2014-15 Progress Review Report of UK Consortium on Turbulent Reacting Flows (UKCTRF)

Introduction

Vision and work programme of UKCTRF

The UK Consortium on Turbulent Reacting Flows (UKCTRF) was launched on the 8th of January 2014 upon the successful outcome of the responsive mode collaborative research grant proposal EP/K025163/1 (involving 15 UK institutions and 1 Principal Investigator and 34 Co-Investigators), which was submitted to the Engineering and Physical Sciences Research Council (EPSRC) in 2013 (differing from other consortia which were funded through the High End Computing (HEC) call of EPSRC). The UKCTRF performs high-fidelity computational simulations (i.e. Reynolds Averaged Navier-Stokes simulations (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulations (DNS)) utilising national High Performance Computing (HPC) resources to address challenges related to energy efficiency through the fundamental physical understanding and modelling of turbulent reacting flows. Engineering applications range from the formulation of reliable fire-safety measures to the design of energy-efficient and environmentally-friendly internal combustion engines and gas turbines. The consortium serves as a platform to collaborate and share HPC expertise within the research community, and help UK computational reacting flow research to remain internationally competitive. The research of the consortium is divided into three broad work packages, which will be continued throughout the duration of the consortium, and which will be reinforced by other Research Council and industrial grants secured by the consortium members. These three work packages concentrate on (i) Fundamental physical understanding based on cutting-edge Direct Numerical Simulations of single- and multi-phase reacting flows, (ii) Applied research and technology development and (iii) Algorithm and architecture development for future platforms, respectively. The major scientific activities in individual work programmes are discussed below.

(i) WP1 Fundamental research: Improved fundamental physical understanding is warranted for turbulent premixed and non-premixed combustion of conventional hydrocarbon fuels and for new fuels. Fundamental research is necessary to explore the physics of combustion involving multiphase systems (e.g. droplet-laden mixtures), new and complex fuels, a range of different combustion regimes, detailed chemistry and molecular transport. The fundamental physical information obtained from WP1 will also provide the data required to develop and validate the models which are used in WP2.

(ii) WP2 Applied research and technology development: In this work package, emphasis is given to providing computational methods that can later be turned into applicable technologies, which will then contribute to improved fire-safety measures and the design of energy-efficient and environment-friendly IC engines and gas turbines. The applied research under UKCTRF will concentrate on LES/RANS simulations of gaseous-phase premixed, non-premixed and partially-premixed combustion, and numerical simulation of multiphase reacting flow simulations.

(iii) WP3 Algorithm and architecture development for future platforms: This work package will focus on providing advanced technical support to the consortium and on the collaborative development of the next-generation software that will provide the foundation for future HPC exploitation. In recent years, computer manufacturers have concentrated on developing hierarchical forms of hardware (e.g. multicore) to deliver performance. This trend is expected to continue and extracting this new level of concurrency from these hardware platforms has emerged as a major technical challenge. In addition, future platforms will see multicore CPUs with floating point accelerators provided by Graphical Processing Units (GPUs). The HPC community need to respond to this challenge by placing emphasis on designing and re-tooling algorithms so that they can address the complex memory hierarchy of these new computing platforms. In WP3, research will be carried out to enable the production codes of the consortium to successfully adapt to the changing hardware and take advantage of future high-end computing. This activity is likely to be relevant for ARCHER, IBM's Blue Joule, located at the Hartree Centre, and HPC platforms available through PRACE.

Progress report

Progress against research objectives

This consortium was formally launched only a year ago so it is still early days for this consortium. However, within this short period, the members of this consortium have conducted numerical simulation based cutting–edge research on turbulent reacting flows relevant to conventional single-phase premixed and non-premixed flames, mutli-phase spray and coal particle-laden combustion, and industrial fires. The aforementioned research has been carried out using state of art advanced Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) codes. A number of high quality journal and conference publications have already arisen since the consortium was launched and the scientific findings in these papers have significantly enriched the existing literature of numerical simulation and modelling on turbulent reacting flows. Moreover, some of the ongoing research will be disseminated in major international conferences such as 7th European Combustion Meeting, 15th International conference on Numerical Combustion, 9th Mediterranean Combustion Symposium in 2015. It is also anticipated that the research conducted in this consortium will lead to further journal publications and give rise to submissions to the 36th International Combustion Symposium, which is to be held in 2016.

