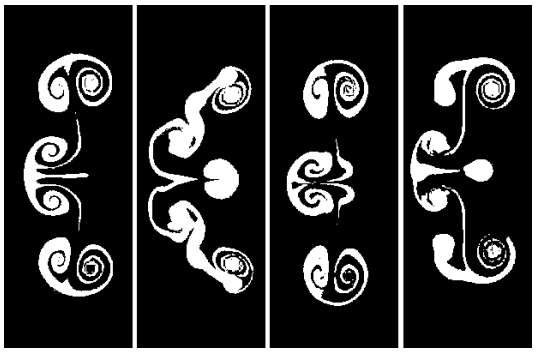
CCS News Bytes

LALP-05-015 **February 2005**



Which of these shock tube morphologies do you think is least similar to the others? Most people choose No. 2. It is now possible for a computer to make the same selection….

CCS-3 Team Can Find 'Needles in Haystack'

Supercomputers make it possible today to generate huge data sets from hydrocodes. It is even possible to create visualizations from the data that can summarize what has occurred.

However, these visualizations are so simplified that they can fail to reveal problems buried deep within the masses of data. By analogy, consider trying to determine from a photograph whether one dime lies hidden in a gymnasium full of pennies.

Now, a team of five people—Michael Cannon, Tony Warnock, Patricia Fasel, Richard Fortson, and John Hogden, all in the Modeling, Algorithms, and Informatics Group of the Computer and Computational Sciences Division (CCS-3)—has developed a mathematical way to reach into these terabyte data sets and find relevant problems.

Their method is already being used in several interesting ways. They are, for example, assisting the Applied Physics Division (X Division) in checking for asymmetries in the computer simulation of imploding pits.

Their method can also be extremely useful in checking terabyte sets of data for transient events. They do this by checking an event to see how many standard deviations out from the mean it lies.

Cannon commented, "We find needles in haystacks!"

The team can also find bad values in mixed cells. Warnock has developed what Cannon called "a mathematical bump detector" that can find "bugs you never knew existed." These bad values would never be revealed in a visual tour of the data.

Consider one more application of the team's work: the ability to compare shapes and determine which ones are alike and which ones are different. The human eye and brain are very good at such discrimination, but in the past, it has been difficult to teach a computer to do it. Now, however, team members can use their mathematical methods to compare photos taken by PHERMEX (the pulsed high-energy radiographic machine emitting x-rays), for example. Their approach involves comparison of histograms of many lines from random point to random point on the surface.

Cannon noted that the method works in both two and three dimensions.

X Division, Physics Division (P Division), and the Dynamic Experimentation Division (DX Division) have expressed interest in this method of determining similarity and difference in shapes.

After a recent briefing on the team's work, CCS Deputy Division Leader Stephen Lee said, "This is very high-impact work with important ramifications in the nuclear weapons program and threat reduction programs."

Donations for Shelter *Poured* into Fisk's Office

Gina Fisk, a computer scientist in the Advanced Computing Laboratory (CCS-1), organized a campaign to collect money and gifts for a homeless shelter in Socorro during the holiday season—and pulled in money and donations that filled two cars.

The shelter she wanted to help was Puerto Seguro (Safe Port) Inc. "Some members of my family had gotten involved in it," she said during a recent interview. What really attracted her, she said, was that 100% of donations to Puerto Seguro go to helping the homeless.

(Please see DONATIONS, page 2.)

Welcome to News Bytes

Hello! My name is Charmian Schaller. I'm a writer-editor from the Communication Arts and Services Group (IM-1), and I am now assigned to the Computer and Computational Sciences Division (CCS).

I will be editing "News Bytes," a newsletter for CCS—writing the stories, taking photos and distributing the publication to all division employees.

I will also be working on a variety of other CCS projects from recruitment brochures to websites. When time permits, I will also be available to help you polish your own papers by checking grammar, spelling, style, and flow.

"News Bytes" will be a nontechnical publication intended to help CCS people located in 10 buildings get to know each other and share more of a feeling of belonging.

