LSU
FOR COMPUTATION
TECHNOLOGY

Cybertools WP4
Application Toolkits

S. Jha, J. Kim, E. Schnetter, M. Tyagi

LSU
FOR COMPUTATION
TECHNOLOGY

WP4: The Mission

- Capture and analyze the application characteristics and requirements of the science drivers
- Facilitate the use of computational infrastructrure, including but not limited to LONI, for advancing science
  - Short-term (6-12 months): help deploy applications and the design of tools to facilitate utilisation of infrastructure
  - Longer-term (1-3 years): design of application managers and toolkits – that abstract the common requirements and usage modes of applications
- Work not only with Science Drivers to provide direct support, but also interface with other Cybertool WPs

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Personnel

Science Drivers:

- Sumanta Acharya, Prasad Kalghatgi
- Don Gaver, Jerina Pillert, Kate Hamlington, Dave Halpe
- Steve Soper, Dimitris Nikitopoulos, Eamonn Walker
- Tom Bishop

HPC/LONI/CyD:

- Honggao Liu (LONI), Dan Katz and Joohyun Kim (CyD)
- Hartmut Kaiser, Sanjay Kodiyalam

WP4 funded personnel:

- Joao Abecasis (GA)
- *Nayong Kim* (USC) and *Jeff Ko* (KISTI, Korea)

LSU
FOR COMPUTATION
TECHNOLOGY

WP4-SD Interaction

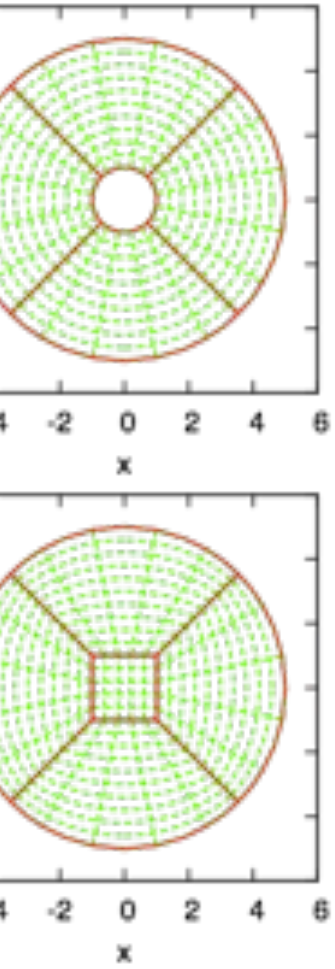
- Analyse the requirements SDs, into existing (fast track) or need-to-be-developed (deep track) capabilities
  - Regular bi-weekly meetings
- SD1 (BioTransport):
  - Multi-block support for implicit solvers [Prasad]
  - Immersed boundary support for moving geometry
- SD2 (Fluid Structure Interaction):
  - OpenMP version for BEM code [Jerina, Kate]
- SD3 (BioSensor):
  - Fast Track: vorticity formulation + driven cavity
  - Deep Track: coupling CFD + MD appropriate interface
- Infrastructure development for all SDs (with WP1,2)
  - Initial sketch of general purpose application manager

	Biotransport	Fluid-Structure Interaction	BioSensor	Capabilites that Exist
Numerical Schemes				
BE Method		Y		
Finite Difference	Y		Y	Y
Finite Volume	Y			Y
Numerical Solvers				
Lapack		Y		SCALAPACK
Hyper	Y			UNiGRID
PetSc				UNiGRID
MultiGrid			Y	MUDPACK
Explicit				
Domain Representation				
Uniform Grid		Y	Y	Y
Single Block			Y	Y
Multiblock	Y			Y
AMR	Y			Y
Unstructured (Meshless)			Y	

Computational Infrastructure	Biotransport	Fluid-Structure Interaction	BioSensor	Work Packag
Parallelization Scheme				
OpenMP		Y	Y	WP4
MPI	Y		Y	WP4
Cactus Features				
Checkpointing	Y	Y	Y	WP4
Error Handling	Y	Y	Y	WP4
Visualization (post-processing)	Y	Y	Y	WP3
Visualization (Steering)			Y	WP3
Distributed Data Mgmt, Handling and Archiving	Y	Y	Y	WP1
Efficient I/O			Y	WP1, WP4
Distributed Job Launch/Mgmt	Y		Y	WP1, WP2, W

LSU
OR COMPUTATION
ECHNOLOGY

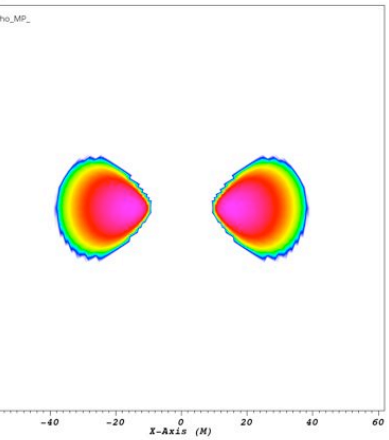
Multi-Patch Systems in the Cactus Framework



- Spherical (smooth) outer and/or inner boundaries
- No coordinate singularities (*z* axis, origin)
- Adapted to interesting features (neutron stars, boundaries, objects and their trajectories)
- Can choose angular and radial resolution independently

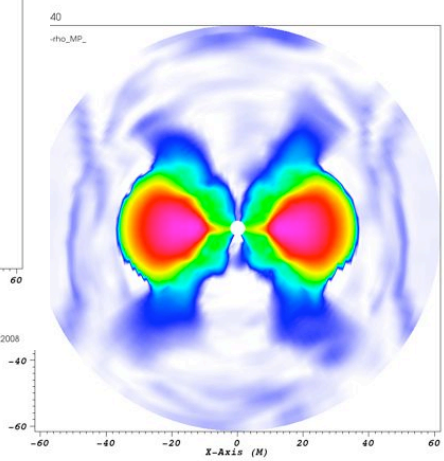
LSU
OR COMPUTATION
ECHNOLOGY

Astrophysical Application: Magnetised Torus

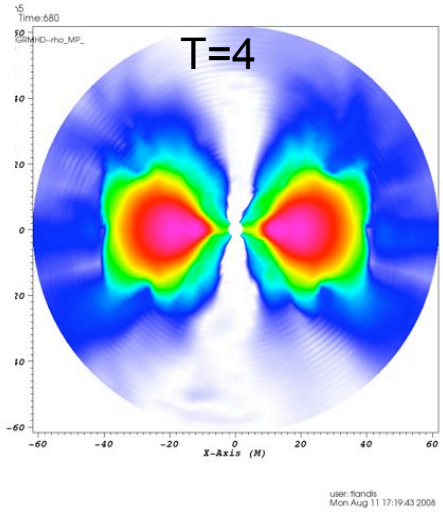


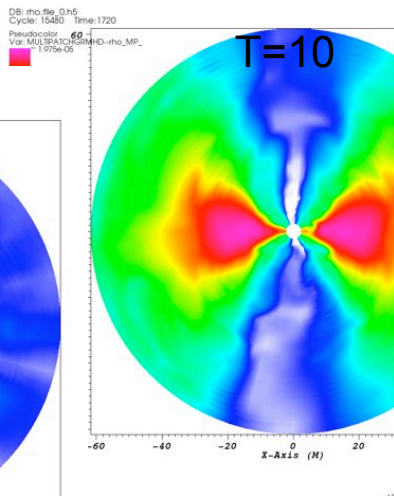
T=0

Schwarzschild (black hole) background



T=2





ur map:

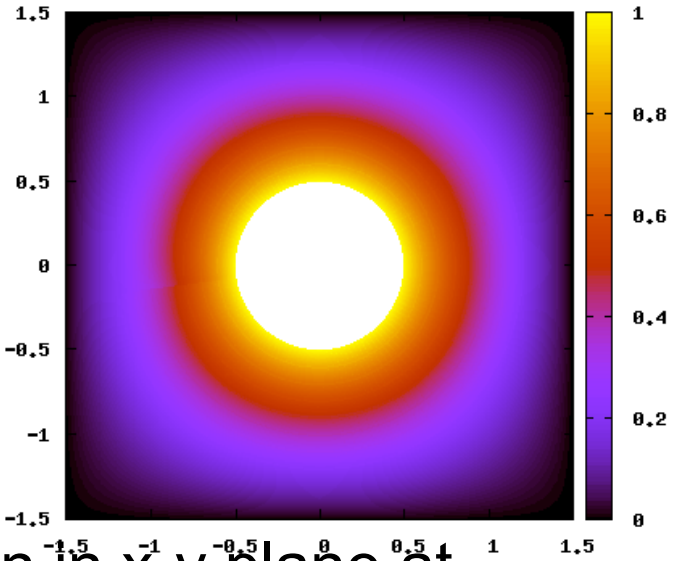
density

ally weak poloidal magnetic field loops
w and make torus unstable

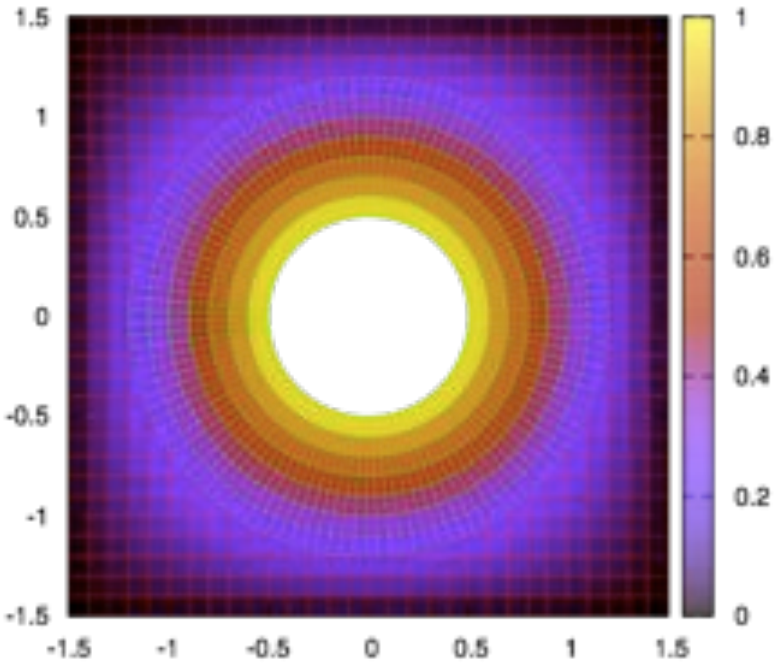
LSU
OR COMPUTATION
ECHNOLOGY

Test Problem: Diffusion Equation

main:
be minus Cylinder



tion in x-y plane at
.5

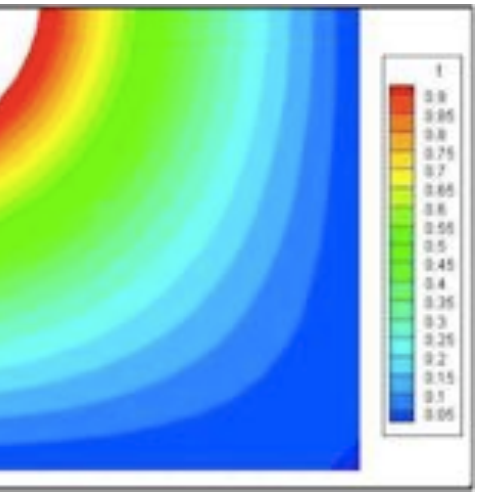


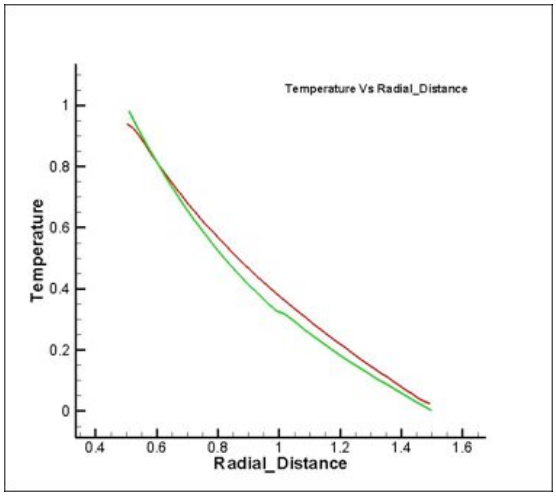
Grid Structure in x-y plane

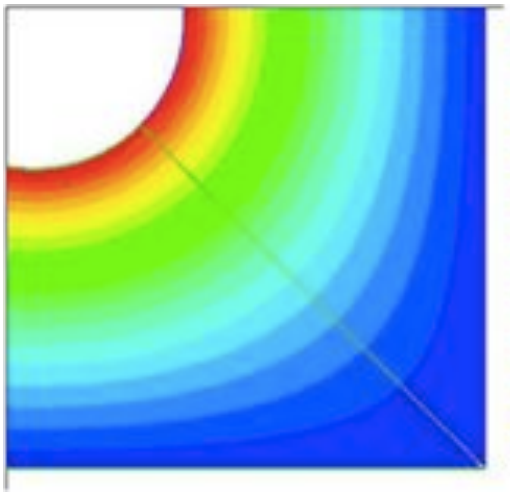
See P. Kalghatgi's poster for a comparison to S. Acharya's Science Driver

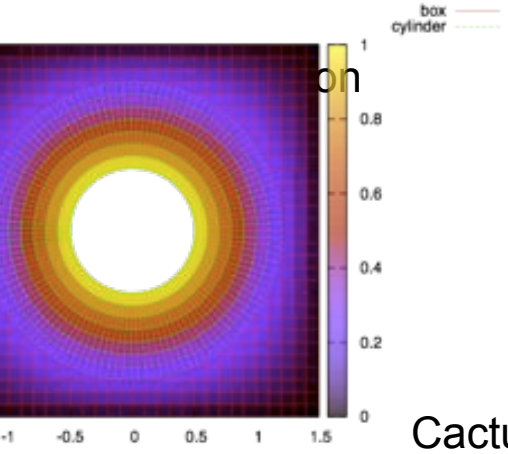
LSU
OR COMPUTATION
ECHNOLOGY

Test Problem: Diffusion Equation









on

Comparison

CFD Module simulation

Courtesy P. Kalghatgi (see pos

Domain (3D):
Cube minus Cylinde
x-y central plane sho

Cactus multi-patch

grid structure

LSU
OR COMPUTATION
ECHNOLOGY

Cactus: Overview

- Cactus (www.cactuscode.org) is a software framework for collaborative development, primarily developed at LSU
- Very successful in astrophysics (used by >200 publications, >30 student theses)
- Provides computational infrastructure and supports application toolkits (e.g. CCTK, Einstein Toolkit)

LSU
OR COMPUTATION
ECHNOLOGY

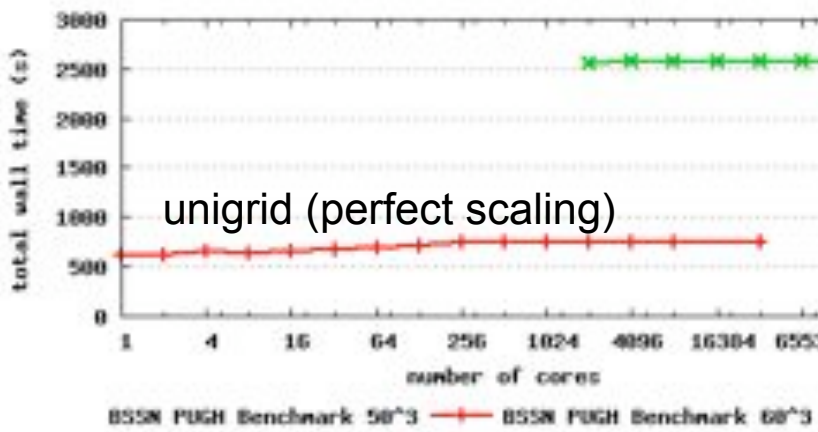
Cactus:
Separation of Concerns

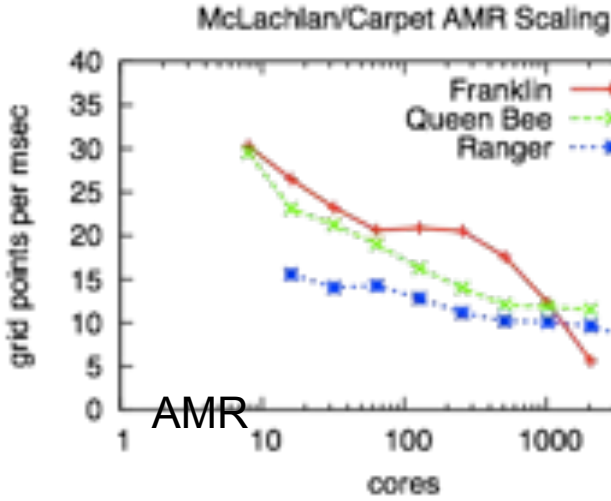
- Physics: equations, stability, modelling
- Discretisation: differencing, numerical analysis, conservation, constraints
- Domain: mesh, parallelisation, load balancing, cache efficiency
- Computer science: module interfaces, scheduling, efficient I/O, visualisation

