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Mechanical Engineering

Particle Formation and Growth in Turbulent Flows

Particle formation and growth play a significant role in a number of natural and industrial processes. One application of particular interest is the conversion of solar energy into fuels using the world's most abundant, but intermittent, source of energy. Of the options for solar fuel production, hydrogen produced from water is arguably one of the most promising options for a clean energy future. The use of concentrated solar energy to drive thermo-chemical water splitting cycles holds great promise for high-efficiency utility-scale fuel production. An intriguing ap-

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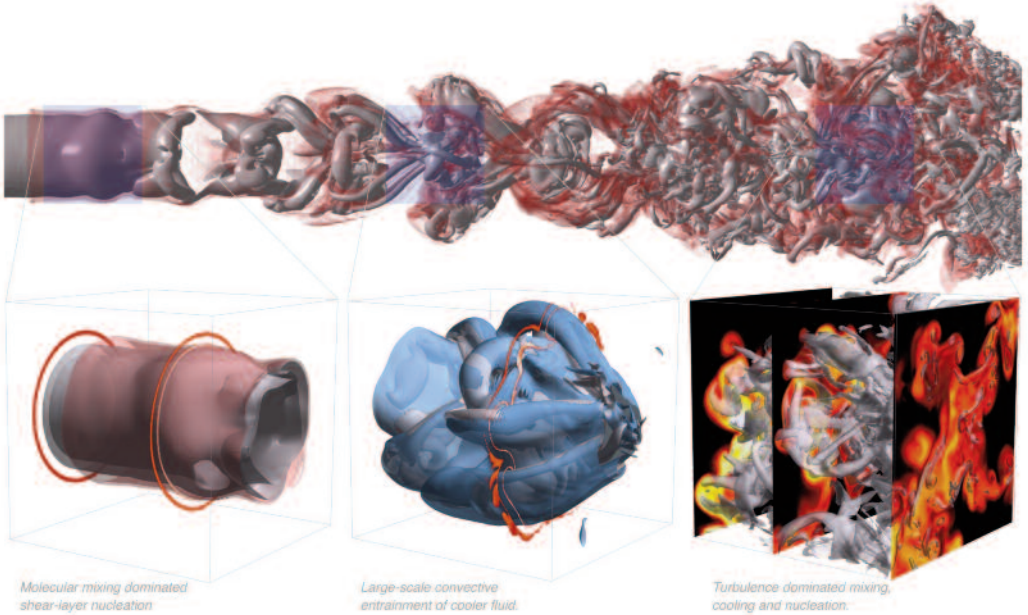


Figure 1: Nucleation of zinc nanoparticles in a turbulent round jet. The gray iso-surface reveals locations in the flow where the vorticity is 1/4 the maximum value. In the top image, the red surface indicates where the nucleation rate is 10^{18} particles per m^3 per second. The area of the red surface increases with mixing and downstream direction. Initially, this is a "cylindrical" surface and nucleation is molecular-diffusion driven (lower left). Further downstream, vorticity acts to entrain the cooler flow and increase the saturation ratio (lower middle). At some point the large-scale structures break down, the flow is fully turbulent, and vortex bending and stretching act to significantly increase fluid mixing, lower the temperature, increase the saturation ratio, and increase the nucleation rate.

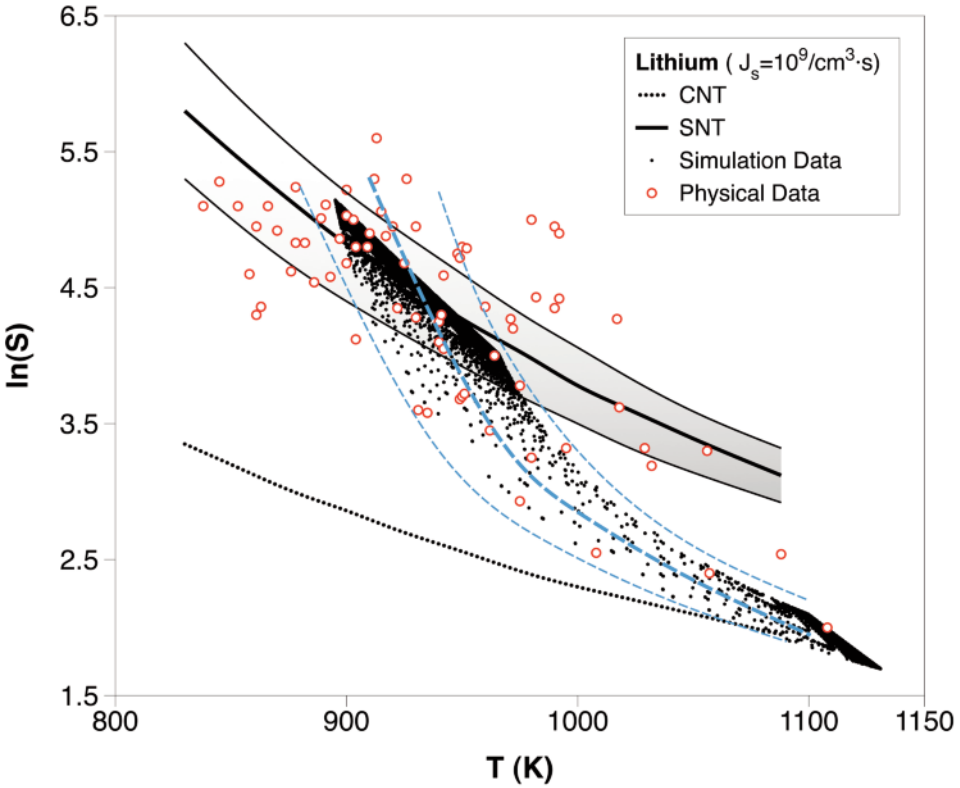


Figure 2: Saturation ratio vs. temperature in the nucleation of lithium nanoparticles. The results (in blue) show improved prediction compared to both classical nucleation theory (CNT) at all temperatures and scaled nucleation theory (SNT) at higher temperatures.

proach involves the use of metallic nanoparticles that act as individual chemical reactors. The surface of the nanoparticles is where water vapor and the metal react to produce the hydrogen gas. A major advantage of using nano-scale particles (as opposed to larger micro-scale particles) is the high specific surface area of the nanoparticles. This favors complete or nearly complete oxidation, and therefore increased hydrogen production. In principle, this is a way to cheaply produce hydrogen, in a carbon-neutral manner.

