

Oak Ridge National Laboratory and Georgia Tech: Productive Collaborations

MARILYN BROWN, BOB MCGRATH, AND DAVID BUCKNALL
GEORGIA INSTITUTE OF TECHNOLOGY

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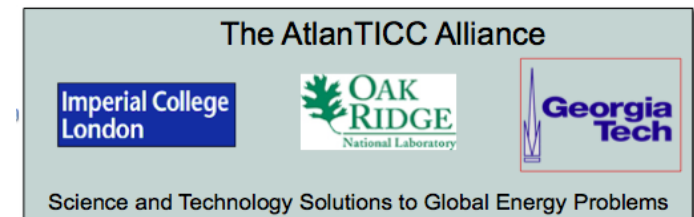
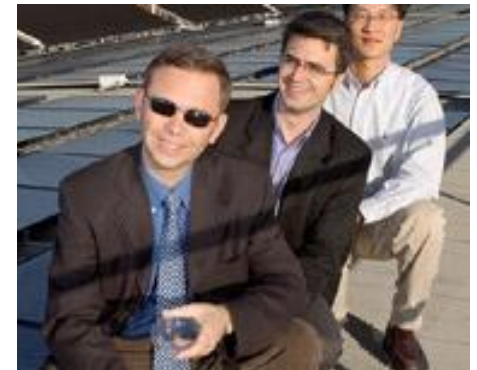


Outline

- Long-Term History of Interactions at all Levels
- Recent history of GT and ORNL contracts
- Researcher collaborations between GT and ORNL:
 - Joint Faculty Appointments
 - Faculty-Student partnerships
 - Postdoctoral Researchers
 - Recent proposals
- Energy Systems Fellowship program
- Collaborative Events

History of Interactions at all Levels

- GT-ORNL interactions have been strong for a decade
- The AtlanTICC Alliance is a past example of such interactions
 - Cross-organizational effort involving GT, ORNL, and the Imperial College of London
 - Involved Jeff Wadsworth (ORNL Lab Director, now President of Battelle Memorial Institute),
 - Also involved Jean-Lou Chameau (GT Provost, now President of Cal Tech), and others
 - ✦ Though the three-way AtlanTICC has ended, bilateral collaborations continue on a project-specific basis

