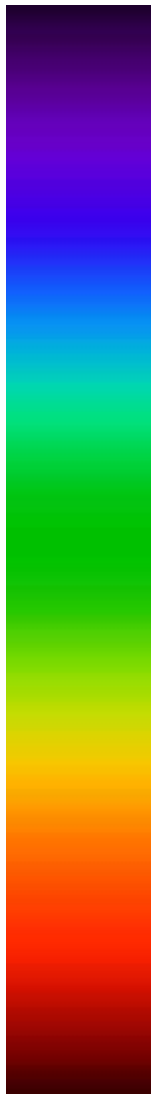
*Michael Polanyi, "The Tacit Dimension" 1967*

**Michael Polanyi (1891-1976)**

# Rainbow Color

How many colors can you see in rainbow?

# Ontology for Rainbow Colors



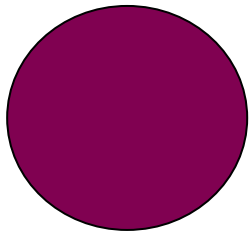
From 360 nm〜400 nm

All the colors you can see with your own eyes!

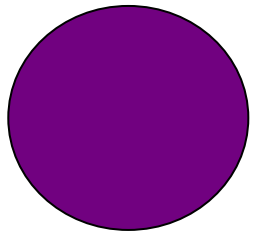
to 760 nm〜830 nm

| | RGB Value |
|---|---|
| **Purple** | **#800080** |
| **Indigo** | **#000080** |
| **Blue** | **#0000FF** |
| **Green** | **#008000** |
| **Yellow** | **#FFFF00** |
| **Orange** | **#FF8000** |
| **Red** | **#FF0000** |

# Which are Purple?



**#800050**



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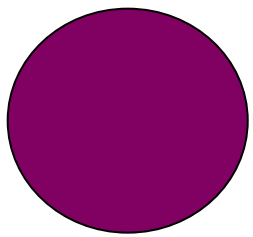

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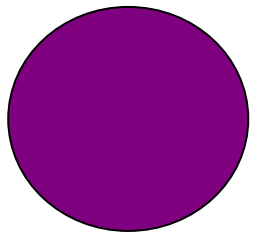

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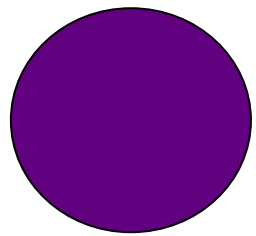
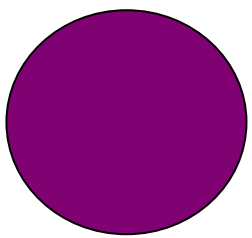


**#600080**



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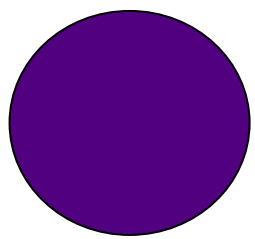
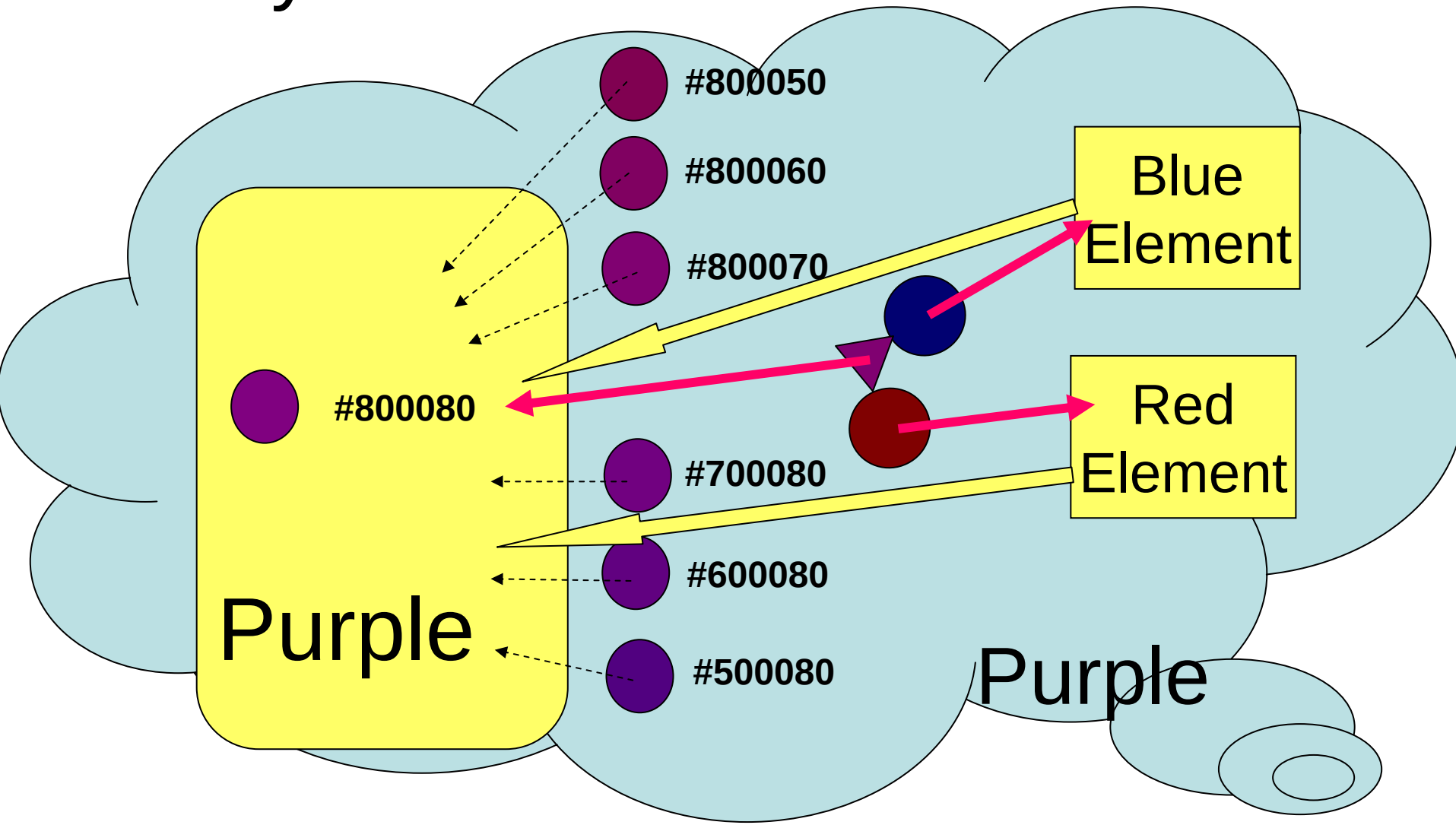


