Argonne NATIONAL LABORATORY

Update

FALL 2006

The Community Newsletter of Argonne National Laboratory

UChicago Argonne, LLC wins management contract

THE Department of Energy has announced that UChicago Argonne, LLC has been awarded the contract to manage Argonne.

The UChicago Argonne, LLC brings together the expertise and experience of The University of Chicago, the sole member of the LLC, with Jacobs Engineering Group, Inc. and BWX Technologies.

UChicago Argonne, LLC is designed to combine the finest scientific leadership with best-practice management methods in order to support innovation and discovery at Argonne that serves the national interest. The University of Chicago is the sole member of the UChicago Argonne, LLC.

"The university's open-minded approach and strong intellectual traditions have fostered an effective and symbiotic relationship that will produce future scientific dividends," said Argonne Director Robert Rosner. "This new team will combine individual strengths to forge a unique and powerful partnership on behalf of the DOE and the nation."

The University of Chicago's new partnership with Jacobs Engineering and BWXT strengthens the university's leadership by bringing outstanding resources to laboratory management. Jacobs Engineering is one of the world's largest and most diverse providers of technical, professional and construction services globally. BWXT is the nation's premier manager of complex, laboratory-owned facilities recognized as a model by the DOE.

UChicago Argonne, LLC is the entity created by the university to be solely responsible for the management of Argonne. The University of Chicago has managed Argonne since 1946. Beginning Oct. 1, 2006, the laboratory will be operated by the LLC together with team members Jacobs Engineering Group Inc. and BWXT Technologies Inc.

UChicago Argonne, LLC will manage the laboratory through its Board of Governors, which consists of leaders in science and technology from industry and universities including the presidents of The University of Chicago, Northwestern University and the University of Illinois. The board's Science Policy Council, which provides strategic and scientific advice, consists of the vice presidents for research of the University of Chicago and Northwestern University, the vice chancellors for research at the University of Illinois at Champaign-Urbana and the University of Illinois at Chicago, and the director and the chief scientist of Argonne. ■

CONTRACT SIGNING

The U.S. Department of Energy (DOE) announced July 31 that a new team assembled by The University of Chicago — UChicago Argonne, LLC — has been selected to manage Argonne. Signing the contract are Thomas F. Rosenbaum, CEO of UChicago Argonne, LLC and vice president for Research and Argonne National Laboratory, and Sergio Martinez, contracting officer for DOE's Argonne Site Office. In the back row are Deputy Laboratory Director Don Joyce, Argonne Director and UChicago Argonne, LLC President Robert Rosner, and Argonne Site Office Manager Robert Wunderlich. *Photo by George Joch.*

World-class science to continue

ROBERT ROSNER, ARGONNE DIRECTOR

IT goes without saying that I am enormously delighted by the U.S. Department of Energy's decision to extend its longtime association with The University of Chicago through the Argonne management contract. The association has many benefits. First, of course, is my firm belief that this decision will ensure the laboratory's continued central role in supporting DOE's missions, advancing the national economic and energy security of the U.S. through promotion of first-rate scientific and technological innovation. Beyond this, there are numerous opportunities for both Argonne and the university to benefit from our continued relationship, and the university's continued management of the lab. We have been laying plans for developing joint programs, for joint appointments, for student experiences and for sharing infrastructure. Moreover, with our new industrial partners, BWXT and Jacobs Engineering and the university's new academic partners — Northwestern University and University of Illinois — I look forward to building on past excellence in research and operations, and renewing the laboratory in order to meet the great challenges of the 21st Century, from understanding the fundamentals of space, time and matter, the origins, structure and evolution of our universe, to the more practical needs of understanding the properties of matter on the atomic and molecular scales, and ultimately meeting the enormous challenge of how to supply the energy needs of our nation in the coming century.

