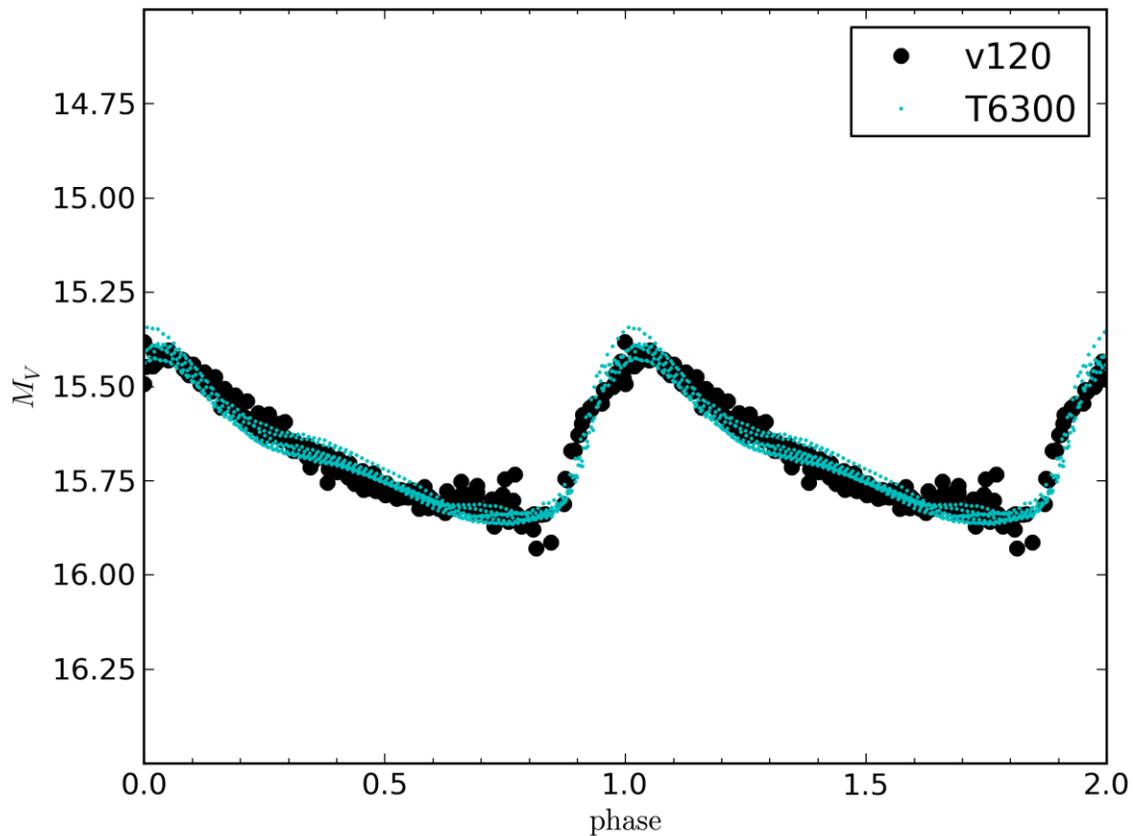


ANNUAL REPORT 2012



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Cover Image: Chris Geroux, Ph.D. student (see next page for caption)

Front Cover Photo Caption

The interaction of radial pulsation and convection has been a long standing problem in stellar astrophysics. This interaction becomes especially important as convection strengthens as the effective temperature of RR Lyrae stars approaches the effective temperature of the "red edge" of the RR Lyrae instability strip from the hotter side. The "red edge" is the cool side of the region in temperature and luminosity space where RR Lyrae stars pulsate. Recent work by Marconi et al. (2007) showed that while a 1D time dependent mixing length theory approach works reasonably well for matching observed light curves of RR Lyrae much hotter than the red edge, it has difficulty reproducing light curve shape and amplitude simultaneously near the red edge, in particular for variable star v120 in M 3 (See figure 17 of Marconi et al. 2007, A&A, 474, 557 for their fit to this star's light curve).

