



Cybertools WP4 Application Toolkits

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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



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)



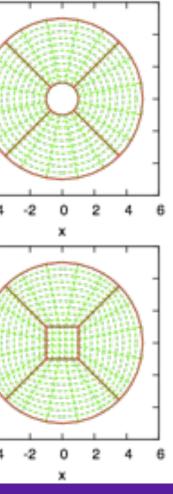
WP4-SD Interaction

- 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			1	
BE Method		¥.		
Finite Difference	۷		Y	Y
Finite Volume	Y			۷
Numerical Solvers				
Lapack		Y		SCALAPACK
Hyper	Y			UNIGRID
PetSc				UNIGRID
MultiGrid			Υ.	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	۷		۷	WP4
Cactus Features				
Checkpointing	Y	Y	Ŷ	WP4
Error Handling	¥	Y	Y	WP4
Visualization (post-processing)	¥	Y	Y	WP3
Visualization (Steering)			Y	WP3
Distributed Data Mgmt, Handling and Archiving	Y	Y	Y	WP1
Efficient I/O			۷	WP1, WP4
Distributed Job Launch/Mgmt	Y		Y	WP1, WP2, V

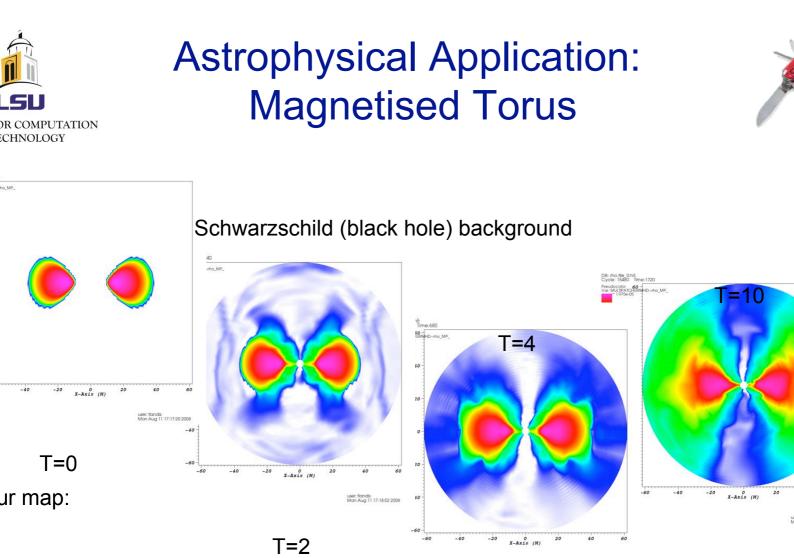




Multi-Patch Systems in the Cactus Framework



- 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