As Argonne celebrates its 60th anniversary, the announcement by DOE emphasizes that Argonne will continue to provide world-class multidisciplinary researchers in energy sciences, physical sciences, biosciences and computational sciences with an environment of open collaboration with state-of-the-art facilities that will result in the brighter ideas for tomorrow. ■

ARGONNE OPEN HOUSE
OCTOBER 7, 2006
9 AM – 4:30 PM
www.anl.gov

Nanotube building blocks may lead to advanced electronics

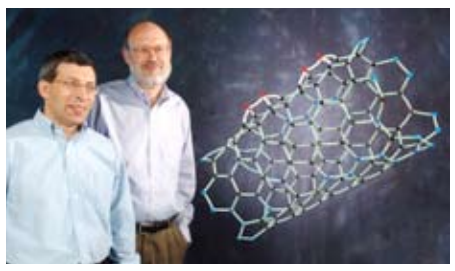
EVELYN BROWN

A new method to systematically modify the structure of single-walled carbon nanotubes could expand their electronic properties and open the path to nano-electronics.

Carbon cylinders a few billionths of a meter in diameter and a few microns long, these nanotubes are one of the strongest structures known and have unique electrical and thermal properties.

This promising method to add defects to carbon nanotube walls was developed by Argonne researchers who are interested in improving the materials for thermoelectric power generation, the use of heat differences to generate electricity. Thermoelectric conversion is the principle behind thermocouples, thermal diodes and solid-state refrigerators.

"If you change the electronic structure," said Argonne chemist Larry Curtiss, "by adding defects in an ordered way, theoretically you can make more efficient thermoelectric materials. So we could produce electricity more efficiently from solar, nuclear or any thermal power generation." Curtiss is group leader of the Molecular Materials Group in Argonne's Materials Science Division.

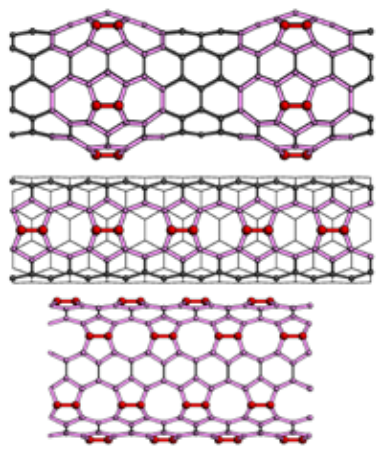


Peter Zapol (left) and Larry Curtiss with a model of the zipper nanotube.

One dimer at a time

Creating defects by adding molecules to nanotubes is challenging because of their extremely small size. Researchers are seeking a controlled, reproducible method. So the Argonne team, which includes Curtiss, Michael Sternberg, Peter Zapol, Dieter Gruen, Gary Kedziora, David Horner and Paul Redfern, used computer simulation tools to learn how to add a single carbon dimer — a molecule of two bonded carbons — to a single-walled carbon nanotube. After they understood how to add one dimer, the researchers began to add dimers in patterns.

The "zipper" structure particularly appeals to Argonne researchers because the atomic spacings in the



Nanotube designs include (from top) "bumpy," "zipper" and "multiple zipper."

openings are just the right size to bond nanotubes to Ultrananocrystalline™ diamond and combine the properties of both. Ultrananocrystalline diamond is a novel form of nanocarbon developed by Argonne that has many of the properties of diamond and can be deposited on a variety of surfaces. Unlike diamond, its properties can be optimized depending on the application.

This research was funded by DOE's Office of Science, Office of Basic Energy Sciences' Division of Materials Sciences and Engineering. ■

Visionary projects receive time on Blue Gene/L supercomputers

BY DONNA JONES PELKIE

COMPUTING projects ranging from understanding Parkinson's disease to modeling climate change have been awarded large amounts of joint time on Blue Gene/L computer systems at Argonne and IBM's T.J. Watson Research Center in Yorktown Heights, N.Y. The computer time is available to researchers through the Department of Energy Office of Science's INCITE program — Innovative and Novel Computational Impact on Theory and Experiment.

"It's good to see the Department of Energy fostering the big ideas, the visionary projects that wouldn't happen otherwise," said Ray Bair, director of the Laboratory Computing Resource Center and Senior Computational Scientist in Argonne's Mathematics and Computer Science Division. "These projects are ones you couldn't approach on a lesser facility. Some of them might even be the wellspring of the next generation for science directions of computation."

