

UT Austin | Portugal

INTERNATIONAL COLLABORATORY FOR EMERGING TECHNOLOGIES, CoLAB

Annual Report 2009 - 2010: ADVANCED COMPUTING



INTERNATIONAL COOPERATIVE RESEARCH AND EDUCATION: Year 4 of 5

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UT Austin | Portugal CoLab: ADVANCED COMPUTING

Strategy

As the UT Austin | Portugal CoLab completes its fourth program year, high focus is placed on results to date and finalizing the program toward sustainability beyond the FCT funded scope of December 2011.

Advanced computing occupies an academic space that intersects both advanced digital media and mathematics—and is increasingly involved in those threads of the CoLab program. Consequently, several of the CoLab Advanced Computing activities were conducted in cooperation with either the CoLab Advanced Digital Media or the CoLab Mathematics programs. To provide accurate reports by program, these interdisciplinary activities are included here, as well as in the annual reports for Advanced Digital Media and Mathematics.

This past year’s results include:

- Four 2-year Advanced Computing collaborative research projects were funded by the FCT
- Seventeen graduate students visited UT Austin to work on advanced research and to audit CS courses.
- Pursuit of research projects that encompass highly advanced computationally-driven visual graphics;
- Student support for doctoral thesis research;
- Summer School in e-Science with many-core CPU/GPU processors;
- Support to the 2nd Cloud Computing Conference, *Cloudviews 2010*;
- Participation in *IBERGRID 2010* Iberian Grid Infrastructure Conference
- Increased cooperation in shared grid computing between Portugal and Spain;
- Pursuit of research projects that encompass highly advanced computationally-driven visual graphics;
- Hosting digital artists in the TACC’s Visualization Laboratory.

These advancements have effectively forwarded the core purposes for which the CoLab Advanced Computing program was established in 2006.

Alberto Proença & Keshav Pingali



RESEARCH & EDUCATION

CoLab sponsored research projects: What constitutes success?

All of the research projects pursued by the Advanced Computing group involve complex mathematical applications, including those with the object of creating animated visual modeling. In order to create these models, mathematical analyses and understanding of the subject's physics is prerequisite to presenting these subjects in meaningful animation—often at a cellular or molecular level, but which might as easily implement large geographic or galactic views—including sequences of events over time. Against all Advanced Computing research projects, classic metrics apply as follows:

- Advancement regarding the mathematical solutions required to meet the need or model the subject;
- Software development against those mathematical solutions;
- Publications describing mathematical advancements achieved, processes in software development, implications that are revealed through modeling processes, etc.

These publications may include papers in journals, book chapters, articles or books edited, conference presentations and proceedings, etc. In the longer term, successful research results may include:

- Broader adoption of the model, or the understanding facilitated by the model, into academic or industrial practices, or product applications;
- Academic, industrial, or societal behavioral changes caused by the understanding facilitated by the model.

A basic purpose of CoLab research projects is increased interaction between universities, and each research project application is required to implement a team-based approach that involves professors from at least two Portuguese universities, as well as one or more professors in the U.S. In addition to dispersing benefits of the research investment more widely across the nation of Portugal, and intrinsically improving inter-university relationships, this also helps increase the possibility of publications and similar diffusion of research results. Similarly, inclusion of graduate students as active research members helps further overall CoLab goals while infusing young talent into cutting edge research projects.

Project: SIMCARD

Patient-specific cardiovascular modeling & analysis

Principal Investigators:

1. Adélia Sequeira, IST
2. Thomas J. R. Hughes, UT Austin
3. Chandrajit Bajaj, UT Austin

Research Team : IST

4. Alberto Massimo Gambaruto
5. Alexandra Bugalho de Moura
6. Angel Rodríguez Rozas, PhD candidate
7. Carlos Alberto Mota Soares
8. Diana Catarina da Fonseca Madeira Nunes, PhD candidate
9. Helder Carriço Rodrigues
10. Jevgenija Pavlova, PhD candidate
11. João Gonçalo Silva Marques, PhD candidate
12. João Manuel Ribeiro da Silva Tavares
13. João Orlando Marques Gameiro Folgado
14. José Carlos Fernandes Pereira
15. José Manuel da Silva Chaves Ribeiro Pereira, PhD candidate
16. Juan Antonio Acebron de Torres
17. Marco Paulo Lages Parente

Research Team: UPorto

18. Francisco Paulo Marques de Oliveira, PhD candidate
19. Ilda Marisa de Sá Reis, PhD candidate
20. Pedro Alexandre Lopes de Sousa Martins, PhD candidate
21. Zhen Ma, PhD candidate

Research Team: UTL

22. João Paulo Vicente Janela

Research Team: Hospital de Santa Maria

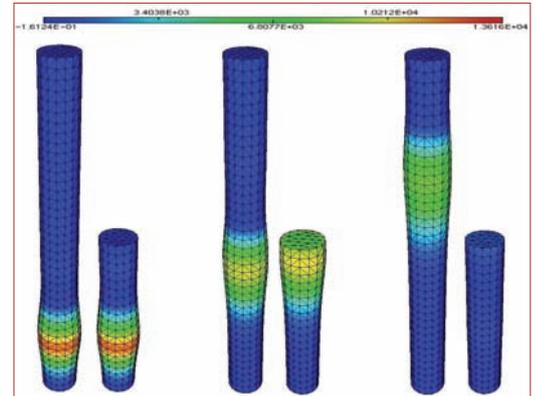
23. Jorge Rodolfo Gil Guedes Cabral Campos
24. Renato Manuel Natal Jorge Rita Fernandes Sousa, PhD candidate

The *Sociedade Portuguesa de Ressonância Magnética* also participates in the SIMCARD project.

The project

SIMCARD is an interdisciplinary project that develops, analyzes, and simulates mathematical models of the cardiovascular system. According to the most recent statistics, cardiovascular diseases represent the major cause of death in developed countries. The important consequences of such diseases at the individual and social levels have a significant impact in the cost and overall status of healthcare. An increasing demand from the medical community for scientifically rigorous and quantitative investigations of cardiovascular diseases has given a major impulse to the development of mathematical models and numerical tools for computer simulation of the human cardiovascular system, in both healthy and pathological states. Since the circulatory system is highly integrated and modeling its various functions is an incredibly challenging problem, which requires many fundamental issues to be addressed.