LSU
OR COMPUTATION
ECHNOLOGY

Cactus: Parallelisation

- Supports both OpenMP (simpler) and MPI (more efficient) parallelisation strategies
- Provides Adaptive Mesh Refinement (AMR) and multi-patch domains with Carpet driver (www.carpetcode.org)
- Can e.g. perform automatic loop optimisations (cache blocking) at run time





LSU
OR COMPUTATION
ECHNOLOGY

Cactus: Job Handling

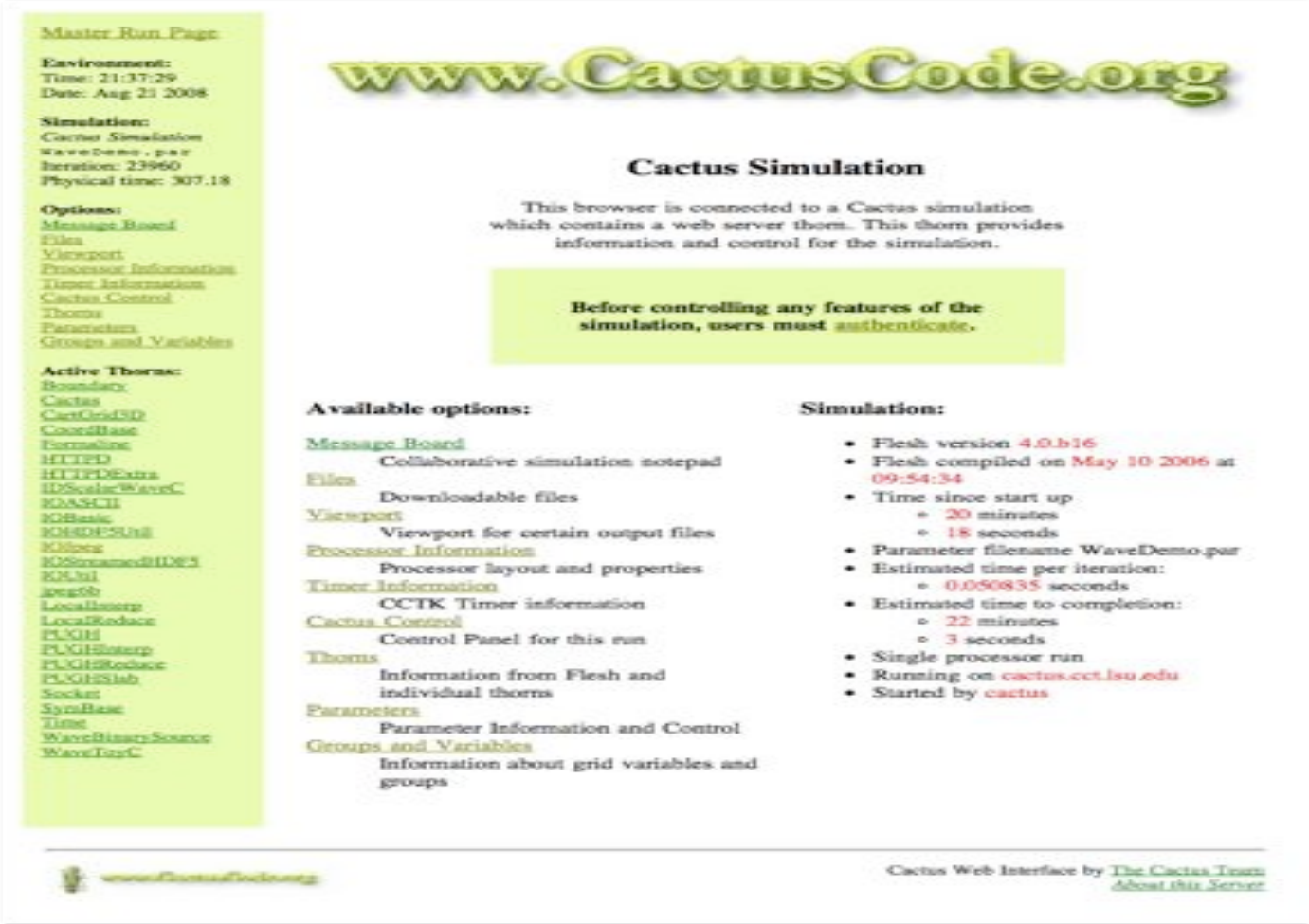
- [Show portal listing Cactus jobs] (http://devportal.cct.lsu.edu:8081/gridsphere/gridsphere)
- [Interact with perpetual Cactus simulation] (http://cactus.cct.lsu.edu:5555/)

LSU
OR COMPUTATION
ECHNOLOGY

Cactus Simulation Portal

LSU

OR COMPUTATION
ECHNOLOGY



Master Run Page

Environment:
Time: 21:37:29
Date: Aug 21 2008

Simulation:
Cactus Simulation
WaveDemo.par
Iteration: 23960
Physical time: 307.18

Options:
Message Board
Files
Viewport
Processor Information
Timer Information
Cactus Control
Thorns
Parameters
Groups and Variables

Active Thorns:
Boundary
Cactus
CartGrid3D
CoordBase
Formaline
HTTPD
HTTPDExtra
IDScalarWaveC
IOASCII
IOBasic
IOHDF5Util
IOJpeg
IOStreamedHDF5
IOUtil
jpeg6b
LocalInterp
LocalReduce
PUGH
PUGHInterp
PUGHReduce
PUGHSlab
Socket
SymBase
Time
WaveBinarySource
WaveToyC

www.CactusCode.org

Cactus Simulation

This browser is connected to a Cactus simulation which contains a web server thorn. This thorn provides information and control for the simulation.

Before controlling any features of the simulation, users must authenticate.

Available options:

Message Board
Collaborative simulation notepad

Files
Downloadable files

Viewport
Viewport for certain output files

Processor Information
Processor layout and properties

Timer Information
CCTK Timer information

Cactus Control
Control Panel for this run

Thorns
Information from Flesh and individual thorns

Parameters
Parameter Information and Control

Groups and Variables
Information about grid variables and groups

Simulation:

- Flesh version 4.0.b16
- Flesh compiled on May 10 2006 at 09:54:34
- Time since start up
  - 20 minutes
  - 18 seconds
- Parameter filename WaveDemo.par
- Estimated time per iteration:
  - 0.050835 seconds
- Estimated time to completion:
  - 22 minutes
  - 3 seconds
- Single processor run
- Running on cactus.cct.lsu.edu
- Started by cactus

Cactus Web Interface by The Cactus Team
About this Server

LSU
OR COMPUTATION
ECHNOLOGY

Cactus: On-Line Visualisation

Master Run Page

Environment:
Time: 21:38:40
Date: Aug 21 2008

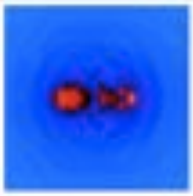
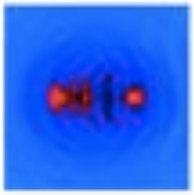
Simulation:
Cactus Simulation
WaveDemo.par
Iteration: 25360
Physical time: 325.13

Options:
Message Board
Files
Viewport
Processor Information
Timer Information
Cactus Control
Thorns
Parameters
Groups and Variables

Viewport

This page displays certain types of the output files from the download page as images (currently only JPEGs [mime type image/jpeg]).

