### Oak Ridge National Laboratory and Georgia Tech: Productive Collaborations

#### MARILYN BROWN AND TIM LIEUWEN GEORGIA INSTITUTE OF TECHNOLOGY

September 24, 2015





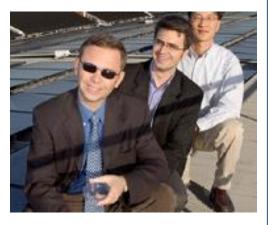
## Outline

- History of Interactions at all Levels
- Recent history of GT and ORNL contracts
- 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 15 years, starting with the AtlanTICC Alliance between GT, ORNL and the Imperial College of London
- Focused on:
  - Biomass to Bioproducts, Biofuels & Biopower
  - Materials for Energy (Organic Photovoltaics & Microbial Fuel Cells)
  - Enabling Technologies (Computing & Networking)

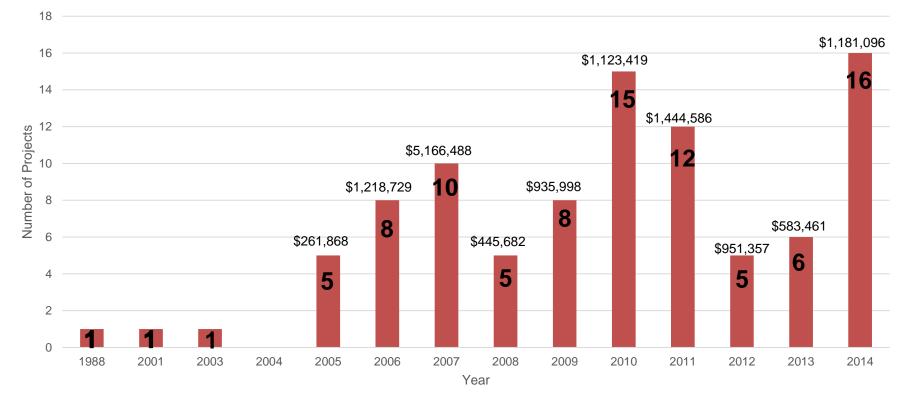






## Recent History of GT+ORNL Contracts

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



Strong history of collaboration between GT and ORNL

- Across the R&D community, the role of the joint faculty continues to grow in prominence and impact
- GT-ORNL Joint faculty have developed long-term partnerships and provide a foundation for growing future collaboration



### Joint Faculty Appointments from GaTech to ORNL:

- × Matthew Wolf [Computing and Computational Sciences]
  - Researching adaptive I/O for exascale systems, metadatarich data services, and fusion of heterogenous data types



- Samuel Graham [Energy & Transportation Sciences]
  - Energy storage and air bearing heat exchangers for thermal energy systems. Two PhD students supported by the GO! Program and a LDRD program.



### Joint Faculty Appointments from GaTech to ORNL:

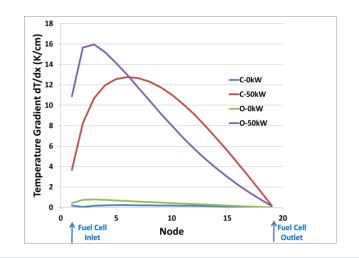
- Nolan Hertel [Nuclear and Radiological Engineering]
  - Radiation detection and shielding, radiation protection and dosimetry



- 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

Summary of Fuel cell test cases (below): Solid temperature gradients for the cases (right)

	LoadFC	LoadT	CA	HA	BA
Nominal	510 kW	50 kW	20%	10%	2%
C-0kW	25 kW	0 kW	0%	2%	2%
C-50kW	562 kW	50kW	0%	2%	2%
O-0kW	25 kW	0 kW	80%	80%	2%
O-50kW	325 kW	50 kW	80%	80%	2%



### Joint Faculty Appointments from ORNL to GaTech:



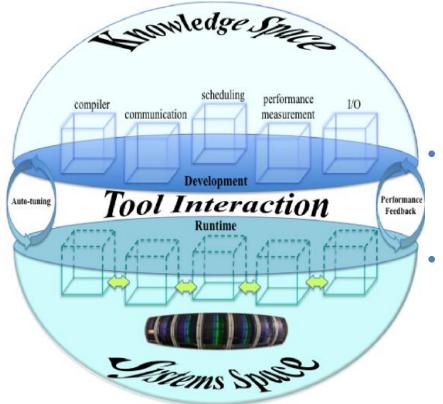
- Costas Tsouris [Energy & Transportation Sciences]
  - Chemical separations for energy applications