The image shows the phased, observed light curve from Cacciari et al. (2005) for v120, doubled to show two cycles for easier comparison. It is matched by the small cyan points for a 6300 K effective temperature model. The model is two dimensional with 20 horizontal zones covering 6 degrees of the simulated star's surface. The model light curve points are from seven consecutive periods at fully amplitude which have been phased and doubled in the same manner as the observations. Bolometric corrections from Bessell et al. (1998) have been used to convert the models absolute bolometric magnitude to absolute visual magnitude and a distance modulus of 15.34 has been chosen to allow comparison with the apparent visual magnitude of the observed light curve. The small spread in the model light curve points indicates how well the pulsation cycles reproduce. In fitting the light curve only the phase shift and distance modulus were adjusted. We also did not perform a detailed parameter search to find the best fundamental model parameters for matching this light curve but rather used values representative of the cluster as a whole. The fit is a noticeable improvement over the 1D time dependent mixing length approach for this cool RR Lyrae star.

These results are based on a 2D hydrodynamic simulation with the SPHERLS code, which is being developed in the ICA by Ph.D. student **Chris Geroux** under the guidance of **Dr. Robert Deupree**, ICA Director.

ICA Annual Report October, 2011 – September, 2012

Introduction

The ICA was created in late 2002 to promote the study of complex astrophysical phenomena by numerical simulation. Throughout the past decade the ICA has acquired access, through ACEnet and Compute Canada (in which several ICA members have played very significant roles), to significant high performance computing resources required for these simulations. In addition the ICA has enriched the environment of the Department of Astronomy and Physics by hiring ten postdoctoral fellows since its inception. A number of graduate students have been part of the ICA, and to date eight MSc. degrees and three Ph. D. degrees have been awarded to ICA students. Several more students are nearing completion of their degree programs at both the MSc. and Ph. D. level. Currently ten of the twelve graduate students in the Department of Astronomy and Physics MSc. and Ph. D. programs have ICA faculty members as supervisors.

The ICA has six full time faculty members, each of whom is also a faculty member in the Department of Astronomy and Physics. They are Dr. Robert Deupree, Director and Tier 1 Canada Research Chair, Dr. David Clarke, Dr. David Guenther, Dr. Marcin Sawicki, Dr. Ian Short, and Dr. Rob Thacker, Tier 2 Canada Research Chair. Drs. Guenther, Short, and Sawicki were on sabbatical for at least part of calendar year 2012. Two postdoctoral fellows, Dr. Fernando Peña and Dr. Taro Sato, completed their terms. Dr. Peña obtained a postdoctoral position at Dalhousie University performing mathematical calculations for medical research and Dr. Sato returned to the USA. Ph. D. student Mr. David Williamson has taken up a position in South Korea teaching English as a second language. Ph. D. student Mr. Chris Geroux has taken up a postdoctoral position with Dr. Isabelle Baraffe at the University of Exeter. Both will be defending their respective theses in January, 2013. Dr. Mike Casey, who completed his Ph. D. degree in the fall of 2011 and chose to remain in Halifax for family reasons, has accepted a research position at the Bedford Institute of Oceanography. Two Master's students, Ms. Anneya Golob and Mr. Diego Castañeda, are expected to defend their respective theses in December 2012 or early January, 2013.

Ms. Florence Woolaver is completing her sixth year as the ICA administrative assistant. Attached to the ICA are three ACEnet employees, Mr. Stephen Condran, Mr. Phil Romkey and Dr. Sergiy Khan. Mr. Romkey is the system administrator for the Mahone computer cluster, and Dr. Khan provides

computational researchers with support on issues related to using the ACEnet clusters. Dr. Khan's background is in astrophysics, and he has helped a number of ICA postdoctoral fellows and graduate students with specific code issues. Mr. Condran arrived in early September and is the system manager for the Brasdor cluster. Ms. Woolaver supplies administrative support to local ACEnet personnel and acts as a key interface between SMU and the ACEnet administration in St. John's and between SMU and the ACEnet Chief Technology Officer located at Saint Francis Xavier University.

