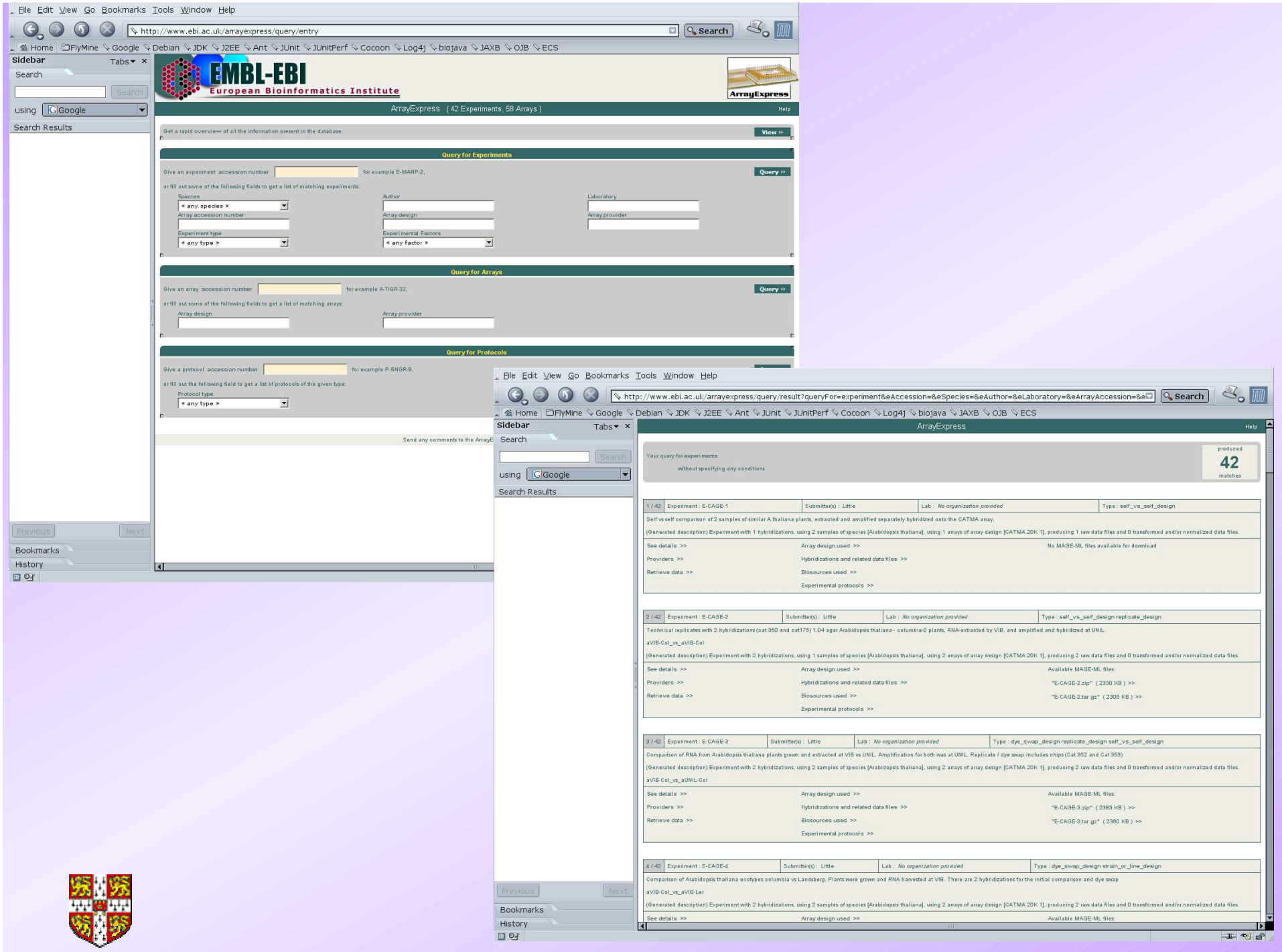
# FlyMine

An integrated database for *Drosophila* and *Anopheles* genomics

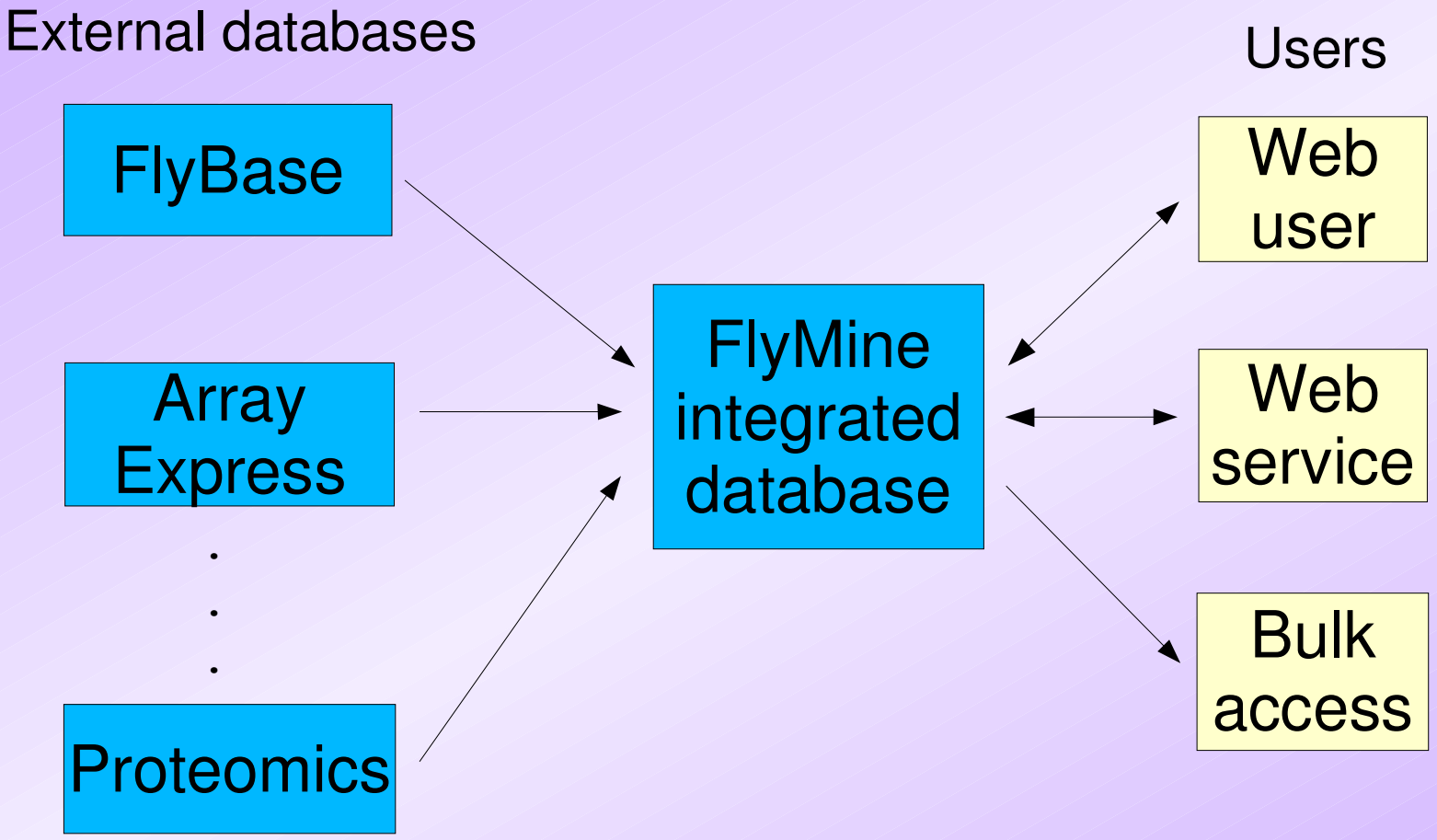
Andrew Varley
24th July 2003

# Why yet another database?

- Currently lots of little databases
  - fine for “browsing”, bad for “querying”
- Hard to query across them
  - lots of “cut and paste” on web pages
- Massive amounts of experimental data (microarray, proteomics) being produced
- Need to tie this information together


File Edit View Go Bookmarks Tools Window Help
http://www.ebi.ac.uk/arrayexpress/query/entry
Search
Home FlyMine Google Debian JDK J2EE Ant JUnit JUnitPerf Cocoon Log4j biojava JAXB OJB ECS
Sidebar
Tabs
Search
using Google
Search Results
Previous
Next
Bookmarks
History
EMBL-EBI
European Bioinformatics Institute
ArrayExpress
ArrayExpress ( 42 Experiments, 58 Arrays )
Help
Get a rapid overview of all the information present in the database.
View »
Query for Experiments
Give an experiment accession number
for example E-MANP-2,
Query »
or fill out some of the following fields to get a list of matching experiments:
Species
« any species »
Author
Laboratory
Array accession number
Array design
Array provider
Experiment type
« any type »
Experimental Factors
« any factor »
Query for Arrays
Give an array accession number
for example A-TIGR-32,
Query »
or fill out some of the following fields to get a list of matching arrays:
Array design
Array provider
Query for Protocols
Give a protocol accession number
for example P-SNGR-8,
or fill out the following field to get a list of protocols of the given type:
Protocol type
« any type »
Send any comments to the ArrayE
http://www.ebi.ac.uk/arrayexpress/query/result?queryFor=experiment&eAccession=&eSpecies=&eAuthor=&eLaboratory=&eArrayAccession=&e
Your query for experiments
without specifying any conditions
produced
42
matches
1 / 42 Experiment : E-CAGE-1 Submitter(s) : Little Lab : No organization provided Type : self_vs_self_design
Self vs self comparison of 2 samples of similar A.thaliana plants, extracted and amplified separately hybridized onto the CATMA array.
(Generated description) Experiment with 1 hybridizations, using 2 samples of species [Arabidopsis thaliana], using 1 arrays of array design [CATMA 20K 1], producing 1 raw data files and 0 transformed and/or normalized data files.
See details >>
Array design used >>
No MAGE-ML files available for download
Providers >>
Hybridizations and related data files >>
Retrieve data >>
Biosources used >>
Experimental protocols >>
2 / 42 Experiment : E-CAGE-2 Submitter(s) : Little Lab : No organization provided Type : self_vs_self_design replicate_design
Technical replicates with 2 hybridizations (cat 350 and cat175) 1.04 agar Arabidopsis thaliana - columbia-0 plants, RNA-extracted by VIB, and amplified and hybridized at UNIL.
aVIB-Col_vs_aVIB-Col
(Generated description) Experiment with 2 hybridizations, using 1 samples of species [Arabidopsis thaliana], using 2 arrays of array design [CATMA 20K 1], producing 2 raw data files and 0 transformed and/or normalized data files.
See details >>
Array design used >>
Available MAGE-ML files:
Providers >>
Hybridizations and related data files >>
"E-CAGE-2.zip" ( 2330 KB ) >>
Retrieve data >>
Biosources used >>
"E-CAGE-2.tar.gz" ( 2305 KB ) >>
Experimental protocols >>
3 / 42 Experiment : E-CAGE-3 Submitter(s) : Little Lab : No organization provided Type : dye_swap_design replicate_design self_vs_self_design
Comparison of RNA from Arabidopsis thaliana plants grown and extracted at VIB vs UNIL. Amplification for both was at UNIL. Replicate / dye swap includes chips (Cat 352 and Cat 353)
(Generated description) Experiment with 2 hybridizations, using 2 samples of species [Arabidopsis thaliana], using 2 arrays of array design [CATMA 20K 1], producing 2 raw data files and 0 transformed and/or normalized data files.
aVIB-Col_vs_aUNIL-Col
See details >>
Array design used >>
Available MAGE-ML files:
Providers >>
Hybridizations and related data files >>
"E-CAGE-3.zip" ( 2383 KB ) >>
Retrieve data >>
Biosources used >>
"E-CAGE-3.tar.gz" ( 2380 KB ) >>
Experimental protocols >>
4 / 42 Experiment : E-CAGE-4 Submitter(s) : Little Lab : No organization provided Type : dye_swap_design strain_or_line_design
Comparison of Arabidopsis thaliana ecotypes columbia vs Landsberg. Plants were grown and RNA harvested at VIB. There are 2 hybridizations for the initial comparison and dye swap.
aVIB-Col_vs_aVIB-Ler
(Generated description) Experiment with 2 hybridizations, using 2 samples of species [Arabidopsis thaliana], using 2 arrays of array design [CATMA 20K 1], producing 2 raw data files and 0 transformed and/or normalized data files.
See details >>
Array design used >>
Available MAGE-ML files:

# Outline

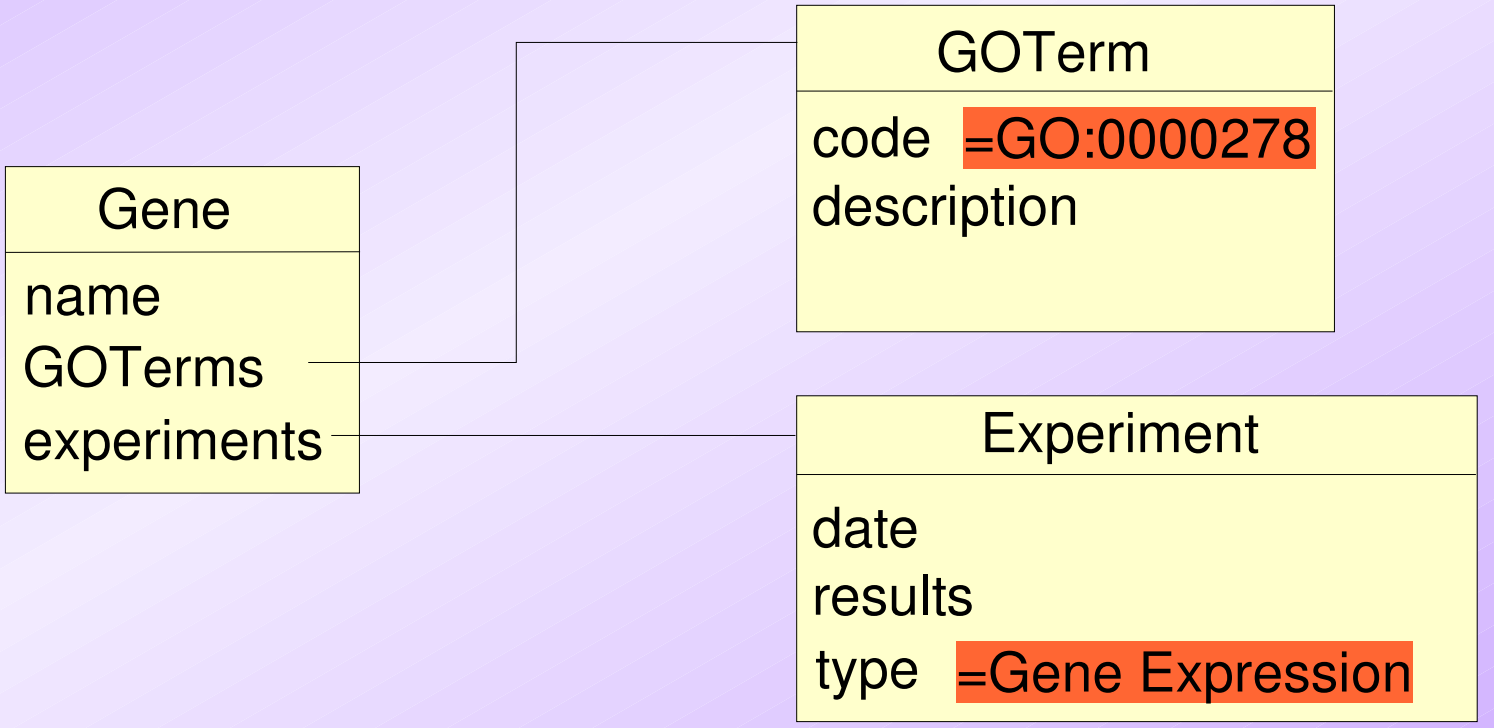

External databases
FlyBase
Array Express
Proteomics
FlyMine integrated database
Users
Web user
Web service
Bulk access

# Aims

- Integrate data from multiple sources
- Allow arbitrary queries from users
- Queries based on objects, not SQL
- Multiple query interfaces (Java, OQL, graphical, etc)
- Different classes of user (web-based, SOAP)
- Open source!

# Query interfaces – graphical

*"Show gene expression data for genes which have GO term GO:0000278 applied"*




# Query interfaces – OQL

*"Show gene expression data for genes which have GO term GO:0000278 applied"*

```
SELECT gene, exp
FROM Gene AS gene, GOTerm AS term,
     Experiment AS exp
WHERE gene.GOTerms CONTAINS term
AND term.code = "GO:0000278"
AND gene.experiments CONTAINS exp
AND exp.type = "Gene Expression"
```

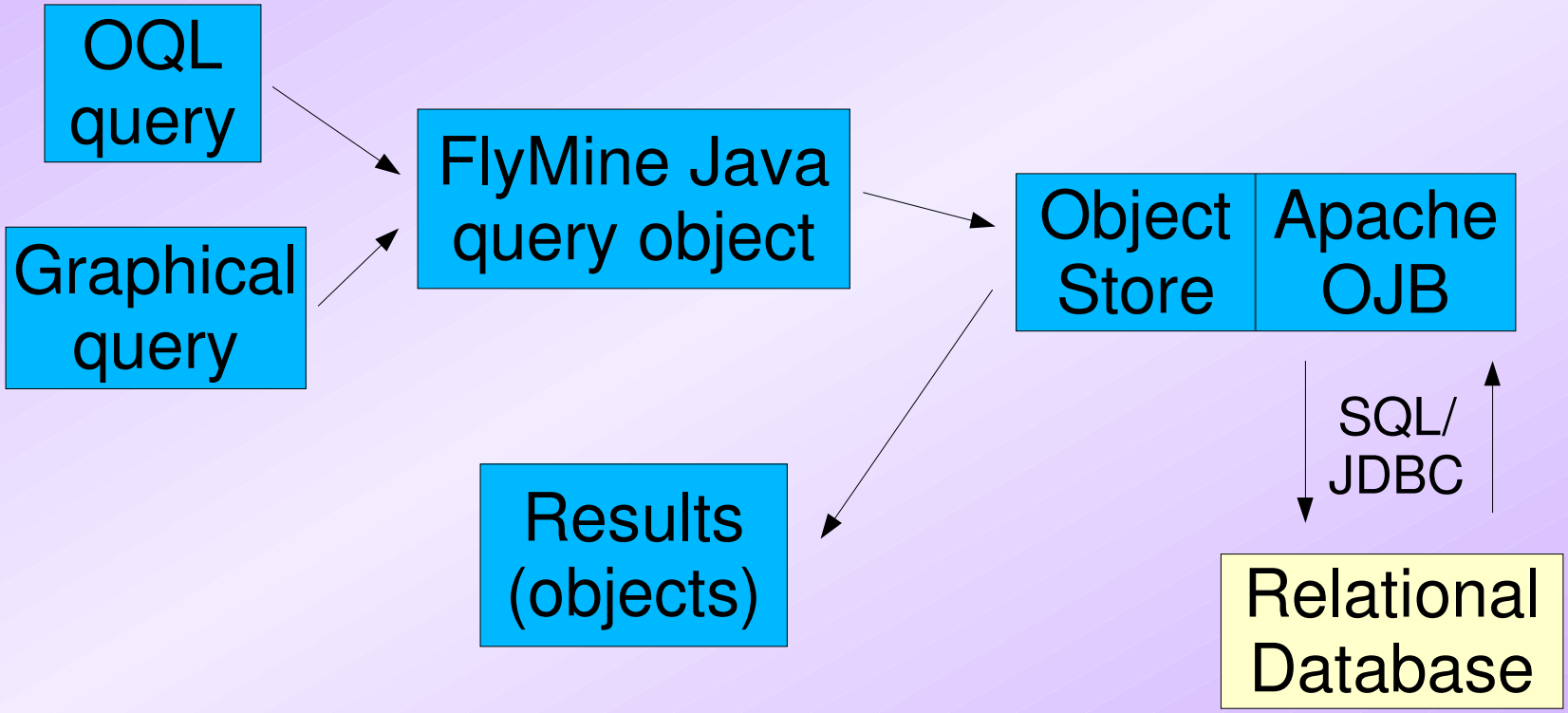
# Query interfaces – Java

*"Show gene expression data for genes which have GO term GO:0000278 applied"*

```
Query q = new Query();
QueryClass qcGene = new QueryClass(Gene.class);
QueryClass qcTerm = new QueryClass(GOTerm.class);
QueryField qfGeneTerm = new QueryField(qcGene, "GOTerms")
ConstraintSet cs = new ConstraintSet();
Constraint con1 = new ContainsConstraint(qfGeneTerm,
                  ContainsConstraint.CONTAINS, qcTerm);
cs.add(con1);
.
.
q.setConstraint(cs);
```

