Information Package: *Conformal Computing* 2005*

From Quantum Computing to Grid Computing:

Common themes united under the theory and practice of the Conformal Computing approach*

Sponsored by:
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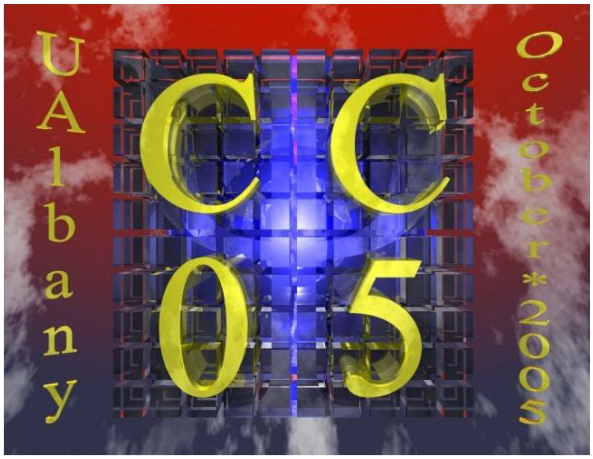
14–15 October 2005



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UNIVERSITY AT ALBANY
State University of New York

General Information

From Quantum Computing to Grid Computing Workshop

This workshop brings together leading researchers in the fields of Scientific, Quantum and Grid Computing. Various aspects of computing, mathematics, and quantum physics will be emphasized. The purpose of this workshop is to bring together researchers who are working on problems that appear to be only tangentially related, but are in fact united in their relation to a newly emerging discipline called Conformal Computing.[1] Conformal Computing is the name given to a uniform, mathematically based theory and software/hardware design methodology for applications to scientific and engineering problems.

This approach has widespread application to a number of important applications from parallel and grid computing to fundamental aspects of quantum computing. At the heart of the theory/design methodology are the two cornerstones: (1) the Mathematics of Arrays (MoA) and (2) ψ-calculus. With the MoA, algorithms are formulated and analyzed in terms of abstract representations in the form of multi-dimensional arrays. Expressions are manipulated into their simplest form in a mathematically provable way. Then using the ψ-calculus such expressions are reduced to an explicit form that is directly translatable into any programming language. The result is an implementation that is extremely efficient and avoids most temporary arrays, and their concomitant computational expense, through the use of direct indexing.

In the domain of parallel and grid computing, each data structure is formulated as a multi-dimensional array.

[1]. The name Conformal Computing is protected. Copyright 2003, The Research Foundation, State University of New York.

Each degree of freedom, such as number of processors, levels of memory, details of the network etc., is represented as an additional dimension of the array. Using various cost functions (cache and memory speed, network speed, latency, etc.) an optimal implementation can be derived and reasoned about in a rigorous mathematical way. The resulting code is flexible and platform independent in that all of the parameters relating to cost functions, dimensionality of arrays, etc. are input parametrically at run time.

In the domain of quantum computing, the generic abstract approach to array representations is shedding new light on fundamental questions. In particular, we find it most natural to represent the various quantities of the theory (e.g. the density matrix, unitary transformation matrices, etc.) in terms of multi-dimensional hypercubes. Such operations as the quantum Fast Fourier Transform are most naturally expressed and reasoned about using such structures. We have also recently discovered important connections between one of the fundamental operations of Conformal Computing (i.e. the *reshape-transpose* operation) and quantum algorithms such as Shor's factoring algorithm.

Workshop Highlights

Featured Speakers:

Professor **Russ Miller**, Director, Center for Computation Research, UBuffalo, SUNY; Professor **Vladimir Privman**, Robert A. Plane Endowed-Chair, Director, Center for Quantum Device Technology, Clarkson University; Professor **Samuel J. Lomonaco,** Department of CS and EE, University of Maryland, author of numerous journal and book publications in the field of Quantum Computing and algorithms.

