CyberTools

Advancing Science through co-development of Cyberinfrastructure and Scientific Applications
Background

*Four Layers: Each Reinforces the Next*

- **Layer 1. 2001-3: Gov. Foster Vision 2020**
  - Bio Initiative
  - $5.7M one time capital outlay; $2.75M recurring
  - IT Initiative: $25M annual across 5 campuses
    - 2003: CCT, $9M annual at LSU

- **Layer 2. 2004: LONI and its impact**
  - Gov. Blanco: $40M + $10M infrastructure
  - NLR Membership

- **Layer 3. 2007: CyberTools**
  - $12M Statewide NSF/EPSCOR CI project

- **Layer 4. 2007: LONI Institute and beyond**
  - $15M Statewide project to recruit people

*Catalyzed many new hires, funding, additional investments*
Layer 2: LONI

LA Tech

Ul-L

SUBR

LSU

Tulane

UNO

Just Equipment: Need More!

~ 100TF IBM, Dell Supercomputers
National Lambda Rail
LONI Creates a Regional Environment

- Suddenly collaborative, competitive
  - Meetings, collaborations between universities: most important!

- Many new multisite projects built on top of LONI
  - NSF ESPCOR RII: CyberTools
    - Common software infrastructure for MD, CFD, Experiment
    - Viz services, data services, computing services, co-scheduling, portals
  - DOE EPSCOR: UCoMS
  - NSF MRI: PetaShare, VizTangibles
  - NIH LBRN, Enlightened, HD Classes, etc...
  - BoR PKSFI: Security CyberSpace Center, LONI Institute
National Infrastructure

- NSF $2.2M HPCOPS Award
  - LONI joins TeraGrid (Jan08)
  - 7 new HPC staff
  - NCSA subcontracted to support

- NSF $208M Track 1 PetaScale Award
  - LSU partners with NCSA; 10PF-class computer
  - LSU focus on applications, tools, outreach

- CCT submitting new $30M NSF Track 2c

We are working to ensure that Louisiana researches can take advantage of all this!
LONI and TeraGrid

Resource Provider (RP)

Software Integration Partner

SDSC
TACC
UC/ANL
NCSA
ORNL
PU
IU
PSC
UNC/RENCI
UW
LSU
UC/ANL
PSC
UW
ORNL
Caltech
NCAR
USC/ISI
SDSC
UC/ANL
Grid Infrastructure Group (UChicago)

LONI and TeraGrid

Resource Provider (RP)

Software Integration Partner

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UW
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PSC
UW
ORNL
Caltech
NCAR
USC/ISI
SDSC
UC/ANL
Grid Infrastructure Group (UChicago)
Layer 4: LONI Institute

- $15M, 5-year project
  - $7M BoR, $8M from LA Tech, LSU, SUBR, Tulane, UNO, UL-Lafayette
  - 12 new faculty, 18 grads, 6 CI staff!

- Built on LONI infrastructure, create bold new inter-university superstructure
  - Faculty, staff, students focus on CS, Bio, Materials, but all disciplines impacted; digital art & media!
  - Promote collaborative research at interfaces for innovation

- Draws on, enhance strengths of all universities
  - Strong groups recently created; collectively world-class
  - Much stronger recruiting opportunities for all institutions

- Create University-Industry Research Centers (UIRCs)
  - Economic development!
Original LONI Vision

- Build LONI infrastructure - create **bold new inter-university superstructure**
  - *All disciplines impacted* -- EPSCoR RII focuses on the development of computational tools in collaboration with biosensor and fluid transport process researchers
  - Promotes collaborative research at interfaces for innovation

- Draw on, enhance strengths of all universities
  - Strong groups recently created; *collectively world-class*
  - Much stronger recruiting opportunities for all institutions

- Transform our state
  - Such committed cooperation between sites extraordinary
State Cyberinfrastructure

