Computer Science

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From the Department Head

As I near the end of my fifth year as department head, it's time to look back on departmental achievements since I came to CS@VT in August 2008. The department has grown stronger in research, in the depth of our graduate program and in our connections to the computing industry. We also have experienced significant growth in undergraduate student enrollment and in repositioning of our graduate program to emphasize PhD and MS thesis studies.

The core strength of any department is its faculty. We are proud to count 12 NSF and DOE CAREER award winners among 39 CS faculty. Since academic year 2008-2009, the achievements of 9 CS@VT faculty have been recognized by College of Engineering Dean's Awards (e.g., Outstanding Assistant Professor, Faculty Fellow). We celebrate that three faculty – Drs. Doug Bowman, Wu Feng and Naren Ramakrishnan – all have been named *ACM Distinguished Scientists* and that Dr. Madhav Marathe became an *IEEE Fellow*.

Our research has been strengthened by increased funding, strategic emphasis on new areas in computing research and reorganization of some traditional areas of strength. In 2010, Dr. Wu Feng led a proposal to obtain $1.4M from NSF to build *HokieSpeed,* a new GPU/CPU parallel computer that allows scientists and engineers to explore heterogeneous computation at a new scale. *HokieSpeed* ranked as 11th on the Green 500 List at its debut. During this period, CS faculty have increased our department research funding by 50% to the level of $30 million at the end of FY12. The department also added two new strategic research areas – data analytics and cyber security. We have a new *Discovery Analytics Center (DAC),* with director Dr. Naren Ramakrishnan. This interdisciplinary center includes faculty from Statistics and ECE as well as two new CS faculty hired last year – Dr. Sanmay Das, Dr. Aditya Prakash -- with a third anticipated hire from this year's search. Dr. Ramakrishanan led a successful DAC proposal obtaining $13.5M from IARPA, with VT as lead institution. Our cyber security focus collaborates with ECE on research, faculty hiring and curriculum. We will soon have an approved cyber security minor for undergraduates and a cyber security certificate for ECE and CS masters degrees. There is new leadership of our *Center for High-End Computing Systems (CHECS,* Dr. Kirk Cameron*)* and our interdisciplinary *Center for Human-Computer Interaction (CHCI,* Dr. Doug Bowman). Adding to our interdisciplinary research commitment, Dr. T. M. Murali is co-director of the new *Center for Systems Biology of Engineered Tissues (SBET).* Three of these centers (DAC, CHCI, SBET) are receiving 'seed funding' from the university through ICTAS (www.ictas.vt.edu).

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From the Department Head, continued from page 1

After an external review in 2010, we introduced many changes to our graduate program to clarify the milestones to a PhD and to augment the feedback received by graduate students on their progress. We added an annual *Green Thursday* review of the progress of each PhD student by the entire CS faculty, instituting annual Student Activity Reports filled out by students and their advisors, and used by the Graduate Program Committee to chart student progress. We started weekly, department-wide research seminars required of all graduate students for their first three semesters, and attended by faculty; these seminars increase the breadth of awareness of the entire field of CS. We hosted 17 Distinguished Lecturers, including two Turing Award winners and 12 ACM Fellows, who have met 1-on-1 with our students during *Meet the Speaker* hours. We have hosted two CS@VT Distinguished Alumni --- Dr. Greg Lavender (now CTO for Architecture and Infrastructure Engineering at Citi) and Dr. Lucy Nowell (Program Manager for the Advanced Scientific Computing Research program office in the Department of Energy's Office of Science). In terms of numbers, we estimate that by May 2013 we will have graduated 93 PhDs and 245 MS degree recipients since August 2008, of which 23%(PhD) and 30% (MS) were female, numbers at or above the national averages.

Our industrial partners program, the Computer Science Research Consortium (CSRC), provides support for our co-curricular CS program and many opportunities for internships and jobs for our students. The CSRC is a unique strength in our department. It has grown to an astonishing 85+ technical companies; they conduct semi-annual job fairs and contribute to CS student co-curricular activities. Our *Investment in Excellence* scholarship fund, under the stewardship of Ms. Libby Bradford, has accumulated an endowment of over $250,000 supported by CSRC funds. Income from this fund is distributed as scholarships annually to excellent CS students.

