InterMine

Object integration and warehousing software

FlyMine

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

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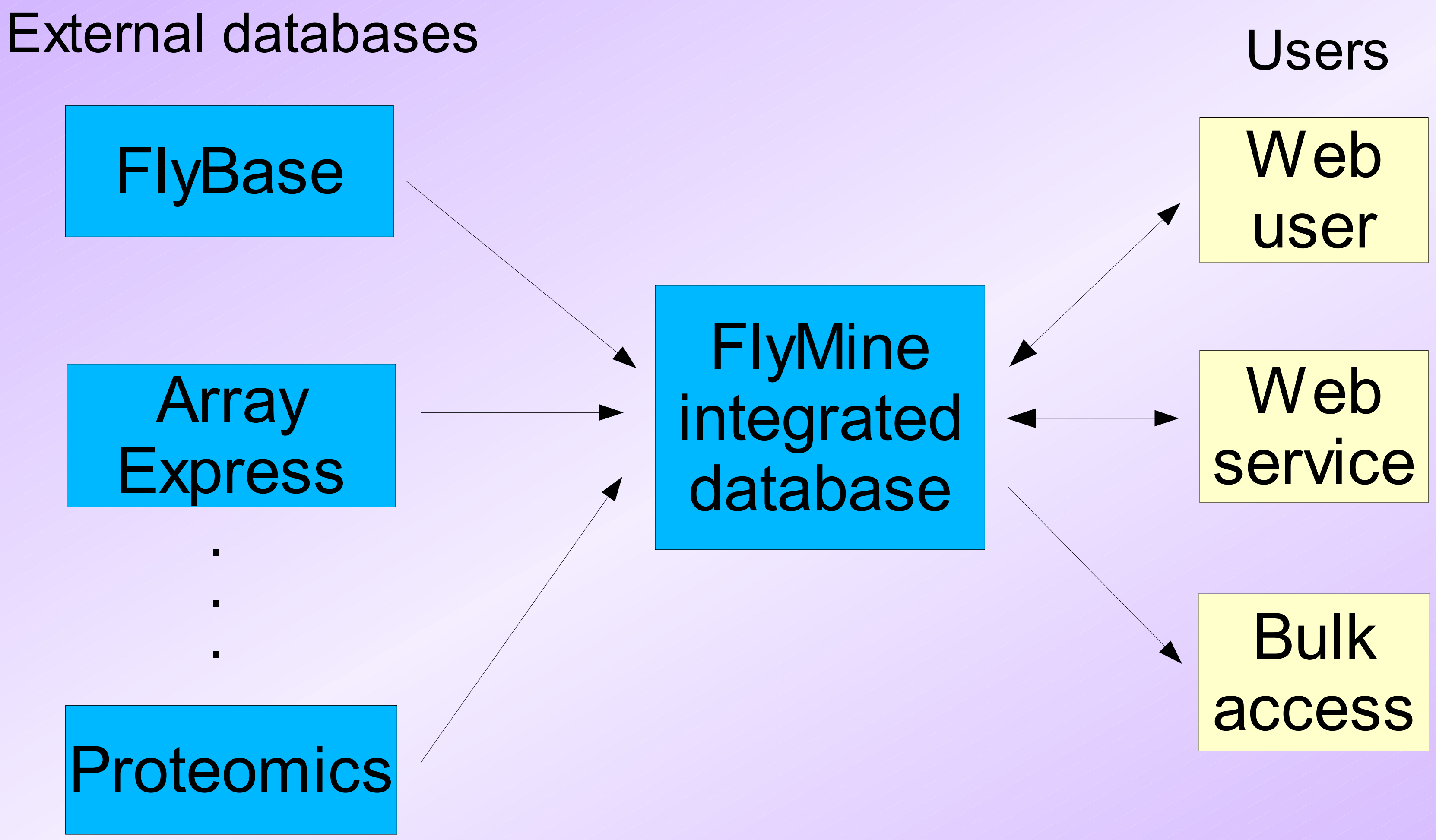
Why yet another database?

- 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

Outline


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

InterMine - aims

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

Query interfaces – OQL

“Show gene expression data for genes which have GO term GO:0000278 applied”

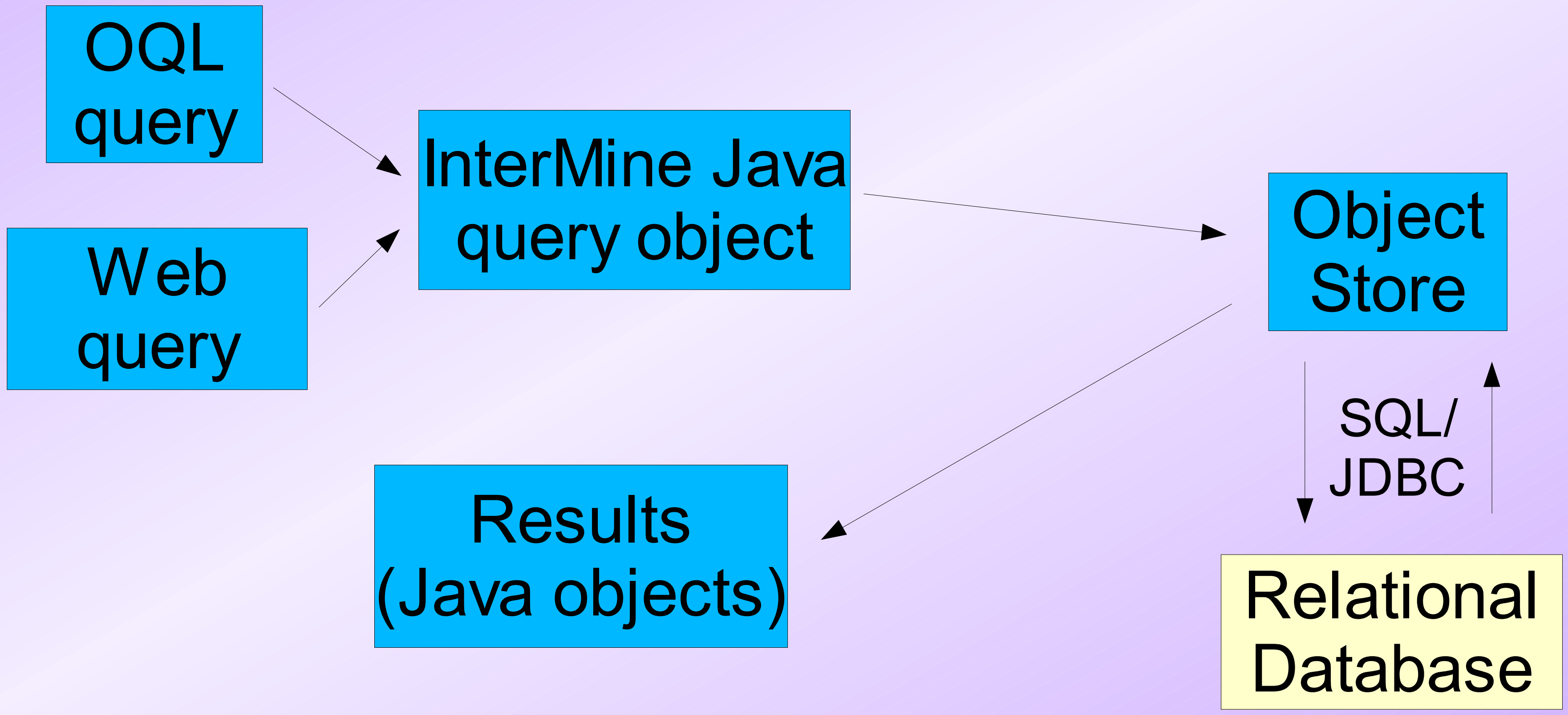
```
SELECT gene, exp
FROM Gene AS gene, GOTerm AS term,
     Experiment AS exp
WHERE gene.GOTerms CONTAINS term
AND term.code = “GO:0000278”
AND gene.experiments CONTAINS exp
AND exp.type = “Gene Expression”
```

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);
```

InterMine ObjectStore

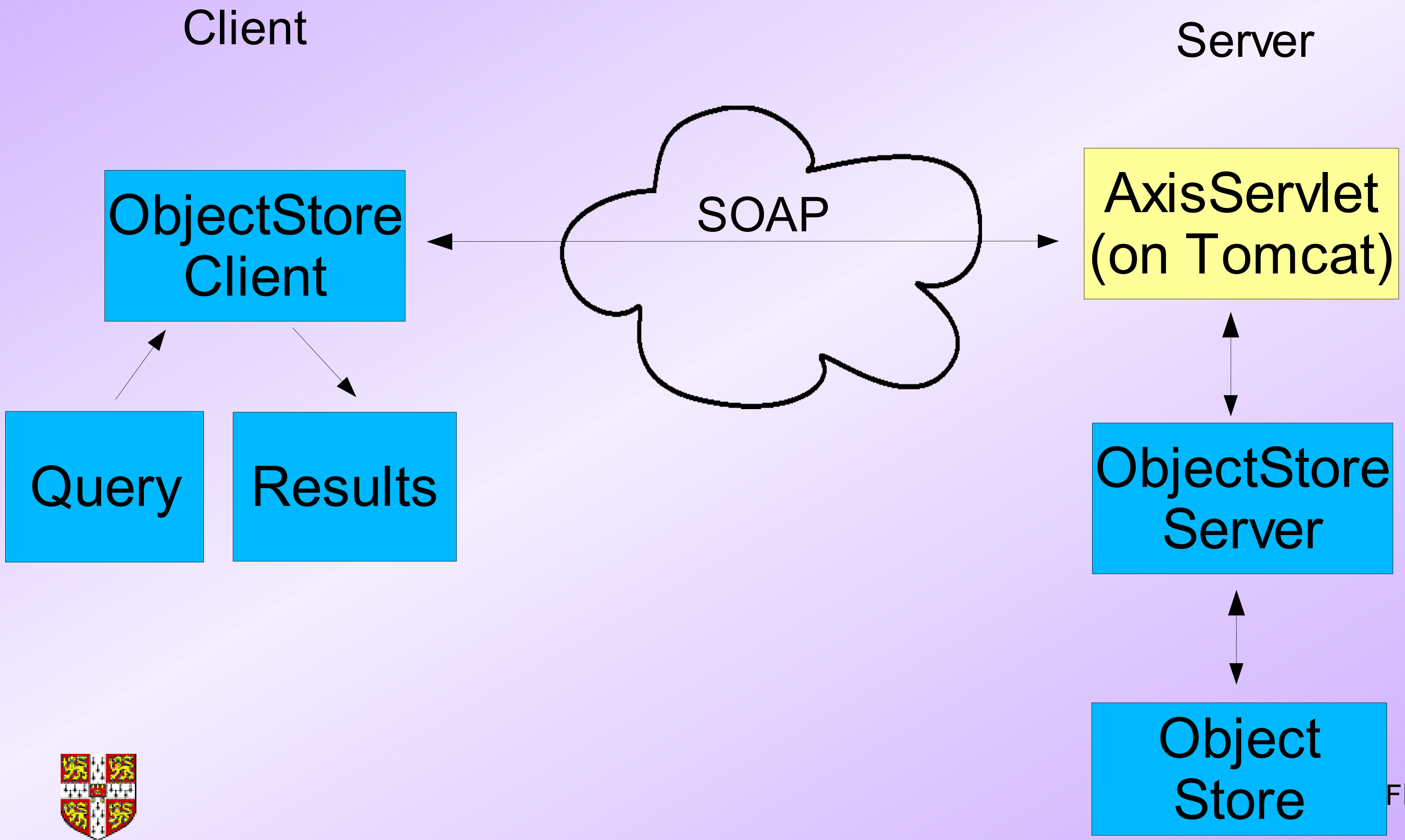


ObjectStore interface