RII Science Drivers
LONI Institute
SCIENCED

CyberTools

LONI
TeraGrid
CyberTools

- We have an emerging website!
- http://cybertools.loni.org
- Thanks Ana!
Integrated with Science Drivers

- Geno/immuno sensors: Cortez
- Small molecule sensors: Soper
- Bio-transport: Gaver
- Environmental transport: Allen

Science Drivers:
- Biosensor Development: Soper
- Transport Processes: Gaver

CyberTools:
- Seidel

Work Packages:
- WP1: Data, Scheduling
- WP2: Information
- WP3: Visualization
- WP4: Application

People:
- K-12
- Undergraduate
- Graduate
- Postdoctoral
- Faculty
Science Driver Needs

- **Bio-Sensors:**
  - Molecular Dynamics (MD) Simulations
  - CFD – Newtonian and Non-Newtonian Fluids; Chemical interactions at surfaces (MD); CFD Flow Simulations (mixed-scale)

- **Bio-Transport**
  - Multiscale large scale simulations, Boltzmann/Particle simulations in capillaries (non-continuum)
  - Mesoscopic simulations for property evaluation (coarse-graining)
  - Coupled atomistic-continuum hybrid model, new hybrid atomistic/coarse-grained/continuum models

- **Environmental Transport:**
  - Storm Surge Simulations: dynamic code coupling, resource allocation, drives DDDAS toolkit development, coupling Cactus-ADCIRC
  - Decision algorithms implemented in toolkits

- **All**
  - Data storage, management, retrieval, visualization
Building on our Strengths in Enabling Software

Very ambitious, could not be done without these

- Cactus Framework
- HARC Co-allocator
- PetaShare Data Management
- Parallel CFD Toolkit
- HA-Oscar Cluster
- SAGA Grid Toolkit
- GridSphere Portal Framework

Leveraging New and Existing Collaborations:

- SPRUCE Urgent Computing (ANL)
- Charm++ (Illinois)
- Globus (Chicago/ANL)
- Condor (Wisconsin)
Synergistic CyberProjects
Partial list...all multinstitutional

- NSF CFD IGERT
- PKSFI LONI Institute
- PKSFI CyberSpace
- NSF TeraGrid
- NSF TangViz
- DOE/BOR UCOMS
- DoD/BOR Epscor
- NSF DynaCode
- DOE UCoMS
- NSF XiRel
- NSF Alpaca
- ...

WPs in a Nutshell

**WP1: Scheduling and Data Services (Dua, Kosar)**
Infrastructure deployment & high availability; scheduling; data archiving & retrieval; metadata

**WP2: Information Services and Portals (Allen)**
Information services (infrastructure, apps, experiments); application interfaces for scientists; portals for information gathering

**WP3: Visualization Services (Cruz-Neira, Ullmer)**
Data/Viz integration; HD streaming viz; advanced viz facilities; integration with application toolkits

**WP4: Application Toolkits (Jha)**
Development of toolkits to support all simulation codes (CFD, MD, other); app manager; SAGA interfaces
WP 1: Data & Scheduling

*Dua/Kosar*

- **Activities**
  - Deployment (Katz, GA)
  - Data generation and management for simulation and experimental data (Kosar/Allen, .5PD*, Soper, .5GA)
  - Resource scheduling/co-scheduling (Kosar/Allen, .5PD*)
  - High availability for on-demand resources (Box, GA)
  - Metadata and information management (Dua, .5PD, Iyengar, GA)

- **Challenges:** Management, retrieval, categorization, mining, scheduling & co-scheduling, metadata, ontologies

- **Components:** Core Grid software, PetaShare, HARC, Spruce, ROAR, task farming, HA-OSCAR

* Mehmet Aktas (Fox student)
WP 2: Info Services & Portals

Allen

- **Activities:**
  - Reliable and up-to-date information services (Dua, .5PD)
  - Portals for discovering, monitoring, and providing information about resources and applications (Allen, GA*, Soper, .5GA, Acharya, .5GA)