# FlyMine ObjectStore

- Based on heavily modified Apache OJB

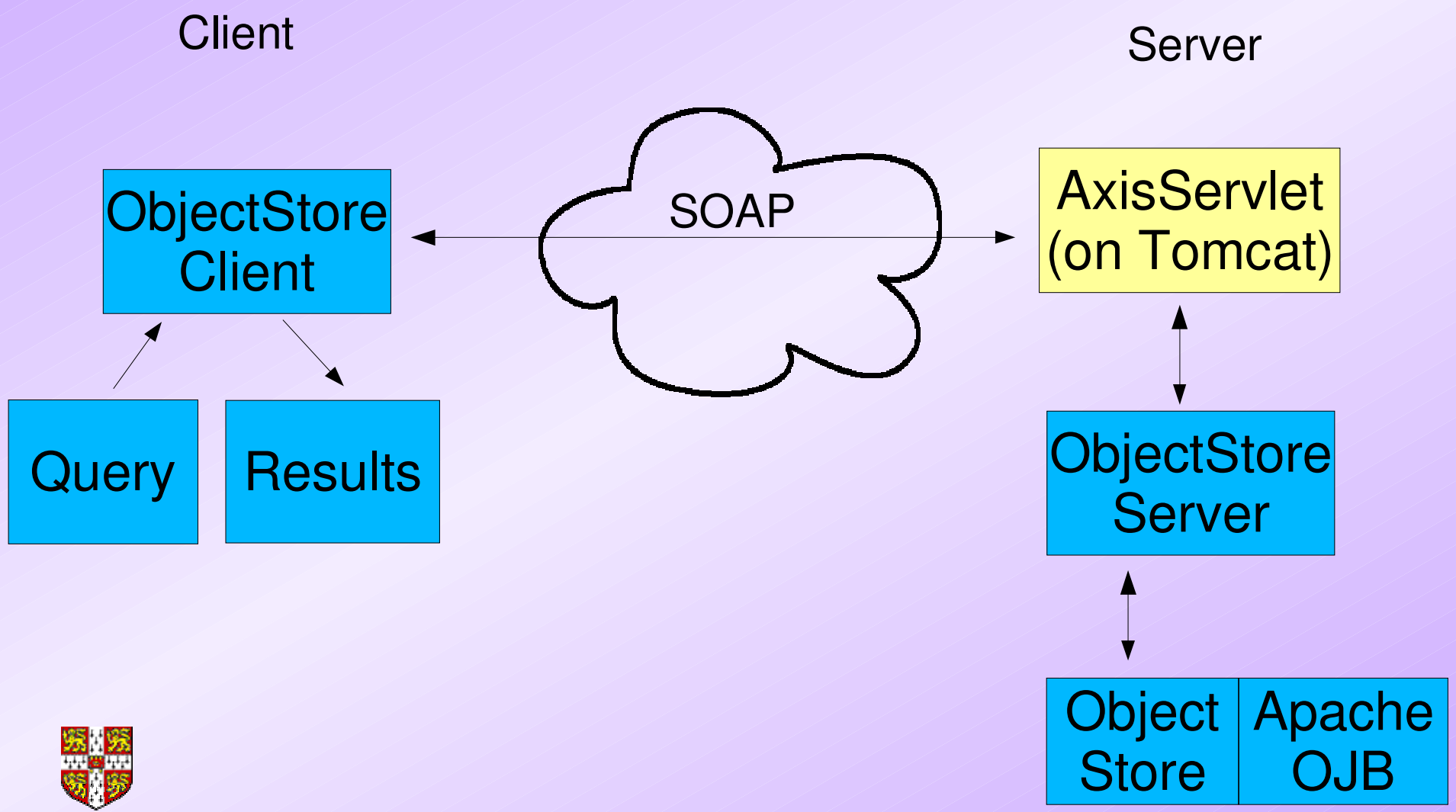



# ObjectStore interface

```
public interface ObjectStore {

  Results execute(Query q);
  List execute(Query q, int start, int limit);
  int count(Query q);
  ExplainResult estimate(Query q);
  Object getObjectByExample(Object obj);
  Model getModel();
}
```

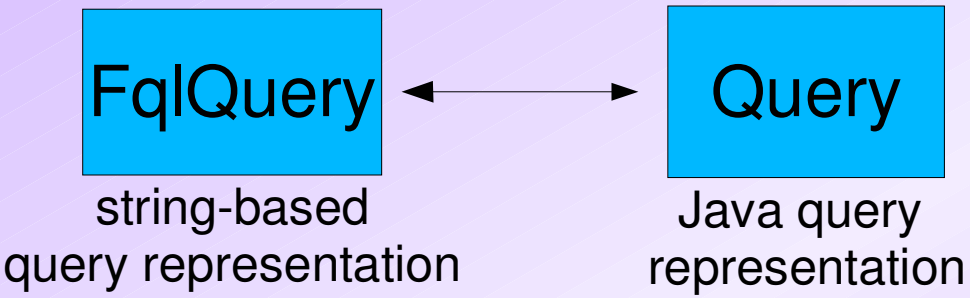
# Web service


Client
Server
ObjectStore Client
SOAP
AxisServlet (on Tomcat)
Query
Results
ObjectStore Server
Object Store
Apache OJB

# Web service

- Objects to encode
  - data objects (all are beans)
  - Query
  - ResultsRow (a list)
  - ExplainResult (a few integers)
  - Model (already have XML format)
  - object proxies

