



Center for  
Molecular Medicine  
& Genetics

# Advances

## Message from the Director



Centers and institutes within Wayne State University are designed to create synergy among the many sources of expertise based within college departments. While much of CMMG's expertise is related to the practice of medicine and medical research, it has much in common with life sciences and other scientific endeavors within the university.

We are pleased that two of our faculty members will be part of the new WSU Institute for Scientific Computing. Drs. Stephen Krawetz and David Womble will contribute their unique biotechnical perspectives as Dr. William Hase shapes what promises to be another great technological asset of our university. Our CMMG staff representatives will help the institute focus on research and educational opportunities in biocomputing and bioinformatics. As we congratulate Dr. Hase's initiative, we also acknowledge the progressive interest Drs. Krawetz and Womble have demonstrated in bioinformatics on behalf of CMMG for several years. It is this intellectual initiative that will help position CMMG, and Wayne State, as one of Michigan's top resources in the evolving Life Sciences Corridor.

This summer, we said goodbye to a valuable colleague and staff member, Dr. Mary Murray. She will remain in Detroit and promises to continue her association with CMMG's graduate education program. David Womble, who performs a variety of administrative functions for the Center, has been selected to replace Dr. Murray as the Center's Graduate Officer. I'm confident David will continue to enhance the quality of our educational programming, which is one of the hallmarks of CMMG's mission.

Sincerely,

George Grunberger, M.D.  
Henry L. Brasza Professor  
Director, Center for Molecular  
Medicine and Genetics

# WSU Institute Creates Synergy Among Computational Scientists

Stephen Krawetz, Ph.D., professor of CMMG, has been aware of the “next big thing” in science for nearly 20 years – bioinformatics. It’s a special capability he brought to Wayne State in 1989, which led to the creation of one of the first courses in the subject and is now a major component of the newly chartered WSU Institute for Scientific Computing (ISC).



William Hase, Ph.D.

The brainchild of William Hase, Ph.D., Distinguished Professor of Chemistry, the Institute was established last fall to create synergy among the university’s scientists who share an interest in scientific computing, promote interdisciplinary research and create educational opportunities. The Institute has two formal goals: work with departments throughout the university to develop interdisciplinary research in scientific computing and encourage the development of an infrastructure that enhances training in scientific computing. In order to enable a new generation of scientists to contribute to the development of these exciting new areas, participants in the ISC see the need for a fresh approach to

training graduate students. The Institute served as a catalyst for the creation and approval of the new Certificate Program in Scientific Computing, which will formally go into effect in the winter semester, 2001.

Dr. Hase sees the Institute as a vehicle to enhance university Centers such as CMMG through the promise of interdisciplinary collaboration among scientists who have an interest in scientific computing.

“There are about 20 to 30 people who specialize in scientific computing spread across the WSU campus,” he says. “Someone said that in this country you could count on one hand those who are highly skilled in biology and computer science.”

Cross-departmental dialogue has already begun to occur, explains David Womble, Ph.D., CMMG faculty member. “It’s getting people talking together instead of people working in different corners of the university not talking to each other. I’ve met a lot of people recently who I haven’t met before. There are people in the Computer Science Department who are very interested in writing programs that will be useful to biologists. The melding of those two is where all the action will be in the next 25 years or so.”

Bioinformatics has been a unique feature of CMMG since Drs. Krawetz and Womble created its post-graduate course – one of the first in the nation. Most recently, the two ISC members created a new course in molecular biology, which is a collaboration with Chemistry and Biology, as well as the Shiffman Medical Library. The

**Professor Hase is the Principle Investigator on an NSF-IGERT Grant entitled “Interdisciplinary Traineeships in High Performance Computing Applications.” This highly competitive grant will enable Wayne State University to provide fellowships of \$23,255 to qualified graduate students who are U.S. citizens (or permanent residents). For detailed information on the Scientific Computing Program (SCP) at WSU, including the Certificate Program and the IGERT fellowships, as well as application forms, please visit the SCP Web site at <http://www.scp.wayne.edu>.**

course is taught in the library, with students using individual computer terminals. Drs. Krawetz and Womble, and Drs. John SantaLucia from Chemistry and Rob Stephenson from Biology, will alternate presentations, while the others circulate among students to answer questions and help with problems. The text for the course, *Bioinformatics Methods and Protocols*, was co-edited by Dr. Krawetz, with two chapters in the book written by Dr. Womble.



David Womble, Ph.D., and Stephen Krawetz, Ph.D.

## The institute will focus on five categories of strategic research:

- 1) Automotive and aerospace systems
- 2) Biocomputing and bioinformatics
- 3) Clinical applications of computing
- 4) Chemistry, physics and materials science
- 5) High-performance computing software tools and numerical algorithms



Drs. Krawetz, Hase, and Womble  
with "Deep Blue"

"When I came to Wayne State I had just finished my post-doctorate developing an imaging company in Canada. We brought to market the first DNA sequence reader." The first thing Dr. Krawetz did when he arrived was organize support throughout the medical school for bioinformatics. "In 1989, we had a full-fledged version of genbank analysis software."