```
public interface ObjectStore {

  Results execute(Query q);
  List execute(Query q, int start, int limit);
  int count(Query q);
  ResultsInfo estimate(Query q);
  Object getObjectById(Integer id);
  Model getModel();
}
```

Web service

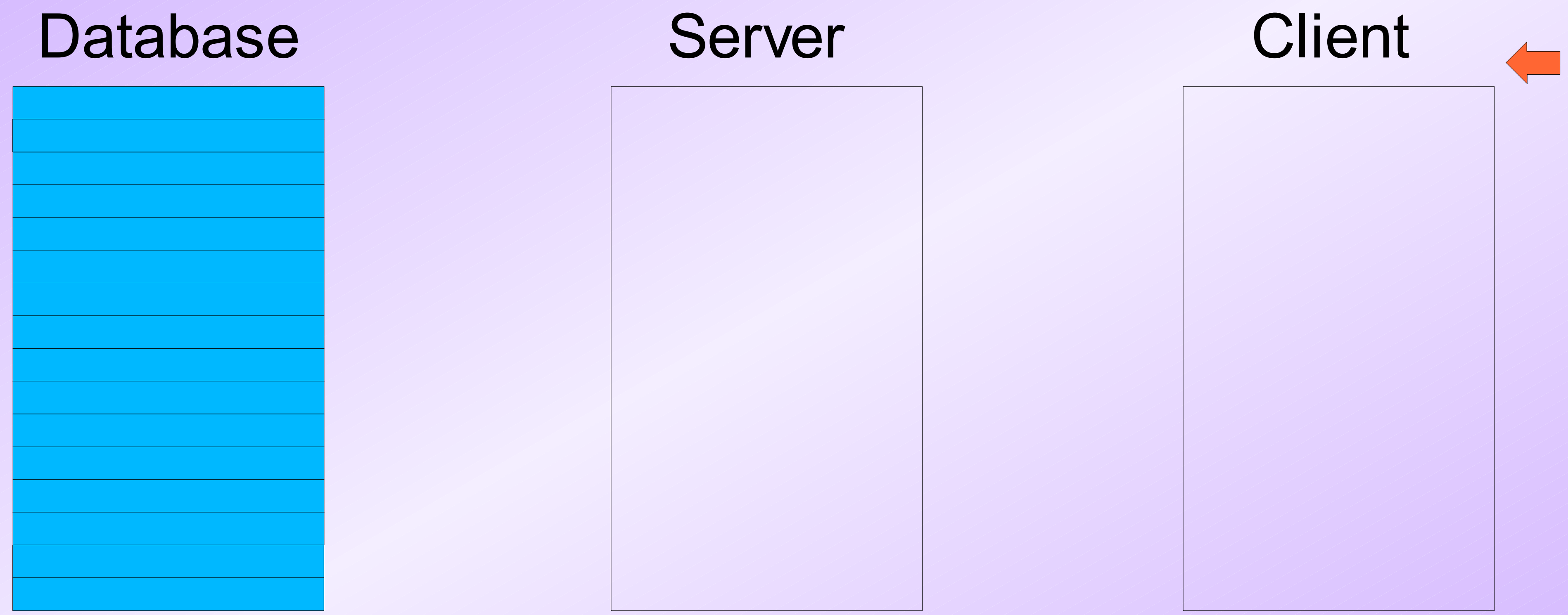


FlyMine

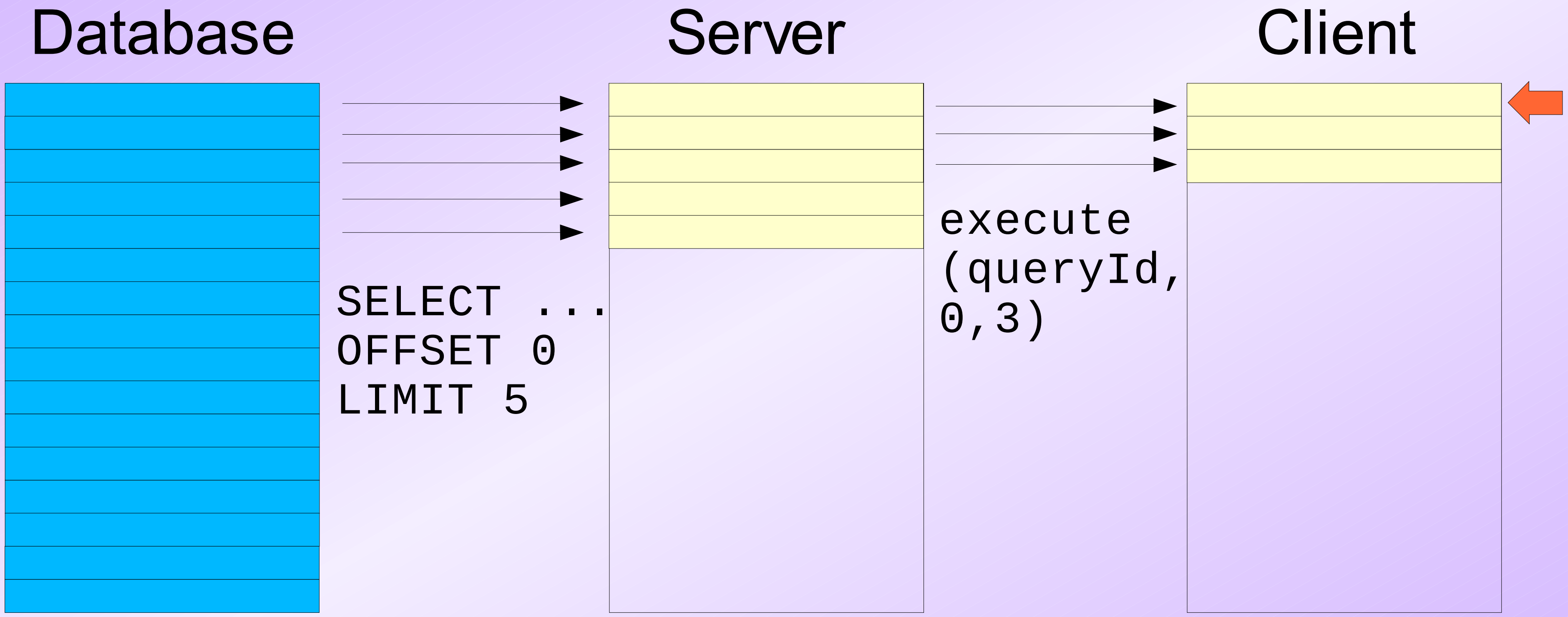
InterMine ObjectStore

- Results are tables of Java objects
  - All collections and references are proxied
- Results rows are fetched in batches from the underlying database server
- Results rows are pre-emptively fetched and cached (per JVM).

Results



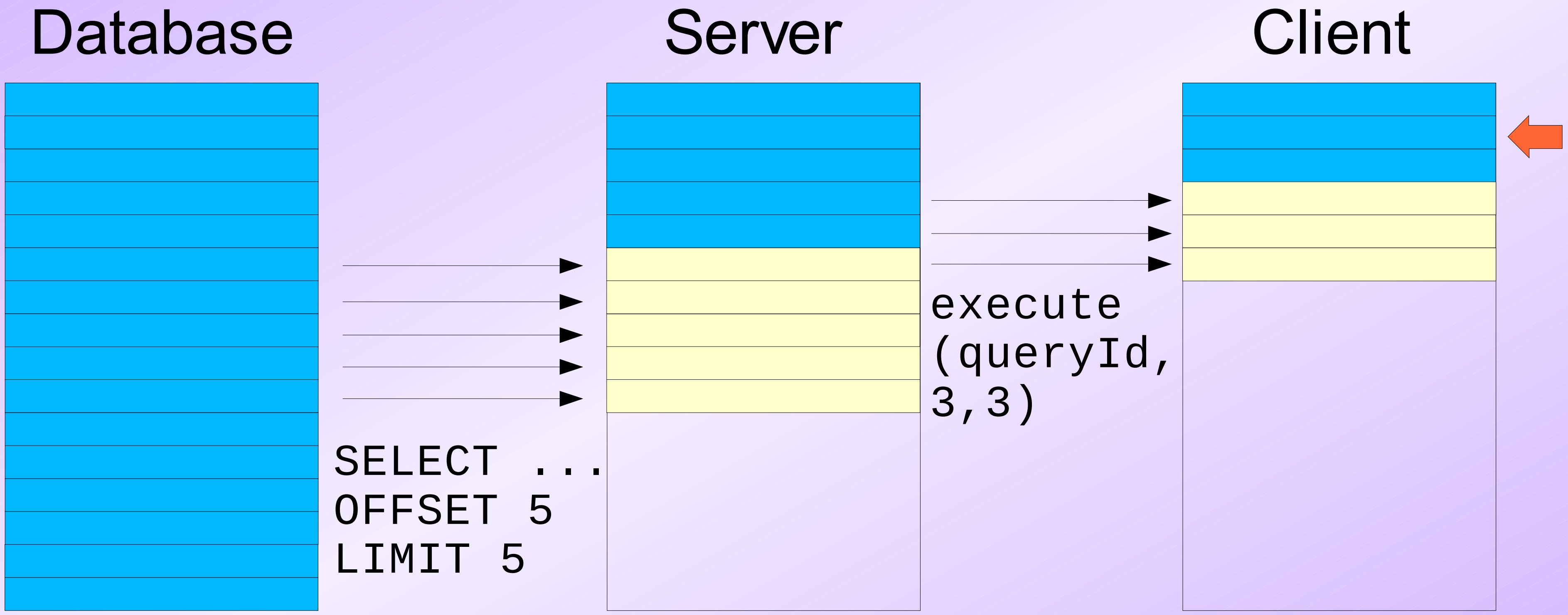
Results