- ✓ Jeff Vetter [Computing & Computational Sciences]
  - Experimental, high-performance computing systems (PI on Keeneland project)

# GT+ORNL JF Highlights: Matthew Wolf

 Dr. Wolf has several multi-year joint projects with ORNL and other institutions, and he has several new proposals under development. Georgia Tech students are involved, both in person and using lab resources in collaboration, resulting in joint software releases. Many of these projects have been organized through Wolf's GT lab, Korvo Research





**The MONA(lytics) project** seeks to understand, evaluate, and ultimately, control the online data flows generated by future exascale applications and the analytics processing applied to those flows

The RSVP project seeks to fundamentally address extreme-scale and exascale data management challenges by developing model in which computational data transformation and data analytic services can be easily and efficiently associated with and applied to science data as part of an end-to-end, in situ "process flow."

More details available at korvo.gatech.edu

# R&D 100 Award for GT+ORNL project



Award Minner

#### 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 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).

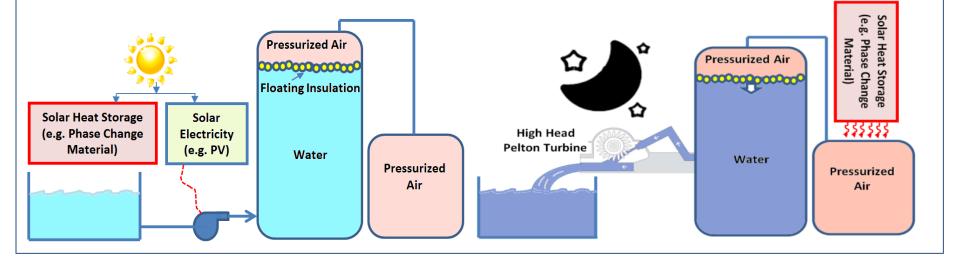
Team led by Scott Klasky (overall leader, ORNL) and Matthew Wolf (GT leader) selected as an R&D 100 award recipient for the ADIOS data I/O system

## Jeff Vetter: Keeneland Project Highlights

- Keeneland project ended in April 2015 after 5.5 years
- Served 942 R&D and education-based users
- Keeneland is a full-fledged, important component of the NSF National XSEDE infrastructure, serving 100s of scientists: <u>https://www.xsede.org/gatech-keeneland</u>.
- 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 <u>367</u> publications, presentations, and software products – see full list at <u>http://keeneland.gatech.edu/publications</u>.

# Sam Graham: GLIDES Energy Storage

- A new method of for energy storage is being developed with ORNL through an LDRD program (GLIDES)
- System stores energy through pressurized fluids that are expanded through turbine to produce energy.
- Models of system have been completed, and all components manufactured.
- 3D printed turbine wheel.
- Currently under assembly at ORNL



### GT Research for Bioenergy Sciences Center focuses on:

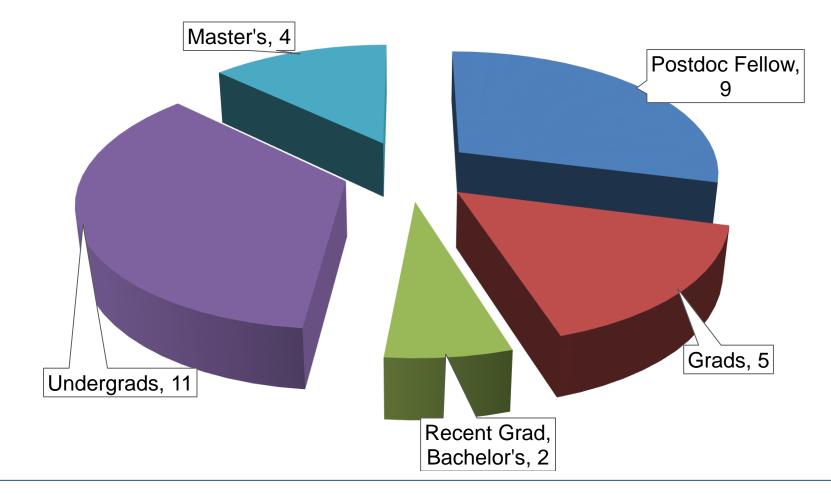
- Developing switchgrass and Populus varieties that are more fermentable for biofuel production
- Studying novel enzymes for biomass deconstruction
- o Improving analytical techniques for biomass research
- Art Ragauskas became a Regents' Professor at UT-ORNL in 2014, after years of work with BESC at Georgia Tech
- Marilyn Brown (GT-Public Policy) serves on the BESC Advisory Committee

