

The Grinder and Gene Sets

Master's Thesis

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November 28, 2007

Points of this talk

- ▶ What is the Grinder.
- ▶ How do you use it.
- ▶ How do you add data and mappings to it.
- ▶ Gene Sets.

What is the Grinder?

The Grinder is a Web accessible database that tracks mappings between Keyspaces.

What is a Keyspace?

- ▶ A set of **unique** identifiers for biological information that can be **mapped** to other biological information.
- ▶ Allowed mappings: 1-1, 1-Many, Many-1, Many-Many.
- ▶ Characteristics:
 - ▶ Name
 - ▶ Description
 - ▶ Species
 - ▶ Type
 - ▶ Source: URL and / or FTP location for origin of the data
 - ▶ Download date

What is a Keyspace?

- ▶ CREATE TABLE KeySpaces (
 - ▶ id INT UNSIGNED NOT NULL AUTO_INCREMENT
DEFAULT NULL,
 - ▶ name VARCHAR(30) NOT NULL UNIQUE,
 - ▶ species VARCHAR(30) NOT NULL,
 - ▶ description VARCHAR(255) NOT NULL DEFAULT ' ',
 - ▶ type INT UNSIGNED DEFAULT NULL REFERENCES
KeySpaceTypes (id),
 - ▶ url VARCHAR(10000) DEFAULT NULL,
 - ▶ ftp VARCHAR(10000) DEFAULT NULL,
 - ▶ lastDownloaded TIMESTAMP DEFAULT
CURRENT_TIMESTAMP,
 - ▶ PRIMARY KEY (id),
 - ▶ INDEX (species))
 - ▶ ENGINE = MyISAM;

What is a Mapping?

- ▶ A one way or bidirectional equivalence between two bits of biological information.
- ▶ Example: GenBank Accession Number U48705 (discoidin domain receptor) maps to LocusLink accession number 780
- ▶ Characteristics:
 - ▶ Name
 - ▶ Description / Provenance
 - ▶ Quality
 - ▶ Source: URL and / or FTP location for origin of the data
 - ▶ Download date

What is a Mapping?

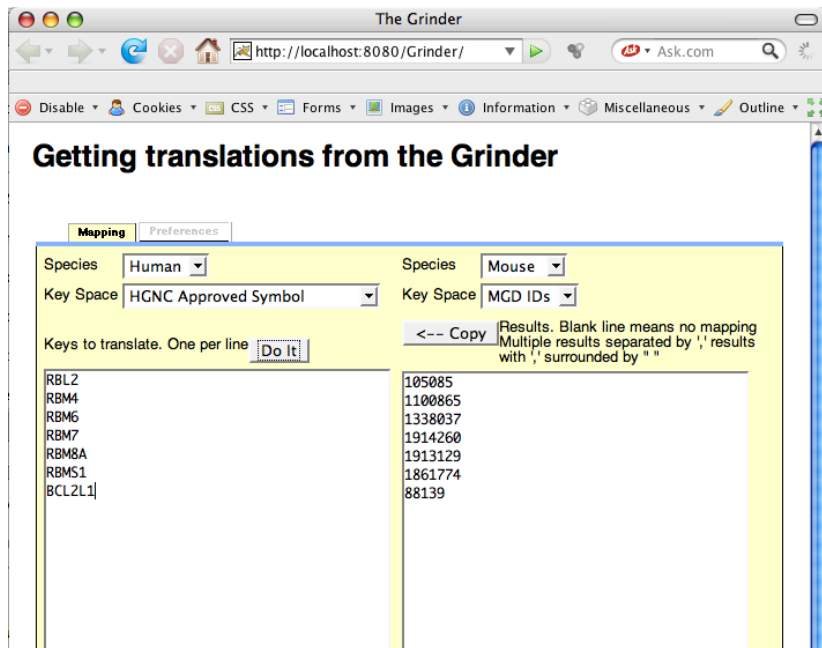
- ▶ CREATE TABLE Mappings (
 - ▶ id INT UNSIGNED NOT NULL AUTO_INCREMENT
DEFAULT NULL,
 - ▶ name VARCHAR(30) NOT NULL UNIQUE,
 - ▶ description VARCHAR(255) NOT NULL DEFAULT ' ', #
AKA provenance. Who did this mapping?
 - ▶ type INT UNSIGNED DEFAULT NULL REFERENCES
MappingTypes (id),
 - ▶ url VARCHAR(10000) DEFAULT NULL,
 - ▶ ftp VARCHAR(10000) DEFAULT NULL,
 - ▶ lastDownloaded TIMESTAMP DEFAULT
CURRENT_TIMESTAMP,
 - ▶ quality INT UNSIGNED NOT NULL DEFAULT 1,
 - ▶ PRIMARY KEY (id))
 - ▶ ENGINE = MyISAM;

What is a Mapping?