```
SELECT ...
OFFSET 0
LIMIT 5
```

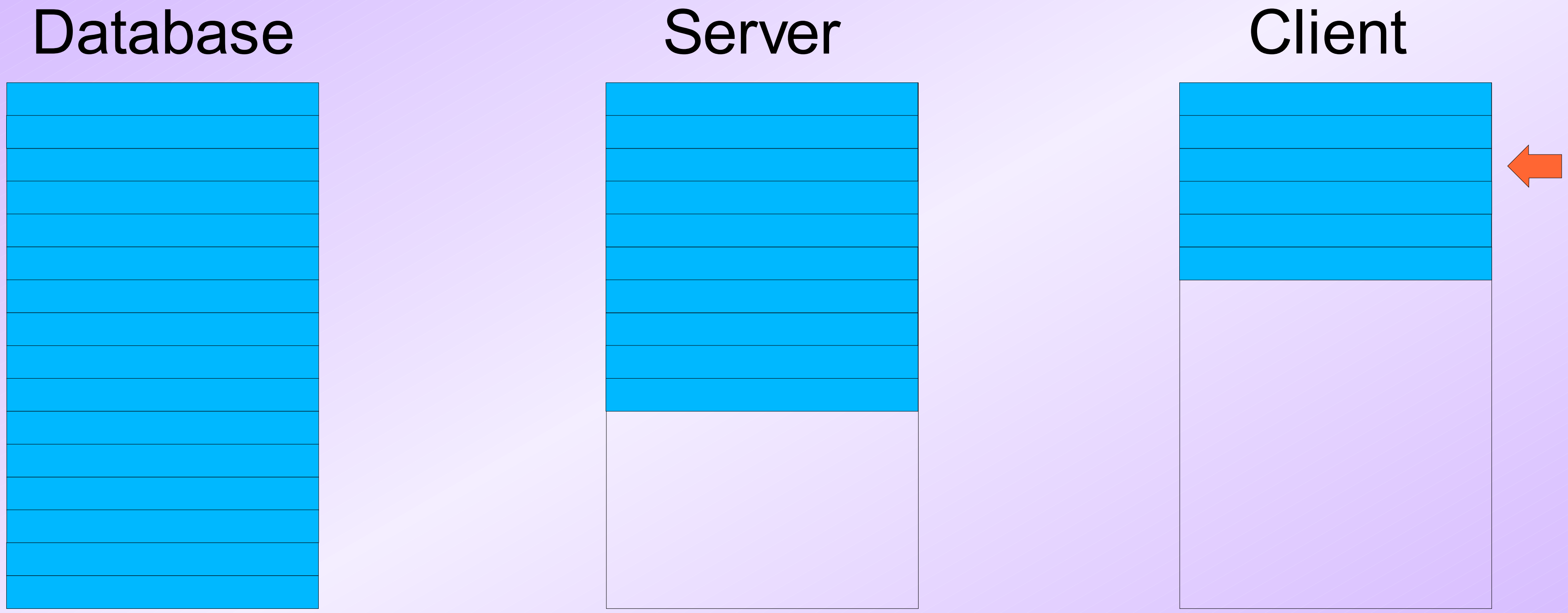
```
execute
(queryId,
0,3)
```

Results

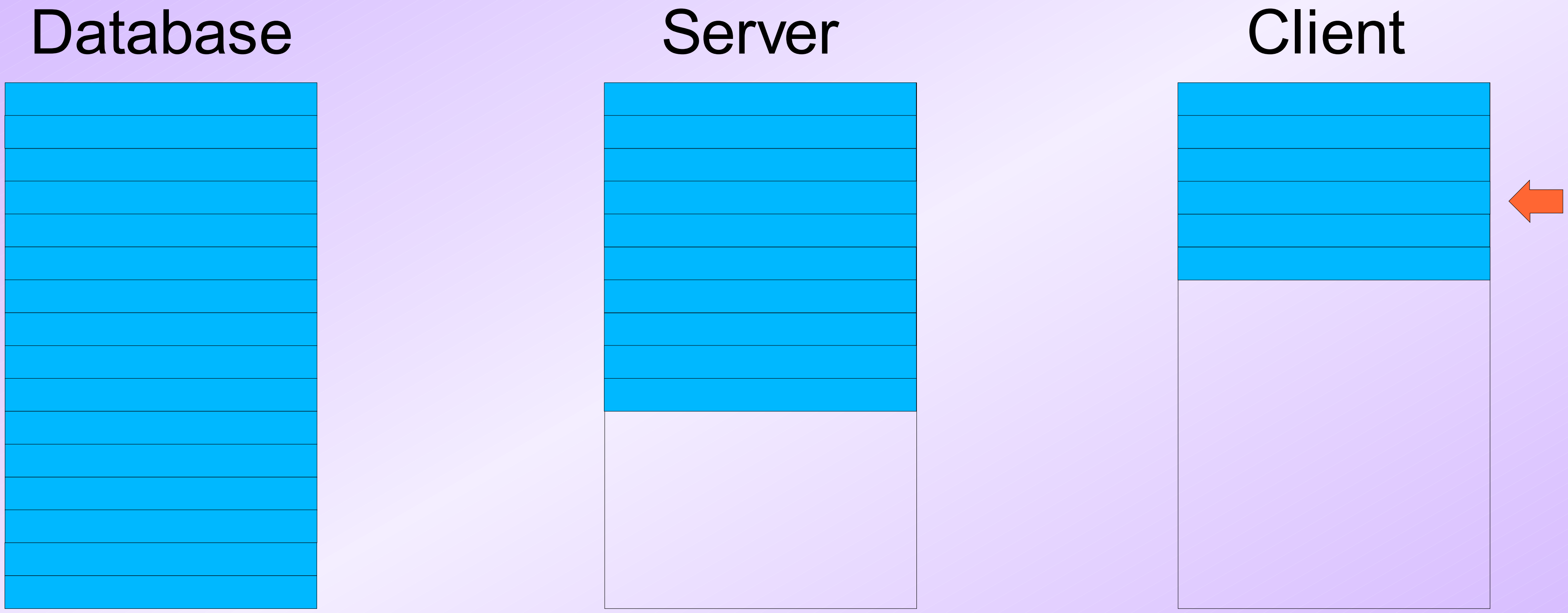


Database
Server
Client
SELECT ...
OFFSET 5
LIMIT 5
execute
(queryId,
3,3)

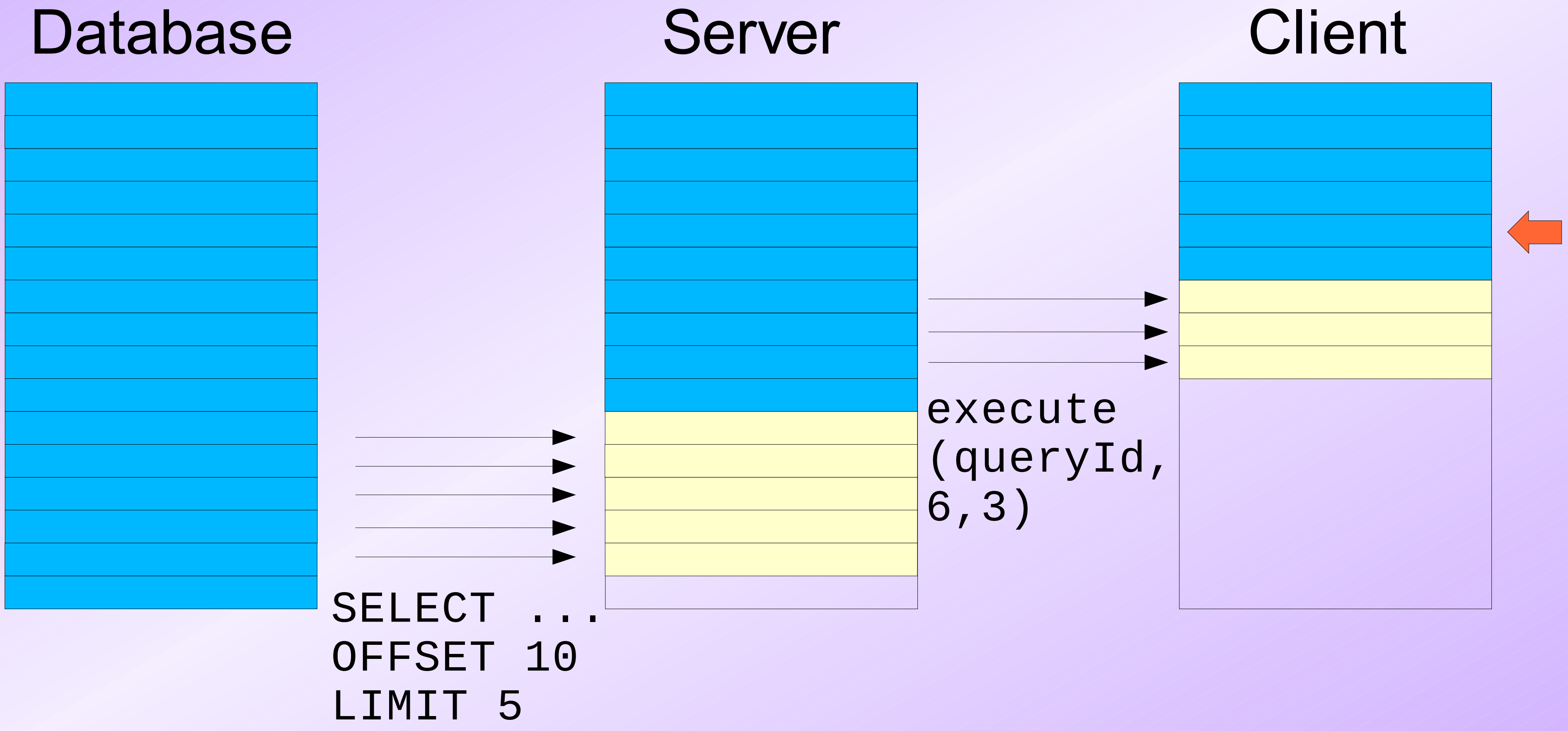
Results

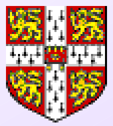


Results



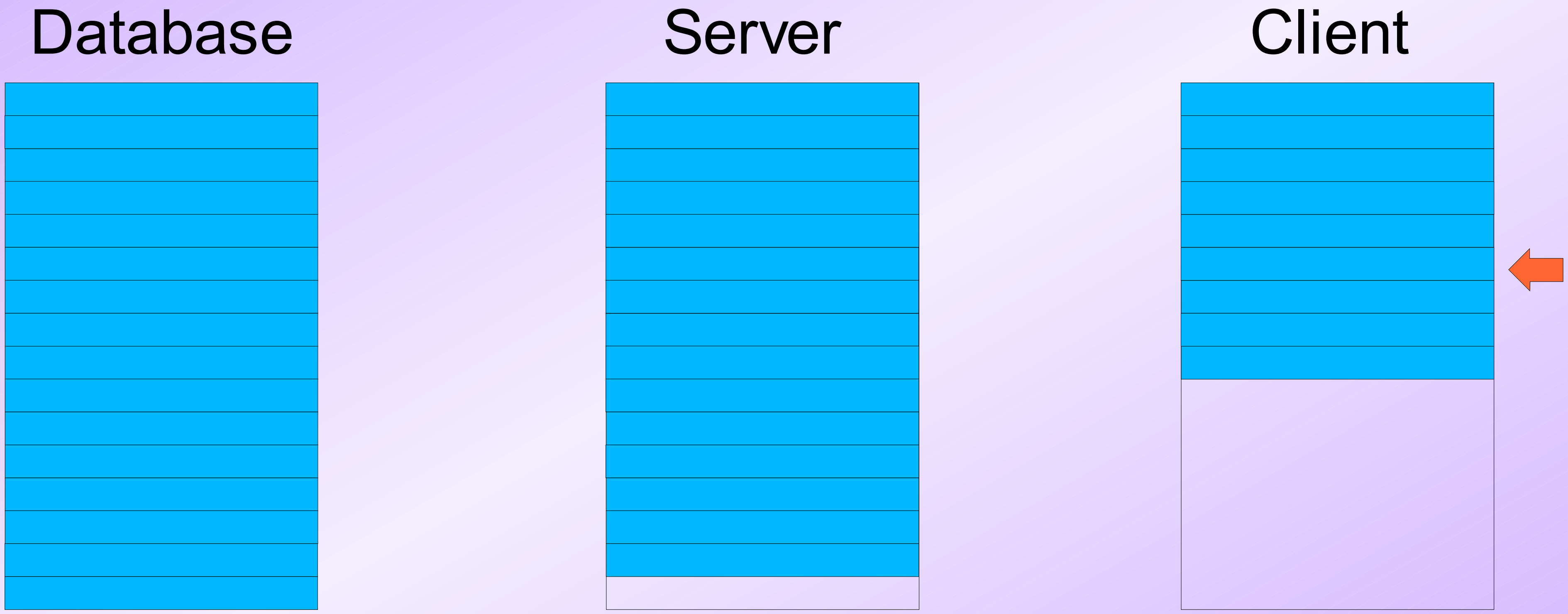
Results



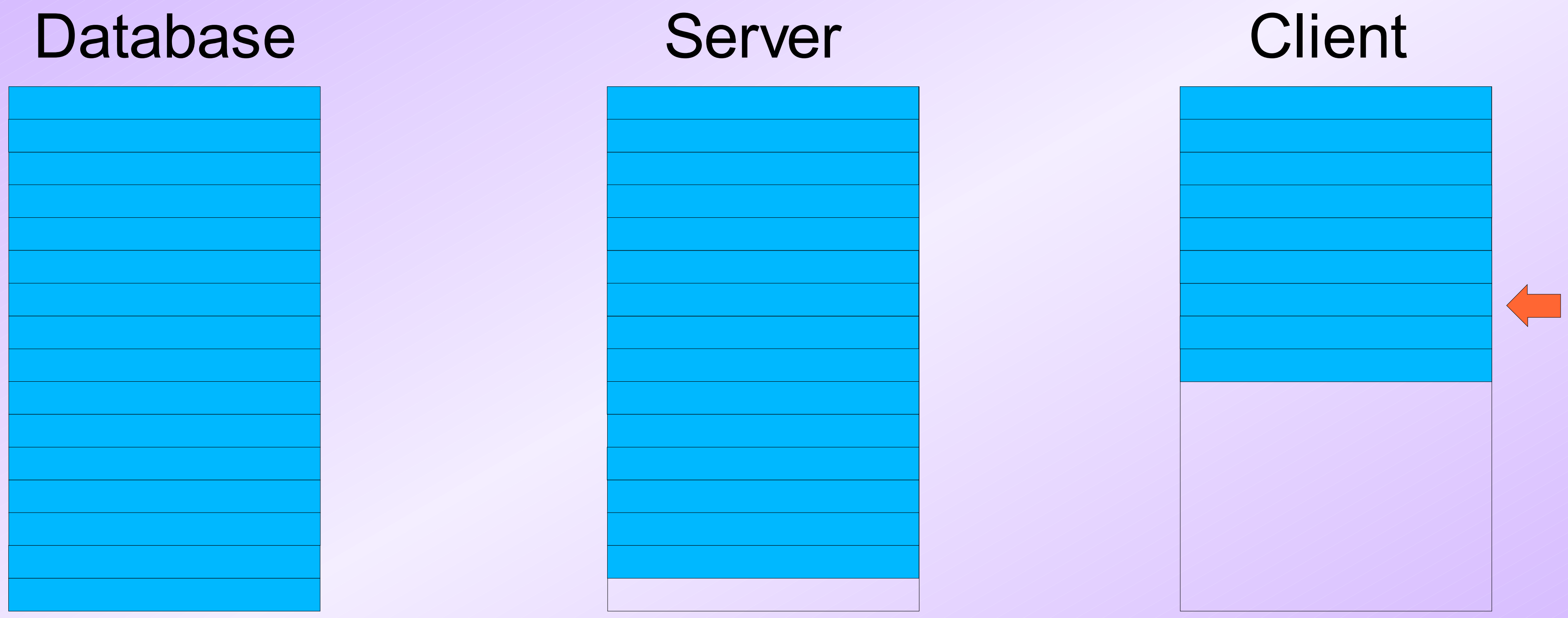


FlyMine

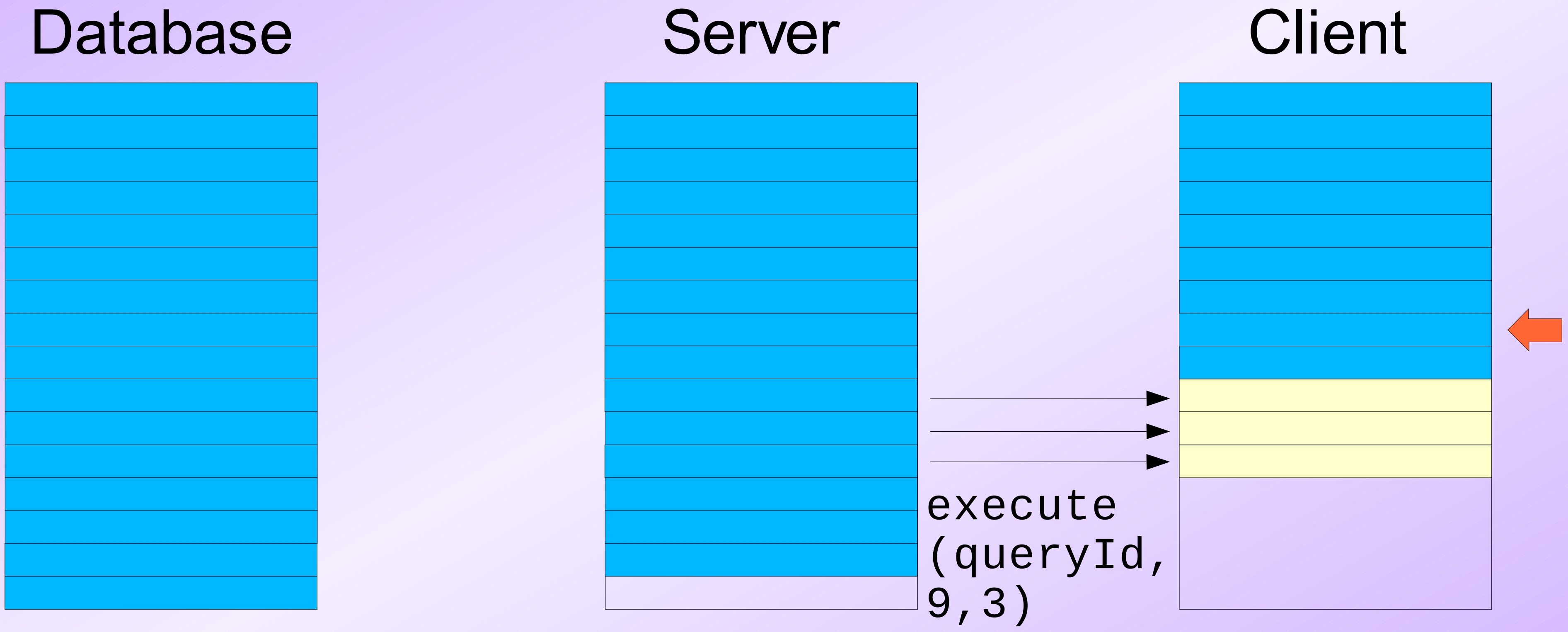
Results



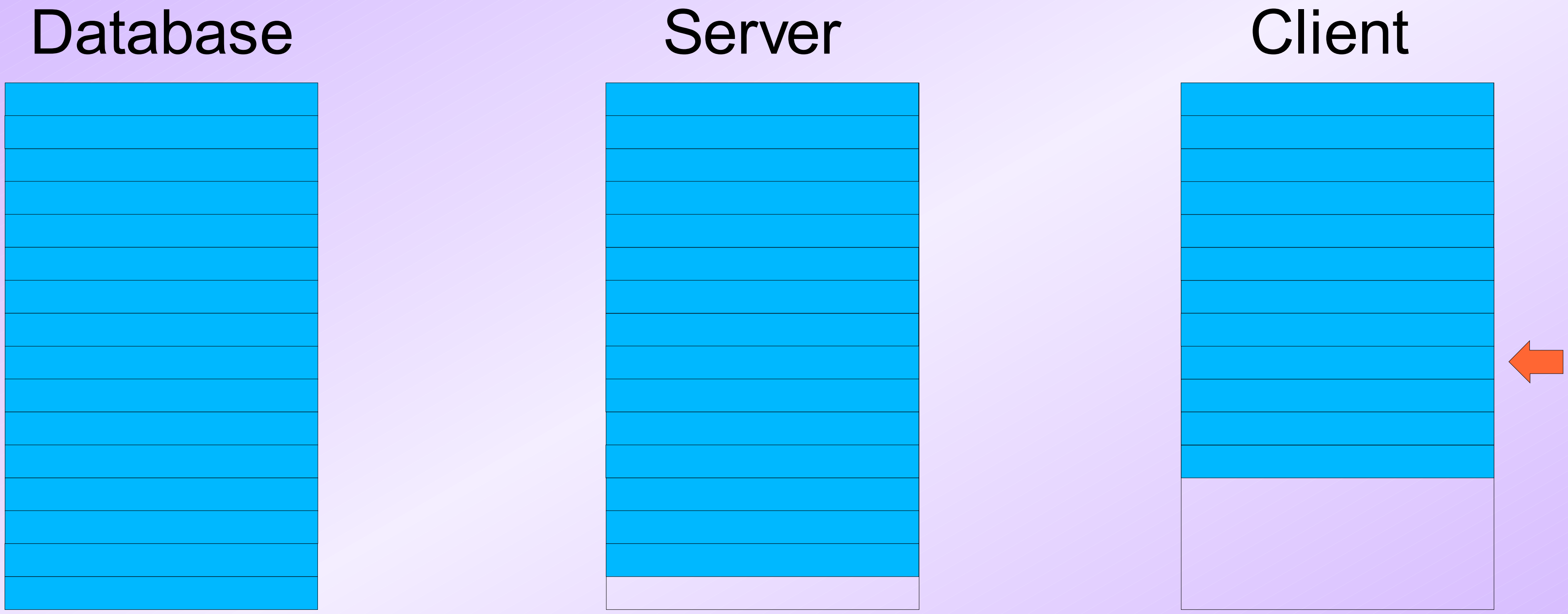
Results



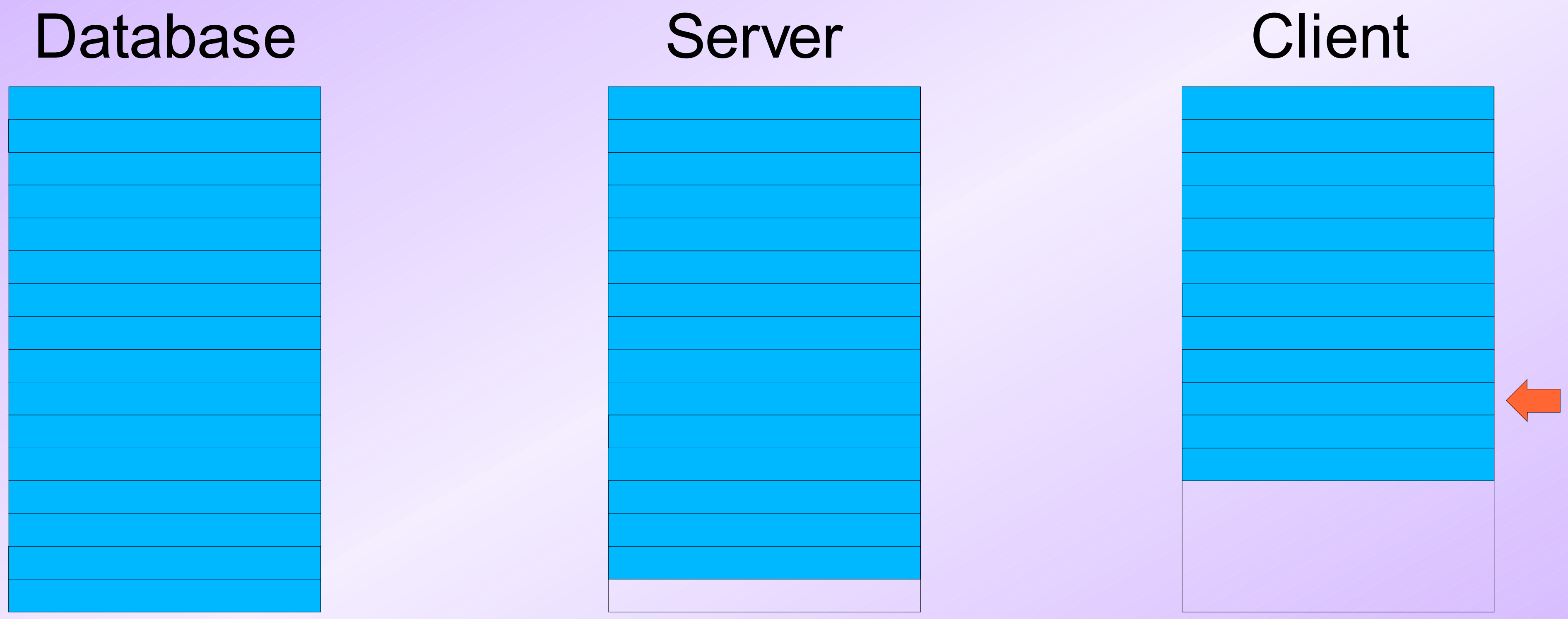
Results



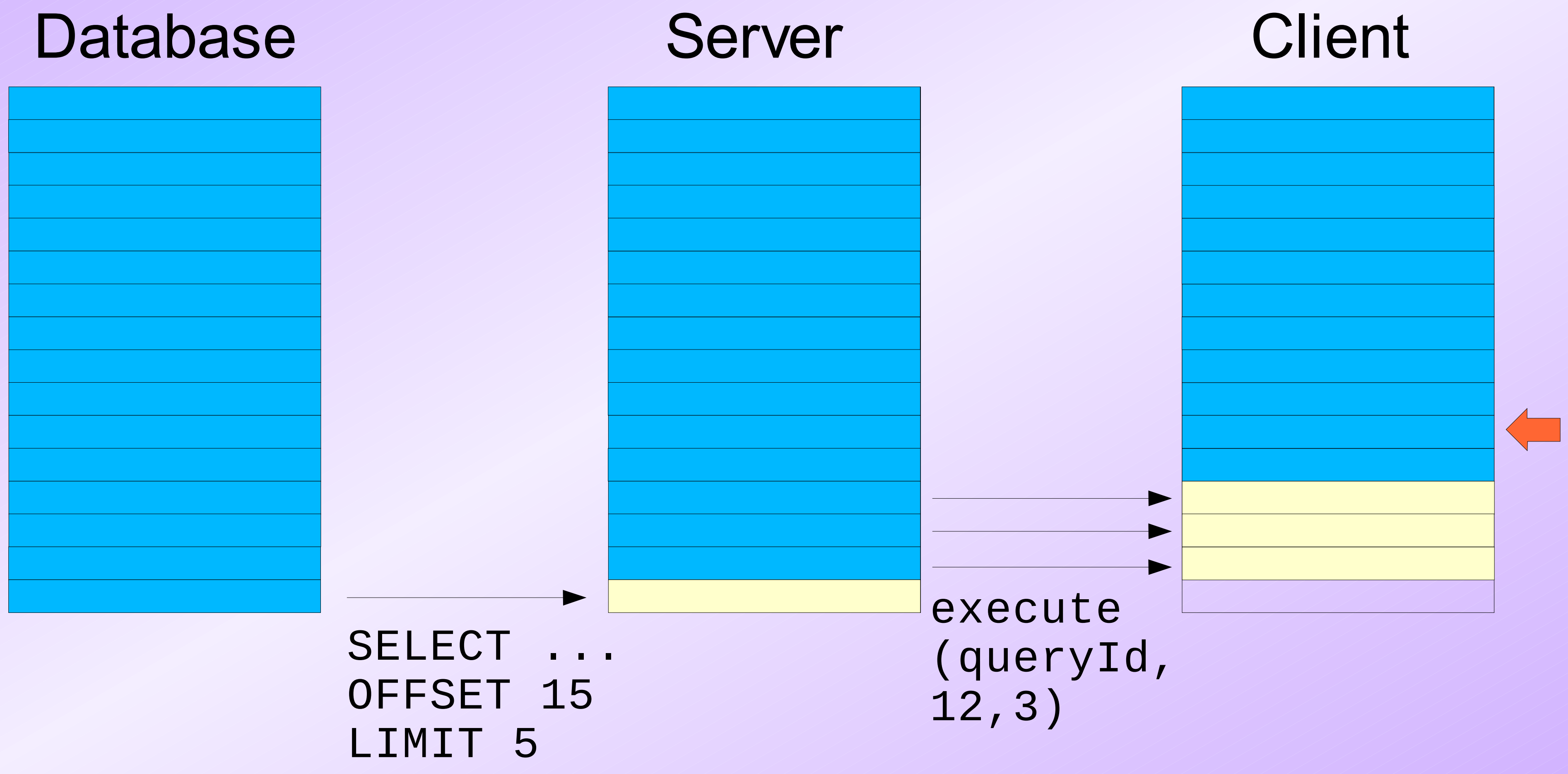
Results



Results



Results



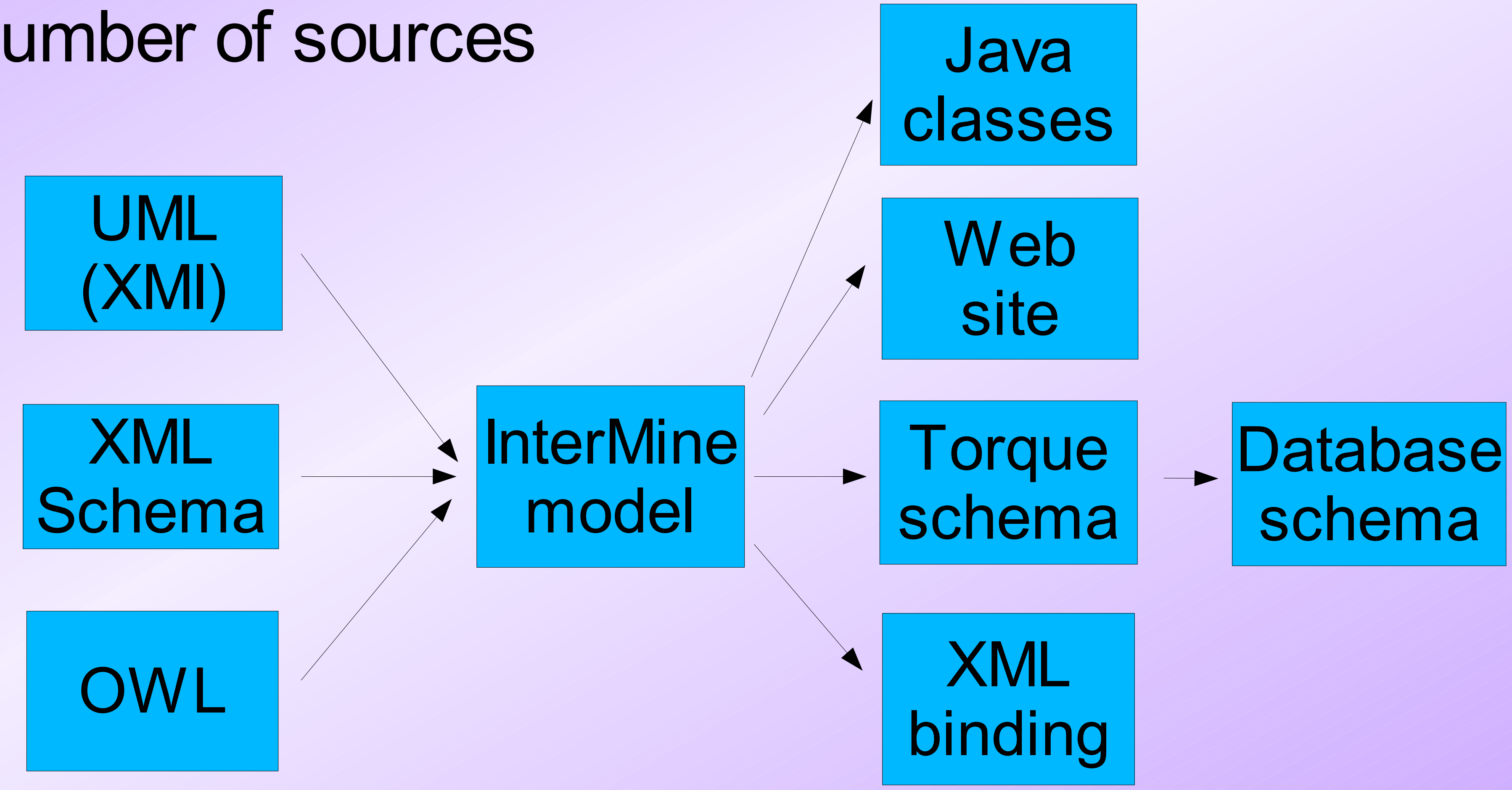
```
SELECT ...
OFFSET 15
LIMIT 5
```

