SnBDCV

Shake-and-Bake

Distributed Collaborative Visualization

By: Amin Ghadersohi
CSE714 – Fall 2006 - Dr. Russ Miller.
Department of Computer Science and Engineering
Distributed Visualization

- Modules run on different machines.
- Distributed resources used in order to visualize large and computationally intensive datasets.
- Only the computation for the visuals is performed on distributed resources.
Collaborative Visualization

- Multiple human participants
- Joint interpretations of visualized data
- However, may still refer to a single view system with multiple people looking “over each other’s shoulders”
Distributed Collaborative Visualization (DCV)

- Collaboration performed both at the system and human levels
- Sharing of resources and data from remote locations
- Common virtual environment
- Grid friendly!
Requirements

- Networking
  - TCP and UDP
- Real-time Distributed Database
  - On top of network
- Data Consistency
  - Function of Real-time Distributed Database
- Scalability
  - Depends of Real-time Distributed Database
- Security
- Portability
- Graphics performance
  - OpenSceneGraph API
- Interaction performance
  - Tradeoff between consistency and interaction performance
Data Consistency

- Central record locking mechanism.
- Performed by a third tier: the bootstrap
- Consistency guarantees
  - Performance tradeoff
    - A client needs to wait for permissions before changing the data
    - Decouple consistency from data distribution
    - The bootstrap is a central, lightweight and fast protocol based on UDP
- Scalable design
SnB DC V
Shake-and-Bake
Distributed Collaborative Visualization

External Data
- Raw Data
- Relational DB
- WWW

DCV Servers
- Server 1
- Server 2
- Server m

Bootstrap
- Record Locks & Keys
- Certificate Validation

DCV Clients
- Client 1: Workstation
- Client 2: Mobile
- Client 3: CAVE VR
- Client n: Tile Display Wall

UDP:
- Authentication
- Authorization
- Server Assignment/Request
- Key Generation/Lease/Return

TCP:
- Distribute data changes

Input Data
- Environment Data
Failure Management

- Network-aware application layer
  - Connection, dropout, and error (lost, corrupt packet) notification.

- Client disconnection
  - Wait for reconnection
  - Exit at user’s will

- Server disconnection
  - Bootstrap re-assigns a new server for the lost server’s clients.
  - If no others servers available, the clients will halt all operations until the server is reconnected, or exit at user’s will.

- Bootstrap disconnection
  - Predetermined server will re-spawn bootstrap from backup data.
Load Balancing

- One server can only serve so many clients
- More servers needed for extra clients
- Servers form a data backbone
- Bootstrap assigns servers to the clients dynamically based on system load statistics
Based on a certificate or proxy from a known and trusted Certificate Authority (CA) that can be verified by the bootstrap.

Maintain a mapping of certificates to a list of valid IP addresses to block intruders with stolen or hijacked certificates.

- Detect spoofing via the routing trace.
Graphics Performance

Video Performance Benchmarks

Frames Per Second (FPS)

- **ATI Radeon 7200 32MB P4 2.0GHz 512MB**
- **ATI Radeon Mobile 64MB Athlon XP 3000+ 512MB**
- **Geforce FX 5600 128MB P4 2.0GHz 1GB**
- **Geforce FX 5200 128MB P4 1.6GHz 256MB**
- **Geforce 3 64MB PIII 900MHz 256MB**
- **ATI Radeon 7200 32MB P4 2.0GHz 512MB**
- **ATI Radeon Mobile 64MB Athlon XP 3000+ 512MB**
- **Geforce FX 5600 128MB P4 2.0GHz 1GB**
- **Geforce FX 5200 128MB P4 1.6GHz 256MB**
- **Geforce 3 64MB PIII 900MHz 256MB**

Cable 5 Mb Ethernet 100 Mb

- **FPS 800x600**
- **FPS 1024x768**
- **FPS 1280x1024**
- **FPS 1024x768 FSAA 2x**
Interaction performance

Bootstrap Request Round Trip Time (Cable 5 Mb/s)

Bootstrap Request Round Trip Time (Ethernet 100 Mb/s)
Shake-and-Bake (SnB)

- *Shake-and-Bake* [Miller et al. 1994] is a state-of-the-art program for molecular crystal structure determination from X-ray crystallographic data.
- **The SnB package:**
  - Distributed to more than 500 laboratories worldwide.
  - Released in the mid-1990s.
    - primitive visualization.
- **Advances in Grid Computing:**
  - the *SnB* package no longer bound to one physical location.
  - Jobs queued/executed from anywhere in the world.
  - Need to monitor intermediate distributed results.
**SNBVIS: Shake-and-Bake Visualizer**

- Visualization of protein structures
- Integrate multiple data sources, such as *SnB* instances running on the Grid
- Monitor progress of structures
- Discuss, annotate, and edit structures as a team
- Used by chemists and the crystal determination community

- Edit structures determined by the *SnB* package:

  - Select atom for deletion
  - Atom deleted
  - Undelete atom
  - Atom undeleted
  - Select atoms to bond
  - Atoms bonded

- Calculate structural properties:

  - Distances
  - Angles
  - Torsion angles

- Future:

  - Molecular Docking
  - Electron Density Fitting
Grid MACE: Grid Monitoring and Administration Collaborative Environment

Distributed Grid Resources

- Visualization of high volume, real-time Grid monitoring data
- Aid to administrators and users of the Grid

ACDC Grid Monitoring Infrastructure

Monitoring Data Storage  Web Server

Bootstrap

Client 1: Workstation
Client 2: Mobile
Client 3: CAVE VR
... 

DCV Servers

DCV Clients
Amir: What's going on with Lennon?
Amir: I'm gonna look at the operations dash for more details on that.
Summary:

- Enable distributed collaboration at both the system and user level via a three-tier software architecture developed at CCR (Center for Computational Research http://www.ccr.buffalo.edu)
- Enable visualization and interaction with data across a geographically disparate network topology
- Integrate multiple data sources:
  - Scientific
  - Multimedia
  - Real-time
- Research and Development:
  - Real-time distributed databases
  - OpenGL 3D programming
  - 3D Modeling
  - Character animation
  - User interaction
  - Virtual Reality (CAVE VR)