

# Supercomputing Institute

## for Advanced Computational Research

a unit of the Office of the Vice President for Research

### Spring 2011 Research Bulletin

Physics and Astronomy

## Simulations of Thermonuclear Supernovae From Very Massive Stars

Understanding the evolution of the first stars in the universe is one of the main frontiers of modern cosmology. The first stars hold the key to understanding the formation of the first heavy elements and the first galaxies in the universe. Current models suggest that the first stars were very massive, with typical masses greater than 100 times the mass of our sun, which suggests that some of them might have died as energetic thermonuclear explosions known as Pair-Instability Supernovae (PSNe).

At the end of their lives, stars with masses of 140–260 solar masses develop a large oxygen core, where high temperatures reach relatively low densities. In

these conditions, photons convert into electron-positron pairs, which reduces the radiative pressure and triggers a rapid contraction of the core. During the contraction, the central temperature and density in-

crease, leading to explosive burning of oxygen and silicon. The energy released by the burning raises the pressure high enough to turn the contraction into an explosion.

By studying PSNe, Professor

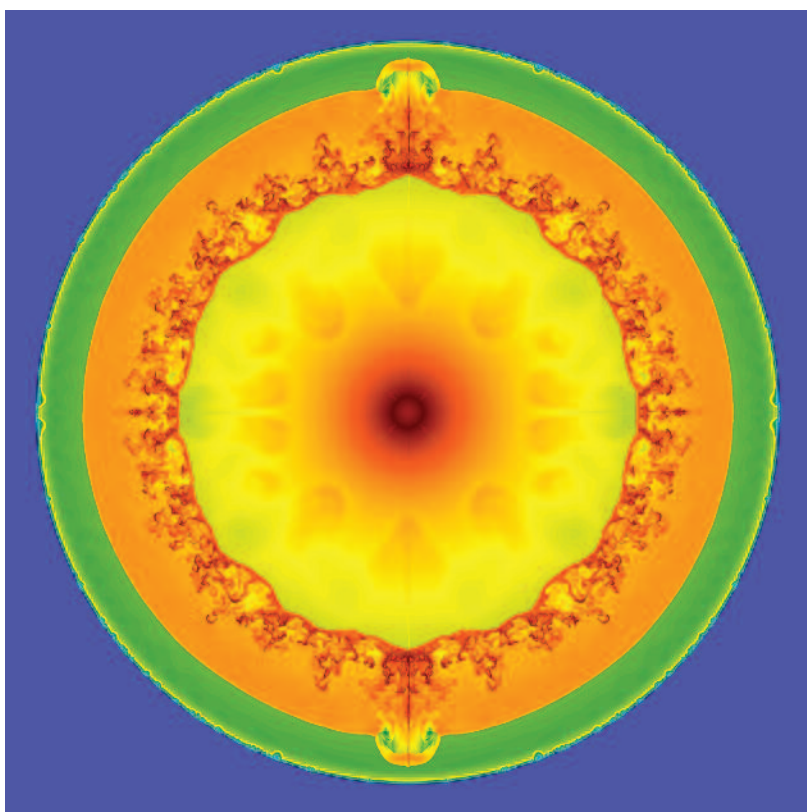


Figure 1. Density snapshot from two-dimensional PSN simulations: Density distribution when the shock is approaching the stellar surface. The strong reverse shock has developed Rayleigh-Taylor instabilities that lead to significant mixing.

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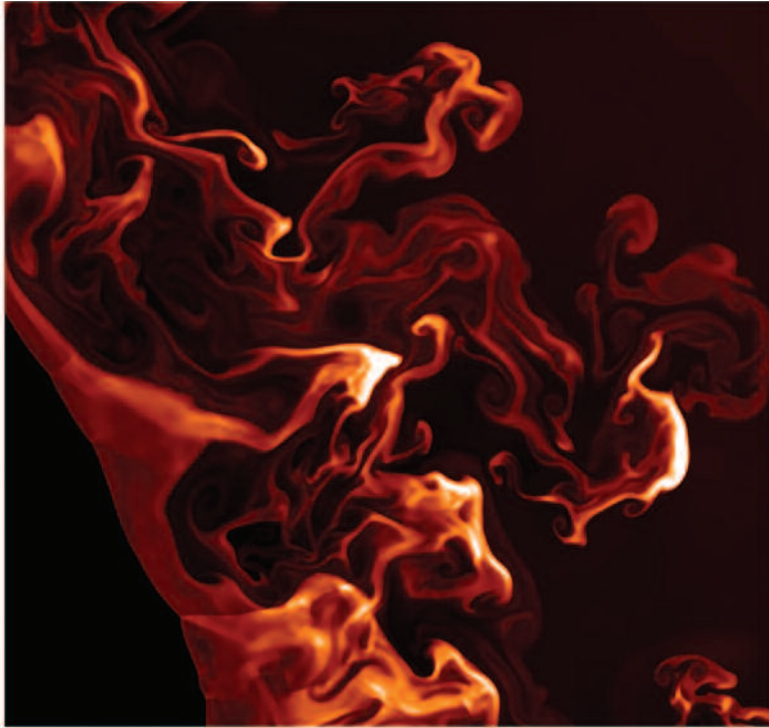


Figure 2: The mixing region: In this zoom-in of the mixing region, the Rayleigh-Taylor fingers have grown into turbulence and formed the vortex patterns.

Alexander Heger of the School of Physics and Astronomy, his graduate student Ke-Jung Chen, and Dr. Ann Almgren of the Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory (Berkeley, California) hope to understand how much energy was released during the explosion, how the first heavy elements were made and what the relative abundances are. Because PSNe usually happen far away from Earth, observational data of PSNe is very rare. So far, few studies of PSNe have been published, and many discrepancies exist between theoretical models and observations. A possible reason may be that most current theoretical models for PSNe are based on one-dimensional calculations. This research investigates PSNe using multidimensional simulations that will lead to a better un-

derstanding of them.

How does one blow up stars in supercomputers? For the sake of computational efficiency, it is first necessary to use one-dimensional calculations to follow a star's evolution until the core starts to collapse. During this period the star is essentially spherical in shape so that a one-dimensional approximation is sufficient. Once the core begins to collapse, the researchers map the one-dimensional profiles onto multidimensional grids where they serve as initial conditions, and follow the evolution until the star explodes. In this stage, multidimensional simulations are essential because, when the star dies in a supernova, the assumption of spherical symmetry of the star breaks down on a large scale due to fluid instabilities generated during the explosion. These instabilities are fundamentally multidimen-

sional.

Large multidimensional calculations require both sophisticated numerical codes and powerful supercomputers. For their simulations, the Heger group uses a code called CASTRO that is being developed at the Lawrence Berkeley National Laboratory. It is a new, massively parallel, multidimensional Eulerian, Adaptive Mesh Refinement (AMR) hydrodynamics code for astrophysical applications. (In AMR, the grid size of simulations is adjusted automatically to enable the use of higher spatial resolution where it is most needed.) They have worked with the code developers to add new physics modules to make it suitable for their simulations. Their calculations include several physics processes, hydrodynamics, gravity, rotation, and nuclear reactions that are very computationally demanding, requiring the use of supercomputers. CASTRO was selected to test MSI's new supercomputer, Itasca, and demonstrated very impressive scaling performance (see Figure 3).