**#500080**

# Representation by Elements and Constructor



# Web Services for Bioinformatics

# Formulation of Community

東京医科歯科大学
Tokyo Medical and Dental University

IBM

科学技術振興事業団
Japan Science and Technology Corporation

NEC
Empowered by Innovation

国立遺伝学研究所
NATIONAL INSTITUTE OF GENETICS

JAIST

GSC RIKEN ゲノム科学総合研究センター


統計数理研究所

大阪産業大学
Osaka Sangyo University

徳島大学

MKI 三井情報開発株式会社
Mitsui Knowledge Industry

SSE

MIZUHO

DOSHISHA UNIVERSITY 同志社大学

Wakayama University
和歌山大学

NTT西日本
"光"、ひろがる。ひびきあう。

東京工業大学
Tokyo Institute of Technology

hp
invent

三菱総合研究所

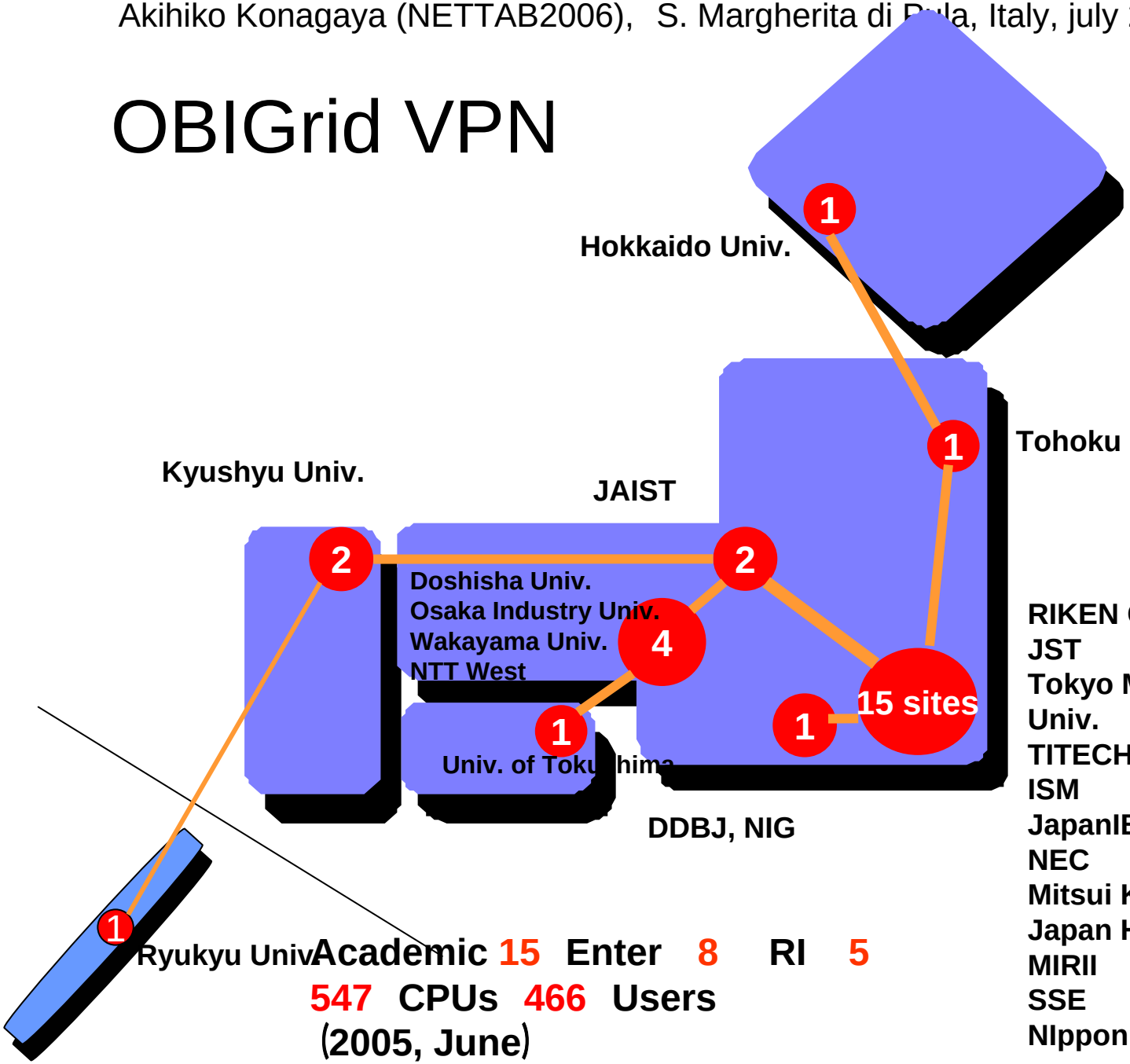
富士総合研究所

九州大学
Kyushu University

日本新薬

琉球大学 University of the Ryukyus

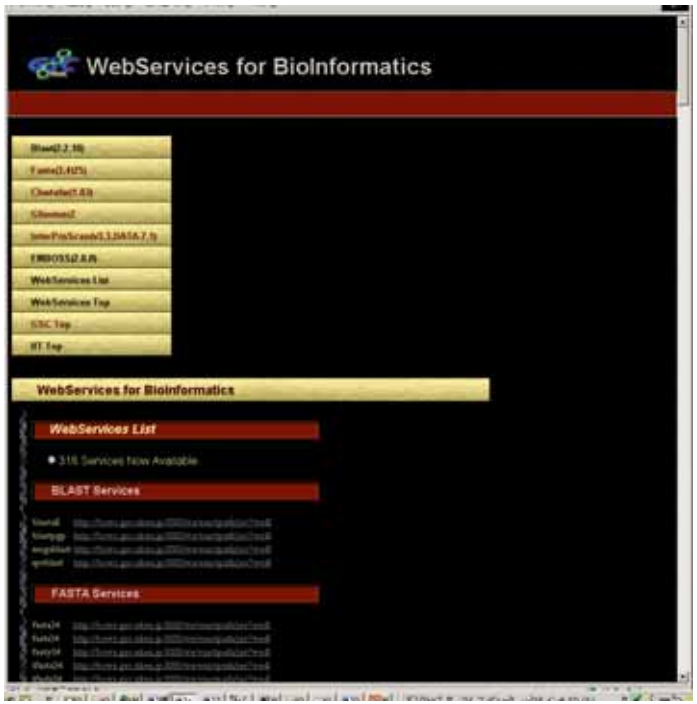
# OBIGrid VPN




RIKEN GSC
JST
Tokyo Medical and Dental Univ.
TITECH
ISM
JapanIBM
NEC
Mitsui Knowledge Industry
Japan HP
MIRII
SSE
NIppon Shinyaku, Co, Lsd

**Academic 15 Enter 8 RI 5**
**547 CPUs 466 Users**
**(2005, June)**

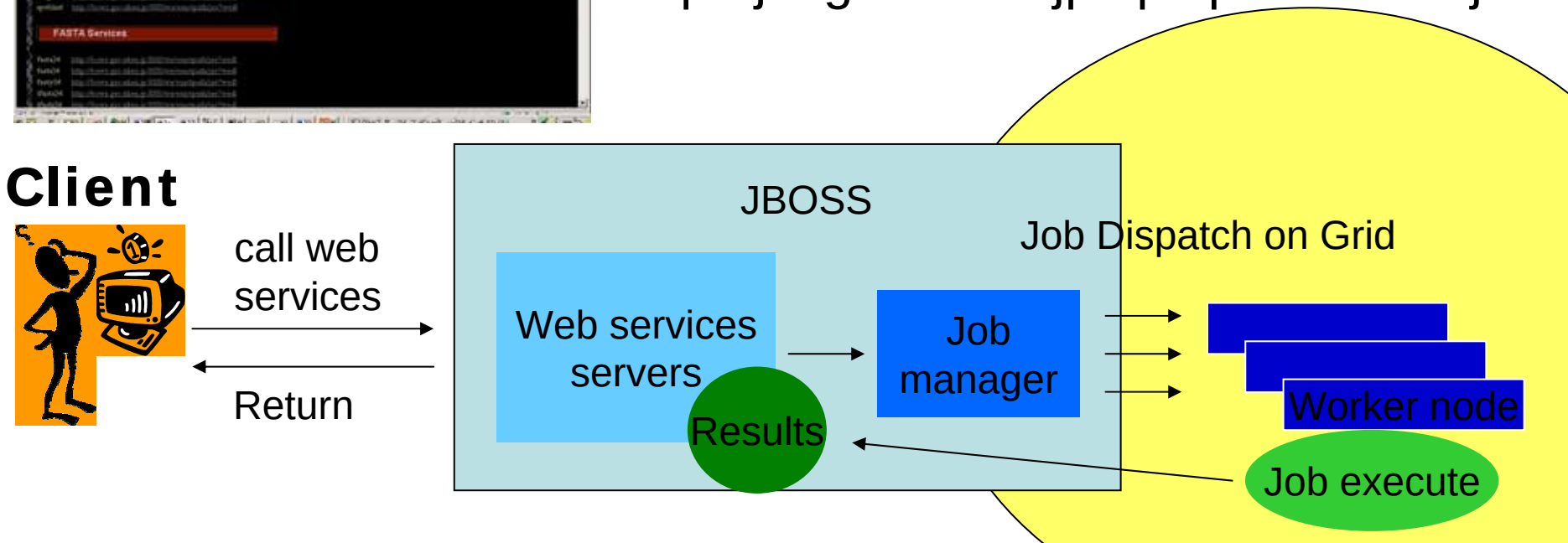
# Bioinformatics Web Services on Grid




**GRIDIFIED**

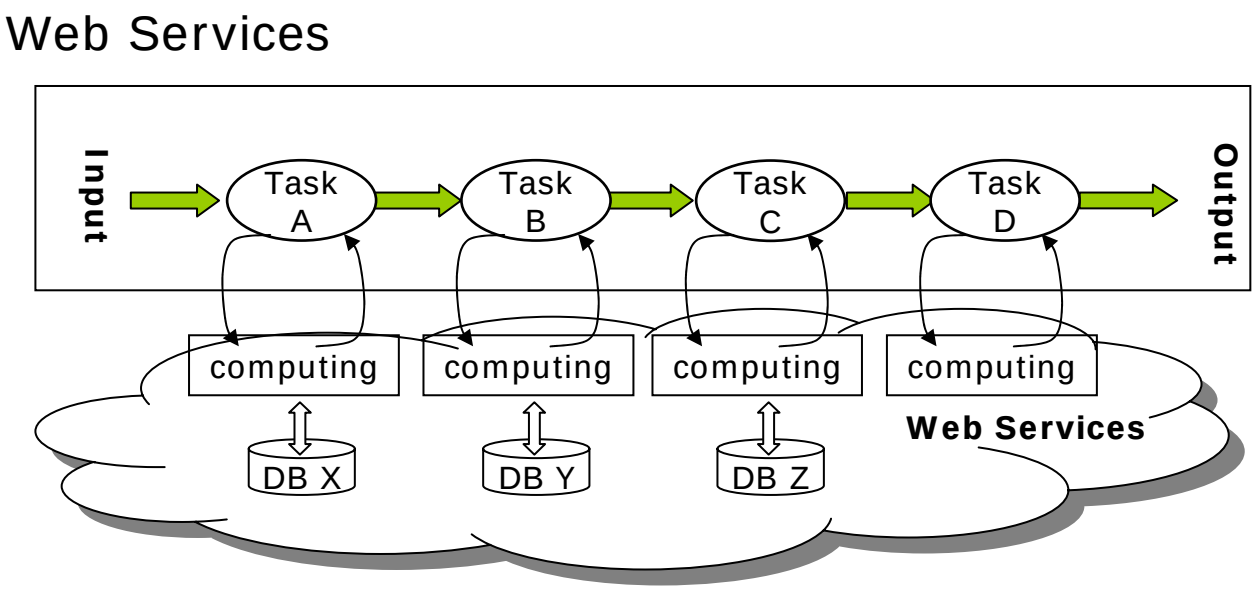
BLAST,FASTA, ClustalW, Glimmer2, InterProScan,

