Institute for Computational Astrophysics ICA

2006 Annual Report

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Institute for Computational Astrophysics

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Institute for Computational Astrophysics

Saint Mary's University

Annual Report

2006

The Institute for Computational Astrophysics (ICA) was formed by an act of the Saint Mary's University Faculty Senate in December 2002 on the basis of a proposal generated by Drs. David Clarke and David Guenther. In July 2005, Dr. Terry Murphy, Vice President Academic and Research submitted the amended ICA Constitution to Senate, on behalf of the ICA. Senate unanimously passed the amended ICA Constitution in July, 2005.

This year saw a number of changes at the ICA. Postdoctoral fellow Dr. Sasha Men'shchikov left in early January for a permanent position at Saclay near Paris. Postdoctoral fellows Dr. Nathalie Toque arrived on March 1 and Dr. Alex Razoumov started on July 1. Mr. Chris Capobianco completed his Master's research with Dr. Joe Hahn and left to begin his Ph. D. studies at Queen's University. Dr. Hahn and his family returned to Texas in early July and Ms. Julee Adams, the ICA administrative support, departed in the middle of August. The search for Dr. Hahn's replacement began early this year, and the ICA is very pleased to submit Dr. Rob Thacker, currently at Queen's, as a Tier 2 Canada Research Chair (CRC) to replace Dr. Hahn. This round of CRC applications is expected to be announced early next year. Dr. Thacker proposes to start at the ICA in July, 2007. The ICA administrative support position was upgraded this year from Secretary III to ICA Assistant. Ms. Audrey Kennedy, Ms. Latoya Perkins, and Ms. Florence Woolaver have provided temporary administrative support during this transition. An extensive search was conducted for a replacement this fall, and Ms. Woolaver will become the permanent ICA Assistant beginning in January. Mr. Nick MacDonald joined the ICA as a graduate student in the fall working with Dr. Clarke. Former ICA postdoctoral fellow Dr. Amanda Karakas received a three year Australian Postdoctoral fellowship from the Australian Research Council and returned to Australia from her post doctoral position at McMaster University this fall. The ICA expects to hire two more postdoctoral fellows early in 2007 through the ACEnet Postdoctoral Fellowship program.

EVENTS in 2006

The ICA participated in three conferences during the spring and summer of 2006. ACEnet was the host of the 20th annual High Performance Computing Symposium at Memorial University in St. John's, Newfoundland in May. Dr. Deupree and Ms. Adams served as the editors of the proceedings of the conference. Unlike many conferences in astronomy, the proceedings were published by the time the conference was held, so it was a busy spring for the editors. The Division of Dynamical Astronomy of the American Astronomical Society held its annual meeting in Halifax during the last week of June, with the ICA and Saint Mary's University as the hosts. The meeting was organized by Dr. Hahn with assistance from Ms. Adams and Ms. Elfrie Waters, the Department of Astronomy and Physics secretary. Finally, there was a three day MOST satellite meeting held at Saint Mary's in June. Dr. Guenther was the host, aided by Ms. Adams.

The ICA had a number of visitors during the past year for periods as short as a few days up to about six weeks. These included Dr. David Ballantyne (University of Arizona), Ms. Houria Belkus (Vrise Universiteit Brussels), Mr. Chris Cameron (University of British Columbia), Dr. Joyce Guzik (Los Alamos National Laboratory), Dr. Falk Herwig (Los Alamos National Laboratory), Dr. Jennifer Hoffman (Berkeley), Dr. Thomas Kallinger (University of Vienna), Dr. Rob Thacker (Queen's University), and Dr. Toru Okuda (Hokkaido University).

Dr. Guenther spent the academic year 2005-6 on sabbatical. He spent three months working with Professor Werner Weiss and the asteroseismology group at the University of Vienna. This included a series of lectures Dr. Guenther presented on asteroseismology. Dr. Guenther also received the Saint Mary's University President's Award for Excellence in Research.