Pair-instability supernovae are powered by purely thermonuclear explosions and can be more easily simulated than the more well-known core-collapse supernovae. After the explosive burning of silicon and oxygen, a large amount of the radioactive nickel isotope  $^{56}\text{Ni}$  is synthesized. It then decays through cobalt ( $^{56}\text{Co}$ ) into iron ( $^{56}\text{Fe}$ ). Because the half-life time of  $^{56}\text{Ni}$  is about seven days, the energy from the  $^{56}\text{Ni}$  decay can power the late-time light curve (the changing brightness of a star with time) of supernovae. At the end of the burning, a strong shock wave is generated that travels out-

ward until it hits the surface. As the shock propagates through the helium and hydrogen envelope, the “snow-plow” in front of the shock slows it down. This sets up a pressure gradient directed outward. In general, the direction of the density gradient points to the center of the star, because the density is larger at the core and smaller at the atmosphere. When the direction of the density gradient is opposite to the pressure gradient, a Rayleigh-Taylor (RT) instability can develop. In this case, the deceleration of material acts like gravity and pulls the matter from higher density into lower density regions. The RT instability is proven to play an important role in different astrophysical mixing processes. In these simulations, one observes that tiny perturbations grow due to the RT instability, leading to significant mixing (Figures 1 and 2). The amount of mixing depends on the stellar structure of pre-supernova models. There is more mixing when the

SN progenitor star is a red supergiant (a very large and luminous star) than when it is a blue supergiant.

The mixing redistributes the elements from their initially spherically symmetric distribution when they are ejected from the supernovae. Some observational quantities are directly affected by the amount of mixing during the explosion. Different elements have different emission and absorption features in the spectrum and changing abundances of those elements can significantly affect the observed spectrum. This is quite relevant for modeling of the PSN candidates observed in the local universe. Also, gamma-ray emission from the decay of  $^{56}\text{Ni}$  may be observed if radioactive  $^{56}\text{Ni}$  was dredged up by mixing at the early stage of explosion. Most important of all, the amount of mixing tells us something about the internal structure of the dying stars. The Heger group is currently calculating both light curves and

spectra from their simulations. This will help them to understand the observational data.

Using modern supercomputers, these researchers have done the most sophisticated multidimensional PSN simulations to date. They have discovered fluid instabilities that occur in multiple spatial dimensions. They have studied how they affect the explosion, dredge-up, and nucleosynthesis of these supernovae as well as possible effects on observations. These models help them to understand the dynamics of PSNe and explain how the first heavy elements in the universe were created. Combining observational results and these simulations can significantly advance the understanding of PSNe. However, PSNe from the first stars are located in the distant universe, which makes them difficult to observe. NASA now is building a new space telescope, the James Webb Space Telescope, which is scheduled to be launched in 2015 ([www.jwst.nasa.gov/](http://www.jwst.nasa.gov/)). These simulations will help to determine what observational signatures to look for then.

The Heger group’s work is supported by the Center for Computational Sciences and Engineering at LBNL (use of CASTRO) and the National Energy Research Scientific Computing Center. Andrea Mehner, Dan Kasen, Adam Burrows, and Stan Woosley also contributed to this article. Funding for this research came from the DOE SciDAC program and the US Department of Energy. A poster about this work was selected as a finalist at the 2010 MSI Research Exhibition (see [www.msi.umn.edu/events/25th/index.html](http://www.msi.umn.edu/events/25th/index.html)).

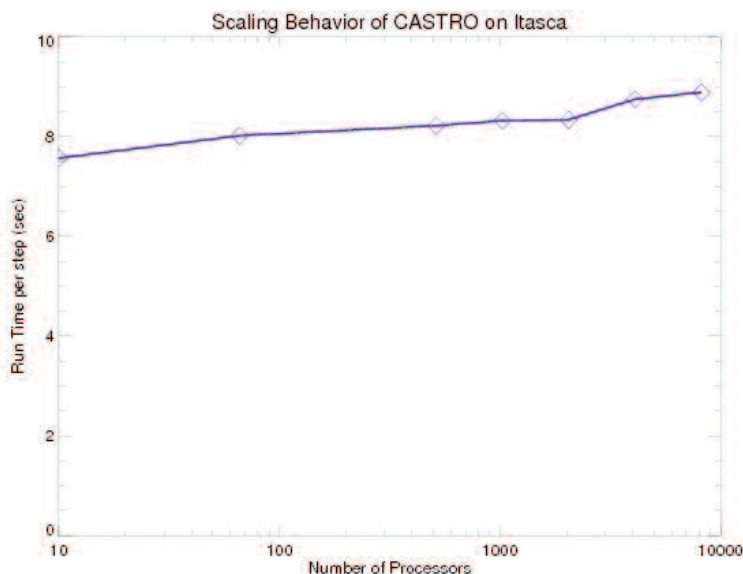


Figure 3: Scaling performance of CASTRO on Itasca. The load of jobs is scaled linearly according to the number of processors. In the case of perfect scaling, the curve would be flat.

# Controlling the Onset of Turbulence by Downstream Traveling Waves

The global energy crisis has increased awareness of the need for renewable energy generation and more efficient transportation means. This motivates research and development of cost-effective wind and tidal energy harvesting as well as fuel-efficient and environmentally friendly vehicles. Understanding and controlling fluid flows plays an important role in all of these applications, and may therefore have critical effects on our economy and environment.

Fluid motion is classified as either laminar or turbulent; flows that are smooth and ordered, lami-

nar, may become complex and disordered, turbulent, as the flow speed increases. This process is known as transition to turbulence. Turbulent flow around cars, airplanes, and ships increases resistance to their motion (drag). For example, about half of the fuel required to maintain the aircraft at cruise conditions is used to overcome the drag force imposed by the turbulent flow. Similarly, in wind farms, turbulence reduces the aerodynamic efficiency of the blades, thereby decreasing the energy capture. In the absence of atmospheric disturbances, flow around an aerodynamically perfect

aircraft wing or wind turbine would remain laminar all the way from the leading edge to the rear. However, disturbances and design imperfections may trigger turbulence (Figure 1). Current practice combines physical intuition with costly numerical simulations and experiments in an attempt to mitigate transition to turbulence. Even though simulations and experiments offer valuable insights into the performance of control strategies, their effectiveness can be significantly enhanced by flow control design based on analytical models and optimization tools.

