Bioinformatics reactivity features through the Semantic Web

Tiago Franco and José Alferes and Ludwig Krippahl and Ricardo Amador CENTRIA - Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa

Abstract

In order to propagate changes in, and between information nodes in the Web, a high-level architecture has been proposed for a reactive framework aligned with the goals and technologies of the Semantic Web – r^3 (see http://rewerse.net/I5/r3/). As part of the validation of this framework, we have used Bioinformatics as a case study. This approach required the design and implementation of a service ontology for the Bioinformatics domain (B-Domain). The ontology describes both the static and dynamic concepts of the domain, enabling reasoning and rule composition, without disregarding language heterogeneity in the Semantic Web.

B-domain example: Reasoning with SPARQL 1 - User registers ECA rule 2 - B-Domain pools PDB for new proteins (3) - PDB returns the IDs of the new proteins (4) - B-Domain queries protein XML in PDB markup 5 - PDB returns XML that is parsed and transformed to RDF by B-Domain 6 - B-Domain triggers Event for ECA rule providing the protein in RDF/XML format B-Domain **6**) - ECA Engine queries SPARQL Broker with Condition PDB Strub 8 - SPARQL Broker returns Condition result ECA Engine executes <u>Action</u> – store protein's RDF/XML in Personalized Mirror Broker User later browses his personalized mirror 9 Condition DESCRIBE ?structure WHERE (structure <http://www.w3.org/1999/02/22-rdf-syntax-ns#type (10) http://ontologies.w4sys.com/2007/b-domain#Dimer

Fig. 1. Validation Scenario: inferring the presence of Dimers in a new PDB structure

The concept was validated with 4 scenarios similar to the one presented in Fig. 1. This particular scenario shows a user being notified whenever a new dimer is published in PDB. To accomplish this task the scenario depicts the use of the B-Domain and SPARQL Brokers and of a Personalized Mirror. The first component integrates information sources relevant to bioinformatics exposing its features through B-Domain's ontology. The second leverages the features of the SPARQL query language to the framework's Enterprise Service Bus. The Event Condition Action (ECA) Engine is an r^3 rule engine that allows the registration and execution of Event-Condition-Action rules. Finally, the Personalized Mirror is a simple component that allows users to store RDF/XML data. The external interfaces of each component are described using the r^3 framework's ontology. The execution of the validation scenarios showed that Bioinformatics would strongly benefit from the features provided by B-Domain. Its characteristics allow the description of the static and dynamic semantic features of the domain, enabling reasoning on top of those concepts. It also offers a way to create and deploy declarative rules (ECA), which can be chained to create complex meaningful rules. The running version of B-domain can be found at http://rewerse.net/I5/r3/TST/install/dev/other/b-domain/.