Vapor-phase synthesis is an economical route for the production of nanoparticles. In its simplest form, hot metal vapor is mixed rapidly with a cooler, inert gas and the metal nanoparticles form. These synthesis processes require large flow rates, which means large Reynolds numbers and turbulent flows. Fluid turbulence acts to increase the rate of cooling, which typically increases the rate of particle formation (Figure 1). According to homogeneous nucleation theory, the appearance of an embryonic nucleus is the result of the aggregation of molecules. If the surface energy binding the molecules is greater than the kinetic energy of the molecules in the cluster, then the cluster will persist and become a stable nucleus. Otherwise, the cluster will degenerate to its constituent molecules. This is all fairly simple. The problem in predicting the number of particles formed is that "all clusters aren't created equal." Some are more stable than others. The result is that theories that do not include some sort of cluster size information in determining particle formation rates are sometimes grossly inaccurate. High-fidelity numerical simulation is promising because it can probe physical and chemical interactions at length and time-scales that are impossible to observe via physical investigation. Approaches such as density functional theory and molecular dynamics techniques are able to describe nucleation processes at the atomic level. While these techniques benefit from the resolution of kinetics, the difficulty associated with extending the techniques to realistic length and time-scales means that they are infeasible for practical systems/processes. There is a need for methodologies that include the advanced physics of these approaches and the well-established benefits of the simple homogeneous nucleation theory.

Professor Sean Garrick (MSI Fellow) and his researchers Jun Liu and Andrew Fager in the Department of Mechanical Engineering are developing models to predict the formation of nanoparticles for a variety of scientific and engineering purposes. Homogeneous nucleation theory is attractive because it is relatively simple to include in computational fluid dynamics (CFD). Starting with relatively simple flows, Professor Garrick and his researchers have shown that including size-dependent properties in the homogeneous nucleation theory yields significantly better results, when compared to traditional classical nucleation theory and scaled nucleation theory (Figure 2). This is significant because CFD is used to study

a wide variety of problems and models which are able to be incorporated in traditional codes will be of great value. The results show that for metal nanoparticles, the number of particles predicted to form using the size-dependent approach may be up to eight orders of magnitude (10^8) less than when classical nucleation theory is used. In terms of solar thermo-chemical synthesis this means that the surface area available for the metal and the water vapor to react to produce hydrogen would be greatly reduced. Even though there are more small particles, the growth of the particles (via coagulation) is proportional to the square of their number concentration. This means that they would not remain "nano-scale" for very long. As if these uncertainties weren't enough, these physico-chemical processes often occur under turbulent flow conditions. Turbulence is typically characterized by the presence of a variety of length- and time-scales plus fluctuations. These fluctuations can change particle formation and growth rates by several orders of magnitude. The sensitivity of the physical phenomena to variations in temperature and chemical histories means that analytical approaches and physical measurement often do not adequately provide a means to characterize the underlying processes. For example, nuclei formation is a strong function of local temperature and chemical concentration, and can occur within micro-seconds (Figure 3). Capturing the fluid, temperature, and chemical dynamics—or their effects—is key to accurate prediction.

Mr. Fager and Professor Garrick are utilizing different combinations of direct numerical simulation (DNS) and large-eddy simulation (LES) to study the effects of turbulence on particle formation. DNS is very useful in elucidating the physical and chemical dynamics—in a spatially and temporally resolved manner—present in multi-scale flows. Unfortunately the compute-times required (hundreds of thousands of CPU-hours) are beyond what most scientists and engineers can afford. A typical DNS of metal vapor nucleation requires roughly 96,000 CPU-hours. The corresponding LES requires roughly 105 CPU-hours. As a result, approaches such as LES, which utilizes sub-models to account for small-scale interactions, are increasingly popular. Recently developed hybrid DNS-LES approaches are useful in illustrating the effect of unresolved, small-scale interactions. The simulations are performed using a fully resolved spatial and temporal discretization. This serves as the benchmark dataset. Additional simulations are performed where one or more of the dependent variables—e.g. temperature and vapor concentration—are not fully resolved. This is accomplished by using a filter to remove the small-scale, high-frequency content typically absent from LES. While these simulations are more computationally expensive (~148,000 CPU-hours) they help to elucidate the effects of both temperature and concentration fluctuations on particle formation. Using 4096 cores on Itasca, one simulation can be completed in roughly 36 hours. The results suggest that the fluctuations act to both increase and decrease temperature. However, the regions where the temperature is decreased have a much more sig-

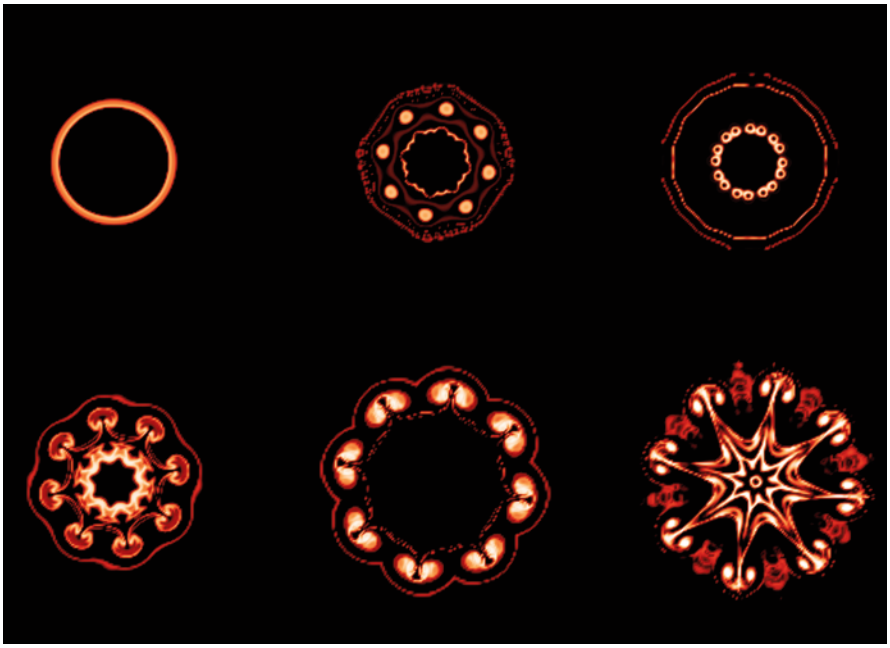


Figure 3: Instantaneous contours of nucleation rate in a round "crowned" jet at different downstream locations. The non-linear nature of the high Reynolds number flow shows that small perturbations grow. Nucleation occurs where the hot metal vapor and cooler background gas (argon) meet. Further downstream all symmetry is broken (as demonstrated in Figure 1).