Six projects were allocated more than 10 million processor hours through the Argonne and IBM collaboration, ranging from a University of Washington project on high-resolution protein structure prediction to aircraft engine maker Pratt and Whitney's high-fidelity simulations of an aircraft engine combustor.

Through this collaboration Argonne will provide 10 percent of its Blue Gene/L hours to INCITE, and IBM will provide five percent of BGW's hours to INCITE. The BGW system is the second fastest computer in the world, with a capacity of 91 teraflops — 91 trillion calculations per second.

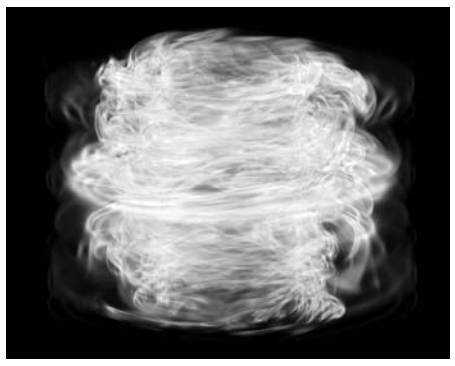
"It's often hard for researchers to get big enough allocations on supercomputers for the most challenging projects," Bair said. "With the extended joint time on the two Blue Gene systems, DOE researchers can attack cutting-edge problems in science and engineering that were previously unfeasible on traditional systems."

A computation needing 500,000 hours could run on 1,000 processors for 500 hours, or about 21 days, he said. Running the same project on a single-processor desktop computer would take about 20 years.

INCITE seeks computationally intensive research projects of large scale that can make high-impact scientific advances through the use of a large allocation of computer time and data storage.

Blue Gene

"Argonne's Mathematics and Computer Science Division," Bair said, "is focusing on petascale computation — creating the tools and applications for addressing the challenges of very large science and engineering problems with computers soon capable of 10^{15} operations per second. Blue Gene has design features that make it especially attractive for computational science. We're evaluating it to see how broadly applicable it is to science and engineering problems."



This visualization of supercomputer data shows a volume rendering of the energy dissipation through the current in the development of magneto-rotational instability, believed to be important in accretion of matter onto a central compact object such as a black hole.

In the past year scientists from across the nation have identified more applications for Blue Gene than originally expected. Such broad applicability indicates that the supercomputer could well become a mainstay for leadership computing.

The Blue Gene/L is the most powerful computer Argonne has ever had. "It's an example of a machine that's opening many doors in science," Bair said. "Of the 100 most powerful computers, 19 are Blue Genes, and of those, one is Argonne's." ■

Local science teacher honored

Mike Kennedy, left, physics teacher at Neuqua Valley High School in Naperville, has received the Ellis P. Steinberg Award for Pre-College Science Teaching. He is pictured with Harold Myron, director of Argonne's Educational Programs. The award, presented by Argonne and Argonne's chapter of Sigma Xi, is given to teachers in the state of Illinois who have shown excellence and innovation in teaching the fundamentals of science. Recipients of this award receive a plaque recognizing their achievements and a monetary award of $500. The Steinberg award commemorates the commitment to excellence in science education exemplified by the late Ellis P. Steinberg who had an illustrious career in nuclear chemistry and was director of Argonne's Chemistry Division from 1982-1988. ■

"It's good to see the Department of Energy fostering the big ideas, the visionary projects that wouldn't happen otherwise."

SAMM TAKES SHAPE

Argonne's Sub-Angstrom Microscopy and Microanalysis (SAMM) facility is beginning to take shape. SAMM, with its four cutting-edge electron microscopes, will be a user facility open to researchers at Argonne and from industry and academia. Its powerful electron microscopes will give researchers atom-scale views of the structure of materials, with a focus on nanoscience. *Photo by Dave Jacqué.*

Combined appeal makes additional donations

THE Argonne Combined Appeal (ACA) steering committee presented one-time donations of $1,000 each to four local agencies. These gifts are made in honor of the laboratory employees who donate to the combined appeal.

The Argonne Combined Appeal is an annual employee contribution campaign supporting more than a dozen charitable organizations.

The donations were presented at a reception attended by the ACA Steering Committee, Argonne Director Robert Rosner, Kelly Mannsfeld, deputy to the laboratory director, as well as the Argonne employees who nominated the agencies to receive the donations.