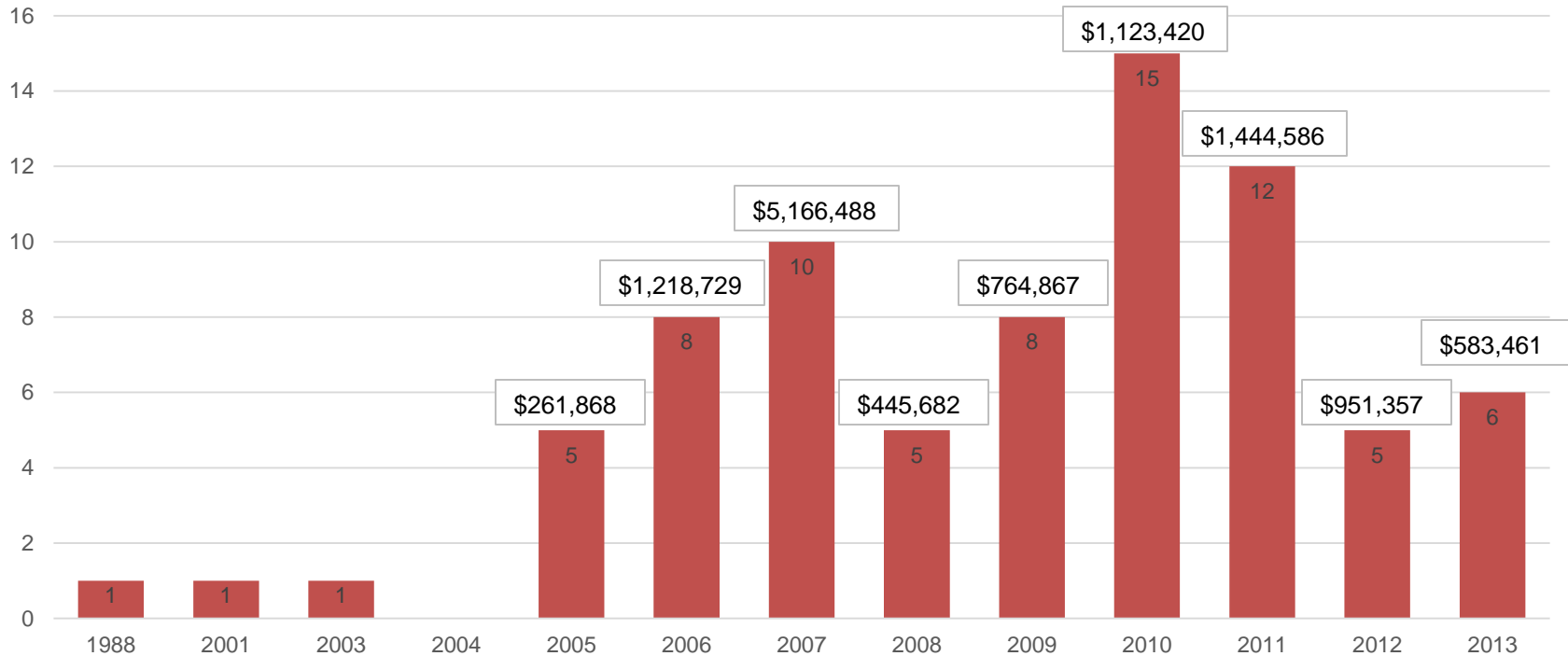


History of Interactions at all Levels

- The AtlanTICC Alliance focused on:
 - Biomass to Bioproducts, Biofuels & Biopower
 - Materials for Energy (Organic Photovoltaics & Microbial Fuel Cells)
 - Enabling Technologies (Computing & Networking)
- Other interactions at the strategic level include
 - GT (Bob McGrath) is a member of the UT-Battelle Board of Governors
 - GT (Marilyn Brown/David Bucknall) serves on the ORNL Core University Liaison Committee

Recent history of GT+ORNL contracts

Number of Projects Started per Year with Total Cumulative Funding for Projects Started in that Year



- Strong history of collaboration between GT and ORNL

GT+ORNL Researcher Collaborations

Joint faculty have developed long-term partnerships and provide a foundation for growing future collaborative research.



- **Joint Faculty Appointments from GaTech to ORNL:**

- ✦ Matt Wolf [Computing and Computational Sciences]
 - Researching adaptive I/O interfaces, metadata-rich data services, and fusion of heterogenous data types
- ✦ Massimo Malagoli [Computing and Computational Sciences]
 - Published in high-molecular-weight polymer brushes and arylamine-based organic light-emitting diodes
- ✦ Sam Graham [Energy & Transportation Sciences]
 - Thermal transport properties in thin films
 - Development of advanced thermal energy storage system



GT+ORNL Researcher Collaborations



Joint Faculty Appointments from GaTech to ORNL:

- ✦ Nolan Hertel [Nuclear and Radiological Engineering]
 - Radiation detection and shielding, neutron spectrometry and dosimetry
- ✦ Glenn Sjoden [Nuclear Security and Isotope Technology Division]
 - Radiation transport, detection, shielding, and integrated systems analysis



Joint Faculty Appointments from ORNL to GaTech:

- ✦ Costas Tsouris [Energy & Transportation Sciences]
 - Chemical separations for energy applications
- ✦ Jeff Vetter [Computing & Computational Sciences]
 - Experimental, high-performance computing systems (PI on Keeneland project)



Keeneland Project Highlights

- Keeneland is a **full-fledged**, important component of the **NSF National XSEDE infrastructure**, serving **100s of scientists**: <https://www.xsede.org/gatech-keeneland>.
- The Keeneland system is located in the **ORNL computer center** to leverage the world-class ORNL facilities, and Keeneland **funds a number of staff members at ORNL**.
- **Seeking an additional supplement from NSF** this fall of ~\$3M in order to upgrade and extend the lifetime of our Keeneland production system, bringing the total funding to ~\$15M.
- Keeneland has served **over 800 users** on KIDS and KFS. This number includes normal users, educational, and training accounts.