Cerebral vasculature pathologies and malformations, including aneurysms and stenoses, are studied from medical images. The work geared towards the study of realistic physiological processes and clinical application is striving for faster and more robust schemes as well as more physiologically accurate mathematical models. This involves virtual model reconstruction from medical images, uncertainty estimation of the virtual model definition, inter-patient characterization, validation of simulations with clinical data and feedback to physicians.



SIMCARD PROJECT:

FSI for idealized geometries of a straight vessel with boundary conditions implemented as 1D network.

Blood flow interacts mechanically with the vessel walls and gives rise to complex fluid-structure interaction problems which require appropriate algorithms to describe the energy transfer between the fluid and the structure. Accurate and efficient computations of the coupled problems are a difficult task due to large displacements and difference between time scales of the main blood flow and of the pulse propagation. The research team proposes to extend the existent results and numerical codes, to couple non-Newtonian models for blood flow with complex models for the vessel wall, using non-standard defective boundary conditions to deal with real geometries reconstructed from medical images and data from measurements. New computational methodologies and models are being developed to analyze:

- the mechanical behavior of structures from medical image sequences;
- biomechanical principles of the segmentation, tracking, and motion analysis of the heart from images;
- the estimation of the mechanical properties of the heart's relevant tissues, by non-invasive techniques;
- and the development of 3D models of the heart.

These research results will contribute to simulation of pathological cases of medical interest at reasonable computational costs. There is an evident bottleneck of computational cost of the described simulations. This is seen especially in the numerical simulations of the non-Newtonian blood flow and the vessel structure dynamics, and their coupling. While some approaches to alleviate the computational costs, such as 0D (lumped parameter) or 1D reduced models can be used for simulating the vasculature far from the region of interest, the more accurate and complex the mathematical models, the more computationally intensive the simulation.

This multi-disciplinary collaborative project involves large-scale computational simulations and requires a synergy of research efforts and knowledge of different fields. Dealing with specific problems of clinical interest, it will benefit from the longstanding national and international collaboration with bioengineers and medical doctors. This project is strongly contributing to strengthen the links between Portuguese researchers from several institutions (IST, UPorto, UTL, HSM) with the research teams of UT-Austin, whose expertise in the field is recognized world wide.

Research metrics

Start date: April 1, 2009

End date: March 31, 2012

The following task set has seen advancement in this research:

- Medical imaging in vivo (MRI, MRA, CT);
- Medical image interpretation;
- Numerical simulations of cerebral vasculature;
- Uncertainty quantification of vessel geometry variability;
- Software development.

Preliminary work has been carried out, and a variety of image interpretation techniques have been studied, and their applications tests, toward the two tasks of:

- Analysis of the behavior of structures and estimation of their mechanical properties from images;
- Experimental properties and reflexive activity of the tissues.

Results remain to be consolidated toward the task of *micromechanical modeling and optimization of cardiovascular stents*. Research publications and presentations directly related to the project by team members, to date, include:

- Books or special issue journals edited: 5
- Papers in international journals or book chapters: 20
- Papers in conference proceedings: 20
- Relevant presentation at conferences and seminars: at least 24;
- One PhD thesis.

In addition to these publications and presentations, project members organized ten special scientific events; and there are five related additional research projects related to the SIMCARD project.

Project: Parallel programming Refinements for irregular applications

Principal Investigators:

1. João Luís Sobral, UMinho
2. Keshav Pingali, UT Austin
3. Don Steve Batory, UT Austin

Portugal Research Team

4. Luis Paulo Peixoto dos Santos, Faculty Researcher UMinho
5. Miguel Jorge Tavares Pessoa Monteiro, Faculty Researcher UNL
6. Diogo Telmo da Sá Lima Pinto Neves, Graduate Researcher, UMinho
7. Edgar Manuel Fernandes da Mota Sousa, Graduate Researcher UMinho
8. Rui Carlos Araújo Gonçalves, Graduate Researcher, UMinho
9. Matheus Barros de Almeida, Graduate Researcher, UMinho
10. Pedro Miguel Ferreira Costa Monteiro, Graduate Researcher, UNL

The project

Given current trends, it can be expected that general-purpose processors will be many-core processors in which the number of cores is likely to double every 1.5 years. Currently, four and eight core processors are on the market, and ten years' time could see development of "kilocore" processors. This move towards many-core architectures has shifted the burden of improving program execution speed from chip manufactures to software developers, requiring a fundamental change in the way software is developed and maintained.

The high-performance computing (HPC) community uses communication libraries, like MPI, to code parallel applications for distributed-memory computers. Their approach to software development is performance-driven, and high software development costs have been hidden behind the high cost of large-scale distributed-memory parallel systems. This approach is too expensive for the mass market.

Most of what we know about parallel programming is confined to "regular programs", which are programs that manipulate dense matrices. Stencil codes and matrix factorizations are examples of regular programs. We know very little about the patterns of parallelism and locality in irregular programs, so there are few languages, constructs, and tools to help programmers to write such programs. Recently, the Galois project, led by Keshav Pingali, performed a number of case studies of irregular programs that show that many of these programs have a generalized form of data-parallelism called "amorphous data-parallelism".

In addition to parallelism, programming models must also permit expression of locality of reference, which is important even on sequential platforms. Programming paradigms promoting strong separation of concerns can play a crucial role to address the development complexity of parallel applications. The decomposition of parallelization concerns into high level features (fine-grained refinements that add implementation detail, such as parallelism or the use of particular data structures) will

make it possible to synthesize/tune applications for each class of target platforms and/or problems by selecting the set of features to attain the best performance.