The newsletter will be bringing you interviews with new people in the division, stories about CCS activities that affect us all, and at least one story per issue explaining (in simple, nontechnical language) the work of one interesting CCS employee or team.

Your help will be essential to making this an enjoyable publication. Please call me with your suggestions for stories—and don't be hesitant about telling me when you have published a paper, won an award, or received an honor yourself. My telephone number is 665-3895; my e-mail address is cosx@lanl.gov; my office is in Room 268 in Building 200—and my door is open.

DONATIONS (Cont'd from P.1)

"They have a shelter that has a kitchen, bathrooms, and a laundry," she said. In an emergency—for example when a family's car breaks down on the highway—the shelter lets the family use Puerto Seguro facilities and then puts them up briefly in a hotel. Puerto Seguro also provides propane and money to pay bills for the poor in the Socorro area.

Puerto Seguro is run by an all-volunteer board of directors. The City of Socorro donates space, and benefactors, donors, and grants cover all costs.

At first, Fisk thought that Laboratory donors might give to a specific family. She contacted Puerto Seguro, and the organization sent her a list of 20 families from which to choose—but when she looked at the list, she found it impossible to select just one family. She decided, instead, to call for donations of gifts, money, and clothing that the shelter could distribute as needed.

The result? "We got a ton of stuff," Fisk said. She began storing donations in an empty cubicle near her office that covers about 150 feet square, and by the end of the drive, it was full. She estimated that approximately 400 items poured in from more than 75 donors. The campaign also drew $500 in cash.

Those who responded worked in five divisions—the Computer and Computational Sciences Division (CCS); the Computing, Communications, and Networking Division (CCN); the Information Management Division (IM); the Applied Physics Division (X); and the Theoretical Division (T).

"I delivered it on Dec. 19," she said. Her husband went along, in part because the donations filled two vehicles. "They were very surprised," she said with a smile. She took in the first box, and people thanked her warmly—and then she told them that the box was just the first of many.

Board members at the shelter subsequently drove to the homes of those in need and delivered the wrapped gifts that had been donated.

Fisk said, "I was really pleased with the turnout." She hopes to repeat the drive next year.

Asked about her own background, she said she is from Edgewood, New Mexico, and has been at the Laboratory for 11 years. She has some past experience in assisting those in need. "I've done a lot of food-drive stuff," she said, and she helped the Red Cross after the Cerro Grande Fire.

Meet Our New People

Four new people have joined CCS since October 1, 2004. Brief biographies of each of them appear on the next three pages. Please make them welcome!

(Please see NEW PEOPLE on page 3.)

NEW PEOPLE (Cont'd from P. 2.)

John Patchett

John Patchett, who recently became a technical staff member and University of California employee at the Advanced Computing Laboratory (CCS-1), has a wealth of experience—including five and a half years as a Butler employee working for the Computer and Computational Sciences Division.

His work in the past has included building a 128-node parallel visualization cluster running Windows 2000. Currently, he is on the systems team in CCS-1, working toward installation of new Linux visualization clusters.

Patchett's background is unusually varied. In 1995, he earned a bachelor's degree in anthropology from the University of New Mexico (UNM) with a minor in geography. In 1996, he received a Basic Management Certificate from UNM's Robert O. Anderson School of Management.

His interest in computers led to a 1995 job as sales manager at "PC Place." He was promoted to assistant sales manager before he changed jobs. In 1997, he began working as a system administrator at PTLA. Looking for a field that was more "exciting and challenging," he came to work at CCS-1 in 1999.

In 2002, he went back to school with the goal of obtaining a master's degree in computer science. He has accumulated 37 additional hours in math and computer science from UNM. He is also a Microsoft certified systems engineer, and he has taken a large variety of computer administration and user courses. In a recent interview, he said he also "reads a lot." His bookshelves prove it. They are crammed with computer-related texts.

Patchett has an interesting personal background. He described himself as a "military brat," born in New Mexico. While he was growing up, he lived on Air Force bases in North Dakota, Utah, and Germany. His family finally returned to Alamogordo, where he graduated from high school. He was the middle child in a family of five children, he said, and, "I was the only one of my mom's kids born in the States." He said he enjoyed his family's frequent moves to new places.

