CyberTools

Advancing Science through co-development of Cyberinfrastructure and Scientific Applications

Background
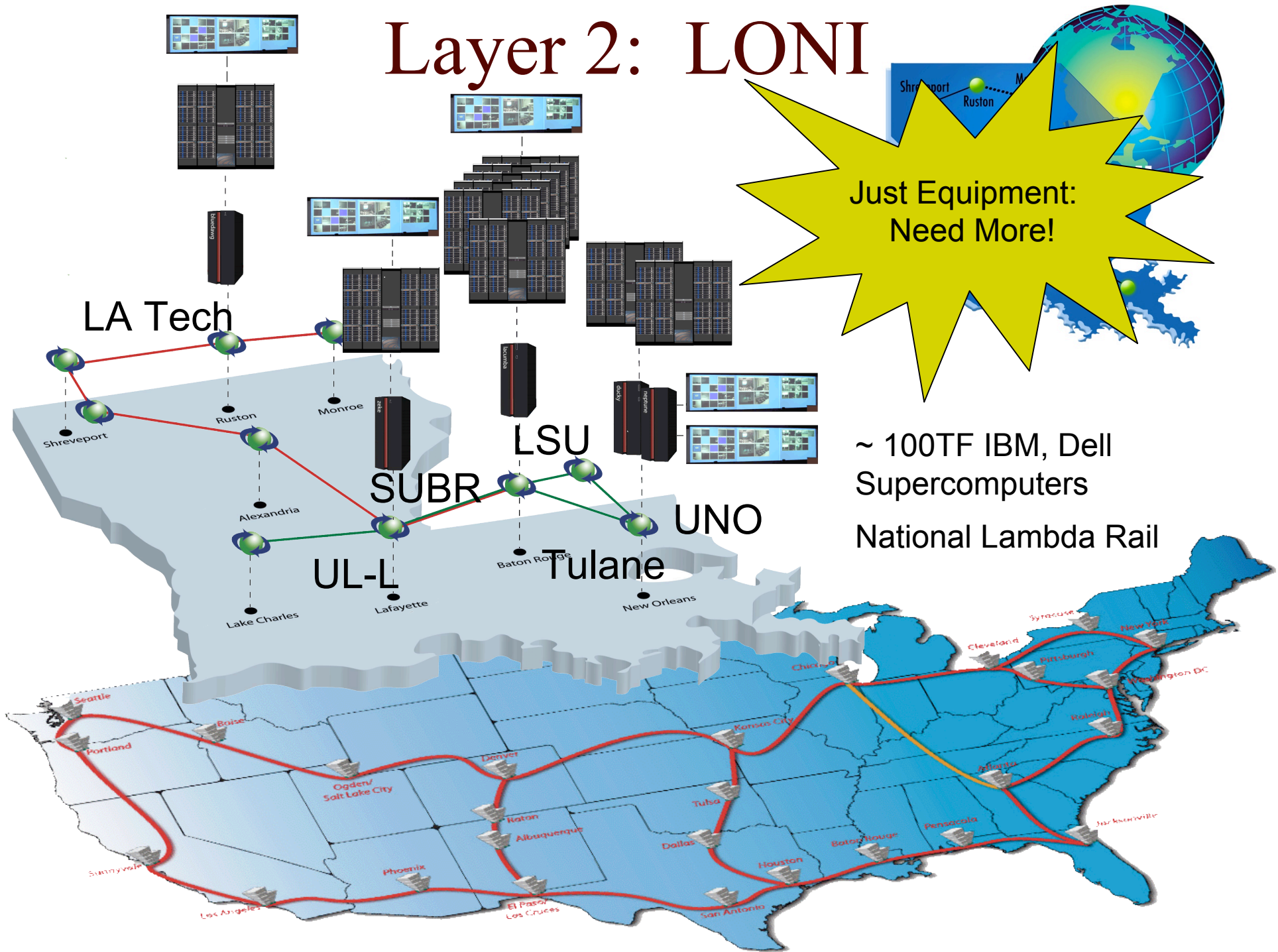## *Four Layers: Each Reinforces the Next*

- □ 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 recrtuit people

Catalyzed many new hires, funding, additional investments

Layer 2: LONI

LA Tech

SUBR

LSU

UNO

UL-L

Tulane

Just Equipment: Need More!

