IGEP on Computational Tissue Engineering (CTE)

Colleges (5): (i) College of Engineering (COE), (ii) College of Science (COS), (iii) College of Agriculture and Life Sciences (CALS), (iv) College of Veterinary Medicine (VetMed), (v) College of Liberal Arts and Human Sciences (CLAHS)

Departments and Offices (8): (i) Chemical Engineering, (ii) Computer Science, (iii) Biomedical Engineering and Sciences, (iv) Biological Sciences, (v) Biochemistry, (vi) Science and Technology in Society, (vii) Biomedical Sciences & Pathobiology, (viii) Office of Assessment and Evaluation

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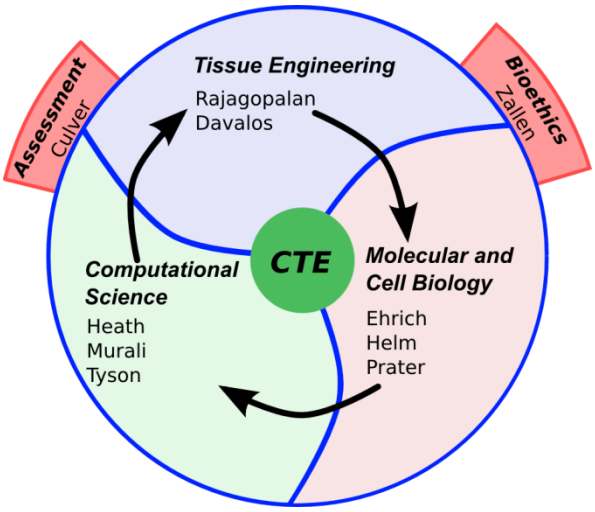
Introduction

Imagine a child with a skin injury who walks into a drugstore to purchase a Band-aid containing cells that will heal the injury. Imagine a patient with a damaged liver not having to wait years for a transplant but having the organ regenerated from his own liver cells. Imagine being able to test the side effects of drugs on artificial tissue cultures *in lieu* of expensive animal testing and complex clinical trials. Such is the promise of the field of tissue engineering [1]. Despite tremendous developments [2], the field requires high-throughput assays and instruments to reduce the cost, time, and complexity; novel biomaterials that support multiple cell types in defined spatial configurations; biochemical assays to monitor the interaction of cells with biomaterials and their environment; and predictive computational models for engineering functional tissues.

Concomitant with the advances in tissue engineering are the genomic revolution of the past two decades and rapid advances in high-throughput experimental techniques in molecular biology [3]. These advances are transforming molecular biology into an increasingly data-driven science, focused on understanding the functioning of the living cell as a complete system. Systems biology approaches have revolutionized the study of cancers and complex human diseases [4].

Scientific goals. So far, the inherently interdisciplinary fields of tissue engineering and systems biology have been developed independently. **The goal of the CTE IGEP is to fruitfully exploit the natural synergy between these two areas to define a new synthesis between tissue engineering and systems biology. We propose to use the computational sciences to drive this synthesis.** In our vision, seamlessly intertwined computational and experimental models will drive the next generation of advances in tissue engineering and in systems biology. Systems biology approaches will underlie predictive computational models of engineered tissues and drive novel experimental analyses of engineered tissues, while the demands of tissue engineering will inspire new experimental methods in systems biology and novel analysis frameworks in computational science.



Educational goals. We will train students at the confluence of tissue engineering, molecular and cell biology, and computational science. **Our vision is that trainees will emerge as the leaders of the new trans-disciplinary field of "Computational Tissue Engineering".** They will be equipped to lead and develop this new field, have the training to span traditional disciplinary boundaries, and to converse in the languages of tissue engineering, molecular and cellular biology, and computational science with ease. These students will be well-equipped to address the current challenges faced by each of these fields. Their future efforts will directly lead to realizing the promises of tissue engineering outlined earlier.

Unique aspects of CTE. Our proposal forges a bond between Virginia Tech's strengths in tissue engineering (School of Biomedical Engineering, Chemical Engineering), systems biology (Genetics, Bioinformatics, and Computational Biology, Biological Sciences, Biochemistry), and Computer Science, creating a partnership that seeks to launch the new field of "Computational Tissue Engineering". Coursework on ethical issues (Science, Technology, and Society) raised by the proposed training and research will enable students to emerge with a holistic understanding of their responsibilities as scientists as well as to their research subjects and to society.

