

Institute for Computational Mathematics
Annual Report
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prepared by

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SECTION I: INTRODUCTION, RESEARCH, AND PRIORITIES FOR 1999-2000

The ICM mission continues to be encouraging, facilitating, and advancing interdisciplinary research involving advanced scientific computing. In support of this mission, ICM acts as a locus for interactions between researchers from the Department, Kent State University, industry and other universities, both in the United States and internationally. Although ICM is a unit within the Department of Mathematics and Computer Science, its associated membership includes faculty from several disciplines within the University. ICM provides its associate and visiting members with excellent computing facilities and a stimulating supporting environment for cooperative scientific efforts in computational mathematics, and we propose to continue supporting and extending these activities.

In particular, we plan to develop stronger bonds with scientists at the Mathematical Mechanization Center or the Chinese Academy of Science in Beijing University. Dr. Wang has NSF funding in "Advanced polynomial computations" with this group in Beijing, and included in this effort is Dr. Iyad Ajwa of Ashland University in Ohio.

Another priority for this period is research and curriculum development, in *Web Publishing*, under the direction of Dr. Wang. Richard Varga and Paul Wang are research directors of ICM. Research and curriculum development for *Web Publishing* involves integrating the design and technology aspects of Web publishing in upper undergraduate and beginning graduate level courses. The effort receives support and cooperation from the College of Arts and Sciences, the College of Fine and Professional Arts, and industry. The curriculum development is conducted by Paul Wang and Professor Sanda Katila from Visual Communication Design with help from instructional design expert, Professor Frank Suzi, and industrial consultants. The curriculum will combine maturing World-wide Web technologies with emerging design principles for creating effective, functional, and attractive Websites.

The Web is the newest medium of mass-communication and human expression in the Nation and the world. The combination and synergy of computing technology with visual design is intrinsically important. The curriculum also addresses a critical need for training personnel with balanced skills in the programming, functional, and artistic design aspects of Web sites.

The project will develop a two-semester sequence of courses, *Introduction to Web Publishing* and *Advanced Web Publishing*, with these major features:

- Combination, integration, and interplay of computer science and visual communication design.
- Team work on design and implementation.
- Critical analysis of requirements, and evaluation of Web site created.
- Developing students' abilities to apply both programming techniques and design principles to achieve Web site goals.
- Project-based, hands-on learning.

Paul Wang continues to nurture and develop industrial connections, student internships with local industry, intensive training courses, and consulting arrangements.

As part of our priorities for this period, we plan to have a number of distinguished scientists visit our Institute, for the express purpose of conducting research with members of our Institute, and also to give enlightening lectures on their research to faculty and graduate students in our Department of Mathematics and Computer Science. These lectures are specifically aimed at broadening the scope of our graduate programs in mathematics and computer science. Visitors to our Institute in this period will include:

1. Dr. Daidong Lin, Institute of Systems Science, Academia Sinica, Beijing (symbolic mathematical computation)
2. Professor Nicolaos Stylianopoulos, University of Cyprus (numerical complex variables)
3. Dr. Vladimir Andrievskii, University of Eichstätt (complex function theory)
4. Professor Igor Pritsker, Oklahoma State University (complex function theory)

Another major priority in this period for the ICM will be on research with respect to *Internet Accessible Mathematical Computation (IAMC)*.

The goal of IAMC is to make mathematical content and mathematical computing power easily and widely available on the Internet and the Web. Accessing a math-oriented computing service should be as simple as entering a command, retrieving a Web page, or sending email. Internet accessibility can make research, experimental, parallel/super computing, one-of-a-kind, demonstration, or commercial software systems that deal with mathematics in any technical discipline easily reachable on a global basis. What's needed is flexible integration of heterogeneous mathematical systems on a distributed basis, involving *data integration*, *control integration*, and *user interface integration*.

The symbolic mathematical computing community has led the way in the critical data integration area. OpenMath is a protocol for representing semantically rich mathematical objects, allowing them to be exchanged between programs, stored in databases, and published in electronic form. The central notions in OpenMath are *Content Dictionaries*, providing standard and application-defined vocabularies and definitions, and *Phrasebooks*, which provide translation between application concepts and those defined in the relevant Content Dictionaries. Translated data may be

exchanged in either binary or XML form. There is a strong relationship to MathML. MathML deals principally with the presentation of mathematical objects, while OpenMath is primarily concerned with the semantic meaning, or content. MP is a mathematical data encoding/exchange format, developed at ICM/Kent, that uses a binary encoded annotated parse tree for efficiency.