Figure 4. Instantaneous contours of temperature for the DNS (upper image) and hybrid DNS-LES (lower image). In the DNS, the temperature field is fully resolved while in the DNS-LES, only the large-scale temperature is resolved, as it would be in LES. While the temperature fields are very similar, the absence of small-scale mixing is quite noticeable in the lower image. This has the effect of altering the particle nucleation rate by 80%.

nificant impact on particle formation. In these regions turbulence acts to augment the molecular-dominated cooling (conduction) and the stable nuclei form more rapidly. This work points to the need for sub-models in order the capture the unresolved particle formation terms in a LES. DNS is only possible for the simplest of flows, such as the one in this study. It quickly becomes impossible for any flow of practical, engineering interest where complex geometries, thermochemistry, and fluid-particle/ particle-particle interactions exist simultaneously. For these engineering flows, LES is attractive as it still captures the large-scale, time-dependent flow features and has a speed up factor of ~1000 when compared to DNS.

Nucleation is only the first step, however. Other important processes include condensation, coagulation, and finite-rate sintering. Consider the more complex problem of particulate generation from combustion processes. The transition of gas-phase species to solid particles is likely the least understood part of the soot formation process. These involve polyacetylenes, ionic species, or polycyclic aromatic hydrocarbons as the key gaseous precursors to soot. Soot comes in all shapes and sizes. Flames act to restructure the soot particles and shear flows increase aggregation as well as de-aggregation. Some agglomerates are hard and others are soft. Being able to better characterize the soot will lead to the development of better filters as well as exhaust gas after-treatments. Physically accurate models and computationally affordable numerical tools will help scientists and engineers tackle problems that pose challenges to current and future energy as well as environmental concerns.

Funding for this research came from the National Science Foundation, the Department of Energy, and the University of Minnesota's Institute on the Environment. A poster on this project was selected as a finalist at the 2011 MSI Research Exhibition (see URL below and page 10 of this publication):

www.msi.umn.edu/events /researchexhibition2011.html

Numerical Simulations of High-Speed Jets in Crossflow

The term "jet in cross-flow" refers to a jet of fluid that exits an orifice to interact with the surrounding fluid that is flowing "across" the orifice. "High-speed jets in crossflow" implies that either the jet or the crossflow is supersonic. Such jets occur in scramjet engine combustors, where sonic jets of fuel are injected into a supersonic crossflow of air. Due to their high speeds, the fuel and the air will reside in the combustor only for milliseconds. Successful operation of the combustor requires the fuel and the air to efficiently mix and burn thoroughly before they exit the combustor. Accurate estimation and detailed physical understanding of the turbulent mixing mechanisms are therefore essential to the design of scramjet combustors.

High-speed jets in crossflow are very complex flows (Figures 1 and 2). The complexity makes detailed measurements difficult, and only limited information is provided by past experimental studies. Traditional engineering simulation tools also experience difficulties in simulating such flows. As a result, basic understanding of high-speed jets in crossflow is severely lacking, and several important questions are yet unanswered. Professor Krishnan Mahesh (MSI Fellow) and his student Xiaochuan Chai in the Department of Aerospace Engineering and Mechanics are developing novel numerical methodologies to perform high-fidelity simulations of high-speed jets in crossflow. The primary objectives of their study are to develop a novel algorithm and large-eddy simulation (LES) capability for high-speed flows in complex geometries, provide a high-fidelity simulation database for high-speed jets in crossflow, and answer specific questions concerning the jet penetration, mixing and turbulent fluctuations.

Professor Mahesh's research group has developed a novel methodology to perform high-fidelity simulations of high-speed complex flows on unstructured grids. Using unstructured grids allows complex geometries to be discretized efficiently. The algorithm developed by the Mahesh group involves a least-square-based flux reconstruction on the faces of control volumes and splitting of the viscous flux, to calculate the derivative terms in the governing equations accurately and stably on unstructured grids. The algorithm also uses a predictor-corrector methodology to resolve shock waves. The predictor step is non-dissipative and designed to accurately represent