Description

At Virginia Tech, we have the unique opportunity and the capability to realize the promise of fusing tissue engineering, molecular biology, and computer science [5,6]. The founding members of CTE have pioneered several fundamental technologies including layered tissue architectures (Rajagopalan), comprehensive and sensitive molecular profiling (Helm), computational mining and modeling of massive datasets (Murali, Heath, Tyson), microfluidic systems (Davalos), toxicological systems (Ehrich), and animal models of disease (Prater). Our group includes a bioethicist (Zallen) who studies social, ethical, and policy issues arising from advances in genetic technologies. In the future, we will invite other VT faculty with relevant expertise to join CTE and contribute to its intellectual vigor and educational breadth.

Intellectual partnership. CTE scientists have highly complementary expertise and an excellent history of collaboration. A core group (Rajagopalan, Murali, Helm, Prater) are founding members of the ICTAS Center for Systems Biology of Engineered Tissues (ISBET). ISBET officially started in July 2010. Discussions to found ISBET started a year earlier, in July 2009. These deliberations directly led to the conception of the CTE IGEP. Our current funding base of $4.5M (see Appendix) provides a firm foundation for the sustainability of this IGEP. Moreover, the support that ISBET receives every year from ICTAS will provide critical funds for materials and supplies required by CTE trainees in their research. The VT Mass-Spec Incubator, directed by CTE member Helm, receives similar support from the Fralin Life Science Institute.

Intellectual Focus of Graduate Training

CTE students will obtain in-depth training at the nexus of three distinct fields of scientific study. *To illustrate the cognitive outcome to trainees, we highlight hypothetical students, the research questions they want to pursue, and how they can collaborate with and learn from CTE faculty.*

Understand the effects of environmental chemicals on humans. A toxicology Ph.D. student advised by **Ehrich** seeks to understand how chemicals released into the environment may harm humans. Since foreign compounds are first processed by the liver, he/she collaborates with a tissue engineer (**Rajagopalan**) to use her liver mimic to address the question. The student exposes the liver mimic to multiple chemicals to obtain a very rich dataset. He/she collaborates with a computer scientist (**Heath**) to analyze the dataset to determine which chemicals induce similar responses in the liver. The student learns how to exploit bioengineered tissues to answer a question of societal importance. Later, he/she uses this expertise in a position at the Environmental Protection Agency.

Study inter-cellular signaling in liver tissues. An SBES student in **Rajagopalan**'s group desires to study how different types of cells in the liver communicate with each other. He/she has identified a few dozen proteins that play critical roles. The student collaborates with a proteomics specialist (**Helm**) to measure the temporal activities of these proteins. Next, he/she collaborates with a computational biologist (**Tyson**) to build ordinary differential equation models of the activities of and interactions among these proteins. Simulations of these models suggest new experiments that shed more light on intercellular interactions. The student gains experience in interdisciplinary research with cell biologists and computational scientists. After leaving Virginia Tech, the student launches a successful career in using tissue mimics and computational systems biology to probe the mysteries of intercellular signaling.

Discover how cells interact with the extracellular matrix. A student in **Rajagopalan**'s group has developed a novel biomaterial that can influence stem cells differentiation. In order to discover the genes and proteins that control the decision at the cellular level, the student performs experiments using DNA microarrays. The resulting data are too large to analyze manually. Meanwhile, a student in **Murali**'s group is developing a new computational method to summarize precisely such datasets in order to ease their interpretation. The two students collaborate with each other to discover previously unknown control mechanisms in stem cells. They move on to cofound a biotechnology company that specializes in stem cell technology.

Structure of Coursework

Core courses. CTE trainees will share a common core of five courses (15 credits), comprised of three foundational courses in tissue engineering, molecular and cell biology, and computational analysis of biological data, a course on bioethics, and a course on interdisciplinary research:

(a) *Introduction to Regenerative Medicine (BMES 5984*): Offered every spring, the course introduces the fundamental principles of regenerative medicine and the current issues in this field. The course discusses how this field integrates the principles from several fields to develop materials and therapies to repair or replace damaged cells, tissue, and organs.
(b) *Biological Paradigms for Bioinformatics (GBCB 5314)*: Offered every fall, the course is an introduction to the central paradigms of molecular cell biology. It presents material from cell molecular biology and genetics and places these in a genomics context. The course prepares students in mathematical disciplines to interact in teams in the pursuit of bioinformatics research.
(c) *Computational Systems Biology* (CS 5854, **Murali**): Offered every spring, this course covers applications of computational, mathematical, and statistical techniques to the modeling and analysis of molecular interaction networks. It emphasizes interaction between biological and computational disciplines in systems biology through semester-long group research projects.
(d) *Issues in Bioethics* (STS 5444, **Zallen**): Offered every semester, this course provides students with in-depth exposure to ethical, social, and policy issues related to experimentation on humans, animals, and genetically modified microbes. Students who complete this course receive certification, now required by the federal government, from the Virginia Tech Institutional Review Board attesting to their training in human-subjects protections. Short modules drawing on specific CTE issues will be incorporated into this course. For more intensive coverage, additional modules will be developed and presented to CTE students using a workshop format held during non-term time (e.g., during the summer).
(e) *Interdisciplinary Research* (GRAD 5134): CTE faculty will team teach this course every alternate year, starting in year three. In every offering, we will focus on an important social or scientific problem relevant to CTE, e.g., how environmental chemicals are processed by the body and can harm it. In studying this problem, students will learn about toxicology (**Ehrich**) functional tissue mimics (**Rajagopalan**), techniques to expose liver mimics to mixtures of chemicals (**Davalos**), using mass spectrometry to measure cellular responses (**Helm**), and analyzing the resulting large datasets to prioritize new experiments (**Murali**).

Elective courses. Students will take elective courses from one or more of the following tracks (courses listed are illustrative rather than comprehensive):
- **Tissue engineering**: Polymeric Biomaterials (CHE 5214, **Rajagopalan**), Biomedical Eng. & Human Disease (BMES 5024), Fundamentals of Tissue Structure (BMES 5424), Biomedical Microdevices (BMES 5714, **Davalos**)
- **Molecular biology:** Biochemistry for the Life Sciences (BCHM 5124), Computational Cell Biology (GBCB/BIOL/CS 5424, **Tyson**), Molecular Biology of the Cell (BIOL 5884)
- **Computer science:** Algorithms in Bioinformatics (CS 5124, **Heath**), Theory of Algorithms (CS 5114, **Heath/Murali**), Numerical Analysis (CS 5465), Data Mining (CS 6604)

We will fine tune the core and electives for each CTE student, keeping in mind their previous educational training, departmental requirements, and research interests. Ultimately, each student will create a personalized plan of study with advice from advisors and the thesis committee.

Building a CTE community

Steering committee. Rajagopalan (chair), Helm, Murali, Tyson, and Zallen constitute the CTE steering committee. CTE faculty will serve three-year rotating terms. The committee will be charged with strategic planning for the IGEP, evaluating graduate students for support by CTE, and organizing CTE events such as journal clubs and annual workshops.
Recruiting graduate students. Apart from the parent departments of the CTE faculty, we will have access to a strong pool of candidates in inter-disciplinary PhD programs including Genetics, Bioinformatics, and Computational Biology (GBCB), Macromolecular Science and Engineering

(MACR), and the School of Biomedical Engineering and Sciences (SBES). Currently, *CTE investigators mentor about 15 students from these interdisciplinary programs*. **Murali** chairs the GBCB admissions committee, a position that streamlines our access to GBCB students. We will also advertise CTE to students enrolled in the new Systems Biology undergraduate major (***Tyson** chaired and **Murali** was a member of the Task Force that created this major*) and students participating in Scieneering, an interdisciplinary undergraduate studies and research program funded by a Howard Hughes Medical Institute Science Education Grant, (***Rajagopalan** serves on the advisory board of Scieneering*). We also plan to attract students from an *annual undergraduate summer institute* starting in Summer 2012 on Computationally Driven Experimental Biology in Engineered Tissues (organized by **Murali, Helm and Rajagopalan**). We will recruit members of underrepresented groups to CTE in coordination with the Graduate School and various programs at VT (e.g., Initiative to Maximize Student Diversity and the Center for Enhancing Engineering Diversity).

Mentoring and advising students. Right from the outset, we will emphasize CTE's inter-disciplinary nature to every student. We will require that each CTE graduate student be co-advised by two faculty from different departments. Furthermore, we will strive to ensure that at least one other CTE investigator is a member of each student's thesis committee. Such relationships will emerge very organically, as suggested by the examples cited earlier.