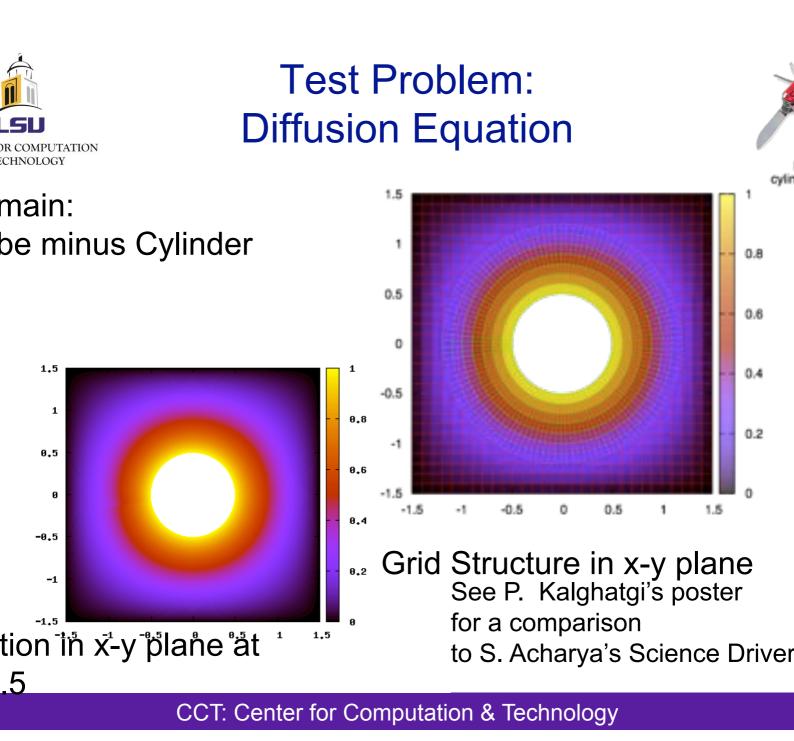


density

ally weak poloidal magnetic field loops wand make torus unstable

CCT: Center for Computation & Technology

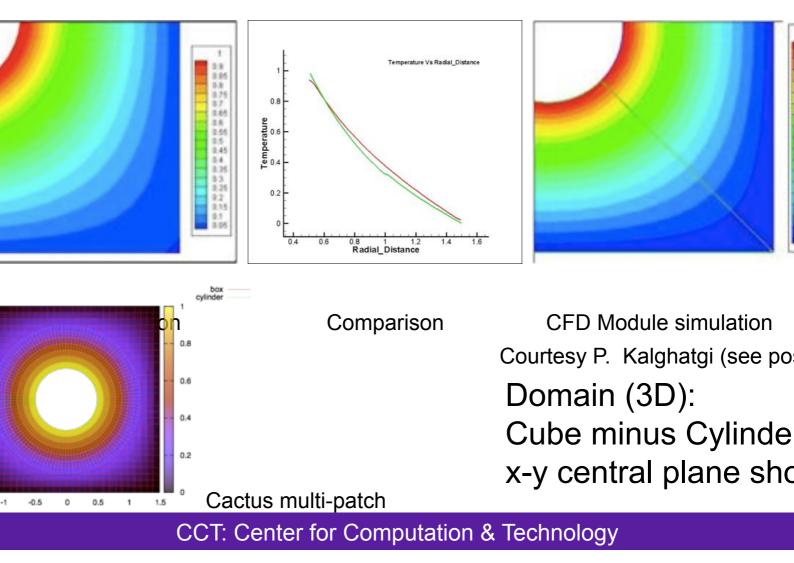
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Test Problem: Diffusion Equation





grid structure





- Cactus (<u>www.cactuscode.org</u>) 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)



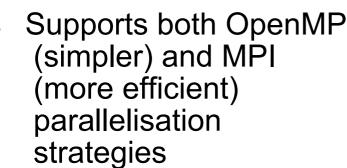
Cactus: Separation of Concerns



- 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



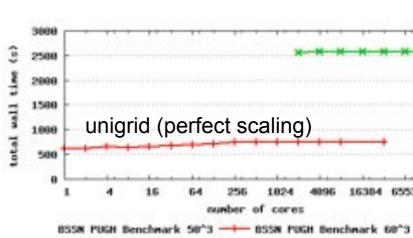
Cactus: Parallelisation

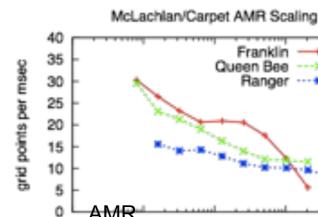


Provides Adaptive Mesh Refinement (AMR) and multi-patch domains with Carpet driver

(www.carpetcode.org)

Can e.g. perform automatic loop optimisations (cache blocking) at run time





1000

100 cores

AM





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/)