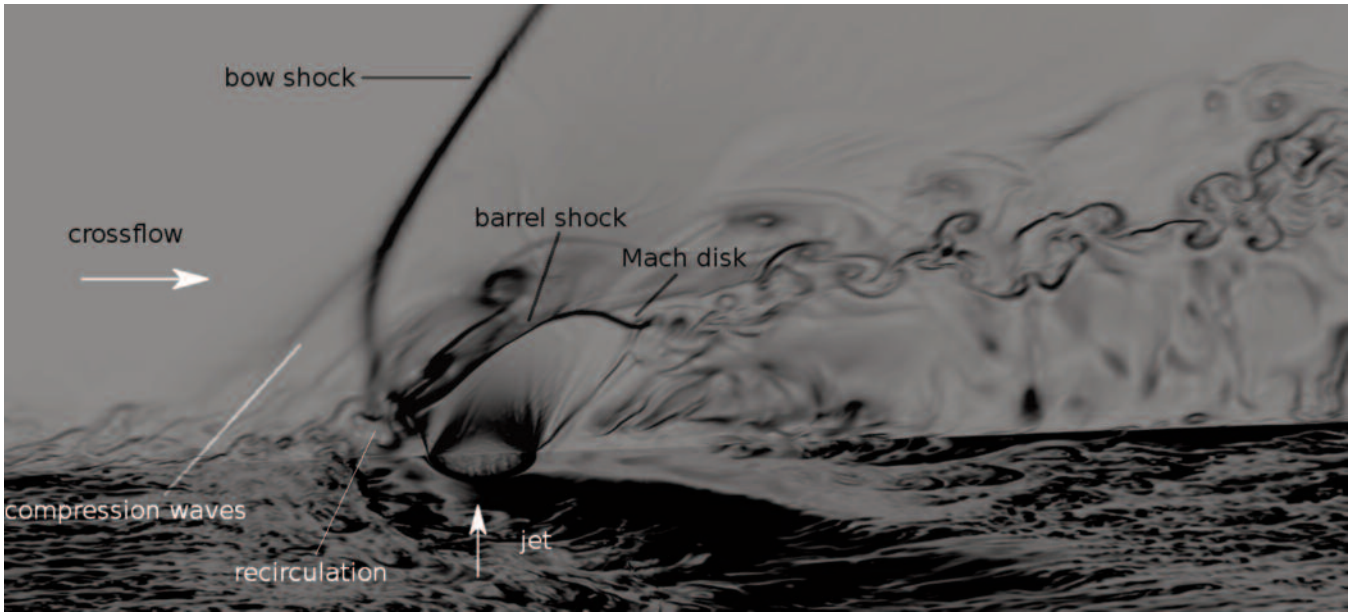


Figure 1. Instantaneous contours of density gradient magnitude in the interaction of a Mach 1 jet with Mach 1.6 crossflow.

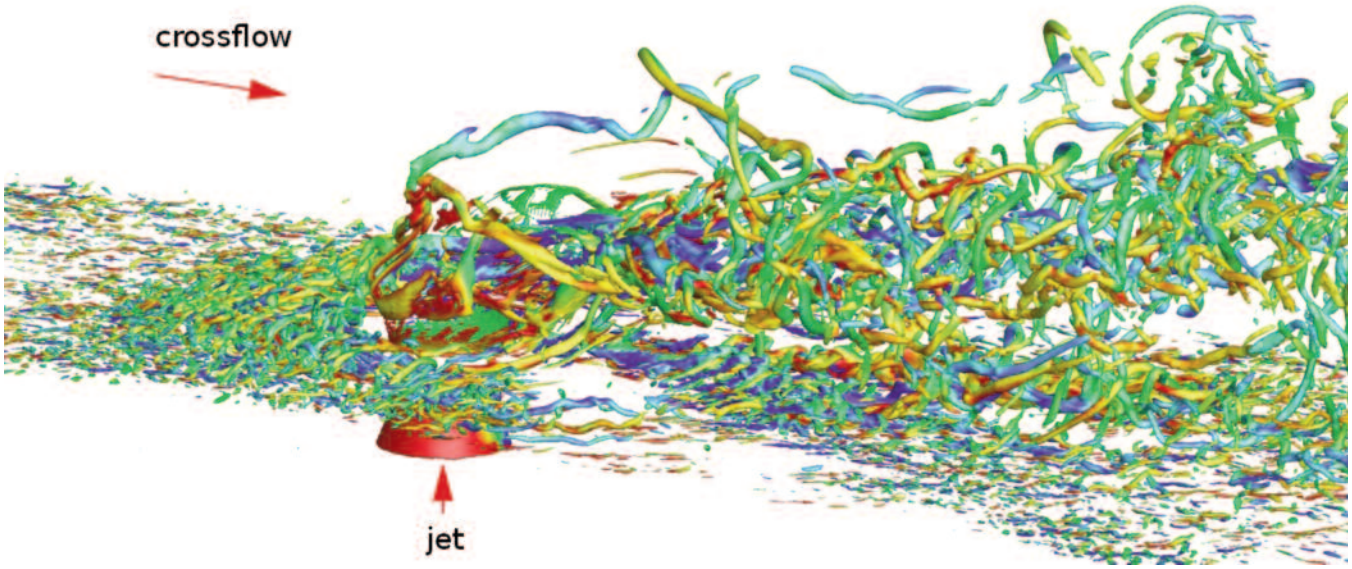


Figure 2. Instantaneous vortical structures visualized for the simulation.

broadband turbulence, while the corrector step is a characteristic-based filter that is localized around shock waves. Thus, the overall scheme avoids unnecessary numerical dissipation, which is required for high fidelity numerical simulations. Recently, Mr. Chai and Professor Mahesh developed a novel sub-grid scale model for LES of complex high-speed flows, which enables the Reynolds numbers in numerical simulations to match the high values found in practical applications. Thus, their work advances simulation capability to practical engineering problems, and marks the early stage of an evolution that will change the way that flow problems will be solved in the future.

Figure 1 shows instantaneous contours of density gradient magnitude from simulations of a sonic jet injected into a Mach 1.6 supersonic crossflow. As shown, the flow field consists of very complex turbulent flow structures and shock waves. The supersonic crossflow travels from left to right and contains a fully developed turbulent boundary layer. It sees the transverse jet as an obstacle, and responds by forming a bow shock, a recirculation region, and a family of compression waves in front of the jet. Exiting the orifice, the sonic jet tries to penetrate and expand, and sets up an inclined barrel shock and Mach disk on its periphery. On the windward side of the jet, the shear layer rolls up into vortices which detach from the jet boundary and are shed downstream. Coherent flow structures

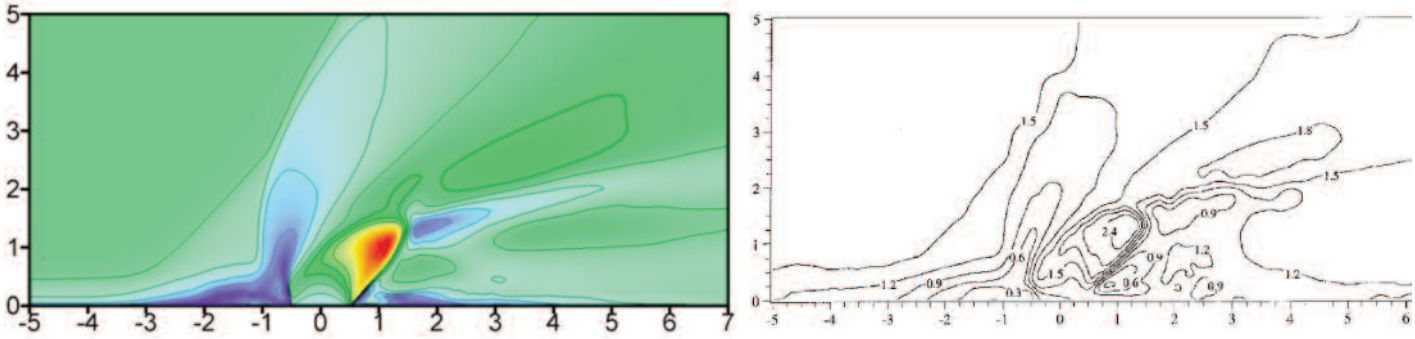


Figure 3. Mean Mach number contour on central plane. At the left is the simulation; at the right are results from experiment (Santiago and Dutton, 1997).

are observed downstream of the jet after the jet/crossflow interaction.