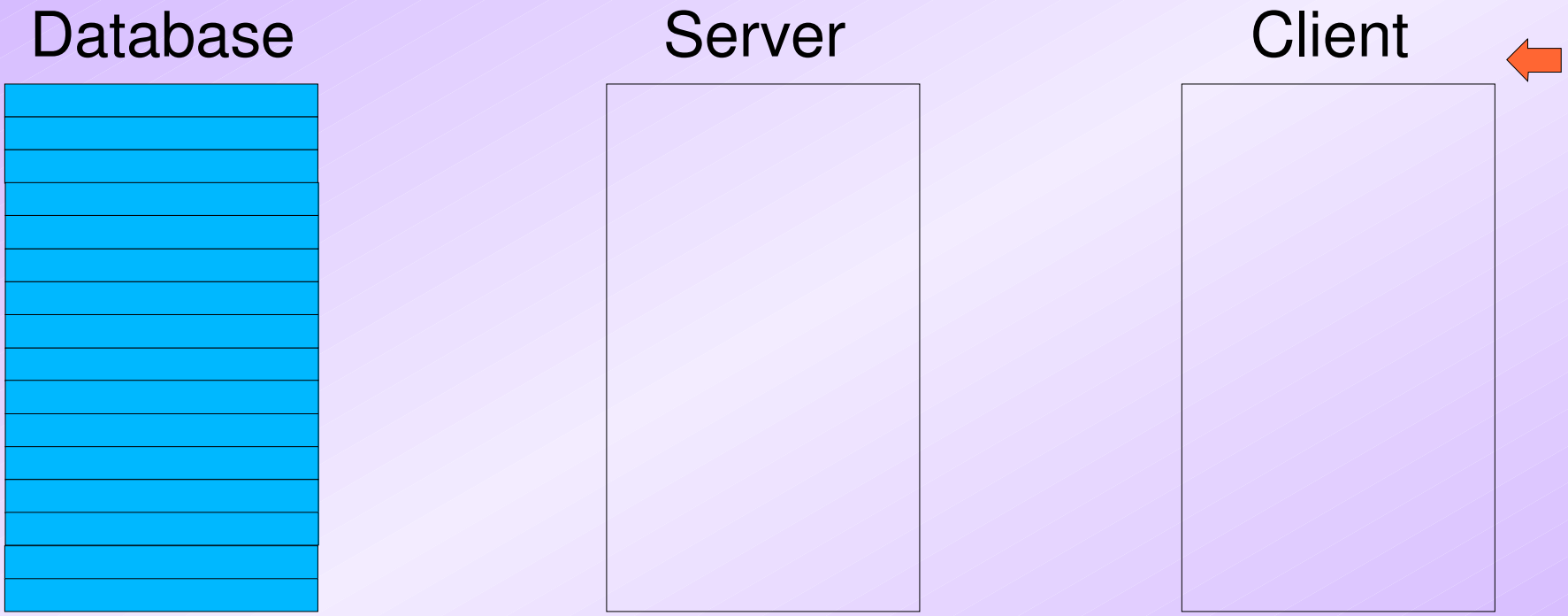
# ObjectStoreServer



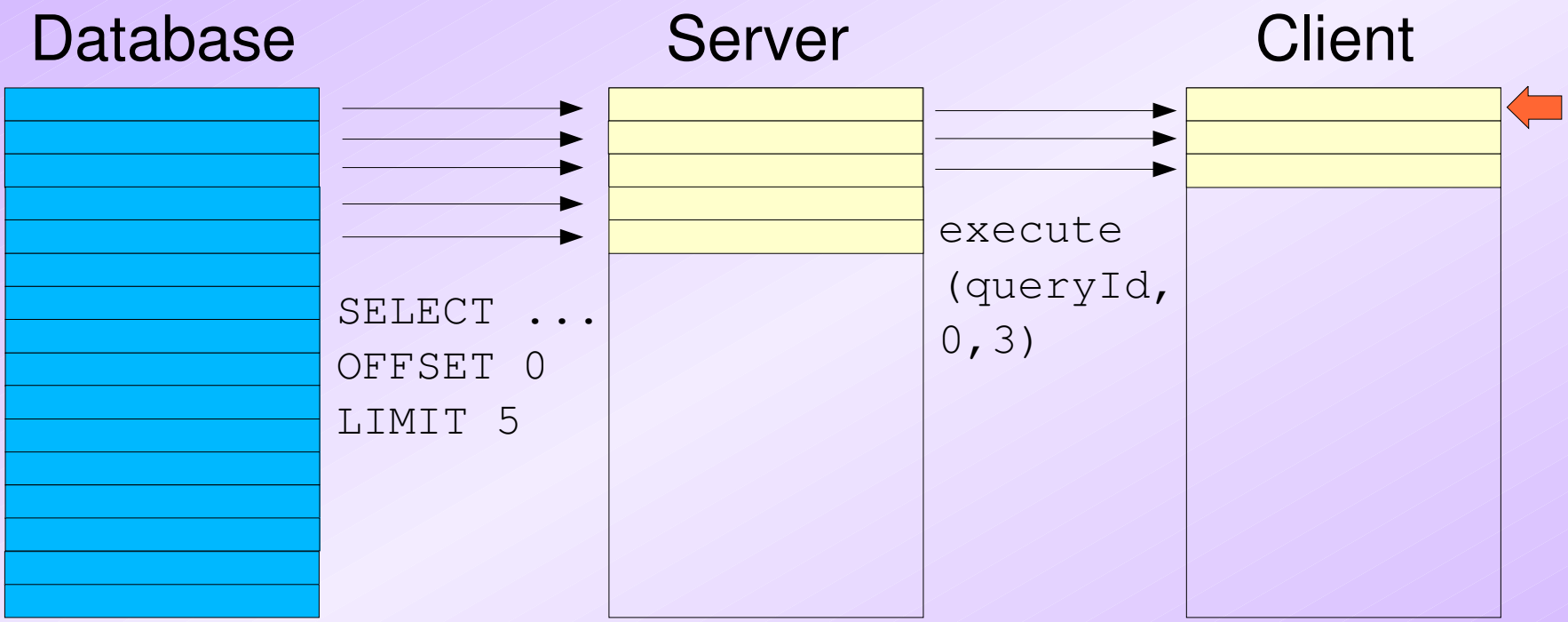

```
public class ObjectStoreServer {
   int registerQuery(FqlQuery q);
   List execute(int queryId, int start, int end);
   int count(int queryId);
   ExplainResult estimate(int queryId);
   Object getObjectByExample(Object obj);
   Model getModel();
}
```

```
 <soapenv:Body>
  <registerQuery
soapenv:encodingStyle="http://schemas.xmlsoap.org/soap/encoding/">
   <arg0 href="#id0"/>
  </registerQuery>
  <multiRef id="id0" soapenc:root="0"
soapenv:encodingStyle="http://schemas.xmlsoap.org/soap/encoding/"
xsi:type="fql-query"
xmlns:soapenc="http://schemas.xmlsoap.org/soap/encoding/">
   <packageName
xsi:type="xsd:string">org.flymine.model.tutorial</packageName>
   <queryString xsi:type="xsd:string">select g from Gene as
g</queryString>
  </multiRef>
 </soapenv:Body>
```

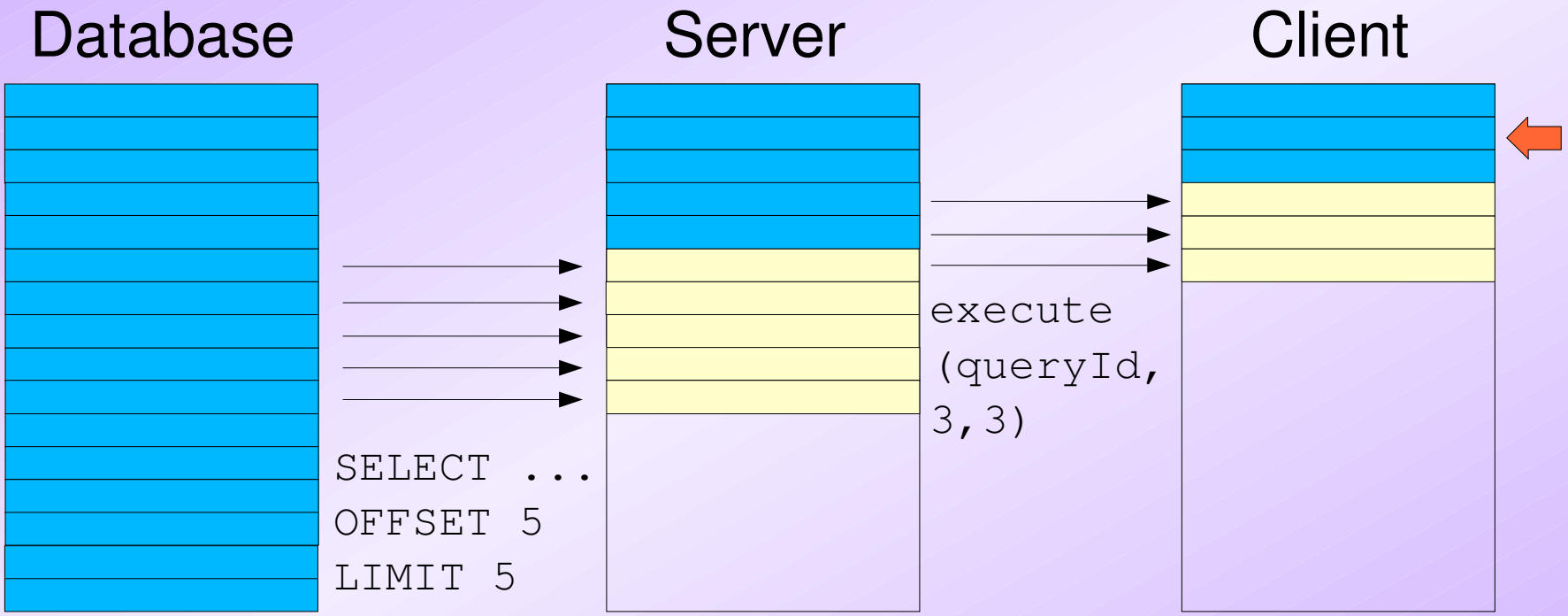
# Results



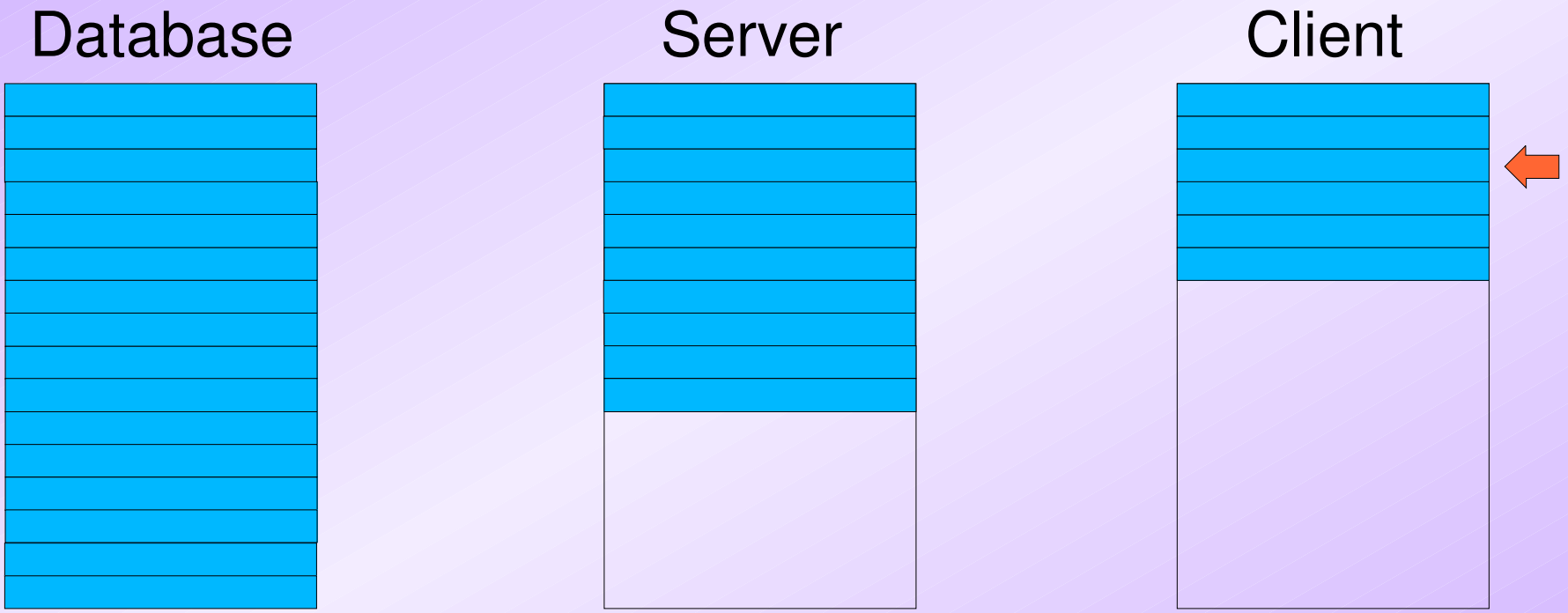

# Results


Database
Server
Client
SELECT ...
OFFSET 0
LIMIT 5
execute
(queryId,
0,3)

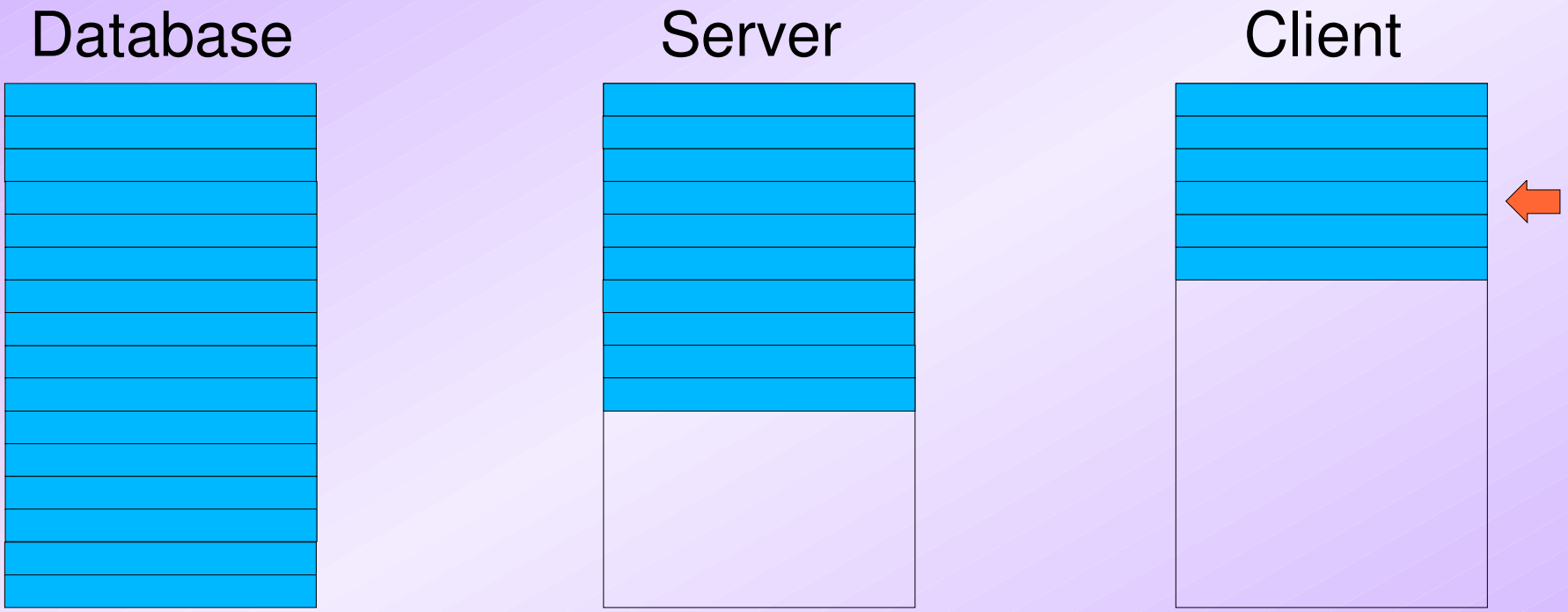
# Results


Database
Server
Client
SELECT ...
OFFSET 5
LIMIT 5
execute
(queryId,
3,3)