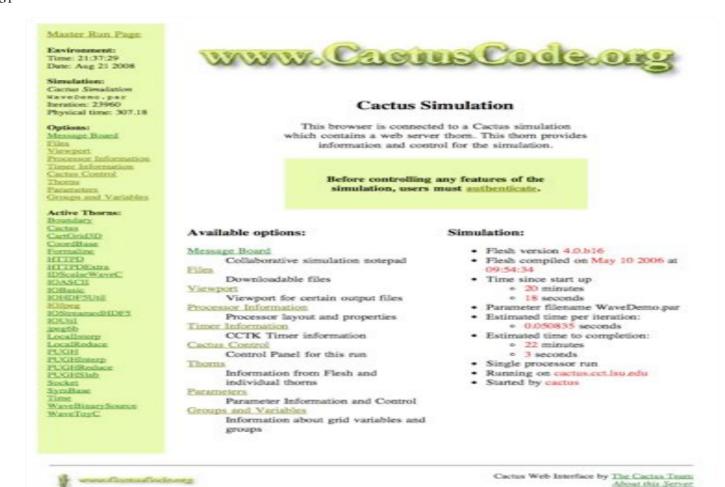


Cactus Simulation Portal

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About this Server



Cactus: On-Line Visualisation

OR COMPUTATION CHNOLOGY

Master Run Page

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Cartar Simulation NavaOuno.par Iteration: 25360 Physical time: 325.13

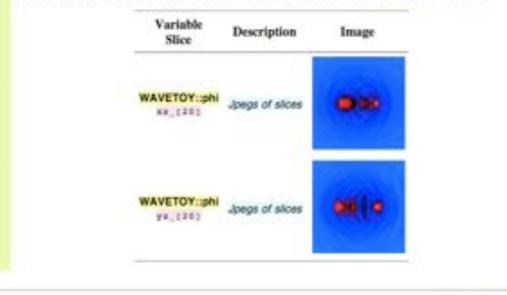
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Viewport

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

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



essoformatistory

Cactus Web Interface by The Cactus Team About this Server



Cactus: Steering, Profiling



Con	ntrol and Status	Page
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	Ran Control	
Select if the run should be p	used, running normally, or termi to the next iteration.	nated. You may also single step
O PAU	SE ® RUN O TERMINAT	E (STUP)
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	Run Until	
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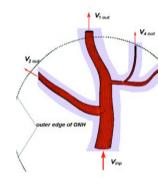


- Benefit from other ongoing Cactus projects:

 XiRel (improve AMR; data handling)
 Alpaca (performance/correctness tools)
 ParCa (connect to PARAMESH solver)
- Generalise elliptic solver interfaces for AMR /multi-patch



WP4: Connection to SD1 (Biotransport)



in driver for "multiblock finite volume method inuum 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 bint method, MPM)

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

continuum Effects

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

Jpscaling or coarse-graining calculations for averaged property informated by the second s



SD2: Flow around Ω-obstructions (slide courtesy: Gaver Group)



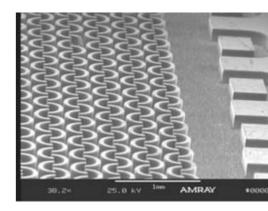
OR COMPUTATION CHNOLOGY

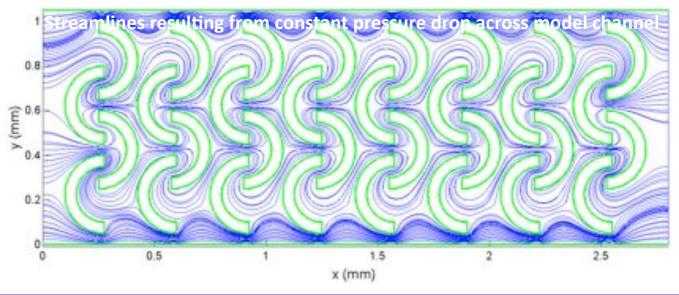
GOAL → Computationally determine the optimal geometric configuration of the omega channel network to enhance mixing of two species.

aminar flow field governed by continuity & Stokes equations: $\nabla \cdot \mathbf{u} = 0$

