















Project Goals (Cooperative Agreement)

- The focus is the development of a multi-functional cyberinfrastructure (CyberTools) to broadly enable significant advances in modern science and engineering. CyberTools will improve methods to manage data, foster development of complex simulations, improve visualization, and mine data. They will also enable co-scheduling of network, data, computational, and visualization resources for complex tasks. The goals of the proposal are to:
- Enhance the scientific capabilities of researchers by linking experimental and computational investigation;
- Enable scientific investigation through the use of advanced computational CyberTools;
- Drive CyberTools development by directly linking to prototype scientific projects.

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WP4: Tasks (2)

•For each Science Driver:

- Understand science problem and scope:

• Define simplest problem capturing "most crucial physics", i.e. Toy problem & derive Toy Model

- Define Grand Challenge Problems?
- Prioritize requirements in between

•...

- Understand current computational methods:

•Describe current code & usage mode? Current tools?

•How effectively are these deployed on LONI?

•Extensible? Scalable? Amenable to coupling with other codes ?

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- Multi-physics, multi-scale simulation ready?

•...



WP4: Tasks (4) Refine Tasks

- •UC for each Science Driver:
- · Is there a multi-physics, multi-scale scenario?
- If so, for every scenario outline:

Coupling requirements, exchange of info/control, codes used, problem sizes, challenges...

- Prioritization and time-lines
- Any Other Info?
- ...

– Q: Would SMS require/involve CFD-MD Coupled Simulations? Or Uncoupled CFD and MD? Does GIS require/involve coupled CFD-MD simulations? If so, how different from SMS?

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•Refine WP4 tasks:

Add here based upon discussions











WP2: Information Services Gabrielle Allen, et al

- We will develop a monitoring infrastructure on LONI with up-to-date relevant information for our applications, and provide generic and application-specific portals to provide scientific gateways into LONI:
- Information services. Review different information services (e.g., MonaLisa, GPIR, NWS) and production HPC services (e.g., Nagios, IPM, Big Brother), deploy as needed for CFD, MD, experimental projects and general applications, and devise mechanisms populated with reliable, up-to-date information. Provide services, schema and interfaces to store and query application monitoring information and to query other information services, to enable DDDAS applications, to allow collaborators to interact in real time with their simulations and experiments, and to prototype and develop new application scenarios.
- Portals. Generic portal interfaces and services with GridSphere that simplify the development, deployment, and reuse of complex application software and new Grid technologies will be developed. A LONI portal, with portlets for HPC (machine, service, job monitoring, job deployment), application specific interfaces (CFD, MD, Coastal) as well as advanced grid services (interacting with metadata, scheduling, data, information, task farming services) will be developed and deployed.

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