Many IO methods have *steerable* parameters which allow you to e.g. add fields and customise behaviour. Depending on your authorisation, you can access the parameter steering page

Variable Slice	Description	Image
WAVETOY::phi xz_[20]	*Jpegs of slices*	
WAVETOY::phi yz_[20]	*Jpegs of slices*	

Cactus Web Interface by The Cactus Team
About this Server

LSU
OR COMPUTATION
ECHNOLOGY

Cactus: Steering, Profiling

		after regridding		
POSTSTEP	HTTPD	Working routine	0.272410	0.151978
POSTSTEP	HTTPD	Convert Working routine	0.156236	0.023994
CPINITIAL	IOStreamedHDF5	Initial data checkpoint routine	0.000010	0.000000
ANALYSIS	Formaline	Put some extra information about the current run into permanent storage	2.736291	0.054092
EVOL	WaveBinarySource	Provide binary source during evolution (C)	1.069777	1.076837
EVOL	WaveToyC	Evolution of 3D wave equation	23.241877	22.937492
EVOL	WaveToyC	Boundaries of 3D wave equation	0.398572	0.361954
EVOL	WaveToyC	Apply boundary conditions	0.000000	0.000000
POSTRESTRICT	WaveToyC	Boundaries of 3D wave equation	0.000000	0.000000
POSTRESTRICT	WaveToyC	Apply boundary conditions	0.000000	0.000000
CHECKPOINT	IOStreamedHDF5	Evolution data checkpoint routine	0.158191	0.021996
TERMINATE	Formaline	Put some extra information about the current run into permanent storage	0.000000	0.000000
TERMINATE	IOHDF5Util	IOHDF5Util termination routine	0.000000	0.000000
TERMINATE	IOStreamedHDF5	Termination routine	0.000000	0.000000
TERMINATE	IOStreamedHDF5	Termination checkpoint routine	0.000000	0.000000
TERMINATE	PUGH	Termination routine	0.000000	0.000000
SHUTDOWN	HTTPD	HTTP daemon shutdown	0.000000	0.000000

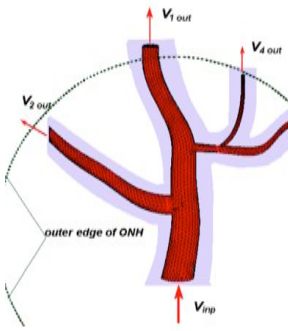
LSU
OR COMPUTATION
ECHNOLOGY

Next Steps

- Benefit from other ongoing Cactus projects:
  - XiRel (improve AMR; data handling)
  - Alpaca (performance/correctness tools)
  - ParCa (connect to PARAMESH solver)
- Generalise elliptic solver interfaces for AMR /multi-patch

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Connection to SD1 (Biotransport)



in driver for “multiblock finite volume method

tinuum flow and FSI calculations

ultiblock structured grid (Biosensors need this capability)

ow-Structure interaction (Science need for BEM also)

article-based meshless calculations for structural deformations (Materia
oint method, MPM)

mmersed Boundary Methodology (IBM) for resolving boundary condition
ong moving interfacial surfaces

-continuum Effects

Atomistic (Molecular-Dynamics) simulations of particle/molecule transp
cross cellular interfaces

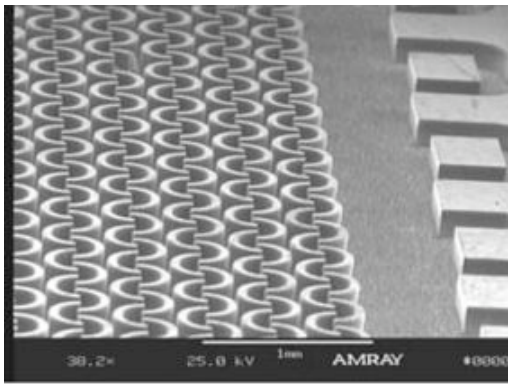
Upscaling or coarse-graining calculations for averaged property informa
eeded for continuum calculations

SD2: Flow around Ω-obstructions

(slide courtesy: Gaver Group)

LSU
OR COMPUTATION
ECHNOLOGY

GOAL ➔ *Computationally determine the optimal geometric configuration of the omega channel network to enhance mixing of two species.*

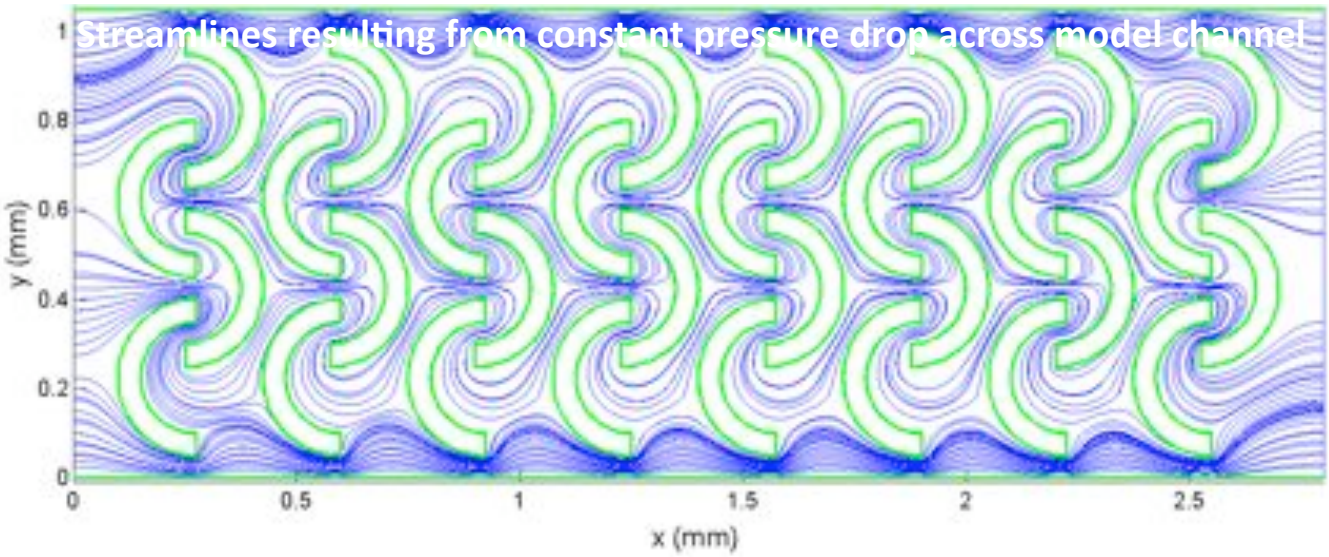


Laminar flow field governed by continuity & Stokes equations:

$$\nabla \cdot \mathbf{u} = 0$$

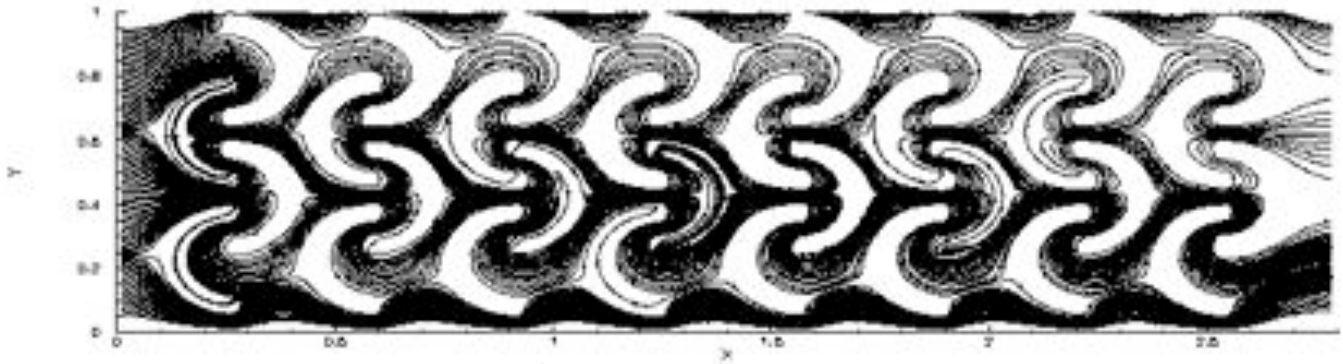
$$\nabla P = \mu \nabla^2 \mathbf{u}$$

Boundary Element Method determines velocities and surface stresses

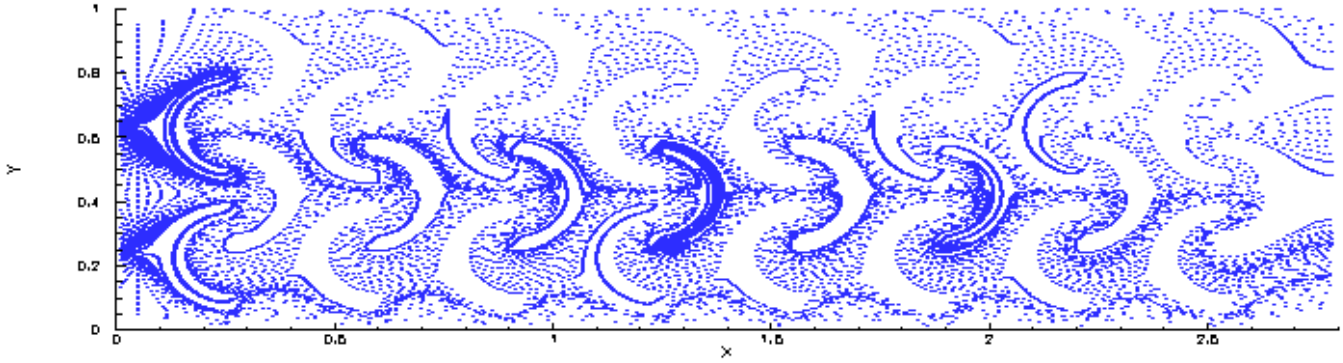


LSU
OR COMPUTATION
ECHNOLOGY

WP4: Link to SD2
Model Microchannel Problem



Streamlines



Particle Traces

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Link to SD2

(slide courtesy: Gaver Group)