"I'm really proud that our employees both donate money and volunteer to coordinate this worthwhile effort," Rosner said before presenting the donations. Mannsfeld thanked the agency representatives for the work their organizations do saying, "This is a token of our gratitude."

Agencies that received donations are:

- The American Lung Association of Metropolitan Chicago
- Edward Foundation's Animal Assisted Therapy program, the first and largest "volunteer dog" program in the region (see photo).
- Hinsdale Community Service, which provides interim assistance to people in their service area in need of food, housing assistance, clothing, counseling and other emergency services.
- Helping Hand Rehabilitation Center, which helps persons with disabilities to achieve their highest level of independence through quality programs and services.

"Organizations such as these do tremendous work in our communities," said Joe Kilar (EQO), ACA co-chair. "We are happy to be able to contribute to that work." ■

Argonne Director Robert Rosner shakes hands with Dharma, a member of Edward Foundation's Animal Assisted Therapy Program, the first and largest "volunteer dog" program in the region. The program provides patients with visits from specially trained dogs and their handlers, providing a therapeutic "touch of home." Dharma and representatives of four area agencies were recently presented donations from the Argonne Combined Appeal (ACA). Also pictured are, standing from left, ACA co-chairs Sheila Rossi and Joe Kilar and Kelly Mannsfeld, deputy to the laboratory director. Seated, from left, are Patty Kaplan of the Edward Foundation; Audrey Eisenberg of the American Lung Association of Metropolitan Chicago; Martina Shera of Hinsdale Community Service; and Keith Williams of Helping Hand Rehabilitation Center. *Photo by George Joch*

Argonne NATIONAL LABORATORY

Argonne News Digest is published every other month by the Communications and Public Affairs. Send news items to Editor Dave Jacqué, Building 201, Room 261(C&PA-201). Voice: (630) 252-5582. Fax: (630) 252-5274. E-mail: *info@anl.gov*. Argonne National Laboratory is managed by the University of Chicago for the U.S. Department of Energy. VOL. 12, NO. 2.

Argonne named one of 'Chicago's 101 Best & Brightest'

ARGONNE has been named one of "Chicago's 101 Best & Brightest Companies to Work For" for the second year in a row by the National Association of Business Resources. The award is made even more significant by the organization's decision to recognize only 60 area organizations this year.

Winners are organizations that "work with imagination and conviction to create organizational value and business results through their policies and best practices in human resources management. This distinction is bestowed in honor of an organization's recognition of its employees as its greatest asset."

The categories in which Argonne was judged include communication, community initiatives, compensation and benefits, diversity and multiculturalism, employee education and development, employee engagement and commitment, recognition and retention, recruitment and selection, and work-life balance. Final judging was based on a detailed description of laboratory business practices and the results of an opinion survey issued to a random sample of 250 Argonne employees.

"This recognition from the National Association of Business Resources reaffirms Argonne's commitment to developing strong leadership, supporting a creative and diverse workforce, recruiting, developing and retaining the talent needed to implement the laboratory's programmatic activities and initiatives," said Argonne Human Resources Director Carol Quinn. "Receipt of this award helps confirm the success of the laboratory in its commitment to continue the reputation of Argonne National Laboratory as 'The Employer of Choice.'"

Family-friendly programs

Argonne was also honored by the Chicago Regional Section of the Society of Women Engineers with the society's 9th annual Golden Family Award for "outstanding support of family issues that includes helping employees with the delicate balance between work and family."

The award recognizes the laboratory's management philosophy and the programs and benefits that accommodate the needs of a diverse workforce and ultimately motivate and help retain highly qualified employees. ■

Lab, Purdue join forces to restore NW Indiana natural resources

ARGONNE will help conduct basic and applied research and develop educational programs related to the restoration of natural resources in northwest Indiana under an agreement signed June 27.