Figure 2 shows the vortical structures in this flow. The flow is highly unsteady and is composed of turbulent eddies of different sizes. The recirculation bubbles wrap around the jet and form horseshoe vortices. Downstream of the jet, there are two regions symmetrically on each side of the center line that contain few turbulent eddies. They correspond to the expansion and acceleration of the crossflow passing by the jet. The jet plume has a very complex structure with different signs of vorticity on each side of the centerline. Statistically, this becomes the contour-rotating vortex pair (Figure 4). Also observed is an increase of turbulent eddy sizes downstream of the jet. These vortical structures are responsible for the mixing of the jet with the crossflow.

The simulation results are validated by comparison to available experimental results (Santiago and Dutton, 1997). Figure 3 compares

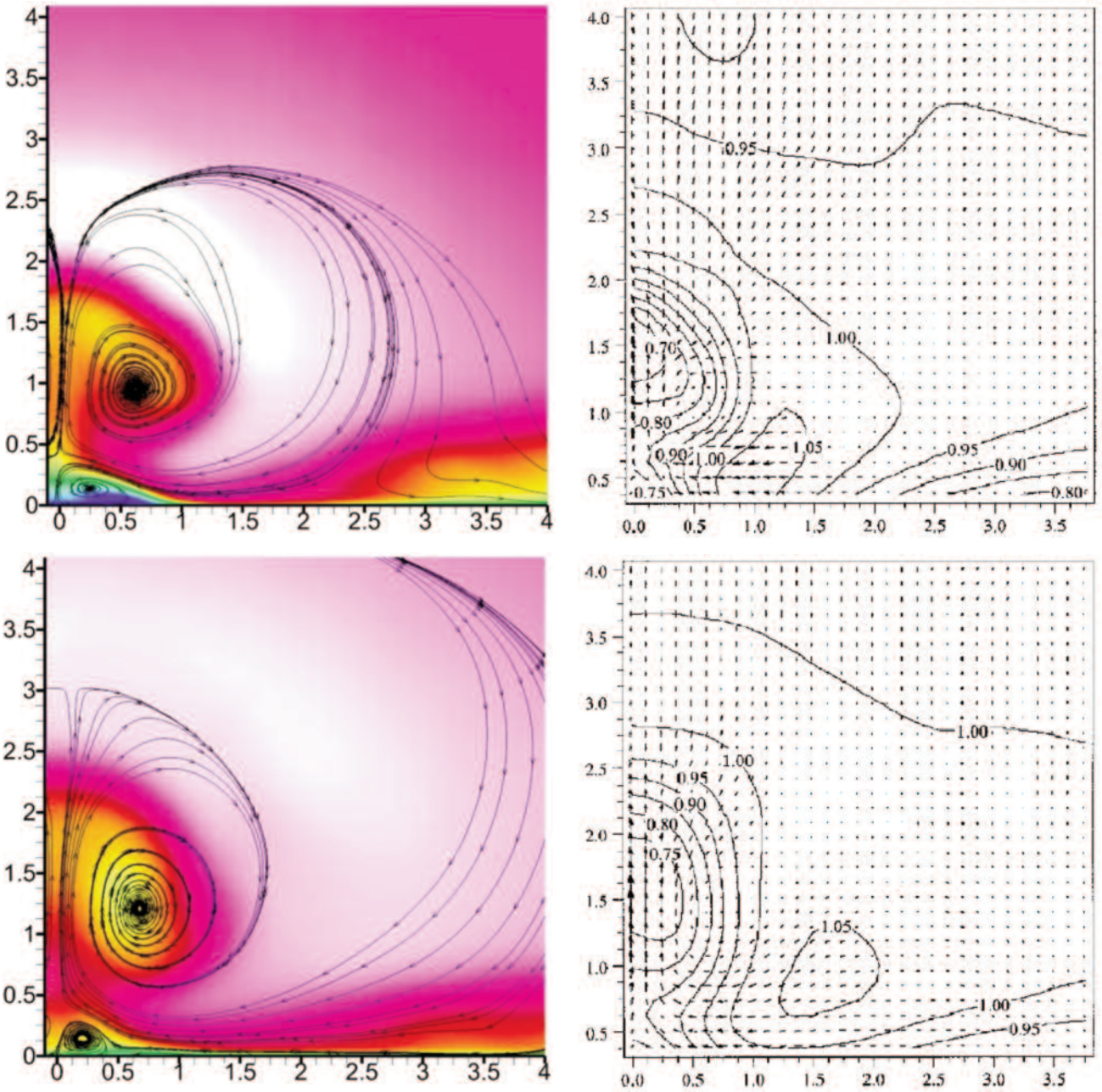


Figure 4. Time-averaged velocity contours on two cross-planes.

