

#### Alma Mater Studiorum · Università di Bologna

Dipartimento di Fisica e Astronomia - DIFA

#### AIM Live Meeting

#### **CHIMeRA**

# Complex Human Interactions in Medical Records and Atlases

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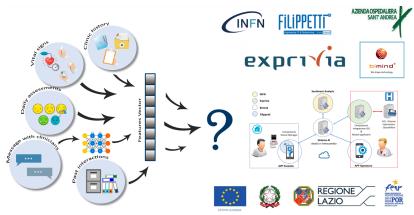
### Aim of Chimera

Build a network-of-networks with different types of biomedical/chemical/genomical information to enhance interpretability of experimental analyses for:

- advanced diagnostics
- novel drug targeting
- patient stratification
- multi-omics annotation



### Prodrome: FiloBLU Project (with INFN))





### Disease Ontology for FiloBlu

Disease-Symptom Network (from Italian language websites)



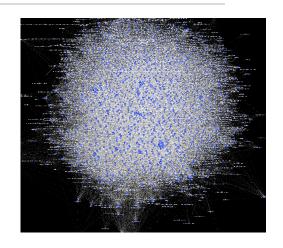
- 1381 nodes;
- 14002 links;



- **1200** nodes;
- 16035 links;

#### Symptoms Network:

- nodes: 2285;
- links: 29557;





### Web Scraping: extracting unstructured data





Web sites with HTML pages & Ajax

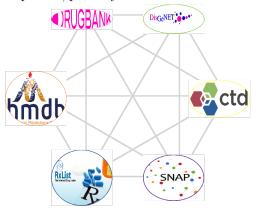
Web Scraping Service

Scructured data



### CHIMeRA network-of-networks structure

Nodes: genes, SNPs, diseases, phenotypes, drugs, metabolites/compounds/pathways





### Mining the Web

#### Database contents

Source Information Data

HMDB

#### Metabolites, Metabolic and Disease Pathways

- 114,003 Metabolites entries with chemical taxonomy
- ~25,000 human metabolic and disease pathways

CTD

#### Diseases, Synonyms and Phenotypes

- 7,212 Diseases with mapped synonyms
- 4.340 Disease Related Phenotypes



**SNAP** 

#### **Disease Ontology and Synonyms**

• 8,803 Disease terms with related synonyms





### Mining the Web

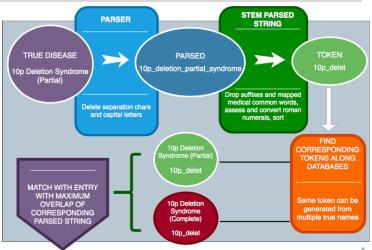
#### Database contents

Source Information **Drugs, Drugs Interactions, Drug-Target Association** DB 11.926 Drugs • 18,969 Drug-Targets Associations Gene-Disease, Disease-Variant Associations **DGNET** • 628,685 associations, between 17,549 genes and 24,166 diseases 210,498 associations, between 117,337 variants and 10.358 diseases Data Diseases, Related, Causes and Drugs · Associations between related disease and **RXLIST** causes Drug-Disease associations



### String Processing

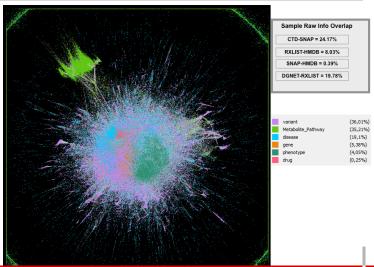
#### Pre-processing Pipeline





### CHIMeRA

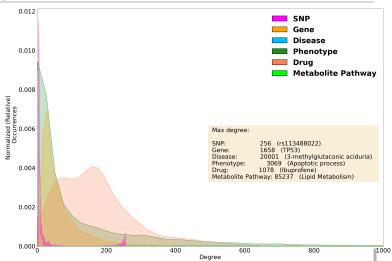
#### Network visualization: 360k nodes, 38M links





### Preliminary Analysis

#### Degree distributions





### CHIMeRA as Service

- Convert Network structure to quearable DataBase (ArangoDB);
- Query node according (disease, gene, SNP, drug, metabolite, phenotype):
  - Query single node: neighborhood, equivalent to single database query;
  - Breadth first search: percolation from a given root node (n-th neighborhood);
  - Query multiple root nodes (in progress);
  - Query shortest paths between two entries (in progress).
- Graphical visualization of resulting networks;



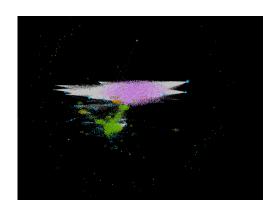
### Example: Leukemia disease

## Looking for "Leukemia" disease into CHIMeRA db:

- 291 types of Leukemia
- 82 connected components

#### Node types:

- 838 diseases (subtypes, related);
- 2463 genes;
- 5195 phenotypes;
- 765 SNPs;
- 154 metabolite pathways;
- 40 metabolites;
- 5 drugs;





### Next

- New build based on enhanced processing
- Network-of-Networks analysis
- Improve query efficiency and user interface.
- Implement as a public querable web service.



### Thanks to the research group