- Nolan Hertel (GT-Nuclear & Radiological Engineering)
  - o 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.

- Costas Tsouris (ORNL) PI on DTRA project and co-PI on DOE projects, investigating:
  - "Renewable Hydrogen Production from Biomass Pyrolysis Aqueous Phase".
    - New 3-year project in Fall 2015:
    - o 2 GT faculty, 1 ORNL researcher, 1 ORNL-GT JF
    - Funded by DOE/EERE; includes ORNL, UT, and GT researchers
  - "Sorption Modeling and Verification for Off-Gas Treatment",
    - Current project: 1 GT faculty, 1 GT Ph.D. student, 1 ORNL-GT JF
    - Funded by the DOE Nuclear Energy University Program; includes Syracuse University, ORNL, Georgia Tech, and Prairie View A&M University
  - **o** "Post-Detonation Behavior of Radiological Debris"
    - Current Project: 2 GT faculty, 2 GT Ph.D. students, 1 UT Faculty, 1 ORNL researcher, 1 ORNL-GT JF
    - Funded by DTRA (Defense Threat Reduction Agency); includes GT, ORNL, and UT

## GT+ORNL Faculty-Student Partnerships

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



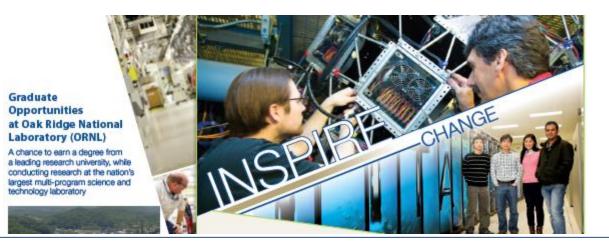
### Science Education Programs at ORNL

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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       • No citizenship requirement	Nuclear Engineering Science Laboratory Synthesis (NESLS)       • 3.0+ GPA         • Duration: 10-weeks to 52-weeks       • Duration: 10- weeks to 52-weeks         • No citizenship requirement       • No citizenship requirement         DOE Office of Science Graduate Student Research Program       • Mean Market Student Strategiese	esearch Experiences	Duration: 8-weeks to 52-weeks, limited extensions	2.5+ GPA prior to graduation     Duration: 8-weeks to 52-weeks	2.5+ GPA     Internship or thesis/dissertation research     Duration: 8-weeks to 52-weeks, limited extensions
DOE Office of Science Graduate Student Research Program	DOE Office of Science Graduate Student Research Program	cience Laboratory	Duration: 10-weeks to 52-weeks		3.0+ GPA     Duration: 10-weeks to 52-weeks
		raduate Student esearch Program	TEOIN LEARNING NORE		For more information, please visit the DOE Office of Science website:

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## 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 faculty, eight students, and seven ORNL mentors participating in the "GO" Program



## GT+ORNL faculty/student affiliation

### Laboratory-directed Research and Development (LDRD) DOE grant

ORNL Mentor/TPO	University Faculty	ORNL Division	Student Name
Panchapakesan Ganesh	David Sholl	Center for Nanophase Material Science	Hakan Demir
Melanie A Mayes	Kostas Konstantindi	Environmental Sciences Division	Eric Johnston
Mina Yoon	Satish Kumar	Center for Nanophase Material Science	Liang Chen
Georgia Tourassi	Jimeng Sun	Computational Science & Engineering	Kunal Malhotra
Panchapakesan Ganesh	Nazanin Bassiri-Gharb	Center for Nanophase Material Science	Jilai Ding
Kurt A Terrani	Bojan Petrovic	Fusion Energy Division	Joseph "Joey" Burns