~ 100TF IBM, Dell Supercomputers

National Lambda Rail

Shreveport

Ruston

Monroe

Alexandria

Lake Charles

Lafayette

Baton Rouge

New Orleans

Seattle

Portland

Boise

Ogden/ Salt Lake City

Denver

Kansas City

Chicago

Cleveland

Syracuse

New York

Pittsburgh

Washington DC

Raleigh

Atlanta

Sunnyvale

Los Angeles

Phoenix

El Paso/ Los Cruces

San Antonio

Houston

Dallas

Tulsa

Baton Rouge

Pensacola

Jacksonville

Albuquerque

Raton

# 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
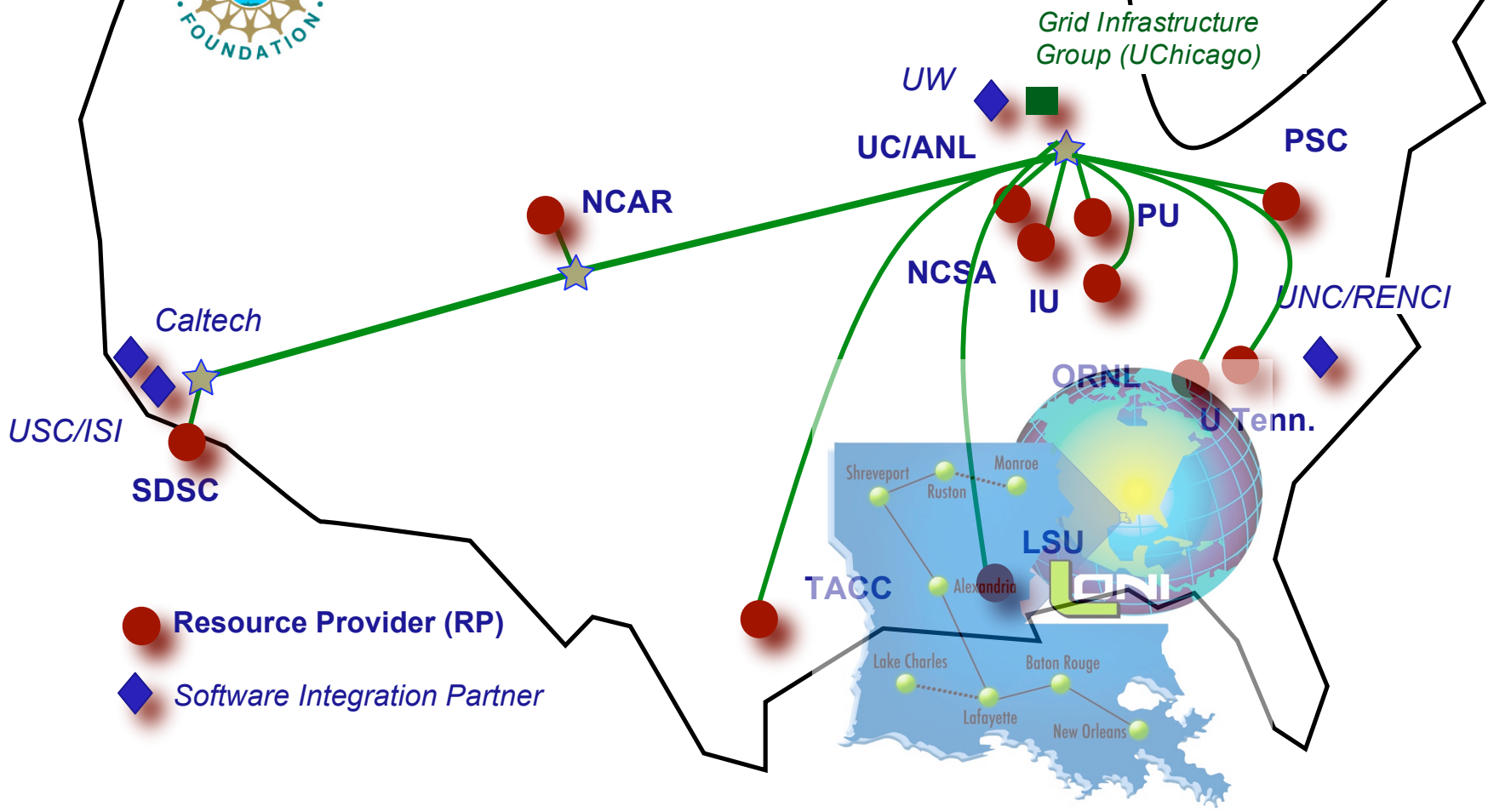
National Infrastructure

- 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
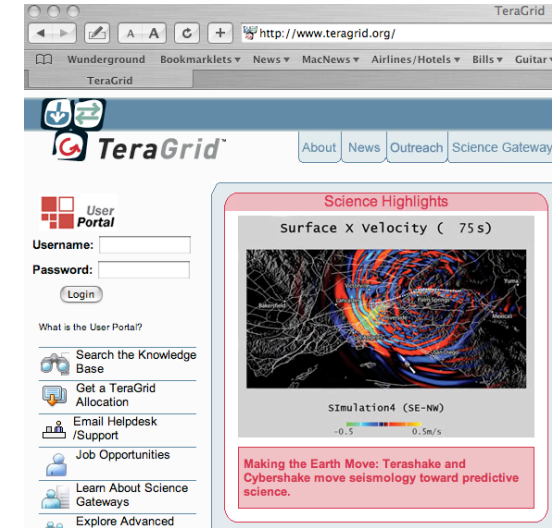