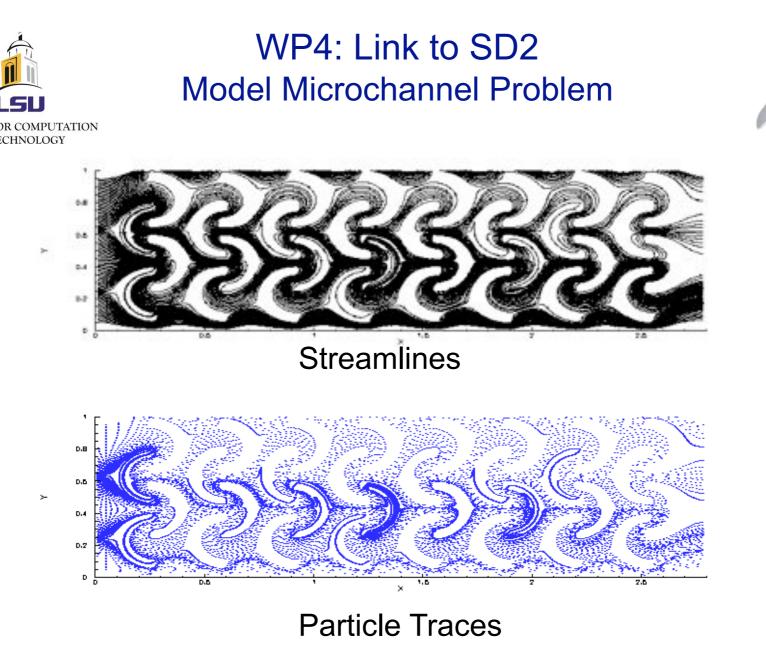
$$\nabla P = \mu \nabla^2 \mathbf{u}$$

Boundary Element Method determines velocities and surface stresses





CCT: Center for Computation & Technology



CCT: Center for Computation & Technology







- 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
- <u>Future Work:</u>
 - Parallelization of source code including transport



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)

Progress

Medium Tern

- 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)



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 parallelization 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



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)

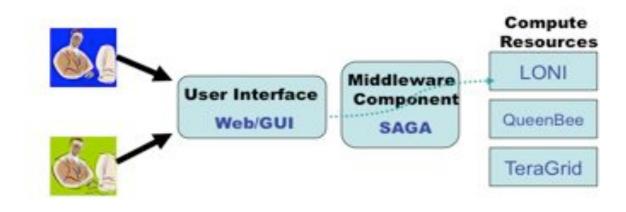


Application Manager



Provides support for uniform usage patterns and interface to heterogeneous resources

Application Manager : NAMD





Application Manager: Sailent Points

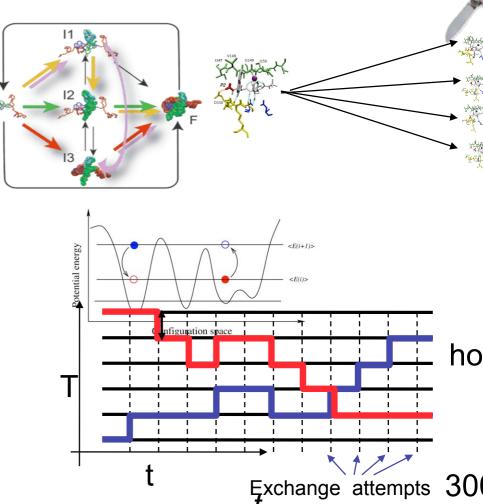
- Uniform: Provides single interface to heterogeneous and distributed resources
- Generic: Infrastructure can be embedded into either a portal or into a GUI
 - Also lightweight, flexible, modular
 - Easy to deploy
 - Can support:
 - Other MD packages (e.g., LAMMPS)
 - Other Usage Modes (e.g., High-throughput)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



Replica-Exchange Application Pattern

OR COMPUTATION

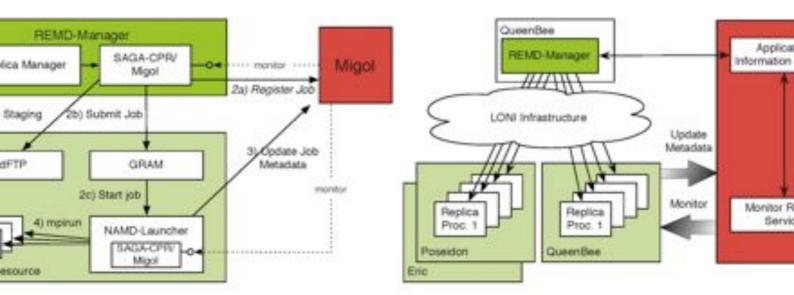
- Task Level Parallelism
 - Embarrassingly distributable!
- Loosely coupled
- Create replicas of initial configuration
- Spawn 'N' replicas over different machine
- Run for time t; Attempt configuration swap
- Run for further time t; Repeat till finish