Technical Sessions:

- Tutorial introduction to Conformal Computing: Applications and Success Stories
- Scientific Program: invited presentations on Scientific, Quantum and Grid Computing
- Tutorial introduction to Grid Computing with demos

Technical Committee (alphabetical)

Professor Saj Alam (Physics, UAlbany)
Professor Timothy Lance (Mathematics, UAlbany)
Mr. Brian Macherone (Research Comp., UAlbany)
Professor Russ Miller (CS, UBuffalo)
Professor Lenore Mullin (CS, UAlbany)
Professor James Raynolds (Nano, UAlbany)
Ms. Anne Shelton (Research Comp., UAlbany)

Registration

The registration fee for the Conformal Computing 2005 workshop is $50 (waived for speakers). A $15 early registration discount will be granted to those registering by **30 September 2005.** Registration includes coffee breaks, lunch, and wine and cheese reception. All attendees must complete and submit the (included) registration form along with the registration fee (make checks payable to the University at Albany). Receipts will be issued at the workshop. For further information please contact Professor Lenore Mullin at 518-442-3332 (ph); 518-442-5638 (fax); lenore@cs.albany.edu

Web Address

Up-to-date information is available at the following web site: www.albany.edu/CC05

Travel and Lodging

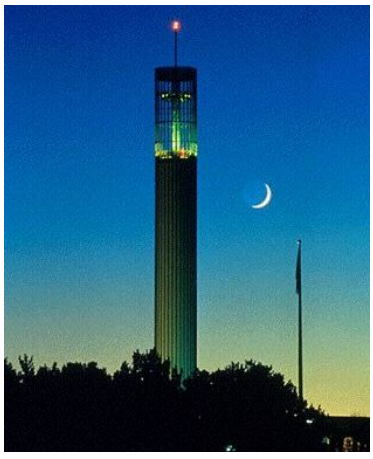
Transportation and lodging for this workshop will be the responsibility of each attendee (featured speakers will be reimbursed). Full details regarding lodging options and directions to UAlbany are available at the conference web site: www.albany.edu/CC05.

Reception and Posters

The first day of this workshop will conclude with a wine-and-cheese reception/poster session to foster interdisciplinary dialog. This reception is included in the registration fee. All attendees are encouraged to share their current research by contributing a poster.

Industry Involvement

The workshop organizers are currently working with the New York State Office of Economic Growth to encourage industry participation.



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From Quantum Computing
To Grid Computing Workshop
14-15 October 2005

Preliminary Agenda

Location: Auditorium, New Life Science Building and Adjacent Conference Room

Friday, 14 October

8:00 – 8:30 Continental Breakfast
8:30 – 8:45 Welcome and opening remarks
Peter Bloniarz, Associate Provost and Dean, College of Computing and Information

Session I (AM) Introduction to Conformal Computing (Chair: Lenore Mullin)
8:45 – 9:15 Geometry of Arrays (L. Mullin)
9:15 – 9:45 Applications of Conformal Computing to Problems in Computational Physics: The Fast Fourier Transform (J. Raynolds)
9:45 – 10:15 Memory Hierarchies and Conformal Computing Applications (H. Hunt)
10:15 - 10:45 Coffee Break and Start of Poster Session

Session II (AM) Introduction to Quantum Algorithms and Simulators (Chair: Timothy Lance)
10:45 - 11:30 **Featured Speaker: Professor Samuel Lomanaco** A Rosetta Stone for Quantum Computing
11:30 - 12:00 Density-Matrix Based Optimizations for Quantum Simulators (L. Mullin)
12:00 - 1:30 Lunch and Poster Session

Session III (PM) Quantum Physics and Large-Scale Simulations (Chair: James Raynolds)
11:30 - 2:15 **Featured Speaker: Professor Vladimir Privman** Effects of Decoherence in Quantum Control and Computing
2:15 - 2:45 Large-Scale Density Functional Calculations (J. Raynolds)
2:45 - 3:15 Coffee Break and Continuing Poster Session

Session IV (PM) Introduction to Grid Computing and Applications (Chair: Brian Macherone)
3:15 - 4:00 **Featured Speaker: Professor Russ Miller** Grid Computing and Buffalo's Center for Computational Research
4:00 - 4:30 NYSernet and New York State Center For Computation Research (T. Lance)
4:30 - 6:00 Wine and Cheese Reception and Poster Session

Saturday, 15 October
9:00 – 12:00 Hands-on Grid Computing Demos (UAlbany Research Computing and UBuffalo Center for Computation Research)

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Please complete this form and return with:

-- $35 before 30 September 2005.
-- $50 after 30 September 2005
-- A limited number of travel stipends for students are available (please inquire)

To: Professor Lenore Mullin **CC05**
Department of Computer Science
College of Computing and Information
1400 Washington Avenue
University at Albany, SUNY
Albany NY, 12222

This form and your check (**credit cards are not accepted**) made payable to the University at Albany.