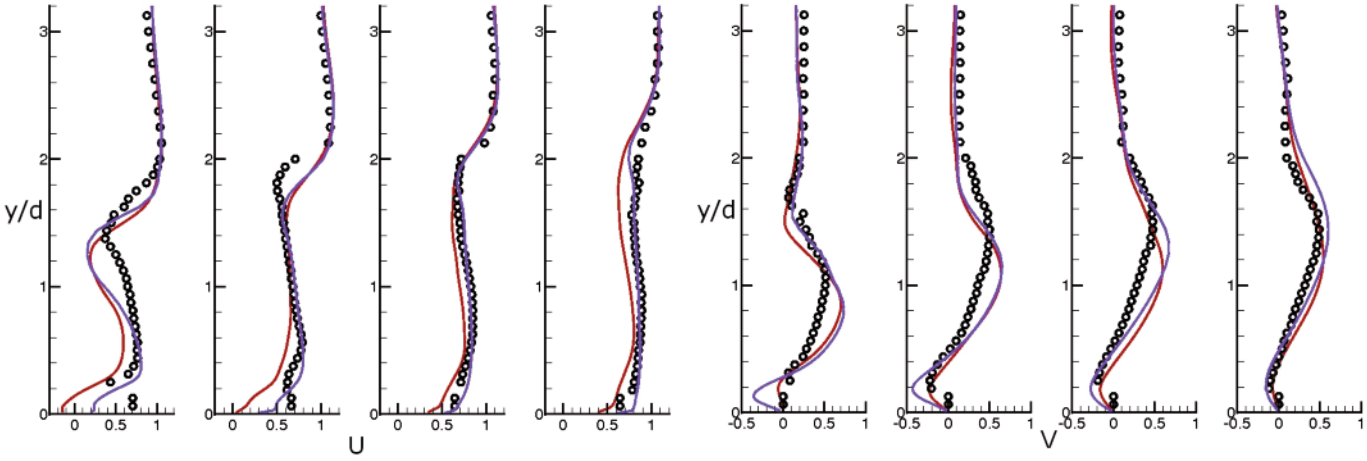


Figure 5. Effects of crossflow boundary layer. Red: laminar; blue: turbulent; symbols: experiment.

the mean central plane Mach number contour with the experiment, and Figure 4 compares the time average velocity contours at two different cross-planes downstream of the jet. Good agreement can be observed.

There are many factors that can affect the accuracy and reliability of the simulations. Therefore, a series of simulations were carried out systematically to study their effects. For example, the effect of the inflow boundary layer was examined. Figure 5 compares the velocity profiles between simulations using a laminar crossflow boundary layer to those using a turbulent boundary layer. While both simulations agree reasonably with the experiment, using turbulent inflow is observed to have better agreement overall, and improves the velocity distributions near the wall. The mixing between the jet and crossflow is also enhanced when the inflow boundary layer is turbulent. Grid refinement was also performed, and more flow details as well as improved agreement with experiment were observed on the fine mesh. Presently, Mr. Chai and Professor Mahesh are evaluating the role of the sub-grid scale model in the simulations. Their next step is to quantify the flow in terms of jet penetration, eddy sizes and frequencies, and mixing properties, and then develop scaling laws that can be useful for practical design. Their work also lays the foundations to include chemical reactions in the simulation, and ultimately enable high-fidelity simulations of the entire scramjet engine.

This research is funded by the National Science Foundation. The simulations are performed on MSI's Itasca supercomputer. The most recent simulation contains 75 million grid points which are distributed over 1024 cores. Resources from MSI's Scientific Visualization and Development Lab are used for computational mesh generation and post-processing. The group's work was presented at the 62nd and 63rd Annual Meetings of the APS Division of Fluid Dynamics, the AIAA 40th Fluid Dynamics Conference and Exhibit, and the 49th AIAA Aerospace Science Meeting including the New Horizons Forum and Aerospace Exposition. Their newly developed LES model has been submitted to the Journal of Fluid Mechanics for publication. A poster about this work was selected as a finalist winner at the 2011 MSI Research Exhibition (see URL below and page 10 of this publication):

www.msi.umn.edu/events/researchexhibition2011.html

In Memoriam: Daniel D. Joseph

Regents Professor Emeritus Daniel D. Joseph, Department of Aerospace Engineering and Mechanics, passed away on May 24, 2011. Professor Joseph was an MSI Principal Investigator for many years, and was named an MSI Fellow in 1999. His recent research at MSI involved direct numerical simulation and modeling of multiphase flows. He and his research group applied theories of viscous potential flow and dissipation method to the study of problems in two-phase fluid dynamics. They also investigated the fundamental dynamics of three-dimensional motions of solid particles in Newtonian and viscoelastic fluids.

The staff of the Institute express their deepest condolences to Professor Joseph's family, friends, and colleagues.

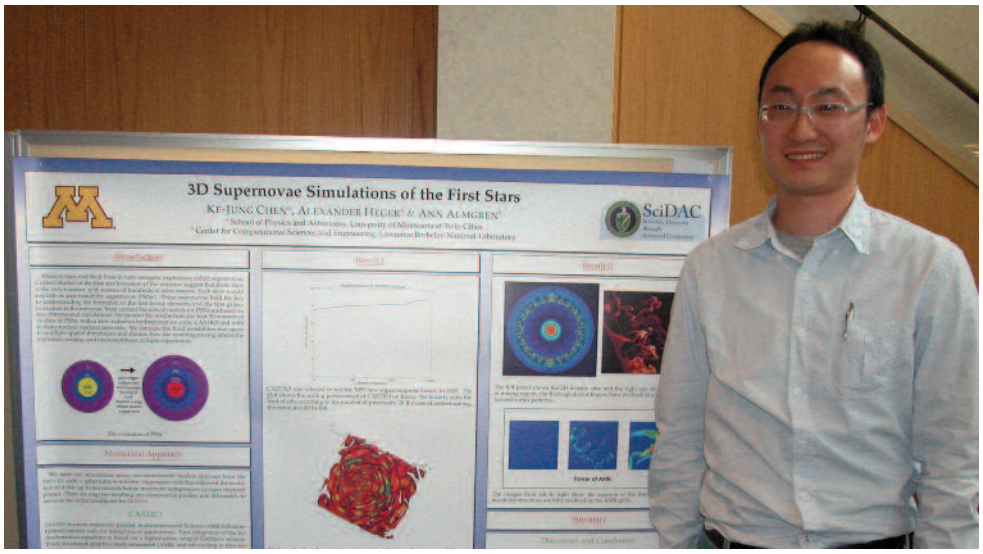
MSI Research Exhibition 2011

The Second Annual MSI Research Exhibition was held on April 25, 2011. The Research Exhibition was an opportunity for MSI researchers to present posters of their work using MSI resources. The posters were judged by a committee of MSI Principal Investigators. The judges chose the six finalists before the event and made the final decision for the Grand Prize winner after talking to the poster presenters that day.