He has now lived in Los Alamos for seven years—the longest he has ever lived in one place in his life.

It was in Los Alamos that he learned scuba diving, an interest that has taken him to the Caribbean three times. (He has a detailed map of the Caicos Islands on his wall.) He has also dived in Puget Sound and in southern California. "There's nothing to stress out about when you're under water," he said. "It's very relaxing."

He is married to a physical therapist, Rita, and they have a son, Michael, who is 20 months old. Another child is due in March. He is so busy at home now that he has no time for scuba diving. "I hang out with my family now," he said. He also does a little bit of walking and hiking.

He used to spend a lot of his free time working with computers, he said, but that has changed. "I found out how to do what I love at work," he explained.

Mark R. Petersen

Mark R. Petersen, a postdoctoral researcher who recently joined Continuum Dynamics (CCS-2), will be participating in the Overflow Project, a problem on the forefront of climate research.

Petersen holds a bachelor's degree in environmental engineering from the University of Nebraska-Lincoln; a master's degree in mathematics and statistics from UN-Lincoln; another master's degree in atmospheric and oceanic science from the University of Colorado-Boulder; and a Ph.D. in applied mathematics from UC-Boulder.

His background includes two years as a project engineer on air pollution control systems at U.S. Filter/RJ Environmental in San Diego, California; two years as a graduate student researcher and instructor at UN-Lincoln; several years as a mentor and consultant for the undergraduate-scientists program at the National Center for Atmospheric Research (NCAR); and three years as a graduate student researcher and instructor at UC-Boulder.

He has wide-ranging interests.

His doctoral thesis at UC-Boulder had two parts, both of which used reduced equations for fluid dynamics. The first part involved ocean and atmospheric models and the study of quasi-geostrophic turbulence. The second studied the formation and longevity of vortices in protoplanetary disks, which are disks of gas that surround young stars. These vortices concentrate dust and rock and accelerate planetary formation. Petersen created computer models to investigate the dynamics of quasi-geostrophic turbulence and protoplanetary disks.

However, during his work at NCAR, he also did considerable statistical research on women and minorities in science and engineering. "In general, the numbers are rising, which is good," he said, but when the statistics are analyzed based on the number of minority-group members per population, the increases aren't as impressive. He found that, "per population, underrepresented minorities receive 40% as many bachelor's degrees in science, math, and engineering as do white students. That has been nearly constant over the last 25 years." Women's graduation rates are highly variable, depending on the field. In 2001, U.S. bachelor's degree recipients were 60% women in biological sciences, 48% in mathematics, 42% in physical sciences, and 20% in engineering." He determined, however, that "women form a smaller proportion of Ph.D. recipients—for example, 28% in physical sciences and 18% in engineering."

Petersen is also interested in music. He plays the accordion and the Bavarian zither—an instrument he learned from his mother, who was Bavarian. He sings bass and knows many German and American folk songs.

(Please see MORE NEW PEOPLE, page 4.)

MORE NEW PEOPLE (Cont'd from P.3.)

Petersen was attracted to Los Alamos National Laboratory because, he said, "I was definitely looking for a place where they create big oceanic and atmospheric (climate) models." He also wanted a small town with good schools for his children, and, he added, "I enjoy the outdoors—camping and cycling." He was impressed by the quality of the work done here by the ocean–modeling group, and he felt that he would have good mentors.

Petersen and his wife, Kimberly, have two children—Theodore, who is 7, and Lillian, who is 2. Readers of *Science* magazine might already know what his children look like. Late in 2004, *Science* held a contest, asking people, "Where do you read your *Science*?" Petersen sent in a photograph that showed him reading the magazine to his children. The advertisement and photo appear on page 1658 in the December 3, 2004 issue. He is quoted as saying, "I read my *Science* with my kids. Theodore and Lillian enjoy the pictures of animals, people and planets as I browse through the magazine. It's a fun way for us all to learn more about science."