The research team from the De-

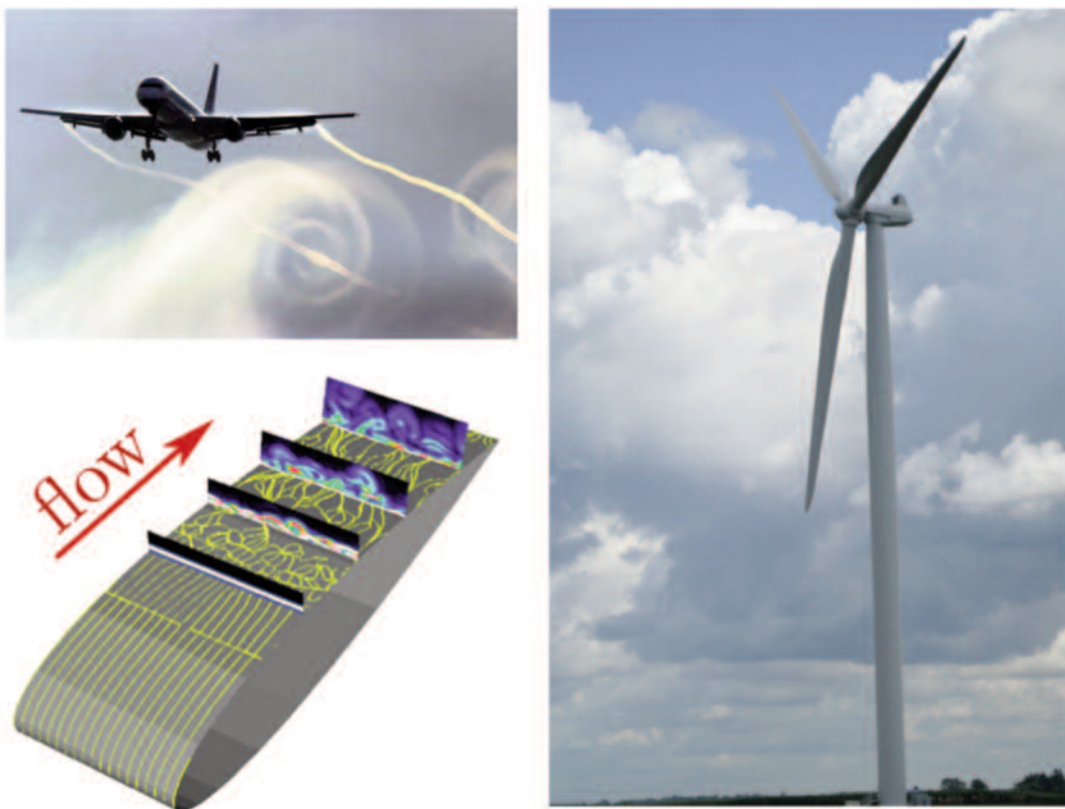


Figure 1. Ordered (laminar) flow around an aircraft wing, or a wind turbine blade, becomes complex and disordered (turbulent) as it moves away from the leading edge. E-fluids photo (bottom left) by Miguel Visbal.

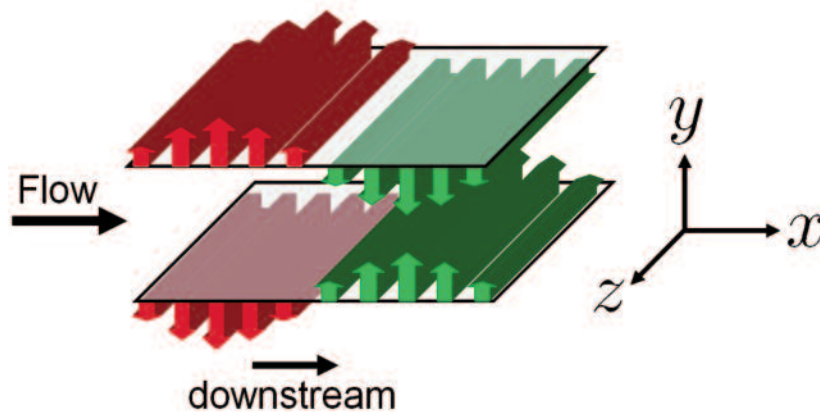


Figure 2. Channel flow with blowing and suction along the walls. Channel flow is commonly used as a benchmark for turbulence suppression studies. In the absence of control, air flows in the downstream direction between two parallel walls. Through wall perforations, control injects (green arrows) and takes out (red arrows) a small quantity of air without introducing additional mass. The actuation is characterized by three design parameters: amplitude, frequency, and speed of the traveling wave.

partment of Electrical and Computer Engineering, led by Professor Mihailo Jovanovic, has developed theory and techniques for sensor-less flow control in order to prevent transition to turbulence. Parallel attempts to control turbulence via surface-mounted arrays of sensors and actuators are often prohibitively expensive as they call for rather sophisticated control mechanisms and information processing. Instead, sensor-less flow control represents a viable and effective alternative with many advantages. Inspiration for this type of control often comes from nature. For example, the skin of sharks is textured with micro-grooves which help them swim with reduced friction. This observation has inspired the development of sharkskin-like surface coatings for drag reduction in vehicles.

In recent *Journal of Fluid Mechanics* papers (vol. 663, November 2010), doctoral students Rashad Moarref and Binh Lieu, together with Professor Jovanovic, have pioneered a model-based approach to sensor-less flow control, where the dynamics are impacted by zero-mean oscillations. Their methodology avoids the need for

expensive numerical simulations and experiments at the early stages of control design. It also facilitates synthesis of superior turbulence suppression strategies compared to what was earlier thought possible.

The methodology has been applied to study the onset of turbulence in a channel flow subject to surface actuation in the form of downstream traveling waves (Figure 2). This study disentangles three distinct effects of blowing and suction on (i) resistance to motion; (ii) cost of control; and (iii) kinetic energy reduction. For small amplitude actuation, a weakly nonlinear analysis was utilized to determine how base-flow is affected, and to assess the resulting cost of control. Sensitivity analysis of the velocity fluctuations around this base-flow was then employed to design the traveling waves. This simulation-free approach reveals that, relative to the flow with no control, the downstream waves with properly designed speed and frequency can significantly reduce high flow sensitivity, making them well-suited for controlling the onset of turbulence. In contrast, the upstream waves increase sensitivity of the velocity fluctuations to disturbances and, consequently,

promote turbulence. The theoretical predictions, obtained by perturbation analysis of the linearized flow equations, have been verified using high-fidelity simulations of the nonlinear flow dynamics. These were conducted using MSI's supercomputing resources and they showed that a positive net efficiency as large as 25% relative to the uncontrolled turbulent flow can be achieved with downstream waves. Furthermore, it was shown that these waves can even re-laminarize turbulent flows. This work has demonstrated that the theory developed for the linearized flow equations with uncertainty has considerable ability to predict full-scale phenomena, and that transition can be inhibited by reducing the tremendous sensitivity of flow dynamics using either active or passive means.

Formulation of the control objective was motivated by recent research showing that high flow sensitivity to disturbances and design imperfections triggers transition to turbulence. For example, surface roughness and free-stream turbulence can introduce departure from laminar flow. The effect of downstream traveling waves on sensitivity is quantified by the energy

$$\begin{aligned} \text{Equation 1: energy amplification} &= \frac{\text{energy of flow with control}}{\text{energy of flow without control}} \\ &= 1 + (\text{wave amplitude})^2 \times g \end{aligned}$$

of velocity fluctuations in stochastically forced flows. For small amplitude actuation, perturbation analysis provided an explicit formula for energy amplification, shown above in Equation 1.

This formula was used to identify the wave frequencies and speeds that reduce flow sensitivity. The plot of the function “g” in Figure 3 reveals the wave parameters that amplify (red regions) or attenuate (blue regions) the most energetic modes of the flow with no control. Further analysis has confirmed that the energy ampli-

fication trends are captured by the second order correction in the wave amplitude. Most notably, all theoretical predictions have been verified using full-scale numerical simulations of the nonlinear flow dynamics (Figure 4, page 7).

The contribution of this work goes beyond the problem of designing transpiration-induced downstream traveling waves. The developed theory and techniques may also find use in designing periodic geometries and waveforms for maintaining the laminar flow or drag reduction in vehicles or

wind turbines. This work suggests that reducing high flow sensitivity represents a viable approach for controlling the onset of turbulence. It also offers a computationally attractive method for determining the energy amplification of flows subject to periodic controls.

Funding for this research came from the National Science Foundation under a CAREER Award and from a 3M Science and Technology Fellowship (to Rashad Moarref).