Retaining CTE students and promoting *esprit de corps* among them. We will take several steps to inspire a shared sense of responsibility among the CTE trainees and faculty. (i) We will organize a bimonthly journal club as a venue for sharing exciting research results in relevant scientific fields. These meetings will also provide opportunities for practice talks before conferences and defenses. (ii) We will make ample use of on-line tools for close coordination among CTE faculty and students, e.g., the CiteULike website for sharing published literature (already used by the Rajagopalan and Murali groups), and a listserv and a Wiki for communication. (iii) We will organize a monthly seminar series where CTE faculty and invited speakers will address topics such as best practices in research, career development, scientific writing, laboratory management, and grantsmanship. (iv) We will organize an annual day-long student research symposium under the auspices of CTE and ISBET to give CTE students opportunities to showcase their research via presentations.

Criteria for success. We aim to reach a steady state of 15–20 graduate students, with 4–5 students graduating every year. We will measure CTE's success based on the number of publications in which at least two CTE faculty are co-authors, whether such joint publications appear in higher impact factor journals, and the number of collaborative proposals involving at least three CTE faculty. We aim to reach a steady state of 5–10 joint publications and 3–4 joint proposal submissions every year.

Assessment of student training. Dr. Steven Culver, Associate Director, Office of Assessment and Evaluation will direct a formal assessment activity that will focus on the development of professional skills, knowledge, and attitudes in a trans-disciplinary context, specifically to (1) document the extent to which CTE has achieved its goals (summative evaluation) and (2) to collect, analyze, and synthesize data to inform revisions and improvements of project activities (formative evaluation). The use of multiple- and mixed-methods approaches will enhance the strength and rigor of the evaluation [7,8,9]. *Results of these assessments will play an important role in developing the planned IGERT and GAANN applications.* The following examples highlight how assessment will proceed:

- *CTE goal*: The program provides a viable curriculum for students to explore trans-disciplinary subjects. *Measures:* number of students entering the program, persistence rates, times of completion, graduation numbers, post-program follow-up for future career pursuits.
- *CTE goal:* Students will appreciate the impact these distinct fields have on their knowledge base and their research. *Measures:* yearly student interviews and focus groups, yearly student reflective report, reports presented in journal club, interviews with faculty.
- *CTE goal:* Students utilize inter-twined disciplinary resources in their research. *Measures:* yearly student activity reports, yearly student reflective report, student-co-authored paper topics, publication and paper reference lists, dissertations completed and references used.

Appendix

The appendix contains the following sections:

1. Current funding base
2. Plan for securing extramural funding
3. Facilitating graduate fellowship applications
4. Plan to incorporate disciplines
5. References
6. Letters of support

Current funding base. Our current research is supported by $4.5M in funding from the NSF, NIH, and EPA. Below, we only list grants that involve at least two CTE researchers.

1. *ABI Innovation: Bridging the Gap between the Transcriptome and the Proteome to Study Inter-cellular Signaling*, NSF Advances in Bioinformatics, 2011/06/01–2014/05/31, T. M. Murali (PI), Rich Helm (co-PI), Padma Rajagopalan (co-PI), $1,102,995.
2. *Integrating Top-Down and Bottom-up Models in Systems Biology with Application to Cell Cycle Control in Budding Yeast*, NIH/NIGMS, 2011/05/01–2016/04/30, T. M. Murali (PI), John Tyson (co-PI), Jean Peccoud (co-PI), $2,090,932.
3. *Multi-scale Modeling of Toxicant Responses in Engineered Liver Mimics: from Genes, Proteins, and Pathways to Cells and Tissues*, EPA, 2011/05/01–2014/04/30, Padma Rajagopalan (PI), T. M. Murali (co-PI), Marion Ehrich (consultant) $750,000.
4. *Transcriptional signatures of 3D liver mimetic architectures*, NSF Biomedical Engineering, 2009/08/01–2012/07/31, Padma Rajagopalan (PI), T. M. Murali (co-PI), $302,860.

Plan for securing extramural funding. We will target both training grants and research grants.

Training grants: To ensure the sustainability of our IGEP, we will apply for funding from the NSF IGERT, DOE GAANN, and the NIH T32 training grant programs. We anticipate submitting these applications after the second year of the IGEP. We will also encourage students to apply for individual fellowships, as described in the next item.

