



Extending Chimera for collaborative molecular visualization

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CHIMERA

Extending Chimera for Collaborative Molecular Visualization

Goals

Tools

Collaboratory

Technologies

Overview

To develop a collaboratory environment for carrying out interactive three-dimensional molecular modeling studies

- * multiple scientists at remote locations to interactively manipulate shared, complex three-dimensional molecular models ('face-to-face')
- * full semantics for the modification of an object by any collaborative participant
 - access to the object's data, not just the object's graphical representation
 - individual participants can perform operations privately first, then present results in collaborative session



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typical scenario

- * type command on keyword on one workstation, display and execute the command on all other participating on-line collaboration workstations
- * display molecules moves in tandem in real-time on all workstations simultaneously in response to input from any participant
- * provide independent control for each participant for a separately shaped or colored mouse cursor
 - highlight interesting facets of a molecular model
 - interactively control rotations, translations and scaling
- * participants can join and/or leave an on-line session at any time



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Computer graphics

- * qualitative
- * generates pictures
- * quality vs. real-time, interaction
- * value lies not in numbers themselves, but insights gained
- * idea generator

Experimental techniques

- * X-ray crystallography
- * NMR
- * Mass spectroscopy



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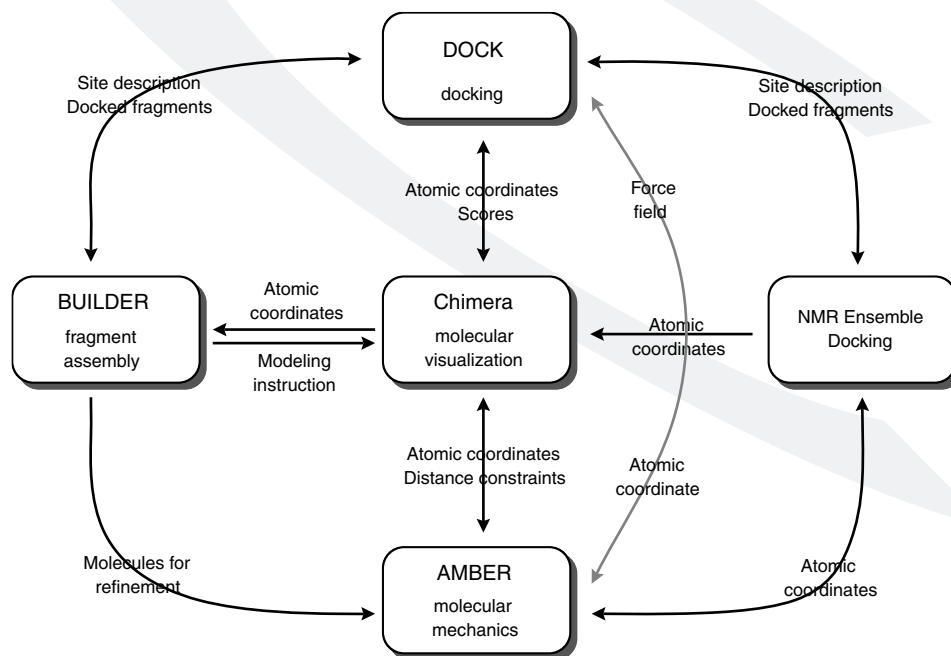
Collaboratory

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Thematic Example: Structure-Based Drug Design

- * Facile and comprehensive system for determining the structures of proteins and nucleic acids in solution and designing new ligands and drugs
- * Integrated Software Tools for Structure-Based Drug Design Applications





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- * data exchange among programs
 - standardized data definitions
 - common I/O routines
 - CHIMERA (C++ and Python)
 - AMBER (FORTRAN)



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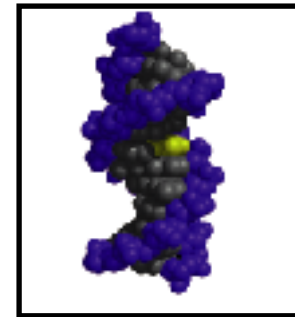
Overview