We are working to ensure that Louisiana researches can take advantage of all this!

LONI and TeraGrid

Grid Infrastructure Group (UChicago)

UW

UC/ANL

PSC

NCAR

PU

NCSA

IU

UNC/RENCI

Caltech

ORNL

U Tenn.

USC/ISI

SDSC

Shreveport Monroe

Ruston

LSU

Alexandria

TACC

LONI

Lake Charles Baton Rouge

Lafayette New Orleans

● Resource Provider (RP)

◆ Software Integration Partner

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	SCIENCE

| CyberTools | | |

LONI	TeraGrid

CyberTools

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

Integrated with Science Drivers
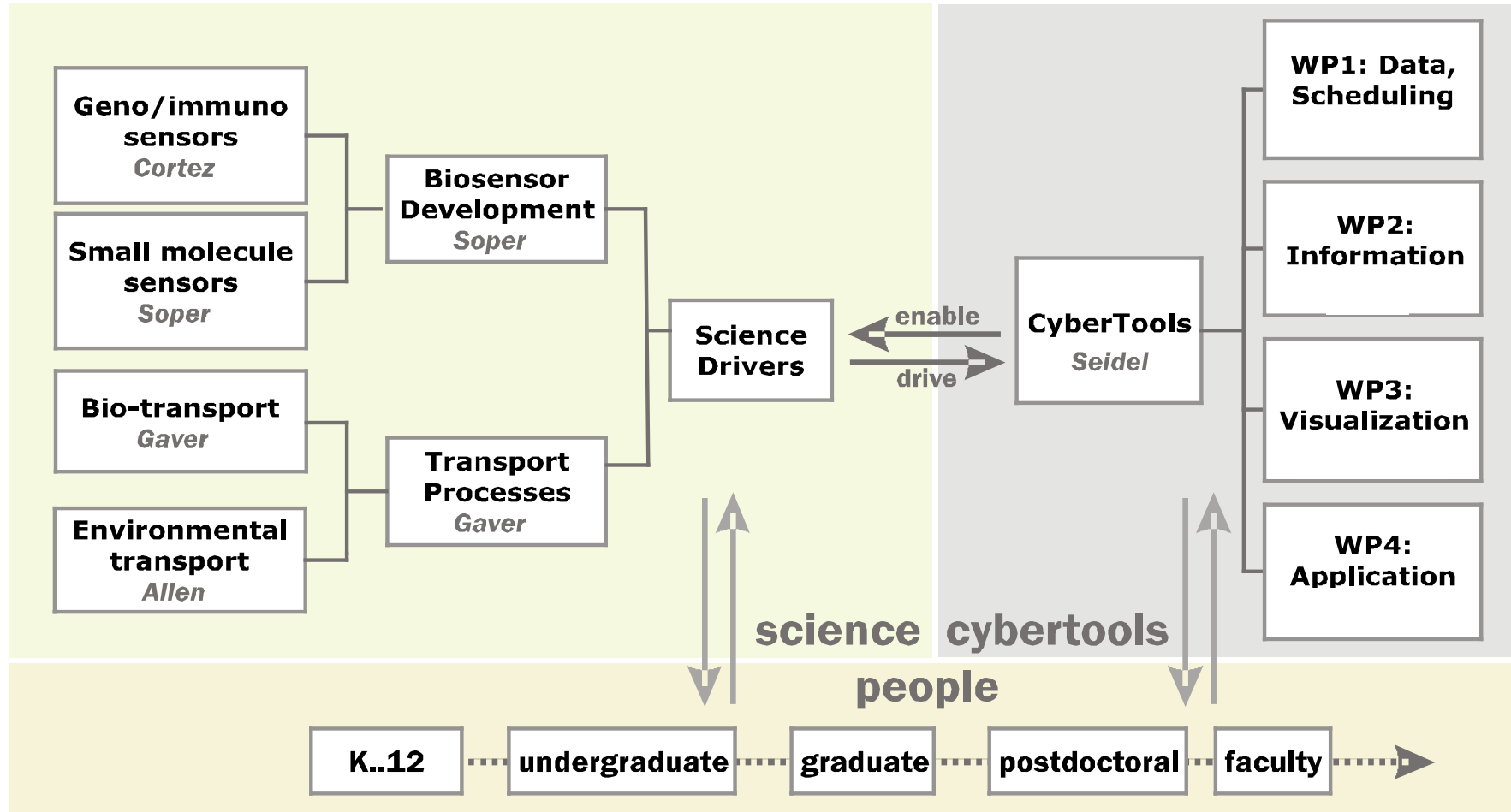
Science Driver Needs