Dr. Deupree's term as the CASCA representative on the CITA Board ended this summer. He began his term on the Advisory Board of the Herzberg Institute for Astrophysics early this year. He continues to serve as the Principal Investigator of ACEnet, the regional high performance computing (HPC) consortium for Atlantic Canada. He acquired the extra duty this year of becoming a member of the National Initiatives Committee (NIC), made up of the principal investigators of the seven regional HPC consortia throughout Canada. The NIC was tasked with writing a proposal for the Canada Foundation for Innovation (CFI) National Platform Fund. The proposal, submitted in June, was for $60M in CFI funds, to be matched by $60M from provincial sources and $30M from vendor in kind contributions. On December 21, 2006 the CFI announced it would fund the proposal in its entirety. Part of the proposal was to develop a national management and governance structure for HPC in Canada. Filling in the details of this management structure is expected to continue for several months, and the NIC will work with several other organizations to determine the final structure.

Looking forward to this new managerial structure, Dr. Deupree joined the board of C3.ca this spring. C3.ca has for a number of years promoted the welfare of HPC in Canada, including the Long Range Plan for HPC which many believe contributed greatly to the establishment of the National Platform Fund call in HPC.

ACEnet was able to obtain all required matching funds to its CFI award in the spring of 2006 and began to build its HPC infrastructure. Significant computational resources were placed at Saint Mary's University, St. Francis Xavier University, and Memorial University of Newfoundland in June. Saint Mary's is host to a 168 node Opteron cluster with Myranet interconnects. Mr. Phil Romkey has been hired as the resident ACEnet system administrator at Saint Mary's, with the ICA supplying his administrative support. During the coming year these clusters will be expanded, and new resources will be placed at Dalhousie University and the University of New Brunswick. It should be noted that all ICA personnel have access to all the ACEnet computational resources regardless of location. The ICA also maintains its own small 48 processor cluster for small projects and for testing. Construction continues on the ACEnet Access Grid and Data Cave rooms at Saint Mary's, and it is expected that the Access Grid multi-site, video teleconferencing system will be installed in early to mid January of 2007. The Data Cave is expected to be installed in the spring of 2007 after the construction residue is completely gone. The Access Grid capability will allow ICA members to interact visually and audibly with researchers at multiple institutions at once. The NIC proposed that all major academic research institutions in Canada acquire Access Grid as part of the National Platform proposal so that we expect to work with other astrophysicists anywhere in Canada within about two years. The ICA will be responsible for the Data Cave, the Access Grid room, and another visualization room which will include several computers with high powered graphics cards and large screens for more traditional visualization needs. ICA members expect to be very heavy users of the Data Cave.

UNDERGRADUATE RESEARCHERS

ICA faculty again hosted several undergraduate researchers during the summer. Dr. Short led Ms. Christine Hiratsuka and Ms. Jayme Derrah in their Honors thesis work on non-LTE analysis of carbon and oxygen in the Sun and Arcturus, respectively. Second year student Mr. James Sherar worked with Dr. Short on producing synthetic photometry with PHOENIX stellar atmosphere models. Mr. Michael Cooper, a third year student from Dalhousie University, worked with Dr. Deupree and Master's student Mr. Chris Geroux on producing synthetic cluster HR diagrams in which individual cluster members may be rotating at any rate. The undergraduate students participated in the Undergraduate Research Symposium, in which all undergraduate students who work in the Department of Astronomy and Physics give papers describing their summer research. Mr. Patrick Rogers completed his undergraduate Honors degree with Dr. Deupree this spring. His thesis work involved computing the gravitational potential at the surface of each member of a binary system and comparing the result to the Roche potential. Mr. Rogers won the Governor's medal for his undergraduate work and began his graduate work at McMaster University this fall.

RESEARCH

Here we present summaries of the research carried out by ICA members during this past year.

Dr. Clarke and fellow researchers are finishing an intensive code development phase, and as a result, there is only one new publication from Dr. Men'shchikov to report this year. AZEuS, the merger of Adaptive Mesh Refinement (AMR) and ZEUS-3D, continues to represent the bulk of their efforts. While much of this work was performed by Dr. Men'shchikov, several important aspects of the code were not complete at the time of his departure. These have been taken over and largely completed by graduate student Mr. Jon Ramsey and Dr. Clarke.

A manuscript entitled "Magneto-centrifugal launching of jets from Keplerian discs, and the use of the polytropic equation of state" by Dr. Clarke and Mr. Ramsey will be revised once some issues related to the boundaries of the problem are resolved.