It is worth noting that a number of young researchers (both PhD students and Research Associates) are involved in the on-going research in this consortium. A large proportion of these young researchers did not have much experience of using HPC on a Tier 1 facility such as ARCHER. One of the major aims/challenges of this new consortium was to involve young researchers, train them and encourage them to use cutting-edge HPC facilities, and this consortium fulfilled its aims in this regard in its first year. In doing so, this consortium generates a growing pool of highly skilled researchers in the UK who will hopefully utilise the current and future advancements of HPC for turbulent reacting flow research to tackle the problems relevant to energy efficiency and environmental friendliness.
The aforementioned activities of the consortium are consistent with the objectives of (i) carrying out world-leading computational research on turbulent reacting flows with direct relevance to energy efficiency and environment friendliness using HPC and (ii) creating a forum for HPC based turbulent reacting flow research in the UK. Furthermore, this consortium lays significant emphasis on the development of highly skilled manpower, which will contribute to the UK economy and research in the future. In the above respects, the work done so far in UKCTRF is consistent with the promised work plan and research objectives. It is anticipated that the user base (already 2 full members have joined since the launch) and collaborative network of this consortium will expand further with time as the research in UKCTRF gains momentum.

Key Scientific output

A number of high quality research outputs in the form of journal and conference papers, awards and grant applications arose from the research undertaken under the umbrella of this consortium. It is worth noting that the subject in these research outputs encompass all three work packages of UKCTRF. The key scientific outputs of this consortium are summarised below:

Journal papers

- Y. Gao, N. Chakraborty, M. Klein, *Eur. J Mech., Fluids-B* (accepted).
- T. Brosh, D. Patel, D. Wacks, N. Chakraborty, *Fuel* (accepted).
- D. Patel, N. Chakraborty, *Int. J. Spray and Combust. Dyn.* (accepted).
- A, Lipatnikov, V. Sabel'nikov, S. Nishiki, T. Hasegawa, N. Chakraborty, *Flow Turb. Combust.* (accepted).
- N. Chakraborty, R.S. Cant, *Numer. Heat Trans. A* (accepted).
- Y.Gao, N. Chakraborty, N. Swaminathan *Combust. Sci. Technol.*, 187(3), 362-383, 2015.
- Y.Gao, N. Chakraborty, M. Klein, *Int. J. Heat Fluid Flow,* 52, 28-39, 2015.
- N. Chakraborty, *J. Energy Res. Technol.*, 137, 032201, 2015.
- J. Shinjo, J. Xia, A. Umemura, *Proc. Combust. Inst.*, 35, 1595-1602, 2015.D. Patel, N. Chakraborty, *Combust. Theo. Modell.*, 18,627-651, 2014.
- T. Brosh, N. Chakraborty, Energy & Fuels, 28(9), 6077-6088,2014.
- Y. Gao, N. Chakraborty, N. Swaminathan, *Flow Turb. Combust.*, 93, 461-486, 2014.
- N. Chakraborty, L. Wang, M. Klein, *Phys. Rev.E* , 89, 033015, 2014.
- K.K. J. Ranga Dinesh, X. Jiang, J.A. van Oijen, *Int. J. Hydrogen Energy.* 39, 6753-6763, 2014.
- M.F.Mohd Yasin, R.S.Cant, C.T.Chong, S.Hochgreb,Fuel 126, 44-54, 2014.
- Y.Minamoto, N.Swaminathan, R.S.Cant, T.Leung, *Combust. Sci. Technol*., 186,1075-1096, 2014.
- Y.Minamoto, N.Swaminathan, R.S.Cant, T.Leung, *Combust. Flame* 161, 2801–2814, 2014.
- M.A. Abdel-Raheem , S.S. Ibrahim, W. Malalasekera, A.R. Masri, Int. J. Hydrogen Energy (in press).
- A. Heidari, J.X. Wen, *Int. J. Hydrogen Energy,* 39 (36), 21317 - 21327 (2014).
- C.J. Wang, J.X. Wen, Z.B. Chen, S. Dembele, *Int. J. Hydrogen Energy* 39 (35), 20560 – 20569 (2014).
- A. Heidari, J.X. Wen *Int. J. Hydrogen Energy,* 39 (11), 6184 - 6200 (2014).
- Z. Chen, J. Wen, B. Xu, S. Dembele *Int. J. Heat Mass Trans.,* 70 389 - 408 (2014).
- B.P. Xu, J.X. Wen , *Int. J. Hydrogen Energy,* 39 (35) (2014).
- B P Xu, H E Jie, J X Wen, *Int. J. Pressure Vessels and Piping,* 123-124 60 - 69 (2014).
- H. Aghajani, S. Dembele, J. X. Wen, *Fire Safety Journal,* 64 1 - 11 (2014).
- D. Petkova, T. Donchev, J.X. Wen *Construction and Building Materials,* 68 55 - 61 (2014).
- Q. Wang, H. Chen, Y. Wang, J. X. Wen, S. Dembele, J. Sun, L. He, *Fire Safety Journal,* 63 113 - 124 (2014).
- C.J. Wang, J.X. Wen, Z.B. Chen, S. Dembele, *Int. J. Hydrogen Energy,* 39 (35), 20560 - 20569 (2014).
- Z. Chen, J.X. Wen, B. Xu, S. Dembele (*Fire Safety Journal,* 64 12 - 26 (2014).
- S. Dembele, J. X. Wen, *Int. J. Hydrogen Energy,* 39 (11), 6146 - 6159 (2014).
- C. Wang, J. X Wen, Z. Chen, *Combust. Sci. Technol.,* 186 (10-11), 1632 - 1649 (2014).
- Sewerein , F., Rigopoulos, S., Combust. Flame (in press).
- Elbahloul S., Rigopoulos S., Combust. Flame (in press).
- K.K. J. Ranga Dinesh, J.A. van Oijen, K.H. Luo, X. Jiang, *Fuel*, 130, 189-196, 2014.
- J. Shinjo, J. Xia, L.C. Ganippa, A. Megaritis, *Phys. Fluids*, 26, 103302, 2014.
- J.Ma, H. Zhao, P. Freeland, M. Hawley, J. Xia, *Proc. SAE Transactions*, 7, 2014-01-9051, 2014.
- K.D. Wan, Z.H. Wang, Y. He, J. Xia, Z.J. Zhou, J.H. Zhou, K.F. Cen, *Fuel*, 139, 356-364, 2014.
- Y. Gao, N. Chakraborty, N. Swaminathan, *Flow Turb. Combust.* (submitted).
- M. Klein, N. Chakraborty, Y. Gao, *Int. J. Heat Fluid Flow* (submitted).
- I. Langella, N. Swaminathan, Y. Gao, N. Chakraborty, *Combust. Flame* (submitted).
- I. Langella, N. Swaminathan, Y. Gao, N. Chakraborty, *Combust. Theo. Modell*. (submitted).
- D. Butz, Y. Gao, A.M. Kempf, N. Chakraborty, *Combust. Flame* (submitted).
- K.K. J. Ranga Dinesh, H. Shalaby, K.H. Luo, D. Thevenin, *Combust. Flame* (submitted).
- K.K. J. Ranga Dinesh, J.A. van Oijen, K.H. Luo, X. Jiang, *App. Energy* (submitted).
- W. Liu, *Combust. Flame* (submitted).
- W. Liu, *Combust. Sci. Technol.* (submitted).
- C.Y.Lee,L..Li, M.P.Juniper, R.S.Cant, Combust. Flame (submitted).
- E.Demosthenous, G.Borghesi, E.Mastorakos, R.S.Cant, Combust. Flame (submitted).

