Oak Ridge National Laboratory and Georgia Tech: Productive Collaborations

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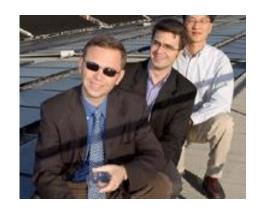
Outline

- History of Interactions at all Levels
- Recent history of GT and ORNL contracts
- o GT&ORNL researcher collaborations:
 - 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 Alliance has ended, bilateral collaborations continue on a project-specific basis

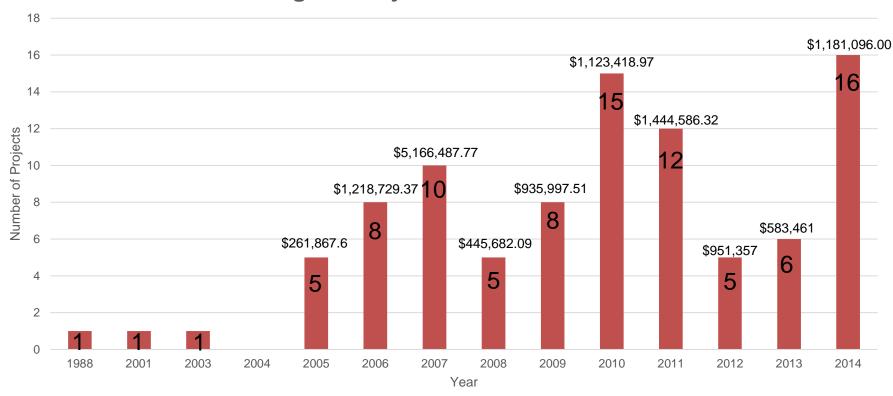






Recent History of GT+ORNL Contracts

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



Strong history of collaboration between GT and ORNL

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 and development of advanced thermal energy storage system



Joint Faculty Appointments from GaTech to ORNL:

- Nolan Hertel [Nuclear and Radiological Engineering]
 - Radiation detection and shielding, radiation protection and dosimetry



- Nazanin Bassiri-Gharb [Micro and Nano Engineering]
 - Ferroelectric thin films and nanostructures: synthesis and characterization; Piezoelectric NEMS/MEMS sensors and actuators



- Comas Haynes [Fuel Cell and Battery Technologies]
 - Modeling steady state and transient behavior of advanced energy systems, thermal management of fuel cells, and the characterization and optimization of novel cycles

Joint Faculty Appointments from ORNL to GaTech:



- Costas Tsouris [Energy & Transportation Sciences]
 - Chemical separations for energy applications



- - 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 GT staff members at ORNL.
- 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.

R&D 100 Award for GT+ORNL project



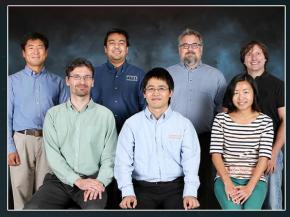
Hward Winner



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 Chol, Hasan Abbasi, 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 Research for Bioenergy Sciences Center 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
- Art Regauskas became a Regents' Professor at UT-ORNL in 2014, after years of work with BESC at Georgia Tech
- Marilyn Brown (GT-Public Policy) serves on the BESC Advisory Committee
- 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

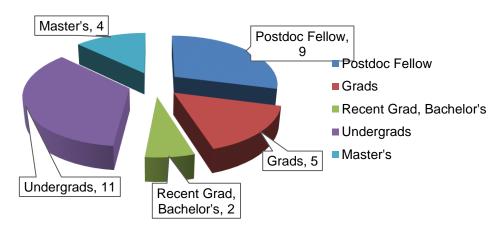
- Nolan Hertel (GT-Nuclear &Radiological Engineering)
 - Acting Director of the Center for Radiation Protection Knowledge
 - Part of ORNL Center for Radiation Protection Knowledge team that is supplying updated radiation dosimetry for the NRC 10CFR20 and 10CFR50 updating.
- Nazanin Bassiri-Gharb recently finished six-month sabbatical at ORNL
 - Studied new ways of exploring phase transitions in ferroelectric materials
 - Explored novel approaches to study the dynamics of ferroelectric materials at nano-, micro- and meso-scale, attempting to separate the domain wall and intrinsic polarization dynamics
 - Probed a new method to process ferroelectrics: an ORNL pulse thermal processing technique that can heat a material up to 600,000 degrees
 Celsius in a second. create ferroelectric materials directly on a polymer substrate, a combination not feasible with other processing techniques.