Mr. Jon Ramsey is beginning to test AZEuS on problems directly relevant to his Ph.D. dissertation research, namely the numerical simulation of a proto-stellar jet from the accretion disc that launches it to observational scales. Such a simulation has never been attempted before because it requires following the same simulation over six orders of magnitude of scale lengths. Indeed, this is one of the drivers for the development of AZEuS.

Mr. Nick MacDonald has begun his M.Sc. thesis work to map jets and lobes of extragalactic radio sources (ERS). Nearly 20 years ago, Dr. Clarke published a couple of papers with Drs. Michael Norman and Jack Burns in which they presented the first "numerical observations" of giant radio lobes from simulations of jets with "passive" magnetic fields. They had a self-consistent description of the magnetic field, but no prescription for the spectrum of the relativistic electrons, and thus our false synchrotron emission images lacked some realism. For example, they had no way to track the "synchrotron aging" of the particles, nor any accurate way to account for re-energisation of electrons at shocks.

Within the past five years, Dr. Tom Jones and his group at Minnesota published some false images of radio jets and lobes with both magnetic fields and a realistic description of the particle spectrum. The latter was accomplished by solving the so-called Skilling equation, which is actually a 4-D problem including three spatial dimensions and one momentum dimension. This work represents a major leap forward in understanding why ERS emit the way they do but, unfortunately, it also requires the solution of a technically difficult equation on a 4-D grid, rendering such simulations impractical for most applications.

Dr. Clarke's and Mr. MacDonald's idea is to model the particle spectrum as a two-index power law (which the Jones' work largely confirms), with the break in the power law being tracked for each zone as a simple advected quantity. With the break in the power spectrum known (and affected by both aging and shock-reacceleration), they hope to reproduce all the qualitative effects found by the Jones group, and much of the quantitative results as well, with a much simpler scheme.

Dr. Clarke, ICA visitor Dr. Toru Okuda, and Dr. Alex Razoumov have made a first attempt at installing a radiative transport module in ZEUS-3D which, when complete, would be migrated to AZEuS. Dr. Okuda is interested in the physics of accretion discs surrounding compact objects, and needs the self-gravity and MHD aspects of ZEUS-3D with his radiative transport modules to advance his investigations. This work is still at a very early stage.

With Dr. Phil Bennett (adjunct faculty at Saint Mary's University) and Dr. Wendy Hagen-Bauer of Wellesley College in Massachusetts, Dr. Clarke is a co-Investigator on a recently submitted NSF proposal to study the peculiar binary system VV Cep. This system consists of two very massive stars, one slightly more massive than the other. The more massive star is a supergiant, while the less massive star is still a compact MS object. While the supermassive star has not filled its Roche lobe (the stars are in a highly elliptic orbit of several thousand AUs), it does launch a significant wind, some of which is trapped and accreted by the compact companion. Dr. Clarke has been asked to help the group understand what role the hydrodynamics of such a complex system might have in modifying the observed spectra and variability, data which will be gathered by extensive HST time. The team also includes Dr. Ted Gull at NASA Goddard, who is the deputy PI of the project that developed the Space Telescope Imaging Spectrograph (STIS), which will play an important role in the observations anticipated for this project.

The paper by Ms. Catherine Lovekin and Drs. Deupree and Short (ApJ, 643, 460) that determines the observed spectral energy distribution for a 2D rotating stellar structure model by performing a weighted integral of the emergent intensity over the stellar disk has been published. The rotating model provides the latitudinal variation of the effective temperature and surface radius, and the intensities are interpolated in effective temperature and gravity through a grid of

PHOENIX model atmospheres. The resultant spectral energy distribution for a given model produces a deduced luminosity and effective temperature as a function of the inclination between the observer and the rotation axis. These results were compared to results calculated using von Zeipel's law and found to disagree noticeably for rapid rotating stars.

Dr. Deupree and Mr. Patrick Rogers expanded the work done by Drs. Deupree and Karakas (ApJ, 633, 418) on 2D binary star evolution. The earlier work had calculated the stellar structure and evolution of each of two members of a binary system assuming that the gravitational potential of the other member could be treated as that of a point source. Mr. Rogers for his Honors thesis wrote a code to take the stellar structure of each of the two stars and their separation and calculate the total gravitational potential on the surface of each star. This potential was compared with the total potential calculated by Deupree and Karakas and was found to agree to with 0.5%. This suggests that the Deupree and Karakas calculations give an acceptable representation of the stellar structure of each of the two binary members.