Recently, the department has experienced significant growth in our undergraduate major --- Fall08 (285) to Spring13 (525) --- an 84% increase! Our enrollments in our first year course for CS majors have risen by 30% in the last two years, tracking a nation-wide trend reported by the CRA Taulbee Survey. Much of our work in diversity has been focused on our undergraduates. We were founding members of the *NCWIT VA/DC Aspirations in Computing Awards* program and the *NCWIT Pacesetters* program, focused on increasing the numbers of net new women in academia (www.ncwit.org/programs/campaigns/pacesetters). Having graduated fewer than 8% women for most years since 2008, we are proud to have increased our percentage of women CS majors enrolled currently to approximately 13% and expect continued growth in the future.

Numbers alone do not tell the entire story of the department. A department is its faculty, its staff and its students – how they interact, how they work hard towards shared goals, how they react to adversity (e.g., budget cuts that we have experienced). CS@VT is a strong community --- in its support of intellectual excellence and state-of-the-art practical experiences for its students, of outstanding CS research and interdisciplinary collaborations across departmental lines, of co-curricular experiences for our students that enhance their 'soft skills' needed in the marketplace, and of working together to enhance the diversity of our faculty and student body.

Dr. Barbara G. Ryder

J. Byron Maupin Professor and Department Head

Fall 2012 CSRC Career Fair

On Monday, September 17, the Computer Science Resources Consortium had its fall luncheon and Career Fair. This fall's career fair, held in Cassell Coliseum, was the largest since the dot.com boom, with 78 companies attending. For the fall 2012 semester, the CSRC welcomed 20 new companies and institutes: Accenture, Agilex, CCS Inc, Digital Receiver Technology, EMC, Excella Consulting, Gannett Co., Georgia Tech Research Institute, Hughes Network Systems, Lutron Electronics, MetroStar Systems, Open Software Integrators, Packet Forensics, Palantir Technologies, PIETECH Inc, Readyforce, Solers, TIBCO Software, Ultimate Software, ViaSat, and Zeta Associates. The CSRC also welcomed back Hughes Network Systems.

The members of the CSRC were on campus to learn more about the department and to recruit students as full-time employees, interns, and cooperative education students. CSRC companies provide support for CS student organizations and student scholarships.

Attending the luncheon in Owens Banquet Hall were 100+ company representatives, CS faculty and undergraduate scholarship winners. Sixty undergraduates were recognized for receiving scholarships for the 2012/13 academic year. The majority of these funds were provided by the College of Engineering, with CGI, the Department of Computer Science, and the CSRC contributing to the total.

CSRC members had the opportunity to visit several classes and speak with Computer Science students to discuss how to prepare for career fairs and interviews, the variety of opportunities in the field, and the abundance of jobs available to CS majors.

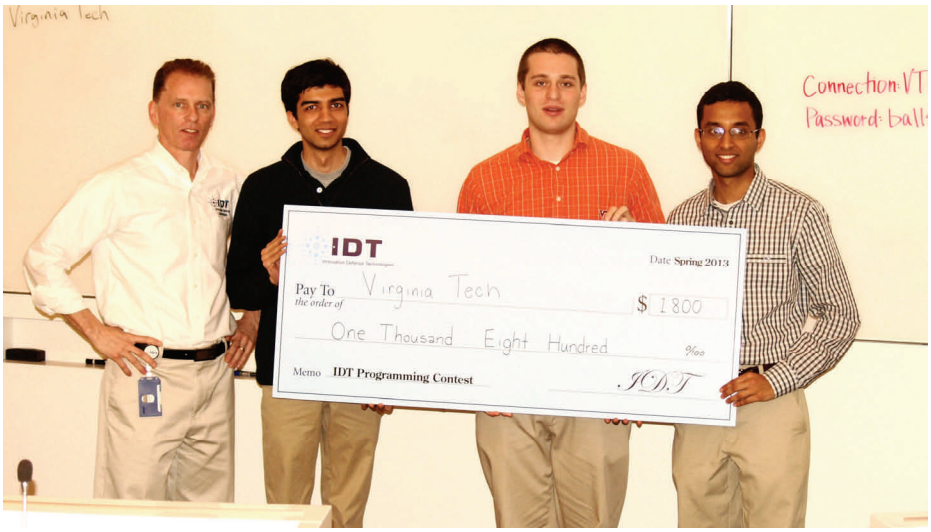
With the number and variety of positions offered by our CSRC partners, it is definitely a great time to be a CS major!