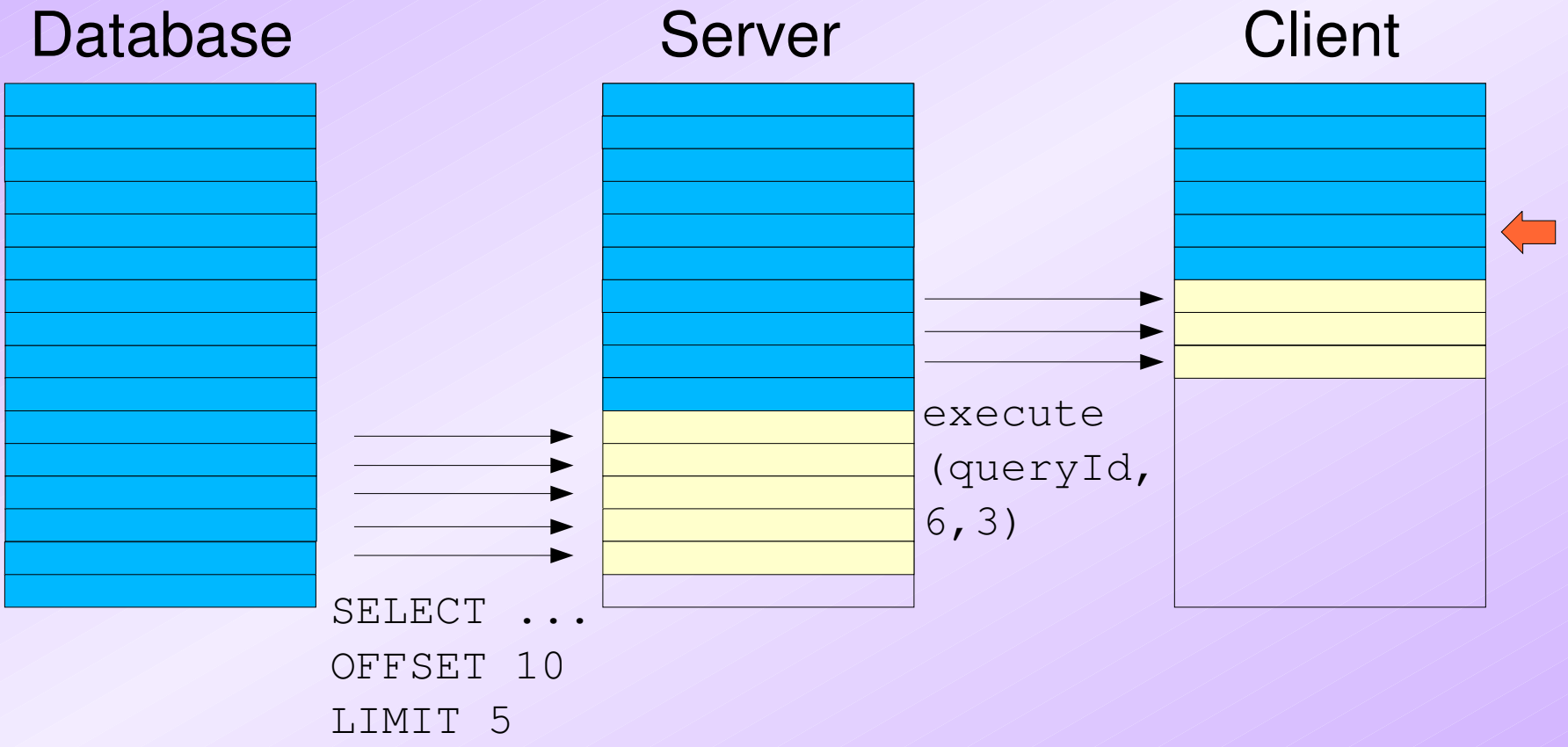
# Results




# Results

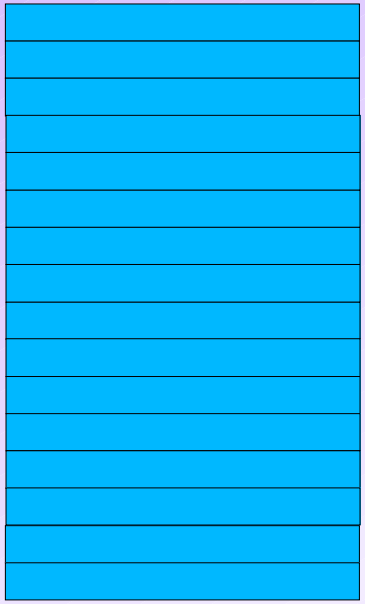



# Results

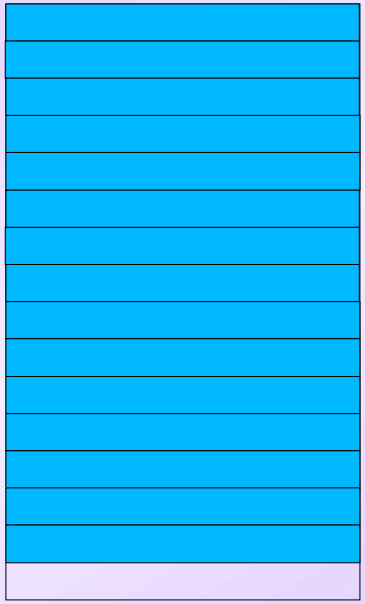

Database
Server
Client
execute
(queryId,
6,3)
SELECT ...
OFFSET 10
LIMIT 5

# Results

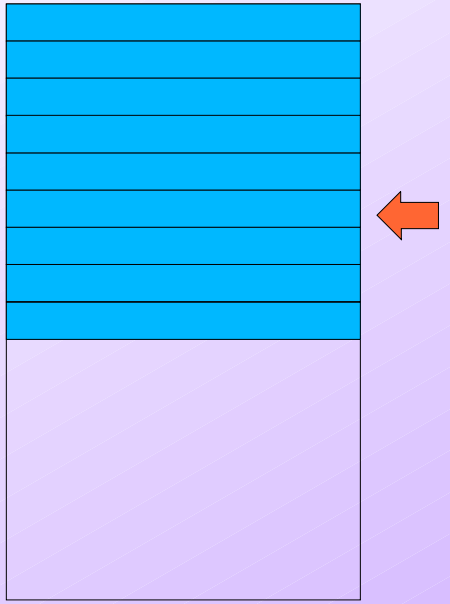
Database



Server

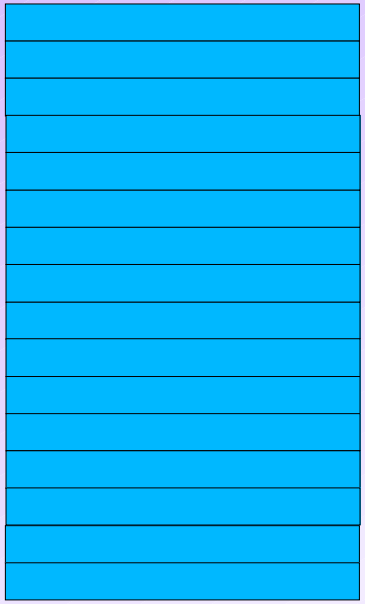


Client

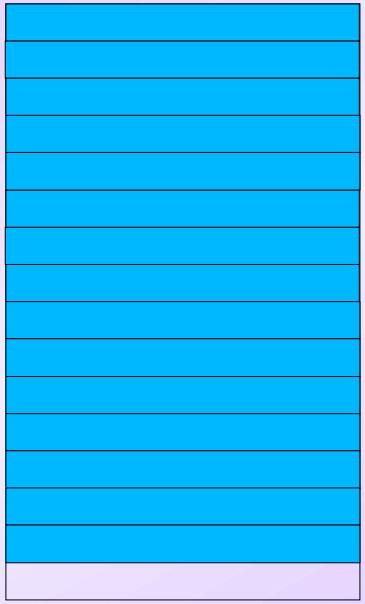


# Results

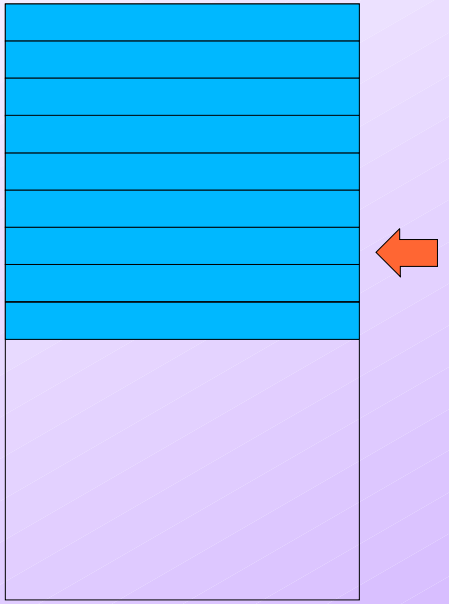
Database



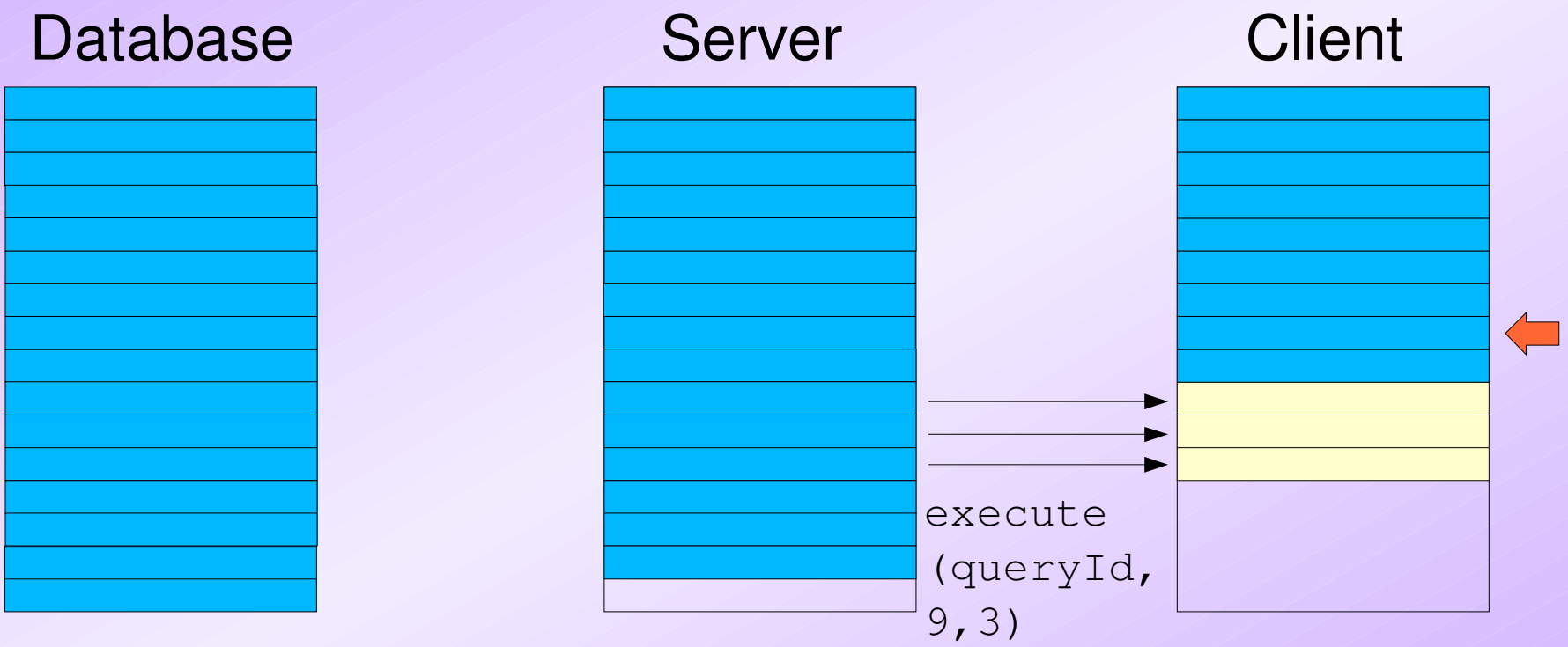
Server



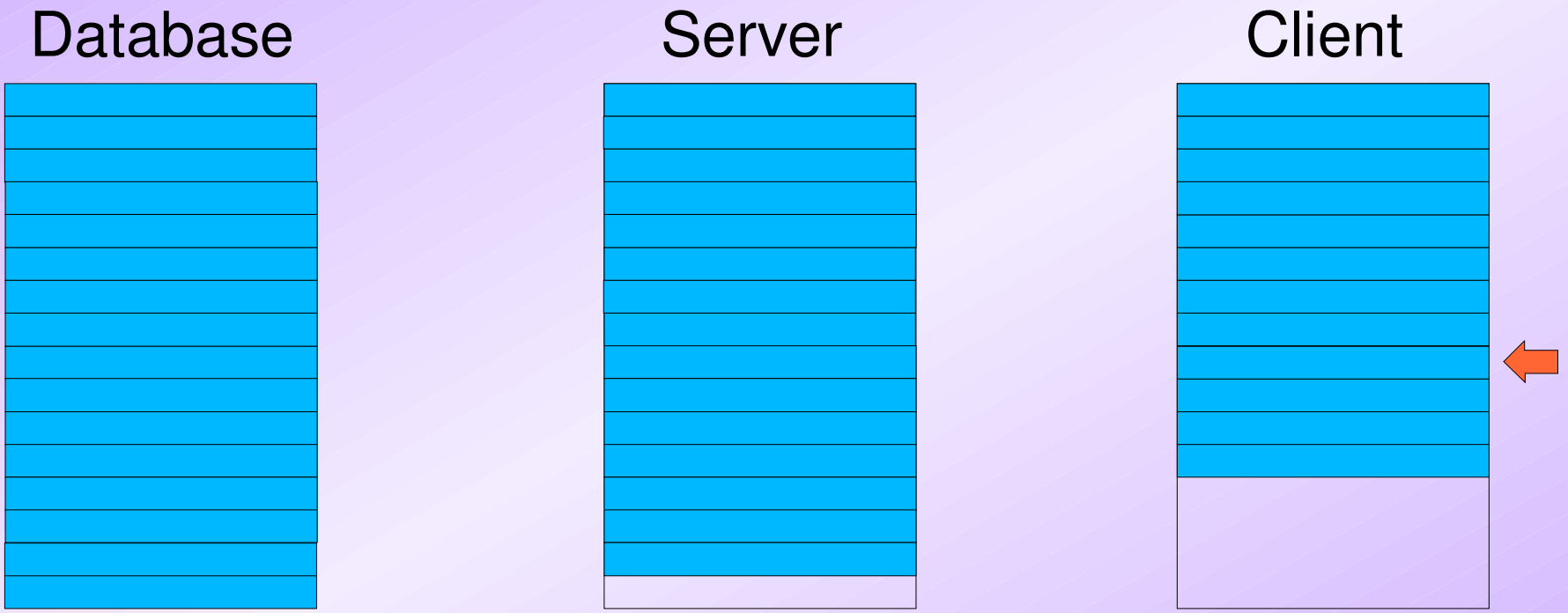
Client



