Semantics and Services Enabled Problem Solving Environment for *Trypanosoma cruzi*

*Amit Sheth, Satya Sahoo, Priti Parikh*

*Kno.e.sis Center*, Wright State University

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Trypanosoma cruzi

- *T. cruzi* is a protozoan parasite that causes Chagas Disease or American trypanosomiasis.
- Chagas disease is the leading cause of death in Latin America where around 18 million people are infected with this parasite.
- Related parasites include, *Trypanosoma brucei* and *Leishmania major* that causes African trypanosomiasis and leishmaniasis, respectively.

*T. Brucei* surrounded by red blood cells in a smear of infected blood. (Copyright: Jürgen Berger and Dr. Peter Overath, Max Planck Institute for Developmental Biology, Tübingen)
Project Outline

Search and Retrieval System

Result
1. Trypomastigote
2. Amastigote

Result browser

Build your query

By navigating through the ontology scheme (i.e., the definition of the possible types and interconnections available in the knowledge base), the system will guide you through the process of posing a question in an intuitive way, e.g., "Person -> family_name -> Cruz".

T. cruzi immunology ontology Parasite Experiment ontology T. cruzi life cycle ontology
aligned ontologies

Ontological infrastructure

UniProt T. cruzi DB NCBI data sources

Data and information sources

Internal Lab Data

PubMed
Project Outline

**Data Sources**

- **Internal Lab Data**
  - Gene Knockout
  - Strain Creation
  - Microarray
  - Proteome

- **External Database**
Project Outline

- **Data Sources**
  - Internal Lab Data
    - Gene Knockout
    - Strain Creation
    - Microarray
    - Proteome
  - External Database

- **Ontological Infrastructure**
  - Parasite Lifecycle
  - Parasite Experiment
• **Data Sources**
  - Internal Lab Data
    - Gene Knockout
    - Strain Creation
    - Microarray
    - Proteome
  - External Database
• **Ontological Infrastructure**
  - Parasite Lifecycle
  - Parasite Experiment
• **Query processing**
  - Cuebee
Project Outline

- **Data Sources**
  - Internal Lab Data
    - Gene Knockout
    - Strain Creation
    - Microarray
    - Proteome
  - External Database

- **Ontological Infrastructure**
  - Parasite Lifecycle
  - Parasite Experiment

- **Query processing**
  - Cuebee

- **Results**
Collaborating Institutions

Tarleton Research Group, Center for Tropical and Emerging Global Diseases (CTEGD), University of Georgia

Large Scale Distributed Information Systems, LSDIS Lab, University of Georgia

National Center for Biological Ontologies, NCBO, Stanford University

The Wellcome Trust Sanger Institute, Cambridge, UK

The Oswaldo Cruz Institute (Fiocruz), Brazil
Project Generated Resources

- **Trykipedia**: Wiki-based discussion and dissemination platform for the parasite community
  - [http://knoesis.wright.edu/trykipedia](http://knoesis.wright.edu/trykipedia)

- **Parasite Knowledge Repository (PKR)**
  - Parasite Lifecycle Ontology
  - Parasite Experiment Ontology

- **Cuebee**: platform that provides intuitive interface to query biological data semantically
Trykipedia - a Wiki-based platform for collaboration of Parasite Research Community

Trykipedia is a Wiki-based resource for the ontologies and other tools being created as a part of the NIH funded project, "The Semantics and Services enabled Problem Solving Environment for Trypanosoma cruzi." This project aims to utilize state-of-the-art semantic technologies for effective querying of multiple databases through creation of a suite of ontologies modeling multiple aspects of T. cruzi research domain. As a part of the project, two ontologies have been created, namely Parasite Lifecycle Ontology (PLO) and Parasite Experiment Ontology (PEO). One of the objectives of the project was to create a platform for lifecycle and Experiment ontologies for T. cruzi that can later be extended for other human parasites with community collaborations. We are currently working with the Sanger Institute (UK) to extend PLO with Plasmodium sp. and other human parasites.

