Working Group 5
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Mission, Activities, and Future Objectives

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WG 5 Meeting: Agenda

- Short overview of the mission, objectives, members, and projects
- Presentation of the working group activities during the past year (Michela Taufer)
- Short presentations:
  - High-Performance Parallel Computing of Pulmonary Air Flow on TeraGrid (Ching-Long Lin)
  - TeraGrid Simulations of the Human Arterial Tree (George Karniadakis)
  - Transparent access to compute resources for multiscale modeling applications (Wilfred Li)
- Discussion and identification of activities for the incoming year

Other topics:

- Merging of WG 5 and WG 7
- Election of new WG lead

Mission and Objectives

- Mission:
  - Addressing challenges in designing and deploying HPC systems for multi-scale modeling applications
  - Sharing knowledge about HPC systems and how they can contribute to the goals of our projects
- Objective - year 1:
  - Spread knowledge in HPC and grid systems for large-scale simulations
- Objective - year 2:
  - Share knowledge among the members of the group about our computing systems used for simulations in our projects

Tools

- Webpage: http://gcl.utep.edu/projects/msm/
    - Advertise the WG activities to the public and the members of the WG
    - Provide members with a password-protected environment to retrieve information / data from Consortium and vice versa
- Phone meetings: http://www.freeconference.com
- E-notebook: http://enotebook.eng.utep.edu/msm/index.html
    - For documents, protected by password access (not successful)

Activities

- Phone meeting June 2006:
    - Discuss of goals and activities of the working group
- Phone meeting Aug 2006:
    - Invited speaker: Charlie Catlett (Argonne National Laboratory)
    - Topic: The TeraGrid initiative - how to join it and use it.
- Phone meeting Oct 2006:
    - Invited speaker: Kelly Gaither
    - Topic: Data visualization and analysis on TeraGrid
- Phone meeting Feb 2007:
    - Invited speaker: David Anderson (UC Berkeley)
    - Topic: Volunteer computing resources for large-scale simulations
- Phone meeting Feb 2007:
    - Invited speaker: Viktors Berstis (IBM)
    - Topics: Support science through the World Community Grid

Meeting

- Two members of the working group have access to TeraGrid
  - On single site: Ching-Long Lin
  - Across sites: George Karniadakis
- Other members will soon be in need for computing power
- User support: good support
- Critical issues that are still open questions:
  - Scalability
  - Time from submission to execution too long and limits in the number of jobs that can be submitted
  - Parallel debugging
- Performance:
  - Tools exist for better understand lack in scalability of applications
  - Working with experts from national labs to address scalability issues as a possible activities for year 2

Performance Issues

- Open-source tools exist for better understanding the lack in scalability in our applications

  - Need to identify the tools

- Working with experts from National Labs to address scalability issues as a possible activities for year 2

  - Need to identify the experts

- Involvement of external experts in our projects to help us addressing performance issues

  - Tutorials and teleconferences

  - Work in small groups to address application specific problems

  - Rewarding experts for their help

Resources

- Need for sharing resources
- Web services to install and manage computation environments across sites:
    - Opal
    - Meta-scheduler across clusters
- Available resources:
    - World community grid
    - Teragrid
    - Local clusters
- Emerging technologies:
    - Are we ready for them?
    - Are they ready for our applications?

Next Steps

- Identify experts
- Characterize specific needs for specific applications within the working group
- Involve experts from e.g., National Labs in our projects for:
    - Advising
    - New collaborations
- Move web-page to wiki where we can also have some sort of forum for discussion and sharing of documents