Dr. Deupree and Mr. Joel Tanner are completing a project examining the radial fundamental mode Beta Cephei stars in NGC 3293. This work combines 2D stellar evolution sequences of rotating stars, the 2D stellar pulsation code of Clement (ApJS, 116, 57) for determining the pulsation modes of rotating stars, and the integration code of Lovekin, Deupree, and Short to properly place the individual stars in the HR diagram as a function of the inclination between the rotation axis and the observer. They show that they can fit the radial fundamental mode for each of the four Beta Cephei stars in the cluster identified to pulsate in that mode, as well as determine the inclination and rotational velocity from the models, and match the observed location in the HR diagram and the observed projected rotational velocity. The results suggest this approach will be useful as a probe in determining the structure and interior angular momentum distribution of rapidly rotating stars.

Dr. Deupree and Mr. Chris Geroux have developed a code for creating synthetic cluster HR diagrams. The code allows for the individual stars to be assigned an arbitrary rotation rate and random inclination between the rotation axis and the observer. The code interpolates among 2D stellar evolution sequences and uses the integration code of Lovekin, Deupree, and Short to determine the deduced effective temperature and luminosity as functions of inclination. Clusters are now being simulated to determine the probability that stars of a given rotation rate dominate a given portion of the observed HR diagram. This may help in being able to determine the relative distribution of angular momentum among stars when compared with observed clusters.

Dr. Deupree and Mr. Aaron Gillich are expanding on the work of Lovekin, Deupree, and Short to include modeling line profiles as well as the entire spectral energy distribution.

Dr. David Guenther continued to analyze the data coming from Canada's first space telescope, MOST. He shares responsibility with the other 7 science team members for the stellar modeling, oscillation modeling, and interpretation of the data obtained from the satellite. He participated in the MOST science team meeting, December 2005 in Vienna.

Dr. Deupree worked with Dr. Nathalie Toque to solve some problems with the 2D stellar evolution code that arose for models with extreme differential rotation. Dr. Toque resolved the issues and the code now produces ZAMS models for models rotating under these conditions. Dr. Toque is now working on evolving the rotating models and including in a realistic way the secular instabilities that can transport both composition and angular momentum from the core to the outer layers.

Dr. Guenther completed his analysis of the sun-like star observations from MOST. Considerable time was spent dealing with a serious contaminant in the data caused by sunlight reflected off of the earth that was leaking into the optics of the MOST telescope.

He studied the data reduction techniques used by the Vienna asteroseismology group. This included reviewing and refereeing a new technique called sigspec, invented by graduate student Peter Regeen (University of Vienna), that assigns a probability function to power spectrum peaks.

Dr. Guenther collaborated with University of Vienna graduate students, Mr. Thomas Kallinger and Ms. Konstanze Zwintz. He showed that their observations of oscillations on pre-main sequence stars (very young stars just recently formed) could be fully explained as nonradial oscillations. The existence of nonradial oscillations on pre-main sequence stars had been speculated before but never established through model fits to the observations.

Dr. Guenther also worked with Mr. Kallinger to show that the oscillations Mr. Kallinger observed on a K giant could be explained as nonradial oscillations. Mr. Kallinger proposed an essential fix to Dr. Guenther's stellar pulsation code that enabled them to compute mixed modes for these evolved stars. Prior to their discovery, it was not believed possible to observe nonradial oscillations on giants.

Based on these discoveries, the MOST science team has agreed to dedicate over two months next year to observing pre-main sequence and giant stars. Dr. Guenther has begun computing pre-main sequence and giant star models and their oscillation spectra to aid in the analysis of these future observations.

Dr. Guenther continued his work with the Yale Convection Group (Dr. P. Demarque, P.I.) on calculating three-dimensional stellar convection zones. They proposed models to explain the unexpected null detection of p-modes on Procyon. They have developed a new technique that will enable them to approximate the detailed (computationally lengthy) solutions from their convection simulations without having to redo the calculation from scratch. They are also in the process of testing an adaptive mesh size algorithm upgrade to their convection code that reduces computation times by up to a factor of 10.