Keeneland Highlights for NSF review

- Keeneland has contributed to over **160 publications and reviewed presentations** including articles in Science, Proc. Natl. Acad. Sci, AIAA, Journal of Physical Chemistry, SC, IPDPS, Journal of Computational Physics, SIAM PP, and many others. See the full list at <http://keeneland.gatech.edu/publications>.
- Keeneland has contributed to over **20 tutorials on heterogeneous computing**: <http://keeneland.gatech.edu/tutorials>.
- Our team has collaborated with users, resulting in improvements to a range of scientific applications include areas like **earthquake prediction, phylogenetics, cancer detection, and materials**, as well as computer science advances in **programming models, libraries, and other software**.
- **KFS** is heavily used by our **XSEDE** users; **system utilization** is almost always **above 90%**, and more recently, it is **more than 98%**.
- Our team has handled **over 630 trouble tickets** over the past year.

R&D 100 Award for GT+ORNL project

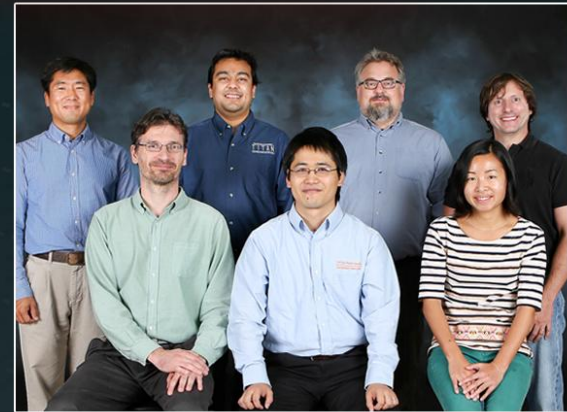


Award Winner

Adaptable I/O System for Big Data (ADIOS)

ADIOS is a portable, scalable, easy-to-use software framework conceived to solve "big data" problems. For scientists making use of high performance computers, ADIOS significantly reduces the input or output complexities typically encountered and reduces the time to solution, so researchers spend less time managing data. The software streamlines workflows and lays the foundation for exascale supercomputers to be able to run multiple tasks simultaneously.

The research was funded by DOE's Oak Ridge Leadership Computing Facility, the Office of Advanced Scientific Computing Research, the Office of Fusion Energy Science, and the National Science Foundation.



The ORNL team consisted of (seated) Norbert Podhorszki, Gary Liu, Yuan Tian; (standing) John Youl Choi, Hasan Abbas, Jeremy Logan, Scott Klasky; and (not pictured) Roselyne Tchoua. Also not pictured are Karsten Schwan and Matthew Wolf (Georgia Institute of Technology), Manish Parashar (Rutgers University), Nagiza Samatova (North Carolina State University), and Jay Lofstead (Sandia National Laboratories).

Team led by Scott Klasky (overall leader, ORNL) and Matthew Wolf (GT leader) selected as an R&D 100 award recipient for the ADIOS data I/O system

GT+ORNL Research Collaborations

Art Ragauskas, a GT Faculty who is currently a visiting ORNL fellow, contributed to the ORNL proposal for the BioEnergy Sciences Center (BESC).

Funding for the BESC was awarded in 2008, and the project is now in its second 5-year term.

- **GT research for BESC focuses on:**
 - –Developing switchgrass and Populus varieties that are more fermentable for biofuel production
 - –Studying novel enzymes for biomass deconstruction
 - –Improving analytical techniques for biomass research
- **Jeff Vetter (ORNL)** is a co-PI on this NSF grant.
- **Marilyn Brown (GT-Public Policy)** serves on the BESC Advisory Committee

GT+ORNL Researcher Collaborations

- **Costas Tsouris (ORNL)** PI on DTRA project and co-PI on DOE projects, investigating:
 - –Post-detonation behavior of radiological debris (DTRA)
 - –Modeling of adsorption processes for off-gas treatment (for the nuclear fuel cycle) (DOE-NEUP)
 - –Renewable hydrogen production from biomass pyrolysis aqueous phase (DOE-EERE)
 - –Capacitive deionization of produced water (DOE-EERE)
- **Vladimir Tsukruk (GT, Material Science)** and his research team collaborate with ORNL for over four years on
 - Spallation Neutron Source (SNS) program with Dr. Anker (ORNL)
 - High Flux Isotope Reactor (HFIR) with Dr. Melnichenko (ORNL)