CS Department celebrates December 2012 Commencement

The Department of Computer Science celebrated 2012 Fall Commencement for undergraduates and graduate students on Thursday, December 20, 2012. December graduates, their friends and family, and CS faculty and staff attended the CS Commencement Reception held in the Computer Science Undergraduate Learning Center. Congratulations to all of our graduates!

CS@VT team takes top prize at IDT Programming Competition for second year in a row

Innovative Defense Technologies (IDT) held the final round of its annual High School and Collegiate Programming Contest on Saturday, March 2, at the Virginia Tech Research Center in Arlington, VA. The competition focused on innovative methods of implementing Automated Software Testing techniques. Several local high school and university teams participated.



Pictured left to right: Thom Garrett (IDT), Eeshan Shah, Ian Davies and Karthik Kumar

In the High School Division, McLean High School won first place (Akshay Karthik, Peter Ott, Drew Sorrels). IDT recognized McLean's coach, Jean Wright, for her 31 years of teaching Computer Science at the high school level. Two teams from Thomas Jefferson High School for Science and Technology (TJHSST) placed second and third.

In the Collegiate Division, Virginia Tech won first place (Ian Davies, Karthik Kumar, Eeshan Shah). Second place went to William & Mary (James Rountree and Gregory Smith). McLean High School team with coach Jean Wright. "The purpose of this type of event is to promote student interest in Automated Software Testing through problem solving, teamwork, and innovative technology," said Thom Garrett, IDT contest chair. The top three high school teams earned cash awards for the Computer Science Departments at their schools, as well as prizes and T-shirts for the participants. The college teams won cash awards for their team members. IDT's annual programming contest is open to teams from high schools and colleges in Virginia, Maryland, and DC.

For more information about future contests, visit contest.IDTus.com.

Article provided by Innovative Defense Technologies.

CSRC makes $75K donation to Investment in Excellence Scholarship

The CS Department's corporate partners program, the Computer Science Resources Consortium (CSRC), made a $75,000 donation to the Investment in Excellence Scholarship fund in December 2012. The Investment in Excellence Scholarship was created in the fall of 2007 by funding provided by the CSRC. The CSRC has been able to make a sizable donation in each year since the endowment was created. With the 2012 donation, the endowment has reached $250,000. The CS Department thanks the corporate partners who made this possible.

Four CS@VT students recognized for "Creativity on Campus"

Four computer science students were recognized for their "Creativity on Campus" by the Institute for Creativity, Arts, and Technology (ICAT). According to the ICAT website: "Creativity on Campus (ConC) challenges all Virginia Tech students to submit anything that speaks to them as an excellent example of creativity. Creativity can come in all shapes and sizes, from songs to graphs, paintings to diagrams, animations to research posters—nearly anything is eligible." Each winner receives a $50 Amazon gift card and has their submission published on the ICAT website.

2012/2013 CS Winners:

- October 2012, Huanqing Liu: Self-Portrait in Sand
- November 2012, Alexandru Cioacia: Picture of Chicago O'Hare Airport
- December 2012, Panagiotis Apostolellis: VIGOR Concept Design
- February 2012, Michael Stewart: Sodoku Game Design

Undergraduate Huanqing Liu selected for National Conference on Undergrad Research and ACC Meeting of the Minds

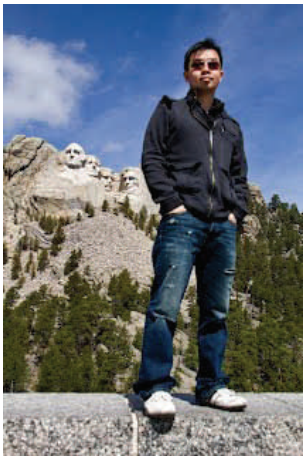
Second year computer science student Huanqing "Quinn" Liu was selected to present his research at the National Conference on Undergraduate Research (NCUR) and at the ACC's Meeting of the Minds (MOM). Liu is mentored by Dr. Anthony Cate, assistant professor of psychology at Virginia Tech. Read more about Liu's research:

Hierarchical Temporal Memory Simulation Using OOD and MVC (presented at NCUR and MOM)