* Test Cases

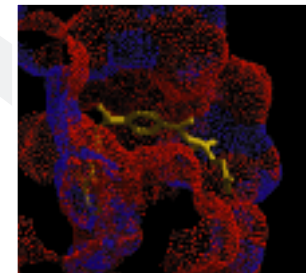
Research

- * 1-1
- * 1-N
- * N-N

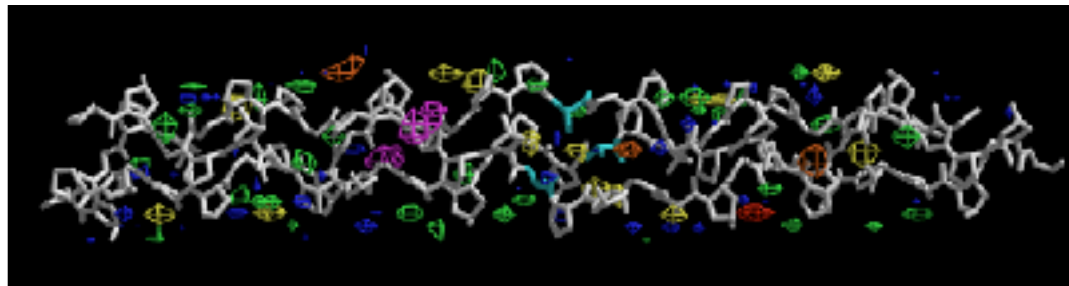
- Molecular Mechanisms of Mutagenesis and DNA Repair: Recognition of Damaged DNA



- Dihydrofolate Reductase



- Structural Aspects of type 1 Collagen in Osteogenesis imperfecta





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Training

- * active learning for local and remote users
 - classroom-style teaching
 - collaboratory-style teaching
- * 1-1
- * 1-N
- * Chimera
 - users local to UCSF
 - users at remote sites with high-speed network access
 - users with today's typical Internet access



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Desktop Videoconferencing

- * real-time, multi-party multimedia application
- * high quality audio
 - better or equal to clear, static free telephone connection
- * be able to discern important facial or hand gestures
 - full-motion video
 - reduced frame video
- * off-the-shelf



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Data Network

- * Parameters affecting network performance
 - bandwidth
 - latency
 - delay variance
 - connection quality
 - multicast support
 - quality-versus-price tradeoffs
- * Collaboratory Data connection characteristics
 - lower bandwidth than videoconferencing
 - higher reliability
 - bursts of activity



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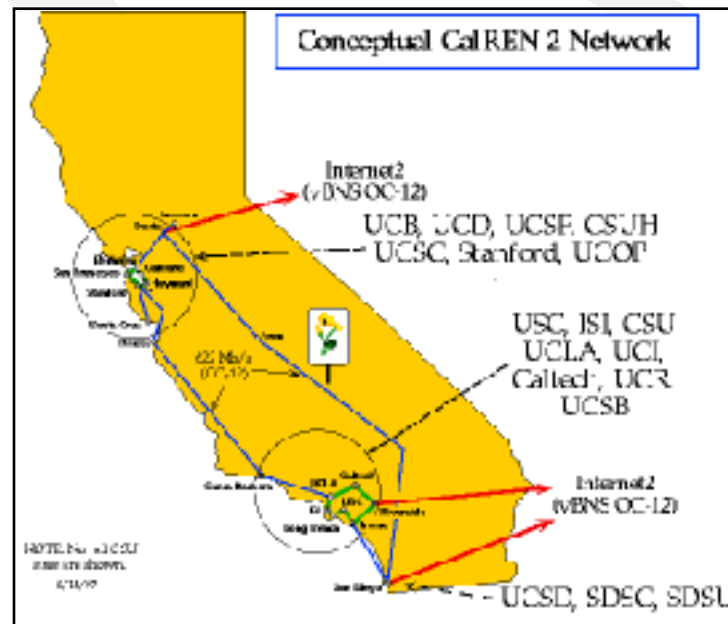
Tools

Collaboratory

Technologies

Overview

- * CENIC/CalREN-2 - high speed backbone network infrastructure serving higher education in California
 - map of CalREN-2
 - state-of-the-art data communications
 - minimum internode network bandwidth OC-12 (622 Mbps)
 - UCSF connected via a dedicated OC-3 (155 Mbps) "Packet-over-Sonet" network interface via Cisco router