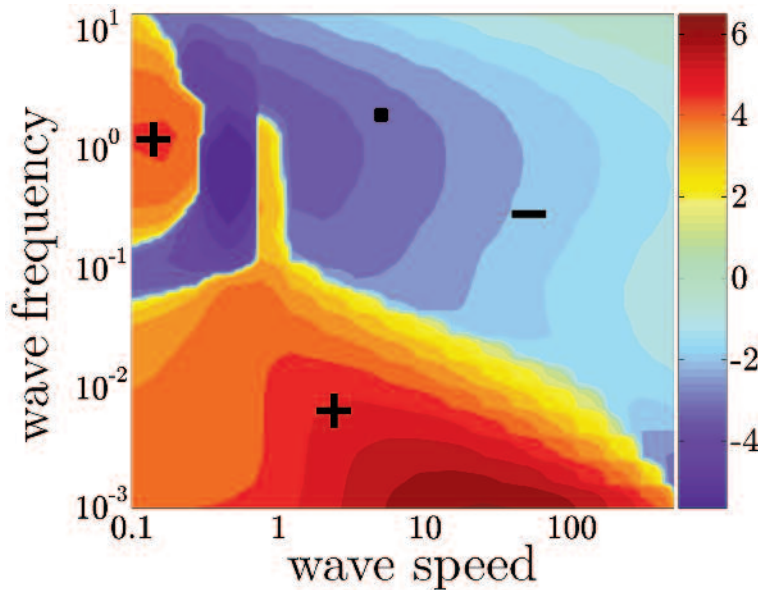


Figure 3. Influence of small amplitude downstream waves on the most energetic modes of the flow with no control is determined by the sign of the function “g”. The Reynolds number (i.e., the ratio of inertial to viscous forces) is set to 2000. The plot is colored using a sign-preserving logarithmic scale. Up to second order in the wave amplitude, the speed and frequency associated with the blue regions reduce the energy amplification. The black square denotes the control parameters that provide a good balance between sensitivity reduction and low cost of control.

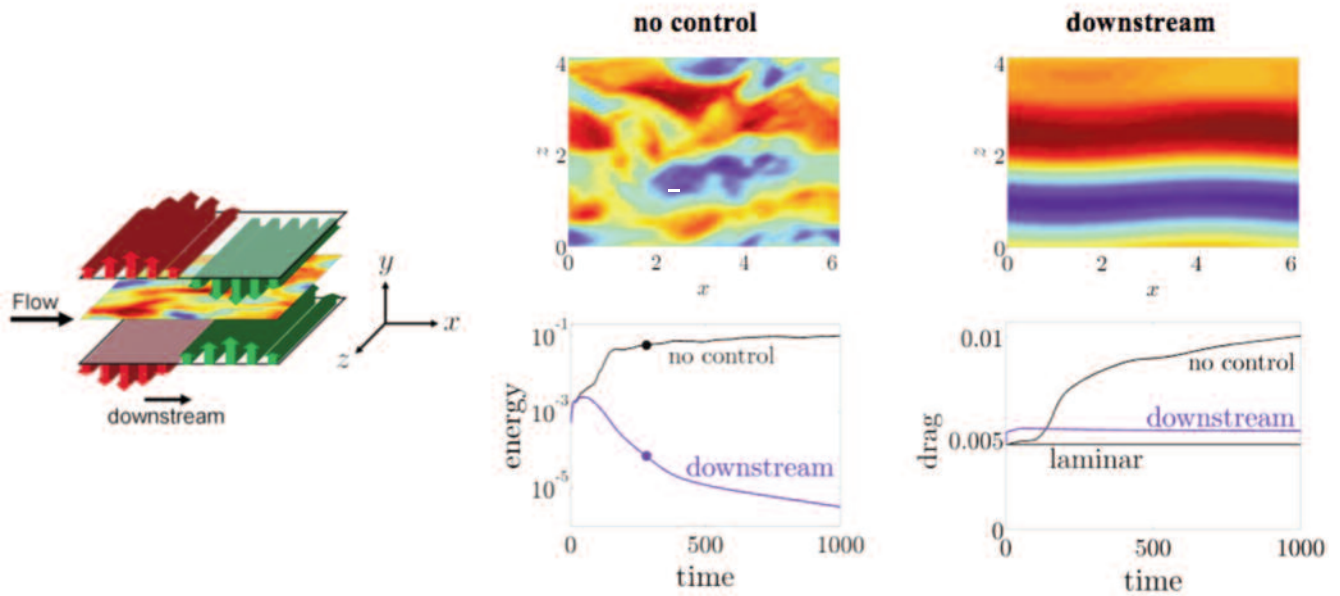


Figure 4. Top row: the stream-wise velocity fluctuations at the channel’s center-plane for the flows with and without control. The uncontrolled flow fluctuations are disordered with a broad range of spatial and temporal scales, and in the controlled flow they are smooth and ordered. Bottom left: the fluctuations’ kinetic energy as a function of time. The downstream waves prevent the flow from becoming turbulent by suppressing growth of energy, while the uncontrolled flow triggers turbulence by promoting growth of energy. Bottom right: the drag coefficient as a function of time. The controlled flow has about 50% less drag than the uncontrolled flow.

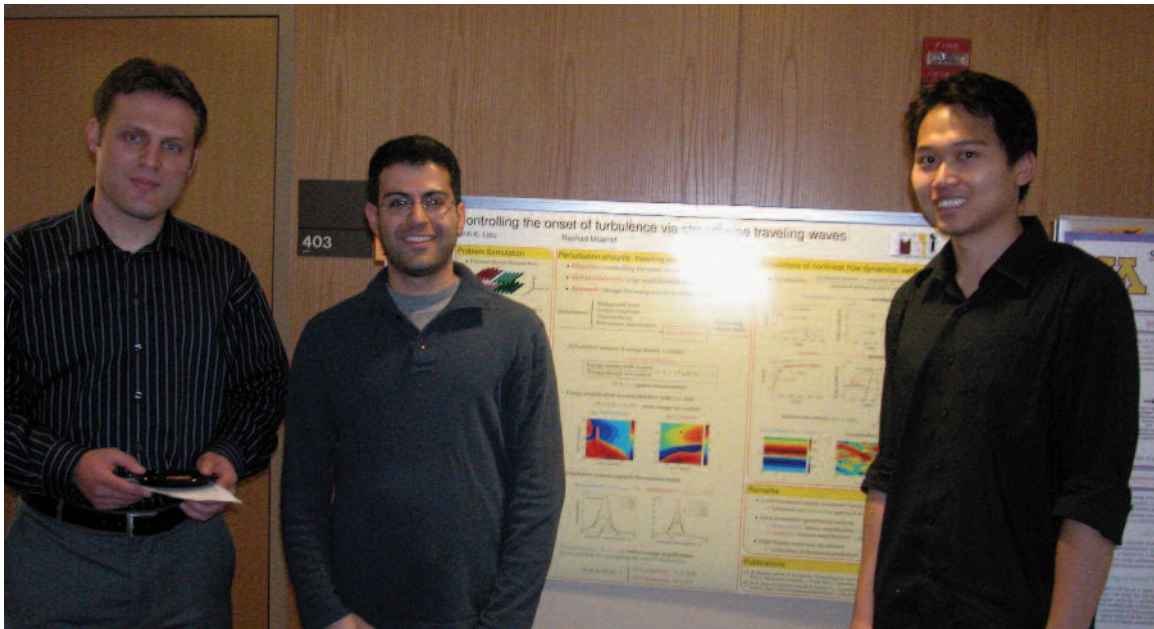


Figure 5. Prof. Mihailo Jovanovic and his graduate students Rashad Moarref and Binh Lieu (from left to right) at the MSI 25th Anniversary Research Exhibition. Their poster, which dealt with the research in this article, was selected as one of the five outstanding posters at the exhibition (see [www.msi.umn.edu/events/25th/index.html](http://www.msi.umn.edu/events/25th/index.html)).