Events in the Past Year

The ICA has organized two meetings on the SMU campus this year. In October 2011 the annual national meeting of the technical support personnel of all Compute Canada consortia was held at Saint Mary's. Dr. Deupree opened the meeting by welcoming the attendees and making some introductory remarks. In July Saint Mary's hosted an ACEnet sponsored introductory course in high level computing (the "Software Carpentry Workshop") given by Greg Wilson. Ms. Woolaver provided the comparatively extensive administrative organizational support required for both meetings. In addition, many ICA faculty and students participated in the second ACEnet annual meeting (at Dalhousie; the first was at Saint Mary's last year) outlining the current state of affairs in ACEnet and Compute Canada and the expectations for the next one or two years.

Dr. Thacker's CRC Tier 2 position was renewed, and he received an associated CFI award of approximately \$90k in computer hardware. In addition, Dr. Thacker is the Principal Investigator of a proposal to Compute Canada that was awarded 2.5 million CPU hours on the WestGrid clusters.

The ICA hosted seven visitors for periods ranging from a few days to about five weeks. Five of the visitors presented colloquia to the Department of Astronomy and Physics weekly colloquium series.

ICA Member Service

Members of the ICA play significant roles in service to the university, the community, and to the astronomical community on both the national and international scale. Here some of these activities are summarized.

Dr. Deupree continues to serve on the Advisory Board of the NRC's Herzberg Institute of Astrophysics. He is now in his second and final term and brings his experience in high performance computing to the Board. He also serves as a member of the ACEnet's Chairs of the Local Users Group and is the Chair of the Saint Mary's Local Users Group. Dr. Deupree also served as the internal chair of the external review of the Saint Mary's Ph. D. program in Management.

Dr. Clarke serves on several university committees, including the Science Curriculum and Science Space Committees. He also organized the Astronomy and Physics Department's Undergraduate Summer Research Mini-Symposium, which included presentations by several ICA related undergraduate students.

Dr. Guenther is a member of the BRITE Constellation consortium. The BRITE Constellation is a proposed set of six nano-satellites designed to observe oscillations on the brightest stars in the sky. The project represents a joint collaboration of Canadian, Polish, and Austrian asteroseismologists. The first four satellites are scheduled for launch in 2012, with the two remaining (Canadian) satellites to be launched in 2013. Guenther will contribute asteroseismic modeling of red giants. Dr. Guenther also continues his collaborations with Dr. Kostanze Zwintz (University of Vienna) on modelling the oscillation spectra of pre-main sequence stars and with Dr. Thomas Kallinger (Belgium) on modelling the oscillation spectra of red giants obtained by the CoRoT and MOST satellites. His collaborations with the MOST Science Team and the Yale Convection Group continue.

Dr. Sawicki continues to serve the profession in a number of ways. Organizationally, he serves as the vice chair of the Association of Canadian Universities for Research in Astronomy (ACURA) Board of Management and on the Board of Directors of the Canadian Astronomical Society (CASCA). He is on the Science Advisory Committees for the Canadian segment of the Canada-France-Hawaii Telescope (CFHT), Gemini, and ALMA. Other service includes membership on the Science Team for the TFI/NIRISS instrument being built by Canada for the James Webb Space Telescope, being the PI of the Canadian Euclid

Science Ground Segment Phase 0 study for the Canadian Space Agency (CSA), and the Canadian collaboration contact for the JAXA sponsored WISH telescope project. He is member of the Extragalactic Science Team for the next generation CFHT project and of the Canadian Space telescope study team for the CSA. Finally, he continues to demonstrate his commitment to the popularization of astronomy through his participation of the Beyond IYA Committee.

Dr. Short continues to serve on the CASCA Awards and Education and Public Outreach committees and has become the Saint Mary's member of the ACEnet Research Directorate. He also served on the time allocation committee for the Canadian share of telescope time on the international offshore facilities of which Canada is a part.

Dr. Thacker continues to serve as the head of the Astronomy and Physics Department and as a member of the Canadian Astronomical Society's (CASCA) Implementation Committee for the Long Range Plan in Astronomy. He has also served as a member of the time allocation committee for the Canadian share of telescope time.