- Current Work:
  - Parallelization of Stokes flow problem for use in the HPC environment (WP4: Mayank Tyagi, Shantenu Jha, Sanjay Kodiyalam, Yaakoub El-Khamra)
    - *OpenMP*
  - Visualization of model problem using TecPlot
  - Generalization of code to develop a *CyberTool* package that solves Stokes flow equations
- Future Work:
  - Parallelization of source code including transport

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Links to SD3

(Slide Courtesy: Dimitris)

- Multi-Phase flow Simulation Tool (WP4, WP3, WP1)
  - Parallelization
    - Implementation of parallelized Multi-Grid solver (WP4)
    - Distribution of different multi-processor simulations to groups of processors for efficient parametric studies (WP1)
  - Advanced interactive visualization tools (WP3)
  - Improvement of Accuracy/Performance
    - Implement Multi-Grid algorithm designed to handle elliptic equations with discontinuous coefficients (WP4)
    - "Poisson" solver for the pressure
  - Extend code capabilities to handle complex Cartesian geometries
    - Domain Decomposition (WP4)
    - Multi-blocking (WP4)
  - Computational Steering (WP1, WP3, WP4)

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Link with SD3 (Coupling CFD-MD)

Basic MD code

- Developed
- Parallelized in one dimension
- Tested on simple 2D flows
  - Couette
  - Poiseulle
- Modification of MD code to accommodate more diverse BC and paralleliza in two dimensions (in progress)
- **Documentation of the code for delivery to WP4 (in progress)**

Continuum 3D N-S Parallel Code (Velocity/Vorticity Formulation)

- Developed (international collaboration)
- Tested on 3D driven cavity test problem - Re[0.1,5000] (in progress)
- **Documentation of the code for delivery to WP4 (in progress)**

Continuum-MD Coupling (In progress)

- **Will work with WP4 to develop tools to**
  - Build a Modular Continuum-MD Parallel Simulation Environment unde CACTUS

LSU
OR COMPUTATION
ECHNOLOGY

WP4: Connection to WP1-3

/P1 (Scheduling and Data Services):

- Work with WP1, CyD, LONI/HPC to define infrastructure and deployment requirements (eg PetaShare, SAGA)
- Facilitating high-throughput MD and other simulations with data-intensive complex data-management needs

/P2 (Info Services and Portals):

- Applications Managers being developed using SAGA, which will integrate with portals and gateways

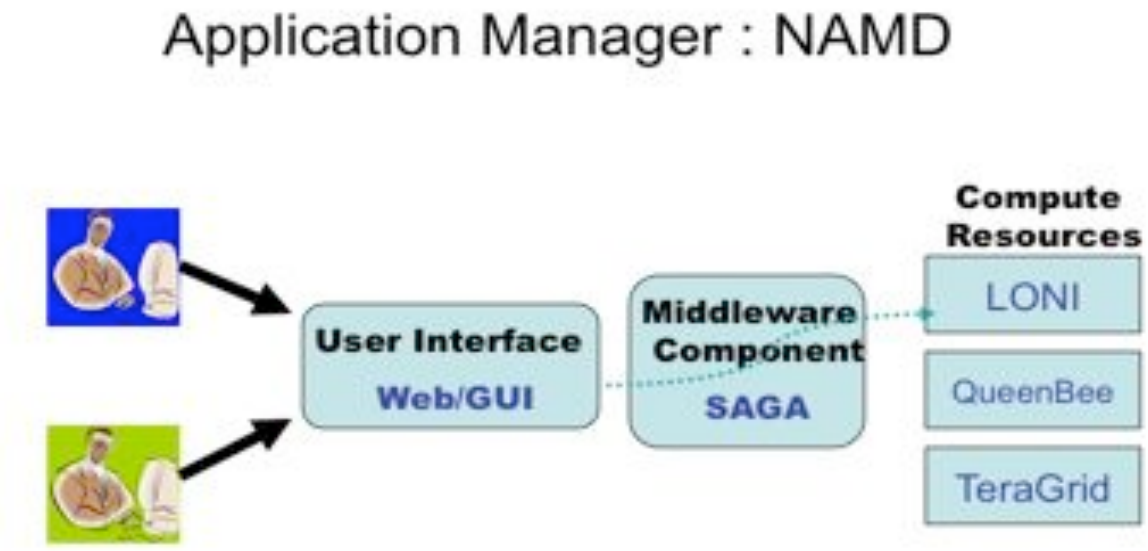
/P3 (Visualization Sevices):

- Exploring with applications use of Vish, VISIT
- Common interface for accessing visualization (SAGA)

LSU
OR COMPUTATION
ECHNOLOGY

Application Manager

Provides support for uniform usage patterns and interface to heterogeneous resources

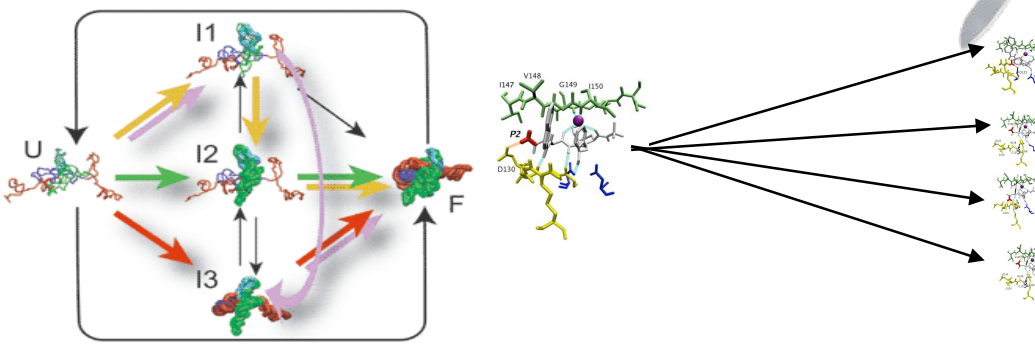


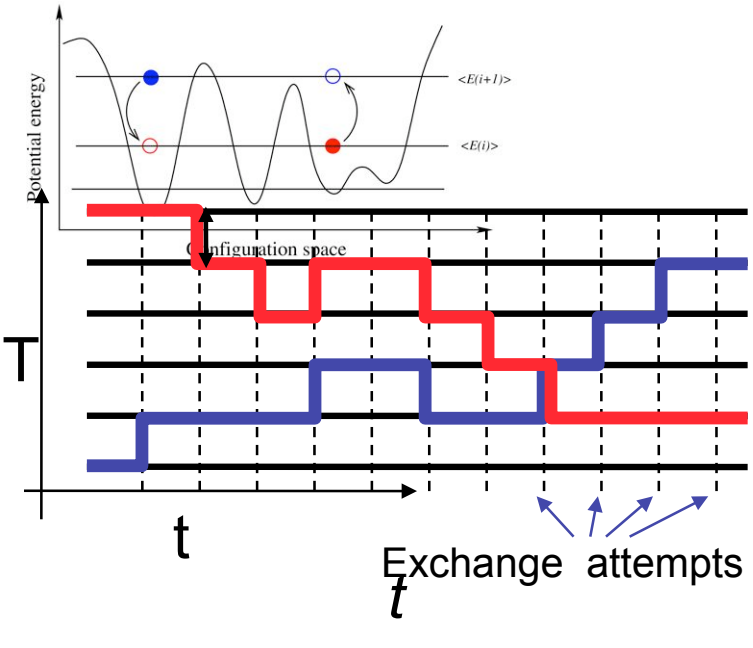
Application Manager: Sailent Points

- Uniform: Provides single interface to heterogeneous and distributed resources
- Generic: Infrastructure can be embedded into either a portal or into a GUI
  - Also lightweight, flexible, modular
  - Easy to deploy
- Can support:
  - Other MD packages (e.g., LAMMPS)
  - Other Usage Modes (e.g., High-throughput) (WP1)
  - Complicated workflow driven computation (WP1)