The Dr. Wang together with collaborators at other institutions, is investigating control and user-interface integration schemes to

- Make math-oriented data and services easily and widely accessible on the Internet – directly, via the Web, and by email.
- Support interactive use of user-designated remote *compute servers* almost as if they were local programs.
- Provide effective and efficient communication of mathematical data over the Internet.
- Allow exchange and further processing of computational results among different compute servers.

To achieve these goals, we devise the architecture, protocol, and implementation of a distributed IAMC system. For the IAMC project, major efforts include defining a *mathematical computation protocol* (MCP), implementing a Java class library for MCP, and building prototypes for a typical IAMC client and a customizable IAMC server.

The IAMC effort is on-going and it involves the overall architecture, designs for the IAMC client, the IAMC server, and the MCP protocol. Results have been reported at ASCM'98 (Lanzhou, China) and ISSAC'99 (Vancouver, Canada).

IAMC Workshop

Dr. Wang has obtained NSF funding to organize a workshop for Internet Accessible Mathematical Computation (IAMC). The IAMC workshop was held on July 28, 1999 at ISSAC'99 (International Symposium on Symbolic and Algebraic Computation), an ACM SIGSAM/SIGNUM Symposium (July 28–31, 1999) at Simon Fraser University, Vancouver, B.C. Canada.

The IAMC'99 workshop offers invited speakers, contributed paper sessions, system demos, and a panel discussion. The workshop attracted over 65 attendees from all parts of the world.

IAMC Web Site

To better organize and promote IAMC research and to increase its visibility, Dr. Wang has established a homepage for IAMC gathering useful information about the research area for easy reference. The site will be used to organize future work in this area at ICM/Kent and cooperation with others in different parts of the world. The URL for the IAMC web site is

<http://monkey.mcs.kent.edu/icm/research/iamc.html>

External Research Cooperations of Dr. Wang involves NSF funded cooperation on “Advanced Polynomial Computations” with the Mathematical Mechanization Center of the Chinese Academy of Science in Beijing. The cooperation also involves Dr. Iyad Ajwa of Ashland University in Ohio.

Dr. Wang also has received NSF funding to cooperate with Dr. Simon Gray at Ashland University on MP, an efficient binary protocol for mathematical data encoding.

Numerical Analysis and Approximation Theory:

Researchers in these areas include Professors Alfred Cavaretta, Paul Farrell, E. Charles Gartland, Lothar Reichel, Arden Ruttan, Meera Sitharam and Richard Varga. The work of Professors Farrell, Sitharam and Varga is described elsewhere in this report.

Professor Alfred Cavaretta's primary mathematical interests are spline functions, numerical analysis, numerical quadrature, differential inequalities, approximation theory, classical analysis and optimization. He is a specialist on subdivision techniques for the computer generation of curves and surfaces, a subject on which he has coauthored a research monograph. Professor Cavaretta continues his collaboration with A. Sharma, Univ. of Alberta, and C. R. Selveraj, Penn. State University, on such subjects as optimal recovery and overconvergence phenomena.

Professor Chuck Gartland continued his research program of investigation of numerical solutions of problems in liquid crystals. His current research projects include investigation of liquid crystal tensor models, stripe phase instabilities in liquid crystals, liquid crystal display optics, nonlinear optics of liquid crystals, and automatic code generations and problem-solving environments for liquid crystals. One doctoral student, Sami Mkaddem, received his Ph.D. in Applied Mathematics, December, 1998; while one doctoral student and one masters student continue their dissertation and thesis research under Dr. Gartland's direction. Dr. Gartland is supported by NSF ALCOM funding (which also supports his current masters student) plus an individual NSF grant. During this reporting period, Professor Gartland delivered three invited talks and one conference presentation on his research activities.

Professor Lothar Reichel's area of research is numerical linear algebra. He has an NSF grant to develop numerical methods for the solution of large scale ill-posed problems, and is a Co-PI on a grant for developing numerical methods for large-scale bifurcation problems. He is currently directing one Ph.D. dissertation and one Master's thesis.

Professor Arden Ruttan is the managing editor for Electronic Transactions on Numerical Analysis (ETNA) and a co-principal investigator of the NSF Science and Research Center for Advanced Liquid Crystalline Optical Materials (ALCOM). His current research is on environments for visualization and interactive computational steering on a network of distributed workstations on a fast network.

Computer Science:

In this area, the major foci of the ICM associated faculty are parallel and distributed computing and scientific computations. Brief descriptions of the activities of these faculty members are given below.

Professor Johnnie Baker's research activities focus on parallel models of computation and parallel algorithms, computational chemistry, and applications of parallel computing to areas such as computational geometry and air traffic control. He has also published in the areas of Banach spaces and general topology.