From the NCUR website: "Currently, the best neural networks have only been successfully applied to specific problems and are fundamentally not how a real brain creates intelligence. In order to further the machine learning field in a more biological direction to allow success for any given input data, I have programmed hierarchical time dependent memory models that are biologically accurate to the human neocortex. To visualize the activity of cells within a lobe of the brain I simulated the known biological behaviors of synapses, axons, cells, columns, and lobes known to neuroscience using object oriented design and graphical user interfaces techniques known to computer science. This interdisciplinary research has produced a new programming library that is based on neuroscience physiology and computer computational efficiency to better understand the brain through modeling. When fully implemented the result will be a new fundamental technology that will be the epitome of time based inference. This will allow understanding of how neurons interact through common learning algorithms by observing small scale brain simulation experiments with object recognition and object prediction. By doing so more efficient and effective brain simulation algorithms that are capable of spatial in-variance and multiple time step predictions can be developed. Furthermore, as the model grows to incorporate biologically accurate feedback algorithms, a detailed theory of consciousness can be added to our understanding of neuroscience."

You can also read more about this and see his artwork on his own homepage: www.walnutiq.com.

Graduate student Chun-Yi Su selected for Lawrence Scholar Program at Lawrence Livermore National Lab



Chun-Yi Su, a PhD candidate in computer science, has been selected for the Lawrence Scholar Program at Lawrence Livermore National Lab (LLNL). Su is advised by Dr. Kirk Cameron, professor of computer science, who reports "that Chun-Yi's application proposed heterogeneous, NUMA memory modeling, analysis and optimization. He is among approximately a dozen students selected nation-wide for this honor. This program allows him to work on his dissertation research at LLNL with a scientist mentor/advisor, Edgar Leon."

Cameron goes on to say "that this award comes with a significant annual stipend and some travel support as well as the chance to work on-site with LLNL personnel for several years. Chun-Yi will work with our group and his LLNL advisor closely on this exciting project in the years to come."

From the LLNL website: "The Lawrence Scholar Program (LSP) and its predecessor programs have played a critical role for many years in helping to recruit new scientific and engineering talent to Lawrence Livermore National Laboratory (LLNL). Top Ph.D. students are granted appointments of up to four years to conduct research of interest to the Laboratory while completing their thesis."

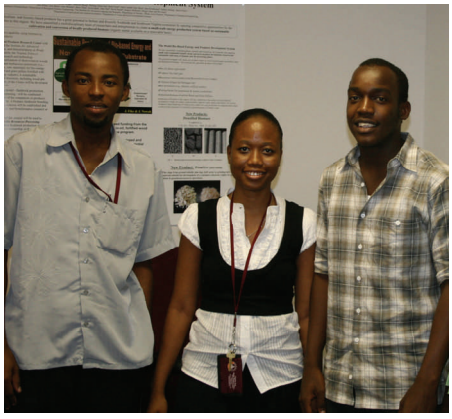
Graduate student Zalia Shams places second in graduate student poster competition at Grace Hopper Celebration of Women in Computing

Zalia Shams, a PhD candidate in computer science, won second place in the graduate division of the poster competition at the Grace Hopper Celebration of Women in Computing for her work entitled "Evaluating Students' Assignments by Running Their Test Cases Against Each Others' Code." She describes the project: "A robust mechanism for evaluating student-written software tests is running one student's solution against others' test-cases. However, in object-oriented languages, tests are commonly included in program codes that may depend on any aspect of author's solution and may not compile against another's program. We present a novel solution for Java that uses bytecode transformation and reflection so tests will run against any other program regardless of compile-time dependencies. Our solution allows automatic evaluation of correctness and test quality of students' solutions even if the solutions are partial or incomplete." Shams is advised by Dr. Steve Edwards.

VT MIT program ranks third in the United States

US News & World Report's Best Online Education publication ranks VT's MIT program as third in the nation. Both the College of Engineering, home to the Department of Computer Science, and the Pamplin College of Business jointly administer this degree program. Virginia Tech placed third behind the University of Southern California and Sam Houston University in Texas. To read more about this ranking, please see the story in its entirety on the College of Engineering's website.

CS@VT graduates return to Haiti to teach the next generation of CS teachers



Mario Calixte, Jennifer François and Fabrice Marcelin

Three graduates of the CS@VT program returned to their native country of Haiti to work and to teach the next generation of computer science teachers. Mario Eliezer Calixte (BS 2010, MAEd 2012), Fabrice Marcelin (BS 2010 and MS 2012) and Jennifer Alexandra François (BS 2010) taught two training sessions for Haitian teachers. (Pictured at left are Calixte, François, and Marcelin.)