## Galaxy Software Release

**W**ith the support of a Minnesota Partnership Grant, an interdisciplinary team at the University of Minnesota has been actively implementing Galaxy, a framework developed at Penn State and adopted for use at the University of Minnesota, as part of its core life-sciences cyberinfrastructure. Dr. Anne-Françoise Lamblin (below left) is the Project Informatics Lead for the project at the University. The Galaxy adoption team was composed of members from the BioMedical Genomics Center, University of Minnesota

Interdisciplinary Informatics, the Masonic Cancer Center Biostatistics and Bioinformatics Division, and MSI.

Galaxy is an informatics tool that will provide the University's researchers with the necessary integrated environment to access data, run analytical workflows or pipelines, and share information. Urgent needs in genomics research, and more specifically Next Generation Sequencing data analysis and data management, is the initial focus of this installation. Galaxy benefits from a thriving, growing community of adopters

and developers, and its development and enhancement is community-driven.

On February 16, 2011, MSI opened Galaxy for general access by University researchers. Dr. James Taylor from Emory University (below right), a member of the original Galaxy team, gave two workshop presentations on Galaxy and its applications in genomics research.

The Galaxy project website can be found at:

*<https://sites.google.com/a/umn.edu/galaxy-umn/about>*





# Blue Waters Proposal Presentation

**B**lue Waters is a petascale computer currently being built at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. It is expected to be one of the most powerful supercomputers in the world. Blue Waters is funded by the National Science Foundation and the University of Illinois, and

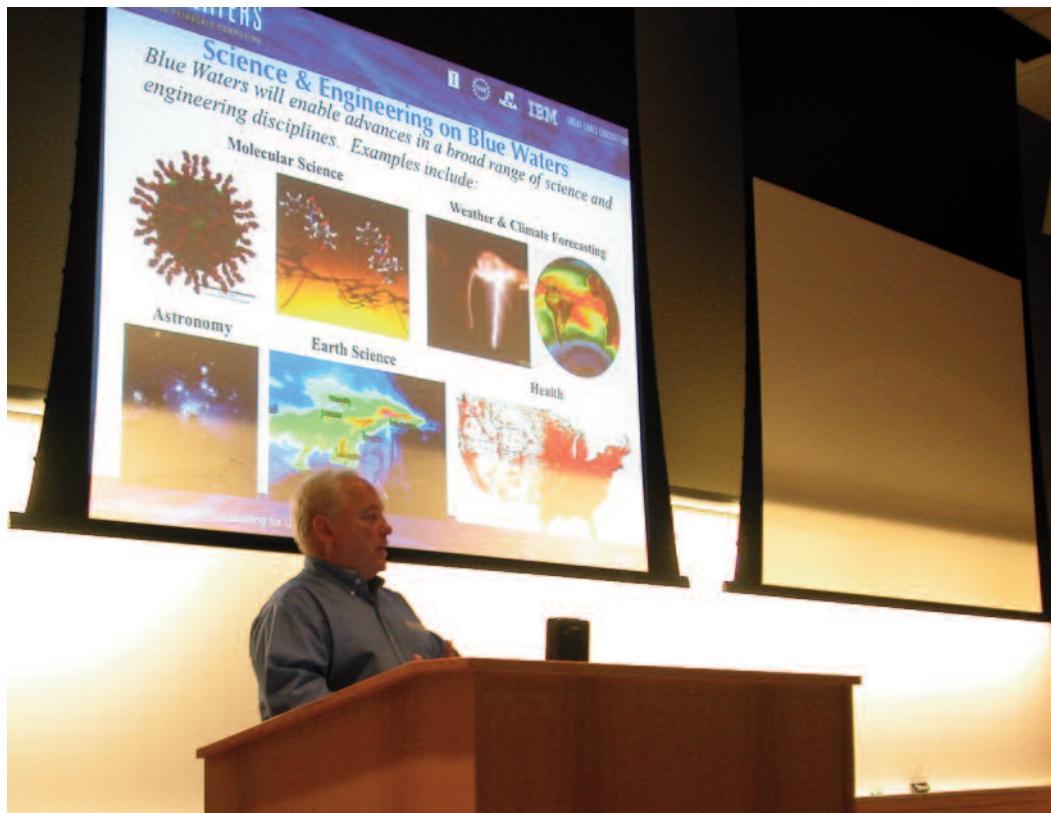
is a joint project of the University of Illinois at Urbana-Champaign, the NCSA, and the Great Lakes Consortium for Petascale Computation, of which MSI is a member.

William Kramer (photo below), Blue Waters Deputy Project Director, NCSA, came to MSI to give a presentation on the Blue Waters architecture and how to submit a successful proposal. The presenta-

tion was held on Friday, February 25, in 402 Walter Library and was attended by approximately 40 MSI researchers.

The Blue Waters website can be found at:

[www.ncsa.illinois.edu/BlueWaters/system.html](http://www.ncsa.illinois.edu/BlueWaters/system.html)



## Aerospace Engineering and Mechanics

- 2010/206  
*Roughness-Induced Transition in High Speed Flows*  
P.S. Iyer, S. Muppidi, and **K. Mahesh**
- 2010/207  
*DNS of Unsteady Shock Boundary Layer Interaction*  
S. Muppidi and **K. Mahesh**

## Animal Science

- 2010/222 and CB 2010-94  
*Development and Application of Bovine and Porcine Oligonucleotide Arrays With Protein-Based Annotation*  
J.R. Garbe, C.G. Elsik, E. Antoniou, J.M. Reecy, K.J. Clark, A. Venkatraman, J.-W. Kim, R.D. Schnabel, C.M. Dickens, R.D. Wolfinger, **S.C. Fahrenkrug**, and J.F. Taylor

## Astronomy

- 2011/4  
*Cluster Turbulence: Simulation Insights*  
**T.W. Jones**, D.H. Porter, D. Ryu, and J. Cho
- 2011/6  
*Radio Galaxy NGC 1265 Unveils the Accretion Shock Onto the Perseus Galaxy Cluster*  
C. Pfrommer and **T.W. Jones**
- 2011/9  
*Synthetic Observations of Simulated AGN Jets: X-ray Cavities*  
P.J. Mendygral, S.M. O'Neill, and **T.W. Jones**
- 2011/24  
*Nonthermal Radiation From Type Ia Supernova Remnants*  
P.P. Edmon, H. Kang, **T.W. Jones**, and R. Ma