Quick Links
- Parasite Experiment ontology - Ontology that models experimental conditions and results
- Parasite Life Cycle ontology - Ontology that models all the lifecycle stages of various kinetoplastids
- Protein Ontology - Upper level provenance ontology
- Publications - conference and journal publications generated from this research
- People - people who are involved in this research

Collaborating Institutions
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- Large Scale Distributed Information System, LDSIS Lab, University of Georgia
- National Center for Biological Ontologies, NCBO, Stanford University
- The Wellcome Trust Sanger Institute, Cambridge, UK
- The Oswaldo Cruz Institute (Fiocruz), Brazil

We invite new members to collaborate with us in extending Parasite Life cycle Ontology (PLO) and/or Parasite Experiment Ontology (PEO).

http://wiki.knoesis.org/index.php/Parasite_Life_Cycle_ontology

Trykipedia - a Wiki-based platform for collaboration of Parasite Research Community

Thursday, January 28, 2010
Parasite Life Cycle ontology

The current Parasite Lifecycle Ontology (shown below) is mainly descriptive of trypanosomatid parasites including *T. cruzi*, *T. brucei*, and *L. major*.

**Contents**
- Introduction
  - 1. Trypanosoma cruzi
  - 2. Trypanosoma brucei
  - 3. Leishmania sp.
- 2 Ontology
- List of ontology classes
- 4 Feedback/Comments

**Introduction**

**Trypanosoma cruzi**

The life cycle of *Trypanosoma cruzi* involves both vertebrate and invertebrate hosts (see figure below). Metacyclic trypomastigotes are deposited on the mammalian (vertebrate host's) skin through the feces of the triatomine bug vector. They have the capacity to penetrate skin through wounds, such as the bite from the bug, and across the mucosal membranes surrounding the eyes and mouth.

Inside the mammalian host, the trypomastigotes penetrate either phagocytic or non-phagocytic cells, in a manner distinct from phagocytosis. Parasites subvert the host cell Ca^{2+}-regulated lysosomal exocytic pathway, literally "hijacking" lysosomes to enable them to invade effectively (Sidney and Andrews, 2000; Tan and Andrews, 2002). Within the host cell, trypomastigotes are initially held within a membrane bound vacuole. They subsequently enter the host cell cytoplasm directly, transforming into amastigotes (the intracellular replicative form) (Tan and Andrews, 2002). Around five days post-invasion, the amastigotes transform back into C-shaped trypomastigotes, and the host cell ruptures, releasing the parasites into the bloodstream. These bloodstream trypanosomatids can then either infect further cells, or can be taken up by a reduviid bug. Within the insect vector, epimastigotes develop in the alimentary tract, taking 10–15 days to replicate and transform into infective stages in the rectum (Kohne and Schaub, 2003). *T. cruzi* can also be transmitted via contaminated blood and infected organs used in transplant operations, or congenitally from mother to child.

**Trypanosomiasis, American (Chagas disease)**

1. Triatomine Bug Stages
   - Triatomine bug leaves a blood meal
   - Tracheal system of triatomine bug
   - Trypcysteine trypomastigotes

2. Human Stages
   - Metacyclic trypomastigotes penetrate various cells at bite migration sites. Inside cells they transform into amastigotes.
   - Amastigotes multiply by binary fission in cells of infected tissues.
   - Trypanosomatids can infect other cells and transform into intracellular amastigotes in new infection sites. Clinical manifestations can result from this parasitic cycle.
Chagas disease

Chagas disease is caused by *Trypanosoma cruzi*, which is a protozoan parasite. The disease was discovered by the Brazilian physician, Carlos Chagas in 1909 and is also known as American trypanosomiasis. It is prevalent in Southern America. It is transmitted to animals and humans through feces of an infected Triatominae bug (also called "kissing" bug). This infection can also be transmitted through: i) contaminated blood or blood products, ii) mother to baby, or iii) an organ transplant from an infected donor.