Conference papers

- D. Wacks, N. Chakraborty, 7th European Combustion Meeting, 30th March-2nd April, 2015.
- D. Patel, N. Chakraborty, 7th European Combustion Meeting, 30th March-2nd April, 2015.
- M. Klein, C. Kasten, Y. Gao, N. Chakraborty, 7th European Combustion Meeting (ECM2015), 30th March-2nd April, 2015.
- J. Lai, N. Chakraborty, 7th European Combustion Meeting, 30th
- K. Fukumoto, J.X. Wen, *6th FM Global Open Source CFD Fire Modelling Workshop*, Norwood MA, USA.C.J. Wang, J.X. Wen, *6th FM Global Open Source CFD Fire Modelling Workshop*, Norwood MA.
- P. Akridis, S. Rigopoulos, Procedia Engineering (accepted).
- F.Sewerin,S. Rigopoulos,9th Mediterranean Combustion Symposium (accepted).

March-2nd April, 2015.
- J. Lai, N. Chakraborty, 9th Mediterranean Combustion Symposium, 8th -12th June, 2015.
- D. Patel, N. Chakraborty, 9th Mediterranean Combustion Symposium, 8th -12th June, 2015.
- D. Wacks, N. Chakraborty, E. Mastorakos, 9th Mediterranean Combustion Symposium, 8th -12th June, 2015.
- Y. Gao, H. Kolla, N. Chakraborty, J.H. Chen, N. Swaminathan, 9th Mediterranean Combustion Symposium, 8th -12th June, 2015.
- K.K. J. Ranga Dinesh, H. Shalaby, K.H. Luo, D. Thevenin, 7th European Combustion Meeting, 30th March-2nd April, 2015.
- K.K. J. Ranga Dinesh, H. Shalaby, K.H. Luo, D. Thevenin, 7th European Combustion Meeting, 30th March-2nd April, 2015.
- W. Liu, 7th European Combustion Meeting, 30th March-2nd April, 2015.
- D. Wacks, N. Chakraborty, SPEIC-2014: Towards sustainable combustion, 19th-21st November, Lisbon, 2014.
- D. Patel, N. Chakraborty, SPEIC-2014: Towards sustainable combustion, 19th-21st November, Lisbon, 2014.
- J. Lai, N. Chakraborty, SPEIC-2014: Towards sustainable combustion, 19th-21st November, Lisbon, 2014.
- Y. Gao, N. Chakraborty, N. Swaminathan, SPEIC-2014: Towards sustainable combustion, 19th-21st November, Lisbon, 2014.
- U. Allauddin, M. Pfitzner, M. Klein, N. Chakraborty, "SPEIC-2014: Towards sustainable combustion, 19th-21st November, Lisbon, 2014.
- D. Wacks, N. Chakraborty, International conference on Heat transfer and Fluid Flow-2014, Prague, 11th-12th August, 2014.
- T. Brosh, D. Patel, D. Wacks, N. Chakraborty, International conference on Heat transfer and Fluid Flow-2014, Prague, 11th-12th August, 2014.
- D. Patel, N. Chakraborty, International conference on Heat transfer and Fluid Flow-2014, Prague, 11th-12th August, 2014.
- N. Chakraborty, M. Klein,CONV-14, Kusadasi, Turkey, 8th -13th June, 2014.
- T. Brosh, N. Chakraborty, Joint meeting of the British Scandinavian-Nordic Sections of the Combustion Institute, Cambridge, UK, 27th-28th March, 2014.
- E.Demosthenous, G.Borghesi, E.Mastorakos, R.S.Cant, 52nd AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics, 2014.
- C.Y.Lee, R.S.Cant, Proceedings of ASME Turbo Expo 2014, ASME paper GT2014-25507, 2014.
- R.A.C.Griffiths, J.H.Chen. H.Kolla, R.S.Cant, W.Kollmann, 35th Symposium (International) on Combustion, San Francisco, 2014.
- C.Bilger, R.S.Cant, 26th Annual Conference on Liquid Atomization and Spray Systems, Bremen, 2014.
- Y. Gao, I. Langella, N. Chakraborty, N. Swaminathan, Joint meeting of the British Scandinavian-Nordic Sections of the Combustion Institute, Cambridge, UK, 27th-28th March, 2014.
- D. Patel, N. Chakraborty, Joint meeting of the British Scandinavian-Nordic Sections of the Combustion Institute, Cambridge, UK, 27th-28th March, 2014.