Cavendish McKay

Cavendish McKay, a new graduate student in the Continuum Dynamics Group at the Laboratory (CCS-2), earned a bachelor's degree in physics from Brigham Young University in 1997 and is now working toward a doctorate in physics with a minor in atmospheric and oceanic sciences at the University of Wisconsin in Madison.

He hopes to complete his degree in May 2005.

His interests and experience are in plasma physics, turbulence, ocean dynamics and ocean modeling, and computational fluid dynamics. He will be working with Balu Nadiga, Daniel Livescu, and others on stochastic modeling for large eddy simulations of ocean flows.

Ocean modeling is important in understanding weather and climate. About half of the heat transport in the world takes place in the ocean. It is more difficult to obtain data in the ocean than in the atmosphere, and, as result, modeling of the ocean is especially important.

McKay's thesis work is somewhat related to the work that he will be doing in Los Alamos. "I'm studying how stratification in the ocean (density in terms of heat and salt) affects wind-driven circulation," he said.

Warmer water is less dense, but the more salty water becomes, the more dense it is. McKay hopes that his work will help scientists understand how changes in the ocean affect climate and vice versa. If the ocean warms up by a few degrees, stratification is affected—and changes in stratification affect circulation.

Asked how he became interested in ocean modeling, McKay said, "It was largely serendipity." His first studies at the University of Wisconsin were in plasma physics. He liked fluid dynamics, however, and he found some "challenging, interesting" aspects to ocean modeling. He also found that fluids were close enough to his background in plasma physics that he was able to transfer a lot of his knowledge.

On the personal side, one of the first things people notice about McKay is his unusual first name. After all, physicist Sir Henry Cavendish measured the gravitational constant. But, McKay said, "As far as I know, I'm not related to him." He is named, instead, for one of his father's uncles, a career diplomat. The name, McKay believes, is from the Isle of Man between Britain and Ireland. "It's good to have a unique name," he said, "I've never met another 'Cavendish.'"

McKay was born and raised in Seattle, Washington. He said that when he first started studying at BYU in Provo, Utah, he didn't fully appreciate the dry environment—but then he started hiking, "and I fell in love with the desert." As a result, when he first visited Los Alamos in November—his first time in New Mexico—he really liked the area. He said he certainly doesn't miss the humidity of Seattle and Madison.

McKay and his wife, Sarah, a Chicago native, have two children—a son named Callister, who is 3, and a daughter named Morgan, who is 18 months old. They moved to Los Alamos January 1. McKay said they enjoyed starting a new year in a new place. They spend their spare time enjoying their children and the out of doors.

Ole Peters

Ole Peters is a new postdoctoral fellow at the Los Alamos National Laboratory (LANL) Center for Nonlinear Studies and at the Santa Fe Institute (SFI).

Peters is originally from Hamburg, Germany, where he went to high school, but he holds an undergraduate degree in physics and a Ph.D. involving the study of nonequilibrium statistical mechanics and critical phenomena from Imperial College in London.

He gave a talk on critical phenomena in March 2004 at the Laboratory and returned in late October as a postdoctoral researcher at LANL (50%) and SFI (50%).

His work in the Computer and Computational Sciences Division (CCS) includes continuing study on critical phenomena. He is doing some work on rainfall. In addition, he is working on avalanche dynamics in neuronal tissue with one of his co-hosts, Luis Bettencourt of the Modeling, Algorithms, and Informatics Group (CCS-3).

Asked what attracted him to the study of nonequilibrium systems, he said he views it as "one big, unresolved problem." He added, "In contrast to equilibrium systems, there's no comprehensive formalism to deal with in nonequilibrium situations." But, he said, such systems are "closer to reality."

"Philosophically, it makes sense to look at nonequilibrium systems," he said

(Please see PEOPLE, page 5.)

PEOPLE (Cont'd from P.4.)

His interest in the field first arose when he was an undergraduate in London.

Asked what drew him to the Laboratory, he said, "I knew people who were here, and they suggested I apply for a position here." He said he is doing "exactly the same work" at SFI, where, he said, the study of self-organized criticality found early support.

His postdoctoral appointment is for two years.