## Biochemistry, Molecular Biology, and Biophysics

- 2010/213 and CB 2010-85  
*Functional Importance of Tyrosine 294 and the Catalytic Selectivity for the Bis-Fe(IV) State of MauG Revealed by Replacement of This Axial Heme Ligand With Histidine*  
N. Abu Tarboush, L.M.R. Jensen, M. Feng, H. Tachikawa, **C.M. Wilmot**, and V.L. Davidson
- 2010/214 and CB 2010-86  
*Cloning, Purification, Crystallization and Preliminary X-ray Diffraction of the OleC Protein From Stenotrophomonas Maltophilia Involved in Head-to-Head Hydrocarbon Biosynthesis*  
J.A. Frias, B.R. Goblirsch, **L.P. Wackett**, and **Carrie M. Wilmot**
- 2010/217 and CB 2010-89  
*Mass Spectrometric Identification of Phosphorylation Sites in Guanylyl Cyclase A and B*  
A.R. Yoder, M.D. Stone, **T.J. Griffin**, and L.R. Potter
- 2010/218 and CB 2010-90  
*Novel In Situ Collection of Tumor Interstitial Fluid from a Head and Neck Squamous Carcinoma Reveals a Unique Proteome with Diagnostic Potential*  
M.D. Stone, R.M. Odland, T. McGowan, G. Onsongo, C. Tang, N.L. Rhodus, P. Jagtap, S. Bandhakavi, and **T.J. Griffin**
- 2010/219 and CB 2010-91  
*Quantitative Nuclear Proteomics Identifies mTOR Regulation of DNA Damage Response*  
S. Bandhakavi, Y.-M. Kim, S.-H. Ro, H. Xie, G. Onsongo, C.-B. Jun, D.-H. Kim, and **T.J. Griffin**

- 2010/220 and CB 2010-92  
*Quantitative Proteomics Reveals Myosin and Actin as Promising Saliva Biomarkers for Distinguishing Pre-Malignant and Malignant Oral Lesions*  
E.P. de Jong, H. Xie, G. Onsongo, M.D. Stone, X.-B. Chen, J.A. Kooren, E.W. Refsland, R.J. Griffin, F.G. Ondrey, B. Wu, C.T. Le, N.L. Rhodus, **J.V. Carlis**, and **T.J. Griffin**
- 2010/221 and CB 2010-93  
*Targeted<sup>18</sup>O-Labeling for Improved Proteomic Analysis of Carbonylated Peptides by Mass Spectrometry*  
M.R. Roe, T.F. McGowan, L.V. Thompson, and **T.J. Griffin**

## Chemical Engineering and Materials Science

- 2010/204  
*The High Pressure Electronic Spin Transition in Iron: Impacts upon Mantle Mixing*  
M.H. Shahnas, W.R. Peltier, Z. Wu, and **R. Wentzcovitch**
- 2010/205  
*A First-Principles Investigation of Hydrated Defects and IR Frequencies in Forsterite: The Case for Si Vacancies*  
K. Umemoto, **R.M. Wentzcovitch**, M. Hirschmann, D.L. Kohlstedt, and A.C. Withers
- 2011/10  
*Spin-State Crossover and Hyperfine Interactions of Ferric Iron in MgSiO<sub>3</sub> Perovskite*  
H. Hsu, P. Blaha, **M. Cococcioni**, and **R.M. Wentzcovitch**

**Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during December 2010—March 2011**

2011/14 and CB 2011-6

*Silica-Nanoparticle Coatings by Adsorption From Lysine-Silica-Nanoparticle Sols on Inorganic and Biological Surfaces*

N. Atchison, W. Fan, D.D. Brewer, M.A. Arunagirinathan, B.J. Hering, **S. Kumar**, K.K. Papas, E. Kokkoli, and **M. Tsapatsis**

2011/22

*A Robust, Practical, and General Method for Coupled Iterations of Black-Box Nonlinear Solvers by an Approximate Block Newton Method*  
**J.J. Derby** and Andrew Yeckel

2011/31

*Anomalous Segregation of Cadmium Zinc Telluride During Electrodynamic Gradient Freeze Growth*  
N. Zhang, A. Yeckel, A. Burger, Y. Cui, K.G. Lynn, and **J.J. Derby**

## Chemistry

2010/209 and CB 2010-82

*An Anionic, Tetragonal Copper(II) Superoxide Complex*

P.J. Donoghue, A.K. Gupta, D.W. Boyce, **C.J. Cramer**, and W.B. Tolman

2010/210

*The cis-[Ru<sup>II</sup>(bpy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sup>2+</sup> Water-Oxidation Catalyst Revisited*

X. Sala, M.Z. Ertem, L. Vigara, T.K. Todorova, W. Chen, R.C. Rocha, F. Aquilante, **C.J. Cramer**, **L. Gagliardi**, and A. Llobet

2010/223

*Microwave Spectrum of (CH<sub>3</sub>)<sub>3</sub>CCN-SO<sub>3</sub>*

G. Sedo and **K.R. Leopold**

2010/224

*Understanding the Structure and Formation of Uranyl Peroxide Nanoclusters by Quantum Chemical Calculations*

B. Vlasisavljevich, **L. Gagliardi**, and P.C. Burns

2010/228

*Infrared Spectroscopy of Extreme Coordination: The Carbonyls of U<sup>+</sup> and UO<sup>2+</sup>*

A.M. Ricks, **L. Gagliardi**, and M.A. Duncan

2011/15

*Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Method for Electronic Excited States: A Benchmark Study*

V. Sauri, L. Serrano-Andres, A.R.M. Shahi, **L. Gagliardi**, S. Vancoillie, and K. Pierloot

2011/16

*Strong Correlation Treated via Effective Hamiltonians and Perturbation Theory*

G. Li Manni, F. Aquilante, and **L. Gagliardi**

2011/17

*Bulky Guanidinato Nickel(I) Complexes: Synthesis, Characterization, Isomerization, and Reactivity Studies*

C. Jones, C. Schulten, L. Fohlmeister, A. Stasch, K.S. Murray, B. Moubaraki, S. Kohl, M.Z. Ertem, **L. Gagliardi**, and **C.J. Cramer**

2011/19 and CB 2011-7

*Influence of C-5 Substituted Cytosine and Related Nucleoside Analogs on the Formation of Benzo[a]pyrene Diol Epoxide-dG Adducts at CG Base Pairs of DNA*  
R. Guza, D. Kotandeniya, K. Murphy, T. Dissanayake, C. Lin, G.M. Giambasu, R.R. Lad, F. Wojciechowski, S. Amin, S.J. Sturla, R.H.E. Hudson, **D.M. York**, R. Jankowiak, R. Jones, and **N.Y. Tretyakova**

## Chemistry and Biochemistry, UMD

2011/35

*Entropy Production in the Driven Lattice Gas on Small Lattices*

S. Kumar, S.K. Ford, K.C. Zielke, and **P.D. Siders**

## Civil Engineering

2010/231

*Geotechnics and Terramechanics*

**A. Drescher** and J.P. Hambleton

2011/29

*Approximate Model for Blunt Objects Indenting Cohesive-Frictional Materials*

J.P. Hambleton and **A. Drescher**

## Computer Science and Engineering

2011/2 and CB 2011-2

*Linear Dimension Reduction for Evolutionary Data*

E. Kokiopoulou, D. Kressner, and **Y. Saad**

2011/12

*Lanczos-Based Low-Rank Correction Method for Solving the Dyson Equation in Inhomogenous Dynamical Mean-Field Theory*

P. Carrier, J.M. Tang, **Y. Saad**, and J.K. Freericks

**Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during December 2010—March 2011**

## Genetics, Cell Biology, and Development

2010/230 and CB 2010-99

*Genome-Wide Analysis of DNA Binding and Transcriptional Regulation by the Mammalian Double-sex Homolog DMRT1 in the Juvenile Testis*

