

SURAggrid Application Description

Application Name		
Application Area	Protein Loop Structure Prediction	
Keywords	Protein Folding, Protein Loop Structure Prediction	
Project/Dept. Affiliation	North Carolina A&T State University	
Specific Objective for Using SURAggrid	Benchmarking the protein loop structure prediction package on a large protein loops Tuning the performance of the protein loop structure prediction package	
Originating institution	North Carolina A&T State University	
Primary Application Contact Name, Email	Yaohang Li, yaohang@ncat.edu	
Technical Contact: Name, Email	Yaohang Li, yaohang@ncat.edu	
Participating sites	North Carolina A&T State University	
Application Description	Collaborating with Dr. Eric Jakobsson's research group at NCSA, we recently develop a new protein loop structure prediction software package based on the residue triplet scoring function and distance-based atom interaction scoring function. The software package has already shown resolution improvement in various difficult protein loops. However, we need to benchmark this software package on a large protein loop structure benchmark with hundreds of loop structures, which is very computational costly.	
Do you have HPC available at your institution?	Yes, I have an 8-node cluster at NCAT for educational purpose.	
Are you interested in contributing a resource to SURAggrid?	Yes. I am currently using this cluster for a class. I would like to contribute when the	
	Initial (Test)	Future (Production)
What are the anticipated system requirements for SURAggrid nodes running this application?	At least 1G memory.	
Have you attended any HPC or Grid training? If so, which ones?	Yes. Several grid computing workshops.	
Grid focus (data sharing, computation, access to unique resources, collaboration)	Computing	
Does your application have any network dependencies (bandwidth, latency, multicast, other)?	No. The application is embarrassingly parallel.	
What is the expected frequency of application run (one-time, occasional, monthly, weekly, daily...)?	Daily.	
Describe expected application invocation mechanism (by user submitting job, programmatically by some event or timing...)	A perl script to submit jobs.	
Estimated start date for application run	ASAP	
Is this application open to others to use with their own data or revisions?	No.	
Do you have an access to a Certificate Authority?	No.	

SURAgriid Application Description

If yes, location is your Certificate Policy and Certificate Practice? Contact for your CA?	
Are you targeting any particular SURAgriid resource? Why?	No
Additional comments	This application requires a lot of memory and it needs a lot of IO operations at the initialization phrase.

SURAgriid Application Description

Application to Join SURAgriid as *Participating Member*

Name of Organization: *North Carolina A&T State University*

Street Address: 1601 East Market St.

City, State, Zip: Greensboro, NC, 27411

Office Telephone: 336-334-7245

Office Fax: 336-334-7244

Organization URL: www.ncat.edu

X *Joining as SURAgriid Participating Member*

Annual renewal of SURAgriid Participating Membership

SURAgriid Participating Members must:

- Participate actively in SURAgriid
- Optionally contribute to the SURAgriid annual report by submitting a Participating Member site annual report

Participating Members effectively acknowledge acceptance of "SURAgriid Participating Member Responsibilities" by submitting to the SURAgriid Governance Committee an Application to Join SURAgriid wherein they describe their institution's interests in joining SURAgriid as a Participating Member. Participating membership is awarded upon review and approval of an Application to Join SURAgriid by the SURAgriid Governance Committee. Each SURAgriid Participating Member will annually renew their participation in SURAgriid by submitting to the SGC an updated Application to Join SURAgriid indicating their institution's continuing activities in SURAgriid for the prior period and confirming their continued participation for the upcoming period.

1. Provide your contact information

Name: *Yaohang Li*

Title: Assistant Professor

Street Address: 1601 East Market St.

City, State, Zip: Greensboro, NC, 27411

Email: yaohang@ncat.edu

Office Telephone: 336-334-7245

Office Fax: 336-334-7244

2. Describe any current activities in SURAgriid:

We have been collaborating with SURAgriid in submitting proposals.

3. Describe your interest in joining (or renewing participating membership to) SURAgriid:

Two primary interests:

1. ***To take advantage of the SURAgriid computational resources to enable scientific discovery in protein loop structure prediction applications.***
2. ***To use SURAgriid community to enhance computer science education.***