- **Challenges:** Application monitoring, steering, production environments, information schema

- **Components:** GridSphere portals for applications and services on LONI

* Kate Stamou, KTH
WP 3: Visualization Services

*Cruz-Neira, Ullmer*

- **Activities:**
  - Data and visualization integration (Cruz/Jindal, GA, Ullmer, GA)
  - HD streaming visualization (Venkataraman, GA, Jana/Ullmer, .5PD, Cruz/Jindal, .5PD)
  - Advanced facilities (Jana/Ullmer, .5PD, Cruz/Jindal, .5PD)
  - Application toolkits (Iyengar/Karki, GA)

- **Challenges:** Data formats and descriptions, HD streaming visualization, leveraging advanced facilities, integrating with application toolkits

- **Components:** LITE, data integration architecture, automation, training, tangibles.

*Additional Application students TBA*
Collaborative interaction devices for visualization; developed w/ NSF MRI for ~8-site deployment.

Above: device for data, parameter control. Right: use with video conferencing, immersion/CAVEs, outreach activities
Viz tangibles technology
WP 4: Application Toolkits

Jha

Activities:
- Cactus CFD Toolkit (Allen, .5PD*, GA, Acharya .5PD, .5GA, Gaver, .5GA, Cortez, .5GA)
- Molecular dynamics toolkit (Allen, .5PD*, Jha, GA, Others)
- Application manager (Kaiser, CCT GAs)
- SAGA adaptors/Cactus SAGA thorns (Allen, GA, Jha, GA)

Challenges: Interfaces for CFD, integration of Cactus and Charm++, application manager.

Components:
- Cactus framework, Charm++, SAGA, CFD Toolkit, partner codes.

*Rene Heinzl, Wien
The Cactus Toolkit- A Unifying Framework for Parallel Computing

- **Physics**
  - Navier Stokes
  - RANS--DNS
  - Boussinesq
- **Meshing Tools**
  - Cartesian, IBM
  - Body-fitted
  - Unstructured
- **Numerics**
  - Finite Diff.
  - Finite Volume
  - Spectral
- **Solvers**
  - Super LU
  - Trilinos
  - PetSc
- **Visualization**
  - Tangible
  - Immersive
  - Conventional

**Application Drivers**
- Storm Surge/Coastal Modeling
- Bio-transport in vessels
- Micro-fabrication
- Microfluidics
- Antibody binding
- Cellular/lipid layer transport

**Multi-Scale Simulation Tools**
- CFD Toolkit
- MD Toolkit

**Physics**
- Force fields
  - CHARMM
  - AMBER

**Structure Tools**
- Molecular Conf.
- PDB Database

**Numerics**
- Integration Meth.
- R-K
- Pred-Corr
- Verlet

**Solvers**
- R-K
- Pred-Corr

**Visualization**
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Management & Work Plans

- **Collaboration**
  - Our WP teams will meet regularly
    - In person, AG, HD (WP3!)
    - Already had WP4 meetings…
  - Collaborative code development
    - CVS, Cactus design, abstraction
  - All hands meetings for real team development
    - WPs, science drivers together for extended period

- **Deployment, Training, & Outreach**
  - LONI, LONI Institute, TeraGrid staff to deploy tools
  - Carry out statewide training to broaden impact
  - Outreach Program: CyberTools down to secondary schools
    - E.g., LIGO portal, high school playstations, Anitra Wilson specifically working on WP3-4 outreach

- **Metrics for success will be monitored carefully!**
Summary

- State has made major investments in information technologies
  - Working hard to make them resonate across state
- NSF is also making major investments
  - We are working hard to align state, prepare for future national CI
- CyberTools is a critical layer
  - It is backed by many ongoing projects, and by numerous experienced staff and faculty at CCT, LITE and CS departments across the state
  - Integrates local CI development with local science projects, national CI
  - Will require much (!) coordination