Prizes for the poster session and refreshments were sponsored by MathWorks. Attendees enjoyed light refreshments as they viewed the posters and talked with the presenters. Information about the event can be found at our website:

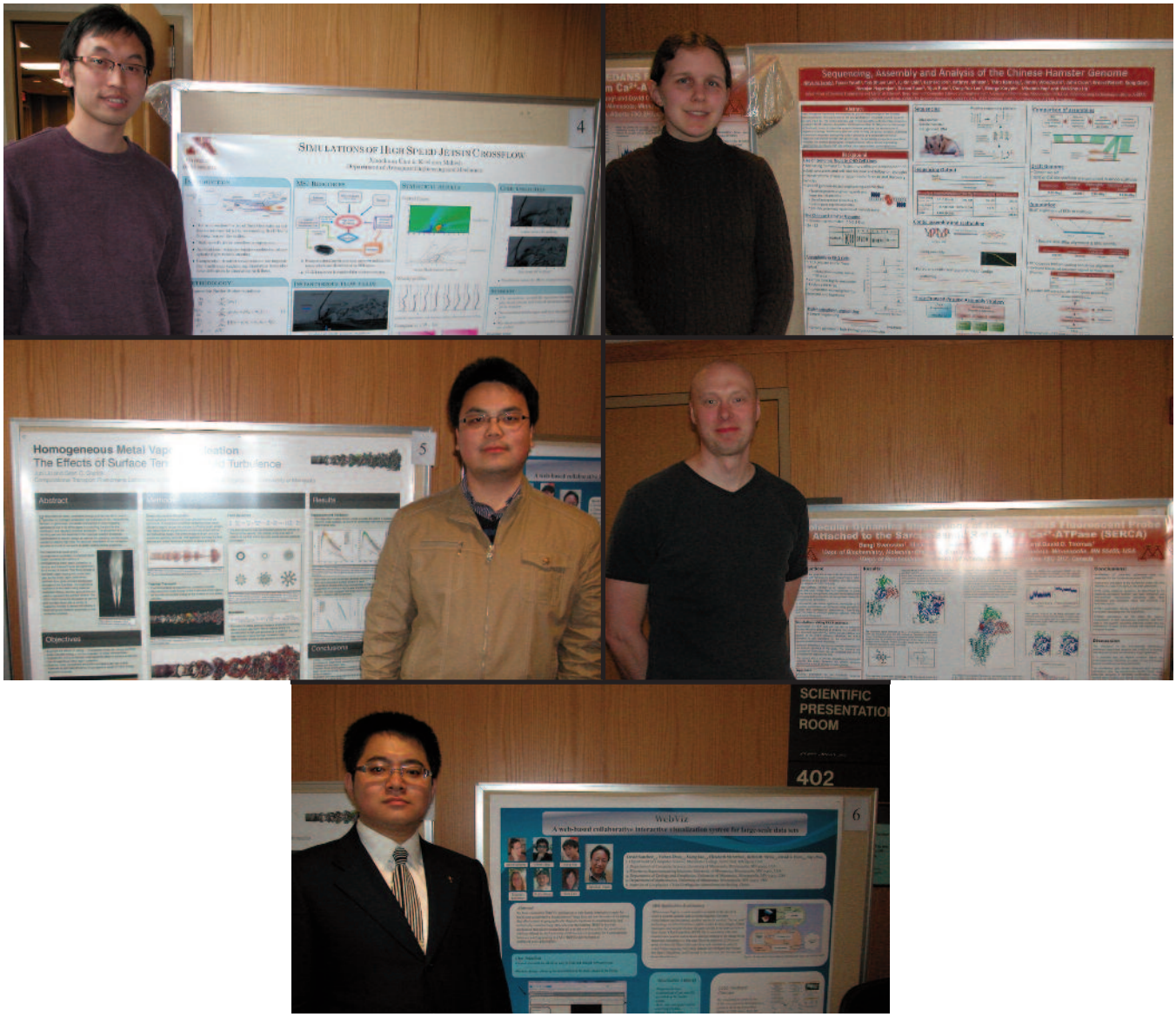
www.msi.umn.edu/events/researchexhibition2011.html

Grand Prize



Left: Ke-Jung (Ken) Chen (Physics; PI: Alexander Heger) with his Grand Prize-winning poster, *3D Supernovae Simulations of the First Stars*. Mr. Chen was also a finalist in the 2010 Research Exhibition and his work was highlighted in the Spring 2010 *Research Bulletin*.

Finalists



Top left: Xiaochuan Chai (Aeronautical Engineering and Mechanics; PI: Krishnan Mahesh), *Simulations of High-Speed Jets in Crossflow* (see article on page 5).

Top right: Kathryn Johnson (Chemical Engineering and Mechanics; PI: Wei-Shou Hu); *Sequencing, Assembly, and Analysis of the Chinese Hamster Genome*.

Middle left: Jun Liu (Mechanical Engineering; PI: Sean Garrick); *Homogeneous Metal Vapor Nucleation: The Effects of Surface Tension and Fluid Turbulence* (see article on page 1).

Middle right: Bengt Svensson (Biochemistry, Molecular Biology, and Biophysics; PI: David Thomas); *Molecular Dynamics Simulations of the IAEDANS Fluorescent Probe Attached to the Sarcoplasmic Reticulum Ca^{2+}-ATPase (SERCA).*

Bottom: Yichen Zhou (Earth Sciences; PI: David Yuen); *WebViz: A Web-Based Collaborative Interactive Visualization System for Large-Scale Data Sets*.