The Indiana Department of Environmental Management, Purdue University Calumet and The University of Chicago, which operates Argonne, entered into a cooperative relationship aimed at economic development and environmental restoration of the Grand Calumet River and Indiana Harbor Canal Riparian Site. The agreement is part of the ongoing collaboration between Purdue Calumet, Argonne and the Purdue Calumet Water Institute. ■

WIST diversifies, strengthens lab's workforce

ESTABLISHED in 1990, the Argonne Women in Science and Technology Program (WIST) supports laboratory goals to diversify and strengthen the scientific and technical workforce at Argonne. WIST activities are facilitated by the WIST Program Initiator under the guidance of a ten-member steering committee; however, the program relies heavily on the volunteer support of hundreds of Argonne employees.

WIST program objectives include promoting and supporting recruitment and hiring of female scientific staff at all levels; retention and professional development of female staff; and encouragement of female students to consider careers in science and technology.

"WIST is not about promoting any one type of person," said WIST Program Initiator Kirsten Laurin-Kovitz (NE). "It's about promoting the diversification of the workforce, and anyone who agrees with that mission can and should be a part of it."

One of Laurin-Kovitz's goals for WIST is to become more strongly aligned with The University of Chicago and its women's initiatives. "It could be a powerful partnership for promoting a climate that's good for women and minorities."

A work environment that is good for women and minorities, she said, includes an acknowledgement that individuals have lives outside of work and that everyone's ideas and work are equally valued. Argonne is taking the right steps in this regard, Laurin-Kovitz said, with the issues and recommendations that have been discussed by the lab's Work/Life Balance Committee for example. Argonne received a 2006 Golden Family Award from the Society of Women Engineers in recognition of its facilities, benefits and programs that encourage a balance between work and family life.

Chemist Katie Carrado Gregar, left, talks to students during the 2006 Science Careers in Search of Women Conference. Each year, hundreds of students attend the conference which aims to encourage young women to consider scientific and technical careers. *Photo by George Joch*

Other priorities for WIST include expanding on its highly successful student outreach programs. Next year will be the 20th anniversary of the WIST-sponsored Science Careers in Search of Women conference, which annually brings hundreds of female high school students to the lab to encourage them to consider scientific and technical careers. A follow-up mentoring program has been initiated in conjunction with Science Careers to track the conference's impact. Argonne received a 2005 Department of Energy Equal Employment Opportunity and Diversity Best Practices Award, recognizing the conference as an innovative and outstanding initiative which should serve as a model for other offices nationwide.

Introduce a Girl to Engineering Day, which pairs middle school students with mentors for a day of job shadowing, tours, activities, and presentations on engineering, had a record number of applicants this year and the goal is to increase the number of participants to 100 over the next two years.

Laurin-Kovitz hopes to involve more Argonne employees — both women and men — in these and other outreach efforts to students and to women and minorities. "There's a lot of untapped potential out there," she said. ■

Argonne technologies win 5 R&D 100 Awards

FIVE of the world's top 100 scientific and technological innovations during 2005, as judged by *R&D* Magazine, came from Argonne.

Argonne has been consistently on the R&D 100 Awards list, having won 95 of the honors since the magazine began presenting them in 1964.

This year's winners from Argonne are:

- The world's fastest commercially producible hydrogen sensor, which will be used in cars to detect unsafe levels of hydrogen.
- Anti-scatter grids for X-ray imaging and collimators for nuclear imaging, developed jointly with Creatv MicroTech, Inc.
- Materials resistant to metal dusting degradation, which will be used to make more durable equipment in plants that manufacture hydrogen.
- Multiport dryer technology for the forest industry, which will improve the efficiency of dryers used in paper mills.
- The separative bioreactor for the production and recovery of biobased products, which will enable biobased chemical products to be used in place of petrochemicals. ■

DOE OFFICIAL VISITS MATT

In front of a 30-kW polymer electrolyte fuel-cell stack, Argonne chemist Deborah Myers explains Argonne's fuel-cell research to Alexander "Andy" Karsner, the DOE Assistant Secretary for Energy Efficiency and Renewable Energy (EERE). Assistant Secretary Karsner reviewed the extensive Argonne Transportation programs supported through EERE's FreedomCAR office. *Photo by George Joch.*

PRESCRIBED BURN

Wild geranium (*Geranium maculatum*) grows in the aftermath of a prescribed burn conducted earlier this year on the Argonne site. The laboratory performed several prescribed burns in the northern and southeastern parts of the site as part of its habitat management program. Prescribed burns help to renew the habitat by reducing invasive species, like multiflora rose, asian bittersweet, honeysuckle and buckthorn, which encourages the growth of native species.