M.W. Murphy, A.L. Sarver, D. Rice, K. Hatzi, K. Ye, A. Melnick, L.L. Heckert, D. Zarkower, and **V.J. Bardwell** (PI: K.A.T. Silverstein)

## Geology and Geophysics

2011/5

*Ascent of Bubbles in Magma Conduits Using Boundary Elements and Particles*

G. Morra, L. Quevedo, **D.A. Yuen**, and P. Chatelain

2011/7 and CB 2011-4

*Interactive Visualization Tool for Planning Cancer Treatment*

R. Weislo, W. Dzwinel, P. Gosztyla, **D.A. Yuen**, and W. Czech

2011/8

*High Throughput Heterogeneous Computing and Interactive Visualization on a Desktop Supercomputer*

S. Zhang, R. Weiss, S. Wang, G.A. Barnett Jr., and **D.A. Yuen**

2011/11

*WebViz: A Web-Based Collaborative Interactive Visualization System for Large-Scale Data Sets*

Y. Zhou, R.M. Weiss, E. McArthur, D. Sanchez, X. Yao, **D. Yuen**, M.R. Knox, and W.W. Czech

2011/25

*Asymmetric Instability From Shear Modulus Contrast Between Oceanic and Continental Lithospheres: Implications for Subduction Initiation*

B.-D. So, **D.A. Yuen**, K. Rege-  
nauer-Lieb, and S.-M. Lee

2011/26

*Support Operator Rupture Dynamics on GPU*

S. Song, Y. Zhou, T. Dong, and **D.A. Yuen**

2011/27

*The Importance of Elastic Property Contrast at Continental-Oceanic Margin on Subduction Initiation*

B.-D. So, **D.A. Yuen**, K. Rege-  
nauer-Lieb, and S.-M. Lee

2011/28

*High Rayleigh Number Mantle Convection on GPU*

D.A. Sanchez, C. Gonzalez, **D.A. Yuen**, G.B. Wright, and G.A. Barnett

2011/30

*Accelerating Swarm Intelligence Algorithms With GPU-Computing*

R.M. Weiss (PI: **D.A. Yuen**)

2011/32

*Impact of Floating-Point Precision on Boundary Layer Instabilities Modeled on Fermi GPU*

D.A. Sanchez, **D.A. Yuen**, Y. Sun, and G.B. Wright

2011/33

*Implementation of a Multigrid Solver On GPU for Stokes Equations with Strongly Variable Viscosity Based On MATLAB and CUDA*

L. Zheng, T. Gerya, M. Knepley, **D.A. Yuen**, H. Zhang, and Y. Shi

2011/34

*Seismic Wave Propagation Simulation Using Support Operator Method on Multi-GPU System*

S. Song, T. Dong, Y. Zhou, **D.A. Yuen**, and Z. Lu

## Integrative Biology and Physiology

2010/225 and CB 2010-95

*Abnormalities in Circadian Blood Pressure Variability and Endothelial Function: Pragmatic Markers for Adverse Cardiometabolic Profiles in Asymptomatic Obese Adults*

A.K. Gupta, **G. Cornélissen**, F.L. Greenway, V. Dhoopati, F. Halberg, and W.D. Johnson

2010/226 and CB 2010-96

*Assessing Variability in Neonatal Blood Pressure, Notably in Hypotensio,*

**G. Cornélissen**, F. Halberg, E.V. Syutkina, G.V. Yatsyk, A.V. Masalov, O. Schwartzkopff, and D. Johnson

2010/227 and CB 2010-97

*Thirty-Five-Year Climatic Cycle in Heliogeophysics, Psychophysiology, Military Politics, and Economics*

F. Halberg, **G. Cornélissen**, R.B. Sothorn, J. Czaplicki, and O. Schwartzkopff

2010/235 and CB 2010-103

*Circadian Dysfrequentia of Cortisol, Melatonin, Dhea, Testosterone and Estradiol*

F. Halberg, **G. Cornélissen**, N. Cegielski, D. Hillman, F. Halberg, O. Schwartzkopff, R. McCraty, J. Finley, F. Thomas, T. Kino, G. Chrousos, R.P. Sonkowsky, M. ElKhoury, and E. Ilyia

2010/236 and CB 2010-116

*The Moon's and the Genes' Tides and Double Tides Pulling the Biosphere*

F. Halberg, **G. Cornélissen**, R.B. Sothorn, F. Barnwell, N. Cegielski, E. Ilyia, and J. Siegelova

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# Research Reports

2010/237 and CB 2010-104  
*Gender Differences in the Chronome of Sudden Cardiac Death Incidence in the Absheron Peninsula, Azerbaijan*  
**G. Cornélissen**, E. Babayev, and F. Halberg

2010/238 and CB 2010-105  
*Grounding or Earthing: Glimpses at Physiology and Pathology*  
**G. Cornélissen**, F. Halberg, F. Guillaume, O. Schwartzkopff, J. Finley, N. Cegielski, P. Rosch, J. Siegelova, and E. Ilyia

2010/239 and CB 2010-106  
*Aeolian Changes and Gender in the Incidence of Cardiac Arrests in Minnesota (1979-2008)*  
**G. Cornélissen**, J. Palermo, and F. Halberg

2010/240 and CB 2010-107  
*Feasible Ambulatory Blood Pressure and Heart Rate Monitoring in American Secondary Schools To Assess Chronomes in Clinically Healthy Adolescents*  
W. Huynh, **G. Cornélissen**, R. Huynh, R. Huynh, and F. Halberg

2010/241 and CB 2010-108  
*The Moon's Image in Prolonged Human Isolation*  
**G. Cornélissen**, F. Halberg, J. Siegelova, and A. Galvagno

2010/242 and CB 2010-109  
*Urinary Output and Geomagnetism Revisited*  
**G. Cornélissen**, F. Halberg, J. Finley, F. Thomas, J. Siegelova, J. Dusek, and B. Fiser

2010/243 and CB 2010-110  
*Circasemidian and Circasemiseptan Gauges of Vascular Adjustment After Transmeridian Crossing of Three Time Zones*  
O. Schwartzkopff, D. Hillman, F. Halberg, **G. Cornélissen**, M. Engbretson, G.S. Katinas, S.M. Chibisov, J. Siegelova, R. Agarwal, and R. McCraty

2010/244 and CB 2010-115  
*A Far-Transyear in the Blood Pressure of A 17-Year-Old Male*  
F. Watanabe, **G. Cornélissen**, Y. Watanabe, and F. Halberg

2010/245 and CB 2010-111  
*Infradian Modulation of the Development of Human True White-Coat Mesor-Hypertension*  
Y. Watanabe, **G. Cornélissen**, F. Halberg, D. Hillman, B. Fiser, J. Dusek, P. Homolka, and J. Siegelova

2010/246 and CB 2010-114  
*Complementary Yet Differing Rhythmic Aspects of A Man's Mood and Vigor in Various Spectral Regions*  
R.B. Sothorn, F. Halberg, **G. Cornélissen**, D. Hillman, G. Katinas, and J. Siegelova

2010/247 and CB 2010-113  
*Night-To-Day Blood Pressure Ratio During Seven-Day Ambulatory Blood Pressure Monitoring*  
B. Fiser, A. Havelkova, J. Dusek, M. Pohanka, **G. Cornélissen**, and F. Halberg