With Dr. Peter Hauschildt (Hamburger Sternwarte) Dr. Short is continuing a program to computationally model the atmospheres and spectra of the recently discovered extremely metal poor (XMP) red giant stars with unprecedented realism in the description of the state of the gas and radiation field. The unique attribute of this modeling is that tens of thousands of the most important spectral absorption lines, including the pervasive veil of Fe I and Fe II lines, are allowed to depart from local thermodynamic equilibrium (LTE). The result will be a more accurate spectroscopic determination of the chemical composition of these primordial stars.

With Ph.D. student Ms. Birgit Fuhrmeister and Dr. Peter Hauschildt (Hamburger Sternwarte) Dr. Short has revived a program to adapt the *PHOENIX* atmospheric modeling and spectrum synthesis code to model the spectrum formation of the atmospheres of stars, such as the Sun, that have a temperature inversion such that the star is surrounded by a chromosphere and corona of much higher temperature than the visible photosphere. The nature of the physical mechanism by which the outer atmosphere is so dramatically heated is one of the main outstanding problems in the astrophysics of late type stellar atmospheres. Unlike previous investigations in which only a few spectral features that diagnose the state of the outer atmosphere could be modeled in non-LTE (NLTE) while most spectral lines were held in unrealistic LTE, *PHOENIX* can model simultaneously tens of thousands of spectral lines in NLTE taking into account NLTE effects among chemical species due to overlapping transitions. Preliminary results indicate that the computed strength of diagnostic spectral lines, and hence the inferred state of the outer atmosphere, depends much more sensitively than previously known on irradiation of the chromosphere from emission lines of the third and fourth ionization stages of elements in the transition region between the chromosphere and corona.

With M.Sc. student Mr. Aaron Gillich and Dr. Robert Deupree, Dr. Short is continuing a program to model the spectra of stars for which the stellar parameters vary continuously as a function of position on the stellar surface as a result of either rapid rotation or tidal distortion in a close binary star system. The unique attribute of this modeling is that the variation of stellar parameters across the stellar surface is specified by stellar interior models that have been evolved with a proper two-dimensional (2D) code (ROTORC - Deupree), and that the atmospheric models and spectrum synthesis incorporate tens of thousands of the most important spectral lines in NLTE.

With Drs. Pierre Demarque and Christian Straka (Yale University) Dr. Short has begun a collaboration to model the outer boundary condition of M dwarf interior structure models more realistically by accounting for hydrodynamic atmospheric turbulence. Dr. Short will be calculating mean radiative opacities suitable for radiation hydrodynamic simulations. The goal is to resolve the discrepancy between the observed and computed mass-radius relation among M dwarf stars.

The relatively cool barely evolved standard star Procyon (α Canis Minoris) has been the subject of much interest recently. It has been the target of a recent interferometric study in the near IR band that has provided unprecedented information of the variation of the visibility with wavelength tantalizingly close to the visible band. This is a major step toward imaging the surface of a dwarf star other than the Sun at optical wavelengths. Moreover, Procyon was a target of the Canadian MOST satellite and was found to have significantly lower amplitude oscillations than expected for a star of its parameters. However, previous analyses of the star’s spectrum and spectroscopic determinations of its atmospheric properties were based on LTE modeling. I have begun a program to model the high resolution Griffin atlas of Procyon with the same type of massively Non-LTE modeling that I have recently applied to the Sun and metal poor red giants to investigate how the inferred atmospheric properties are affected when more realistic modeling is applied.

Dr. Alexei Razoumov's research is focused on high-resolution numerical models of galaxy formation, more specifically on the accurate treatment of radiative and mechanical feedback from star formation and understanding how this feedback affects the thermal state of the interstellar and intergalactic gas out of which these stars form in the first place.

Dr. Razoumov collaborated with Jesper Sommer-Larsen from the University of Copenhagen to calculate the ionization structure of gas in high-redshift star forming regions. Using results from high-resolution (15 pc) galaxy formation simulations in a standard Lambda-CDM cosmology and a fully conservative multi-resolution radiative transfer code around point sources which Dr. Razoumov wrote in 2005, they computed the escape fraction of ionizing photons from a large number of star forming regions in several dozen galaxies (covering a wide range of galaxy types and masses) as a function of redshift from z=3.8 to 2.39. While their results agree well with observational findings on the redshift evolution of the escape fraction in the same redshift interval, their longer term-goal is to try to understand the physical condition for high-redshift star formation which is currently implemented into simulations in a crude phenomenological way.