http://jkt.gsc.riken.jp/sp/spbio/wslist.jsf

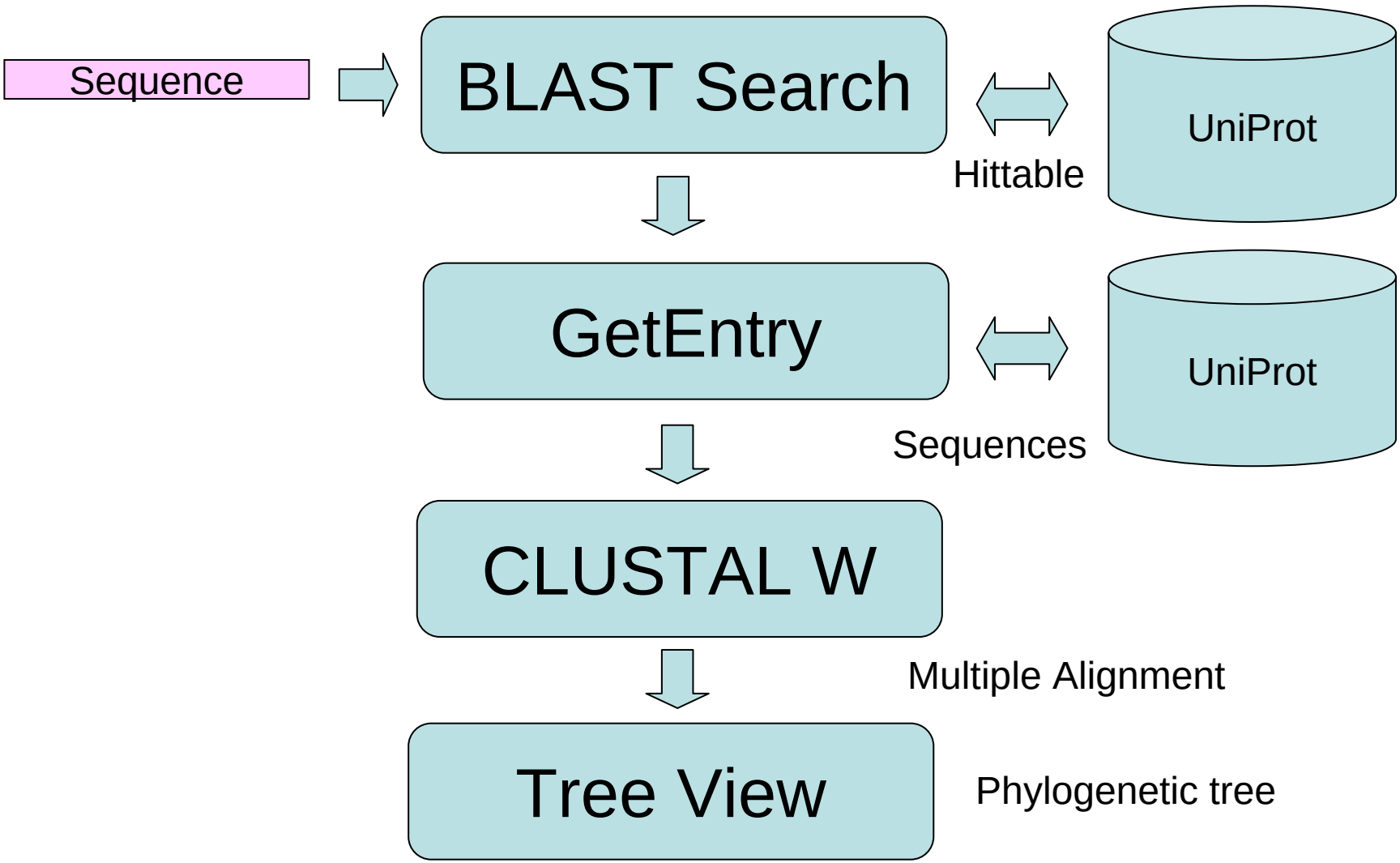


# Advantages of Web Services

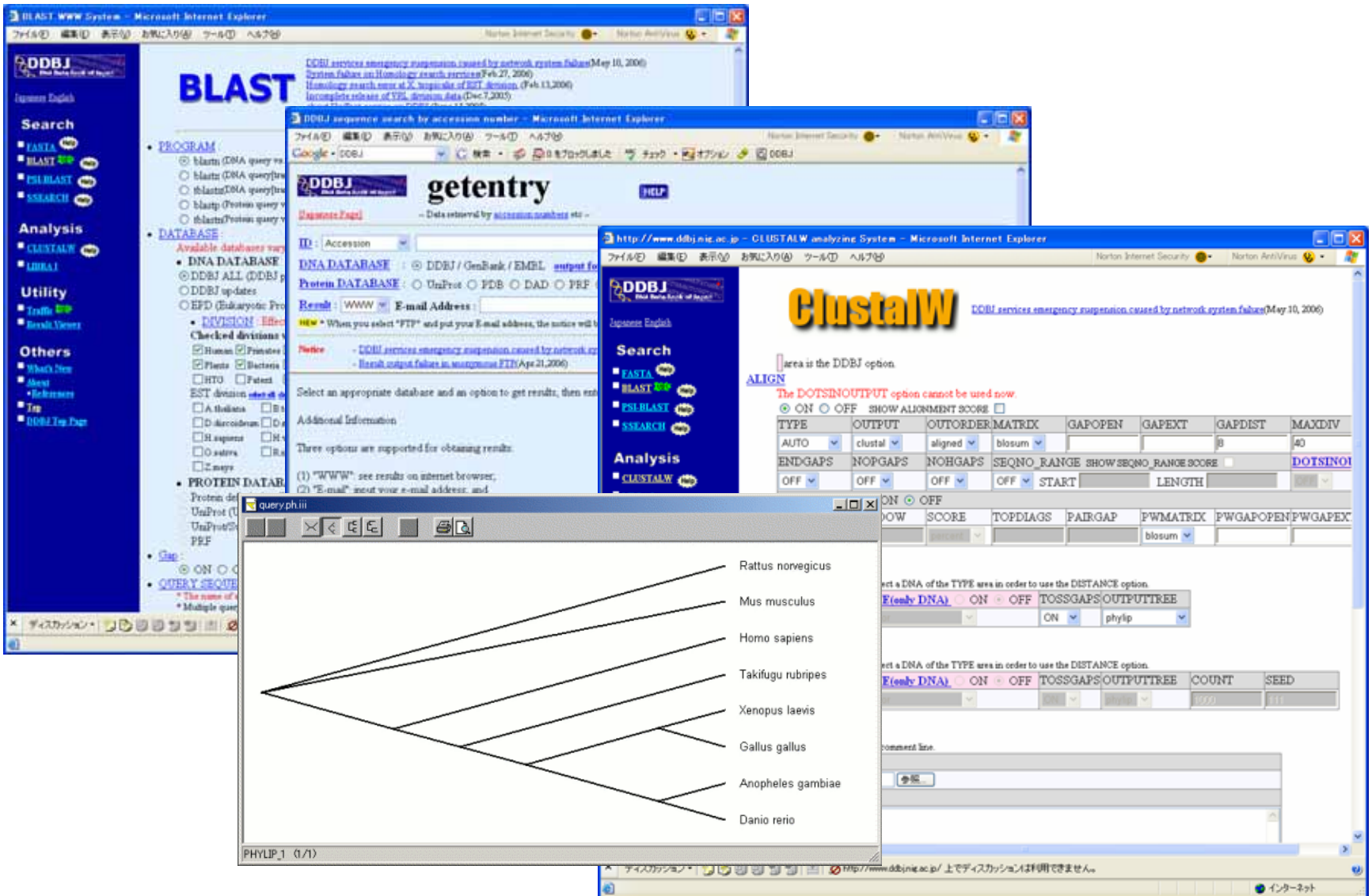
- Liberating from the maintenance of biological databases and tools
- Scalability of computational resources
- High-level application programming interface