```
execute
(queryId,
12,3)
```

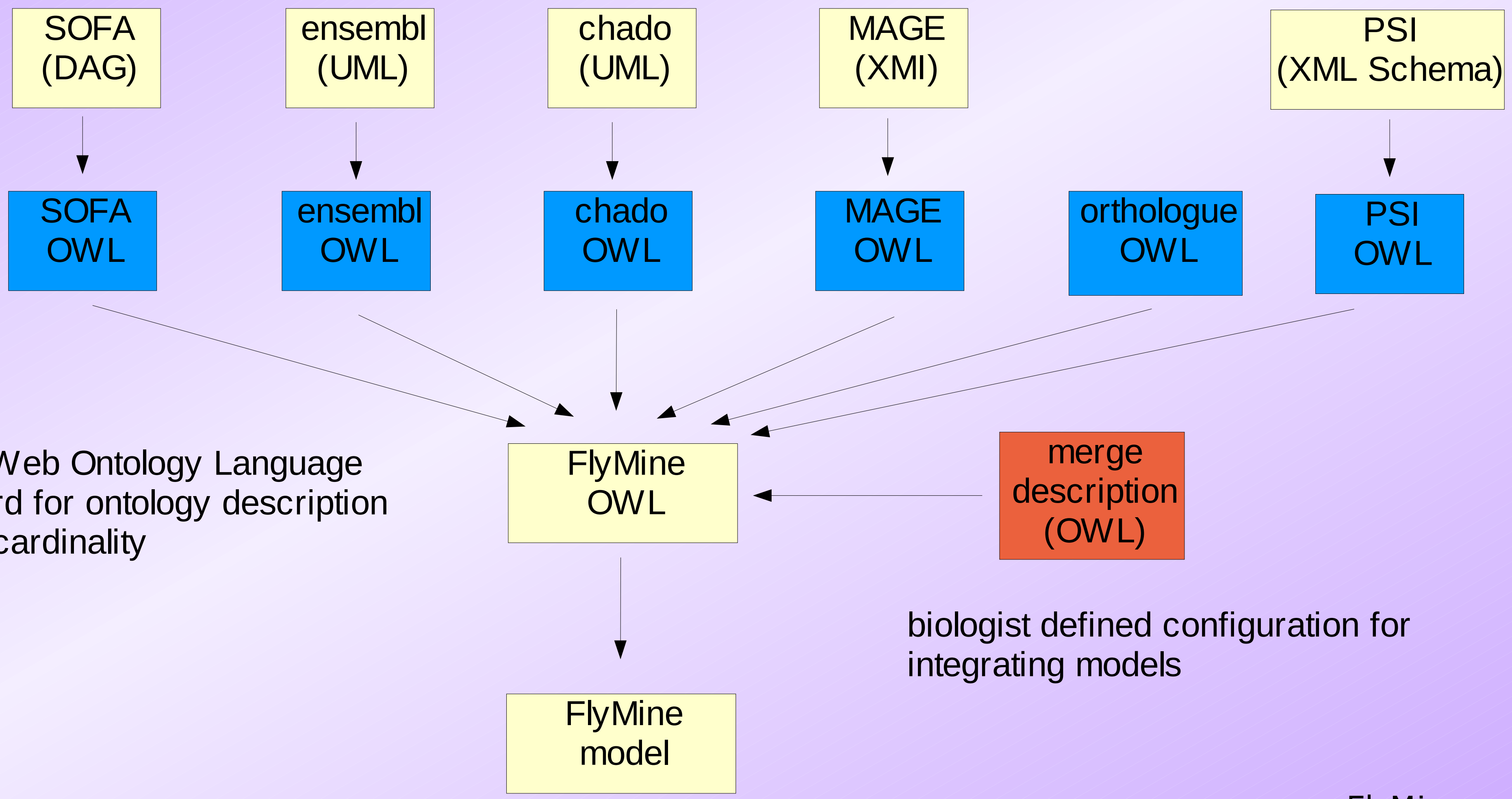
FlyMine

Data model

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



Model Integration



OWL – Web Ontology Language
- standard for ontology description
- allows cardinality

biologist defined configuration for integrating models

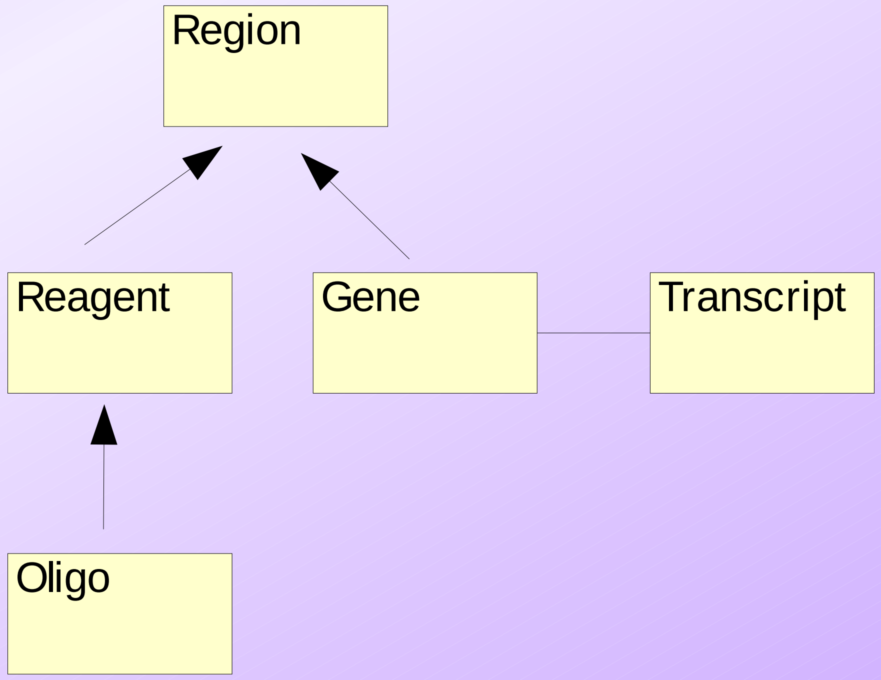
Integrate existing standards

- Link existing and emerging standards to define FlyMine model
  - e.g. SO, MAGE, PSI,GO, other ontologies
- Avoids creating a 'schema of everything'
- Easy to add new types of data
- Evolve as standards change

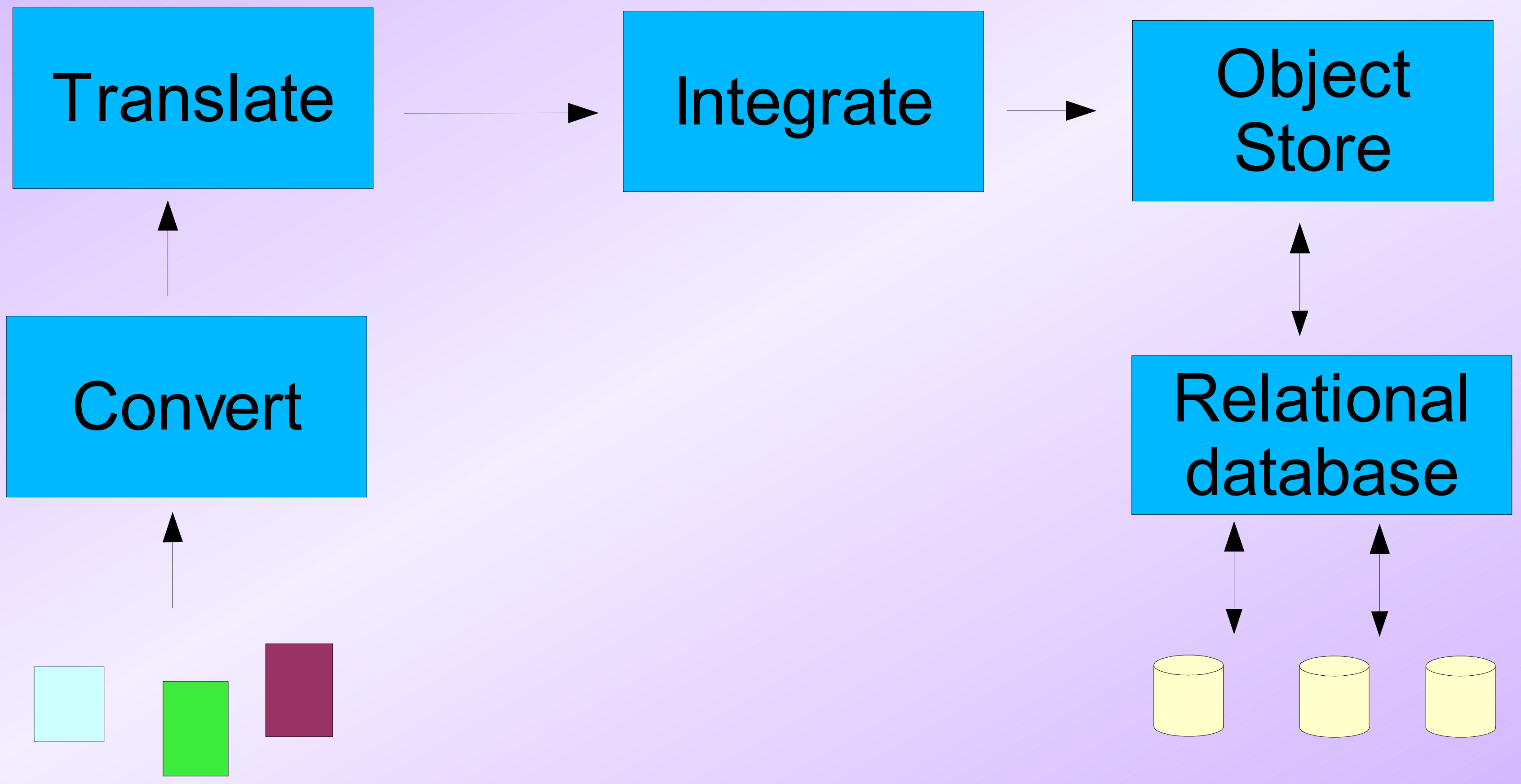
Example – Sequence Ontology

- All terms in ontology become classes in model