- D. H. Wacks, N. Chakraborty, Joint meeting of the British Scandinavian-Nordic Sections of the Combustion Institute, Cambridge, UK, 27th-28th March, 2014.
- I. D. Udechukwu, S. Dembele, A. Heidari, K. N. Volkov, J. X. Wen, 6th. Eur. Conf. Comput. Fluid Dyn. (ECFD VI), Barcelona, Spain.
- C. J. Wang, J. X. Wen, 16th Int. Colloquium on Dust Explosions and 11th Colloquium on Gas, Vapour, Liquid and Hybrid Explosions) , Bergen, Norway.
- I. D. Udechukwu, S. Dembele, A. Heidari, K. N. Volkov, J. X. Wen, CFD Society of Canada, 22nd Annual Conference , Toronto, Canada.
- C. Wang, J.X. Wen, S. Lu, 6th FM Global Open Source CFD Fire Modelling Workshop , Norwood MA , USA
- P.Akridis, S. Rigopoulos, 9th Mediterranean Combustion Symposium (accepted).
- P. Akridis, S. Rigopoulos, 7th European Combustion Meeting (accepted)
- P.Koniavitis, S. Rigopoulos7th European Combustion Meeting (accepted).
- K.K. J. Ranga Dinesh , K.H. Luo, J.A. van Oijen, Joint meeting of the British Scandinavian-Nordic Sections of the Combustion Institute, Cambridge, UK, 27th-28th March, 2014.
- K.K. J. Ranga Dinesh , E.S. Richardson, E.S., J.A. van Oijen, K.H. Luo, and X Jiang, 12th International Conference on Combustion and Energy Utilization, Lancaster, UK, 29th Sep – 3rd Oct 2014.
- K.K. J. Ranga Dinesh , E.S. Richardson, E.S., J.A. van Oijen , K.H. Luo, and X Jiang, 12th International Conference on Combustion and Energy Utilization (ICCEU), Lancaster, UK, 29th Sep – 3rd Oct 2014.
- J. Shinjo, J. Xia, A. Megaritis, L.C. Ganippa, 26th Annual conference on liquid atomisation and spray systems, Bremen, Germany, 8th-10th Sept. 2014.
- L. Zhou, J. Xia, J. Shinjo, A.Cairns, L.Cruff, H. Blaxill, 26th Annual conference on liquid atomisation and spray systems, Bremen, Germany, 8th-10th Sept. 2014.
- D. Wacks, N. Chakraborty, E. Mastorakos, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- D. Patel, N. Chakraborty, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- J. Lai, N. Chakraborty, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- T. Brosh, F. Cavalllo-Marincola, D. Patel, D. Wacks, N. Chakraborty, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- D. Patel, N. Chakraborty, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- K.K. J. Ranga Dinesh, H. Shalaby, K.H. Luo, D. Thevenin, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 (submitted).
- C.Y.Lee, R.S.Cant, 15th International Conference on Numerical Combustion, Avignon, April 2015.
- R.Griffiths, H.Kolla, W.Kollmann, J.H.Chen, R.S.Cant, 15th International Conference on Numerical Combustion, Avignon, April 2015.
- R.S.Cant, 15th International Conference on Numerical Combustion, Avignon, April 2015.
- C.Bilger, R.S.Cant,15th International Conference on Numerical Combustion, Avignon, April 2015.
- G.V.Nivarti, R.S.Cant, 15th International Conference on Numerical Combustion, Avignon, April 2015.
- E.Demosthenous, E.Mastorakos, R.S.Cant, Mediterranean Combustion Symposium 9, Rhodes, June 2015.
- C.F.Quaglia, R.S.Cant, ASME paper GT2015-43804, ASME Turbo Expo 2015, Montreal, June 2015.
- G.V. Nivarti, R.S.Cant, ASME paper GT2015-43416, ASME Turbo Expo 2015, Montreal, June 2015.
- G.V. Nivarti, R.S.Cant, 25th International Colloquium on Dynamics of Explosions and Reactive Systems, Leeds, August 2015.