Replica-Exchange Application Pattern

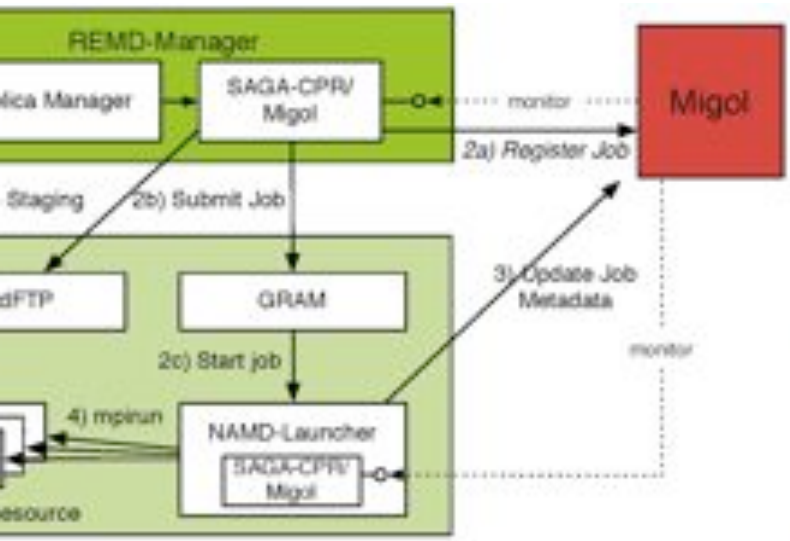
- Task Level Parallelism
  - Embarrassingly distributable!
  - Loosely coupled
- Create replicas of initial configuration
- Spawn 'N' replicas over different machine
- Run for time *t ;* Attempt configuration swap
- Run for further time t; Repeat till finish