ICA Member Research Contributions

All of the ICA faculty members maintain very active research programs involving not only themselves, but also postdoctoral fellows, graduate students, and occasionally undergraduate summer researchers. All participate in publishing papers, as well as serving as referees for various astrophysical journals. Here we present a brief summary of ICA members' research accomplishments for the past year.

Dr. Deupree, along with postdoctoral fellow Dr. Fernando Peña, MSc. student Diego Castañeda, and Dr. Ian Short, performed numerous calculations related to the rapidly rotating, pulsating δ Scuti star, α Oph. Dr. Deupree first computed evolutionary models which could match the observed oblateness, approximate effective temperature, and a number of the oscillation frequencies of the star. These results were not overly satisfactory from an intellectual point of view because the models were not sufficiently constrained to allow conclusions about the nature of α Oph. The research was then expanded to include computing the spectral energy distribution of the models and comparing that the observed

spectral energy distribution. This suggested that the original models had too high effective temperatures. Further models were computed which did match the observed spectral energy distribution and most of the observed oscillation frequencies. All of the models to date had assumed uniform rotation, unlikely given that the star is near the end of its core hydrogen burning phase. Dr. Deupree and Mr. Castañeda computed three models with differential rotation which bridged the region between uniform rotation and the rotation profile one would expect for a model which locally conserved angular momentum. Spectral energy distributions and line profiles were then computed from these models. These calculations show that the results are not much changed from those of the uniformly rotating model. This unfortunately implies that the observed information is probably not going to be very useful in constraining the rotation law of stars of this sort.

Dr. Deupree and Mr. Castañeda also computed spectral energy distributions for a large number of uniformly rotating Zero Age Main Sequence models published last year by Dr. Deupree. In that work it was found that the surface effective temperature, radius, and rotational velocity as functions of latitude were scalable between two models as long as the surface shape remained the same (it is implicit in this that the rotation law remains the same except for a scaling factor). A study has begun to discover whether this means that the observable properties one would deduce from the spectral energy distribution, such as the effective temperature and luminosity, are scalable as well. Because these depend on the inclination between the rotation axis and the observer, such scaling should aid in isolating what models are appropriate for a given observed star.

Mr. Chris Geroux, supervised by Dr. Deupree, has completed his Ph. D. research. He has performed a number of 1D, 2D, and 3D numerical simulations of pulsating RR Lyrae stars. The multidimensional models allow convective motions to be generated naturally in convectively unstable regions and enable the study of the interaction of convection and stellar pulsation without resort to a phenomenological approach to convection such as the local mixing length theory. While the 3D calculations are more realistic, of course, the relationship between convection and pulsation phase is nearly the same in both 2D and 3D calculations. Convection significantly reduced the pulsational growth rates from the 1D (no convection) calculations. The effect of convection on decreasing the pulsation growth rates is only very slightly larger with the 3D models than the 2D models. One of the main goals of the research was to be able to perform these multi-dimensional calculations to full amplitude pulsation. This has been completed for the 2D models with the result that the agreement for relatively blue fundamental mode pulsator models, in which convection is relatively ineffective, is relatively

good both with observations of RR Lyrae stars in M3 and with 1D mixing length calculations performed by Marconi, et al. (ApJ, 596, 299). The RR Lyrae stars chosen for a given model had nearly the same amplitude as the model, and the temperatures were characteristically well within 100 K of those of the model. The agreement with observations for models closer to the red edge is better than that obtained with 1D mixing length full amplitude calculations, even though the parameter space explored with the 1D calculations was appreciably larger than for the 2D calculations. As one can imagine, the required computer time, even with appreciable parallel processing, for the 3D calculations to reach full amplitude is formidable, and the 3D full amplitude solutions will not be a part of the thesis. They are expected to be completed sometime in the spring, 2013.

