

Supercomputing Costa Rica Summer Workshop

Computational Science in Engineering: Bio-informatics and Nanotechnology
Costa Rica
Proposed dates: July 13th - July 19th

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Introduction

Computational Science is a tool for discovery in the XXI century. Their successful application has proved to be a key element for science and technology in different arenas. Costa Rica has been deploying a cyberinfrastructure effort designated to help local scientists and technology experts place their work in the current international state of research. This workshop, *Computational Science in Engineering: Bio-informatics and Nanotechnology*, aims at giving the people theoretical and practical resources for improving the quality of their work and access high level computing resources as those provided by TeraGrid. In general, the workshop will consist of a core set of lectures and hands-on sessions in computational science and domain-dependent activities that will frame the resources within specific research areas.

Bio-informatics and Nanotechnology have been chosen as the main tracks of the workshop due to their pertinence to (a) the local development of science and technology, (b) existing collaborations with institutions in the US and Europe in both areas, (c) existence of local data and scientific resources and (d) compliance with a national strategy for the advancement of Science and Technology, namely, the XXI Century Strategy.

Facilities

The TeraGrid workshop will be held at the National Center for Advanced Technology Studies (CeNAT). It is located in Pavas, San Jose at a 40 minutes drive from the Juan Santamaria airport. Tropical weather will welcome the visitors in the range of 70F minimum and 90F maximum. During the proposed dates –summer in the US- local weather is toward the end of the dry season with a steady 80F to 85F and occasional rains. Participants are advised to carry or buy raincoats in the case of excursions to the rain forest.

Local Staff

Support staff will be composed of four people from the National Center for Advanced Technology Studies and students from the state universities. Each staff member will receive a stipend of \$150 for the entire week.

Workshop instructors

Four instructors will be required for the two parallel sessions. Also, the workshop will be divided in two main sections:

- Core activities, designated to give the necessary computational background to the participants
- Domain-specific activities, demonstrating how the computational tools can be used in the context of discipline-dependent problems

As an important component, two keynote speakers, one for each domain both domains will introduce the workshop. Finally, an introduction to TeraGrid resources will provide attendees with the necessary knowledge of the existing hardware and software architectures for high-end problem solving.

Participants

The workshop will accept between 20 and 25 participants from the United States, Central America and South America. The profile of each participant is that of faculty, researchers, and graduate students in physics, chemistry, biology, and computer science; researchers that want to apply computational tools in their research or researchers related to projects that involve bio-informatics or nanotechnology.

In terms of space a full auditorium and two computer labs will be used at CeNAT.

Travel, Room and Board

Participants should use the Juan Santamaria International Airport (SJO) located in Alajuela Costa Rica, from which ground transportation will be provided appropriately by the local organization. Participants will be housed in executive one and two bed-room apartments. In the case of locals lodging will not be required.

During the stay, all amenities will be available in the residential complex in different modalities in the case of children or spouses for free. Participants can stay an extra day with an extra cost of \$85.00. Amenities allow children room with parents. There will be no parking costs due to in-house parking space and all state universities are in a range of no more than 15 miles from CeNAT where libraries and research laboratories can be found. Recreational facilities are within a range of 5 to 10 miles, including attraction parks, museums and the rain forest.

There is a wide selection of local dining options, including vegetarian and non-vegetarian food as well as traditional dishes from the Costa Rican cuisine. Friday dinner is to be hosted at Machu Picchu restaurant in Santa Ana, a 30 minutes drive from the main building and a 5 minutes drive from the housing facilities.

Classroom and Laboratory Spaces

Each classroom in the building can accommodate a group of 15 people, including laptop space. There is no overhead projector, but a computer projection unit can be easily installed and deployed. Wired and wireless Internet access is available via the building infrastructure as well as Internet2 wired access. The classrooms are open from 8:00am to 6:00pm, but hours can be adjusted as needed with the administration.

Each computer lab in the building can accommodate a group of 16 people with space for laptop computers. Projection units for computer presentations will be provided. Wired and wireless Internet access is available via the building infrastructure as well as Internet2 wired access. Both laboratories have printers and one of them has a 42-inch plotter for high-resolution materials on glossy and non-glossy papers. There is no charge for printing. Also, access to the local HPC clusters will be provided.

Software installation requires three weeks for deployment, testing and creating of accounts for visitors and instructors. Three staff members will be available for technical support in case of any eventualities. An additional room will be available for break refreshment as well as an additional room for breakout sessions.

Workshop Materials and Supplies

Santiago Nunez-Corrales will receive the materials at the following address:

Centro Nacional de Alta Tecnologia
Antiguo AID
1200 N de la Embajada de Estados Unidos de America
Rohrmoser, Pavas
San Jose, Costa Rica

A FedEx delivery is preferred. UPS can be also used for sending the workshop materials.

Photocopying facilities are located at CeNAT as well, with an additional photocopying facility at walking distance. Additional supplies such as erasers, staplers, hole punch and pens can be provided by the local organization. White boards are available for use.

Cost-Sharing

The attached budget indicates a difference in the SC contributions and workshop expenses of \$1,600.00 This difference will be cost shared by the Advanced Research and Technology Collaborative for the Americas (ARTCA).

Workshop program

The program for the workshop will be organized as follows, considering sessions and social activities. Core activities are those shared by both groups, and domain-specific activities are

Sunday

Welcome Dinner and reception

Monday (core: introduction)

Keynote speakers
Introduction to Computational Sciences
Introduction to TeraGrid resources

Tuesday (core: simulation and modeling)

Introduction to mathematical modeling for engineering
Simulation tools for (nanotechnology/bioinformatics)

Wednesday (core: parallel and grid computing)

Introduction to parallel computing
Grid computing and cyberinfrastructure
Introduction to Job submission systems

Thursday (domain-specific activities)

Research in (nanotech/bioinformatics): tools and methods, I part
Dinner at Pueblo Antiguo

Friday (visit)

Research in nanotechnology/bioinformatics: tools and methods, II part (half day)

Visit to INBio Biological Park (half day)

Formal dinner, Machu Picchu

Saturday (wrap-up)

Closing session