# Very Simple Work Flow



# Manual Workflow on Web Apps

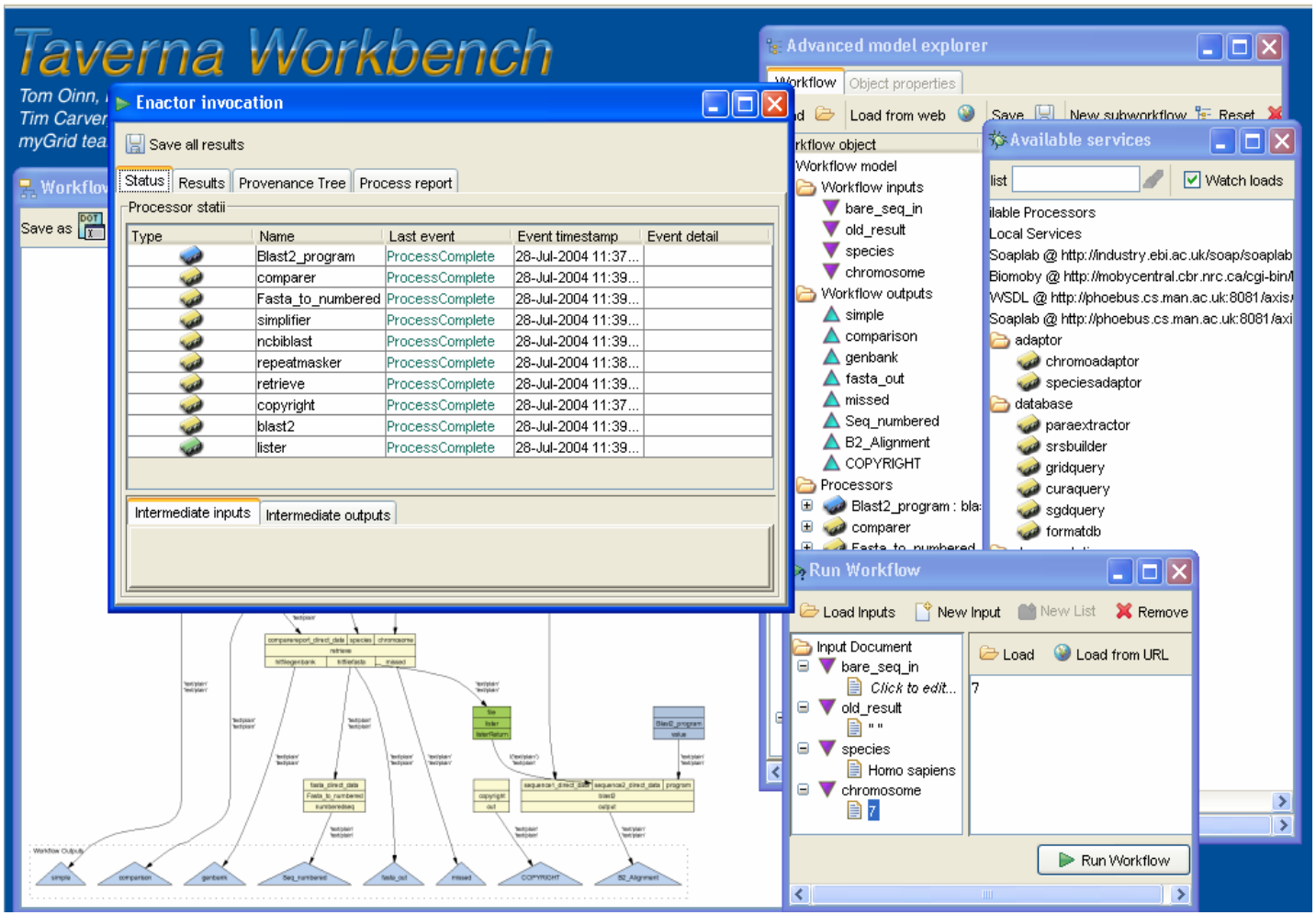


# Web Service Programming

```
#!/usr/bin/perl

use SOAP::Lite;

# SOAP API
# specify WSDL
my $service = SOAP::Lite-> service('http://xml.nig.ac.jp/wsdl/GetEntry.wsdl');

# call web service
$result = $service->getXML_DDBJEntry("AB000003");

# print result
print $result;
```

http://www.xml.nig.ac.jp/perl.txt

# Why don’t we use workflow tools?




http://www.cyclonic.org/Taverna_and_myGrid.ppt

# Needs Automatic Workflow Generate Tool from Very High Level Specification

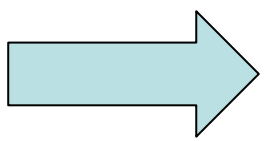
apply **Blastp** to **UniProt**

**GetEntry** from **UniProt**

apply **CLUSTALW**

apply **TreeView**

Automatics Generation

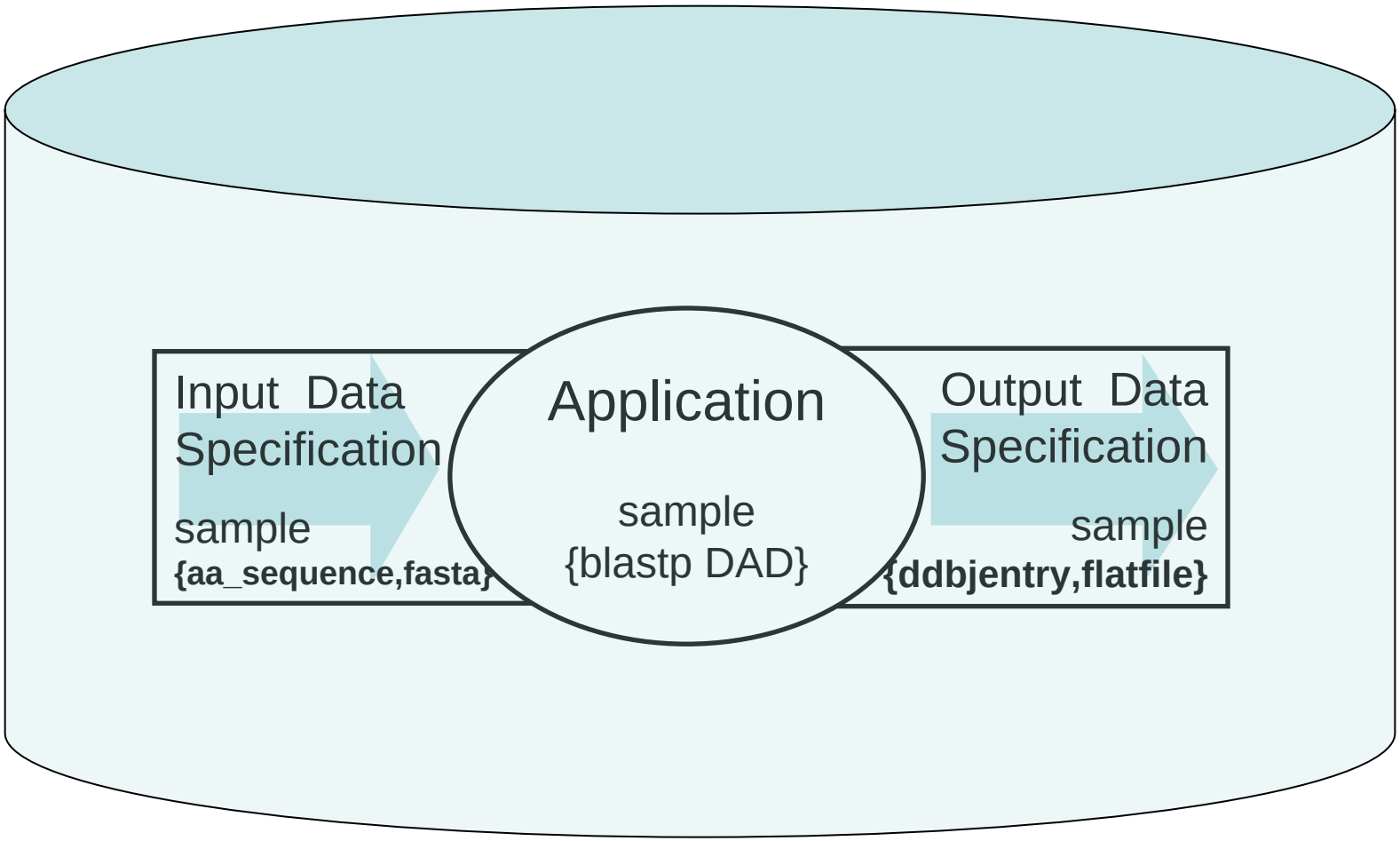


**?**

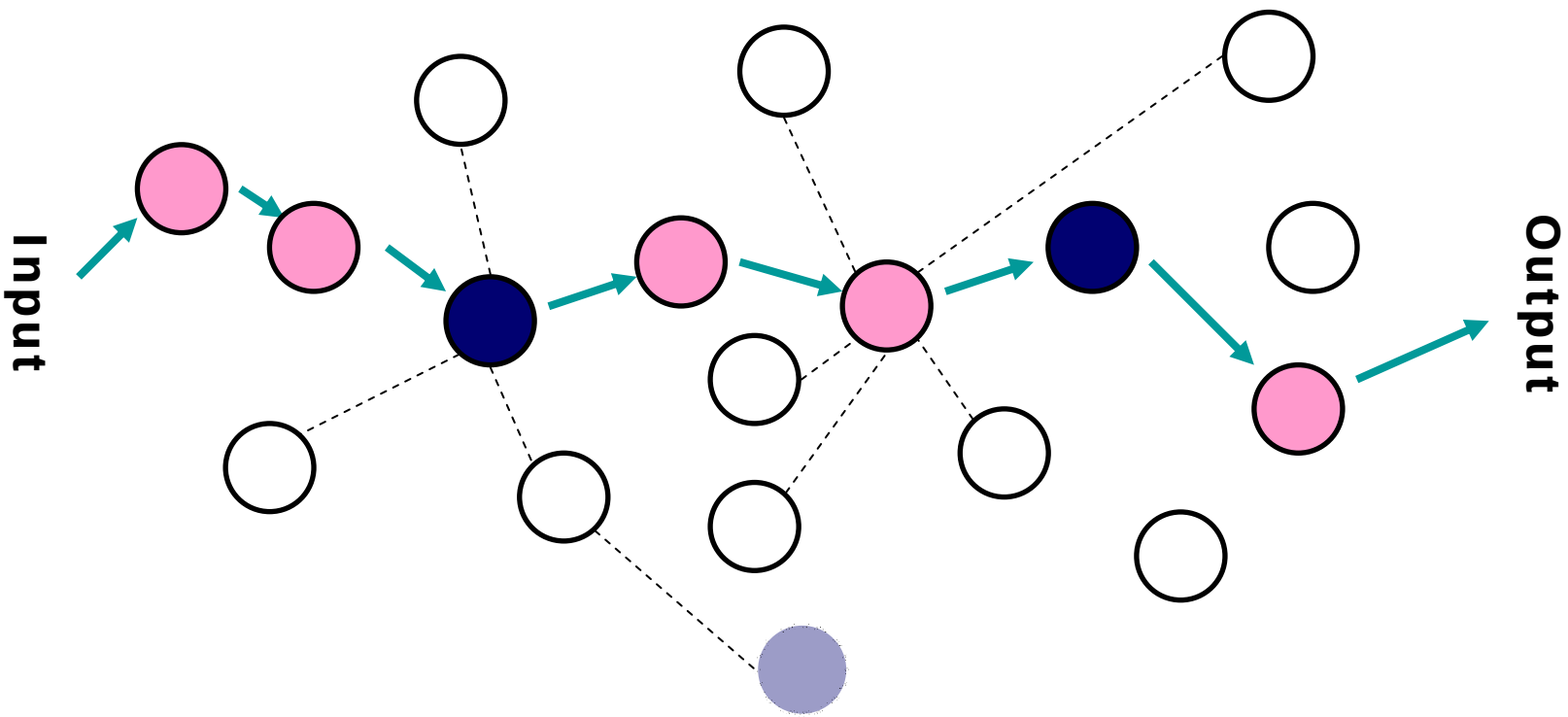
**Workflow for Bioinformatics Web Services**