To be completed by the attendee (please print):

Name: _____

Last (Title) First Middle Initial

Organization and Mailing Address:

_____

_____

E-mail Address: _____

Telephone: Fax:

I plan to attend the Workshop on:

-- 14 October 2005 -- 15 October 2005

-- I plan to attend the reception on 14 October 2005

Signature: _____

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Featured Abstracts

Professor Russ Miller, Ph.D., Director, Center for Computation Research, University at Buffalo, State University of New York

Grid Computing and Buffalo's Center for Computational Research

In this talk, we give an overview of Buffalo's Center for Computational Research (CCR), one of the leading academic supercomputing sites in the world. CCR supports work in the physical sciences, engineering, life sciences, and visualization.

We will also present an overview of our design and implementation of the ACDC-Grid, an extensive, multi-institutional proof-of-concept grid that we have implemented in New York State. This includes our efforts in grid monitoring, predictive scheduling, grid-enabling application templates, backfill detection and optimization, data repositories and operations, dynamic and automated allocation of resources, and our dynamic firewall, to name a few.

Further, we will discuss the functionality of the ACDC-Grid that enables a cost-effective and transparent solution to a critical application that we have developed to solve a key problem in structural biology. This application (SnB) is used to determine molecular structures from X-ray crystallographic data. The grid-based implementation includes grid-enabled optimization via data repositories, data mining, and intelligent generation of jobs to be run by the daemon overseeing the parameter optimization routine.

Professor Vladimir Privman, Robert A. Plane Endowed-Chair, Director, Center for Quantum Device Technology, Clarkson University

Effects of Decoherence in Quantum Control and Computing

This talk will describe approaches to defining measures of decoherence caused by quantum noise, when the time-evolution of a controlled quantum system deviates from ideal evolution, due to system's interactions with the environment. Issue related to scalability and entanglement will be discussed.

Professor Samuel J. Lomonaco, Department of CS and EE, University of Maryland,

A Rosetta Stone for Quantum Computing

This talk will give an overview of quantum computation in an intuitive and conceptual fashion. No prior knowledge of quantum mechanics will be assumed. The talk will begin with an introduction to the strange world of the quantum. Such concepts as quantum superposition, Heisenberg's uncertainty principle, the "collapse" of the wave function, and quantum entanglement (i.e., EPR pairs) are introduced. This part of the talk will also be interlaced with an introduction to Dirac notation, Hilbert spaces, unitary transformations, quantum measurement.

Simple examples are then given to explain and illustrate: (1) Quantum teleportation, (2) The Deutsch-Jozsa algorithm and (3) Shor's algorithm

Poster Titles

Quantum eXpress: An Extensible Gate-Level Simulator Melvin K. Simmons and Kareem Aggour (GE Global Research) Michael Simon (Lockheed Martin)

Improving Quantum Simulations Through Conformal Computing Robert M. Mattheyses and Michael Lapinski (GE Global Research) Lenore R. Mullin (The University at Albany)

Industrial Applications of Semiconductor Quantum Dots, Michael LoCascio (Evident Technologies)

Recent Success with the Albany-Buffalo Grid Connection, Brian Macherone (Research Computing, University at Albany)

Grid Demonstrations

Grid-Enabled "Shake and Bake" Molecular Structure Optimization and the State-Wide Grid Initiative, Russ Miller, (Center for Computation Research, University at Buffalo)

Large-Scale Grid-Enabled Density Functional Calculations for First-Principles Simulations in Materials Science, James E. Raynolds (College of Nanoscale Science and Engineering, University at Albany)

Atlas (particle physics) Simulations Over Workstation Clusters and Grids, Saj Alam, (Department of Physics, University at Albany)

Analysis of Grid Performance, Eric Wencke (Research Computing, University at Albany)