Dr. Clarke continues to work with Dr. Jon Ramsey, former ICA Ph. D. recipient and current postdoctoral fellow at the University of Heidelberg, on papers related to Jon's thesis. This research investigated the relationship between the site where protostellar jets are launched, and the much larger scale (by about five orders of magnitude) where they are routinely observed. This entire range was computed in one simulation. They have discovered a hitherto unknown relationship between the jet's advance speed and its rotation speed, the consequences of which are currently being investigated. They also find that observable properties of the jet, such as the advance speed, mass flux, and angular momentum are all related by a power law to the strength of the magnetic field near the origin of the jet. However, the jet radius and even the magnetic field strength in the large scale jet are not strongly related to the magnetic field at the base of the jet; all jets appear to evolve into a $\beta \approx 1$ plasma. Finally, a simple harmonic knot generator is established near the launch site of the jet whose period is tightly coupled with the magnetic field strength. For future, high-resolution observations, this may provide a means by which the magnetic field strength can be measured.

Dr. Clarke is also working on a new numerical algorithm for his 3D hydrodynamics code, ZEUS-3D. He has found algorithmic solutions to long-standing issues with the main ZEUS-3D algorithm that prevented the code from performing seemingly "simple" 2-D advection tests satisfactorily. The problem has to do with the sequencing of the various sub-algorithms that make up the "Consistent Method of Characteristics" (CMoC) algorithm used in the code since 1994 (Clarke, 1996, ApJ, 457, 291). It seems likely that with these modifications, ZEUS-3D can be rendered fully second-order accurate and conservative in both total energy (already implemented) and momentum (to be implemented) while still maintaining its traditional staggered-mesh, non-Godunov approach.

With Dr. Zwintz, Dr. Guenther is modeling current observations on pre-main-sequence pulsating stars from the ground, MOST, and CoRoT. Based on a technique developed by Dr. Guenther's Ph.D. student, Mr. Mike Casey, they have been able to untangle the unique oscillation spectra of several types of pre-main-sequence stars.

With Dr. Kallinger, Dr. Guenther is modeling the oscillation spectra of red giant stars observed by CoRoT, Kepler, and MOST. Dr. Guenther contributed a new method to compute directly the observable oscillation modes in red giants, uncontaminated by the thousands of unobservable mixed modes.

Dr. Guenther is supervising his graduate student, Mr. Michael Gruberbauer (an NSERC Vanier Fellowship holder), in developing Bayesian techniques to determine corrections for non-specific surface layer effects on the oscillation modes observed in stars. They published the techniques paper and are now working on several application papers, including a detailed re-examination of the oscillation spectrum of the Sun and its deduced age and composition.

Dr. Guenther has developed a combined pulsation and evolution computer code (*YJG*). The code can compute pulsation spectra of models of evolving stars. The code incorporates components from the Yale Rotating Evolution Code (Drs. Demarque, Guenther, and Pinsonneault) and Dr. Guenther's nonadiabatic, nonradial stellar pulsation code. The updated code also includes new routines to compute convective core overshoot using more realistic physics based on the Kuhfuss treatment. With Professor Demarque (Yale) and graduate student Mr. Michael Gruberbauer, they are exploring the effects of core overshoot on models of Procyon.

Mr. Gruberbauer is also investigating surface effects in asteroseismology. He has presented results of his research at several conferences including the Kepler workshops. He has published one paper on his thesis work, with two more papers in preparation.

Dr. Guenther supervised Ph.D. candidate Mr. Mike Casey. Mr. Casey completed his studies of the seismic properties of pre-main sequence stars. He has presented results of his research at several conferences, including the PMS workshop, Vienna, and CASCA, London, Ontario and has a paper based on one of the results of his thesis submitted to the MNRAS.

