INTERNET TOOLS FOR COMPUTATIONAL BIOLOGY

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Electronic access to computational tools in Biology is more important than ever. Electronic mail servers have been in use for a very long time already in order to access large archives of molecular biology data, such as the sequence data providers. The expansion of campus information systems (e.g., Gopher) allowed to implement immediate, interactive access to resources in both query and retrieval. More recently, the burst of World Wide Web has accomplished to make data accessible on networks which have never been visible in this kind of presentation before. Currently, 'the Web' is the most sophisticated tool for information handling which can be accessed by novices. Even more sophisticated tools allow to gather information and computations more specifically, but require to employ specific client software rather than common-purpose browsers. The most important development today is to enhance the access protocol for client-server applications and to expand server-server communication for data update and data presentation issues.

1 Overview

Information in Biology is growing rapidly. There are various areas of information processing which benefit from networked information. Table 1 lists the methods and tools in use today. It is important to realize that the end user is mostly affected by the client-server communication which implies that the browser or special access program will need to run on desktop equipment. Sophisticated computational work is performed on the remote server with very little use of networking, and the work load is shifted to the remote end entirely. The server-server communication, however, becomes increasingly important for database maintenance and requires that both ends are computationally active.

2 End-user aspects

The World Wide Web Virtual Library Biosciences page\(^a\) soon became the reference point of many servers. The page was split into subsections, and various curators now maintain the biology area in a coordinated, collaborative effort. Site presentation, teaching, discussion forums and database access are the main domain of WWW access tools.

\(^a\)http://golgi.harvard.edu/biopages.html
Table 1: Current Methods and Tools for Networked Biology

<table>
<thead>
<tr>
<th>Feature</th>
<th>Community</th>
<th>Purpose</th>
<th>Protocol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Teaching</td>
<td>beginner</td>
<td>learning</td>
<td>various</td>
</tr>
<tr>
<td>Data mining</td>
<td>beginner, casual user, researcher, provider</td>
<td>information, retrieval, resource discovery</td>
<td>http (WWW) and various specialized</td>
</tr>
<tr>
<td>Discussion forums</td>
<td>end user, provider</td>
<td>discussion</td>
<td>nnftp (NEWS)</td>
</tr>
<tr>
<td>Computational analysis</td>
<td>researcher</td>
<td>remote resource utilization</td>
<td>http (WWW) and various specialized</td>
</tr>
<tr>
<td>Data synchronization</td>
<td>provider</td>
<td>maintenance</td>
<td>specialized</td>
</tr>
</tbody>
</table>

Numerous computational tools are available. Some are implemented as stand-alone application using a specific client/server protocol. If WWW is used, the state of a multi-query dialogue has been transmitted using various approaches, such as retransmission of all data, the transmission of a 'identifier' and a stateful engine at the server site which inherits communication via WWW.

A very interesting approach is to utilize tools like the Moo, a virtual reality world which can be operated by keyboard and normal internet access. Those meeting places can be supplemented with WWW pages as discussion basis. More recently, tools became available to expand WWW into three dimensions. The Virtual Reality Modeling Language (VRML) extends the World Wide Web (WWW) interface with the additional ability to visualize three dimensional (3D) object oriented scenarios. Since most of the models in molecular science need 3D representations the new technique can be applied very effectively in biochemistry information networks.

3 Provider aspects

The time-dependency of databases in biology (exponential growth has been observed in the past) raises the difficult problem of synchronization. Quality control and multi-site updates are tackled with dedicated, special purpose protocols. Besides proper characterization of the data set itself as a function of time, the main challenge of synchronization will be an important issue in future biocomputing research on the internet.