# Results

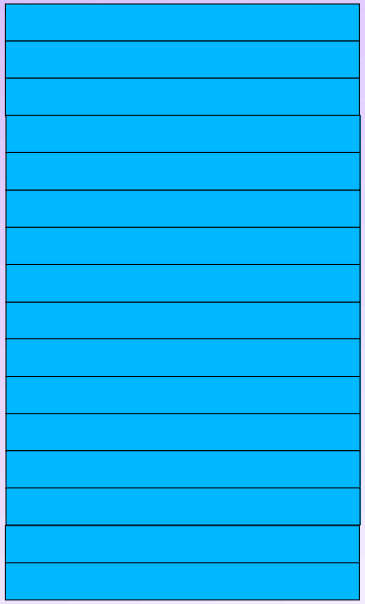



# Results

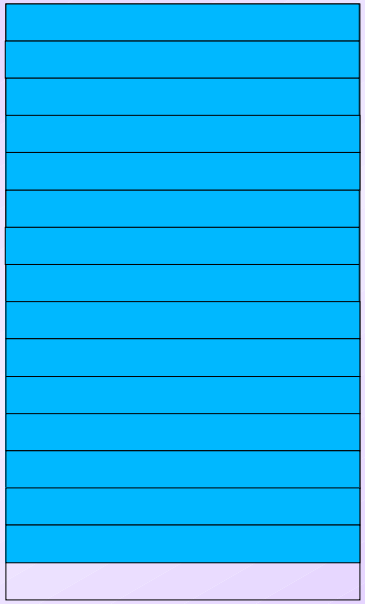



# Results

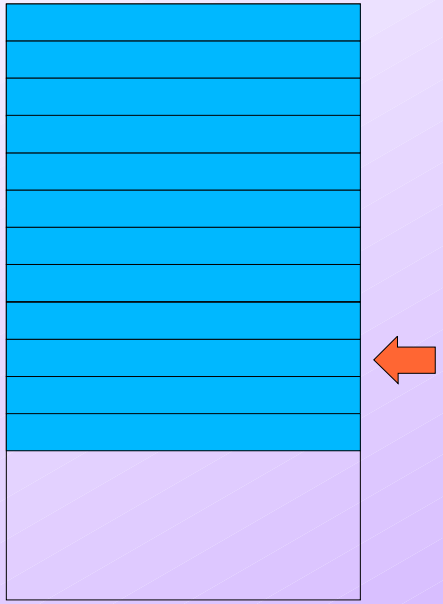
Database



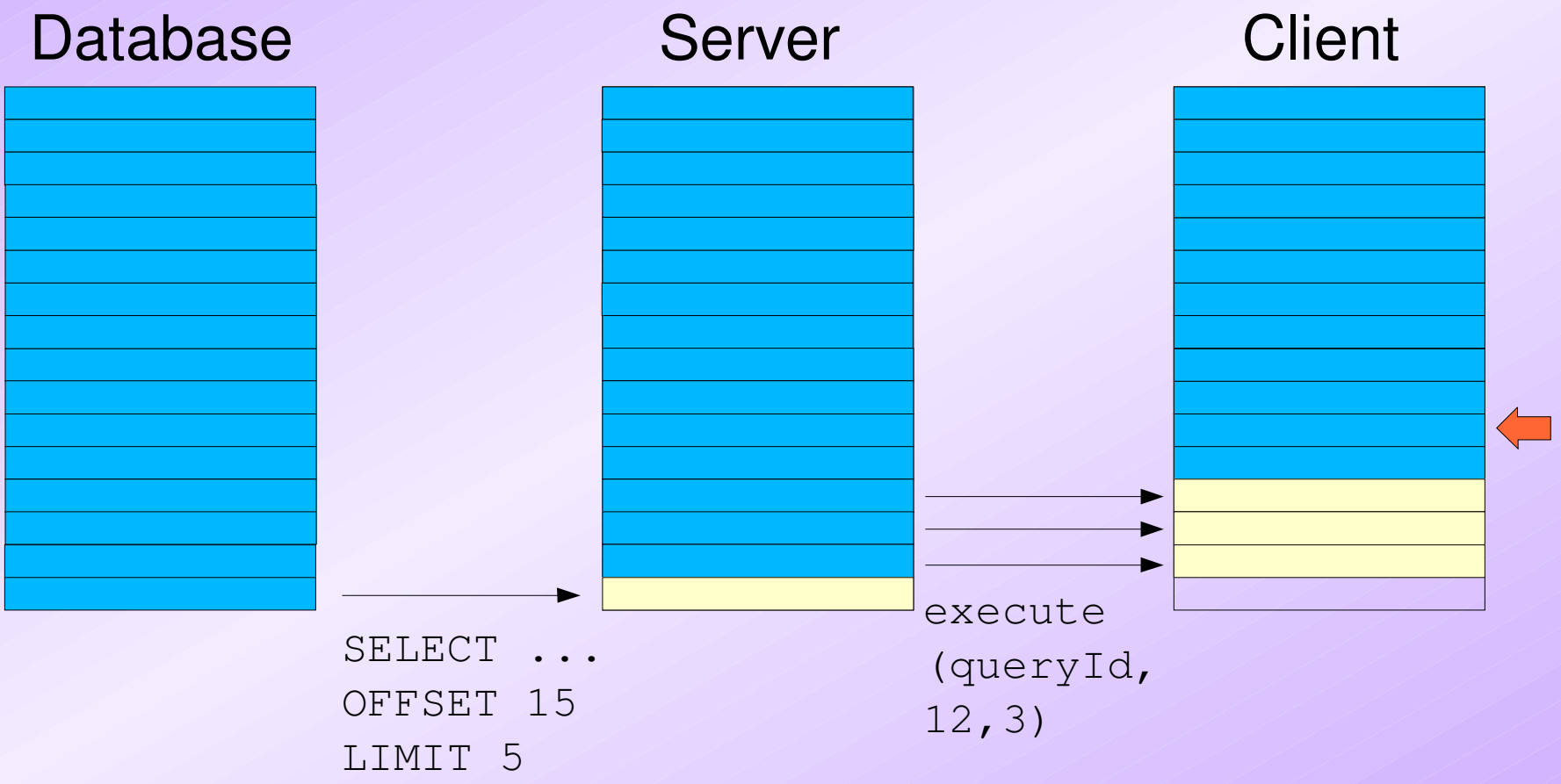
Server



Client



# Results


Database
Server
Client
SELECT ...
OFFSET 15
LIMIT 5
execute
(queryId,
12,3)

# Arbitrary queries – problems

- Badly formed queries may overload database server
- Difficult to optimise database for all queries
  - Which indexes to use?
  - Slow response to complex queries involving multi-table joins

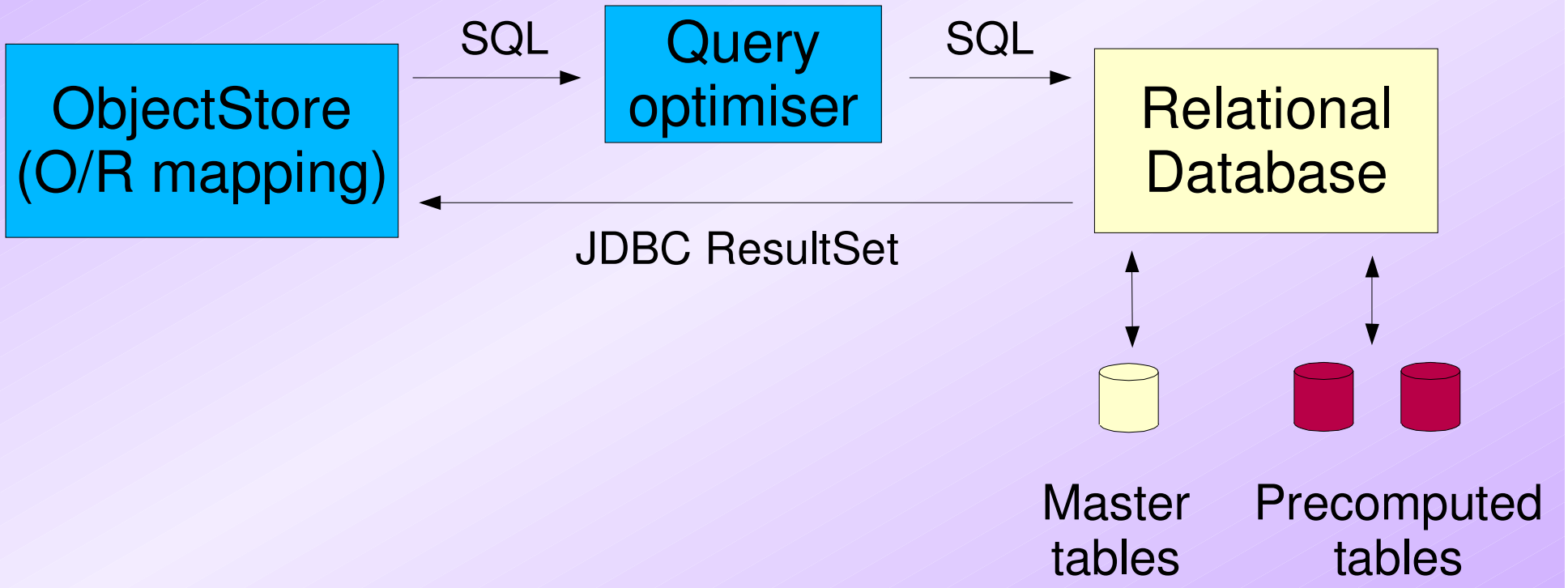