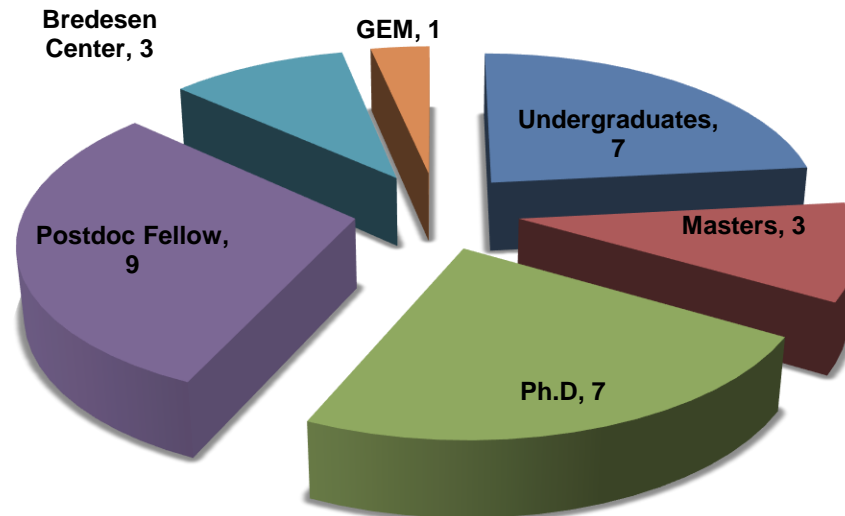
GT+ORNL Researcher Collaborations

- Dr. Jeffrey Vetter [Computing & Computational Sciences] is PI on Georgia Tech's Keeneland Project
 - Supported by the National Science Foundation
 - Keeneland funds 4 full time research scientists at GT in addition to several students and additional faculty members.
- Project includes GT professors Karsten Schwan and Sudha Yalamanchili, plus seven GT grad students

GT+ORNL Faculty-Student Partnerships

- Adewale Odukumaiya (GT-ME) is a GEM fellow (Graduate Degrees for Minorities in Engineering) working with Samuel Graham (GT-ME) and Roderick Jackson in the ORNL Building Technology Program
- The partnership is growing strong

In 2012, 21 students & 9 post-docs conducted research at ORNL



GT+ORNL Faculty-Student Partnerships

- Nolan Hertel's group
 - One Ph.D student was given a fulltime staff position at ORNL, starting early 2013
 - Two Ph.D students did their Ph.D work at ORNL in the past 2 years
 - One Ph.D student is funded through the safeguards program to stay up to 50 days at ORNL over the next 3 years for his Ph.D research
- David Rosen (GT-ME) and Chad Duty (ORNL) had a GT summer student
 - ✦ discussing a broader GT-ORNL faculty/student event to spur further research collaborations.
- Grid Innovation Leaders Fellowship in 2011 included three GT grad students:
 - ✦ Nathan Ainsworth, Alexander Smith, and Dustin Howard

GT+ORNL Faculty-Student Partnerships

- Evan Redd (GT Mechanical Engineering PhD, supervised by Glenn Sjoden) has worked with Dr. Vince Jodoin at ORNL Nuclear Security and Isotope Technology Division (NSITD) in 2013 summer, and will be collaborate again in 2014 summer.
- Glenn Sjoden's "Elements of Nuclear Safeguards, Non-proliferation, and security" class travelled to IAEA and CTBTO in 2013.
 - This trip is made available through collaboration with NGSi and ORNL's Dr. Kim Gilligan and others in the NSIT division.