- ☐ 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

PetaShare

HAoscar — High Availability Open Source Cluster Application Resources

Contact Us

Leveraging New and Existing Collaborations:

SPRUCE Urgent Computing (ANL)
Charm++ (Illinois)
Globus (Chicago/ANL)
Condor (Wisconsin)

3 gridsphere

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.
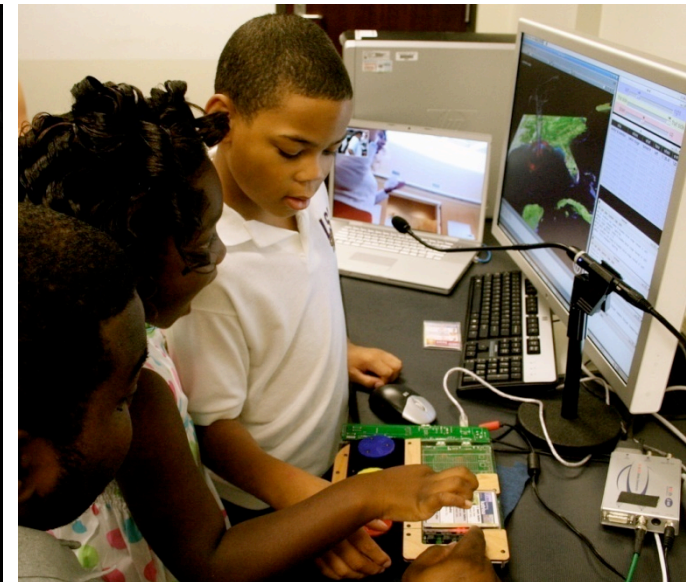
Additional Application students TBA