# Automatic Generation of Bioinformatics Workflow

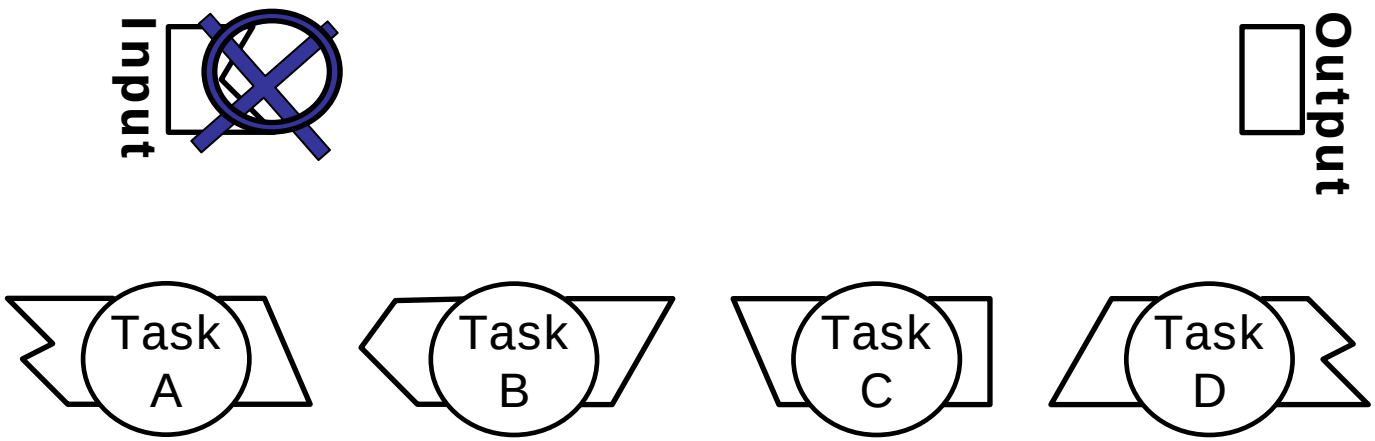
# Task as Atomic Component of Workflow



# Workflow as a Sequence of Tasks

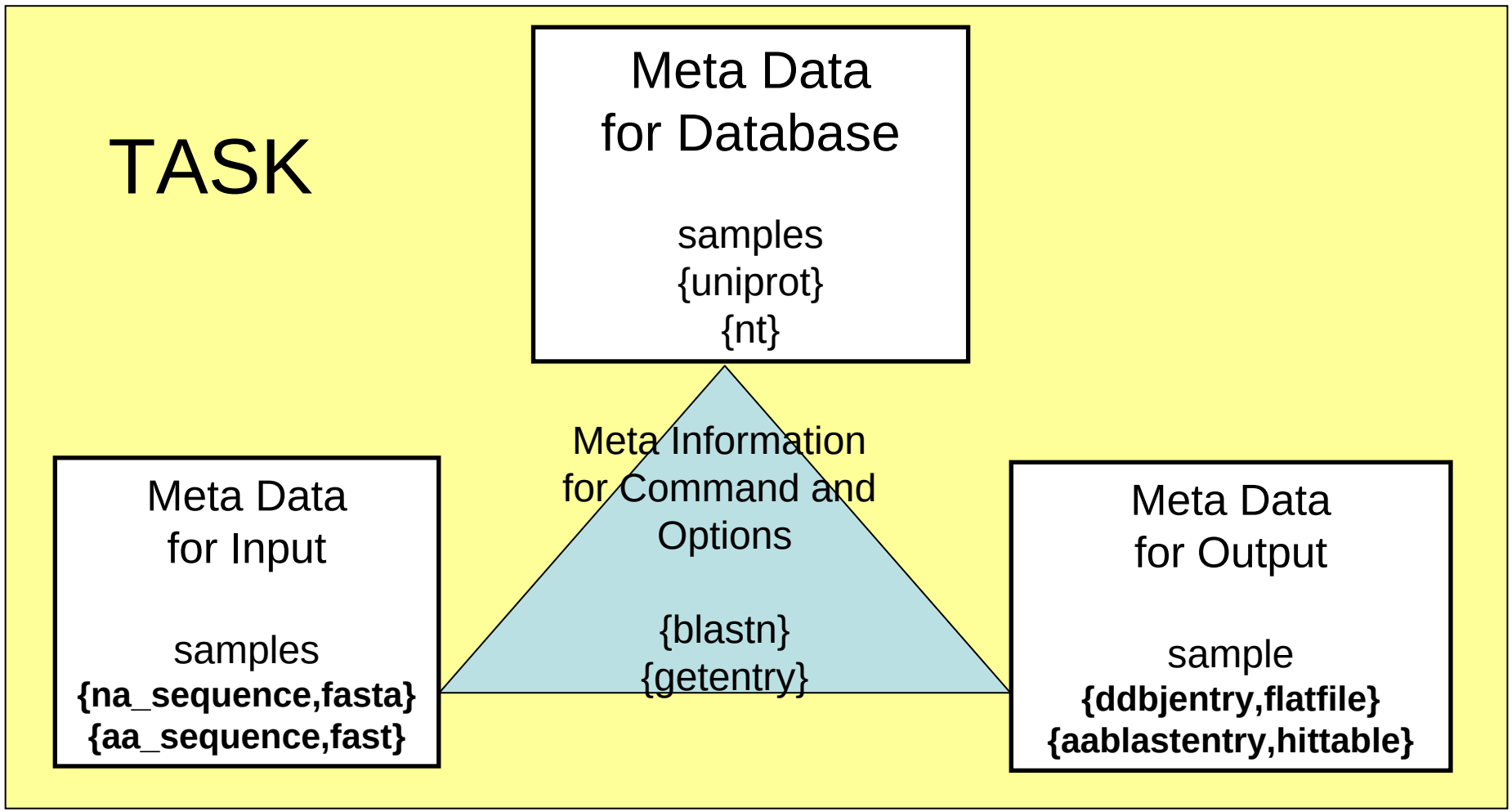


# Automatic Generation of Workflow from Given Input and Output Data Specification and Tasks

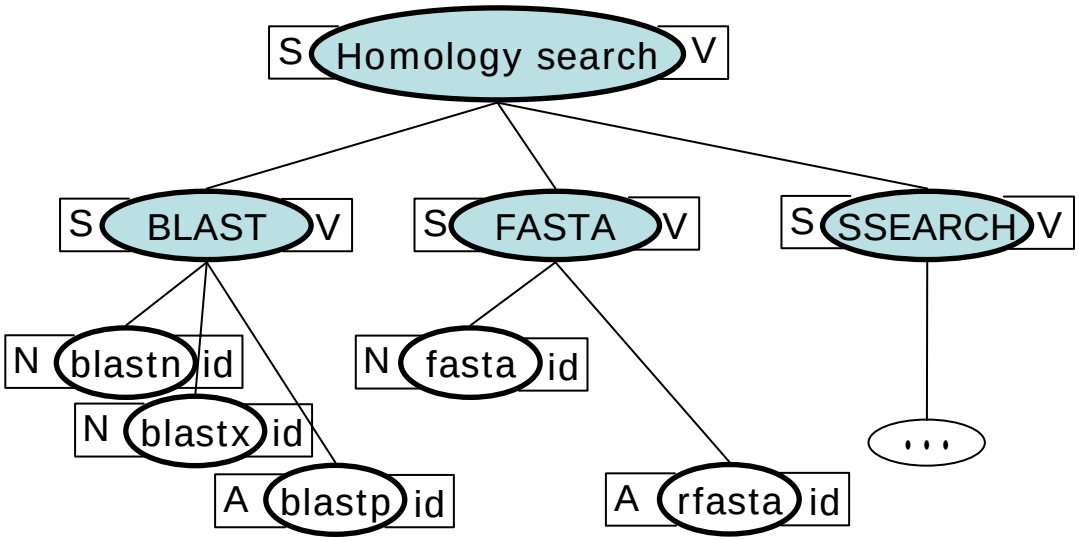


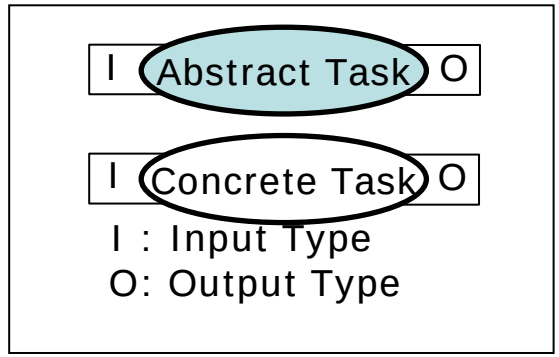

- Path Finding using Meta Information

# Meta Information to Specify the Functionality of Task



# Task Hierarchy (is_a)




S : Sequence or Sequence Name