Dr. Sawicki's research interests are the formation and evolution of galaxies in the distant universe. His research is on the observational side and he and members of his research group use HPC to process and analyze large observational datasets and carry out associated simulations. Under Sawicki's supervision, Ms. Liz Arcila-Osejo and Dr. Taro Sato have been using the Canada-France-Hawaii Telescope Legacy Survey (CFHTLS) data to characterize the populations of passively-evolving and actively-star-forming galaxies at redshift $z \sim 2$; Ms. Anneya Golob worked on the characterization of extreme, blue "BX galaxies" also at $z \sim 2$; and Mr. Robert Sorba is working on spatially-resolved spectral energy distribution (SED) fitting of galaxy images. All these projects make extensive use of ACENet computers. This year also saw the finalization of a paper on Sawicki's "SEDfit" software which forms the foundations of much of his and his group's research, and the delivery to NASA of JWST's FGS/NIRISS instrument, on whose science team Dr. Sawicki is a member. During the first half of 2012 much of Dr. Sawicki's time has been consumed by efforts to enable Canadian participation in the European-led Euclid dark energy mission; while the Phase-0 study that he led was selected by the Canadian Space Agency (CSA) as their top choice for Canadian participation in Euclid, severe budget cuts suffered by the CSA this year put any such plans on hold. In the second half of 2012 (and continuing into 2013) Dr. Sawicki was on sabbatical research leave at Tohoku University in Sendai, Japan, to collaborate with Dr. Toru Yamada and other staff members on the WISH space telescope project and other endeavors.

Dr. Short, working with undergraduate students Mr. Eamonn Campbell and Ms. Heather Pickup and collaborator Dr. Peter Hauschildt (Hamburger Sternwarte), showed that computational models of red giant atmospheres and spectra with hundreds of atomic opacity sources treated with the PHOENIX code in more realistic non-local thermodynamic equilibrium (Non-LTE) leads to effective temperatures inferred from spectral energy distributions (SEDs) that are about 50 K cooler than those derived from the more common LTE modelling. Dr. Short has extended his grid of NLTE models of late type giant stars by including two competing solar abundance distributions (Grevesse and Sauval 1998 ("GS98"), used previously, and Grevesse, Asplund, Sauval, and Scott 2010 ("GASS10")), and to include non-solar abundance distributions that include enhancement of the alpha-process elements for the metal poor (1/3 solar metallicity) grid. He has also increased the effective numerical resolution of the SED grid by quadratic least-squares interpolation in the logarithmic flux to achieve $\Delta T_{\text{eff}} = 25 \text{ K}$ and $\Delta \log(g) = 0.25$. Comparison to a special library of observed SEDs for G8 to K4 III stars indicates that the adoption of the GASS10

abundances lowers the inferred T_{eff} by 25 to 50 K, in addition to the 50 – 75 K reduction due to Non-LTE (NLTE) effects.

Dr. Short also worked with a sizeable array of collaborators to perform a critical comparison of three of the world's leading stellar atmosphere and spectrum synthesis codes, PHOENIX, MARCS, and ATLAS9, by performing a blind experiment where groups using each of the three codes independently derived stellar parameters from observed spectra of known stars of concealed identity. The results show that there are still significant differences among these codes.

Dr. Short is working with MSc. student Mr. Mitch Young in combining 1D model atmospheres to simulate 3D atmospheres with horizontal inhomogeneity in the "1.5D" approximation to explore the biases introduced into stellar parameter (both spectroscopic and photometric) determination with 1D models. This is guided by recent results from 3D hydrodynamic simulations for select stars, but can be applied to a much larger number of stars quickly. The unique feature of this work will be an exploration of the degeneracy between 3D effects and NLTE effects on parameter determination from fitting spectral energy distributions (SEDs).

Mr. Chris Cooke, jointly supervised by Drs. Short and Guenther, is investigating methods for interpolating the Rosseland-optical-depth versus temperature relation among atmospheric models at canonical grid points in stellar parameter space to determine how to best determine the upper boundary condition needed for the calculation of asteroseismological modes of stellar structure models. This will include an investigation of NLTE effects on the optical-depth versus temperature relation and its significance for the predicted frequencies of asteroseismological models.

Dr. Thacker is involved in a collaborative project lead by Dr. Diego Saez (Universidad de Valencia, Spain) on weak lensing of the Cosmic Microwave Background (CMB). Dr. Saez and collaborators developed a numerical analysis tool for predicting the impact of weak lensing by foreground galaxy clusters on measurements of the CMB. Dr. Thacker provided a parallel version of the simulation code they have been using and together they are now running a series of simulations to make predictions for the Planck satellite. The overall impact of weak lensing on the CMB is actually comparatively small and restricted to small scales ("high ℓ 's"); however, Planck will be the first space-borne experiment capable of measuring the impact of weak lensing. The primary motivation for making these measurements is that accurate estimation of cosmological parameters

depends on being able to disentangle the impact of weak lensing on the primary CMB signal.