The research team aims to identify and modularize refinements (a.k.a. patterns, skeletons) that parallelize computations in programs, and to compose such refinements to map base programs to efficient, platform-specific, parallel applications. Researchers start with a base program, specified in a platform independent manner, and progressively increment its functionality towards a more platform specific version. Thus, in the proposed approach, parallel programming abstractions are application refinements that will be validated by making Galois an extensible runtime platform, by allowing the addition of new program refinements and identifying the conditions under which such refinements can be effectively used. Researchers use existing case studies of Galois, as well as new case studies, where parallelism and locality of references will be expressed as program refinements.

Research metrics

Start date: June 1, 2009

Completion date: May 31, 2011

In early research planning meetings, it was decided to initially focus on two key research areas:

- Classification of parallelization patterns for irregular application;
- Parallelization refinements.

These two areas were the main focus of the first year of the project. Currently a catalogue of parallelization patterns is concluded and an initial assessment of techniques to implement parallelization refinements is also concluded. The results obtained so far are at an early stage. Future research falls in three areas:

- Searching for new parallelization patterns in irregular applications;
- Working on the concept of refinement;
- Applying refinement-based programming approach to concrete case studies.

There are several project member publications directly related to the themes under investigation, including two new joint papers describing the most important results from the first year, that are being prepared for publication.

There are three ongoing PhD theses, jointly advised. These three Portuguese researchers spent 6 months at Austin (from February to July 2010). Moreover, one MSc was concluded and another will be concluded this year.

Project: INTELLIPave

Principal Investigators:

1. José Carlos Ferreira Maia Neves, UMinho
2. Jorge Aberto Prozzi, UT Austin

Portuguese Research Team

3. António Carlos da Silva Abelha
4. Austin José Manuel Ferreira Machado
5. Manuel Filipe Vieira Torres dos Santos
6. Renato André Morgado Leite da Costa
7. Reus Salini, PhD candidate
8. Ricardo Gomes de Faria
9. Victor Manuel Rodrigues Alves
10. Helder Manuel Ferreira Coelho

11. João Carlos Balsa da Silva
12. Luis Alberto dos Santos Antunes
13. Paulo Jorge Cunha Vaz Dias Urbano
14. Luis Alberto dos Santos Antunes

The project

The INTELLipave project applies advanced techniques in artificial intelligence and soft-computing to provide a more scientifically accurate, modelling-based approach to evaluate the potential behaviour and durability of asphalt pavements. This approach, being holistic and systemic, is expected to provide much more accurate results than the methods currently employed, which were developed half a century ago (or more) and which are based on empiric and empiric-mechanistic methods.

To meet this objective, researchers are referencing data collected in the Mn/Road Project (Minnesota, USA), which provides a detailed history of the service life for instrumented test sections of asphalt pavements that provides details sufficient for the needs of this approach. The relative data includes records taken by electronic sensors over the service life cycle of the relative asphalt pavements, taken over ten years, with the transit of about 100 million vehicle axles, with the capture of over two billion data terms. This detailed data includes vehicular information (date, time, axle configuration, weight by axle, speed, tire type and pressure, stresses in the tire-pavement contact area), environmental information (air temperature, pavement temperature, precipitation, wind speed, solar and UV radiation, humidity in the granular pavement layer), and structural information (strains and stresses in key points of the asphalt concrete and granular layers).

This wide database allows for the creation of a new modelling method that considers all these variables in an explicit way, without simplification or concession. The modelling method under development will also allow the addition of other variables that are not yet known as significant. Database information will be filtered, qualified, and organized to create a numerical matrix that will be optimized through the use of advanced soft computing techniques (e.g. particle swarm optimization; SOMA, evolutionary genetic algorithms, logic-mathematic functions) and equation systems to determine the contribution of each variable and each vehicle toward the ruin of the pavement. This optimization will populate a “matrix of performance” that will be used as a source of “experiences, knowledge, and intelligence” to program a neural network set that will be able to predict the behavior of asphalt pavements. These predictive qualities will be valuable for projecting design, life expectancy, and maintenance of both new and existing pavements, with the input of information including proposed vehicular traffic, climate, and structural data. Therefore, this research will allow simulation of the life cycle of proposed pavement designs to be modelled against projected use, to secure the maximum design efficiency against projected traffic flow for its climate.

The innovation and flexibility of this modelling approach is based in its potential application against multiple parameters, objective and subjective, to evaluate pavement quality against different future scenarios, including need vs. cost. The following criteria will be included:

- Percentage of cracked pavement area;
- Structural capacity;
- Depth of wheel track;
- Roughness of the road as related to driver comfort;
- Macro texture as related to tire adherence and driver security;
- The value of the property for the highway.

Further, the approach will provide for the addition of new data parameters that are not yet described. Another benefit of this approach is the potential for the accumulation and cross-referencing of knowledge in a scientific way to provide a basis for the development of a matrix of pavement performance: and a foundation by which this body of knowledge can increase continuously over time.

The scope of this work is believed to be sufficient to coalesce a new field of interdisciplinary research in which the fundamentals and practices of Extended Logic Programming Languages, Evolutionary Intelligence, and Soft Computing might help to effectively solve engineering and other problematic aspects of asphaltic pavements. This project coordinates international researchers from Brazil, Italy, Argentina, Portugal, and the U.S.A., to help develop a productive network of expertise in this field, with high potential for expansion. This is also interested in establishing a Society of Pavement Researchers based on the results of this work, and this project has been entered into the Project on the Society of Collaborative Networks (SOCOLNET).