In his spare time in northern New Mexico, Peters, who is single, is snowboarding—"but just because there's no ocean." The sports he enjoys most, he said, are windsurfing and sailing. (On the day of his interview, he was wearing a T-shirt from Hawaii, where he recently spent more than a month with friends.)

Hamburg, a city founded in the ninth century, is one of the largest ports in Europe and is situated at a major river that flows into the North Sea, he said. Sailing is very important there. (His parents and his sister and her husband and son still live there.)

He did a great deal of windsurfing on the North Sea, he said, but he added, "I went windsurfing almost everywhere in Europe." He taught the sport in France.

Asked if he is finding ways to meet people in Los Alamos, he said most of the friends he has made are at work. In fact, he said, at this point, like many postdoctoral researchers, he is spending most of his time working.

Holm Is Teaching Math in London

But He Still Found Time to Compare EPDiff and Tsunami Results

Darryl Holm, a Los Alamos National Laboratory Fellow and employee of the Continuum Dynamics Group (CCS-2), is teaching graduate-level mathematics at Imperial College in London this year.

The job came about because of professional connections developed during almost 15 years of working on turbulence in ocean circulation, and, specifically, years of working on the Parallel Ocean Program (POP) at the Laboratory.

Holm said he was interested in the modeling of geophysical fluids, and he found that Cambridge University does that very well. He became involved with the Isaac Newton Institute for Mathematical Sciences at Cambridge, went to their programs, served as a scientific advisor, and worked on developing a technique for modeling turbulence that would preserve the Kelvin Circulation Theorem.

"Turbulence modeling," Holm said, "is about describing what cannot be computed"; it is "about modeling the sub-grid-scale activity." He added, "The circulation theorem is the fundamental property of fluid dynamics, which should be preserved in this modeling."

Through his work, he met many people at Cambridge and elsewhere around the United Kingdom (UK). For 10 years, starting in the mid-1990s, he was at Cambridge nearly every summer. He found Cambridge to be "the perfect setup" because the university is so prestigious that one can invite people to come and speak, and they will almost always say yes.

Cambridge "gave me a good reputation," he said, and he became known because of his work at "the Newton."

When the Imperial College position became available, he said, "They already knew me and what I do." His work on ocean circulation and his experience at the Laboratory had given him an international reputation, he said, adding, "LANL is very well known around the world. It is a mainstream actor in the international science community."

Holm is teaching "Geometry, Mechanics, and Symmetry," part of the fourth-year mathematics curriculum at Imperial College. "Modeling gets into it," he said, "because the modeling I do is based on exactly those three things."

He started teaching at the college in January 2004. This year, he will be teaching during the "spring term," which runs from Jan. 10 through March 18, and then he will be back at the Laboratory for a month. After this break, he will return to Imperial for the summer term from April 23 through July 1. He will be in Los Alamos in July, August, and September, and then he will return to London to teach again during the "autumn term" from October through mid-December."

The position is renewable. He doesn't know yet exactly when he will return to Los Alamos for good.

The students he is teaching are first-year graduate students. He explained that in the United Kingdom, college students graduate after three years. Graduate students then spend another three years in specialized schools to earn a Ph.D.

Imperial College, he said, "only teaches science, technology, and medicine. All they do is science. They work very hard."

Holm has taught at the University of Minnesota and at the University of California-Santa Cruz as well as in London. Asked how the students at Imperial College compare to those he has taught in the United States, he said they are "more or less the same as U.S. students, but they're under a lot of time pressure." They take classes without tests during the year, then do all their preparation and take all of their examinations during the spring terms. "It's a do-or-die situation," he said. "They take exams, and if they don't do well, they don't come back."

(Please see HOLM, page 6.)

HOLM (Cont'd from P.5.)

Although he is teaching in London, Holm is still very much in touch with his own research in Los Alamos—specifically, EPDiff, a model of shallow-water motion with a free surface. Holm said, "It includes internal waves in the ocean in which the waves are so nonlinear that their kinetic energy is more important than their potential energy. Such a situation is called a 'geodesic flow' on the space of smooth maps, which take the initial position of a fluid particle as it is mapped to its present position."