Awards

W. P. Jones, A. J. Marquis, D. Noh, Proc. Combust. Inst., 35 (2015) 1685-1691 was selected as the most distinguished paper in the Spray and Droplet Combustion Colloquium in the 35th International Combustion Symposium

Research grants

- High Hydrogen Content (HHC) Fuel Burning at High Pressure (EP/L025051/1, PI: KK.J. Ranga Dinesh)
- Ultra efficient engines and fuels (EP/M009424/1, CI: J. Xia)
- Consequence analysis for fire and explosion hazards on offshore installations (KTP with DNV-GL, PI: J.X. Chen)
- Innovative low carbon high fuel efficiency power generation technology (TSB TS/M0011194/1, CI: J. Xia)
- Numerical characterization and simulation of the complex physics underpinning the Safe handling of Liquefied Natural Gas (Funded by: European Commission FP7, Marie Curie ITN, Innovative Doctoral Training, PI: J.X. Chen)

Progress of software development activities

Generic porting and optimisation of major UKCTRF codes have already taken place for ARCHER. Other general porting of codes will be requested through the ARCHER help desk. Support regarding optimisation of an adaptive grid based DNS code (i.e. HAMISH) is being carried out in Daresbury Laboratory as part of the activity of the consortium. The development of a module for noise generation prediction in Code_Saturne has already been submitted for eCSE support by Daresbury Laboratory and this activity is closely aligned with thermo-acoustic instability related research in this consortium. A dedicated postdoctoral researcher, Dr Jian Fang, joined Daresbury in November (2014) and will be working with partners to develop the capabilities of HAMISH.