Research grants: We will also aggressively pursue other funding opportunities for our research. Small-to-medium scale ($500K–$2M) programs that are relevant are the NIH R21 mechanism, the NSF programs in Biomedical engineering, Biomaterials, and Information integration. Larger-scale programs ($2M–$3M) we will apply to include the NSF's Cyber Enabled Discovery and Innovation, the NIH Transformational R01, and the multi-agency Predictive Multiscale Models for Biomedical, Biological, Behavioral, Environmental and Clinical Research. In the longer run (5–10 years), as we cement our collaboration and improve our reputation, we will apply for much larger-scale grants such as NIH Program Projects and NSF Engineering Research Centers. Proposals currently in review include:

- *Spatial and Temporal Inter-Cellular Signaling in Microfluidic Tissue Mimics*, PI: Padma Rajagopalan, co-PIs: Rafael Davalos, Rich Helm, and T. M. Murali, William M. Keck Foundation, 3 years, $1M.
- *Investigating the Effects of Gold Nanoparticles on Hepatic Phenotype using 3D Liver Mimics*, PI: Padma Rajagopalan, co-PI: Renee Prater, NIH/NIDDK, 2 years, $500,000.

Facilitating graduate fellowship applications. To seek additional funding for this project, we will develop processes that will assist graduate students (U.S. citizens and permanent residents) in our groups to apply for national fellowships at the NSF, NIH, DoE, DoD, and the EPA. We will also support CTE students from underrepresented groups to apply for fellowships at the NIH and the Southern Regional Education Board. Since 2010, Murali has coordinated a presentation on fellowship opportunities and a review panel in the Department of Computer Science to give

feedback to students on draft applications to the NSF Graduate Research Fellowships (GRFs). The review panel includes faculty and previous fellowship winners. The success rate in 2010 and 2011 was 50% (4 out of 8). We will offer this program to IGEP graduate students and strongly encourage them to apply in the first year itself. We will recruit reviewers from among the IGEP scientists and our close collaborators. Not only will this initiative augment the pool of students who can participate in the project, it will also expose them to proposal writing early in their graduate careers, thereby preparing them for independent research careers in the future.

Plan to incorporate disciplines and integrate within the proposed curriculum. Right from its inception, CTE will establish strong ties with the social sciences. **First**, the CTE core courses include one on bioethics taught by Zallen. As mentioned in "**Core courses**," Zallen will modify the course to include short modules that drawing on specific CTE issues. Moreover, she will prepare additional modules to be incorporated into an intensive workshop held during non-term time. **Second**, systematic evaluation performed by the Office of Assessment and Evaluation is an integral component of CTE. We plan to use the results of these evaluations (i) to improve and refine our course offerings and graduate experience and (ii) as motivating factors for a future IGERT application on "Computational Tissue Engineering". In the longer term, we will add the following **third** link to the social sciences. We will develop a graduate certificate in CTE. To design the curriculum for this certificate, we will collaborate with curriculum development experts at VT. We have started discussions with Dr. Brenda Brand and Dr. George Glasson, faculty members in the Science Education Program at the School of Education. We expect to start planning the certificate in 2014 or 2015, after we have obtained assessment data from two to three cohorts of graduate students.

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Letters of support (3). (a) COE, COS, CALS, and VetMed, and the Departments of Chemical Engineering, Computer Science, Biomedical Engineering and Sciences, Biological Sciences, Biochemistry, and Biomedical Sciences & Pathobiology; (b) CLAHS and the Dept. of Science in Technology and Society; and (c) ICTAS and the Fralin Life Sciences Institute.

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Karen DePauw, Dean
Graduate School
Virginia Tech
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October 31, 2011

Dear Dean DePauw,

We are writing to express our enthusiastic support and commitment to the IGEP on "Computational Tissue Engineering" proposed by a university-wide team of researchers led by Prof. Padma Rajagopalan. This well-designed program seeks to train graduate students at the confluence of three fields of scientific enquiry: tissue engineering, systems biology, and computer science. By harnessing the rich interplay between these fields, graduate students will be well-equipped to launch the new inter-disciplinary field of "Computational Tissue Engineering", thus paving the way for new developments in engineered replacements for tissues and organs that have been damaged in patients.

The scientists participating in this IGEP come from multiple colleges and departments at Virginia Tech. These researchers have pioneered several approaches that lie at the foundation of the IGEP. They have complementary expertise and a history of successful collaborations. We are very confident that this IGEP will significantly enhance the landscape of inter-disciplinary graduate education at our university.