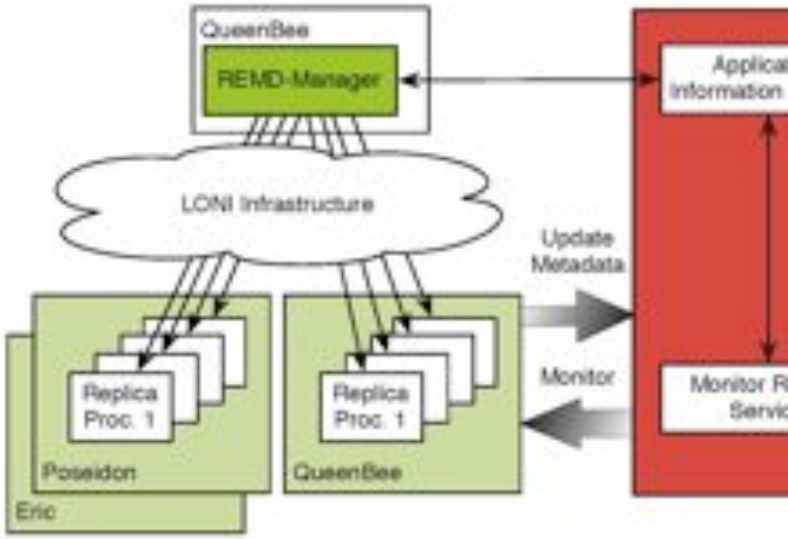




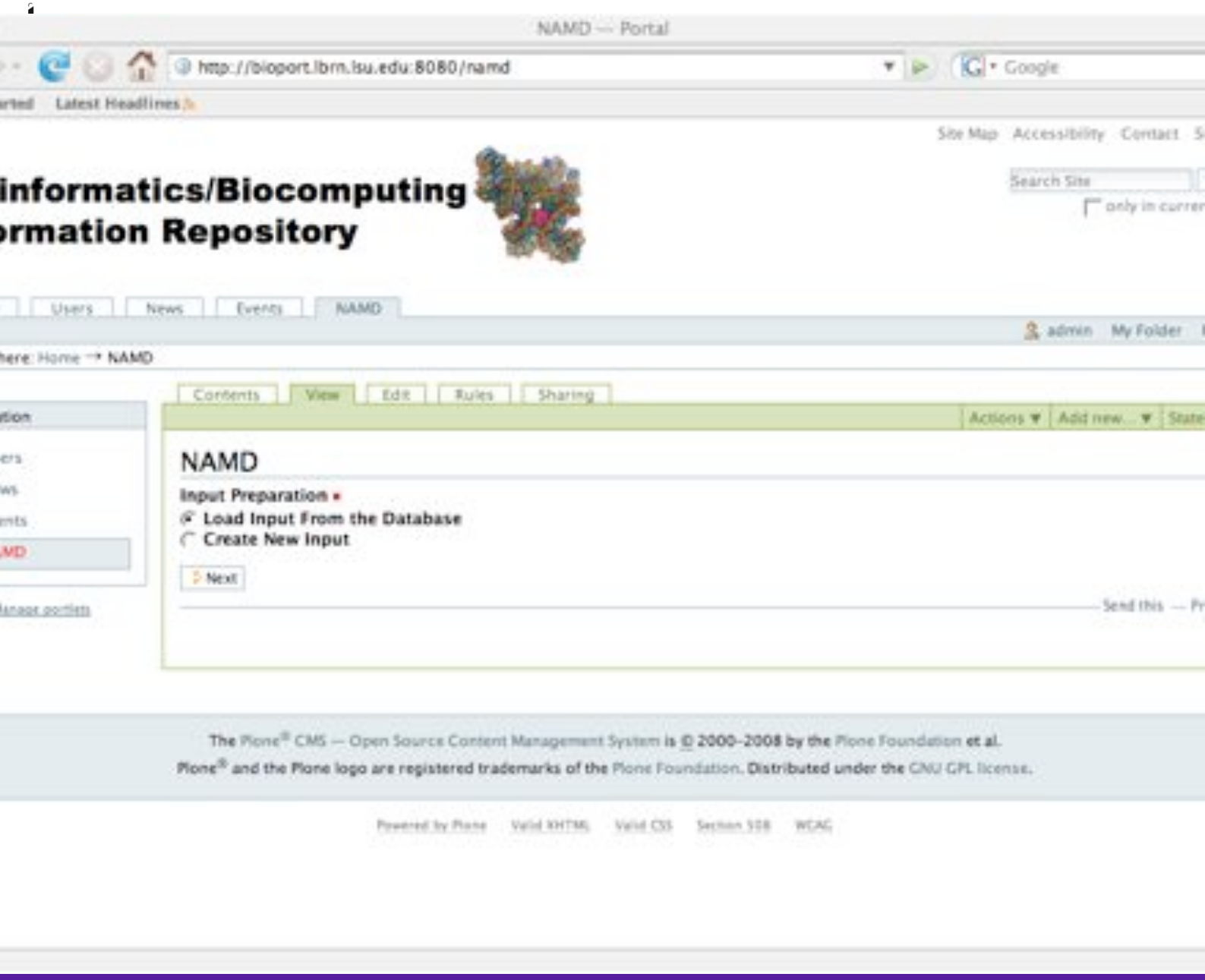
LSU
OR COMPUTATION
ECHNOLOGY

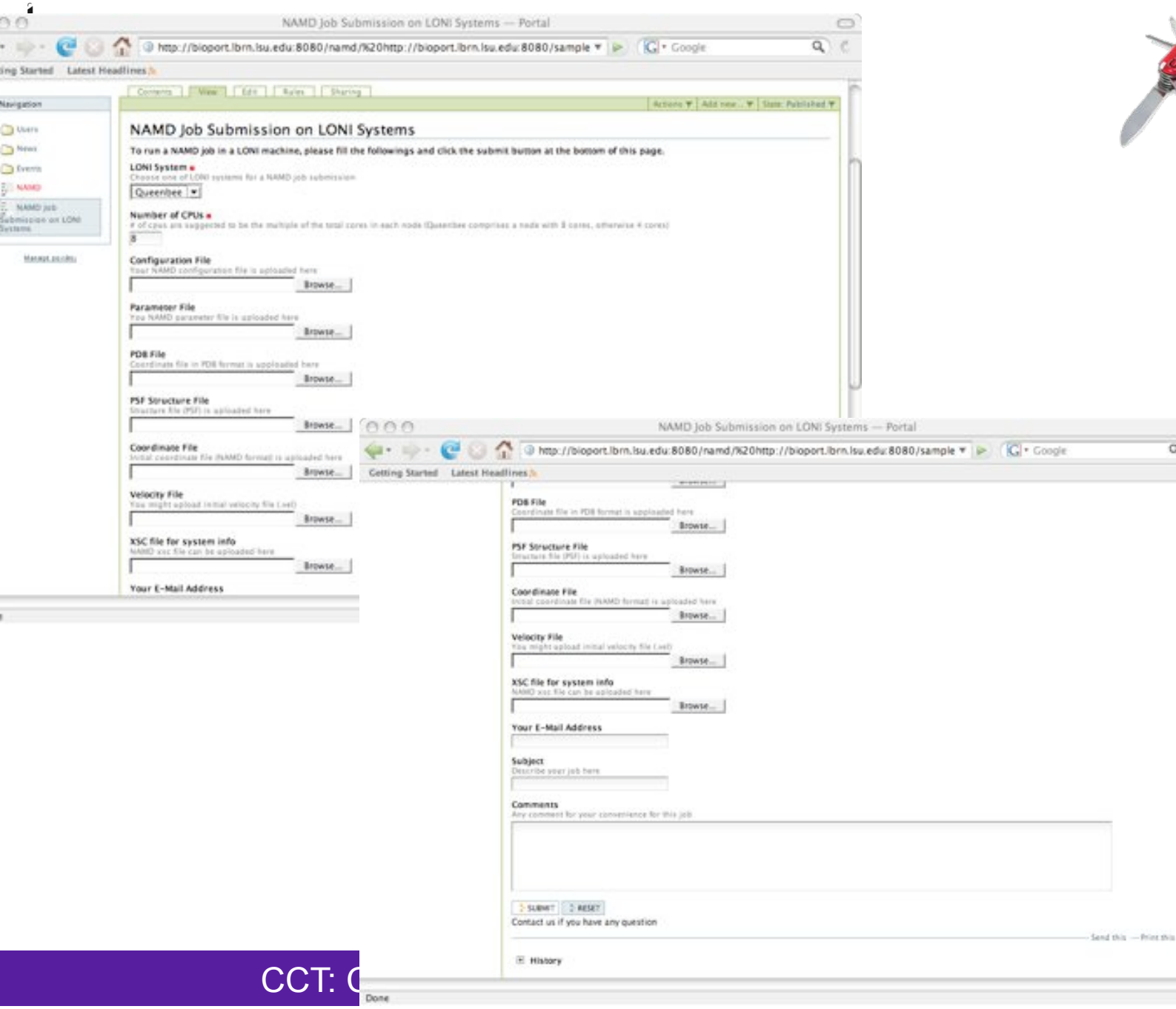
Replica-Exchange Manager

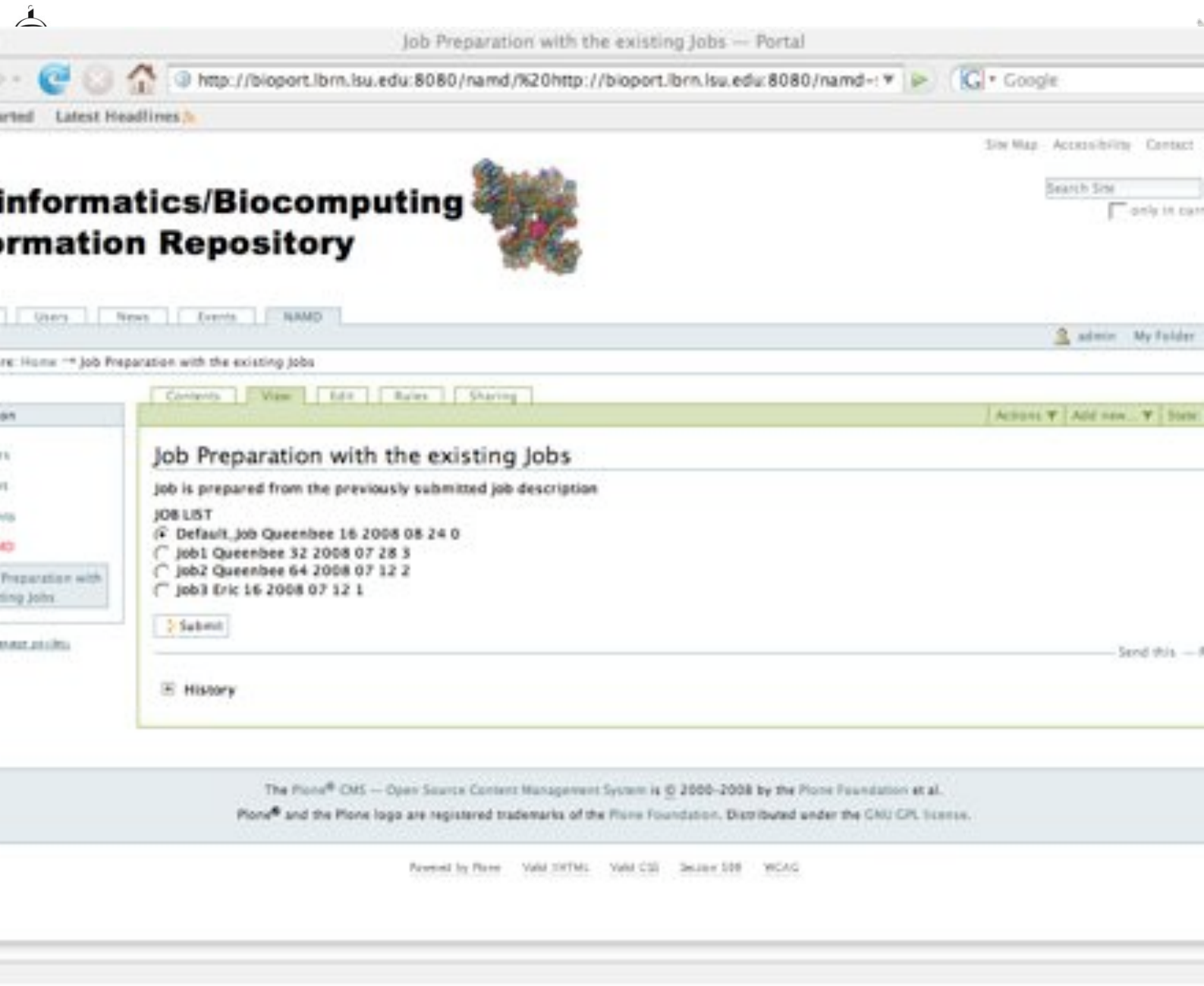





Welcome to Bioinformatics/Biocomputing Information Repository — Portal
http://bioport.lbrn.lsu.edu:8080/
Google
Latest Headlines
Site Map
Accessibility
Contact
Search Site
Users
News
Events
NAMD
admin
My Folder
Contents
View
Edit
Rules
Sharing
History
Display
Add new...
Welcome to Bioinformatics/Biocomputing Information Repository
Also available in presentation mode...
Overview
(Any questions regarding this site, HPC resources and softwares are welcome and send them to
This site provides
A. Useful information about computing resources/application packages available on LONI (www.loni.org) machines
B. Useful links for bioinformatics/biocomputing tools
C. Science gateway providing LONI resources (HPC systems and application softwares for biocomputing)- At the mome
Application Manager Environment for Molecular Dynamics (MD) simulations are provided.
Getting Started
1. How to get an account and an allocation on LONI machines


NAMD — Portal
http://bioport.lbm.lsu.edu:8080/namd
Latest Headlines
Site Map
Accessibility
Contact
informatics/Biocomputing
ormation Repository
Search Site
Users
News
Events
NAMD
admin
My Folder
here: Home → NAMD
Contents
View
Edit
Rules
Sharing
Actions
Add new...
NAMD
Input Preparation *
Load Input From the Database
Create New Input
Next
The Plone® CMS — Open Source Content Management System is © 2000-2008 by the Plone Foundation et al.
Plone® and the Plone logo are registered trademarks of the Plone Foundation. Distributed under the GNU GPL license.