Management of allocation

Current application procedure

The management of a consortium involving 15 institutions is an important and crucial role, and the day-to-day UKCTRF activities are led by Prof. Nilanjan Chakraborty (PI) of Newcastle University with the support of a secretary and the Management Team (MT). Profs. R.S. Cant (Cambridge University), D. Emerson (Daresbury Laboratory), W.P. Jones (Imperial College), E. Mastorakos and N. Swaminathan (Cambridge University) form the MT, which assesses requests for HPC time allocation applications from UKCTRF members. The applications are invited on a continuous basis. The applicants need to complete a simple pro-forma which is available on the consortium website (http://forms.ncl.ac.uk/view.php?id=5420). During the review process the MT ensures that the work is aligned with the goals of the consortium and meets any necessary technical standards. For most cases the decision was reached and computation time was allocated within 10 days of the application. It has been found to be a lightweight process that is not only efficient, fair and robust, but also maintains a high-quality of research.

The MT welcomes the applications for new membership on a continuous basis. However, the new prospective member needs to supply some information regarding the code which his/her research group is going to use and the information related to its bench-marking. At the first instant, the applicant is induced as an associate member and he/she is required to present in the next available consortium meeting so that MT gains a better idea about the current and future research plans of the associate member. The research by the associate member is reviewed by the MT at the end of one year from the commencement of the associate membership and the individual in question is inducted as a full member upon receiving the positive recommendation from MT.

The UKCTRF will maximise the impact of the proposed research activities and has established an Impact Advisory Panel (IAP). The IAP contains three eminent international combustion scientists who are experts in experimental techniques (Prof. W. Meier, DLR, Germany) and numerical simulations of turbulent reacting flows with applications in IC engine, gas turbine and fire prevention (Prof. T. Poinsot, CNRS, France and Prof. D. Roekaerts, Technical University, Delft, Netherlands). The IAP also includes industrial representation from Alstom, Health and Safety Laboratory, MMI Engineering, Rolls Royce, Renuda and Shell and is chaired by Dr. M. Zedda (Rolls Royce Plc.). The role of the IAP is to: (i) offer advice on the research activities in the consortium; (ii) support research activities by disseminating information and sharing experimental and computational data from their research group (as appropriate); and (iii) indicate any avenues of research which need immediate attention from the point of view of fundamental understanding and industrial requirements. The IAP meets along with the MT in the annual progress review meeting to provide an impartial assessment of the activities of the consortium.

The consortium has a website (www.ukctrf.co.uk) where the objectives, aims and work packages of the consortium are clearly described . In addition to this, the information regarding the members and organisational structure of UKCTRF, and the weblinks for the forms for the application for computational time allocation and travel cost reimbursement are also available on the consortium website. This website also contains the pdf versions of the presentations of the speakers of the meetings, which were organised under the umbrella of the consortium.

So far, two meetings have been organised under the umbrella of UKCTRF – the kick-off meeting on the 8th of January 2014 at Newcastle, and the first annual progress review meeting on the 11th of September 2014 in Selwyn College, Cambridge. These two meetings are consistent with the Workplan of UKCTRF. The first annual review meeting was preponed because this is a relatively new consortium so it was felt to be necessary by the MT in order to monitor progress closely, so that actions could promptly be taken to rectify any aspect of the functioning of the consortium where there was scope of improvement. The next annual review meeting will take place in Imperial College, London in September 2015

Current level of usage

It is important to note that the UKCTRF is not funded through EPSRC's HEC funding call but instead is funded through a collaborative responsive mode proposal. As a result, this consortium was launched later than other consortia. The UKCTRF was originally allocated 233,946.6 kAUs until 30th March 2015 and the first call for applications for computational time was issued on 23rd January 2014. To date, 231,321.13 kAUs have been allocated. The cumulative usage profile between 23rd January 2014 to 1st February 2015 is shown below in Fig. 1, which shows a steep increase in kAUs usage by the consortium members.

Plans for increasing the level of usage

It is important to note that UKCTRF was launched much later (about 6 months) than other consortia which were funded through the HEC call.. This research community did not have access to high-end computational resources for a long time so the members of the consortium were reliant on regional HPC facilities (e.g. N8, Cambridge HPCS facility etc.) and on computational time allocations from their existing research grants. Thus, some research groups within the consortium are

using the computational time allocation in their own research grants before applying for computational time from the consortium. However, with time, more users will apply for computational time from the consortium. Furthermore, most applications so far have come from WP 1 and 2, but it is anticipated that applications related to WP 3 will be submitted in the near future.
The MT is closely monitoring the usage of kAUs by the consortium members and there is reason to believe (a couple of big applications are on the way) that the whole computational time allocation until March 2015 will be committed by that time. The MT is in close contact with EPCC's consortium contact for ARCHER to arrange for training sessions for consortium users. It is anticipated that these training sessions will help to increase the number of users and make the existing users to use the facility in a more efficient manner. These training sessions will also help the consortium users to utilise the RDF facility as well. The MT also plans to hold a training session for the new users alongside the annual workshop in September 2015.Based on the above measures, it is anticipated that the level of usage of the UKCTRF will only increase with time.