#### GT+ORNL GO! Program

ORNL Mentor/TPO	University Faculty	ORNL Division	Student Name
Bobby G Sumpter	David Sholl	Center for Nanophase Material Science	Brandon Plaisance
Omar A Abdelaziz	Samuel Graham	Energy & Transportation Science	Anne Mallow
Roderick K Jackson	Samuel Graham	Energy & Transportation Science	Adewale Odukomaiya
Richard W Leggett	Nolan Hertel	Environmental Sciences Division	Lauren Finklea

## Energy Systems Fellowship

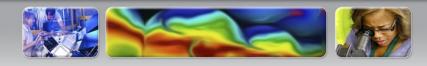
#### Apply now for the exciting new Energy Systems Fellowship!



- Joint-Ph.D. program between GT and ORNL
- Started Spring 2013
- o The first two GT Students:
  - Nathan Ainsworth
    - Has graduated with a Ph.D.
  - × Anne Mallow
    - o Will graduate soon

#### World Class Science. Big Ideas.

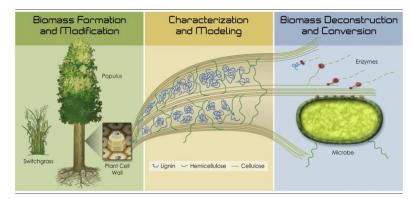
It all starts with YOUR Ph.D.



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

TITAN, the world's most powerful supercomputer

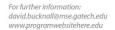
- CDIAC, the Department of Energy's primary climate-change data analysis center
- The Spallation Neutron Source and High-Flux Isotope Reactor, two world-class facilities for exploring materials and neutron science
- The National Transmission Technology Research Center
- The Center for Nanophase Materials 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.

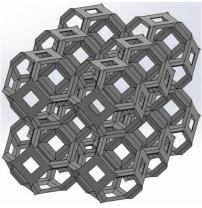




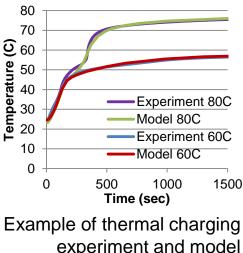
## **Energy Systems Fellowship**

### 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
- Coupled COMSOL modeling with SolidWorks aluminum foam models to develop a methodology for predicting thermal charging <sup>70</sup>/<sub>70</sub> and discharging of various phase change composites
- Next effort will focus on design of air bearing heat exchangers for refrigeration



Aluminum foam model



## 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.
- Adewale Odukomaiya (GT-ME) is a GEM fellow (Graduate Degrees for Minorities in Engineering)

### **GT+ORNL** Postdoctoral Research

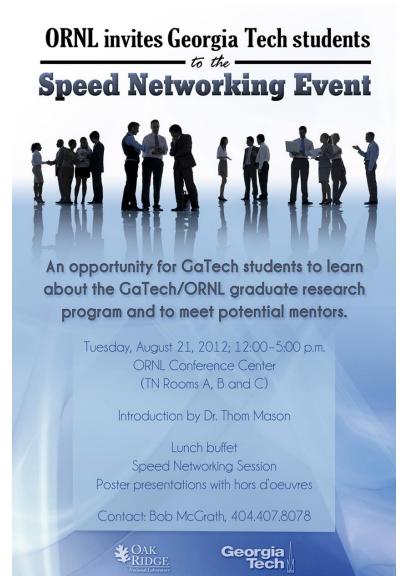
### 70% of ORNL's early career hires have been post-

docs

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.
- 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) have submitted proposals to the DOE Policy Office on Enhancing the National Energy Modeling System's Capacity for Policy Research.



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



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 – Summer 2014

- 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

### 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)









# **Use of ORNL Research Facilities**

- GT is a frequent user of HFIR, SNS, and the National School on Neutron and X-ray Scattering (NXS)
  - 16 users in 21 sessions in 2014.
- 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



### 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

### **University Liaison Committee**



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