# Arbitrary queries – solutions

- Close relationship with database server query planner
  - ask how long a query will take before attempting to run it (~3ms)
  - Disallow queries that will take longer than a certain threshold
- Store data massively redundantly in “precomputed tables” and rewrite incoming queries on-the-fly.

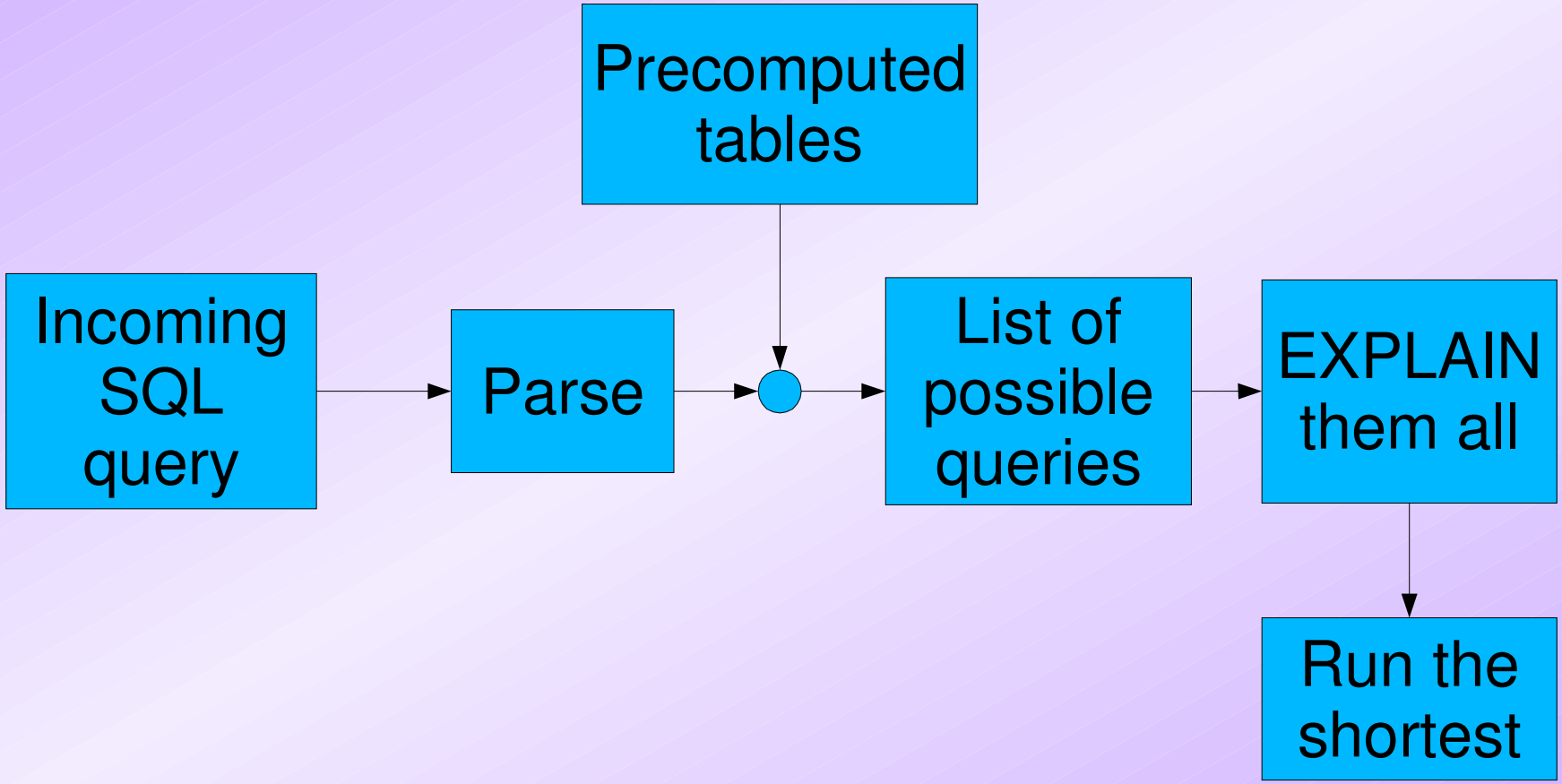
# Query optimisation – aims

- Provide a generic way of speeding up complex queries to any read-only SQL database
- Minimal parsing/computational overhead
- Transparent to users/applications
  - no new schema/model to learn
- Make available as standalone module