External Links

- Chagas disease at the Centers for Disease Control
- Chagas Disease, from Discovery to Control - and Beyond: History, Myths and Lessons to Take Home

This child from Parana is suffering from Chagas disease. The infection manifested as an acute infection with swelling of the right eye. Photo courtesy by CDC and Parana HEI, University of Illinois http://www.choosereducationalhealthcare.org/ Chagas.jpg

Categories: Trypanosoma cruzi | Parasite Life Cycle ontology
Parasite Knowledge Repository (PKR)

- PKR will support complex biological queries related to *T. cruzi* drugs, vaccination, or gene knockout targets; for example,
  - Find all genes with *proteomic expression* in mammalian *lifecycle stage* with GPI *anchor* or signal peptide predictions.
  - Find *genes* annotated as potential *vaccine* candidates.
  - Find all genes with *proteomic expression* evidence in the mammalian host *lifecycle stages* for *T. cruzi*

- Data
  - Internal lab data (from Tarleton Research Group)
    - Gene Knockout, Strain Creation, Microarray, and Proteome
  - External databases (*TriTrypDB, ProtozoaDB, Drug Bank, etc.*)

- Ontologies:
  - Parasite Lifecycle Ontology (PLO)
  - Parasite Experiment Ontology (PEO)
Parasite Lifecycle Ontology (PLO)

- Models lifecycle stages of *T. cruzi*, *T. brucei*, and *L. major* in OWL
- All the entities are linked to each other by explicitly modeled named relationships, for example, *T. cruzi*→*has_vector_organism*→*triatominae*
- Currently has 41 classes and 5 properties with a description logic expressivity of ALU.
- Collaboration with the Sanger Institute (UK) and Oswaldo Cruz Institute (Brazil)
Parasite Experiment Ontology (PEO)

- Models gene knockout, strain creation, microarray, and proteomics experiments data
  - Process, instruments, parameters, and sample details to annotate experimental results with provenance metadata

- 110 classes and 23 properties with a logic expressivity of ALCHQ(Δ)

- Named relationships, for e.g.,
  Tcruzi_lifecyclestage_subsample \( \rightarrow \) part_of \( \rightarrow \) Tcruzi_sample, and
  Tcruzi_lifecyclestage_subsample \( \rightarrow \) is_located_in \( \rightarrow \) spatial_parameter
  - Provides important information about research and Provenance
Provenance for GKO and SC Protocols

KO Project Protocol

KO Region Construct Protocol

Region

Sequence Extraction

5'
Region

3'
Region

Drug Resistance Region

Plasmid Construction

preceded_by

Knock Out Construct Plasmid

Plasmid Construction step

status

Researcher

Allele Designation

Gene Name

Strain Project Protocol

Tcuzi sample

Knock Out Construct Plasmid

Transfection

Transfected Sample

Drug Selection

status

Experiment Notes

Organism Strain

Selected Sample

status

Date Started

Date of last Update

Cell Cloning

Cloned Sample

Experiment Notes
Provenance for GKO and SC Protocols

KO Project Protocol
KO Region Construct Protocol

- Region
  - Sequence Extraction
  - Region
  - Drug Resistance Region
  - Plasmid Construction
    - Plasmid Construction step
    - Knock Out Construct Plasmid
    - status
    - Researcher
    - Allele Designation
    - Gene Name

Strain Project Protocol

- Tcuzi sample
  - Knock Out Construct Plasmid
  - Transfection
  - Transfected Sample
    - Drug Selection
    - Selected Sample
    - Cell Cloning
      - Cloned Sample

New Parasite Strains

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**T. cruzi** Provenance System (TPS) for GKO and

- **Capture**
  - Web pages used in experiments
  - Transform data into RDF instance data corresponding to PEO schema

- **Modeling**

- **Storage**
  - Oracle 10g (release 10.2.0.3.0) RDF database management system (DBMS)

- **Query Analysis**
  - Provenance query operators
Gene Knockout and Strain Creation*
Provenance in Parasite Research

* T. cruzi Semantic Problem Solving Environment Project, Courtesy of D.B. Weatherly and Flora Logan, Tarleton Lab, University of Georgia

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Provenance in Parasite Research

Related Queries from Biologists

- Gene Name
- Sequence Extraction
- Drug Resistant Plasmid
- T. Cruzi sample
- 3' & 5' Region
- Plasmid Construction
- Knockout Construct Plasmid
- Transfection
- Transfected Sample
- Drug Selection
- Selected Sample
- Cell Cloning
- Cloned Sample

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Related Queries from Biologists

- List all groups in the lab that used a Target Region Plasmid?
Provenance in Parasite Research