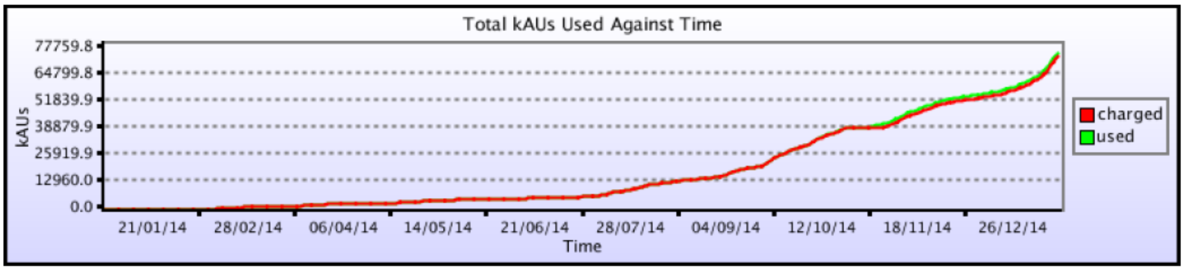

Fig. 1: Cumulative kAUs usage with time by UKCTRF users between 21st January 2014-1st February 2015.

Future Plans

Plans for completing the proposed research program

The current kAU usage of UKCTRF on ARCHER includes fundamental investigation of high Karlovitz number turbulent premixed combustion, dual fuel droplet-laden combustion using advanced three-dimensional detailed chemistry Direct Numerical Simulations from WP 1, and LES simulations of turbulent stratified flame, gas turbine combustion and fire safety applications from WP 2. All of these are currently in progress and some of the outcomes of this research will be disseminated in major international conferences such as 7th European Combustion Meeting, 15th International conference on Numerical Combustion, 9th Mediterranean Combustion Symposium in 2015. It is also anticipated that this research will lead to journal publications and submissions to 36th International Combustion Symposium.
The work is under way in WP 3 to enable consortium codes to successfully take advantage of the changing hardware and future advancements of high-end computing. In particular, the work undertaken focuses on:

- Use of directives, such as OpenMP and OpenACC, to exploit multicore and GPU-based accelerators for discretisation techniques such as finite difference and finite volume methods.
- Implications of implicit and explicit time advancement on massively parallel systems and the optimisation of communication strategies for inverting large algebraic systems.

The current research activities are consistent with the original work schedule and the aims and objectives of the consortium.

New directions that evolved from the project

The UKCTRF builds on the foundations of the successful Consortium of Computational Combustion for Engineering Applications which ran between 1994 and 2010, and makes a focussed effort to address the global and UK challenges of energy efficiency, environmental friendliness and high-fidelity fire safety. This consortium is investigating on the following timely and relevant topics which were absent in the earlier incarnations of this consortium:
Multi-phase reacting flow simulations: It is now possible to carry out simulations of combustion involving liquid and solid fuels using DNS due to recent progress in computational techniques and available computational power. As a part of this work programme, break-up of the primary fuel jet, staged injection, localised ignition of droplet-laden flows are studied using DNS data along with the analysis of the effects of droplet size, equivalence ratio, group number, volatility, turbulence intensity on flame propagation, heat release and pollutant (e.g. NO_x) emission characteristics. DNS data of droplet-laden turbulent reacting flows and use the data to create new RANS and LES modes in the context of PDF and CMC methodologies. Some of these methodologies (e.g. the stochastic field, and Conditional Moment Closure (CMC) methods) have already been implemented for LES of spray flames. The micro-scale combustion systems involving droplet-laden mixtures are expected to be simulated and analysed during the course of this consortium.
The advancement of computational infrastructure enabled the consortium members to carry out DNS and LES of oxy-fuel combustion of pulverised coal particles. The fundamental physical insight extracted from DNS is in the process of being analysed for the development of high-fidelity models for coal combustion.
Thermo-acoustic instabilities: To date, most analyses of combustion instabilities have been carried out based on a linearised system, often relying on strong assumptions and ignoring the effects of viscous damping. With the advancement of computational power, it is now possible to carry out three-dimensional compressible LES simulations of the whole burner

and identify the fluid-dynamic mechanism which leads to thermo-acoustic instability. Moreover, these three-dimensional simulations enable devising high fidelity transfer functions for simplified engineering calculations. Although most analyses in this regard are currently being carried out based on LES simulations, DNS based analyses are under way to analyse acoustic emissions from combustion systems and their interaction with heat release in premixed flames.