Research metrics

Start date: June 1, 2009

End date: October 31, 2010

Project: Applications to combustion Modeling the sub-filter scalar dissipation near the Turbulent/Non Turbulent interface in jets

Principal Investigator:

1. José Carlos Fernandes Pereira, AFFILIATION?

Portuguese Research Team

2. Carlos Frederico Neves Bettencourt da Silva, IST
3. Gwenael Hauet, IST
4. José Manuel da Silva Chaves Ribeiro Pereira, IST
5. Carlos Gonçalves Rossa, UCoimbra
6. Domingos Xavier Filomeno Carlos Viegas, UCoimbra
7. Miguel Abrantes de Figueiredo Bernardo de Almeida, UCoimbra

Please identify University Affiliation

8. Diogo Gomes Almeida Chambel Lopes
9. Rodrigo Miguel Ribeiro Taveira

The Project

Many industrial and transportation devices involve combustion in jet diffusion flames where the combustion reaction takes place at edge of the jet where fuel and oxidizer interface. Improving the understanding and the accuracy of the simulations of turbulent reactive jets is therefore crucial to improve the fuel economy and to decrease the emissions in numerous combustion systems. The study of scalar transport is hugely important in these flows since ultimately it is the evolution of scalar fields governed by transport equations that determines the rates of turbulent mixing, combustion and pollutant dispersion. An important physical quantity in this context is the scalar dissipation which represents the rate at which the scalar fluctuations are dissipated by molecular effects. It acts mainly at the small scales of motion and its dynamics is closely associated with the final stages of the energy cascade mechanism for the scalar field. Regions of intense scalar dissipation tend to form very thin sheet like structures in isotropic turbulence. Due to its high relevance to both theory and applications much work has been done in the characterization of the statistics, topology, and geometry of this quantity (Overholt and Pope 1996, Vedula et al. 2001, Schumaker et al. 2005, Schumaker and Sreenivasan 2005).

On the other hand, it has been recognized for some time that from the existing numerical techniques only large-eddy simulations (LES) can accurately describe the complexities of the flow in turbulent jet diffusion flames. In LES the large, energetic scales of motion are explicitly computed while the effect of the small scales of motion is modeled. A quantity of much interest for large-eddy simulation (LES) of turbulent combustion is the sub-filter scalar dissipation which is needed as a parameter in flamelet models of non-premixed combustion (Cook 1997). It appears also in the transport equation of the sub-filter scalar variance. Thus, in large-eddy simulations (LES) involving scalar transport such as in turbulent mixing or combustion, the sub-filter scalar dissipation has to be modeled (e.g. Pierce and Moin 1998, Cook and Bushe 1999, Grimaji and Zhou 1996).

Since the most important contribution to the sub-filter scalar variance comes from the small scales, its modeling is particularly challenging. Despite its importance many aspects of the sub-filter scalar dissipation are not well understood. In particular, the detailed characterization of the topology of the sub-filter scalar dissipation is still incomplete even in isotropic turbulence. The regions of intense sub-filter dissipation also exhibit a sheet like structure that can be quantified using the surface area, the thickness of the surfaces, and its curvature. Moreover the fractal dimension of these structures can also be computed.

Another important aspect of turbulent jets that is receiving much attention recently is the mechanism of "turbulent entrainment." Turbulent entrainment that takes place in all free shear flows such as mixing layers, wakes and jets and largely governs the transfers of mass, momentum, heat, and other active or passive scalars across the sharp edge of the jet, which in jet diffusion flames separates the fuel from the oxidizer. It has been shown recently that the physical mechanisms occurring at this region are considerably different from previously thought. In particular, recent works show that turbulent entrainment is mainly caused by small scale motions ("nibbling") and not by large-scale eddy motions ("engulfment").

Moreover, the classical turbulent variables displays sharp gradients and a very particular dynamics to this region. Moreover, it has been shown that scalar gradient, its production, dissipation and convective transport are particularly intense near the fuel/oxidizer interface. A detailed study of the sub-filter dissipation in this context is both useful and urgent for the scientific community and the industry. One related application of this knowledge of high interest to the research team is in understanding the action of embers produced during a forest fire which can be transported by thermal plume to create secondary fires, thus complicating fire suppression and very often endangering lives. This process of fire propagation is not well understood, and one of the objects of this research is to apply the knowledge gained against this need.

The goal of this research is to (i) analyze the dynamics of the scalar field across the fuel/oxidizer interface, (ii) study the Lagrangian statistics of the particle trajectories across the fuel/oxidizer interface, (iii) characterize the detailed geometry e.g. the surface, thickness, curvature, and fractal dimension of the structures of intense sub-filter scalar dissipation in turbulent plane jets in the context of the turbulent entrainment and, (iv) develop and assess a new model for the sub-filter scalar dissipation to use in LES based on this information, (v) apply this modeling to predict ember production and transport during forest fires.

Research metrics

Start date: June 1, 2009

End date: December 31, 2011



Edgar Sousa, Diogo Neves, João Barbosa and Rui Gonçalves.

Student Visiting Scholars & Intern Visits

Visiting Scholars

This spring the CoLab Advanced Computing program welcomed Rui Gonçalves, Reus Salini, Edgar Sousa, João Barbosa, and Diogo Neves as Visiting Scholars to study at UT Austin and to collaborate with the departments of Computer Science, Electrical and Computer Engineering, the Institute for Computational Engineering and Sciences (ICES), the Texas Advanced Computing Center (TACC) and the Center for Transportation Research (CTR). Visiting Scholar status at The University of Texas at Austin is a specific accommodation that grants students entry to interact directly with the university for up to two years. Their research covers a broad range of topics in the field of advanced computing. João Barbosa is currently examining high-performance computer graphics: “My focus is heterogeneous and core platforms for real-time ray tracing. The goal of my research is to explore and develop efficient scheduling mechanisms for distributed heterogeneous platforms for real-time problems, such as ray-tracing and ray casting (volume rendering).”

Reus Salini contributes to the INTELLIPave research project: work that may save countries millions of dollars in infrastructure costs. He is researching the application of neural networks to the modeling of asphalt pavement, hoping to make breakthroughs in longstanding civil engineering problems through recent advances in computing power.

Several of the students are working on the parallel programming project. “I am working on parallel programming methodologies that improve modularity and promote the incremental development of parallel applications,” Rui Gonçalves said. Diogo Neves’ focus is “to raise the abstraction level of parallel programming by developing a new set of constructs that promote a stronger separation of concerns in parallel computing. The idea is to separate the domain-specific code from parallelization issues—that is, to hide the complexity of parallel programming as much as possible.”