V : Various Type

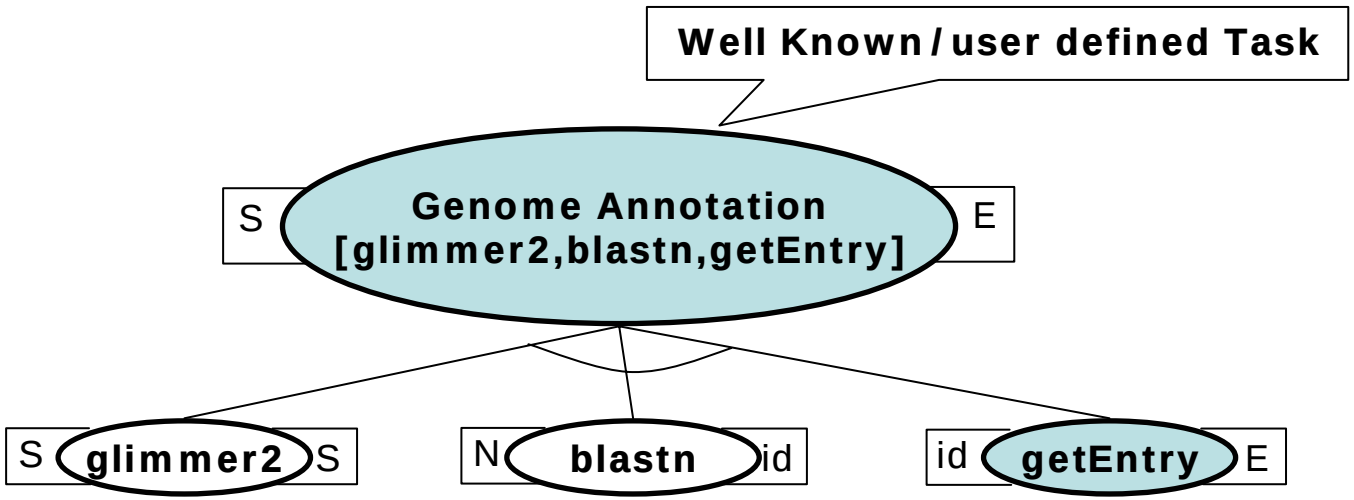
N : Nucleoside Sequence

A : Amino acid Sequence

id : Accession ID

E : Database Entry

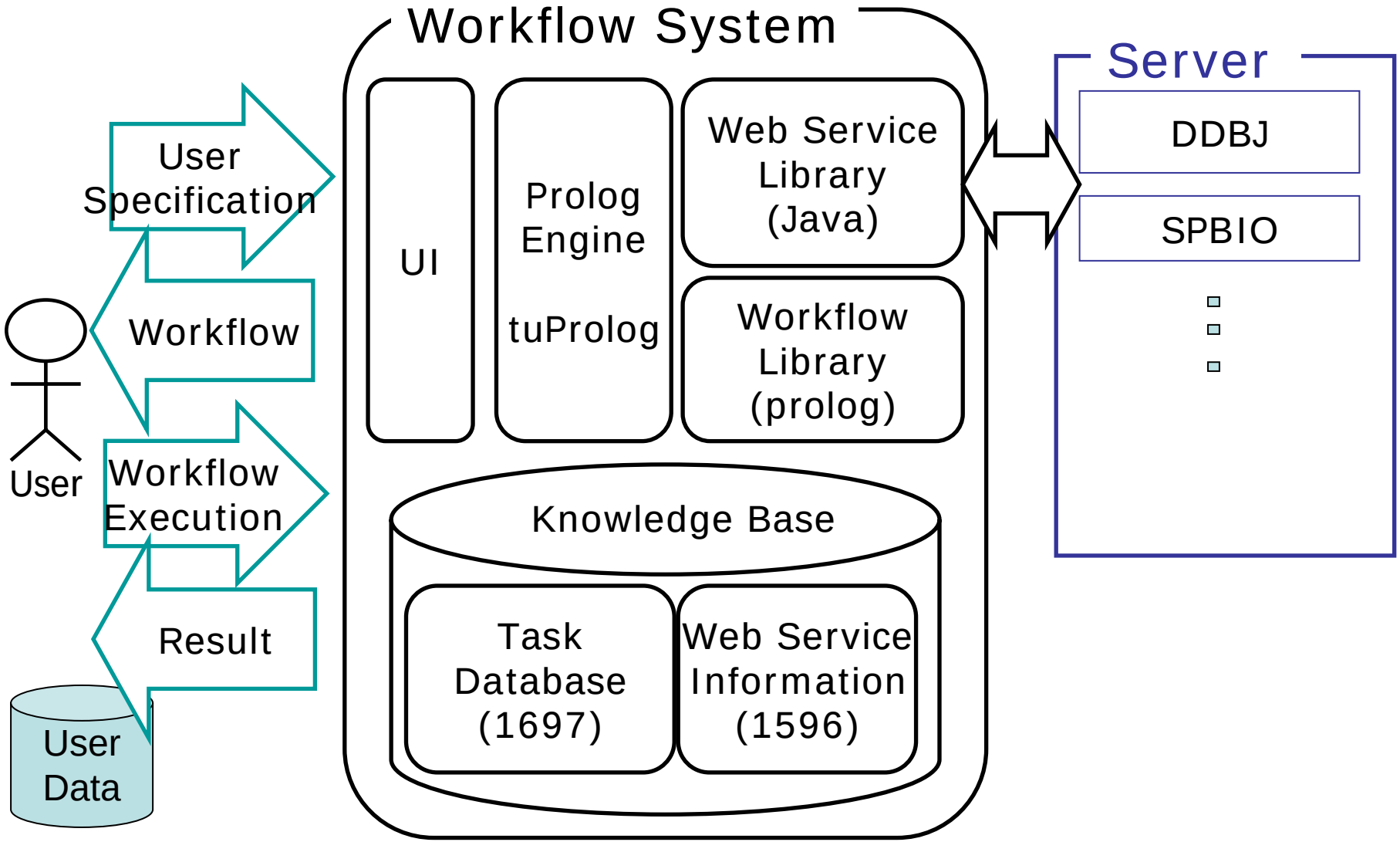
# Task Hierarchy (has_a)



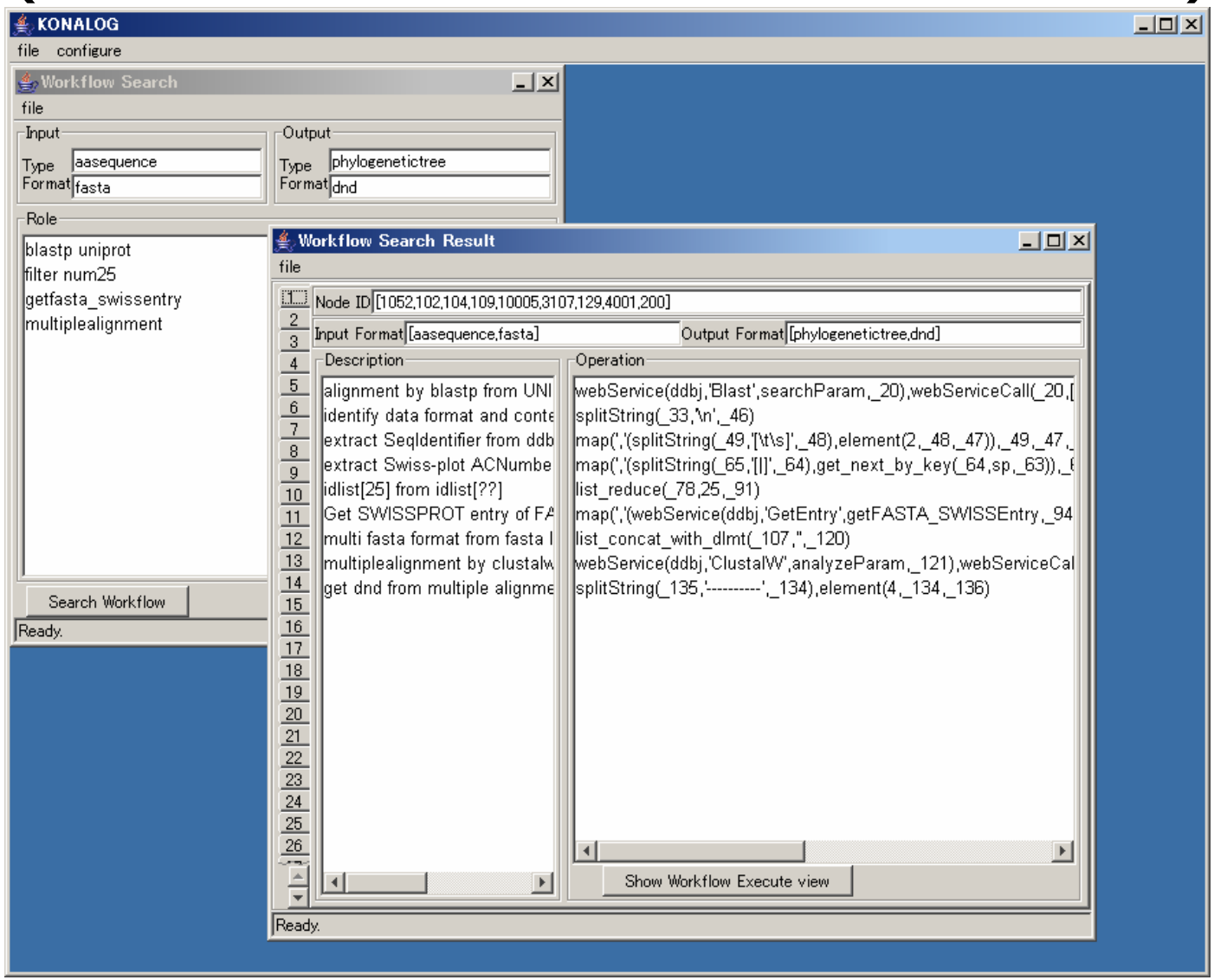
# Prototype for ‘Proof of Concept’

- Language tuProlog
  - Java to Prolog
  - Prolog to Java
    - Web Service Interface through JAVA API
- Task Database
  - Prolog Clause Database
- Optimal Path Finding
  - Bidirectional Breadth First Search Algorithm