In the early 1990s, he was introduced to Dr. Womble. "At the time, there was a real need to start training people. So, we developed one of the first courses in the United States in bioinformatics. It's been extremely successful since its inception."

Today, Dr. Krawetz's laboratory work begins with the computer. "First, we build a computer model and do as much as we can in the dry lab before we actually go to the bench and test our hypothesis. It's a lot more productive that way."

Scientific computing allows scientists to conduct molecular modeling and simulation. "It allows you to make an atomic scale model of a molecule of an enzyme or protein and simulate the motion of that protein and how it interacts with other species, how the enzyme catalyzes a reaction – all modeled at the atomic level," explains Dr. Hase.

Simulation is particularly helpful in determining how a new drug might interact at the atomic level motion with an enzyme, he says. "That takes extraordinarily high-perfor-

mance computing." To meet this need, the university recently announced the installation of IBM's most powerful computer, the RS/6000 SP "Deep Blue" super computer.

"There are simulations that one can do that cannot be tested by experiment, but the simulations can give the science extraordinary insight. You can use that to generate new ideas and new experiments that you wouldn't have thought of had you not conducted the simulation. The simulation tells you something that your mind might not have been able to conceive. So it directs you to do a certain kind of experiment."

This capability will allow CMMG researchers to move into the next era of molecular biology and genetics, says Dr. Krawetz. "With the human genome project finished, the bioinformatician is going to be where the next demand will be. It's already there, but it's going to be heightened. All the sequencing will be done. You're going to divide out the biological science problem into different parts. You'll still have the typical wet bench researcher who will look at a very specific problem. Then you'll have the bioinformatician who tries to actually model the problem. That's where the future is and this fills the need, at least from a teaching perspective."

"If I were starting out all over again I would be in this area," says Dr. Hase. "I'm trying to encourage computer scientists and mathematicians to engage in research that supports CMMG because I think there is a lot of opportunity for

grant support there. But the mathematicians and computer scientists need to learn molecular biology and need to learn the kind of questions CMMG is trying to answer. If the application people want to do cutting-edge research, they have to do cutting-edge computing and cutting-edge mathematical applications. Or else they will be using someone else's software, which is okay; but when you build your own software, you can do what someone else can't."

### **Announcing the ISC Workshop on Bioinformatics October 26, 2000**

**This workshop will bring together many leading researchers in this field for a day of intense discussion on many aspects of this exciting new research area. Visit <http://www.scp.wayne.edu> for more information.**

Dr. Hase believes the Institute has the potential of achieving recognition as a Center by the National Institutes of Health. And, in time, it has the potential to raise the profile of Wayne State as a research university.

"I view my role as someone who is going to lead teams of people from different departments who are submitting research proposals and try to facilitate development of new training programs. Wayne has a number of fine computational scientists."

"I want Wayne to be a great university."

## CMMG Appoints New Graduate Officer

David D. Womble, Ph.D., has been appointed Graduate Officer of the Center's Graduate Training Program in Molecular Biology and Genetics, announced George Grunberger, M.D., Professor and Director of CMMG. Dr. Womble replaces Mary Murray, Ph.D., who left the Center this summer.

Dr. Womble is also Director of Bioinformatics for the Center and has recently been named as faculty with the new Wayne State University Institute for Scientific Computing.

A member of the WSU graduate faculty and affiliated with the Center since 1991, Dr. Womble received his doctorate in Biochemistry from the University of Wisconsin, Madison. He was a postdoctoral research associate and

NIH postdoctoral trainee in the Laboratory of Molecular Biology at Wisconsin.

Dr. Womble's primary research interests include regulation of DNA replication and segregation of bacterial antibiotic resistance plasmids, and the coordination of those events with the cell division cycle. In addition to his educational and scientific endeavors, Dr. Womble is an editor of *Advances* and previously was manager of Web-Based Research and Education Services for the WSU School of Medicine.

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This newsletter is edited by:

**Anne E. Greb, M.S.**

313-577-6298

agreb@cmb.biosci.wayne.edu

**David D. Womble, Ph.D.**

313-577-2374

dwomble@cmb.biosci.wayne.edu

The online version of the newsletter and other information about CMMG are available at the CMMG Web site: <http://cmmg.biosci.wayne.edu>

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Center for  
Molecular Medicine  
& Genetics

Wayne State University School of  
Medicine  
3216 Scott Hall  
540 East Canfield  
Detroit, MI 48201  
313-577-5323  
cmmg@cmb.biosci.wayne.edu  
cmmg.biosci.wayne.edu

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