Of blackboards and computer screens: scientific programming in the 21st century

By Karen McWilliams

Since he was a college student, Damian Rouson (8351) has been fascinated by the intersection of science and computing. Computers have transformed scientific research, yet the fields still exist on separate planes. He takes on the challenge of rendering computer languages, so vital to scientific advancements, more expressive and easier to read in a new book *Scientific Software Design: The Object-Oriented Way*, published by Cambridge University Press this spring.

Everyone is familiar with old black-and-white photographs of physicists working out difficult theories at a blackboard. To the layperson, those cryptic equations strewn across the board look like gibberish, but to fellow scientists it is a perfectly understandable code. These scientists used common mathematical expressions that provided a concise, expressive, and clear way of communicating the intricacies of their abstract theories.

The 21st-century equivalent of the blackboard could be the computer screens that are so much a part of today's world. Complex computer programs are used in most of today's scientific research. However, the commonly understood mathematical symbols from 50 years ago have given way to incredibly complex computer languages that often look like gibberish even to fellow scientists. Most computer languages such as Fortran and C++ are not expressive: code written in these languages is hard to decipher even to fellow researchers.

"This book comes out of my experience as a graduate student, 15 years ago," Damian explains. "I took a class in software engineering from the computer science department, and none of the examples used in the class had any relationship to science. By contrast, if you take scientists, even those who are computationally oriented, they really don't talk about the *writing* of the program. They talk about the mathematical algorithms and it's assumed that the translation of the basic algorithm into code—into a program—is straightforward and doesn't deserve much discussion. They don't get down to the practices for writing the code."

The expressive style of programming outlined in the book provides a way to shorten the development time dramatically, because researchers can use familiar expressions, what they'd write on the blackboard. "That can be translated directly into code that runs on these massive platforms," says Damian. "Our hypothesis is that you ultimately can get the same level of speed and scalability with the code, but you can shorten the development cycle—the time it takes you to get there."

As a visiting faculty member at the University of Cyprus in the fall of 2006, Damian taught a course on scientific software design that eventually formed the basis of this book. Writing the book was straightforward, but issues surrounding the computer languages proved more difficult.

"The book deals a lot with Fortran and C++, the two dominant languages in scientific programming. A lot of the Fortran language features we use today weren't available five years ago, when I started writing," Damian notes. Initial reviews from the publisher indicated that the book would have far more lasting value if it used the recently released Fortran 2003 instead of the more commonly used Fortran 95.

This necessary adaptation proved the biggest challenge in the whole project—finding a compiler that could translate the high-level code added another year's worth of work. Damian drew upon the expertise of co-authors Jim Xia (IBM Canada Lab in Markham) and Xiaofeng Xu (General Motors Corp.) to attune the material to Fortran 2003. Jim is on IBM's XL compiler test team and on the international Fortran language standards committee.

With this book, he hopes to introduce design by way of diagramming in a way that most scientific programmers don't currently use; a very up-to-date version of Fortran, also not yet in use by most scientific programmers; and the expressive style of programming. "The idea is to go behind the curtain and see how, by using some nice features of modern programming languages, you can give your own code the same level of expressiveness that is currently attainable with some proprietary solutions, but do so in a more open, scalable manner," he says.

Now that the book is published, Damian is moving into a new phase of research. The first was developing the style of programming itself. The second was demonstrating that it can produce publishable science—in other words, papers that focus on the science, not the code. "This third phase is showing that we can get it to scale, that we can write, not just pretty code, but fast code, and that some of what makes it pretty also makes it fast," he says.

After coming full circle, Damian has returned as a visiting professor to the University of Cyprus to begin putting together what should be the first truly scalable demonstration of this programming style. "Ideally, this visit will demonstrate the ability to run problems that matter to scientists, on systems that matter, in a national lab-type setting," he says.

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Damian in Cyprus with his son

Eating Well in Season

By Allison Doughty

The health of America can be changed with a good chef's knife, a cutting board and a salad spinner.

That was the message Dr. Preston Maring of Oakland's Kaiser Permanente Hospital shared at his "Eating Well in Season" presentation given on June 23rd. He firmly believes that these basic culinary items are the best public health tools.

Dr. Maring explained that the real healthcare competition is making people understand how to live healthier. Twenty thousand Kaiser members were asked does diet and exercise matter for your health in a recent survey, and shockingly, almost half of the older population did not believe these were important factors. Furthermore, only one-third surveyed are eating 3 servings of fruits and vegetables per day in one of the best agricultural countries in the world.

He also addressed the conflicting messages we receive about our food choices explaining that a whole population is not eating well, many people are way overweight and are getting diabetes and other diseases that are associated with that and aren't eating fruits and vegetables, but what about the chemicals and pesticides that are used on our supposedly healthy food?

