

**LIST OF AWARD RECIPIENTS**  
**UB2020 RESEARCH AND DEVELOPMENT ACTIVITIES FUND (IRDF)**

**Corresponding Investigators  
and Co-Investigators  
May 2009**

**“Characterization of Vascular Flow”**

Corresponding Investigator

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Co-Investigator's

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Project Description

Calculation of blood flow patterns in vessels before and after treatment could improve treatment decisions and outcomes. These blood flow patterns can be calculated using computational fluid dynamics (CFD) and the three-dimensional (3D) vessel geometry generated from computed tomography or magnetic resonance imaging. Unfortunately, the time required for the CFD calculations is too long to be used during treatment procedures.

In this project, we will investigate approaches to speed up CFD calculations. The basic idea is that if you have a CFD solution for a similar type of vessel geometry, that CFD solution can be used as a starting point for our CFD calculations to reach a solution more quickly. Thus, we will generate a database containing a variety of vessels with different vessel geometries, various

amounts of narrowings, various branchings, and various aneurysms. For these various vessels, we will obtain CFD solutions for various initial flow conditions. We will then determine the relationships between the vessel parameters and the parameters describing the CFD solutions and store the data in a rapidly searchable database. When patient comes in, the 3D of the vessels of interest will be generated, the vessel parameters will be determined, the database will be searched, similar vessels will be identified, and the CFD solutions will be generated. These solutions will be used to jumpstart the CFD calculations. As the database grows, the identified solutions will be ever closer to the true solution, and so allow ever more rapid convergence to the true solution.

**“A Dynamic approach to strategic market segmentation: an application of data mining techniques”**

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Program Description

Market segmentation is the cornerstone of a customer oriented business strategy which recognizes that customers differ in terms of their preferences and behavior in the marketplace. In today's highly dynamic and competitive market place no single firm can afford to serve all segments or ignore such diversities. The challenge for most businesses is to identify the segments and to evaluate their relative attractiveness and profitability so that marketing strategy may be focused to maximize return for the firms and satisfaction for consumers. Business practitioners currently use various analytical techniques (e.g., clustering algorithms) to identify groups of customers using some form of similarity/dissimilarity measures. However, the reliability and applicability of the above techniques becomes limited since many assumptions need to be imposed for tractability reasons to reliably estimate such models. This results in sub-optimal outcomes for firms and consumers. The data mining tools developed in engineering and sciences (e.g., computer science) offer some of the missing links to understanding the behaviors of consumers in this context. We propose to develop novel, sophisticated algorithms and techniques to successfully classify, estimate, predict, cluster, and more accurately describe the purchase behavior of customers so as to lead to superior managerial decision making using state of the art data mining techniques. We will use a unique data set comprising detailed consumer purchase transactions over multiple years to develop and elaborate on new data mining techniques that will be relevant for business practice. Our large proprietary data sets provide the opportunity to also perform various natural experiments to assess the optimal outcomes. The innovative methodologies that we would develop will be beneficial for industries and business across a wide spectrum and will provide unique insights and advances for many industries including locally based ones.

## **“Toward the first-principles calculation of bulk-phase thermophysical properties”**

### Corresponding Investigator

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### Co-Investigator's

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### Project Description

For many engineering applications it is necessary to know material properties, such as the pressure for given conditions of temperature and density, or the conditions under which a gas will condense into a liquid. It is impossible to measure these properties experimentally at all physical conditions and for all materials of potential interest, so it is important to be able to predict these properties from theoretical considerations. While the means to do this are known in principle, in practice it has not been possible to make such predictions without considerable input from experimental data. Our aim in this work is to address this deficiency. Key to the approach is the need to perform first-principles quantum chemistry calculations for only a few interacting molecules at once, applying the leverage of statistical mechanics to obtain results suitable for bulk phases. The proposed outcome is like no other treatment of fluid properties. Unlike molecular simulation, which typically simulates thousands of mutually interacting atoms to provide properties at a single state point, our aim is to produce an analytic equation of state, which can be easily applied at any physical condition of interest. The underlying methods were developed independently by the project investigators and have a synergy that can produce transformative advances to both fields. The specific aims of this IRDF-funded work are to conduct proof-of-concept calculations using small-molecule systems to show that the idea is sufficiently feasible to justify additional funding to develop applications to broader classes of systems and phenomena

## **“Stress, Depression and Autonomic Dysregulation: Effects on Cardio-Respiratory Function”**

### Corresponding Investigator

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### Co-Investigator's

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### Project Description

Recently Miller and Wood demonstrated that in depressed asthmatic children, stressful emotional states disrupt normal regulation of autonomic nervous system (ANS) processes controlling airway function. IRDF funding will support the combination of clinical science (Miller and Wood, psychiatry) and basic science (Pendergast, physiology) to track down with greater specificity the mechanisms by which this ANS dysregulation takes place. Pendergast investigates cardiovascular/ANS and respiratory psychophysiology under physical stress conditions. His knowledge base and methods will combine with Miller's and Wood's laboratory-based methods of evoking emotional stress to study ANS and respiratory function in pediatric asthma. Depressed and non-depressed adolescents, with and without asthma, aged 14-17, will be studied. The studies will employ the tilt table and exercise stress challenge tests (Pendergast), in addition to a laboratory based emotional film stress (Miller and Wood), to test whether physical stressors evoke the same patterns of ANS dysregulation as emotional stressors. In addition, by comparing groups with and without depression and asthma, the researchers will test whether such patterns are specific to depression, asthma or both. The long term goal of these studies is to elucidate pathways and mechanisms by which ANS dysregulation influences disease processes and translate that information into targeted treatment and prevention approaches.

### **“Children's Stress and Intima Media Thickness”**

#### Corresponding Investigator

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#### Co-Investigator's

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### Project Description

Cardiovascular disease (CVD) is a leading cause of mortality in developed nations. The antecedents of atherosclerosis and CVD occur during childhood, emphasizing the importance of understanding factors associated with the early pathogenesis of CVD. Reactivity to psychological stress is pathogenic for CVD. The carotid artery intima-media thickness (IMT) is a valid index of diffuse subclinical atherosclerosis. Acute cardiovascular reactivity to laboratory stressors and daily real world stress are positively associated with carotid artery IMT and atherosclerosis in adults and children. Individuals who experience the greatest cumulative stress load during daily life are most at risk for developing CVD. Differences in the cardiovascular reactivity of youth to laboratory-based psychological stressors predict blood pressure (BP) responses to daily stress and are stable over time. Thus, youth who have the greatest BP reactivity to laboratory stressors may be most at risk for the pathogenesis of CVD, if they incur much stress during their daily lives. However, the interactive relationships of individual differences in stress reactivity and daily stressors on IMT have not yet been investigated in youth. School transitions, such as those from

middle school to high school result in great amounts of stress. The specific aim of this research is to determine the relationships between individual differences in cardiovascular stress reactivity and the amount of daily stress with longitudinal changes in IMT during the transition from middle school to high school.