GT+ORNL Postdoctoral Research

- 70% of ORNL's early career hires have been post-docs
- ORNL hosted nine postdoc fellows from Georgia Tech in 2012
 - 8 under ORNL Postdoc program:
 - 1 under ORNL Advanced Short-Term Research Opportunity (ASTRO) program: Abhijit Joshi

GT Postdocs at ORNL

Name	Doctorate Degree From GT	Affiliation at ORNL
Melanie Kirkham	Materials Science and Engineering	Neutron Sciences
Grady Nunnery	Materials Science and Engineering	Carbon Materials Group Materials Science & Technology Division
Charlotte Kotas	Computer Science	Center for Engineering Science Advanced Research
Alfred Park	Computer Science	Modeling and Simulation Group, Computer Science and Engineering Division
Dinesh Bansal	Mechanical Engineering	Surface Processing and Mechanics Group
Kee Sung Han	Chemical Engineering	Fluid Interface Reactions, Structures and Transport (FIRST) Energy Frontier Research Center
Hui Lin	Geochemistry	Environmental Science Division
Willis Shem	Earth and Atmospheric Sciences	Climate Change Science Institute

GT+ORNL Recent Proposals

- David Rosen (ME) and Chad Duty (ORNL) are working with a broader team that includes Ohio State and Colorado School of Mines on a NSF Engineering Research Center (ERC) proposal in additive manufacturing.
- Glenn Sjoden led as PI for a Consortium for Verification Technologies proposal to NNSA, in collaboration with ORNL
- Glenn Sjoden is working on seed funding proposals with ORNL NSITD members.
- Sotira Yiacoumi (GT) and Costas Tsouris (ORNL-GT) have submitted a proposal the DOE Nuclear Energy University Program.
- Marilyn Brown (GT) and Melissa Lapsa and Roderick Jackson (ORNL) submitted a proposal to the DOE Policy Office on Enhancing the National Energy Modeling System's Capacity for Policy Research.

Energy Systems Fellowship

Apply now for the exciting new
Energy Systems Fellowship!



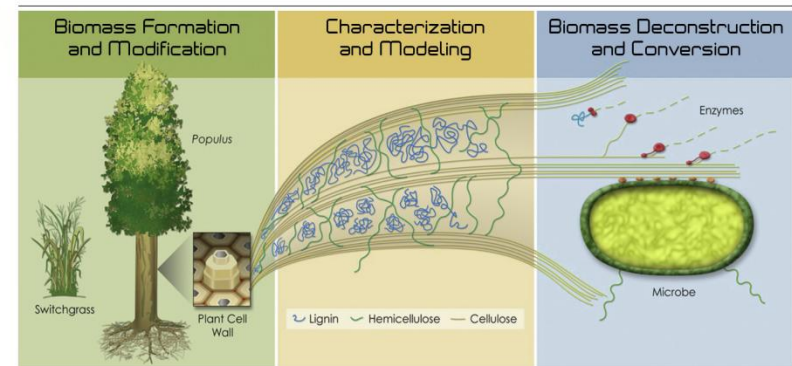
- **Joint-Ph.D. program between GT and ORNL**
- **Started Spring 2013**
- **Two GT Students accepted thus far**
 - ✦ **Nathan Ainsworth**
 - ✦ **Anne Mallow**

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Oak Ridge National Laboratory offers access to world-class research facilities, including:

TITAN, the world's most powerful supercomputer
CDIAC, the Department of Energy's primary climate-change data analysis center
The Spallation Neutron Source and High-Flux Isotope Reactor, two world-class facilities for exploring materials and neutron science
The National Transmission Technology Research Center
The Center for Nanophase Materials Sciences
The Building Technologies Research and Integration Center
BESC, a national center for accelerating cost-effectiveness of biofuels



Energy Systems Fellows will be supported by a generous stipend that recognizes the high caliber of students selected for the fellowship. For the first two years of the fellowship, Energy Systems Fellows will work at Georgia Tech during the Fall and Spring semesters and will participate in summer research programs on-site at the ORNL campus. Subsequent years of the fellowship will involve substantial time at the ORNL campus.