Viz Tangibles

Collaborative interaction devices for visualization; developed w/ NSF MRI for ~8-site deployment.
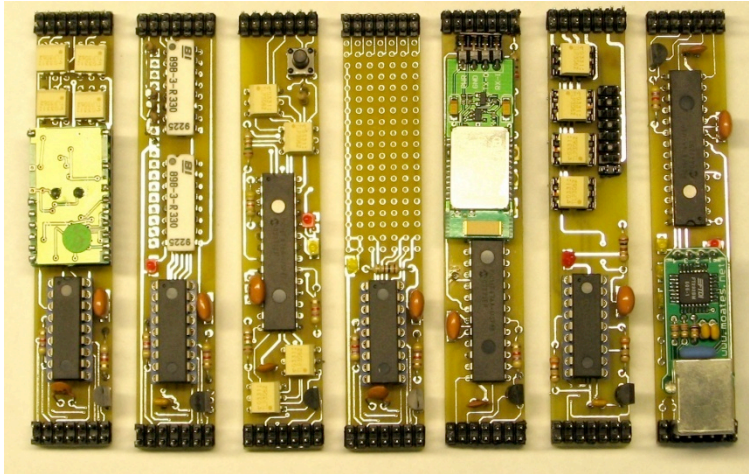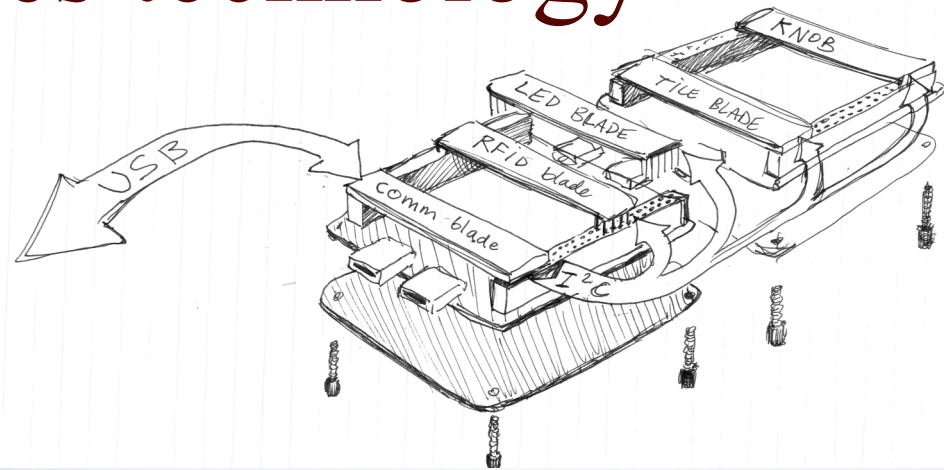
Above: device for data, parameter control. *Right:* use with video conferencing, immersion/CAVEs, outreach activities
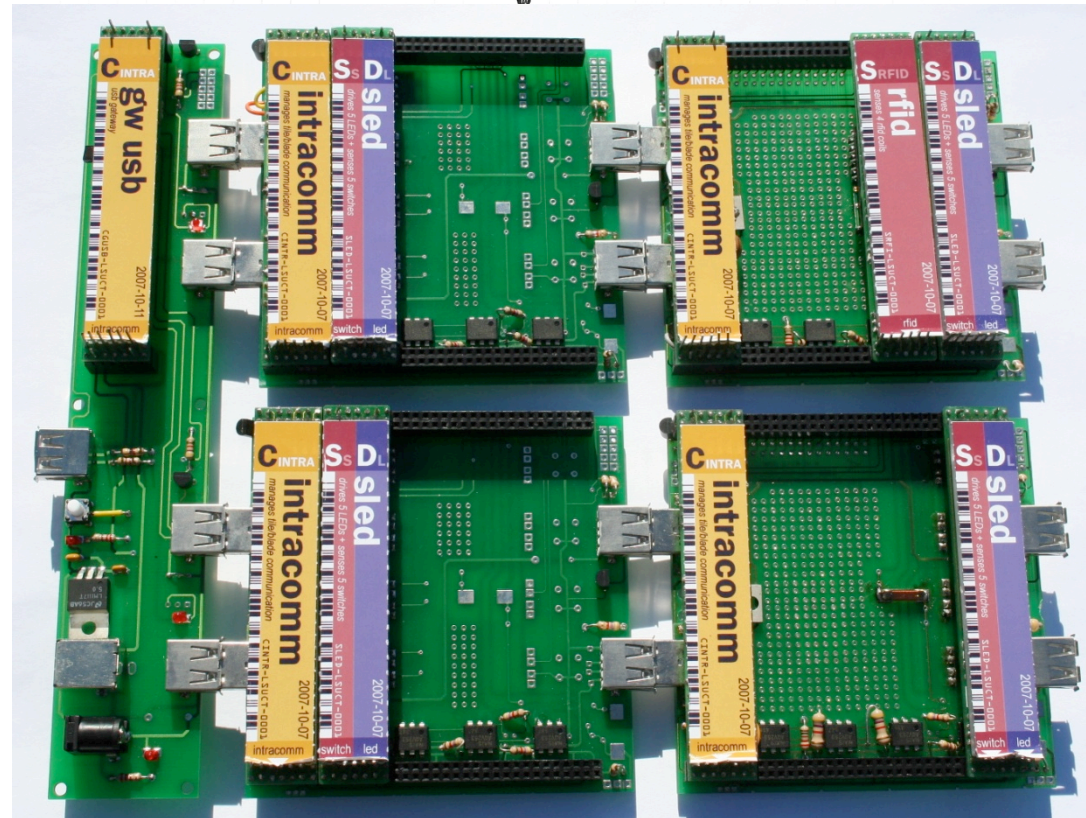
Viz tangibles technology

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

Application Drivers

CFD Toolkit

Multi-Scale Simulation Tools

MD Toolkit

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
Conventionlal

Flow-Structure
Physics, ALE, FEM, MPM

Meso-scale/ Coarse Graining/ Upscaling/Hybrid Tools

WP4
WP4
WP4
WP4

WP3
WP3
WP3
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WP3

Physics
Force fields
CHARMM
AMBER

Structure Tools
Molecular Conf.
PDB Database

Numerics
Integration Meth.

Solvers
R-K
Pred-Corr
Verlet

Visualization
Tangible
Immersive
Conventionlal

WP1

CYBER INFRASTRUCTURE (LONI, TERAFLOPS)

Storm Surge/
Coastal Modeling

Bio-transport in
vessels

Micro-fabrication

Microfluidics

Antibody binding

Cellular/lipid
layer
transport

WP2

Management & WorkPlans

- ☐ 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