- Keeneland is a full-fledged, important component of the NSF National XSEDE infrastructure, serving 100s of scientists: https://www.xsede.org/gatech-keeneland.
- 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)
 - Optimizing Polymer-Grafted Amidoxime-based Adsorbents for Uranium Uptake from Seawater (for Fuel Resources) (DOE-NEUP). The GT PI is Sotira Yiacoumi.
- 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 Faculty-Student Partnerships

- Adewale Odukomaiya (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

Research and Event Participants at ORNL in Programs Administered by ORISE, FY2013



Science Education Programs at ORNL

Opportunities

Undergraduates

Recent AS or BS Grads

Graduate Students

Higher Education Research Experience -Entering Freshman

- · Entering college freshman only
- . 2.5+ GPA
- · U.S. high school diploma
- · Duration: 10-week, summer
- U.S. citizen/LPR
- DOE Community
 College Internship (CCI)
- · Community college students only
- . 3.0+ GPA
- Minimum credit hours
- Duration: 10-week, summer
- · U.S. citizen/LPR
- Laboratory Technology Program (Lab Tech)
- · U.S. CRIZEN/LPR
- Minimum credit hours
 Duration: Up to 5 years, depending on academic level
- · U.S. citizen/LPR
- DOE Science Undergraduate Laboratory Internships (SULI)
- Academic status of sophomore or higher
 3.0+ GPA
- 3.0+ GPA
- Duration: 10-week, summer or 16-week, fall or spring
- · U.S. citizen/LPR
- Higher Education Research Experiences (HERE)
- . 2.5+ GPA
- Duration: B-weeks to 52-weeks, limited extensions
- · U.S. citzen/LPR
- Nuclear Engineering Science Laboratory Synthesis (NESLS)
- 3.0+ GPA
- Duration: 10-weeks to 52-weeks
- · No citizenship requirement

DOE Office of Science Graduate Student Research Program (SCGSR)







- · Recent AS or BS graduate
- Duration: Up to 5 years, depending on academic level
- · U.S. citizen/LPR
- · Recent BS graduate
- · 3.0+ GPA prior to graduation
- Duration: 10-week, summer or 16-week, fall or spring
- · U.S. citizen/LPR
- · Recent A5 or B5 graduate
- · 2.5+ GPA prior to graduation
- · Duration: 8-weeks to 52-weeks
- · U.S. citizen/LPR



- Current graduate student
- . 2.5+ GPA
- · Internship or thesis/dissertation research
- Duration: 8-weeks to 52-weeks. Imited extensions.
- · U.S. citizen/LPR
- Current graduate student
 3.0+ GPA
- · Duration: 10-weeks to 52-weeks
- No citizenship requirement
- Graduate student currently pursuing a Ph.D. degree in areas related to Office of Science missions
- For more information, please visit the DOE Office of Science website:

www.science.energy.gov/wdts/scgsr/

Each year, we host over 1,000 educational participants from more than 40 countries to work on cutting-edge research side-by-side with ORNL scientists and engineers at the U.S. Department of Energy's largest science and energy laboratory.

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GT+ORNL Faculty-Student Partnerships

- Nolan Hertel's group
 - 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
 - One M.S. student funded by the ORNL Environmental Science Division (summer intern for last two summers) and will complete her M.S. thesis on the project)
- 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).
- Glenn Sjoden's "Elements of Nuclear Safeguards, Non-proliferation, and security" class travelled to IAEA and CTBTO in 2013.
 - This trip was 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 postdocs

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 before he became chief scientist at Air Force Technical Applications Center
- 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
 - Has graduated with a Ph.D.
 - **★ Anne Mallow**

World Class Science. Big Ideas.