Some students assist UT professors with their research. Edgar Sousa’s interests lie in “aspect-oriented programming to develop tools for (semi-) automatic parallelization of legacy scientific codes,” he said. “I am working closely with Professor Keshav Pingali and his research team and taking part in the development of the Galois framework.”

Whereas the students know and love their research, the CoLab program introduces them to unfamiliar topics. Diogo Neves explained how his time with CoLab changed his understanding of UT’s reputation. “Before attending UT, I knew that it was recognized as a top university. After being here, I’m realizing that it’s at the top because” it’s home to great scientists and “several top research groups, such as Dr. Keshav Pingali’s group, with whom I am developing my work. It seems that tight relations between UT and the outside world exist which enable UT scientists to perform applied science,” Neves said. According to Rui Gonçalves, UT researchers focus on smaller problems than their Portuguese counterparts but are able to explore the problems more deeply. However, the biggest difference between graduate education programs in both countries is the amount of time spent in classrooms. In Austin, students “spend less time listening to the professor in a classroom” and more time doing homework and other assignments outside of class, Gonçalves said. Variety is another differing factor. “The freedom of choice related to the curriculum” is much greater in Austin, João Barbosa said.

There are more educational and research-related resources at UT, Barbosa added. Many UT researchers and visitors from other institutions give talks outside of class schedules. Neves elaborated, “Is there a day without a seminar? No! It is really awesome!” Another benefit of CoLab participation is the development of professional soft skills. Edgar Sousa plans to use the

teamwork and team management skills he is learning from CoLab in his future work with Portuguese research teams.

Technical resources offer another appeal for many CoLab participants. Reus Salini plans to use TACC's supercomputer to process his "large databases and, together with UT's team, start a deep cooperation between the advanced computing and pavement engineering areas," Salini said. "While Portugal is just starting to create its own infrastructure, UT has a rock-solid infrastructure with which to develop world-class research." CoLab offers students the opportunity to come to Austin under several different initiatives: as members of FCT-funded R&D projects, as students formally accepted into UT Austin PhD programs, or as participants in CoLab's professional internship program. João Barbosa puts it this way, "Prepare yourselves for a different reality."

Summer interns

Nine Portuguese PhD candidates attended a shorter summer intern session in August. Some students worked alone with their faculty mentors and others joined research project teams. Topics varied from software development to computer reproductions of bio-molecular motion.

Luís Correia worked with protein dynamics research. "The thing I liked the most was that I needed to learn about all kinds of physics – keywords, behavior in fluids, all kinds of forces that explain molecular behavior – and more math than what I already knew just to understand the phrases that people in the lab kept saying to me," stated Correia. "Now that I look back to that first week and see myself having to read books and papers just to understand small details, I think it must have been very frustrating. But then again, isn't that the definition of a good challenge? Now that I'm done and can read related work papers, understanding basic implications in molecular dynamics, I feel much more confident, happy (I really like physics), and I am looking forward to finding a place where I can apply what I learned and expand my knowledge."

Other students researched topics with which they were more familiar. "I liked the opportunity to work in my field of study," Luís Miranda said. He and Nuno Barbosa focused on parallel and distributed computing. Filipe Brunido analyzed "ways to parallelize streamline calculations across multiple GPUs and multiple compute nodes. The research mainly focused on two technologies, NVIDIA's CUDA and MPI."

Some students learned different ways to view their courses of study. "The main benefit was that I learned a new perspective of computer science where it can be used as a tool for other sciences," André Lourenço said. He teamed with Luís Correia. "My task was to implement an algorithm in MOIL. The main difference between the existing algorithm and the one that André Lourenço and I implemented is the increased precision of the calculations without adding too much stress to the system," Correia said.

Roberto Ribeiro and Rui Magalhães da Costa explored a topic that consisted of "simulation and numerical experiments with materials with microscale structure—namely, heat conductivity," Ribeiro said. "The experience in Austin was quite profitable because I learned and developed several research methods and capabilities... I was also quite surprised with the mentoring. Very experienced supervisors were always supporting us which was quite helpful in achieving the project goal in five weeks."

André Rocha and Nuno Faria temporarily joined the "computational visualization center (CVC) crew," Rocha commented. "Our main goal was to enhance a software project by adding additional features that would increase the software's performance significantly." Faria said that he and Rocha worked with a team that developed "an application for volume rendering. More specifically, we helped develop the I/O module of HDF5 files in the Volume Rover application. I noticed that the available projects



Summer Interns



Summer Interns

are important and the results that we reach may have a very important role in someone else's research. I started having a new perspective on how to manipulate very large scientific data, and I think it will come in handy in the future."

Students stayed in a UT Austin dorm. Most of them secured their research opportunities by telling their supervising professors in Portugal that they were interested in studying abroad, writing a CV, and submitting a motivation letter. Dr. Keshav Pingali, a computer science professor at UT Austin, selected the students.

"I met Dr. Pingali in a summer school that he [facilitated] in Portugal," Correia said, "I found out about this opportunity and asked a professor in my university about the chance to come to the U.S." To Portuguese students interested in researching with UT Austin, Barbosa advises, "Sometimes the offers aren't public. You need to search and investigate. Speak with your supervisor or with a teacher who is close to you to find out if it is possible to visit." Magalhães da Costa suggests, "Be professional with your work, bring comfortable summer shoes, and maybe some hankies in the first few days until you get used to the thermal shocks of going into and out of buildings in Austin!"