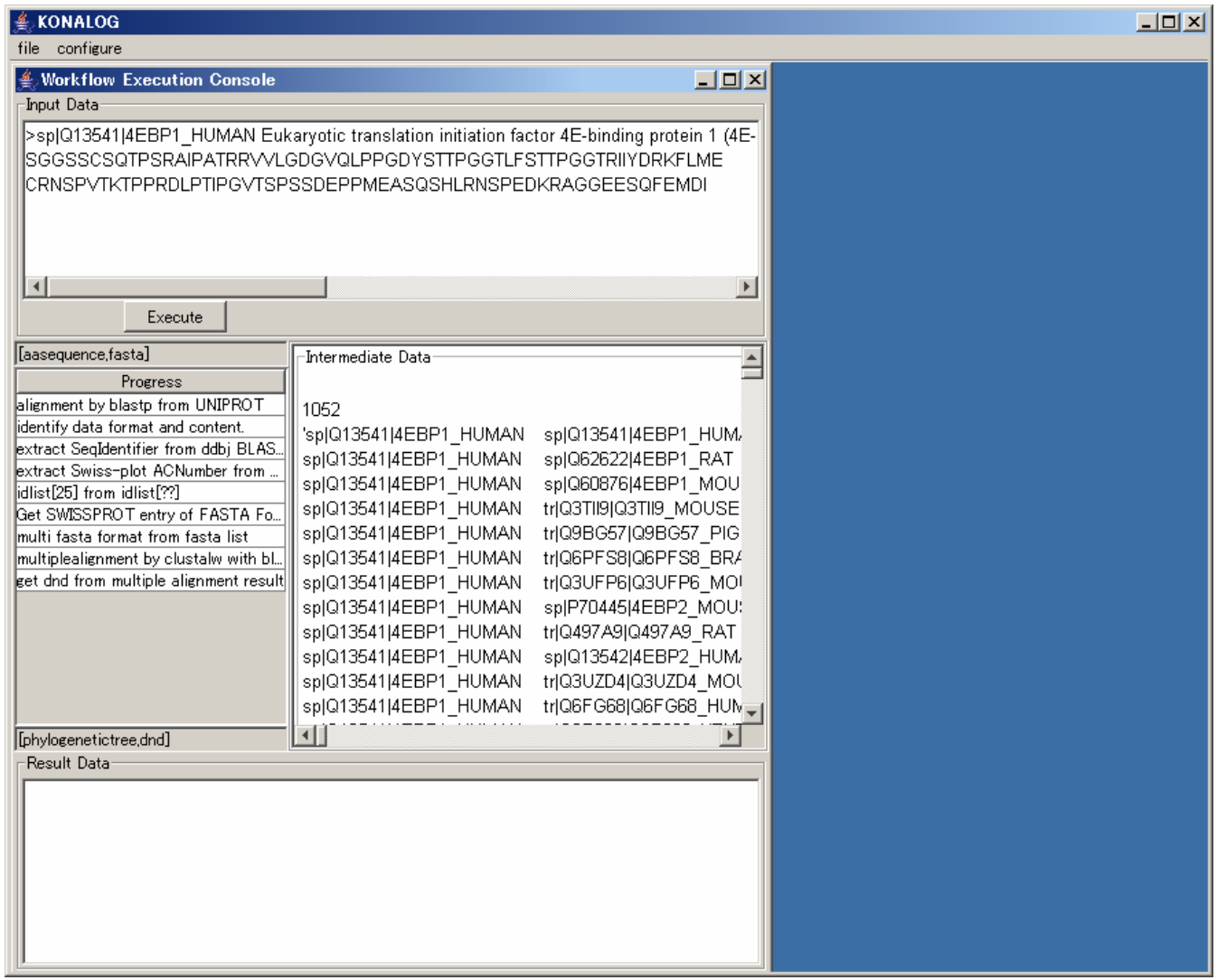
# System Overview



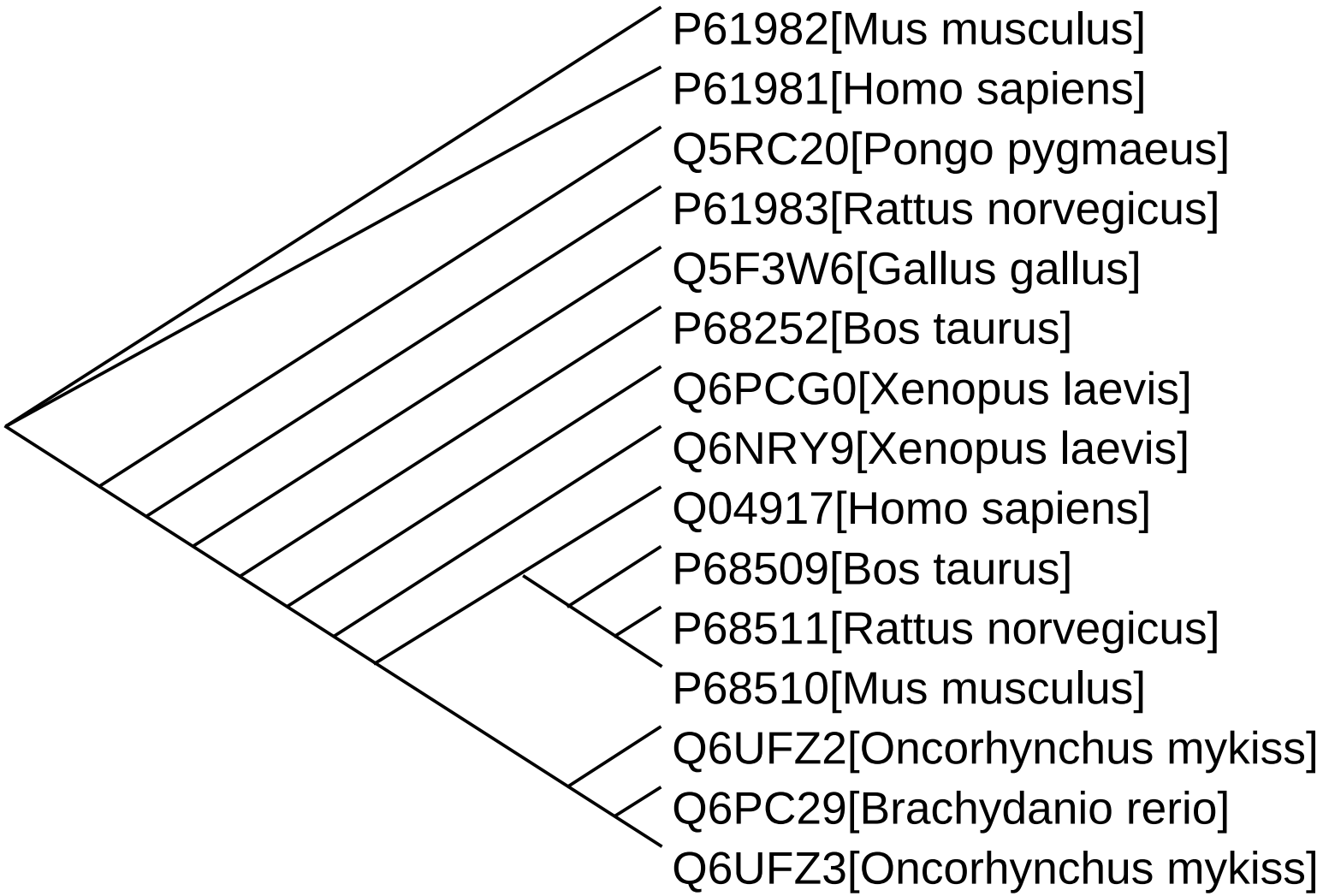
# Screen Snapshot (Workflow Generation Phase)



# Screen Snapshot (Workflow Execution Phase)



# Obtained Phylogenetic Tree by a generated workflow when applying to a Human Insulin Sequence



# Lessons from our First Experience

# Task Database (prototype)

| | | |
|---|---|---|
| Web Service Call | | |
| | DDBJ Blast | 453 |
| | DDBJ SRS | 638 |
| | DDBJ GetEntry | 38 |
| | DDBJ ClustalW | 62 |
| | SPBIO Blast | 405 |
| Format Transformation | | 56 |
| Data Selection | | 45 |
| In Total | | 1697 |