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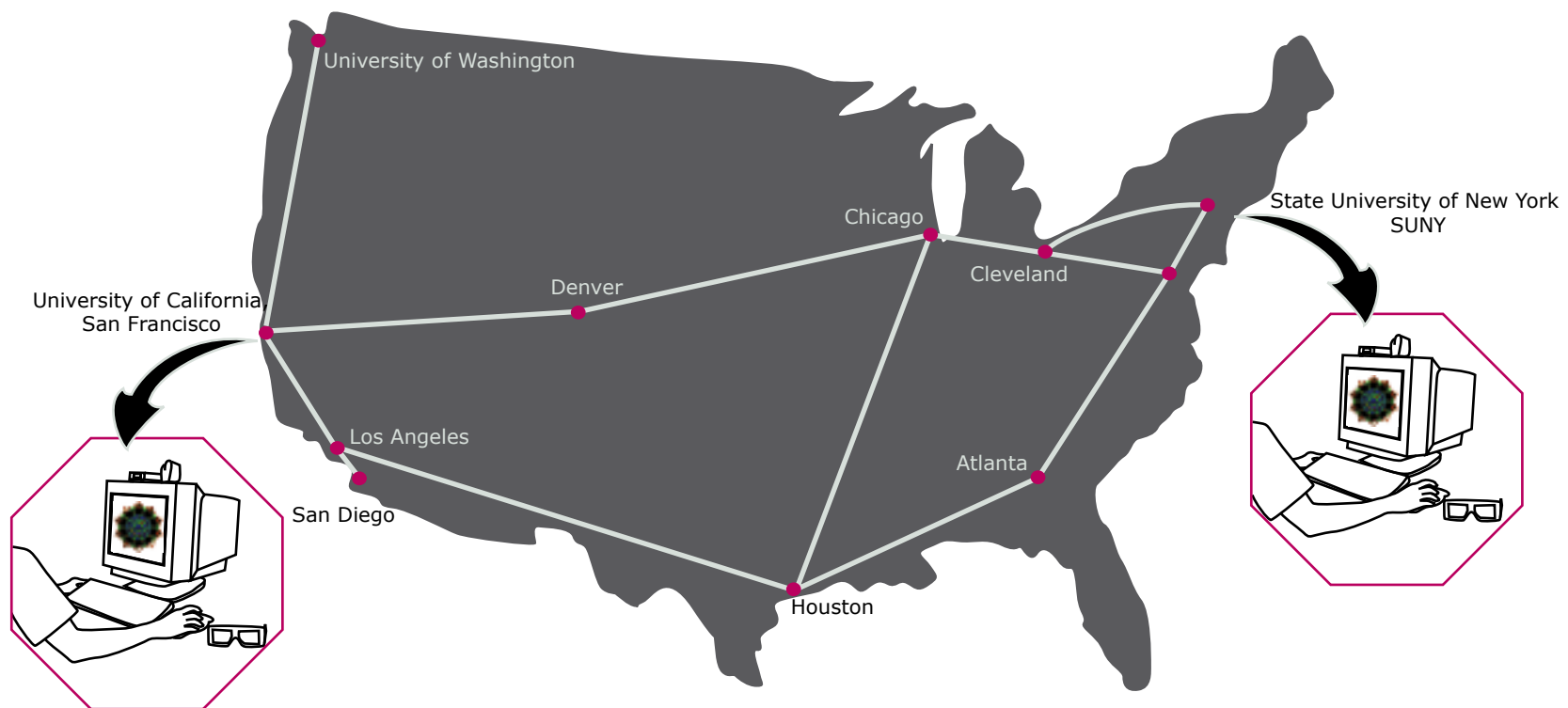
Tools

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Overview

- * CENIC/CalREN-2 connected to vBNS via multiple OC-12 connections
- map of vBNS





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Example of another Collaboratory

- * Molecular Interactive Collaborative Environment (MICE)
 - stores molecular scenes in a relational database and queried
 - rendered in VRML
 - does not allow for modification of an object
 - for further information, see <http://mice.sdsc.edu>



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Background

Extensibility

Chimera

Modeling semantics verses graphics only

Utilize widely available software packages

- * TK (graphical interface)
- * OpenGL (three-dimensional graphics)
- * Python (command language)
 - syntax is straightforward
 - facilitates use by non-programmers
 - embodies object-oriented features
 - extensive libraries available for handling strings, sets, files and graphics
 - source and binaries freely available
 - Copyright allows for free use, even commercial and resale
 - See <http://www.python.org>