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- List all groups in the lab that used a Target Region Plasmid?
- Which researcher created a new strain of the parasite (with ID = 66)?
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- List all groups in the lab that used a *Target Region Plasmid*?
- Which researcher created a new strain of the parasite (with ID = 66)?
- An experiment was not successful – has this experiment been conducted earlier? What were the results?
Provenance Management for Scientific Data

- Provenance from the French word “provenir” describes the lineage or history of a data entity
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Provenance Management for Scientific Data

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• For Verification and Validation of Data Integrity, Process Quality, and Trust

• Issues in Provenance Management
  ➢ Provenance Modeling
  ➢ A Dedicated Query Infrastructure
  ➢ Practical Provenance Management Systems
Ontologies for Provenance Modeling

• Advantages of using Ontologies
  ➢ Formal Description: Machine Readability, Consistent Interpretation
  ➢ Use Reasoning: Knowledge Discovery over Large Datasets
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• **Problem:** A *gigantic*, monolithic Provenance Ontology! – not feasible
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Provenir Ontology
Provenir Ontology Schema

AGENT

DATA COLLECTION

DATA

PARAMETER

PROCESS

has_agent

is_a

is_a

participates_in
Provenir Ontology Schema

[Diagram of ontology schema with labeled nodes and edges: agent, process, data collection, parameter, spatial parameter, domain parameter, temporal parameter, has parameter, located_in, has_agent, participated_in, preceded_by, has_temporal_value, is_a, contained_in, transformation_of, part_of, derived_from, has_participant.
Domain-specific Provenance: Parasite Experiment ontology

*Parasite Experiment ontology available at: http://wiki.knoesis.org/index.php/Trykipedia*
Domain-specific Provenance: Parasite Experiment ontology


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Domain-specific Provenance: Parasite Experiment ontology


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Domain-specific Provenance: Parasite Experiment ontology


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Classified Provenance Queries into Three Categories
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- **Type 1: Querying for Provenance Metadata**
  - Example: *Which gene was used create the cloned sample with ID = 66?*
Classified Provenance Queries into Three Categories

• **Type 1: Querying for Provenance Metadata**
  
  ○ Example: *Which gene was used create the cloned sample with ID = 66?*

• **Type 2: Querying for Specific Data Set**
  
  ○ Example: *Find all knockout construct plasmids created by researcher Michelle using “Hygromycin” drug resistant plasmid between April 25, 2008 and August 15, 2008*
Classified Provenance Queries into Three Categories

- **Type 1: Querying for Provenance Metadata**
  - Example: *Which gene was used create the cloned sample with ID = 66?*

- **Type 2: Querying for Specific Data Set**
  - Example: *Find all knockout construct plasmids created by researcher Michelle using “Hygromycin” drug resistant plasmid between April 25, 2008 and August 15, 2008*

- **Type 3: Operations on Provenance Metadata**
  - Example: *Were the two cloned samples 65 and 46 prepared under similar conditions – compare the associated provenance information*
Four Query Operators – based on Query Classification
Provenance Query Operators

Four Query Operators – based on Query Classification

- `provenance()` – Closure operation, returns the complete set of provenance metadata for input data entity
Provenance Query Operators

Four Query Operators – based on Query Classification

• \textit{provenance}() – Closure operation, returns the complete set of provenance metadata for input data entity

• \textit{provenance\_context}() - Given set of constraints defined on provenance, retrieves datasets that satisfy constraints
Four Query Operators – based on Query Classification

- `provenance()` – Closure operation, returns the complete set of provenance metadata for input data entity
- `provenance_context()` - Given set of constraints defined on provenance, retrieves datasets that satisfy constraints
- `provenance_compare()` - adapt the RDF graph equivalence definition
Provenance Query Operators

Four Query Operators – based on Query Classification

- **provenance ()** – Closure operation, returns the complete set of provenance metadata for input data entity
- **provenance_context()** - Given set of constraints defined on provenance, retrieves datasets that satisfy constraints
- **provenance_compare ()** - adapt the RDF graph equivalence definition
- **provenance_merge ()** - Two sets of provenance information are combined using the RDF graph merge
Answering Provenance Queries using \textit{provenance} () Operator

Query-1

Query-2

Query-3
Provenance Query Engine

• Available as API for integration with provenance management systems
Provenance Query Engine