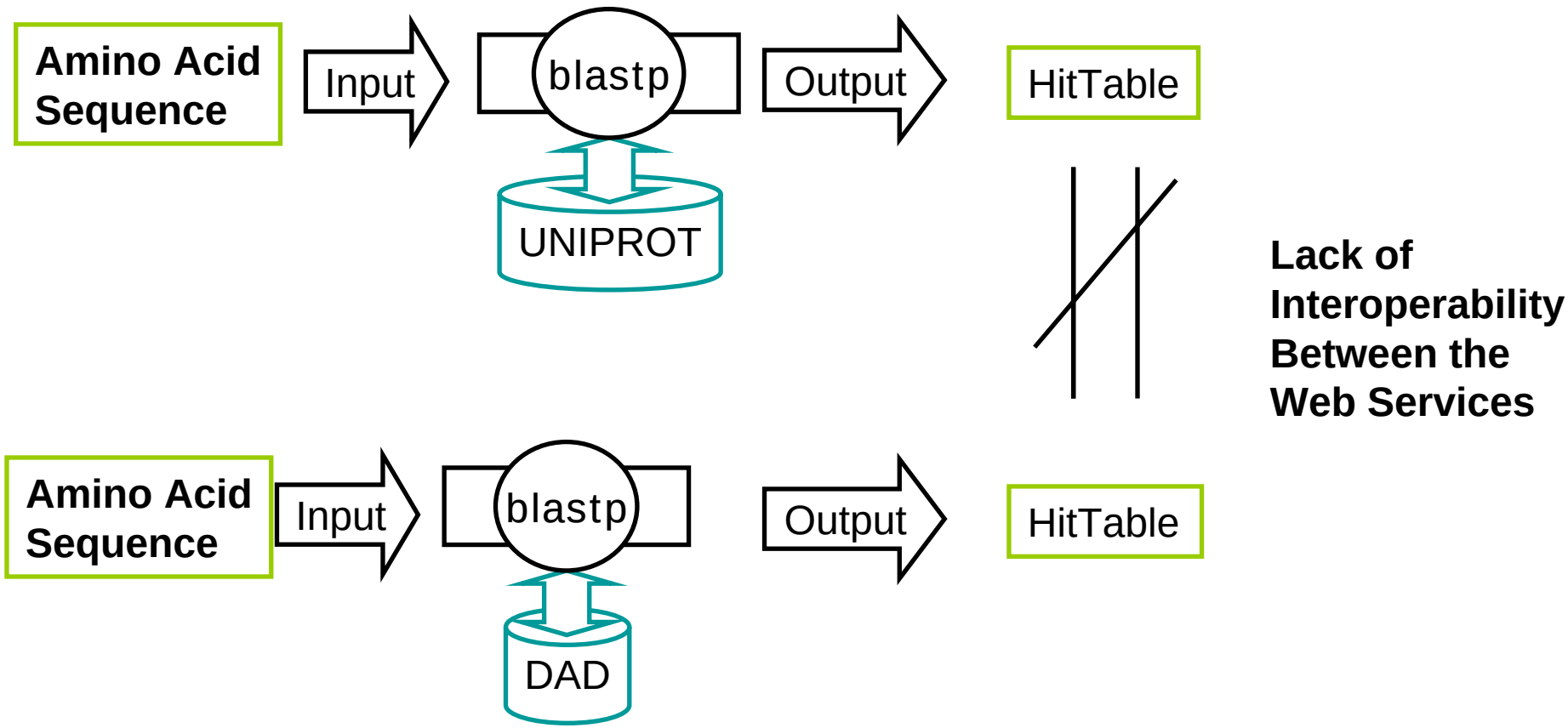
# Test Set of Specification

| No | Workflow | | | | |
|---|---|---|---|---|---|
| | Input | | Output | | Aplications |
| | Format | Type | Format | Type | |
| 1 | fasta | aasequence | gde | aamultiplealignment | blastp uniprot<br>filter num25<br>getfasta_swissentry<br>multiplealignment |
| 2 | | | | | blastp uniprot<br>filter num25<br>getfasta_swissentry<br>multiplealignment |
| 3 | fasta | aasequence | gde | aamultiplealignment | alignmentsearch<br>filter<br>getentry<br>multiplealignment |
| 4 | fasta | aasequence | | | filter<br>getentry<br>multiplealignment |

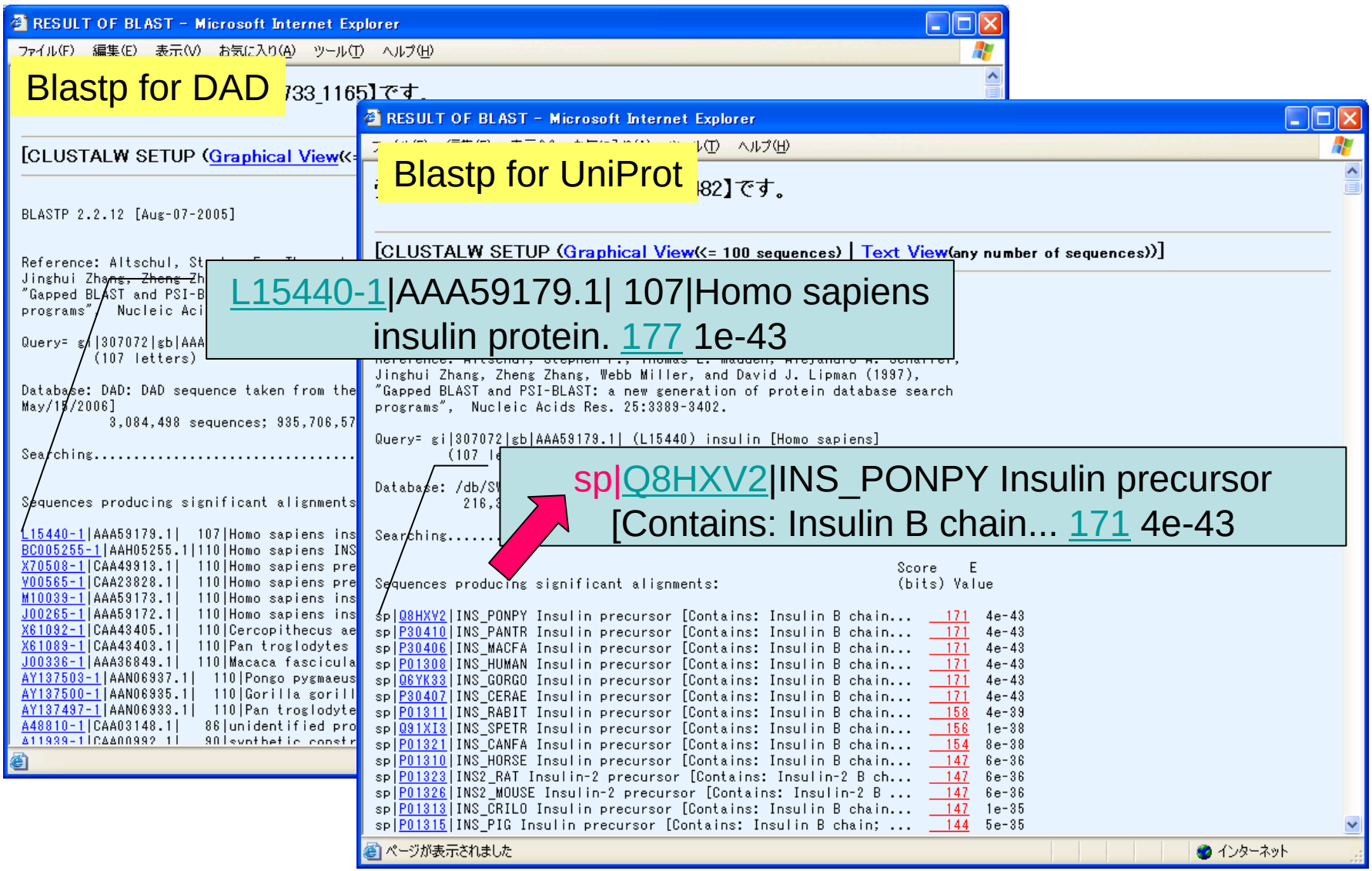
# Differences of Generated Workflow

| Meta Data | No. | Solution Num | time(ms) | First Match WebServiceCall | | |
|---|---|---|---|---|---|---|
| | | | | ID | Description | |
| Input Database Output Full Cmds | 1 | 8 | 11266 | 1052 | alignment by blastp from UNIPROT | ○ |
| | | | | 102 | identify data format and content. | |
| | | | | 104 | extract SeqIdentifier from ddbj BLAST result record | |
| | | | | 109 | extract Swiss-plot ACNumber from SequenceIdentifier | |
| | | | | 10005 | idlist[25] from idlist[??] | |
| | | | | 3107 | Get SWISSPROT entry of FASTA Format by Accession Number. | |
| | | | | 129 | multi fasta format from fasta list | |
| | | | | 4018 | multiplealignment by clustalw with blosum | |
| No input Database No output Full Cmds | 2 | 41 | 46704 | 1052 | alignment by blastp from UNIPROT | ○ |
| | | | | 102 | identify data format and content. | |
| | | | | 104 | extract SeqIdentifier from ddbj BLAST result record | |
| | | | | 109 | extract Swiss-plot ACNumber from SequenceIdentifier | |
| | | | | 1005 | idlist[25] from idlist[??] | |
| | | | | 3107 | Get SWISSPROT entry of FASTA Format by Accession Number. | |
| | | | | 129 | multi fasta format from fasta list | |
| | | | | 4001 | multiplealignment by clustalw with blosum | |
| Input No DB Output Partial Cmds | 3 | 100 over | 249906 | 1043 | alignment by blastp from DAD | X? |
| | | | | 102 | identify data format and content. | |
| | | | | 104 | extract SeqIdentifier from ddbj BLAST result record | |
| | | | | 109 | extract Swiss-plot ACNumber from SequenceIdentifier | |
| | | | | 10001 | idlist[25] from idlist[??] | |
| | | | | 3107 | Get SWISSPROT entry of FASTA Format by Accession Number. | |
| | | | | 129 | multi fasta format from fasta list | |
| | | | | 4018 | multiplealignment by clustalw with blosum | |
| input No DB No output Partial Cmds | 4 | 100 over | 25297 | 1043 | alignment by blastp from DAD | X? |
| | | | | 102 | identify data format and content. | |
| | | | | 104 | extract SeqIdentifier from ddbj BLAST result record | |
| | | | | 109 | extract Swiss-plot ACNumber from SequenceIdentifier | |
| | | | | 10001 | idlist[5] from idlist[??] | |
| | | | | 3107 | Get SWISSPROT entry of FASTA Format by Accession Number. | |
| | | | | 129 | multi fasta format from fasta list | |
| | | | | 4001 | multiplealignment by clustalw with blosum | |

# Why Failed?


Amino Acid Sequence
Input
blastp
Output
HitTable
UNIPROT
Lack of Interoperability Between the Web Services
Amino Acid Sequence
Input
blastp
Output
HitTable
DAD

# Very Similar but not the Same Format



# Conclusion

- Web Services have great potential to share Bioinformatics Data ant Tools in all over the world
- Needs Automatic Workflow Generation Tools to make full use of Web Services
- Bioinformatics Ontology is a key to establish Interoperability among Bioinformatics Web Services

# Acknowledgement


- Daisuke Shinbara Tokyo Institute of Technology (Hitachi, ltd.)
- Sumi Yoshikawa RIKEN GSC, TITECH


# References


Akihiko Konagaya: “Bioinformatics Ontology: Towards the Automatics Generation of Bioinformatics Workflow for Web Services,” in Proc. of Distributed Applications, Web Services, Tools and GRID Infrastructures for Bioinformatics (NETTAB2006), S. Margherita di Pula, Italy (http://www.nettab.org/2006/), pp.75-82 (2006)

Akihiko Konagaya: “OBIGrid: Towards the 'Ba' for Sharing Resources, Services and Knowledge for Bioinformatics”, in Proc. of Fourth International Workshop on Biomedical Computations on the Grid (BioGrid), Singapore (CCGRID 2006), 37 (2006)

# Thank You for Listening