2010/248 and CB 2010-112  
*Day and Night Blood Pressure Variability During Seven-Day Ambulatory Blood Pressure Monitoring*  
J. Siegelova, A. Havelkova, B. Fiser, J. Dusek, M. Pohanka, M. Masek, L. Dunklerova, **G. Cornélissen**, and F. Halberg

## Laboratory Medicine and Pathology

2010/229 and CB 2010-98  
*MicroRNA miR-183 Functions as an Oncogene by Targeting the Transcription Factor EGR1 and Promoting Tumor Cell Migration*  
A.L. Sarver, L. Li, and **S. Subramanian** (PI: **K.A.T. Silverstein**)

## Masonic Cancer Center

2010/229 and CB 2010-98  
*MicroRNA miR-183 Functions as an Oncogene by Targeting the Transcription Factor EGR1 and Promoting Tumor Cell Migration*  
A.L. Sarver, L. Li, and **S. Subramanian** (PI: **K.A.T. Silverstein**)

2010/230 and CB 2010-99  
*Genome-Wide Analysis of DNA Binding and Transcriptional Regulation by the Mammalian Double-sex Homolog DMRT1 in the Juvenile Testis*  
M.W. Murphy, A.L. Sarver, D. Rice, K. Hatzi, K. Ye, A. Melnick, L.L. Heckert, D. Zarkower, and **V.J. Bardwell** (PI: **K.A.T. Silverstein**)

2011/19 and CB 2011-7  
*Influence of C-5 Substituted Cytosine and Related Nucleoside Analogs on the Formation of Benzo[a]pyrene Diol Epoxide-dG Adducts at CG Base Pairs of DNA*  
R. Guza, D. Kotandeniya, K. Murphy, T. Dissanayake, C. Lin, G.M. Giambasu, R.R. Lad, F. Wojciechowski, S. Amin, S.J. Sturla, R.H.E. Hudson, **D.M. York**, R. Jankowiak, R. Jones, and **N.Y. Tretyakova**

## Pharmacology

2011/13 and CB 2011-5  
*Cross-Crystal Averaging with Search Models to Improve Molecular Replacement Phases*  
W. Li and **F. Li**

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## Physical Medicine and Rehabilitation

2010/212 and CB 2010-84  
*MEFS - MIND Electrical Impedance Tomography Forward Solver*  
 F. Yang, J. Zhang, and **R. Patterson**

## Physics, UMD

2011/23  
*A First Nonperturbative Calculation in Light-Front QED for an Arbitrary Covariant Gauge*  
 S.S. Chabysheva and **J.R. Hiller**

## Plant Biology

2010/211 and CB 2010-83  
*Molecular Phylogenetics of Porcini Mushrooms (Boletus section Boletus)*  
 B.T.M. Dentinger, J.F. Ammirati, E.E. Both, D.E. Desjardin, R.E. Halling, T.W. Henkel, P.-A. Moreau, E. Nagasawa, K. Soyong, A.F. Taylor, R. Watling, J.-M. Moncalvo, and **D.J. McLaughlin**

2010/215 and CB 2010-87  
*Pervasive Gene Content Variation and Copy Number Variation in Maize and its Undomesticated Progenitor*  
 R.A. Swanson-Wagner, S.R. Eichten, and S. Kumari (PI: **N.M. Springer**)

2011/3 and CB 2011-3  
*Molecular Phylogenetics and Historical Biogeography of Porcini Mushrooms (Boletus section Boletus)*  
 B.T.M. Dentinger, J.F. Ammirati, E.E. Both, D.E. Desjardin, R.E. Halling, T.W. Henkel, P.-A. Moreau, E. Nagasawa, K. Soyong, A.F. Taylor, R. Watling, J.-M. Moncalvo, and **D.J. McLaughlin**

## Plant Pathology

2010/216 and CB 2010-88  
*Comparative Genomics Reveals Mobile Pathogenicity Chromosomes in Fusarium*  
 L.-J. Ma, H.C. van der Does, K.A. Borkovich, J.J. Coleman, M.-J. Daboussi, A. Di Pietro, M. Dufresne, M. Freitag, M. Grabherr, B. Henrissat, P.M. Houterman, S. Kang, W.-B. Shim, C. Woloshuk, X. Xie, J.-R. Xu, J. Antoniw, S.E. Baker, B.H. Bluhm, A. Breakspear, D.W. Brown, R.A.E. Butchko, S. Chapman, R. Coulson, P.M. Coutinho, E.G.J. Danchin, A. Diener, L.R. Gale, D.M. Gardiner, S. Goff, K.E. Hammond-Kosack, K. Hilburn, A. Hua-Van, W. Jonkers, K. Kazan, C.D. Kodira, M. Koehrsen, Lo. Kumar, Y.-H. Lee, L. Li, J.M. Manners, D. Miranda-Saavedra, M. Mukherjee, G. Park, J. Park, S.-Y. Park, R.H. Proctor, A. Regev, M.C. Ruiz-Roldan, D. Sain, S. Sakthikumar, S. Sykes, D.C. Schwartz, B.G. Turgeon, I. Wapinski, O. Yoder, S. Young, Q. Zeng, S. Zhou, J. Galagan, C.A. Cuomo, **H.C. Kistler**, and M. Rep

2011/1 and CB 2011-1  
*The Transcription Factor FgStuAp Influences Spore Development, Pathogenicity, and Secondary Metabolism in Fusarium graminearum*  
 E. Lysøe, M. Pasquali, A. Breakspear, and **H.C. Kistler**

## Veterinary Clinical Sciences

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*Gene Expression Profiling Identifies Inflammation and Angiogenesis as Distinguishing Features of Canine Hemangiosarcoma*  
 B.A. Tamburini, T.L. Phang, S.P. Fosmire, M.C. Scott, S.C. Trapp, M.M. Duckett, S.R. Robinson, J.E. Slansky, L.C. Sharkey, G.R. Cutter, J.W. Wojcieszyn, D. Bellgrau, R.M. Gemmill, L.E. Hunter, and **J.F. Modiano**

2010/232 and CB 2010-100  
*Detection and Molecular Characterization of Enteric Viruses from Poultry Enteritis Syndrome in Turkeys*  
 N. Jindal, D. P. Patnayak, Y. Chander, A.F. Ziegler, and **S.M. Goyal**

2010/233 and CB 2010-101  
*Full Length Sequencing of all Nine Subtypes of the Neuraminidase Gene of Influenza A Viruses Using Subtype Specific Primer Sets*  
 Y. Chander, N. Jindal, D.E. Stalcknecht, **S. Sreevatsan**, and **S.M. Goyal**

2010/234 and CB 2010-102  
*Detection and Molecular Characterization of Enteric Viruses in Breeder Turkeys*  
 N. Jindal, D.P. Patnayak, Y. Chander, A.F. Ziegler, and **S.M. Goyal**

2011/20 and CB 2011-8  
*Targeting Tumor-Related Lymphoid Progenitors in B-Cell Lymphoma*  
 D. Ito, A. Avery, N. Mason, R. Thomas, M. Beall, L. Honigberg, J. Buggy, M. Breen, T. O'Brian, and **J. Modiano**

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2011/21 and CB 2011-9

*Shared Properties of Tumor-Initiating Cells Defined by Sphere-Forming Culture of Ontogenetically Distinct Cancers*

A.M. Frantz, B.H. Gordon, E.B. Dickerson, T.D. O'Brian, and **J.F. Modiano**

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1–3:30 p.m.  
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