```
@is_a@region
   @is_a@gene
      @part_of@transcript
   @is_a@reagent
      @is_a@oligo
```

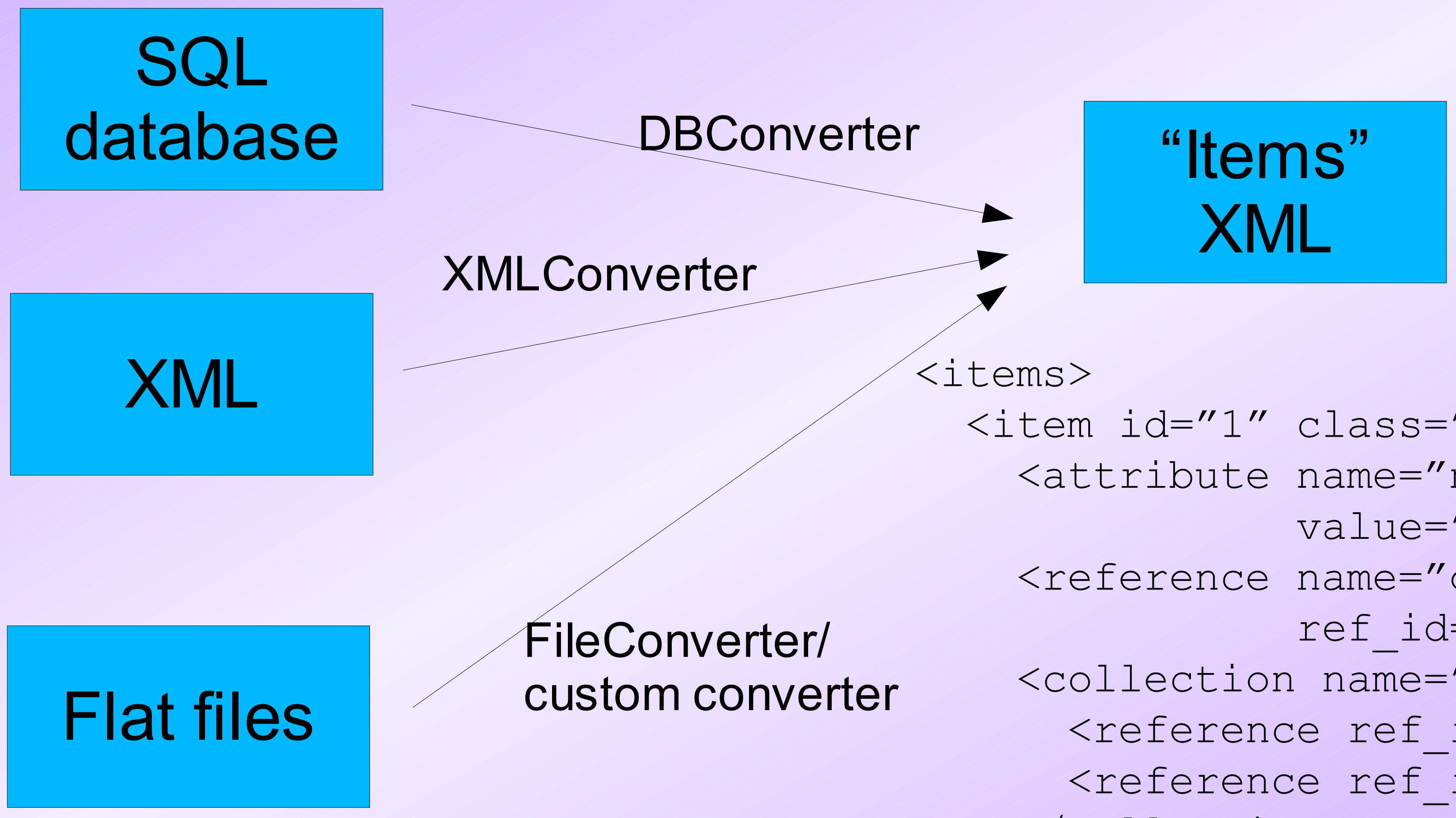


Data loading pipeline



External data sources

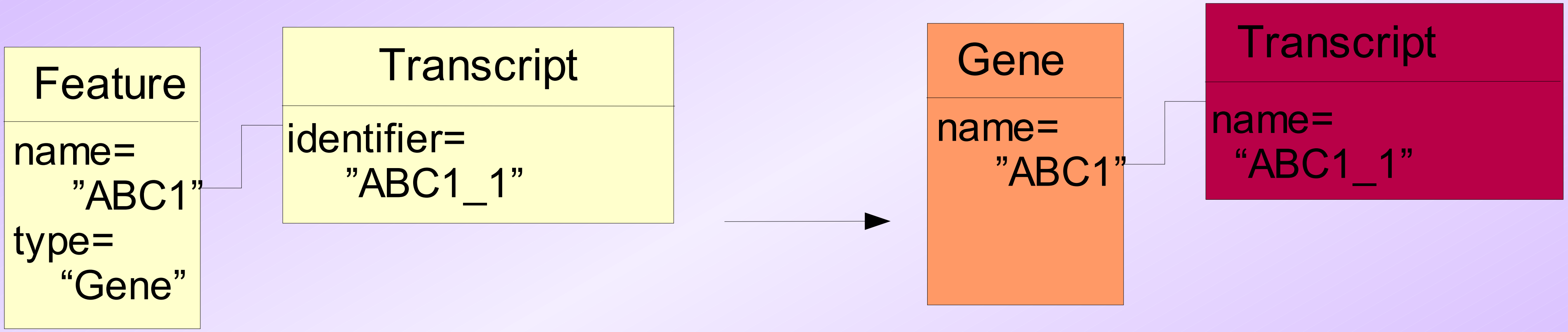
Conversion from external sources