# Query optimisation architecture




# Query optimisation




# Query optimisation – example

## Master tables

Genes

| id | name |
|---|---|
| | |

GOTerms

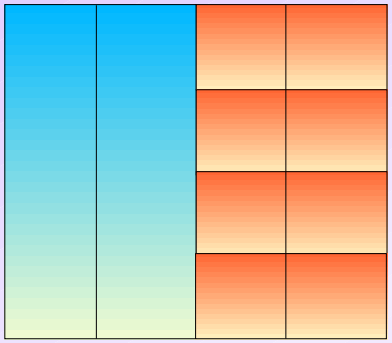
| geneid | code |
|---|---|
| | |

Experiments

| geneid | date | type |
|---|---|---|
| | | |

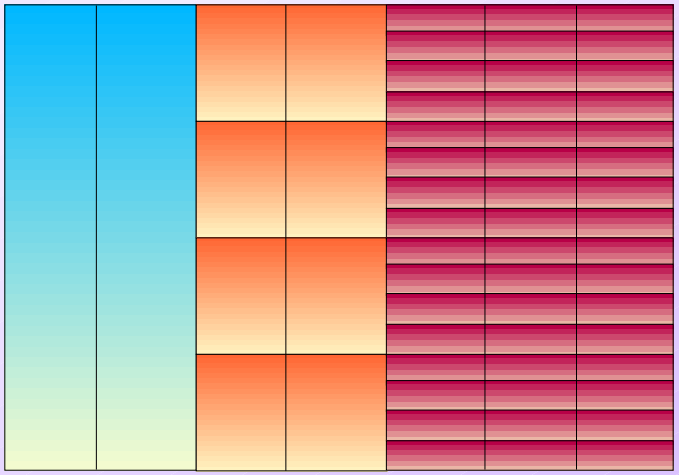
## Precomputed tables

GenesGOTerms



```
CREATE TABLE genesgoterms AS
SELECT genes.id AS genes_id,
       genes.name AS genes_name,
       goterms.geneid AS goterms_geneid,
       goterms.code AS goterms_code
FROM genes, goterms
WHERE genes.id = goterms.geneid
```

GenesGOTermsExperiments



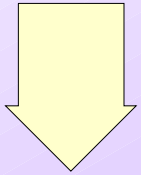
```
CREATE TABLE ....
SELECT ....
FROM genes, goterms, experiments
WHERE genes.id = goterms.geneid
AND genes.id = experiments.geneid
```

FlyMine

# Query optimisation – example

*"Show dates that gene expression experiments were performed on genes which have GO term GO:0000278 applied"*

```
SELECT genes.name, experiments.date
FROM genes, goterms, experiments
WHERE genes.id = goterms.geneid
AND genes.id = experiments.geneid
AND goterms.code = "GO:0000278"
AND experiments.type = "Gene Expression"
```

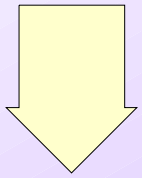


EXPLAIN

5 seconds

# Query optimisation – example

```
SELECT genes_name AS name,
       experiments.date
FROM genesgoterms, experiments
WHERE genes_id = experiments.geneid
AND goterms_code = "GO:0000278"
AND experiments.type = "Gene Expression"
```

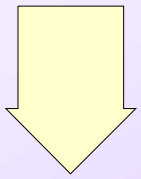


EXPLAIN

1 second

# Query optimisation – example

```
SELECT genes_name AS name,
       experiments_date AS date
FROM genesgotermsexperiments
WHERE goterms_code = "GO:0000278"
AND experiments_type = "Gene Expression"
```



EXPLAIN

200ms

# Query optimisation – example

- Without optimiser

  Time = 3ms + 5 seconds

  (EXPLAIN) (EXECUTE)

- With optimiser

  Time = 9ms + 100ms + 200ms

  (3 EXPLAINs) (PARSE) (EXECUTE)

# Query optimisation – summary

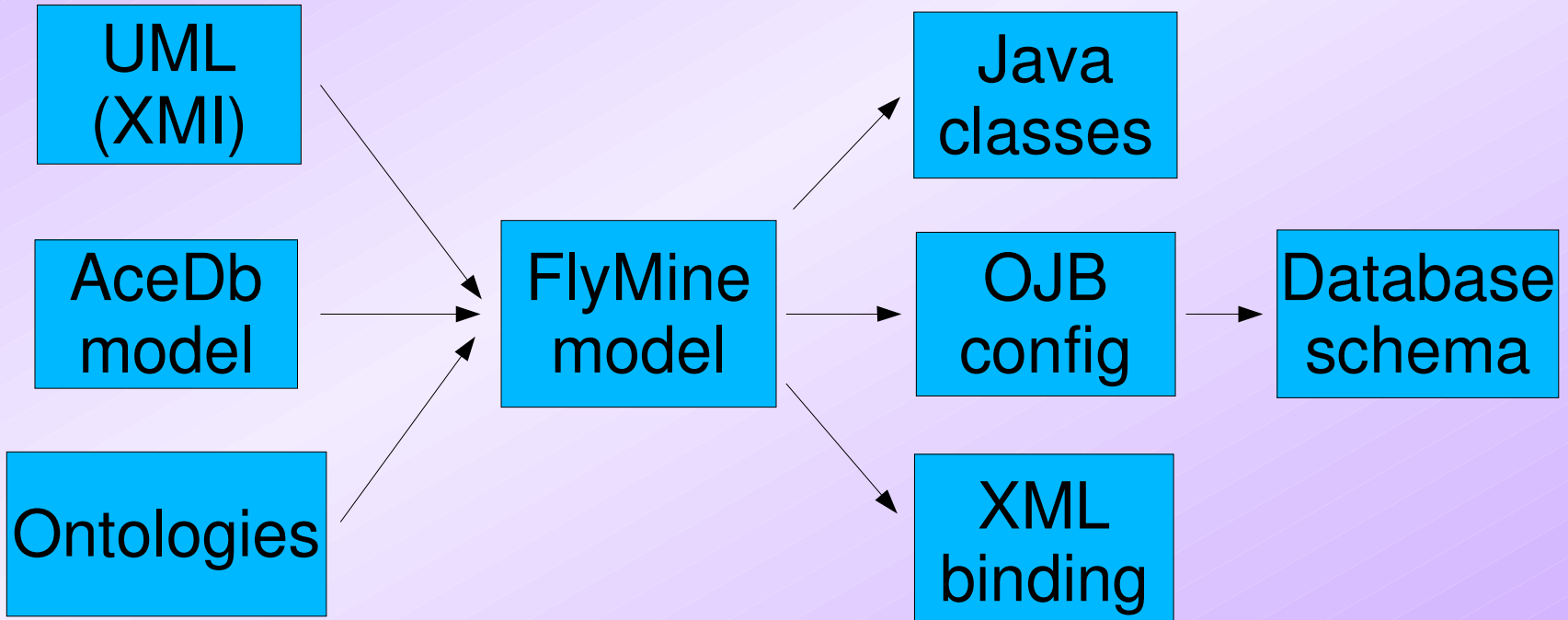
- For complex queries, the SQL optimisation module can produce large speed increases
- Optimisation is transparent to the user or application generating the SQL.
- Choosing which precomputed tables to store is important – may need to analyse incoming queries.

# Query optimiser – summary

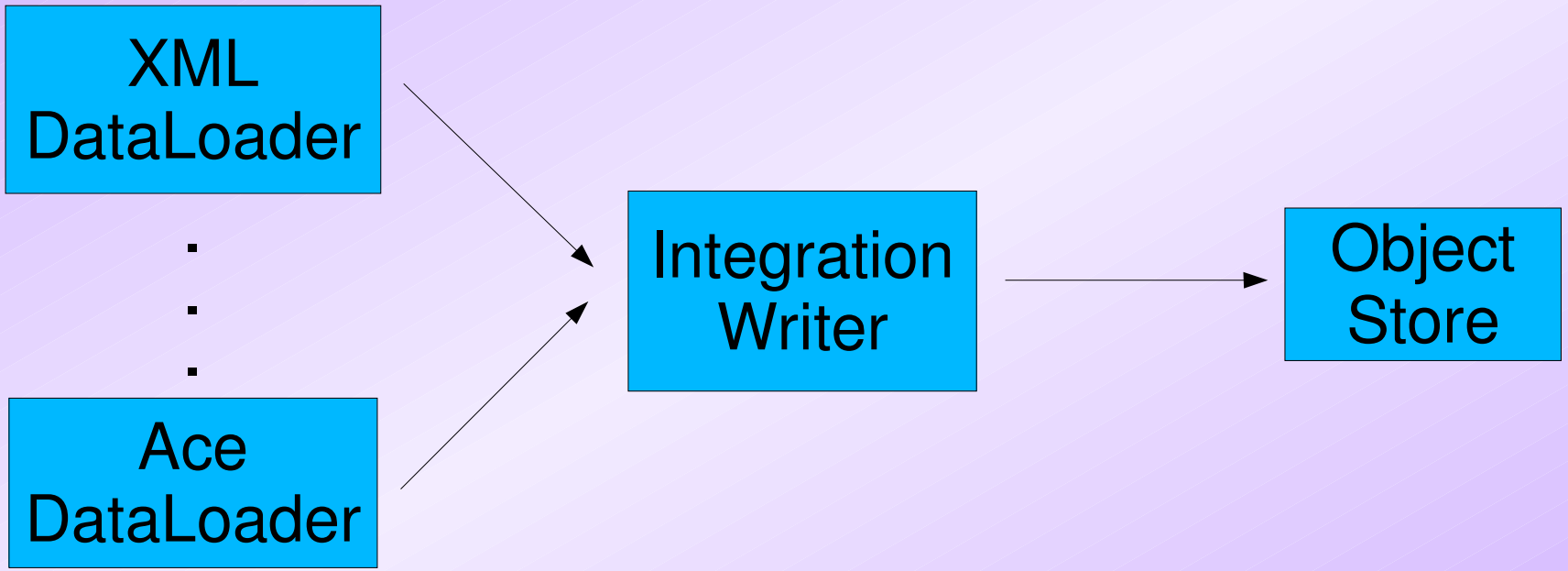
- Optimiser trades off disk space for improved query performance.
- Schema independent.
- Can be used in conjunction with P6Spy to intercept JDBC calls from existing software to a database.
- Available from www.flymine.org !!

# Data model

- Data model can be generated from one of a number of sources




# Data loading and integration




# Summary

- Current status
  - generic SQL query optimiser
  - powerful object database
  - 2 query interfaces (OQL + Java)
  - web service
  - framework for data loading/integration
  - autogeneration of model-dependent parts from UML or Ace model

# Summary

- Coming up
  - graphical query interface
  - web front end
  - integrated Drosophila/Anopheles database (genomics, microarray, proteomics, etc)
  - tools for auto-generation of best set of precomputed tables

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Gos Micklem

Download FlyMine from www.flymine.org


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