The Chimera Collaboratory

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We create innovative computational and visualization-based data analysis methods and algorithms, turns these into easy-to-use software tools, and apply these tools for solving a wide range of genomic and molecular recognition problems within the complex sequence → structure → function triad
Application areas

Gene characterization and interpretation
Drug design
Variation in drug response due to genetic factors
Protein engineering
Biomaterials design
Prediction of protein function from sequence and structure
Motivation for Collaboratories

Science today, especially that which is biology-related, REQUIRES collaboration for success
  • Multi-institution papers the norm
  • Solid evidence of the benefits of “face-to-face” collaborations
  • Testimony from researchers that “collaboration promotes new ideas”

Desire to extend this productive environment to remote scientists
  • Promote more frequent and spontaneous collaborative projects
  • Encourage new collaborations

Desire to utilize remote collaborative environments in new ways
  • Training
  • Improved feedback for software development
Collaboratory Goals

Create an interactive three-dimensional graphics application to support collaborative studies of molecular sequence/structure/function among scientists at multiple remote locations for research and training

- Multiple scientists at remote locations able to interactively manipulate shared, complex three-dimensional molecular models (as similar as possible to “face-to-face” collaborations)
- Full semantics for the modification of an object by any collaborative participant
  - access to the underlying molecular data, not just the molecule's graphical representation
  - individual participants can perform operations privately first, then present results in collaborative session
- Small number (n<4) of participants for collaborative research
- Modest number (10-20?) of participants for training
Chimera Molecular Modeling System

Chimera is an extensible interactive 3-D modeling system designed to allow developers to quickly incorporate novel algorithms and analysis tools.

- Extensions can control standard user interface features (e.g. camera, help, menus, toolbar) as well as their own custom interfaces.

- Extensions are written in the Python programming language:
  - Python easy to learn, even for novice programmers
  - Python is object-oriented and provides features needed for development of complex codes
  - ~30 extensions written to date
Sample Chimera Extension

Multalign Viewer
• simultaneous display of protein sequence and structure
Sample Chimera Extension

Volume Viewer
  • an extension for visualizing three-dimensional (3D) numerical data sets

Electrostatic potential (surfaces)
Electron density (mesh)
Electrostatic potential (solids)
Sample Chimera Extension

**ViewDock**
- rapid screening of promising drug candidates found with the UCSF DOCK program
Sample Chimera Extension

Collaboratory
- supports collaborative studies of molecular structure among scientists at multiple remote locations
Chimera Collaboratory Features

Commands input on one workstation (typed keywords or menu selections), are displayed and executed on all participating workstations
- Molecular models are displayed on all workstations simultaneously in response to input from any participant

Model control provided for each participant
- Interactive control of rotations, translations, scaling, ...
- Colored “telepointers” used by participants to indicate particular regions of interest
- “Private window” for testing ideas
- Participants can join and leave an on-line session at any time
Technologies Employed

**Chimera**
- Collaboratory implemented as an extension to the basic system

**CORBA**
- Common Object Request Broker Agent - used to construct rendezvous service for sessions

**COTS desktop videoconferencing**
- Prefer standards-based tools (e.g. Polycom’s ViaVideo)
- High quality audio imperative, low frame rate video just fine

**Low-latency / modest-bandwidth networking**
- Initial session startup requires data be replicated remotely, but otherwise only modest bandwidth required
Status

Two-participant version largely complete and in active use by our collaborators

Synchronization mechanism being generalized to work with other Chimera extensions

Refinement of user interface on-going

Scaling number of participants just got underway
  • Social interaction issues may complicate this

Formal evaluation not yet begun
Continuing Challenges

Lack of good quality desktop VTC for Macintosh
Session setup (Chimera + VTC) still awkward
Difficult to troubleshoot where network bottlenecks occur (e.g. high latency) and what to do about them
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Further information:
- www.cgl.ucsf.edu