The press release from Higher Education for Development, part of the US Agency for International Development (USAID): Following a devastating 2010 earthquake, Haiti received donations of all kinds and funding from several countries to support its recovery and rebuilding process. When Literacy Volunteers of Fauquier County (LVFC) in Warrenton, Va. donated and installed computer labs with Linux-Mint operating systems throughout Haiti, the group faced one major hurdle: The Haitian teachers and computer lab managers were familiar with Windows, but not with Linux. Determined to put their donations to use, Denny Baumann of LVFC contacted Virginia Tech faculty and requested computer training support for the recipients in northern Haiti. However, the solution was already in-country: Three computer science graduates, Mario Eliezer Calixte, Fabrice Marcelin, and Jennifer Alexandra François, had returned to Haiti months earlier upon graduation from Virginia Tech. "As Haitians, we are well aware of how difficult it is to get either prime education or training, so we felt that it was our right and duty to teach such skills and share our knowledge with the teachers and students in Haiti," stated François, a recent Virginia Tech graduate and new employee at Ericsson, a telecommunication company.

Calixte, Marcelin, and François applied skills and techniques acquired through their education at Virginia Tech to create and facilitate training sessions in their home country. They are among the five graduates whose bachelor's degrees were funded by the U.S. Agency for International Development through a Higher Education for Development (HED) partnership between Virginia Tech and Ecole Supérieure d'Infotronique d'Haïti. As trainers, the three Haitian computer science engineers collaborated on curricula development and led two one-day computer skills sessions in September 2012 in Terrier-Rouge and Port-au-Prince. "This opportunity matched my vision to use technologies to bring educational resources and training into the hard-to-reach area of Haiti," stated Calixte. A total of 14 teachers from schools in Terrier-Rouge, Capotille, Ouanaminthe, Fort-Liberte, Port-au-Prince, and Petit Goave attended hands-on sessions to learn basic navigation skills, application information, and the difference between Linux, Windows and Mac computer operating systems. Calixte and Marcelin also worked individually with each participant and tailored instructions to each person's level. "With my vast knowledge of Linux-Mint, I know I would be a valuable asset to the team," stated Marcelin.

Fulfilling local community needs is not a new endeavor for Calixte, Marcelin, and François. While at Virginia Tech, they were members of the student group, "Computer Science Community Service," which is dedicated to teaching computer skills to U.S. youth and adults alike. Their spirit of global community service is rooted in their international higher education partnership. "The experience at VT had a great impact in our involvement in this project," stated François. "As strong believers of Virginia Tech's motto 'Ut Prosim—That I May Serve,' giving back to the community is now second nature to us."

Eli Tilevich seeks to improve portability of mobile device applications.

Dr. Eli Tilevich, associate professor of computer science, recently received an award from the Microsoft Research Software Engineering Innovation Foundation (SEIF) for his work on mobile device applications. Tilevich's work seeks to improve porting applications across different mobile devices and platforms. This Microsoft award was one of only 10 world wide.

To read more about Dr. Tilevich's research, please see the article by Lynn Nystrom at http://bit.ly/P9PC44.

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Deborah Tatar co-PI for REU "Hands-on, Minds-on: Multidisciplinary Approaches to Understanding and Preventing Society Violence"

Dr. Deborah Tatar, along with colleagues in the Undergraduate Research Institute, Communication, Human Development, and Psychology, were awarded a $365,000 grant from the National Science Foundation for this REU. Read more about this exciting project on the VT News website: http://bit.ly/13pGRWI.

TM Murali, PhD students Ahsanur Rahman and Chris Poirel, and David Badger win best paper award

TM Murali, PhD students Ahsanur Rahman (first author) and Chris Poirel, and group member David Badger won the Best Paper Award at the ACM Conference on Bioinformatics, Computational Biology and Biomedicine 2012. Murali describes the paper: "Analysis of molecular interaction networks is pervasive in systems biology. This research relies almost entirely on graphs for modeling interactions. However, edges in graphs cannot represent multi-way interactions among molecules, which occur very often within cells. Hypergraphs may be better representations for such interactions, since hyperedges can naturally represent relationships among multiple molecules. In this paper, we propose using hypergraphs to capture the uncertainty that is inherent in reverse engineering gene-gene networks from large-scale datasets. We provide a novel formulation of hyperedges to capture this uncertainty. We propose the first algorithm in the literature to discover hyperedges from systems biology datasets."

Read more about this at http://bit.ly/WsSYm9.