```
<items>
  <item id="1" class="Feature">
    <attribute name="name"
               value="ABC1"/>
    <reference name="organism"
               ref_id="2"/>
    <collection name="synonyms">
      <reference ref_id="3"/>
      <reference ref_id="4"/>
    </collection>
  </item>
        .
        .
</items>
```

FlyMine

Translation



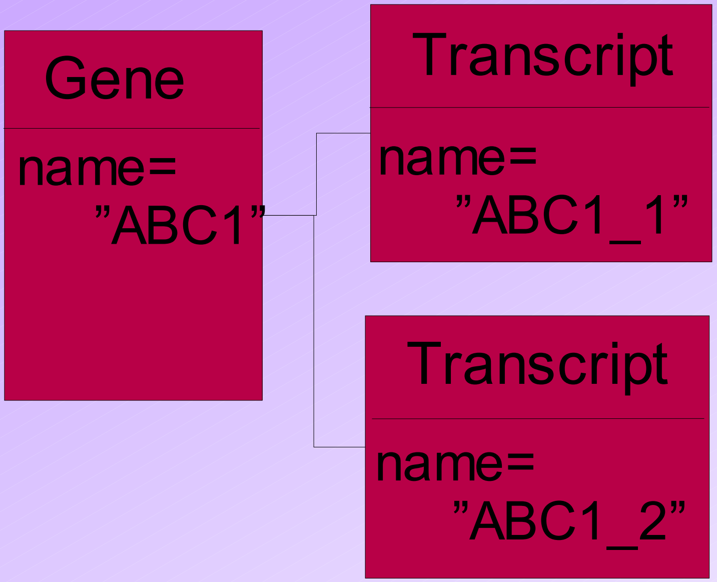
Translation

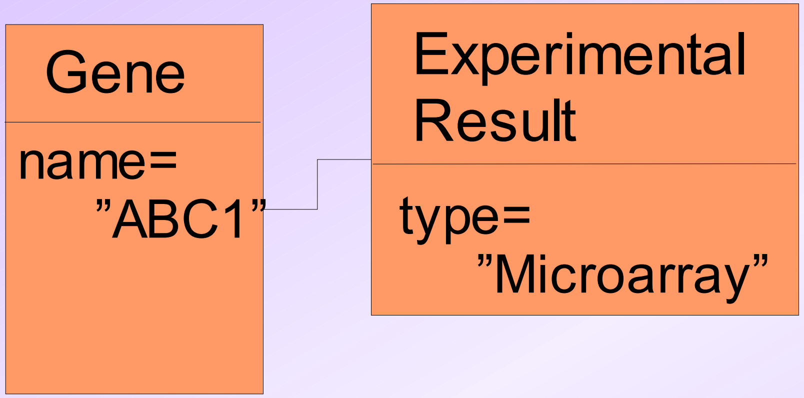
- Controlled by OWL “merge description”