Professor Arvind Bansal's research contribution during 1998-99 has been in the areas of developing algorithms for genome comparison, understanding the genome structure, understanding gene functionality in newly sequenced genomes, the use of the internet as a large virtual computer for fast multimedia knowledge retrieval, and the use of distributed computing to develop internet based distributed simulation of combustion engines. He has collaborated and published with researchers from European Molecular Biology Laboratory, Heidelberg, Germany and Protein Institute, Moscow. He has also taught an interdisciplinary graduate level course on Computational Biology to train students to do multidisciplinary research to apply computational tools to understand the cause of genetic and bacterial diseases.

Professor Kenneth Batcher and his students continue research on the automated restructuring of serial code to extract parallelism. A search for faster sorting networks has also been initiated.

Professor Paul Farrell is currently the sole investigator on a NSF Computational Mathematics and International Programs Divisions grant, principal investigator on a joint grant from the NSF CISE New Technologies Program (with co-PIs Mike Lee, Lothar Reichel, and Arden Ruttan), and on a joint equipment grant from the NSF CISE Research Equipment Program (with co-PIs Steve Chapin, Mike Lee, and Arden Ruttan). He is a member of the IMACS Technical Committee on Partial Differential Equations. His research interests are distributed and parallel computation and algorithms, high speed networking, computational steering and visualization, application of numerical methods to liquid crystal problems, singularly perturbed differential equations, Navier-Stokes equations and semi-conductor devices, automatic code generation for parallel architectures, and application of expert systems in numerical computing. During the reporting period he published one research paper, had four others accepted for publication, was an organizer and invited speaker of Workshop'98 on Methods for Singular Perturbation Problems, Losnetz, Bulgaria; was invited to serve on the organizing committee of the Second Conference on Numerical Analysis and Applications (NAA'2000), June 11-15, 2000, Rousse, Bulgaria; and attended the Fall Joint NLANR/Internet 2 Tech Workshop, an NLANR Workshop, the Internet 2 Annual Meeting, and Networks+Interop. He also had the following grants which are active:

1996, PI, *Uniform Numerical Methods for Singularly Perturbed Equations*, NSF Computational Mathematics and International Programs Divisions, 9/1/96–8/31/99, \$66,000.

1996, PI, *A High-Performance Network for Distributed Computation and Visualization*, NSF CISE Research Equipment Program for \$135,000, with co-PIs Arden Ruttan, Steve Chapin and Mike Lee.

1997, PI, *A Steering and Visualization Environment*, NSF CISE New Technologies Program, 1997–2000, \$395,003, with Mike Lee, Lothar Reichel and Arden Ruttan.

Professor Cheng Lu's research interests are data compressions, image processing and document image processing.

Professor Hassan Peyravi's research focuses on interconnection networks for large scale parallel and distributed processing, and on computer communications networks. During this reporting period, he has published five articles, attended four international conferences and obtained a university research grant.

Professor Jerry Potter's research interests include the continuing development of the associative computing paradigm, the integration of associative SIMD computers with other architectures in a heterogeneous supercomputer environment, the development of techniques for compilation on massively parallel SIMD computers, natural language and artificial intelligence processing on SIMD computers, and the development of techniques for the introduction of parallel programming at the high school level. Professor Potter published six research papers in 1997-1998, and he is currently directing three doctoral students and 4 master's students. Dr. Potter was awarded a grant from AFRL Rome, NY, in April 1999.

Professor Michael Rothstein directs his research activities toward algorithms and systems for symbolic and algebraic computation, parallel computations, symbolic-numeric interfaces, high-level languages, object-oriented programming, scientific user interfaces, and functional language implementations.

Tetsuji Ueda's research interests are in applied mathematics, in particular the mathematical modeling of physical phenomena, asymptotic methods, and scientific computations. His current projects include the dynamics of liquid-crystalline filament immersed in fluids and the high-speed spinning of polymer fibers. These works involve collaborations with researchers at the Courant Institute at New York University, the Mathematics Department at the University of North Carolina–Chapel Hill, and the Liquid Crystal Institute at Kent State University. One research paper has been accepted for publication, and another has been submitted for review.

Computational Chemistry:

This interdisciplinary research program continues in cooperation with Upjohn Laboratories. **Professor Victor Nicholson**, ICM, and Professors C. Tsai and R. Gregory of the KSU Chemistry Department are conducting this research in which the emphasis is on the development and application of computer algorithms and software to investigate the relationship between molecular structure and chemical activity. This effort involves applications of topology, graph theory, organic chemistry and biochemistry.