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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

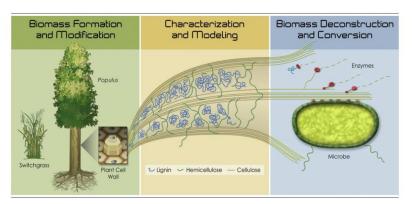
The Spallation Neutron Source and High-Flux Isotope Reactor, two world-class facilities for exploring materials and neutron science

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 End during the Fall and Spring semesters and will participate in summer research programs on-site at the ORNIL campus. Subsequent years of the fellowship will involve substantial time at the ORNIL campus. Subsequent years of the fellowship will involve substantial time at the ORNIL 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

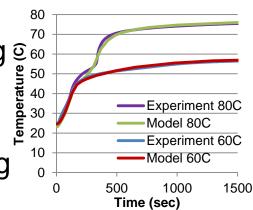
Anne Mallow

 Student of Samuel Graham (ME) collaborating with Omar Abdelaziz (ORNL's Building Technology Center)

 Currently focused on the development of aluminum and graphite based phase change composites for thermal energy storage heat exchangers

O Coupled COMSOL modeling with SolidWorks aluminum foam models to develop a methodology for predicting thermal charging and discharging of various phase change composites

 Next effort will focus on design of air bearing heat exchangers for refrigeration



Aluminum foam model

Example of thermal charging experiment and model



 Speed networking events joint effort between UT Knoxville and GT to network with ORNL

GT Energy Club

- ORNL Deputy Director of Science Ramamoorthy Ramesh was Keynote speaker at Energy Expo in April 2014 at the invitation of the GT Energy Club
- Assistance provided by Shannon Yee (Energy Club Advisor)









- 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





Organized by Georgia Tech's IGERT NESAC Fellows:

Integrated Graduate
Education and Research
Traineeship focusing on
Nanomaterials for Energy
Storage and Conversion

Georgia Tech Southeastern Regional Symposium

 Presenting energy and sustainability-related research to REU minority students and students from universities in the Southeast

Plenary Speakers included:

- Dr. Roderick Jackson, Oak Ridge National Lab
 - Modeling residential energy use behaviors in advanced model homes at ORNL and highlighted the potential of distributed PV.
- Dr. Nancy Jackson, US State Department and Sandia National Lab
 - Discussed how good scientific leadership is manifested through international cooperation
- Dr. Peter Evans, Center for Global Enterprise
 - Focused upon drivers of the future energy systems in the age of gas, big data, & shocks to major infrastructure.



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

Graduate Opportunities ("GO") Program

- ORNL has extended its energy-campus to many top research universities across the southeastern United States including Georgia Tech through the "GO" Program
- Georgia Tech boasts six members of university faculty, eight students, and seven ORNL mentors/TPO through three divisions participating in

the "GO" Program

ORNL Mentor/TPO	Division	University Faculty	Student Name
Bobby Sumpter	CNT for Nanophase Matls Sciences	David Sholl	Hakan Demir
Panchapakesan Ganesh	CNT for Nanophase Matls Sciences	Satish Kumar	Zhequan Yan
Karren More	CNT for Nanophase Matls Sciences	Nazanin Bassiri- Gharb	Jilai Deng
Roderick Jackson	Energy & Transportation Science	Godfried Augenbroe	Michael Street
Roderick Jackson	Energy & Transportation Science	Samuel Graham	Adewale Odukomaiaya
Omar Abdelaziz	Energy & Transportation Science	Samuel Graham	Anne Mallow
Wilson McGinn	Environmental Science Division	Nolan Hertel	Finklea

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 (e.g., the new "GO" program)
- Recruitment joint faculty hires
- Degrees to ORNL employees (GT is second to UT)
- Jobs for GT graduates at ORNL as post docs and fulltime employees
- Increased national and international prestige for energy research