The students and their mentors included:

Nuno Miguel Monteiro Barbosa, University of Porto
Supervising Professors, Porto: Verónica Orvalho, Álvaro Reis Figueira
Supervising Professor, Austin: Paul Navratil

Filipe Brunido, University of Coimbra
Supervising Professor, Coimbra: Luís Moura e Silva
Supervising Professor, Austin: Paul Navratil

Luís Filipe Pinho Correia, University of Porto
Supervising Professor, Porto: Miguel Dias Costa
Supervising Professor, Austin: Ron Elber

Rui Sérgio Magalhães da Costa, University of Minho
Supervising Professor in Minho: Alberto Proença
Supervising Professor in Austin: Ivo Babuska

Nuno Filipe Monteiro Faria, University of Minho
Supervising Professors, Minho: João Luís Sobral, Rui Ralha, Alberto Proença, António Pina
Supervising Professor, Austin: Chandrajit Bajaj

André Pereira dos Santos Lourenço, University of Coimbra
Supervising Professor, Coimbra: Luís Moura e Silva
Supervising Professor, Austin: Ron Elber

Luís Filipe Teixeira Miranda, University of Minho
Supervising Professor, Minho: Alberto Proença
Supervising Professors, Austin: Donald Nguyen, Mario Méndez

Roberto Carlos Sá Ribeiro, University of Minho
Supervising Professors, Minho: João Luís Sobral, Rui Ralha, Alberto Proença, António Pina
Supervising Professors, in Austin: Ivo Babuska, Karl Schulz

André Silva Rocha, University of Minho
Supervising Professor, Minho: Alberto Proença
Supervising Professors in Austin: Chandrajit Bajaj

AC EVENTS

CloudViews cloud computing conference

April 20-21, 2010, Porto. CoLab joined in support of the CloudViews 2010 conference as it convened IT professionals, researchers, and service providers in the cloud computing field. Organized by EuroCloud Portugal, CloudViews 2010 was the second annual edition of the conference purposed to help cloud computing achieve its main goal—to transform IT platforms in elastic, highly available, fault tolerant, secure, and multi-tenant platforms, and to increase Portugal’s capacity to build a true Computing ecosystem in the Cloud: encryption mechanisms, predictability and provision platforms, SLAs monitoring and agreements contracts, AAI, elastic networks, interoperability frameworks, schedule mechanisms, etc. This year’s theme is the “Cloud Ecosystem” and discussion topics included:

- Cloud elasticity;
- Cloud computing platforms interoperability;
- Data management;
- IT departments and cloud computing integration;
- User perspective – how Internet (the cloud) will become our PC;
- Encryption and security technologies;
- Predictability and provision platforms;
- SLAs monitoring and agreements contracts;
- Elastic networks;
- Companies and startup opportunities: How to become a cloud computing provider and how to use cloud computing to add (real) value to business.

These conference presentations were followed by a Business Opportunities Forum to review topics including:

- Business angles, opportunities, and role: Design partnership for success;
- Web based collaborative editor for LaTeX documents;
- Using private clouds to increase service availability and reduce operational costs;
- Privacy for Google docs: Implementing a transparent encryption layer;
- Managing cloud frameworks through mainstream and emerging NSM platforms;

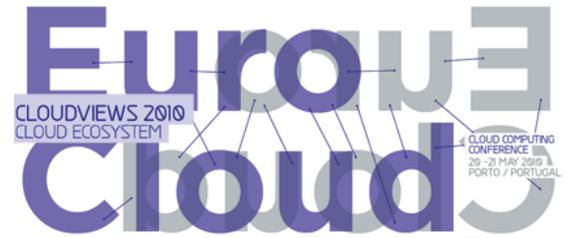
These business-oriented sessions were also presented as a road show of informal sessions around Portugal in April and May.

IBERGRID: 4th Iberian Grid Infrastructure Conference

May 24-28, 2010, Braga. “Bridging the gap between European e-Science and Iberian America.

CoLab also provided support to IBERGRID’2010, the fourth Iberian Grid Infrastructure Conferences, initiated within the framework of the bilateral agreement for science and technology signed between Portugal and Spain. The aim of IBERGRID’2010 was to leverage the construction of a common Iberian Grid Infrastructure and to foster cooperation in the fields of grid computing and supercomputing.

The original IBERGRID agreement between the Ministers of Science of Portugal and Spain, which called for stronger cooperation in grid computing, has grown to include supercomputing and e-Science, specifically HPC activities in computational engineering and science. This year’s conference in Braga had a strong connection to CoLab as Advanced Computing CoLab



IBERGRID 2010



IBERGRID 2010



IBERGRID 2010



Summer School 2010

Director, Alberto Proença, served as Conference Chair; and a hands-on session by Paul Navrátil, on the world's largest GPU cluster for data analysis and scientific visualization, the Longhorn cluster.

The Portuguese Minister of Science, Technology and Higher Education, José Mariano Gago, opened the event, together with the representative of the Spanish Ministry of Science and Innovation (José Manuel de Labastida), the Scientific Coordinators of the e-Science programs in Portugal (Luís Magalhães) and Spain (Vicente Hernandez), the Director of the Emerging Technologies and Infrastructures, DG-INFISO/F, at the European Commission (Mário Campolargo), and the Rector of University of Minho (António Cunha). The Conference Chair during his intervention challenged this political panel to be more active at IBERGRID by funding concrete actions in a fashion similar to the ones already running on CoLab: on researcher mobility and on joint projects.

Organized events included an International Conference with several parallel Thematic Sessions, an HPC Workshop, and a one-day Hands-on Tutorial for researchers in computational science and engineering. This tutorial addressed issues related to access different types of remote HPC facilities, from thin-node-distributed-memory clusters (such as Ranger at TACC), to fat-node-SMP clusters (Finis Terrae at CESGA, Galicia, with up to 1TB of shared RAM) and to CPU_GPU clusters. This latter topic was covered by Paul Navratil from UT Austin, who discussed CUDA and demonstrated access and use of the Longhorn cluster at TACC, the largest visualization and data analysis GPU-cluster system in the world.

In course of the conference, the decision to open a call for e-Science researcher mobility was signed by both Ministers. This call was then opened simultaneously in Portugal and Spain from July 1 till July 23, and the Ministers agreed to open an additional call for collaborative projects later this year, for projects to start early 2011.

Summer School 2010: e-Science with Many-Core CPU/GPU—with NVIDIA and more

June 14-19, Braga. UMinho and UT Austin organized this year's CoLab Summer School. In addition to knowledge-sharing, the program provided hands-on experience in developing applications software for many-core processors with massively parallel computing resources, to provide participants the ability to:

- Understand algorithm styles that are suitable for accelerators.
- Understand the most important architectural performance considerations to developing applications.
- Be exposed to computational thinking skills for accelerating applications in science and engineering.
- Gain ability to engage computing accelerators on science and engineering breakthroughs.