SECTION II: ETNA

An on-going effort in the ICM is the publication of the totally electronic journal Electronic Transactions on Numerical Analysis (ETNA), which was created by ICM members Lothar Reichel, Arden Rutten, and Richard Varga in 1993. Since its inception, eight volumes of ETNA have appeared, covering 1489 pages of new research.

ETNA has been a ground-breaking journal which has set the standard for electronic journals, both with regard to paper quality and to electronic formats. In addition, ETNA is fully reviewed by Mathematical Reviews.

SECTION III: SymbolicNet

SymbolicNet is a World Wide Web (WWW) service for information related to symbolic computation. It was established (Fall 1994) by the ICM under the support of a specific NSF grant. The SymbolicNet web site is now recognized as the leading information center in the area of Symbolic Computing and is used regularly by researchers world-wide.

ICM is responsible for the continued maintenance and upgrade of SymbolicNet. Under the supervision of Dr. Wang, graduate student, WeiDong Liao, performs the day-to-day operations of the site. SymbolicNet has put in innovative interactive demonstrations of mathematical computing systems which are now being upgraded to the new HTTP 1.1-level Web server. A redesign of the site in terms of graphical presentation and better content organization is underway.

SECTION IV: ICM TECHNICAL REPORTS

As of September 1995, ICM technical reports are available on the World-Wide Web. Address is <http://monkey.mcs.kent.edu/icm/tr/index.html>.

ICM-199807-0005 On the Instability of Radial Hedgehog Configurations in Nematic Liquid Crystals under Landau-deGennes Free-Energy Models, E. C. Gartland, Jr. and S. Mkaddem.

ICM-199901-0001 Design and Protocol for Internet Accessible Mathematical Computation, Paul S. Wang.

ICM-199901-0002 Chebyshev Polynomials and Primality Tests, Mohamed O. Rayes, Vilmar Trevisan and Paul S. Wang.

SECTION V: PUBLICATIONS

A. Bansal

A. K. Bansal, P. Bork, and P. Stuckey, "Automated Pair-wise Comparisons of Microbial Genomes," Mathematical Modeling and Scientific Computing, Publisher: Principia Scientia, Vol. 9, 1998,

pp. 1-23.

A. Vitreschak, A. K. Bansal, and M. S. Gelfand, "Conserved RNA Structures Regulation Initiation of Translation of *Escherichia Coli* and *Haemophilus Influenzae* Ribosomal Protein Operons," First International Conference on Bioinformatics of Genome Regulation and Structure, Novosibirsk, Russia, August 24-31, Vol. 1, 1998, p. 229.

A. K. Bansal and P. Bork, "Applying Logic Programming to Derive Novel Functional Information in Microbial Genomes," Proceedings of the First International Workshop on Practical Aspects of Declarative Languages, Lecture Notes Series of Springer-Verlag, LNAI 1551, January 1999, pp. 274-289.

S. Ryan and A. K. Bansal, "Applying Java for the Retrieval of Multimedia Knowledge Distributed on High Performance Clusters on the Internet," Proceedings of the International Conference on Practical Applications of JAVA, 1999, London, UK, pp. 193-203.

S. Ryan and A. K. Bansal, "A Scalable Distributed Associative Multimedia Knowledge Base for the Internet," Proceedings of the 8th International Conference on Intelligent Systems, Colorado, USA, June 1999, pp. 1-6.

E. C. Gartland

"Multidimensional director modeling in a liquid crystal cell using the Q tensor representation," with H. Mori, J.R. Kelly, and P.J. Bos, *Jpn. J. Appl. Phys.*, 38 (1999), pp. 135-146.

"Instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models," with S. Mkaddem, *Phys. Rev. E*, 59 (1999), pp. 563-567.

"Comparison of analytical calculations of finite-difference time-domain simulations of one-dimensional spatially varying anisotropic liquid crystal structures," with C.M. Titus, P.J. Bos, and J.R. Kelly, *Jpn. J. Appl. Phys.*, 38 (1999), pp. 1488-1494.

H. Peyravi

"An Approach Towards Adaptive Routing Using Traffic Intensity Threshold Points," Proceedings of International Conference on Modeling and Simulation on Networks and Communications, pp. 79-84, May 1998, (with Ashish Agarwal).

"Delay and Queue Size Analysis of TDMA with General Traffic," Proceedings of the International Symposium on Modeling, Analysis and Simulation of Computer and Communication Systems, pp. 217-225, July 1998.

"Medium Access Control Protocols for Space and Satellite Communications," *IEEE Communications*, Vol. 37, No. 3, pp. 62-71, March 1999.

“Simulation Modeling and Comparison of Multiple Access Protocols,” *Intl. J. Simulation* Vol. 72, No. 4, pp. 221-237, August 1998, (with Don Wieser).