```
:Gene a owl:Class;
  rdfs:subClassOf exampleSrc:Feature ;
  rdfs:subClassOf
    [ a owl:Restriction;
      owl:onProperty exampleSrc:Feature__type
      owl:hasValue “Gene”
     ] .
:Transcript a owl:Class;
  owl:equivalentClass exampleSrc:Transcript .
:Transcript__name a owl:DatatypeProperty;
  owl:equivalentProperty exampleSrc:Transcript__identifier
```

Integration

- Define “primary keys” for each object type
- Define “primary keys” that each source uses
- Define priorities for fields from different sources
- IntegrationWriter keeps track of originating sources for each field of each object



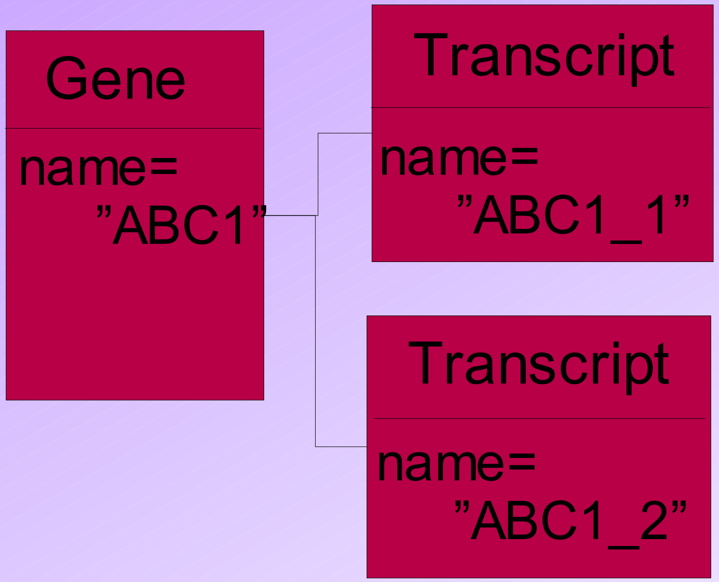


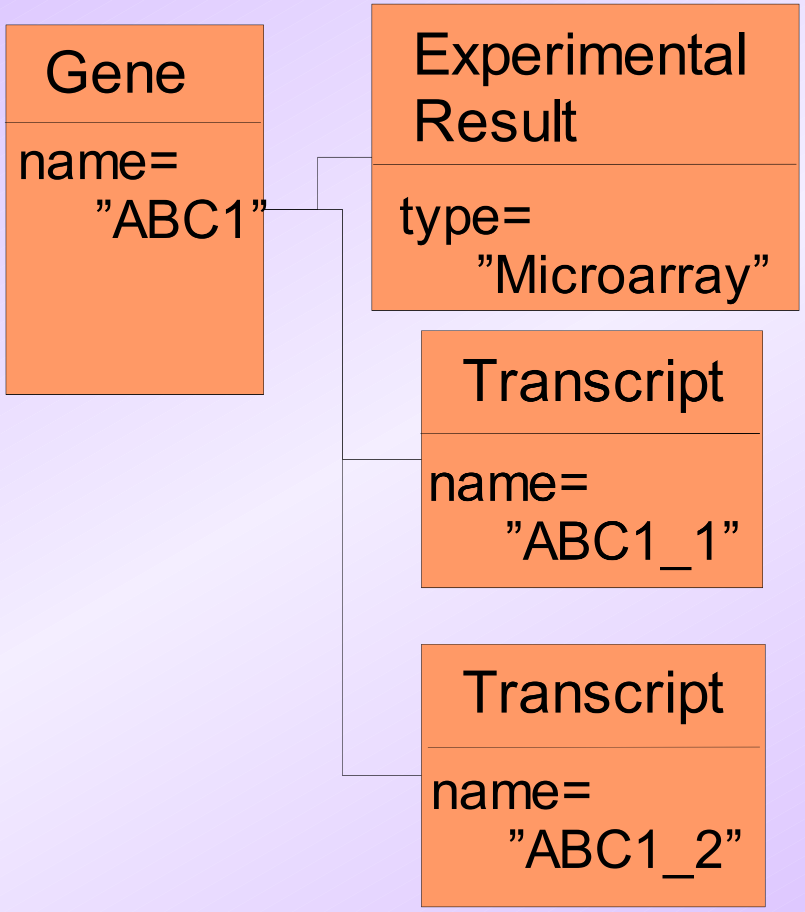
```
Primary keys:
  Gene: name
  Gene: flyBaseName
  Transcript: name,gene
```

New objects

Currently in database

FlyMine





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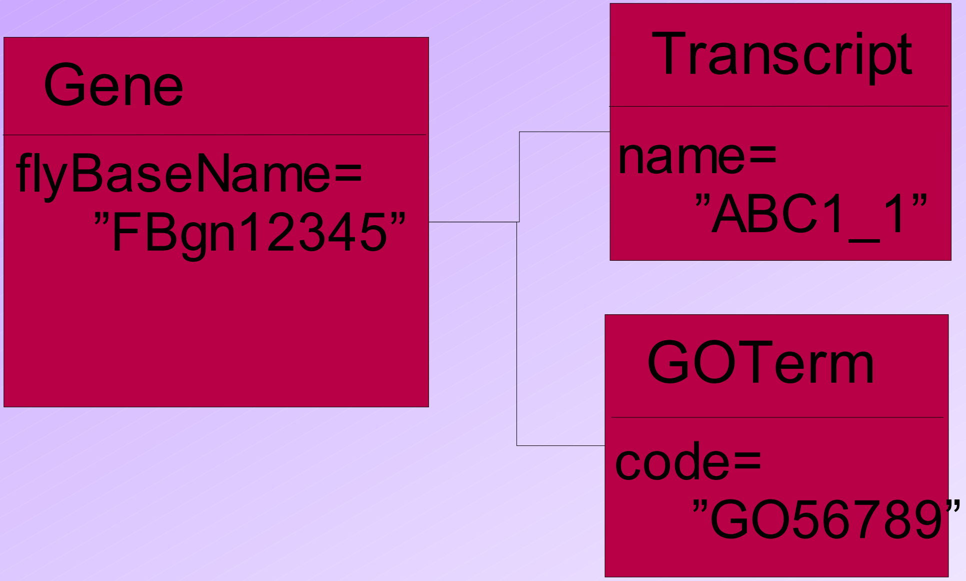

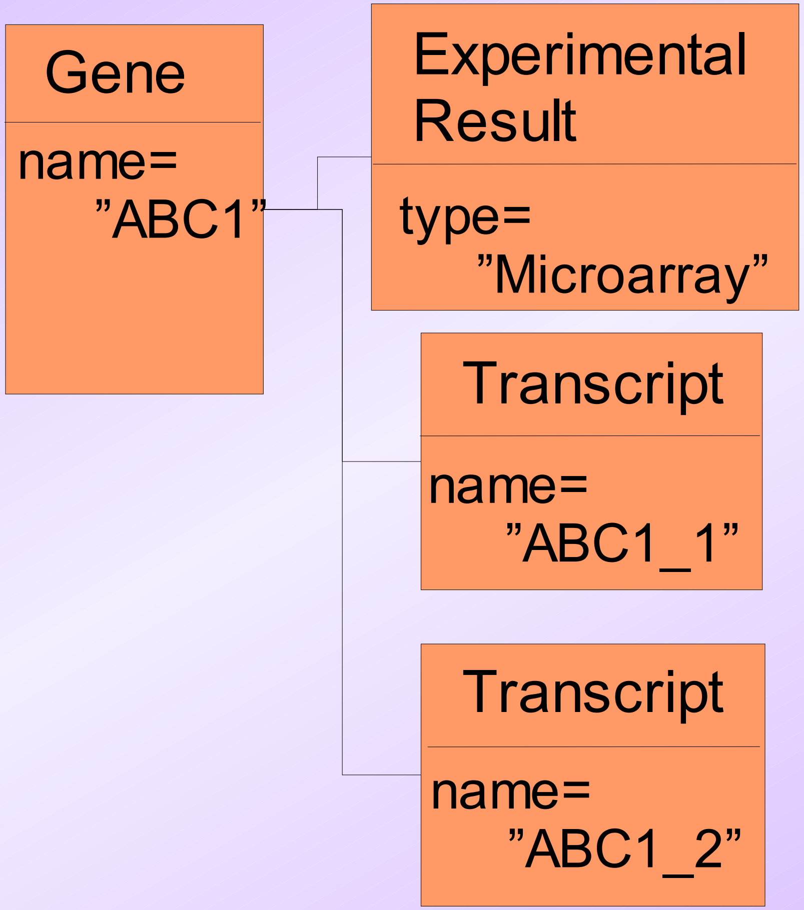

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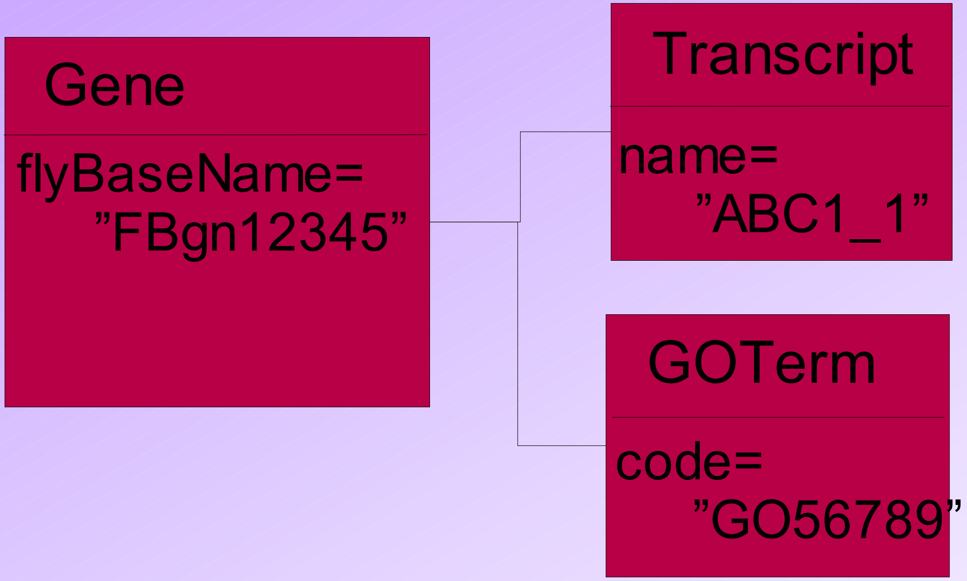

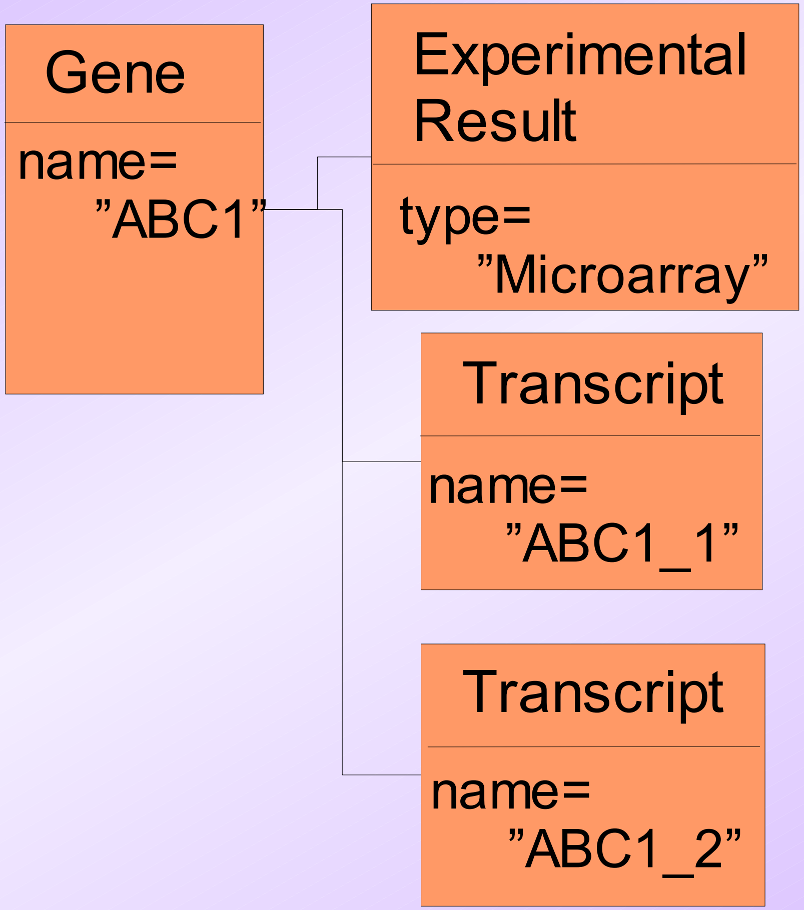

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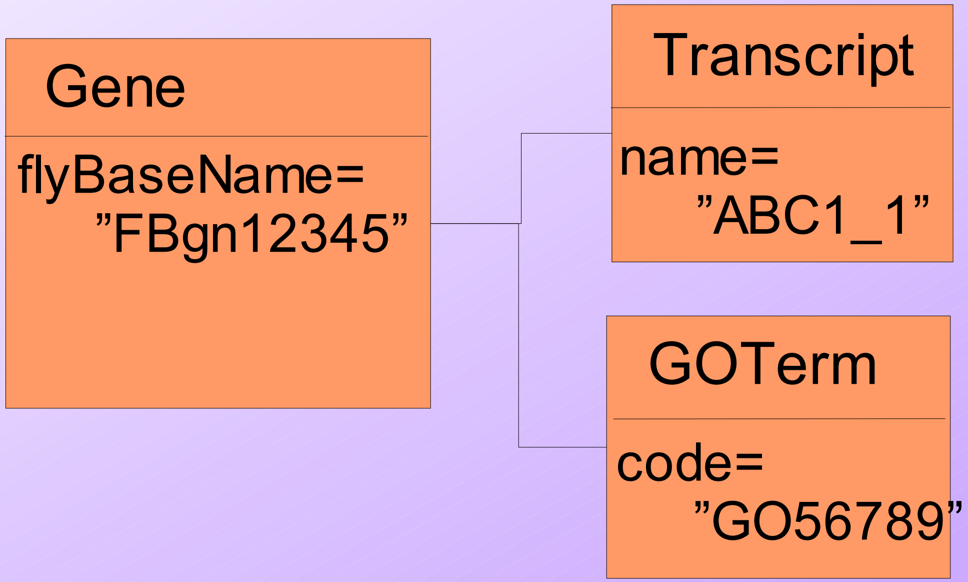

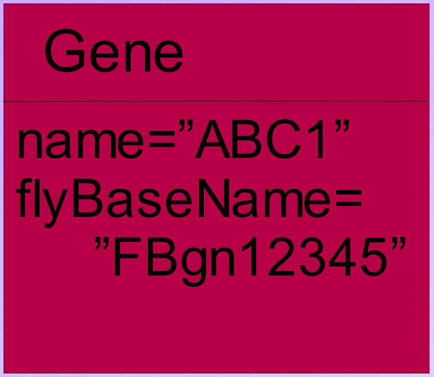

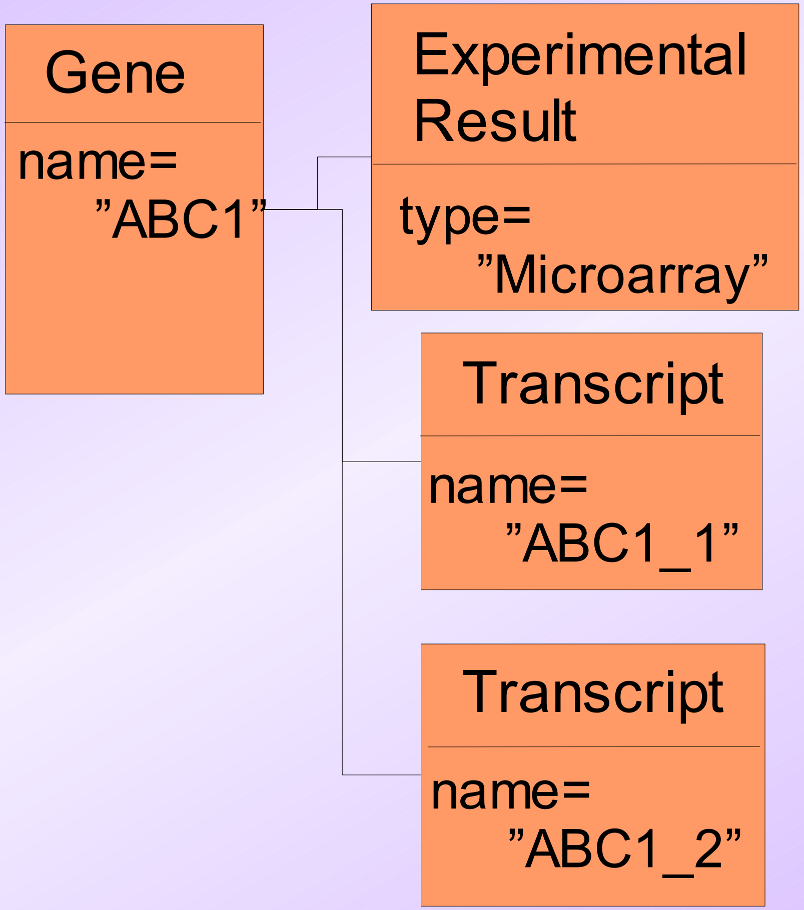

Primary keys:

```
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  Gene: name
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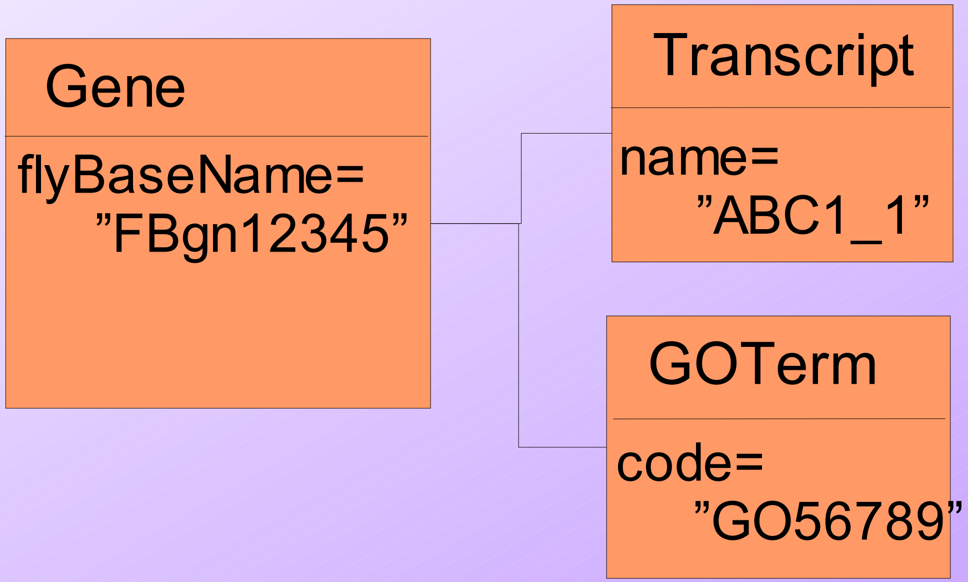
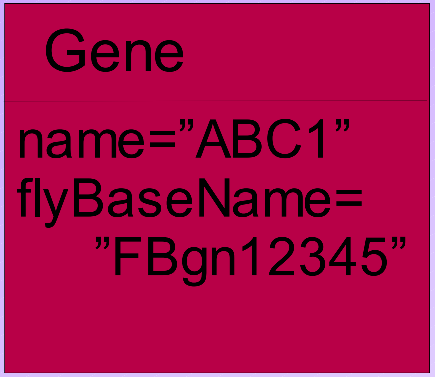
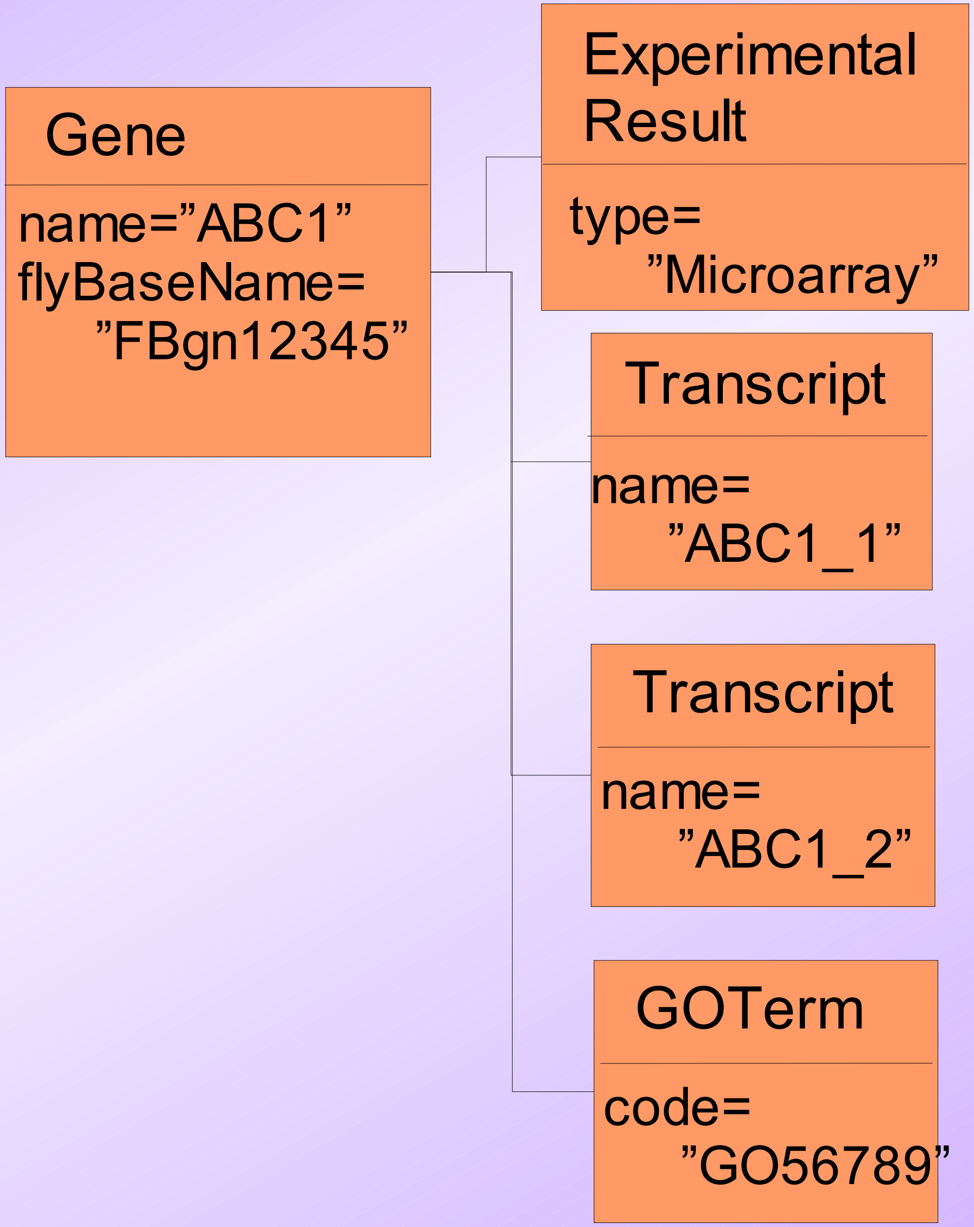






```
Primary keys:
  Gene: name
  Gene: flyBaseName
  Transcript: name,gene
```

New objects

Currently in database

Lessons learned

- Need to batch database reads and writes to avoid round trip time
  - without: 6 months to load
  - with: 6 hours to load
- Cache objects to avoid database lookups
- Use multi-thread model
- GB ethernet link between computational and database machines useful

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

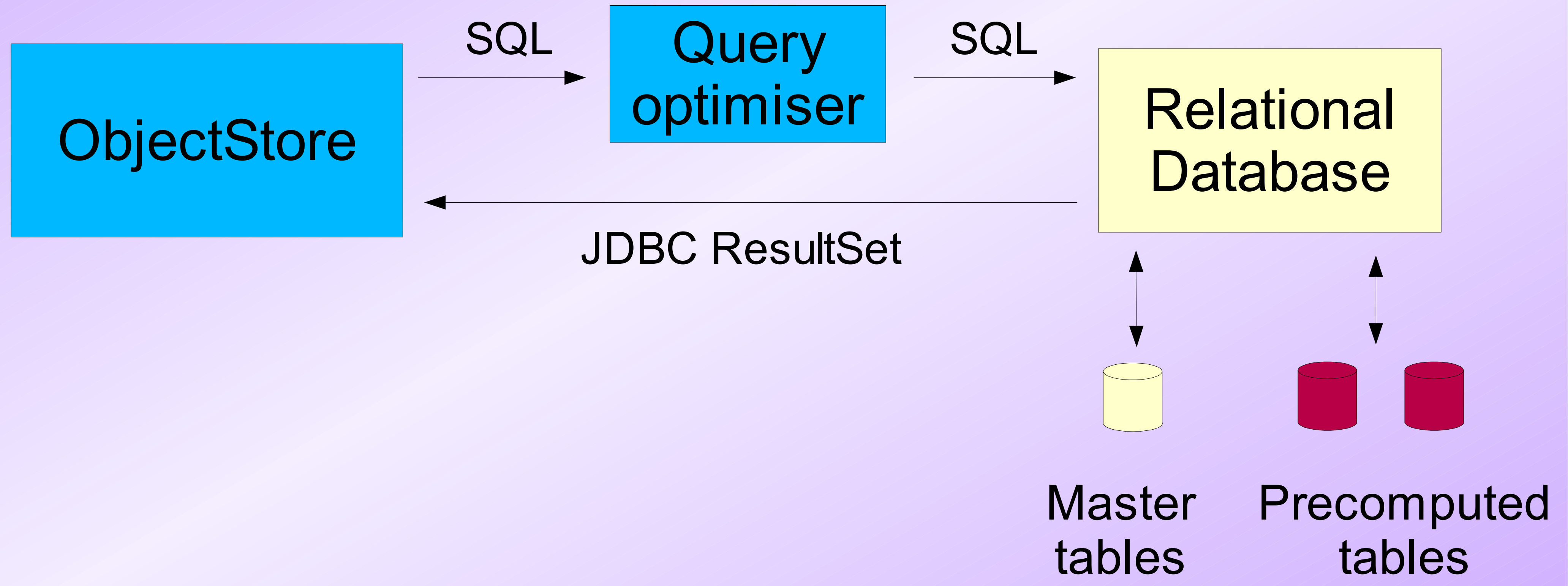
Arbitrary queries – solutions

- 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.

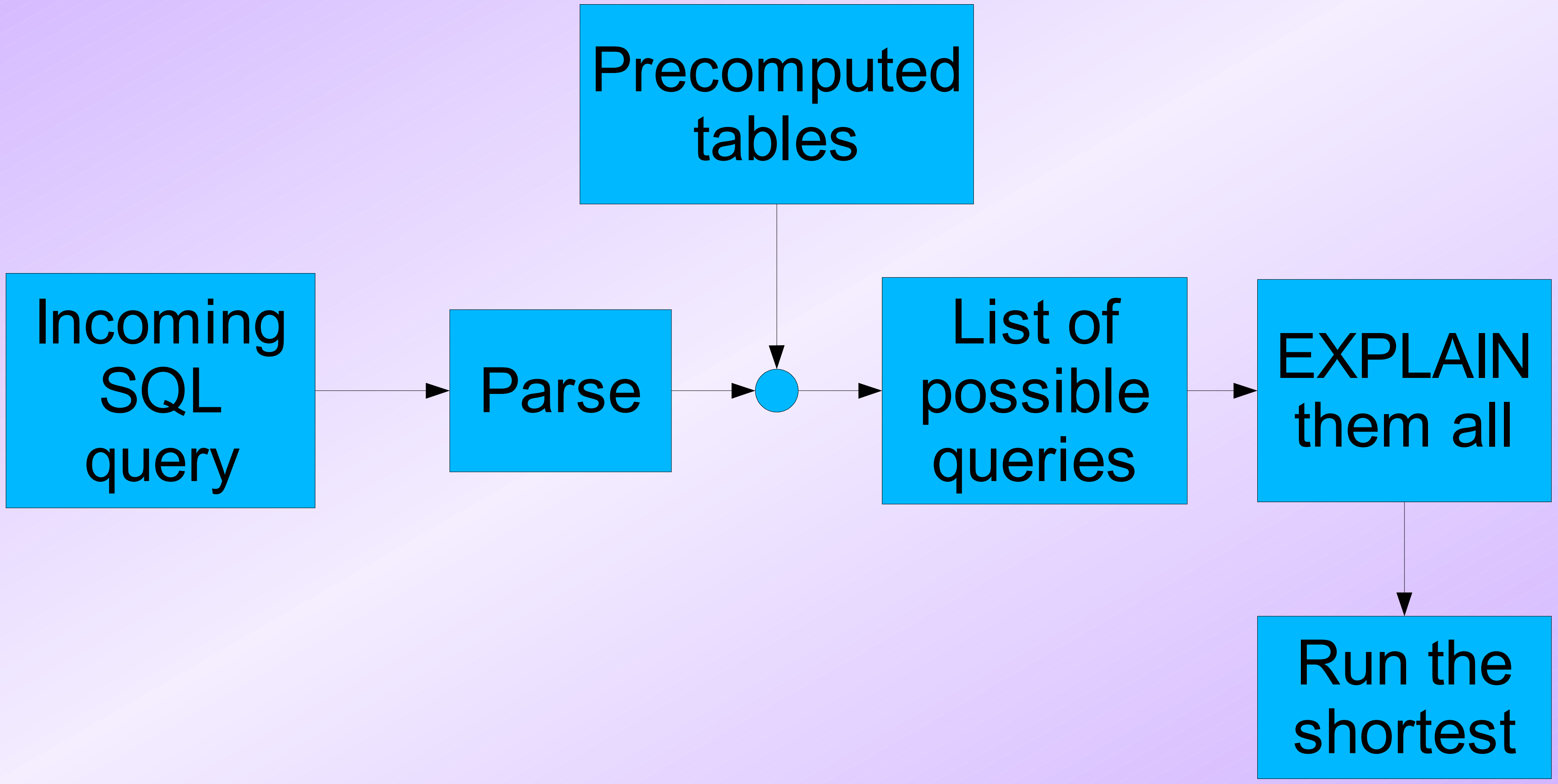
Query optimisation – aims

- 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



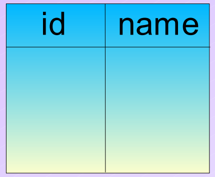
Query optimisation



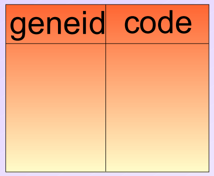
Query optimisation – example

Master tables

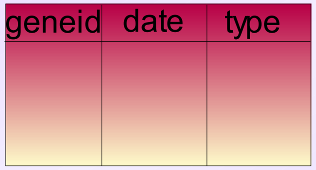
Genes



GOTerms

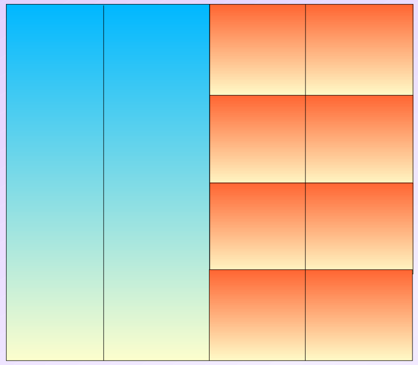


Experiments



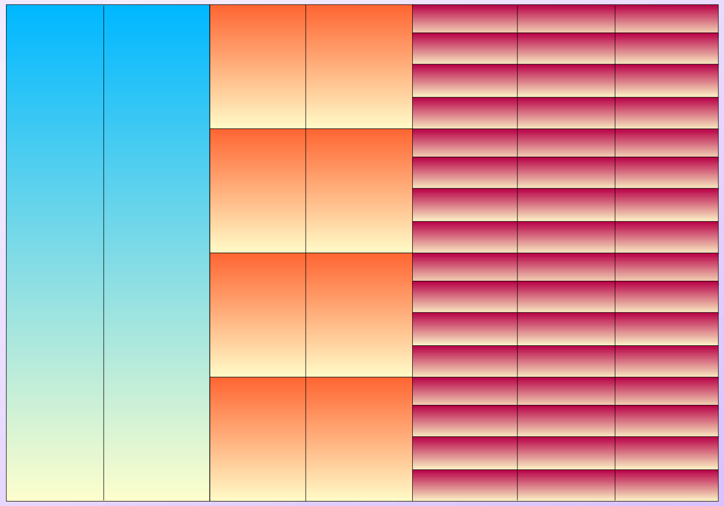
Precomputed tables

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
```

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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”
```

$\Downarrow$ 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

FlyMine

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.intermine.org !!

Summary

- Current status
  - generic SQL query optimiser
  - powerful object data warehouse
  - 2 query interfaces (OQL + Java)
  - web front end
  - web service
  - framework for data loading/integration
  - no model-specific code
  - FlyMine database alpha release

Summary

- Coming up
  - graphical query interface
  - tools for auto-generation of best set of precomputed tables
  - manual curation tools

Acknowledgements

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Richard Smith	Rachel Lyne
Matthew Wakeling	Kim Rutherford
Mark Woodbridge	Gos Micklem

More information and download at www.intermine.org

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