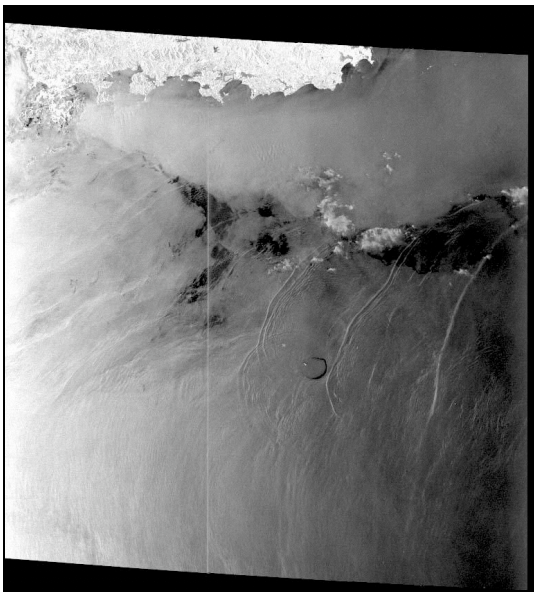
"This is where geometry and symmetry come into the description of the wave," he added. "The solutions of this equation concentrate into waves, which appear, for example, as curved lines on the sea as observed from the Space Shuttle."

Holm said, "The motion of these waves is very similar to the tsunami calculations done by the National Oceanic and Atmospheric Administration (NOAA) as a result of the recent earthquake (in the Indian Ocean)."

Holm has studied the NOAA simulations and noticed many similarities to the solutions of EPDiff. "EPDiff provides a promising long-wave description of the propagation of tsunamis over large distances," he concluded.

(Holm said that persons interested in seeing a NOAA simulation of the tsunami should go to http://www.pmel.noaa.gov/tsunami/Mov/TITOV-INDO2004.mov. Those with Laboratory computers who are interested in more information about EPDiff should go to the EPDiff website recently posted by Holm's colleague, Martin Staley, T-7, at http://t7.lanl.gov/~staley/animations.shtml.)

Holm provided the picture in the next column, which shows a satellite image using 30-centimeter synthetic aperture radar (SAR) of a sequence of internal waves propagating from east to west across the South China Sea. The coastline of South China is seen at the top of the figure. Hong Kong is at top left. The internal waves are seen as "lines on the sea" about 200 kilometers long and separated by about 75 kilometers. These lines are the SAR signatures of internal waves generated by tides in the Luzon Straight between Taiwan and the Philippines a few hundred kilometers further to the east. Internal waves move much more slowly than tsunamis, but they have many of the same properties in their interactions. For example, they merge together when they interact, as seen in the interaction of internal waves to the west of Dong-Sha atoll in the center of the figure. The solutions of EPDiff mimic this behavior accurately, as shown in two-dimensional numerical simulations of EPDiff performed by Staley at Los Alamos. Holm is working with observers and modelers sponsored by the U.S. Office of Naval Research to investigate the three-dimensional aspects of this wave merger.



This satellite image shows a sequence of internal waves on the South China Sea.

In Case You Missed It....

Division Leader William Feiereisen pointed out during the December 2004 all-hands meeting that this has been a year of "amazing accomplishments" in the Computer and Computational Sciences Division (CCS).

As we move into a critical new year—the year of the Laboratory management contract award, it's important to remind ourselves of just how much good work CCS actually did in 2004. Just a few points from Feiereisen's talk:

CCS produced more than 250 refereed publications in 2004, including one in *Nature*.

The division hosted more than 50 invited talks.

It earned six Laboratory Directed Research and Development awards.

And it claimed three out of the five winning Laboratory R&D 100 awards.

The January 2005 *Physics Today* included an interesting article entitled "Computational Science Demands a New Paradigm" by Douglass Post of the Laboratory's Plasma Physics Group (P-24) and Lawrence Votta of Sun Microsystems Inc.

One of the sidebars to the story discussed the successes and failures of the Accelerated Strategic Computing Initiative and included some familiar names including that of Richard Kendall of the Computing, Communications, and Networking Division.