“Distribution of time slot assignments in DAMA with nonuniform traffic,” *Proceedings of the International Conference on Parallel and Distributed Computing Systems*, August 1999, (with K. Khan).

L. Reichel

“Computation of a few close eigenvalues of a large matrix with application to liquid crystal modeling,” *J. Comp. Phys.*, 146 (1998), pp. 203-226. (with J. Baglama, D. Calvetti and A. Ruttan).

“Fast Leja points,” *Elec. Trans. Numer. Anal.*, 7 (1998), pp. 126-140. (with J. Baglama and D. Calvetti).

“Smooth or abrupt: a comparison of regularization methods,” in *Advanced Signal Processing Algorithms, Architectures and Implementations VIII*, (F.T. Luk, ed.), *Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE)*, vol. 3461, The International Society for Optical Engineering, Bellingham, WA, 1998, pp. 286-295, (with D. Calvetti and B. Lewis).

“On the solution of the single input pole placement problem,” in *Mathematical Theory of Networks and Systems*, (A. Beghi, L. Finesso and G. Picci, *Il Poliografo*, eds.), Padova, 1998, pp. 585-588, (with D. Calvetti and B. Lewis).

“Application of anti-Gauss quadrature rules in linear algebra,” in *Applications and Computation of Orthogonal Polynomials*, (W. Gautschi, G. H. Golub and G. Opfer, eds.), Birkhauser, Basel, 1999, pp. 41-56, (with D. Calvetti and F. Sgallari).

“A computable error bound for matrix functionals,” *J. Comput. Appl. Math.*, 103 (1999), pp. 301-306, (with D. Calvetti and G. H. Golub).

R. S. Varga

“Zero distribution, the Szegő curve, and weighted polynomial approximation in the complex plane,” *Modelling and Computation for Applications in Mathematics, Science and Engineering* (J. W. Jerome, ed.), pp. 167-188, Oxford University Press, 1998, jointly with I. E. Pritsker.

“Weighted rational approximation in the complex plane, *Journal de Mathématiques Pures et Appliquées*, ” 78(1999), 177-202, jointly with I. E. Pritsker.

“On Geršgorin-type problems and ovals of Cassini,” *ETNA*, 8(1999), 15-20, jointly with A. Krautstengl.

“Rational approximation with varying weights in the complex plane,” *Computational Methods and Function Theory (CMFT’97)* (N. Papamichael, St. Ruscheweyh, and E. B. Saff, eds.), 437-448, World Scientific Publishing, NJ, 1999, jointly with I. E. Pritsker.

P. Wang

“Tools for Parallel/Distributed Mathematical Computation,” *Proceedings, PASCO ’97* (July 20-22) Maui, HI, pp. 188-195.

“Applying Parallel/Distributed Computing to Advanced Algebraic Computations,” (with Iyad A. Ajwa), *Proceedings of IEEE National Aerospace and Electronics Conference (NAECON ’97)*, pp. 156-164, Dayton, OH, July 14-18, 1997.

“PvmJobs: A Generic Parallel Jobs Library for PVM,” (with Hong H. Ong and Iyad A. Ajwa), *Proceedings of IEEE National Aerospace and Electronics Conference (NAECON ’97)*, pp. 165-172, Dayton, OH, July 14-18, 1997.

“Design and Implementation of MP, a Protocol for Efficient Exchange of Mathematical Expressions,” (with S. Gray and N. Kajler), *Journal of Symbolic Computation*, Vol. 25, No. 2, Academic Press, Feb. 1998, pp 213-238.

SECTION VI: GOALS

Future Plans

A continuing goal for ICM is to raise its level of visibility both internally and externally and increase its level of financial support through some additional internal funding and major external funding. The emerging IAMC research area is a promising direction to pursue.

ICM will facilitate a broader scope of interactions and research collaborations among departments within Kent, with local industry, nationally, and internationally. Emphasis will be on scientific computing, distributed/parallel computing, and application of new computing technologies in different disciplines.

ICM will also increase and expand its industrial contacts through consulting, custom training courses, the ICM Web site, and other means. The hope is to increase opportunities for student placement, faculty consultation, and industrial research cooperation through ICM. Joyce Fuell, the administrative assistant at ICM, has the responsibility of managing and advancing this activity.

The ICM research directors and associated faculty will continue to seek external funding and to advance the reputation of the Institute. Our current budget for the ICM is at an all-time low of \$5,000/year. Our belief is that great benefits to Kent State University would result if this budget could be doubled to \$10,000 for the next period, and an increased budget would materially aid us in achieving our priorities for the future!