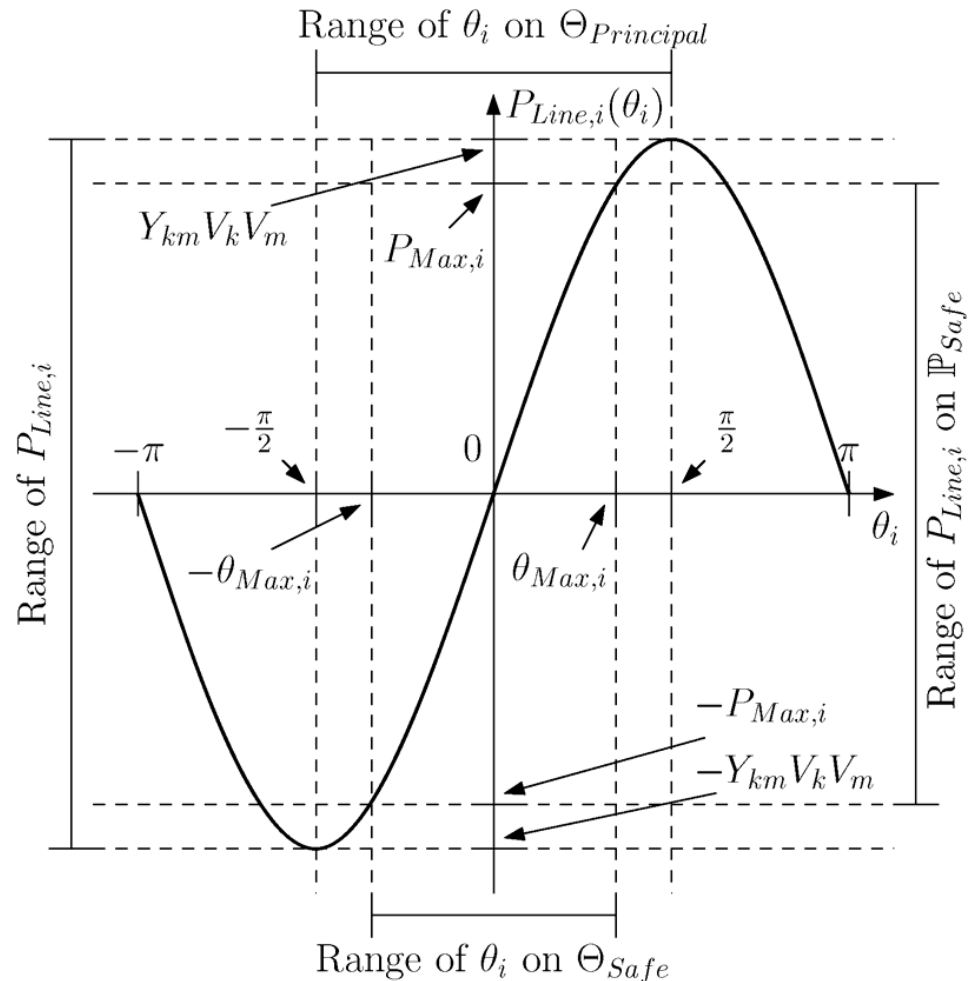
Applications will be reviewed on a first-come, first-served basis. The selection process will be highly competitive, involving interviews by both Georgia Tech and Oak Ridge National Laboratory researchers.



For further information:
david.bucknall@mse.gatech.edu
www.programwebsitehere.edu

Energy Systems Fellowship

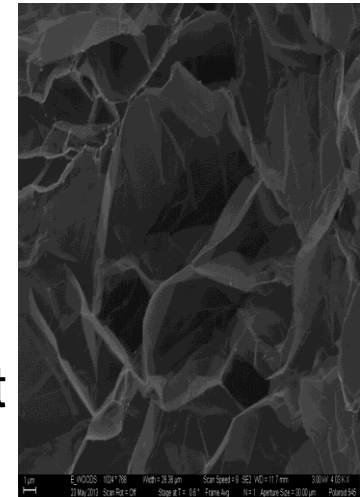
- Nathan Ainsworth
 - Using multi-agent system techniques to develop a Stability Constraint-enforcing Droop (SCED) controller
 - This research contributes to development of ultra-reliable inverter-based microgrids, which allow higher penetration of inverters in traditional utility networks



Energy Systems Fellowship

- Anne Mallow

- Student of Samuel Graham (ME) collaborating with Omar Abdelaziz (ORNL's Building Technology Center)
- Currently focused on the development of aluminum and graphite based energy storage materials
- Continued efforts include the computational analysis of advanced room-temperature thermal energy storage devices with COMSOL and ANSYS FLUENT
- This work supports the development of a stable, cost-effective, non-corrosive, non-toxic latent heat storage system for waste heat recovery



Collaborative Events

ORNL invites Georgia Tech students *to the* **Speed Networking Event**



An opportunity for GaTech students to learn about the GaTech/ORNL graduate research program and to meet potential mentors.