We affirm our full commitment to this IGEP.

Sincerely,

John Lesko, Associate Dean
College of Engineering

John Walz, Head
Dept. of Chemical Engineering

Barbara Ryder, Head
Dept. of Computer Science

Stefan Duma, Head
School of Biomedical Science and Eng.

Nancy Ross, Associate Dean
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October 18, 2011

Professors P. Rajagopalan and T.M. Murali
Virginia Tech
Blacksburg, VA

Dear Professors Rajagopalan and Murali:

With this letter, we confirm the strong support of the Department of Science and Technology in Society (STS) and the College of Liberal Arts and Human Sciences for your proposed IGEP on "Computational Tissue Engineering".

We are pleased that STS Professor Doris Zallen has agreed to be on the faculty of this innovative interdisciplinary program and that students in the program will be required to take the course that she teaches: STS 5444, Issues in Bioethics. To tailor this course to meet specific educational needs of your students, Zallen is prepared to develop modules that can be incorporated into STS 5444 or that can be used separately in a workshop format. If STS is able to hire another ethicist, one whose interests focus on environmental topics, that individual will also be involved in teaching the STS 5444 course. Thus, your students will be able to explore, in depth, both the medical and environmental implications of their research.

We understand that you will provide the STS graduate program with GTA positions on an as-needed basis should any additional Departmental or College resources be required to support your program (such as offering STS 5444 each semester to meet increased student demand).

The humanistic and social-science components that STS and our College can offer should enrich your curriculum and enhance the overall education of your students. We very much look forward to working with you.

Sincerely,

Ellsworth Fuhrman, Ph.D.
STS Department Chair

Dean Sue Ott Rowlands
College of Liberal Arts and Human Sciences

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Karen DePauw, Dean
Graduate School
Virginia Tech
Blacksburg VA 24061

November 1, 2011

Dear Dean DePauw,

We are delighted to write in support of the IGEP on "Computational Tissue Engineering" (CTE) proposed by a university-wide team of researchers from five colleges and seven departments led by Prof. Padma Rajagopalan. This program will offer an integrated education and research experience at the nexus of three important scientific fields: tissue engineering, systems biology, and computer science. CTE graduate students will learn how to harness the synergies between these fields, thereby obtaining the skills to launch the new inter-disciplinary field of "Computational Tissue Engineering".

As directors of the Institute for Critical Technology and Applied Science and the Fralin Life Science Institute, two interdisciplinary institutes at Virginia Tech, we fully support this IGEP. This IGEP's goal aligns very well with the mission of the Fralin Institute to bring scientists from different disciplines together to solve the most complex challenges in biology. Similarly, ICTAS aims to bring together faculty for interdisciplinary research pursuits. One of ICTAS's research thrusts is in the domain of nano-bio interfaces, which matches the scientific themes of the CTE IGEP.

Both ICTAS and Fralin already work closely with many of the CTE faculty. ICTAS support includes the Center for Systems Biology of Engineered Tissues, directed by Prof. Padma Rajagopalan, who is also leading this IGEP. The Center receives funding from ICTAS every year. ICTAS has also dedicated approximately 1100 sq ft of laboratory and office space for the Center. In addition Prof. Rajagopalan and CTE faculty Prof. Rafael Davalos have their personal laboratory and office space in the ICTAS 1 building. The Fralin Life Science Institute provides materials, supplies, and space for the Virginia Tech Mass-Spec Incubator, directed by CTE faculty Prof. Richard Helm. Taken together, this support from the institutes for office and laboratory space and for equipment, materials, and supplies are important and valuable resources that will be available to CET graduate students for conducting their graduate research.

We have the highest confidence in the scholars involved with this proposal. They truly represent the high caliber of scholarship, research, education, and outreach that our institution should strive to support, nurture, and engage. We trust that you will find this IGEP proposal to be as worthy as we do.

We affirm our full commitment to this IGEP.

Sincerely,

Digitally signed by Roop Mahajan
DN: cn=Roop Mahajan, o=ICTAS, ou, email=mahajanr@vt.edu, c=US
Date: 2011.11.02 11:51:47 -04'00'

Roop Mahajan
Director
Institute for Critical Technology and Applied Science

Dennis Dean
Director
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