Participants developed applications software for many-core processors with massively-parallel computing resources. By the end of the event, participants gained an understanding of algorithm styles that are suitable for accelerators and the most important architectural performance considerations for developing applications. Instructors shared computational thinking skills for accelerating science and engineering applications. Participants learned how to engage computing accelerators on science and engineering breakthroughs. This event presented the first course in Europe provided by NVIDIA senior members, which in addition to David Kirk, included Michael Garland and Wen-mei W. Hwu of the University of Illinois at Urbana-Champaign.

David Kirk is an NVIDIA Fellow and served from 1997 to 2009 as NVIDIA's chief scientist, a role in which he led the development of graphics technology for today's most popular consumer entertainment platforms. Wen-mei W.

Hwu is the Walter J. ("Jerry") Sanders III-Advanced Micro Devices Endowed Chair in Electrical and Computer Engineering in the Coordinated Science Laboratory of the University of Illinois at Urbana-Champaign. Michael Garland is currently a research scientist with NVIDIA Research and an adjunct professor in the Department of Computer Science at the University of Illinois, Urbana-Champaign.

The Summer School also had other experts in Graphics Computing as well as from other Scientific Computing areas, to present their views and experiences in using CUDA in the development of their libraries or scientific applications. As a follow-on of the Summer School, researchers from 14 Higher Education institutions in Portugal took an active role in creating the GPU Computing Portugal community, using as a communication forum the GPU computing.net website. A testbed facility with 4 Fermi devices and 40 CPU-cores was deployed at UMinho for the Portuguese community that came out of the Summer School.

Ciência 2010

July 4-7, 2010, Lisboa/ CoLab AC students presented scientific posters related to their PhD theses and the work they are developing in the CoLab program. The posters were on display for the length of the conference. One conference session was organized to provide students an opportunity to answer questions on their work.



Summer School 2010



Summer School 2010

Agenda: Summer School 2010, e-Science with Many-Core CPU/GPU Processors

Monday, June 14:

Welcome by Alberto Proenca and Keshav Pingali
 Beginner's Tutorial on Many-Core Processors, Multi-Core Processors, and C Programming, Michael Garland, NVIDIA
 Introduction to Many-Core Processors, David Kirk, NVIDIA
 Introduction to CUDA, Wen-mei Hwu, University of Illinois U-C

Tuesday, June 15:

CUDA Threading Model & CUDA Memory Model, David Kirk, NVIDIA
 Algorithm Design for Many-Core GPUs, Michael Garland, NVIDIA
 Hands-on lab classes (Problems, Qsub script, Makefile.mac)
 Multiple GPU's in a MPI cluster, Wen-mei Hwu, University of Illinois U-C

Wednesday, June 16:

CUDA Performance Considerations, Wen-mei Hwu, University of Illinois U-C
 CUDA and Higher-level Tools, Libraries and Software Resources, Michael Garland, NVIDIA
 Teacher track (discussion on how to best use the textbook, resource sites, and labs)

Thursday, June 17:

Case Study 1: Dense Linear Algebra for Hybrid GPU-Multicore Systems, Marc Baboulin, Universidade de Coimbra
 Case Study 2: The Power of Heterogeneous Computing in Future Generations of Computer Graphics Systems, David Kirk, NVIDIA
 Case Study 3, Part I: Calculation of Electrostatic Potential Using Direct Summation - Steps of Performance Optimization, Wen-mei Hwu, University
 Case Study 3, Part II: From Direct Summation to Cut-off Binning - Achieving Data Scalability in a Massively Parallel Computation, Wen-mei Hwu, University of Illinois U-C
 Hands-on lab classes
 New Fermi and CUDA 3.0 features, David Kirk, NVIDIA

Friday, June 18:

Case Study 4: Molecular Simulation Strategies for Next-Generation Streaming Architectures, Erik Lindahl, University of Stockholm
 Project proposals: Short presentations about how attendees would CUDA-ize their applications, followed by discussion and suggestions)

EVENTS at the INTERSECTION of Advanced Computing, Digital Media, & Mathematics

Nomadic 0910 in Porto

September 2009, Porto. Stories of Art and Science is an international conference exploring the relationships between art and science, their intersections, and contrasts. Focused on the comprehensive understanding of these questions and on the narrative of specific collaboration episodes, the conference aims to bring people from the visual and performing arts, the natural sciences and the humanities together around the proposed event aims of exploring the dynamics of knowledge production and, more specifically, to sort out the ways art and science foster each other's development, their open and hidden connections.

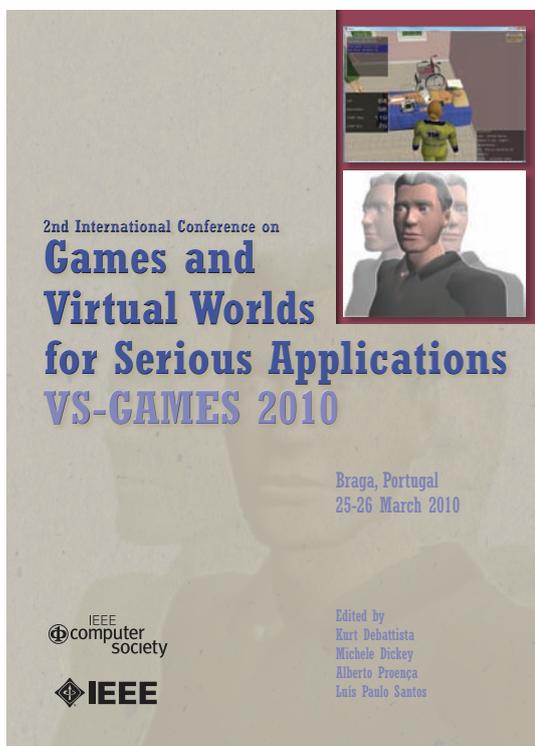
The UT Austin|Portugal Program was represented by Maria Esteva, a Research Associate/Data Archivist in the Visualization and Data Analysis group, of the Texas Advanced Computing Center (TACC), University of Texas at Austin, USA, who provided a lecture on "Endless possibilities: digital collections as crossroads between the Humanities and the Sciences." This theme is related to her professional activity, since her research interests focus on digital archives and preservation, being involved in developing scientific data collections, implementing digital archiving and preservation strategies for scientific data-sets, and the use of information visualization as a tool for archival processing.