Eighty-five percent of the lettuce eaten in the United States is grown in the Salinas Valley. The Salinas River changes from the beginning of the river where it is vibrant and full of animals, to the middle where all frogs have mutated into hermaphrodites, to the end of the river in Monterey Bay where it is silent and still because of the levels of organophosphate pesticides present.

"We want you to eat fruits and vegetables, but look what our agricultural system is doing." This is why he stresses buying healthy, organic food as close to the source as you can. Good health comes from our farmers, so it's best to buy directly from them. Not only do the markets help the community, the farmers, and help to reduce our carbon footprint, but it helps protect your health and the health of your family.

Preventive Health Educator and Program Coordinator, Morgan Edwinson believes the most valuable information from the presentation was how the Farmer's Markets help on several different fronts including the community and local farmers, as well as the doctor's cooking tips. Dr. Maring explained, "I'm not saying at all that the organic Farmer's Market is the answer to the country's food system, but it is a place where you begin to focus on a different way."

Dr. Maring has 40 years of experience at Kaiser Permanente. In May 2003, his first Fresh Friday Farmer's Market opened in the Oakland Medical Center and 24 more Kaiser Farmer's

Markets have opened in Northern California alone and there are now 39 markets in 5 states. Dr. Maring mused about a lady who hurriedly approached him at his Oakland market asking how much longer it would be open. After he replied at least another hour, she told him great, I just have to drop my husband off at the ER and I'll be right back. It's good to know that some people really do get excited about fruits and vegetables.

Dr. Maring authored Eating Well in Season: The Farmer's Market Cookbook. There are also 500-600 of Dr. Maring's delicious, quick recipes and the locations of organic Kaiser Farmer's Markets at kp.org/farmersmarket.

Morgan Edwinson came into contact with Dr. Maring after speaking to her contact at Kaiser about starting a Farmer's Market at Sandia. Lucky for us, this led to Dr. Maring's presentation and advice on how to start our own market. A date has yet to be selected, but the SNL and LLNL Farmer's Market will open in the GAA in front of Post 17 and the CRF (where the Health Fair was held) the week of July 25th. To start, the market will be once a month, and depending on the support from both sites, it may occur more frequently. The market will run from July to October, and then start again in the spring.

The live presentation can be found at :
http://as54snlnt.sandia.gov/mediasite/Viewer/?peid=d2dfc1ba6be446a6a6000d0a093167ea1d
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How to Build Your Dream House

Building a house, at first glance, involves the usual construction trades—a general contractor, electrician, plumbers, painters, and the like. But look at the process from a broader view, and architects, designers, structural engineers, interior designers, landscape architects, and city planners enter the picture.

During the past school year, Gabe Gutierrez and Kari Neely (both 8514) were involved in an innovative education outreach effort designed to get high school students thinking about that broader view and where they might see themselves in the future. They visited Kimball High School in Tracy regularly through the school year to teach "How to Build Your Dream House," curriculum designed by Michael T. Martin, a construction manager at Lawrence Livermore National Laboratory (LLNL) and freelance architectural designer.

“The idea is to give these kids something to think about,” explains Martin. “That they don’t necessarily have to go to college to get into a field with good jobs. I want them to start thinking about what vocation they might see themselves in.”

As the outreach chair for LLNL’s Amigos Unidos Hispanic Club, Martin has been involved in numerous education outreach efforts. So when the Kiwanis Club of Tracy was looking for help with a career education program, they turned to him.

Martin spent last summer designing the curriculum, which was taught at three high schools: Stein High School, the Academy for Business at Law at Merrill F. West High School, and Kimball, which had two sessions. He taught one session and recruited a shop carpenter from Site 300, a general contractor in Tracy, and Gabe and Kari to teach the other three.

“The idea was to make them aware of everything that goes into building a house from the ground up,” explains Gabe. “We had them look at the room they were sitting in and then break it down by components.” Over the school year, the students looked at material samples, watched videos on different utilities, measured their own house to calculate square footage, and learned how to lay out a site for a home.

Both Gabe and Kari found the experience rewarding. “I try to stay involved with outreach, especially at the high schools to keep kids in school,” says Gabe, who also coaches baseball at Livermore High School. “The idea is to encourage kids to find something they enjoy and pursue that as a career.”

Kari spends some of her free time tutoring math. “I think there were parts of this course that were pretty eye opening,” she says. “Occasionally you’d see a light bulb turn on.”

Martin will be organizing the program in the 2011/12 school year, which in Tracy begins in early August. Anyone interested in participating can contact him at martin21@llnl.gov or 925-423-6580.

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