Tuesday, August 21, 2012; 12:00–5:00 p.m.
ORNL Conference Center
(TN Rooms A, B and C)

Introduction by Dr. Thom Mason

Lunch buffet
Speed Networking Session
Poster presentations with hors d'oeuvres

Contact: Bob McGrath, 404.407.8078



- Speed networking event – joint effort between UT Knoxville and GT to network with ORNL
- Coordinated by GTRI's Bob McGrath and Marilyn Brown

Collaborative Events

- GT Energy Club visited ORNL in Spring 2013
 - Coordinated by Ian Anderson (ORNL) and Sofiane Boukhalfa (President of GT Energy Club)
 - Assistance provided by Santiago Grivalja (Energy Club Advisor)
- Eight GT students with research interests in energy fields toured multiple ORNL facilities, including
 - SNS
 - [more details to come]



Collaborative Events

- Novice Workshop on Neutron Scattering
 - Attended by GT's Baratunde Cola (right)
 - Helped develop Cola's proposal for use of the neutron beam line
 - Established key contacts at ARCS neutron beam line



Collaborative Events

Southeast Regional Energy Symposium

Georgia Institute of Technology July 14-15, 2013

A symposium with a focus for

- Georgia Tech undergraduate summer interns and graduate students in energy related fields
- Student residents at other Atlanta area institutions
- Teachers and Faculty from Atlanta area schools interested in the technology-policy interface

Plenary Speakers



Ian S. Anderson
Director, University Partnerships
Oak Ridge National Laboratory



Peter Green
Department Chair
Materials Science and Engineering
University of Michigan



Ken Ostrowski
Director
McKinsey and Company



Esther Takeuchi
Professor
Materials Science and Engineering
and Chemistry
Stony Brook University

Reasons to Attend

- Gain a broader perspective on the energy sector
- Learn about opportunities for energy related studies in graduate school
- Learn about graduate research at Georgia Tech
- Try out interactive demos on energy policy and technology
- Present your research and reach out to potential future graduate students

Poster Session (GT Grad)

- 1st Place: \$250
- 2nd Place: \$150
- 3rd Place (2 prizes): \$50

Abstract Deadline: June 30, 2013

Further Information

Date: July 14-15, 2013

Location: Georgia Institute of Technology

July 14: Klaus Computer Science Building

July 15: Marcus Nanotechnology Building

Website: <http://nesac.gatech.edu/igert-events/gt-seres/>

Register by July 5, 2013



- GT Southeastern Regional Energy Symposium
 - Presenting energy research to REU minority students and students from the metro Atlanta-area Universities
 - Ian Anderson, ORNL Director of Graduate Education, is a key plenary speaker at GT SERES
- Organized by GT's NESAC IGERT – “Nanomaterials for Energy Storage and Conversion Integrated Graduate Education and Research Traineeship”

Collaborative Events



Shreyes Melkote briefing core university representatives during tour of additive manufacturing facilities at GT

- GT hosted Core University Liaison Meeting in May 2013
 - Toured additive manufacturing facilities
 - Discussed ways to expand GT's partnership with ORNL and UT-K on jointly offered energy courses

Summary:

How GT Benefits from Partnering with ORNL

- Opportunity for discovery through expanded interactions with world-class scientists
- Capacity building through exchange of faculty and students in education and research
- Expansion of R&D resources – access to new programs, especially DOE based
- Access to unique, world-class research equipment and cyber-infrastructure-assisted collaboration
- Expanded resources for dissertation research by GT PhD students at ORNL
- Recruitment – joint faculty hires
- Degrees to ORNL employees (GT is second to UT)
- Jobs for GT graduates at ORNL as post docs and full-time employees
- Increased national and international prestige for energy research