As part of this effort, in the summer of 2006 Dr. Razoumov included a radiative transfer module into a cosmological structure formation code Enzo which would allow coupled radiation-hydrodynamics modeling of galaxy formation. In hierarchical models of structure formation in the universe small objects form first, and later they merge into larger galaxies. Since small galaxies are particularly susceptible to radiative feedback, it is of crucial importance to include it into numerical models of the early stages of galaxy formation. In addition, such models examine a link between the first stars and the physical properties of the surrounding gas and thus provide a framework to interpret forthcoming observational data on the very high-z universe.

Dr. Razoumov also worked on the effect of star formation on the properties of damped Ly-alpha (DLA) systems at z=3. Earlier in 2006 he published a paper showing the need for accurate radiative transfer to reconstruct the column density distribution of high-z absorbers. However, these models cannot explain the observed velocity width distribution of DLAs, and in the past 12 months Razoumov has put a lot of effort into improving these models, from working with various prescriptions for star formation to including molecular hydrogen. However, these simulations are extremely resolution dependent as one needs to resolve the multiphase interstellar medium while capturing the statistics on cosmological scales, and this work will certainly extend into 2007.

Dr. Joris Van Bever continues to work on the development of his spectral synthesis/N-body code, which is to be used to study the evolution of the observable properties of young, massive starbursts and their populations of massive stars and compact remnants. The code includes a detailed treatment not only of single stars but of binary stars as well, especially as far as the evolution of close binaries (i.e. interacting binaries) is concerned. Most of the parallellization of the code has been performed and is now being debugged for use on the ACEnet clusters.

As a subproject, and in collaboration with members of the Brussels (Belgium) research group (Dr. Dany Vanbeveren and PhD student, Ms. Houria Belkus), Dr. Van Bever has studied the evolution of extremely massive stars (initial mass of the order of hundred to a thousand solar masses, also referred to as very massive objects, VMOs). VMOs can be formed in the cores of dense stellar clusters (ρ = 10^5 stars/pc^3 or more) through a number of collisions between the most massive stars that were initially present in the cluster (usually as a result of the so-called core collapse stage of the cluster).

Stellar wind mass loss determines the evolution and final fate of these VMOs, and decides whether they form black holes (with normal mass or with intermediate mass) or explode as a pair instability supernova. A good knowledge of this aspect of stellar evolution is extremely important for a correct assessment of not only the behaviour of the VMO itself but also of its impact on the overall dynamical evolution of the cluster. This collaboration resulted in a paper that was submitted to ApJ.

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COLLOQUIA GIVEN BY ICA MEMBERS

Ian Short, "Data needs for stellar atmosphere and spectrum modeling", Invited review paper, NASA Laboratory Astrophysics Workshop 2006 (NASA LAW 2006), Las Vegas, February 2006.

Ian Short, "Stellar atmospheric models and the problem of chemical composition", Saint Mary's University Astronomy and Physics Colloquium, March 2006.

Ian Short, Acadia University Physics Department Colloquium, "Stellar atmospheric models and the problem of chemical composition", March 2006.

Robert Deupree, "Deconstructing Rotating Stars", Yale University Astronomy Department Colloquium, April 2006.

Robert Deupree, "Future of High Performance Computing in Canada", Invited talk, High Performance Computing Symposium, St. John's, NL, May 2006.

Ian Short, "Stellar atmosphere and spectrum modeling", Invited talk, Undergraduate Workshop of CASCA 2006 Annual Meeting, Calgary, June 2006.

Ian Short, Yale University Astronomy Department Colloquium, December 2006.

CONCLUDING REMARKS

This year is probably the most hectic that the ICA has faced. The time required in planning and running three conferences, in finalizing the ACEnet financial issues, and in the preparation of the National Platform Fund proposal has been significant. Yet both the addition of a third post doctoral position and the increased research potential of the ICA graduate students are helping the ICA make progress on the research front as well. The coming year will see continued growth in our capital resources through the arrival of the Data Cave, the high quality visualization computers, and more computational power through ACEnet. The anticipated arrival of Dr. Thacker next summer and two more post doctoral fellows in the next few months through the SUN-ACEnet post doctoral fellowship program will continue to energize the institution.