Feng and Sandu awarded grant for hardware/software co-design project

Dr. Wu Feng, PI, Dr. Adrian Sandu, co-PI, and co-PIs at Virginia Tech Eric de Sturler (Math), Chris Roy (AOE), Danesh Tafti (ME) and co-PIs at NC State Jack Edwards (ME), Hong Luo (ME), and Frank Mueller (CS) were awarded $3.5 million in funding from the AFSOR Basic Research Initiative program. The grant is titled "Co-Design of Hardware/Software for Predicting MAV Aerodynamics."

Dr. Feng describes the project: "While Moore's Law theoretically doubles processor performance every 24 months, much of the realizable performance remains untapped because the burden falls to the (less informed) domain scientist or engineer to exploit parallel hardware for performance gains. Even when such untapped hardware potential is fully realized, it is often not coupled with advances in algorithmic innovation, which can deliver further (multiplicative) speed-up beyond Moore's Law. Building on our past success in adapting our CPU-based parallel implementations of n-body methods and spectral methods onto the GPU via an ad-hoc hardware/software co-design process, we seek to formalize the aforementioned co-design process and apply it to the structured/unstructured grid motifs found in computational fluid dynamics (CFD) in support of aerodynamic predictions for micro air vehicles (MAVs). While many past efforts to develop such CFD codes on accelerated processors have shown limited success, our proposed hardware/software co-design approach will create malleable algorithms that can be mapped and optimized onto the right type of processing core at the right time, and in turn, deliver orders of magnitude better performance than would have otherwise been possible by Moore's Law alone."

Read more at http://bit.ly/12er3H5.

Madhav Marathe named IEEE Fellow

In late 2012, Madhav Marathe, deputy director of the Network Dynamics and Simulation Science Laboratory and professor of computer science at Virginia Tech, of Blacksburg, Va., was named an Institute of Electrical and Electronics Engineers (IEEE) Fellow. He was recognized for "for contributions to the development of formal models and software tools for understanding socio-technical networks." To read more about Marathe's accomplishments, please see the press release on the Virginia Bioinformatics Institute's homepage.

Steve Edwards wins Virginia Outstanding Faculty Award

Steve Edwards, associate professor of computer science, received one of the State Council for Higher Education in Virginia (SCHEV) awards for Virginia Outstanding Faculty on February 12, 2013. This award is the "highest honor for Virginia Faculty."

"Stephen H. Edwards is an Associate Professor in the Department of Computer Science at Virginia Tech, where he has taught since 1998.

"Dr. Edwards' research interests are in software engineering, the use of formal methods in programming languages, automated testing, and software components. In addition, he is internationally known as a researcher in computer science education, and one of the leading advocates of teaching software testing to students of computing.

"In 2012, Dr. Edwards was appointed as the W.S. "Pete" White Chair for Innovation in Engineering Education by the Virginia Tech Board of Visitors. This endowed chair was created by American Electric Power to honor Pete White, in order to 'celebrate and illustrate innovative approaches to teaching using technology.'"

"Dr. Edwards actively serves as an associate editor for *Transactions on Computing Education*, the flagship professional society journal for educational research articles in his field.

"Dr. Edwards' research group at Virginia Tech has produced a number of educational tools for classroom use, the most well-known of which is Web-CAT: The Web-based Center for Automated Testing. This tool, which is designed to give computing students feedback about the quality of computer programs they write, is the most widely used open-source educational tool of its kind, with over 10,000 users at 75 schools at present. Web-CAT won the Premier Award in 2006, given by the NEEDS consortium to recognize high-quality, non-commercial courseware designed to enhance engineering education.

"Dr. Edwards received a B.S. in electrical engineering from the California Institute of Technology in 1988, an M.S. in computer and information science from The Ohio State University in 1992, and a Ph.D. from The Ohio State University in 1995, where he majored in software engineering, and minored in both formal methods in programming languages and in information retrieval and databases. He is married to Diane M. Hodge, Professor in the School of Social Work at Radford University, and they have two children, Matthew and Amanda."

Article from SCHEV website: http://www.schev.edu/AdminFaculty/OFA/2013/13Edwards.asp.