Mapping sources

- ▶ Hugo
- ▶ Geo
- ▶ InParanoid
- ▶ MultiInparanoid
- ▶ OrthoMCL
- ▶ Rio

How do you use the Grinder?



The screenshot shows a web browser window titled "The Grinder" with the URL `http://localhost:8080/Grinder/`. The browser's address bar and menu bar are visible. The main content area displays the heading "Getting translations from the Grinder". Below the heading, there are two tabs: "Mapping" (selected) and "Preferences". The "Mapping" tab contains a form with the following fields:

- Species: Human (dropdown)
- Key Space: HGNC Approved Symbol (dropdown)
- Species: Mouse (dropdown)
- Key Space: MGD IDs (dropdown)

Below these fields, there is a text input field labeled "Keys to translate. One per line" with a "Do It!" button next to it. To the right of this field is a "Copy" button and a tooltip that reads: "Results. Blank line means no mapping. Multiple results separated by ';' results with ';' surrounded by ' '".

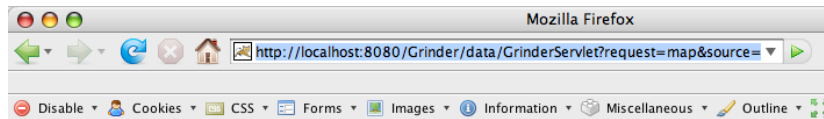
Two text areas are shown below the form, representing the input and output of the mapping process:

RBL2	105085
RBM4	1100865
RBM6	1338037
RBM7	1914260
RBM8A	1913129
RBMS1	1861774
BCL2L1	88139

How do you use the Grinder? The web page

1. Choose the Starting Species
2. Choose the Starting Keyspace
3. Choose the Ending Species
4. Choose the Ending Keyspace
5. Enter keys to map
6. Hit "Do It"

How do you use the Grinder?



105085
1100865
1338037
1914260
1913129
1861774
88139

How do you use the Grinder? The Servlet

How to talk directly to the servlet

```
http://disco.cse.ucsc.edu:8089/Grinder/data/GrinderServlet?  
request=map&source=HGNC%20Approved%20Symbol  
&target=MGD%20IDs  
&ids=RBL2,RBM4,RBM6,RBM7,RBM8A,RBMS1,BCL2L1
```

- ▶ Servlet Address: <Grinder Address>/data/GrinderServlet
- ▶ Query marker: '?'
- ▶ "request="
 - ▶ species: Get a list of all available species
 - ▶ keyspaces: Get a list of all keyspaces for a species, or all species
Optional param: "species=" to restrict to one species
 - ▶ map: Map ids from one keyspace to another
Parameters: "source=", "target=" : Source and target keyspaces
"ids=" : Comma separated list of ids
- ▶ Result : Text file, one id per line

Adding Information to the Grinder

Control Files

- ▶ XML Format
- ▶ Lets you add Keyspaces, Mappings, or Both
- ▶ Can add to existing ones, and / or create new ones
- ▶ One Data File per Control File
- ▶ Can define specific one way or bidirectional Mappings
- ▶ Can also define N-way bidirectional Mappings
- ▶ Format defined in the file ControlFile.xsd
- ▶ Requires User ID and Password to the Database

What are GeneSets?

- ▶ A collection of items from one or more KeySpaces.
- ▶ The collection can be, but doesn't have to be, ordered.
- ▶ The items can have, but don't have to have, values.
- ▶ Can be part of a SetFamily.
- ▶ Can be loaded into the DB via a data file and an XML description file for the data.
- ▶ Characteristics:
 - ▶ Name
 - ▶ Description
 - ▶ Family

What are GeneSets?

- ▶ CREATE TABLE GeneSets (
 - ▶ id INT UNSIGNED NOT NULL AUTO_INCREMENT
DEFAULT NULL,
 - ▶ family INT UNSIGNED NOT NULL REFERENCES
GeneSetFamilies (id),
 - ▶ name VARCHAR(1000) NOT NULL UNIQUE,
 - ▶ description VARCHAR(255) NOT NULL DEFAULT ' ',
 - ▶ installTime TIMESTAMP DEFAULT
CURRENT_TIMESTAMP, (User Sets: 2 weeks w/o use
gets killed)
 - ▶ PRIMARY KEY (id))
 - ▶ ENGINE = MyISAM;

What are GeneSets?