Following publication of their first work in this field they are now investigating the possibility of extending their work to investigate the impact of physics on the CMB. In particular they are interested in further detailing the impact of AGN on both lensing and the Sunyaev-Zel'dovich effect. This would be an extension of previous work conducted in 2006, and would also be the most advanced simulation of these effects to date.

Mr. James Wurster is just about finished with a paper on AGN feedback algorithms. Both he and supervisor Dr. Thacker have presented this research at a number of different conferences (Numerical Cosmology 2012, CASCA 2012 (Thacker), and Turbulence in Cosmic Structure (Arizona State University, March 2012, Wurster). In addition to this work he has also implemented a new feedback algorithm which introduces a number of new features and we have begun an informal collaboration with Dr. Frazer Pearce (U. Nottingham) on the details of this.

Mr. Dave Williamson published his results on effective viscosities in galactic disks due to molecular cloud collisions. This paper rectified a number of problems in earlier analytic work (essentially predicting the time scale was far too long). He presented this work at the turbulence conference in Arizona as well.

More recently Mr. Williamson has implemented models of subgrid turbulence within the FLASH code to examine their impact on modelling gas outflows due to star formation from galactic disks. These simulations are now being written up. We have found that while these models show promise for modelling the intracluster medium in galaxy clusters, they do not seem to be appropriate for modelling the small scale variation in gas structure seen in outflows. Mr. Williamson will be defending his Ph. D. thesis in early January when he returns from Korea.

Appendix 1: Publications and Talks of ICA Members

October 2011 – December 2012

Refereed Publications

- Appourchaux, T., Benomar, O., **Gruberbauer, M.**, Chaplin, W. J., García, R. A., Handberg, R., Verner, G. A., Antia, H. M., Campante, T. L., Davies, G. R., Deheuvels, S., Hekker, S., Howe, R., Salabert, D., Bedding, T. R., White, T. R., Houdek, G., Silva Aguirre, V., Elsworth, Y. P., van Cleve, J., Clarke, B. D., Hall, J. R., Kjeldsen, H., "Oscillation mode linewidths of main-sequence and subgiant stars observed by Kepler", 2012, A&A, 537A, 134
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- Calura, F., **Gibson, B. K.**, Michel-Dansac, L., Stinson, G. S., **Pilkington, K.**, House, E. L., Brook, C. B. & **Few, C. G.**, "The stellar metallicity distribution of disc galaxies and bulges in cosmological simulations", 2012, MNRAS, 427, 1401
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Colloquia and Presentations Given by ICA Members

- Dr. Robert Deupree, Los Alamos Stellar Hydrodynamics Workshop, Santa Fe, NM, "Computational Methods for the Evolution and Hydrodynamics of Rotating Stars", 2-4 April 2012
- Mr. Chris Geroux, Los Alamos Stellar Hydrodynamics Workshop, Santa Fe, NM, "3D Simulations of Convection-Pulsation Interaction in RR Lyrae Stars", 2-4 April 2012
- Dr. Ian Short, Mt. Allison University, Sackville, NB, "Non-LTE modelling of Red Giant Spectra", 4 November 2011
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- Dr. Robert Thacker, Numerical Cosmology 2012 Workshop, University of Cambridge UK, "A Comparative Study of AGN Feedback Models", 17-20 July 2012
- Dr. Robert Thacker, Monash University, Melbourne, Australia, "Skeletons in the AGN modelling cupboard", April 2012
- Dr. Robert Thacker, Swinburne University, Melbourne, Australia, "Skeletons in the AGN modelling cupboard", April 2012
- Mr. Dave Williamson, Saint Mary's University, "Do collisions between molecular clouds make a significant difference on a galactic scale?", 25 November 2011

Contributed Poster Papers

- C. Ian Short, "Modeling the near-UV band of GK stars: NLTE models", Cool Stars 17, Barcelona, 24-28 June 2012