Aditya Prakash and co-authors win Best Paper Award at 21st ACM CIKM

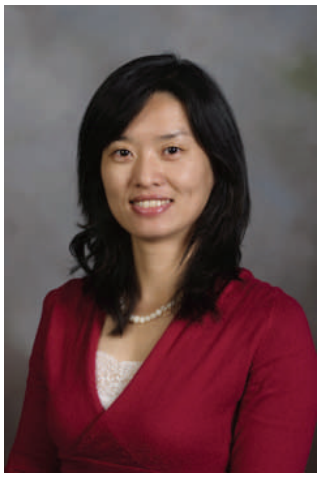
Aditya Prakash, assistant professor of computer science, and his co-authors won the Best Paper Award at the 21st ACM International Conference on Information and Knowledge Management. The CIKM is a major conference in informational retrieval and data mining. Read the paper in its entirety, which Prakash has posted on his web-page: http://bit.ly/15QJXud.

Naren Ramakrishnan featured in ASEE December issue of PRISM

Naren Ramakrishnan's research was featured in the cover story on data analytics in the ASEE December issue of Prism. Read the article on the ASEE PRISM website.: http://bit.ly/17AOhx9. Ramakrishnan's research was also featured on the CCC CRA blog (http://bit.ly/PakLSM), which was picked up by ACM TechNews.

Read more about the IARPA project at: http://bit.ly/12yAnYa.

Danfeng Yao wins best paper award at ICNP; receives 3 year grant from ONR



Dr. Danfeng (Daphne) Yao, assistant professor of computer science, and her collaborators at the Chinese Academy of Sciences and Michigan State University won the Best Paper Award at the International Conference on Network Protocols (ICNP) 2012 held in Austin, Texas in November. Their paper is on reverse engineering unknown network protocols, specifically how to analyze patterns in network traffic in order to extract protocol specifications. Daphne and her collaborators drew parallels between the natural language processing and network traffic analysis, and experimentally demonstrated the accuracy of data mining methods used with large-scale datasets.

Dr. Yao also received a three year grant from the Office of Naval Research for her project titled "Real-Time Anomaly Detection and Quantitative Assurance For Securing Systems." Yao describes her project "We aim to answer the question of whether a complex computer system is running normally as intended by its owner. We will design novel quantitative system assurance models and principles, as well as developing scalable measures and prototypes for practical real-time monitoring."

Read more about this award at http://bit.ly/19A4y1S.

Paper by Alexey Onufriev selected as featured article in Nucleic Acids Research

Alexey Onufriev's paper, "Automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations," was selected as a featured article in Nucleic Acids Research, a journal with an impact factor of 8. Featured articles in this journal represent the top 5% of NAR papers in terms of originality, significance and scientific excellence. A "lay synopsis" of the article is as follows:

"The accuracy of biomolecular modeling and simulation, such as molecular dynamics (MD) depends on the accuracy of the input structures. Preparing these structures can involve the use of a variety of different tools for: correcting errors, adding missing atoms, filling valances with hydrogens, predicting pK values for titratable amino acids, assigning predefined partial charges and radii to all atoms, and generating force field parameter/topology files. H++ automates the above key steps and performs extensive error and consistency checking, providing error/warning messages together with suggested corrections. H++ is available at http://biophysics.cs.vt.edu/."

Onufriev also has a new PNAS (Proceedings of the National Academy of Science) article, "Two-phase stretching of molecular chains." This article reports on work from a US-Russian research collaboration funded by CRDF Global and the Russian Federation for Basic Research. According to the CRDF website:

"The project's goal was to clarify the impacts of nonlinear effects on DNA structural transformations and the formation of its physical and mechanical properties. These properties are important for fundamental understanding of DNA as the basis of heredity and mutagenesis, and thus the existence of congenital diseases and cancer. Potential use of DNA in nanotechnology applications also requires deep understanding of its physical properties at single molecule level, often different from expectation."

Wu Feng and Steve Edwards named Teacher of the Week

The Center for Instructional Development and Educational Research (CIDER) offers the "Teacher of the Week" program, which is "designed to recognize effective, engaged, and dynamic teachers."

Dr. Wu Feng was named a Teacher of the Week in August 2012. According to the CIDER news announcement, Dr. Feng was recognized "for his effort in inspiring students by presenting content that is at the forefront of the computer science industry, his outstanding teaching and presentation skills, and his ability to present difficult topics in a comprehensible manner."