2nd Int'l Conference on Games & Virtual Worlds for Serious Applications (VS-GAMES 2010)

March 25, 26, 2010, Braga. The International Conference on Games and Virtual Worlds for Serious Applications (VS-GAMES 2010) is the primary conference dedicated to serious games and virtual worlds presenting state of the art methods and technologies in the multidisciplinary fields outlined above. The aim of this international conference is to encourage an exchange of knowledge and experience in this cross-disciplinary area and its application to all aspects of the use of games and virtual worlds in serious applications.

The use of virtual worlds and games for serious applications has emerged as a dominating force in training, education and simulation due to the focus on creating compelling interactive environments at reduced costs by adopting commodity technologies commonly associated with the entertainment industries. This field is informed by theories, methods, applications and the state-of-the-art in a number of areas based on technological principles and innovation, advances in games design, pedagogic methodologies and the convergence of these fields. While the serious games community has made it possible to bring together such diverse fields, further academic and industrial collaboration is needed in further defining, formalising and applying the standards and methodologies for the future. Keynote speakers included:

- Prof. Sara de Freitas, Serious Games Institute, Coventry, UK (<http://www.seriousgamesinstitute.co.uk/>)
- Prof. Kathleen Tyner, Assistant Professor, Department of Radio-Television-Film, The University of Texas at Austin, (<http://rtf.utexas.edu/faculty/ktyner.html>)



A call for papers went forth, seeking papers subjects such as, but not limited to:

- Game design
- AI applications for serious games
- Serious games methodologies
- User-modelling in serious games
- Pervasive gaming
- Interactivity issues
- Game modelling
- Alternate reality games
- Virtual environments
- Augmented reality
- Visualisation techniques
- Human-computer interaction
- Mobile games
- Education and learning
- Case studies in serious games and virtual worlds
- Methodologies, theories and frameworks.

The following paper awards were recognized:

- Best Paper Award: *Animating Gaze Shifts for Virtual Characters based on Head Movement Propensity*, Christopher Peters
- Honorary Mentions: *Assessing nurses' acceptance and perceived usefulness of a serious game for emergency medical services*, Alberto Cabas Vidani, Luca Chittaro & Elio Carchietti; and *Attentional Cueing in Serious Games*, Erik Van der Spek, Herre Van Oostendorp, Pieter Wouters and Laurens Aarnoudse
- Best Short Paper Award: *Augmented Reality Game Design for Upper-Limb Stroke Rehabilitation*, J. Burke, M. McNeill, D. Charles, P. Morrow, J. Crosbie and S. McDonough.

Explore Creativity in Digital Space

April 29, 2010, Austin. The Texas Advanced Computing Center (TACC) Visualization Laboratory boasts the world's highest resolution tiled display wall, as well as high-definition video and multiple large-scale graphics displays. In conjunction with the UT Department of Art & Art History and the Austin Museum of Digital Art (AMODA) the TACC VisLab presented an evening of photography and video works by Austin artists including: Lawrence McFarland, Trey Ratcliff, Robert Melton, Ricardo Meleschi and Morgan Gaither. Participants were able to meet and interact with the artists as their work was viewed.

Verónica Costa Orvalho Speaks on Advances in Facial Animation

August , 2010, Austin. Dr. Verónica Costa Orvalho, Assistant Professor of computer science at the University of Porto, as well as founder of the Porto Interactive Center (PINC) and Face in Motion, presented "Facial Animation, Fast and Easy" at UT Austin's Department of Electrical and Computer Engineering on August 10. Dr. Orvalho's software, Fimmie, makes the process of animating facial expressions up to 99 percent faster than animation by traditional methods, according to the Face in Motion site.



Verónica Orvalho



Verónica Orvalho

Before developing Fimmie, Dr. Orvalho spent 18 months asking film production studios about areas in which they could use improved methodologies. During Dr. Orvalho's research, many studio employees described traditional rigging methods as very time-consuming. Artists rig by identifying key points on the face. Key points include areas that govern a lot of movement, such as around the lips and in the corners of eyes. These points are used to create a mesh which is like a computer-generated cheesecloth. The mesh stretches or compresses and gives resolution to 3-D characters.

"Artists currently rig by hand," Dr. Orvalho said, "and this causes bottlenecks in any computer graphics production. I asked the artists why rigging was so slow, but they could not really define it for me. I had to figure out the reasons on my own." Dr. Orvalho determined that accurate geometric deformation was essential to automating facial animation. Through a series of mathematical algorithms, she "created a program that bridges the gap between modeling and animation," she said. Fimmie allows artists to create several characters from one rig. Animation for one character can be automatically applied to animation for other characters that use the same rig.

Dr. Orvalho is the recipient of a €230,000 R&D award through CoLab and the Portuguese Foundation for Science and Technology, together with her collaborators at UT Austin, Dr. J.K. Aggarwal of the Department of Electrical and Computer Engineering and Dr. Yan Zhang of the School of Information. Their project, entitled "LIFEisGAME: Learning of Facial Emotions Using Serious Games," will embed real-time facial analysis and synthesis into a video game for people with autism spectrum disorders (ASDs). According to Portugal's Telecommunication Institute site, "The ability of socially- and emotionally-impaired individuals to recognize and respond to emotions conveyed by the face is critical to improving their communication skills. LIFEisGAME (will help people with ASDs) to recognize facial emotions using real-time synthesis and automatic facial-expression analysis."

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