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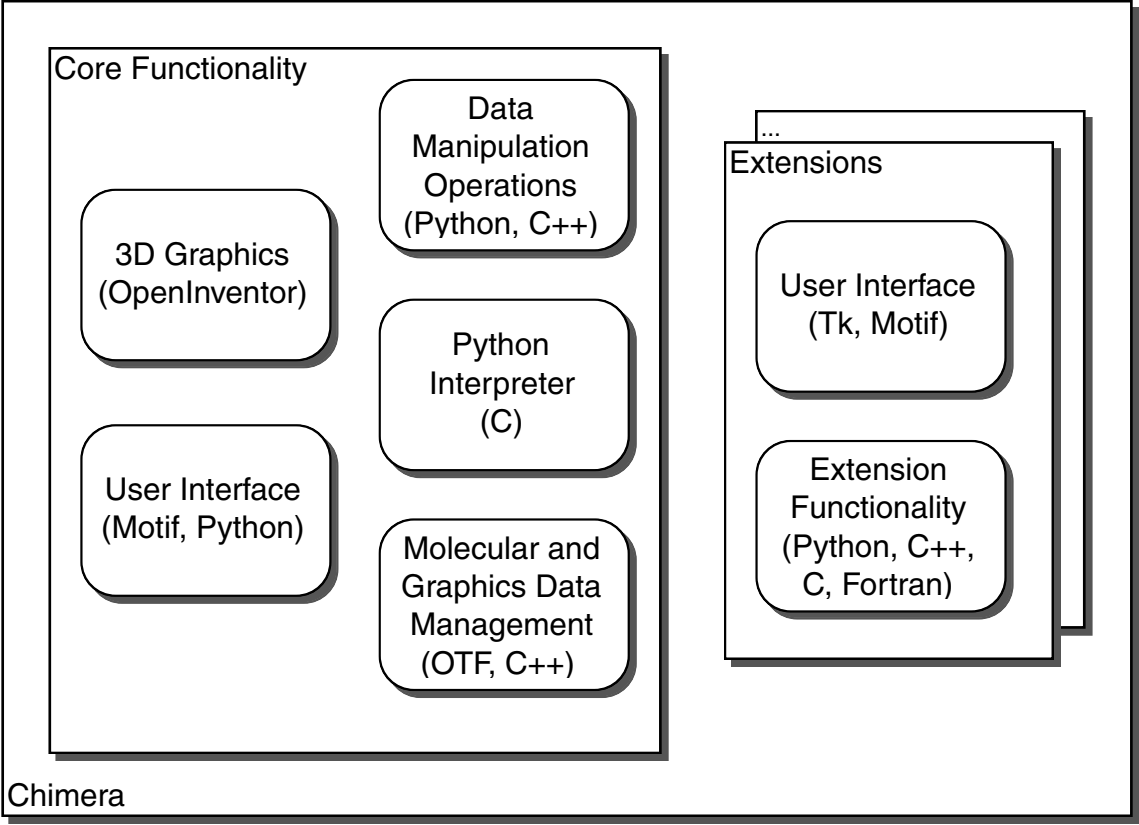
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Background

Extensibility

Chimera

Chimera Software Architecture





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Background

Extensibility

Chimera

Core Functionality

- * data management
- * user interface and methods of user interaction
- * three-dimensional interactive graphics
 - geometric representations of molecules (wireframe, spheres, ball-and-stick, ribbon)
 - molecular surfaces (wireframe, polygonal mesh)
 - text mapping
 - coupling of geometric representations and graphical properties (color and translucency)
 - volume rendering (three-dimensional fields)
 - protein solvent density
 - ensemble probability distributions
 - occupancy distributions from molecular dynamics trajectories
 - isosurface generation



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Background

Extensibility

Chimera

- * interpreted command language
- * infrastructure support
- * hypertext Help system
- * single user system

Extensions

- * written in Python, C, C++, Fortran, etc.
- * built on top of the core functionality
 - World Wide Web capabilities
 - GRAIL (Python web browser)
 - * standard web-browsing capabilities
 - * download and execute Python (similar to Netscape and Java)
- * provide graphical user interface (GUI) for user extensions to basic menu-driven interface
- * interaction communications protocol (run CHIMERA on several workstations simultaneously)



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Prototype

Development

Implementation

Prototype in MidasPlus

- * Proof of concept
 - requires identical setup (both software and user data)
- * 1-1
- * Uses custom protocol over network connection
- * Only commands are transmitted (no bulk data)

Development in Chimera

- * Solutions for 1-1, 1-N and N-N
 - may be different due to different requirements (e.g. reliability, speed, etc.)
- * Communication among participating software clients is central to collaborative design
- * Different technical solutions satisfy different requirements



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* Solutions under consideration:

- CORBA

- Common Object Request Broker Architecture
- From Object Management Group (OMG)
 - * consortium of vendors and end users
- Distributed objects (similar to remote procedure calls [RPC])
- Very good for 1-to-1
- See <http://www.corba.org>

- Multicast

- Many implementations (lots of research articles)
- Most famous is MBONE
- Good for 1-N where reliability requirements is low
- Efficient use of network bandwidth

* Target 1-1 first



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Summary

Designed a real-time, interactive molecular modeling collaboratory to be used for research and training

Currently being implemented as an extension to the new molecular modeling software Chimera

See <http://cgl.ucsf.edu> for updates and availability



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