Dr. Steve Edwards was named a Teacher of the Week in November 2012. From his nomination packet: "One student this spring said of Dr. Edwards' class, "I've always enjoyed your style of lecture where you speak very clearly, are comfortable repeating/re-explaining concepts that are difficult, and make students feel more relaxed in the classroom. While it sounds cheesy, I appreciate professors that put effort into the classes that they teach." Cal Ribbens, the associate head for undergraduate studies in the Department of Computer Science, described Dr. Edwards as "easily one of the most innovative and energetic faculty members I have known in my 25 years at Virginia Tech."

Alumnus Hussein Ahmed named one of GAP 50 Entrepreneurs in 2012

A 2010 graduate of the CS@VT PhD program, Dr. Hussein Ahmed was named as one of the 2012 50 GAP Award Winners by the Center for Innovative Technology (www.cit.org). According to the CIT GAP website, these winners are "most likely to build Virginia's next generation life science, technology, and energy companies." Read more about this on the 2012 CIT GAP page:

www.cit.org/service-lines/gap-50-entrepreneur-award-winners

Ahmed also won the Devcup Silver prize at the Evernote Devcup 2012. Read more about his entry at http://bit.ly/YwoH5a. Devcup is gearing up for the 2013 event, mentioning the top entries from last year's event.

Jody Humphreys receives Leadership Excellence Certificate

Jody Humphreys, administrative assistant to Dr. Barbara Ryder and CS@VT staff member, received a Leadership Excellence Certificate from the University Organizational and Professional Development Office on January 23, 2013. This certificate represents the successful completion of 8 professional development courses offered by the university.

CS@VT is part of NCWIT's Pacesetters Program

With CS Department Head Dr. Barbara Ryder as the department's executive champion, CS@VT renewed its membership in the National Center for Women in IT (NCWIT) Pacesetters program. Ryder will be joined by change agents Dr. Scott McCrickard, associate professor of computer science, and Ms. Libby Bradford, director of external relations and undergraduate studies in the computer science department. Read more about the Pacesetters program (http://bit.ly/10uPLVp) and CS@VT's involvement. (http://bit.ly/10TgXik) with the program.

How you can help CS@VT!

The generosity of alumni, parents and friends of CS@VT allows us to fund many special activities in the department. The budget cuts over the past 6 years have resulted in the department not having sufficient funds to flourish and grow to world-class stature, a goal we aim to achieve.

In the past, we have concentrated on building a departmental scholarship fund, the Investment in Excellence Scholarship fund first endowed in 2007. Today, through the tireless stewardship of Ms. Libby Bradford, Director of External Relations for CS@VT, this fund generates about $12,000 annually for scholarships. We also have special named scholarships, including the George Gorsline Scholarship, the Anne & George Gorsline Scholarship, the Griffith-Strader Christian Scholarship and the CGI Scholarship (see www.cs.vt.edu/undergraduate/scholarships for more details). We would welcome your contributions in support for any of these fine scholarship funds. Please see our scholarship donation page for more information.

However, in order to achieve our goal of ranking among the top 10% of CS departments in the US, we need additional funds to attract outstanding graduate students (e.g., fellowships), to retain outstanding faculty members active in cutting edge research, to maintain state-of-the-art research facilities and to encourage exploration of high risk, high payoff research ideas. We need to start an endowment for CS@VT that will support these goals, and eventually grow into support for endowed faculty fellowships and named chairs.

With your help, together we will accomplish these goals. We are embarking on a fundraising campaign to establish an endowment for our department. Of course, we welcome your financial support at any level. Nevertheless, we urge you to consider a 5-year pledge of a gift at the $300, $600, or $1200 level annually. Such gifts will be acknowledged publicly on our *CS@VT Benefactors* wall in McBryde 106.

How to make a pledge

To make a pledge, please go to www.cs.vt.edu/donations and look for "How to Give to Computer Science" at the bottom of the page. To ensure the department receives your gift, please follow these instructions:

We ask you to specify the Department of Computer Science as the recipient of your gift. To ensure this happens when you use the online gift form, in the section entitled "Gift Information" please select "Other Designation" and type "Departmental Programs - 875766."

You can securely make a pledge, make a payment on an existing pledge, make a gift using your credit card, or request information on donating securities, making a planned gift or using electronic funds transfer from your checking account, via the online pledge form.

Many employers will match donations from employees. To see if your employer will match your donation, please see the Matching Gifts page.

When you make a donation, please send e-mail to donations@cs.vt.edu to notify us of your gift. We would like to promptly acknowledge your gift!

To make sure the CS Department has your current information, please click here. If you know of other CS@VT alumni who are not getting our newsletter, please share the link with them.