- ▶ CREATE TABLE GeneSetLinks (
 - ▶ family INT UNSIGNED NOT NULL REFERENCES GeneSetFamilies (id),
 - ▶ setID INT UNSIGNED NOT NULL REFERENCES GeneSets (id),
 - ▶ geneKS INT UNSIGNED NOT NULL REFERENCES KeySpaces (id),
 - ▶ geneID INT UNSIGNED NOT NULL,
 - ▶ theOrder INT NOT NULL,
 - ▶ value DOUBLE PRECISION DEFAULT NULL,
 - ▶ INDEX fgg (family, geneKS, geneID),
 - ▶ INDEX sgg (setID, geneKS, geneID),
 - ▶ INDEX ki (geneKS, geneID),
 - ▶ UNIQUE INDEX fsgg (family, setID, geneKS, geneID))
 - ▶ ENGINE = MyISAM;

What are GeneSetFamilies?

- ▶ A collection of GeneSets.
- ▶ System Sets: GO (Yeast, what other species?), KEGG, Others?
- ▶ User Sets: Whatever you want to add. Has your user name attached to it.
- ▶ Characteristics:
 - ▶ Name
 - ▶ Description
 - ▶ Source: URL and / or FTP location for origin of the data
 - ▶ Kill Date

What are GeneSetFamilies?

- ▶ CREATE TABLE GeneSetFamilies (
 - ▶ id INT UNSIGNED NOT NULL AUTO_INCREMENT
DEFAULT NULL,
 - ▶ name VARCHAR(255) NOT NULL UNIQUE,
 - ▶ description VARCHAR(255) NOT NULL DEFAULT ' ',
 - ▶ url VARCHAR(10000) DEFAULT NULL,
 - ▶ ftp VARCHAR(10000) DEFAULT NULL,
 - ▶ killTime TIMESTAMP DEFAULT 0,
 - ▶ PRIMARY KEY (id))
 - ▶ ENGINE = MyISAM;

Gene Sets Commands

The screenshot shows a web browser window with the title "Beginning tests of NetworkVisualization package - SeaMonkey". The address bar shows "http://disco.cse.ucsc.edu:8089/". The browser tabs include "solutions8.html", "Beginning tests of NetworkVi...", and "Nested effects models for hi...".

The application interface has a top navigation bar with "Network", "Heat Map", and "Gene Sets" tabs. Below this is a "Display" and "Log" section. The main content area is currently empty, showing a "60 Years" logo.

On the left side, there is a sidebar menu with the following sections:

- Entity Tracks
- Organism & Entity Type
 - worm
 - genes
- Search
- Recommender
- GO Sets
- User Input

A dropdown menu is open over the "Gene Sets" tab, listing the following commands:

- Create Gene Set
- Create Gene Set Operation
- Create Gene Set Transformation
- Create Gene Set Family
- Create Gene Family Operation
- Set User ID
- Set Default Threshold Value
- Set Password
- Set Default p Value
- Get System Set From Database
- Get User Set From Database
- Get Set Family From Database
- Hide Labels
- Hide Sets
- Hide Arrows

Gene Sets in Action

Beginning

Back Forward Reload Stop <http://localhost:8080/ib/>

Entity Tracks

Organism & Entity Type

worm genes

Search

Recommender

GO Sets

User Input

Network Heat Map Gene Sets

Display Log

```
graph TD; A((GO Yeast)) --> B[GO Yeast And Scott Loki's Drugs]; C((Scott Loki's Drugs)) --> B; B --> D[GO Yeast And Scott Loki's Drugs And 232chemdiv-new-het_2]; E((232chemdiv-new-het_2)) --> D; D --> F((Result Family))
```

GO Yeast

Scott Loki's Drugs

GO Yeast And Scott Loki's Drugs

232chemdiv-new-het_2

GO Yeast And Scott Loki's Drugs And 232chemdiv-new-het_2

Result Family

©

Gene Sets

- ▶ Gene Sets allow us to represent organizations of genetic information, such as GO categories.
- ▶ Circles are Gene Sets put together by the User.
- ▶ Triangles are Binary Set operations, and the results of those operations.
- ▶ Doubled figures involve families of sets, rather than individual sets.
- ▶ Will be able to group arbitrary Sets into a Family, or show the top 'n' Sets from a Family.
- ▶ Will be able to Load and Save layouts to / from your file system, and / or the DB.

Where to go for more

The complete documentation for the Grinder is online at the Grinder Wiki page:

<http://wiki.soe.ucsc.edu/bin/view/SysBio/Grinder>

Points of this talk

- ▶ The Grinder is a one stop location for all your mapping needs
- ▶ It's easy to use
- ▶ It's easy for authorized users to add data to it
- ▶ **You** should use the Grinder
- ▶ Gene Set manipulation is also easy to use. Build a pipeline once, use it forever more.