Non-Profit Organization
U.S. Postage Paid
LEMONT, IL
PERMIT #87

Argonne NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Update

The Community Newsletter of Argonne National Laboratory

Argonne NATIONAL LABORATORY

FALL 2006

ARGONNE OPEN HOUSE
OCTOBER 7, 2006
9 AM – 4:30 PM

Argonne will celebrate its 60th anniversary by welcoming the public to an Open House Saturday, Oct. 7, from 9 a.m. to 4:30 p.m.

Tours, displays and demonstrations will feature research on energy, environment, chemistry, physics, biology, computing, materials science, transportation and nuclear engineering. The open house is geared to visitors of all ages.

For more details, see the Argonne Web site at **www.anl.gov** or call (630) 252-2525. Argonne is located on Cass Ave., just south of I-55, between Darien and Lemont.

Honors

MATHEMATICIAN RECEIVES INTERNATIONAL HONOR

Leyffer

COMPUTATIONAL mathematician Sven Leyffer received international recognition for two papers he co-authored on techniques for solving problems arising in situations as important to everyday life as air crew scheduling and finding how much power a nuclear reactor can safely produce. Along with Roger Fletcher of the University of Dundee in Scotland and Philippe Toint of the University of Namur in Belgium, Leyffer received the Lagrange Prize in Continuous Optimization at the Society for Industrial and Applied Mathematics' annual meeting in Boston this July.

RESEARCHER WINS PRESTIGIOUS PRESIDENTIAL AWARD

COMPUTATIONAL Scientist Todd Munson has been honored with a Presidential Early Career Award for Scientists and Engineers. These awards are the highest honor the U.S. government bestows on outstanding scientists and engineers beginning their independent careers. Munson is a member of Argonne's Mathematics and Computer Science Division, where he has made significant contributions in the areas of large-scale continuous optimization and nonlinear complementarity problems.

Munson

CHIARIZIA HONORED FOR ACTINIDE SEPARATION WORK

Chiarizia

AN Argonne chemist has been honored at the 30th Actinide Separations Conference in Richland, Washington for his innovative research on processes that can be used to recycle and dispose of nuclear waste. Argonne Chemistry Division Senior Scientist Renato Chiarizia received the Glenn T. Seaborg Actinide Separations Award. The award recognizes a scientist or engineer who develops a new or improved method of recovery, separation and purification of the actinide elements on a laboratory or productions scale; develops new or improved methods for the plant-scale recovery, separation and purification of actinide elements; or conducts basic research that is directly and clearly related to the separation of actinide elements.

Actinides are a series of radioactive elements, which include uranium and plutonium. Separating these elements from fission products and other elements in nuclear fuel has applications such as recycling and storing nuclear fuel.

Chiarizia is the fifth Argonne scientist to receive the award since it was created in 1984.

LARSEN LAUDED FOR CONTRIBUTIONS TO AUTO INNOVATIONS

TOP General Motors Co. executives recognized the extensive contributions of Argonne's Bob Larsen to university student engineering competitions at the closing ceremonies of the 2006 Challenge X Competition, June 8 in Mesa, Ariz.

Larsen has worked with the U.S Department of Energy and U.S. car companies for two decades to provide collegiate competitions that challenge engineering students to develop vehicles with lower emissions and higher fuel efficiency by tapping into their creativity and using next-generation technology.

WANG HONORED FOR 'ENVIRONMENTAL EXCELLENCE IN TRANSPORTATION'

MICHAEL Wang was honored as the runner-up in the "New Methods and Tools" category of the prestigious Society of Automotive Engineers' International Environmental Excellence in Transportation Awards. The awards, established in 2000, recognize individuals who contribute significant innovations to reduce the environmental impact caused by the transportation industry.

Wang, of Argonne's Center for Transportation Research, received the award for his development of Argonne's GREET software tool, which is used to evaluate the energy and emission impacts of advanced vehicle technologies and new fuels. ■

Argonne... "For a brighter future"