THANK YOU
to our judges:

Matteo Cococcioni
Chemical Engineering and Materials Science

Barry Finzel
Medicinal Chemistry

Krishnan Mahesh
Aerospace Engineering and Mechanics

Alon McCormick
Chemical Engineering and Materials Science

Gary Muehlbauer
Agronomy and Plant Genetics

Fotis Sotiropoulos
Civil Engineering and St. Anthony Falls Laboratory

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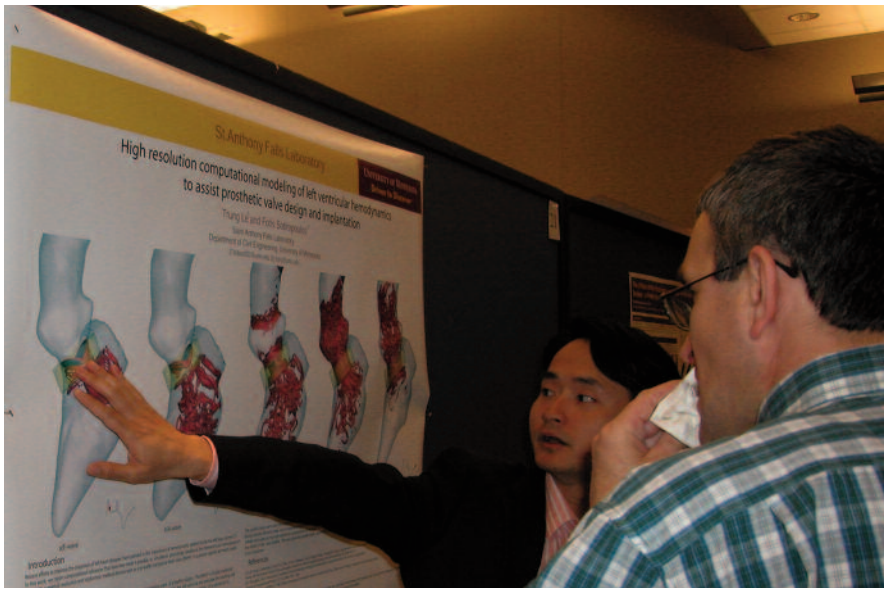
Above: Ken Cleveland, Mathworks Educational Sales Account Manager (left), and Saket Kharsikar, MathWorks Application Engineer, attended the Research Exhibition.

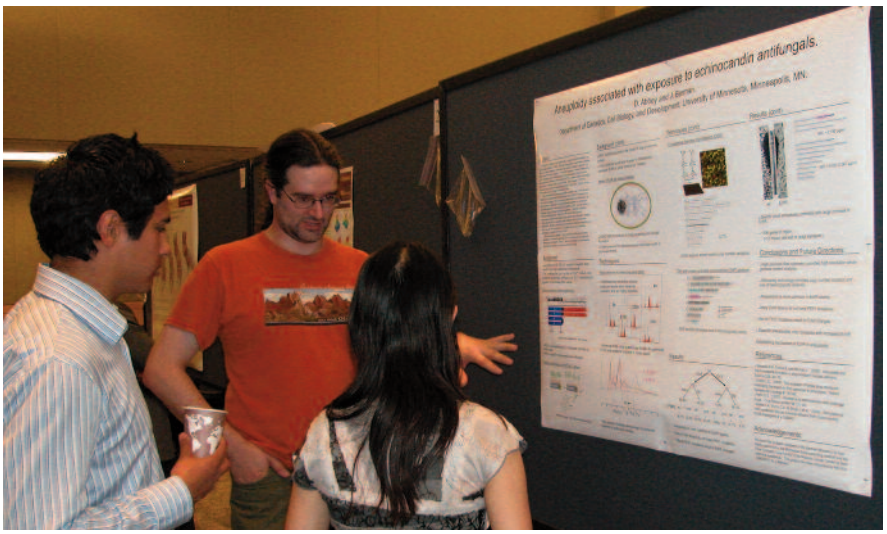
Poster authors describe their research to Research Exhibition attendees.

Right: Erik O.D. Sevre (Earth Sciences; PI: David Yuen)

Below left: Trung Le (Civil Engineering and St. Anthony Falls Laboratory; PI: Fotis Sotiropoulos)

Below right: Darren Abbey (Genetics, Cell Biology, and Development; PI: Judith Berman)





Aerospace Engineering and Mechanics

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L. Shi, N. J. Traaseth, R. Verardi, M. Gustavsson, **J. Gao**, and **G. Veglia**

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Center for Drug Design

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3-Hydroxypyrimidine-2,4-diones as an Inhibitor Scaffold of HIV Integrase
J. Tang, K. Maddali, M. Metifiot, **Y.Y. Sham**, R. Vince, Y. Pommier, and Z. Wang

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pH-Dependent Transport of Pemetrexed by Breast Cancer Resistance Protein (BCRP)
L. Li, **Y.Y. Sham**, Z. Bikadi, and W.F. Elmquist

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A Continuous Fluorescence Displacement Assay for BioA: An Enzyme Involved in Biotin Biosynthesis
D.J. Wilson, C. Shi, B.P. Duckworth, J.M. Muretta, U. Manjunatha, **Y.Y. Sham**, **D.D. Thomas**, and **C.C. Aldrich**

Chemistry

2011/39 and CB 2011-12
Paramagnetic-Based NMR Restraints Lift Residual Dipolar Coupling Degeneracy in Multidomain Detergent-Solubilized Membrane Proteins
L. Shi, N. J. Traaseth, R. Verardi, M. Gustavsson, **J. Gao**, and **G. Veglia**

Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during April–July 2011.

2011/40 and CB 2011-11
Polarized Molecular Orbital Model Chemistry. 1. Ab Initio Foundations
L. Fiedler, **J. Gao**, and **D.G. Truhlar**

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Polarized Molecular Orbital Model Chemistry. 2. The PMO Method
P. Zhang, L. Fiedler, H.R. Leverentz, **D.G. Truhlar**, and **J. Gao**

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Flickering Dipoles in the Gas Phase: Structures, Internal Dynamics, and Dipole Moments of β-naphthol-H_2O in its Ground and Excited Electronic States
A.J. Fleisher, J.W. Young, D.W. Pratt, A.Cembran, and **J. Gao**

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Molecular Dynamics Simulations of the Intramolecular Proton Transfer and Carbanion Stabilization in the Pyridoxal 5´-Phosphate Dependent Enzymes L-Dopa Decarboxylase and Alanine Racemase
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Dipole Preserving and Polarization Consistent Charges
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Insight Into Phosphodiesterase Mechanism From Combined QM/MM Free Energy Simulations
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Adequate Representation of Charge Polarization Effects Leads to a Successful Treatment of the CF_4 + $SiCl_4$ - CCl_4 + SiF_4 Reaction by Density Functional Theory
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Convergent Partially Augmented Basis Sets for Post-Hartree-Fock Calculations of Molecular Properties and Reaction Barrier Heights
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