New fuels: New generation combustion systems are expected to include a large proportion of hydrogen to reduce the emission of CO_2, and pollutants such as CO and soot. New fuels will also improve flame stability, so that flames can be operated in cleaner modes such as lean premixed combustion. A number of collaborative works is under way in the consortium on hydrogen blended hydrocarbon combustion which will include detailed chemical reaction mechanisms.

Detailed chemical mechanisms: Detailed chemistry must be considered to improve the accuracy of all simulation methods. As a part of this work chemical reaction mechanisms for higher hydrocarbon fuels, including surrogate fuels representative of Diesel and Kerosene are being developed alongside refinement of existing mechanisms with emphasis on generic issues concerning hydrogen chemistry, bio-derived oxygenated fuels (including a range of alcohols) and on mechanism reduction for computational efficiency. The physical processes associated with fluid flow-chemistry interactions for bio-derived fuels and nano-particle and soot formation in turbulent non-premixed flames are addressed for the first time in this consortium.

New combustion regimes: New combustion regimes such as mild, stratified, and lean premixed combustion permit the fuel to burn with lower emissions of Nitric Oxides and unburned hydrocarbons. In the consortium, DNS simulations are being carried out for turbulent stratified flames and for mild combustion. The fundamental understanding obtained from DNS data will be used to develop new and improved models for unsteady RANS and LES simulations.

Fire simulations: Fire simulation is often required to approve major new public buildings and ships. Ignition and extinction of fires, fire spreading mechanism, radiative heat transfer due to fire, atmospheric chemical pollution, and environmental effects of industrial releases, fires and explosions are analysed in this consortium. The applied fire research will also focus on the issues of fire-safety and explosion hazards and fire simulations will be performed for accurate predictions of forest, tunnel and pool fire spreading and release of toxic species.

Strategic direction

The consortium recognises the importance of maximising the impact and dissemination of their work and thus established an IAP to ensure a strong knowledge-exchange activity with industrial partners (Rolls Royce Plc., Siemens Plc., Shell Plc., Alstom Plc., MMI Engineering and Renuda Ltd.), and international academic experts (Dr. W. Meier from Institute of Combustion Technology, DLR, Germany, Prof. T. Poinsot from CNRS, Toulouse, France and Prof. D. Roekaerts, Technical University, Delft, Netherlands). The IAP is currently chaired by Dr. M. Zedda from Rolls Royce Plc. who are actively involved in RANS and LES simulations of turbulent reacting flows in complex engineering configurations for the purpose of designing new generation energy-efficient and environment-friendly industrial combustion devices for automotive and gas turbine applications.

The role of the IAP is to: (i) offer advice on the research activities in the consortium; (ii) support research activities by disseminating information and sharing experimental and computational data from their research group (as appropriate); and (iii) indicate any avenues of research which need immediate attention from the point of view of fundamental understanding and industrial requirements. The IAP provides an impartial assessment of the activities of the consortium. Consortium members and colleagues from relevant industrial sectors (Rolls Royce, Shell, Alstom, Siemens etc.) are invited to present their research findings and exchange ideas with the consortium and advisory panel members in these annual progress review meetings.

The industrial colleagues of IAP identified that focused research is needed on explosions modelling, spray and soot modelling, bio-fuel combustion and thermo-acoustic interaction. This industrial view is consistent with the priority areas identified by the consortium. There is a possibility that the IAP members of Shell will be able to provide some experimental data on their explosions test cases and constant volume Diesel spray combustion. Rolls Royce and Siemens have offered to provide test cases with experimental data for validating RANS/LES simulations. Siemens is also willing to share some experimental data on thermo-acoustic interaction. Two academic members of IAP (i.e. Dr. W. Meier and Prof. D. Roekaerts) offered to share some experimental data with UKCTRF members for validation of simulation results. It was felt by industrial colleagues and the members of UKCTRF that it will be useful if the models developed using fundamental insights obtained from DNS data can be implemented in an open-source code such as OpenFOAM or Code_Saturne to demonstrate its validity. This will help the assimilation of research outcomes of UKCTRF members into the industrial sector relatively quickly, and contribute towards the development of the next generation energy-efficient and environment friendly combustion devices. It is recognised that this exercise will require interactions between various research groups and their concerted efforts, and will be a desired outcome at the end of this consortium. This exercise will also help identifying those methodologies which will be useful for pre-processing and post-processing of industrial simulations.