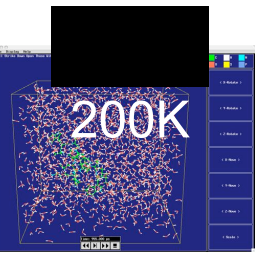

NAMD Job Submission on LONI Systems — Portal
http://bioport.lbrn.lsu.edu:8080/namd/%20http://bioport.lbrn.lsu.edu:8080/sample
Google
Getting Started
Latest Headlines
NAMD Job Submission on LONI Systems
To run a NAMD job in a LONI machine, please fill the followings and click the submit button at the bottom of this page.
LONI System
Queenbee
Number of CPUS
Configuration File
Parameter File
PDB File
PSF Structure File
Coordinate File
Velocity File
XSC file for system info
Your E-Mail Address
Subject
Comments
SUBMIT
RESET
Contact us if you have any question
History
Done

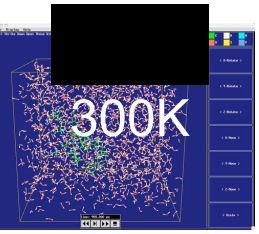

Job Preparation with the existing Jobs — Portal
http://bioport.lbrn.lsu.edu:8080/namd/%20http://bioport.lbrn.lsu.edu:8080/namd-
Google
Latest Headlines
informatics/Biocomputing
ormation Repository
Job Preparation with the existing Jobs
Job is prepared from the previously submitted job description
JOB LIST
Default_Job Queenbee 16 2008 08 24 0
job1 Queenbee 32 2008 07 28 3
job2 Queenbee 64 2008 07 12 2
job3 Eric 16 2008 07 12 1
Submit
History

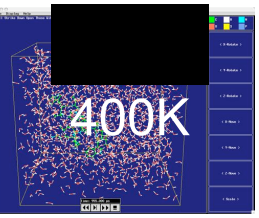
Application Manager: Sailent Points

- Uniform: Provides single interface to heterogeneous and distributed resources
- Generic: Infrastructure can be embedded into either a portal or into a GUI
  - Also lightweight, flexible, modular
  - Easy to deploy
- Can support:
  - Other MD packages (e.g., LAMMPS)
  - Other Usage Modes (e.g., High-throughput) (WP1)
  - Complicated workflow driven computation (WP1)

REMD for β-hairpin folding

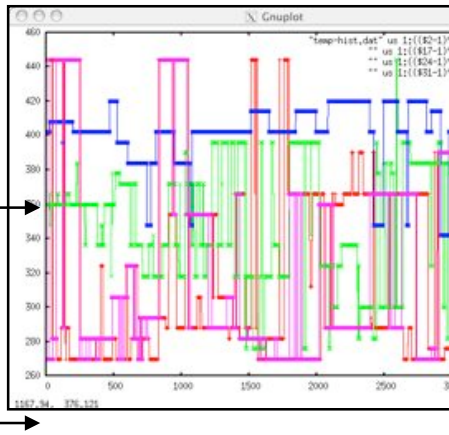






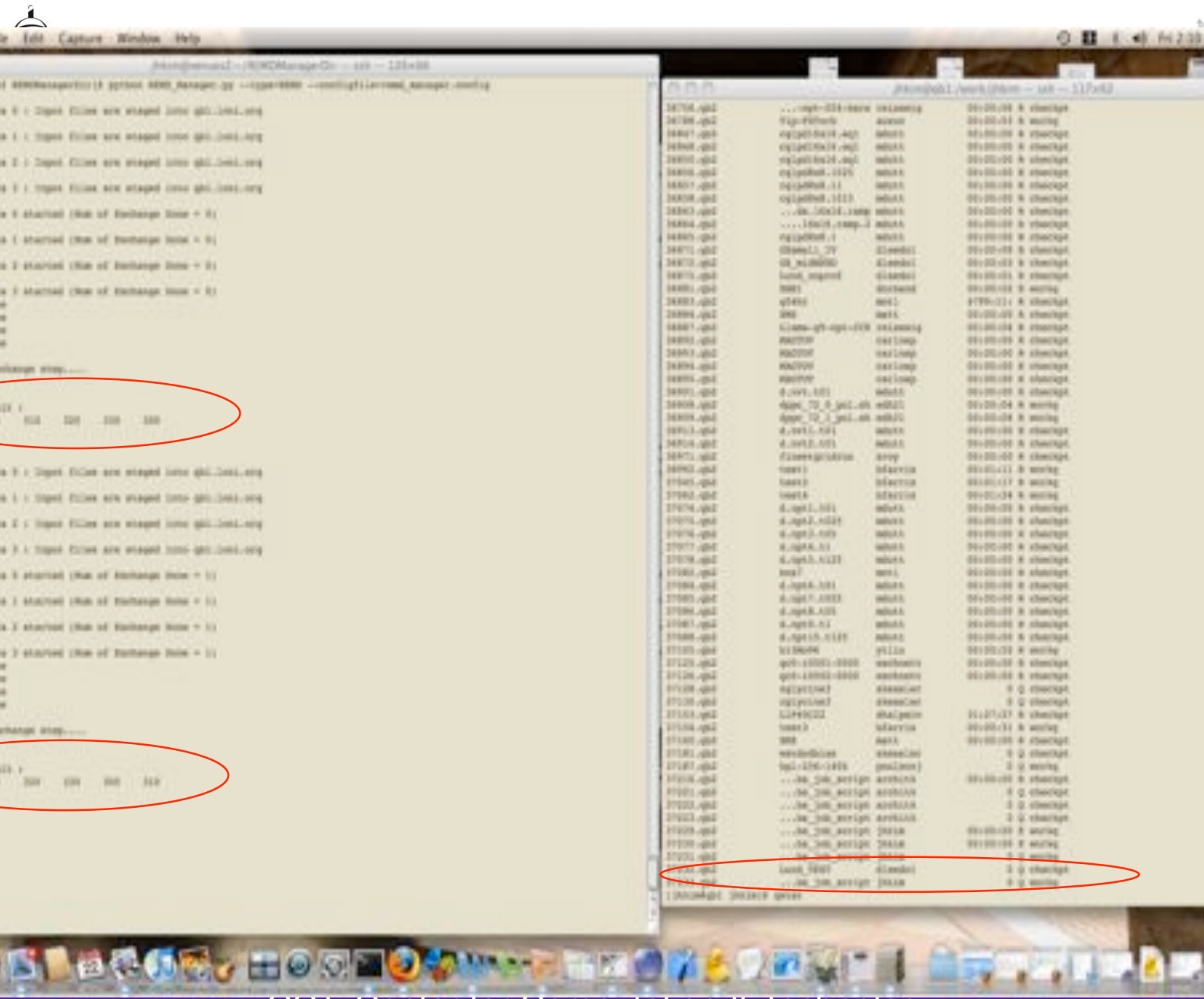
Temperature exchange

$$P_{prob} = min[1, exp[-(\beta_i - \beta_j)(U_j -$$



- 16-64 replicas
- 250K-500K
- More than 10ns
- PMF via. WHAM or Probability
- Free Energy Surface along a reaction coordinate

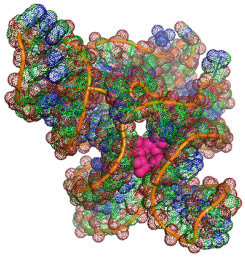
3ns, 30 replicas



```
eplica 1 done
eplica 2 done
eplica 3 done
eplica 4 done

INFO) Now exchange step....


xchange result :
   2-th EX :    320    330    300    310



INFO) Replica 0 : Input files are staged into qb1.loni.org

INFO) Replica 1 : Input files are staged into qb1.loni.org

INFO) Replica 2 : Input files are staged into qb1.loni.org

INFO) Replica 3 : Input files are staged into qb1.loni.org

INFO) Replica 0 started (Num of Exchange Done = 2)

INFO) Replica 1 started (Num of Exchange Done = 2)

INFO) Replica 2 started (Num of Exchange Done = 2)

INFO) Replica 3 started (Num of Exchange Done = 2)
eplica 3 done
eplica 1 done
eplica 2 done
eplica 4 done

INFO) Now exchange step....


xchange result :
   3-th EX :    330    320    310    300



INFO) Replica 0 : Input files are staged into qb1.loni.org
```

LSU
OR COMPUTATION
ECHNOLOGY

REMD Simulation



RNA Riboswitch (SAM-I)

- 50,000 atoms (explicit water)
- 16-32 replicas (2-3 LONI/TeraGrid)
- Each replica : 48-64 cpu mpi job (total : more than 1000 cpus)
- 2-3 days : 10-20 ns for a replica (total : 160 ns-600 ns)

➔ Provides information corresponding to multi-n time scale dynamics