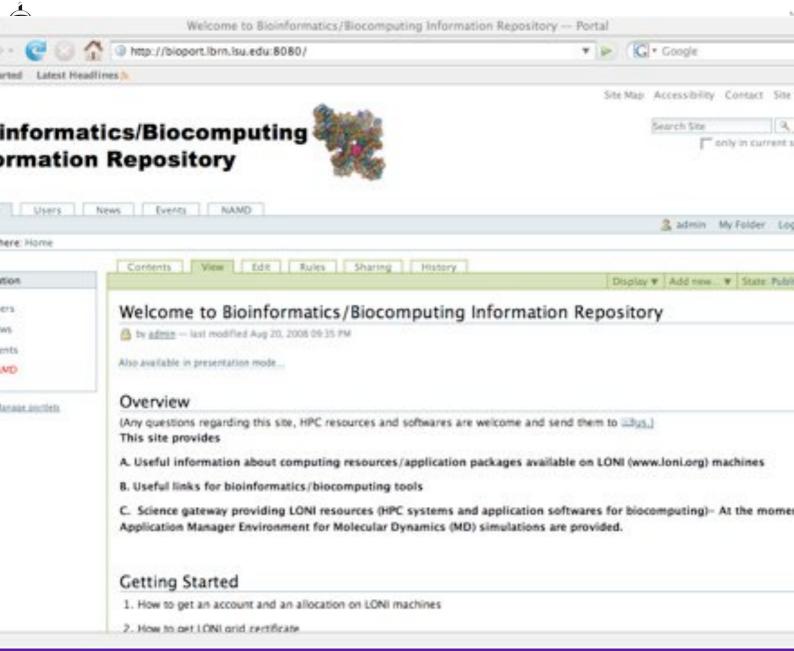


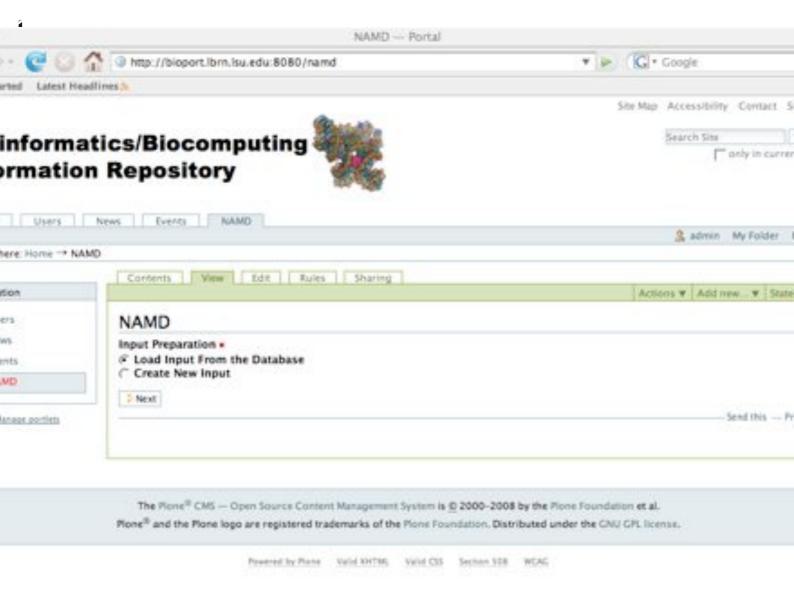


Replica-Exchange Manager

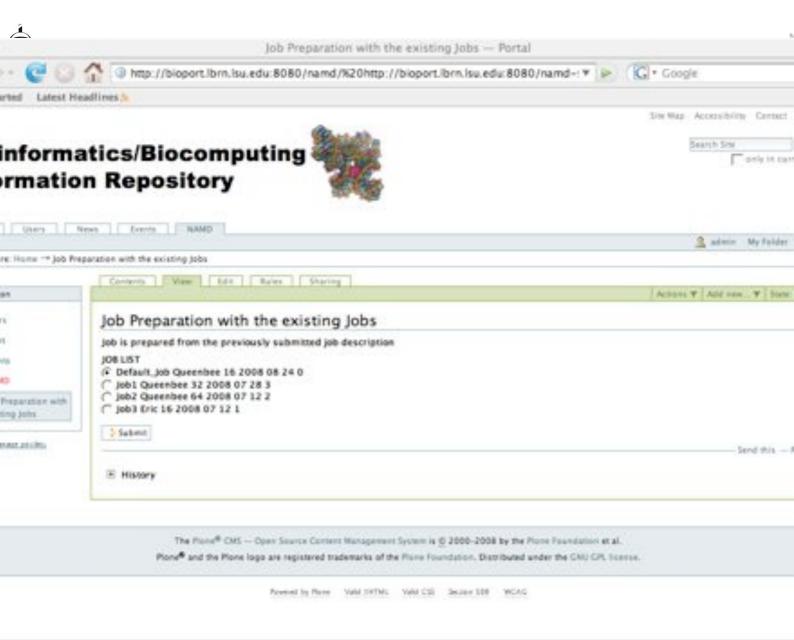








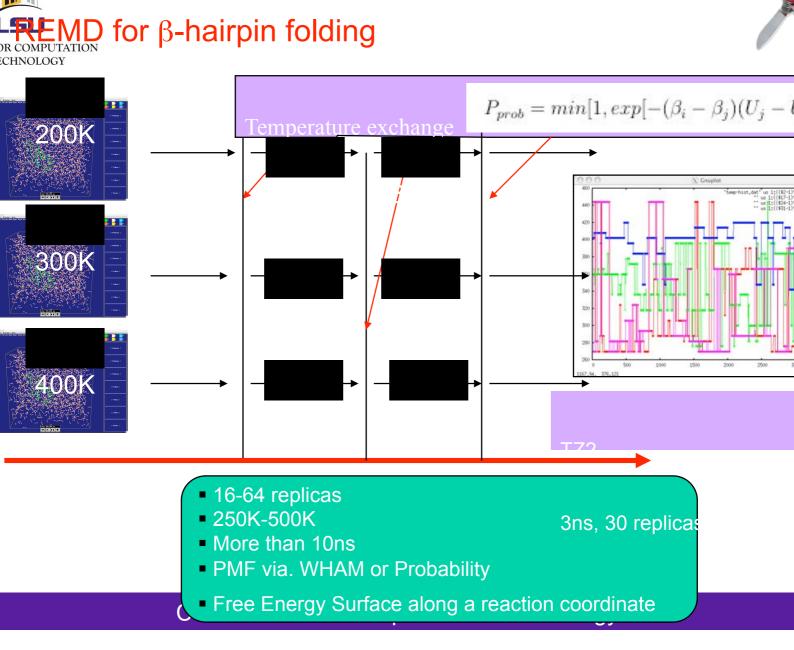
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Application Manager: Sailent Points

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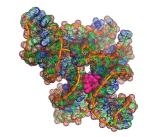
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plica 1 done
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plica 3 done
plica 4 done
(NFO) Now exchange step ....
schange result :
2-th EX : 320 330 300 310
(NFO) Replica 0 : Input files are staged into gbl.loni.org
(NFO) Replica 1 : Input files are staged into qbl.loni.org
(NFO) Replica 2 : Input files are staged into gbl.loni.org
DHFO) Replica 3 : Input files are staged into qbl.loni.org
(NFO) Replica 0 started (Num of Exchange Done = 2)
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(NFO) Replica 2 started (Nam of Exchange Done = 2)
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plica 3 done
plica 1 done
plica 2 done
plica 4 done
INFO) Now exchange step....
schange result :
3-th IX : 330 320 310 300
DEFO) Replica 0 : Input files are staged into qbl.loni.org
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REMD Simulation



NA 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