- Available as API for integration with provenance management systems
- Layer on top of a RDF Data Store (Oracle 10g), requires support for:
  - Rule-based reasoning
  - SPARQL query execution
Provenance Query Engine

- Available as API for integration with provenance management systems
- Layer on top of a RDF Data Store (Oracle 10g), requires support for:
  - Rule-based reasoning
  - SPARQL query execution
- Input:
  - Type of provenance query operator: `provenance()`
  - Input value to query operator: `cloned sample 66`
  - User details to connect to underlying RDF store
<table>
<thead>
<tr>
<th>Query ID</th>
<th>Number of Variables</th>
<th>Total Number of Triples</th>
<th>Nesting Levels using OPTIONAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Query 1: Target plasmid</td>
<td>25</td>
<td>84</td>
<td>4</td>
</tr>
<tr>
<td>Query 2: Plasmid_66</td>
<td>38</td>
<td>110</td>
<td>5</td>
</tr>
<tr>
<td>Query 3: Transfection attempts</td>
<td>67</td>
<td>190</td>
<td>7</td>
</tr>
<tr>
<td>Query 4: cloned_sample66</td>
<td>67</td>
<td>190</td>
<td>7</td>
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</tbody>
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Evaluation Results

- Queries expressed in SPARQL
- Datasets using real experiment data

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<tr>
<th>Dataset ID</th>
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<th>Total Number of RDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>DS 1</td>
<td>2,673</td>
<td>3,553</td>
</tr>
<tr>
<td>DS 2</td>
<td>3,470</td>
<td>4,490</td>
</tr>
<tr>
<td>DS 3</td>
<td>4,988</td>
<td>6,288</td>
</tr>
<tr>
<td>DS 4</td>
<td>47,133</td>
<td>60,912</td>
</tr>
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Evaluation Results

(a) Dataset Identifiers

(b) Query Identifiers
- Materializes a single logical unit of provenance
Query Optimization: Materialized Provenance Views

- Materializes a **single logical unit of provenance**
- Does not require query-rewriting
Query Optimization: Materialized Provenance Views

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- Does not require query-rewriting
- View updates: addressed by characteristics of provenance
Query Optimization: Materialized Provenance Views

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- Does not require query-rewriting
- View updates: addressed by characteristics of provenance
- Created using a memoization approach
Provenance Query Engine Architecture

**Provenance Query Classification**
Type of provenance query operator

**SPARQL Query Composer**
PREFIX ro: <http://obioum. #>
CONSTRUCT
{ ?p ro:has_participant trident:Ch
  ?i ro:has_process_process .
  .
} WHERE
{ OPTIONAL
  { ?p ro:has_participant trident:Ch
    ro:has_process_process .
  }
  OPTIONAL
  }
}

**TRANSITIVE CLOSURE**
Transitive Closure ("process", "preceded_by")

**Oracle 10g RDF Database**

**PROVENANCE QUERY ENGINE**

**Data Value Index**
Input value lookup
1 1 1 1 1 1

**Materialized Provenance Graphs**

**Data Source for Query Execution?**

**Result**

**Index data value from new materialized graph**

**To materialized graphs**

**To underlying database**

**Materialize Result Provenance Graph?**
Yes
No
Evaluation Results using Materialized Provenance Views

(a) Dataset Identifiers

(b) Query Identifiers
Semantics and Services Enabled Problem Solving Environment for *T. cruzi*

**Work Done**

- **PKR**
  - Development of ontologies
  - Conversion of internal lab data to RDF
  - Modeling of internal lab data to PEO

- **Cuebee**
  - Formulation of simple queries

- **External Collaboration**
  - Initiated with the Sanger Institute (UK) and Oswaldo Cruz Institute (Brazil)

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**Future Work**

- **PKR**
  - Addition of external databases, for e.g., TriTrypDB, Drug Bank, etc.
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  - Extensive collaboration on Semantics-driven Web services using SA-REST and APIHut
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- **External Collaboration**
  - Extensive collaboration to extend PLO with other human parasites
  - Expand the scope of PKR to support queries related to drug targets or repositioning (Oswalso Cruz, Brazil)
Semantics and Services Enabled Problem Solving

Questions?
http://knoesis.wright.edu/trykipedia

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