Annual Report for EPSRC High End Computing Consortia

Reporting Period: February 2015 - January 2016

HEC Consortia: **UK Consortium on Turbulent Reacting Flows (UKCTRF)**

Consortia Chair: **Prof. Nilanjan Chakraborty (Newcastle University)**

Allocation and Usage profiles during the reporting period

EPSRC to complete when template has been submitted.

Summary (max. 2 pages):

Background

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, 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 and pollutant emission 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) WP1: Fundamental physical understanding based on cutting-edge Direct Numerical Simulations of single- and multi-phase reacting flows, (ii) WP2: Applied research and technology development and (iii) WP3: Algorithm and architecture development for future platforms, respectively.

Highlights for the Current Reporting Period

Invited lectures by consortium members*:* Prof. N. Chakraborty (Keynote lecture: 29th Israeli Combustion Symposium, Tel-Aviv,2015), Prof. W.P. Jones (Plenary lecture, Clean Air conference, Lisbon, 2015); Prof. E. Mastorakos (7th European Combustion Meeting, Budapest, 2015); Prof. N. Swaminathan (2nd National Propulsion Conference and Combustion Workshop, Indian Institute of Technology-Bombay, India)

Scientific committee of international conferences: Prof. N. Chakraborty (One of the coordinators of 1st International Workshop on Coal and Biomass Conversion 21st April, Avignon, France; Clean Air 2015, 5th-9th July, Lisbon, 2015; Workshop of turbulent premixed combustion, Cambridge, UK, 26th June, UK); Prof. E. Mastorakos (9th Mediterranean Combustion Symposium); Prof. N. Swaminathan (Workshop of turbulent premixed combustion, Cambridge, UK, 26th June, 2015, UK; International Forum on Multidisciplinary Education, Hawaii -Dec. 2015); Dr. J. Xia (International workshop on multiphase flows and phenomena, 7th-8th September, 2015, Brunel, UK).

Awards: The image entitled “Music, order and chaos in a combustion chamber” by I. Langella (a PhD student of Prof. N. Swaminathan, University of Cambridge) received the 1st prize ARCHER image competition and arose from the research carried out in this consortium. This image also appeared in 2016 ARCHER calendar.

Publications: Altogether 120 journal and 150 conference publications by consortium members

Workshops and New Opportunities

The 2nd annual progress review meeting of the UKCTRF and the meeting between the Management Team (MT) and the Impact Advisory Panel (IAP) members took place on 22nd -23rd September 2015 in Imperial College, London. There were 2 invited keynote lectures (45 min) and 16 contributed oral presentations (15 min each) in the aforementioned meeting and the invited keynote lectures were delivered by Dr. M. Zedda

from Rolls Royce Plc. and Prof. D. Roekaerts, Delft University, Netherlands. The next annual progress review meeting and the meeting between MT and IAP will take place in the University of Durham in September 2016. The exact dates and the keynote speakers are currently being finalised. It is anticipated that the number of speakers will grow considerably for the next meeting because of the increasing number of users of ARCHER in the consortium. In order to showcase the diverse range of ongoing research within the consortium in the next annual progress review meeting it is planned that the next meeting will involve shorter oral presentations but will have accompanying poster presentations so that more detailed discussion can take place during the course of the meeting according to the convenience of the attendees. The MT is also considering about having a joint meeting with UKTC during the course of this consortium

The biennial International Symposium on Combustion is the premier conference in the field of combustion and regularly attracts over 2,000 delegates. Papers presented at the symposia are of the highest quality following a strict full-scale peer reviewing process, and the interactions with the peers during the symposium are often intellectually stimulating. UKCTRF members in the past have been successful in getting papers accepted in a very competitive environment, especially as the publications from this conference carry a high impact factor. However, the high cost of attending the symposia due to high registration fees, long haul international flights, accommodation etc, is discouraging. To help members to maximise the impact of disseminating their results, partial funding for attending the 36th International Combustion Symposium (to be held in 31st July-5th Aug., 2016, Seoul, Korea) will be provided, at a rate of £500 per UKCTRF academic member, who has a paper accepted for oral presentation.

Issues and Problems

It took some time and the sustained effort of the management committee before the level of utilisation of the allocated computational time by the UKCTRF users reached a satisfactory level in the previous year. At the end of August 2015 the percentage usage of the computational time allocation was equal to the percentage of time elapsed but at the end of the allocation period about 90% of the allocated computational time for the period was utilised. The deadline for the submissions to the 36th International Combustion Symposium was on the 3rd of December 2015 and thus most users of the consortium were busy writing papers for the symposium rather than running jobs on ARCHER.

The day-to-day UKCTRF activities are led by Prof. Nilanjan Chakraborty (PI) of Newcastle University with the support of a secretary and the 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. The allocation for the period December 2015-May 2016 got assigned to the consortium members based on the applications within 10 days. However, there are some users who need more computational time than they have received so at the moment the demand is higher than the availability. The MT is exploring the avenues of coming up with a new allocation strategy so that all the interested parties receive at least some computational time even if it is not the entire allocation requested by them, and 100% utilisation of the allocation is ensured.

Membership

(New members are shown in bold and the Management team members are indicated by the underlines) Newcastle University: Prof. N. Chakraborty (Consortium chair and PI); University of Brunel: Dr. J. Xia; University of Cambridge: Profs. R.S. Cant, E. Mastorakos, M. Kraft, and N. Swaminathan; University of Central Lancashire: Prof. G.M. Makhviladze, Drs. W. Liu, and **J. Mai** ;City University, London: **Dr. K. Vogiatzaki**; Cranfield University: Drs. C. Armitage and K.W. Jenkins ; Daresbury Laboratory: Prof. D. Emerson, Drs. C. Moulinec and X. Gu; University of Edinburgh: Prof. J. Torero, Dr. S. Welch, and **D. Hyuk Shin**; Imperial College, London: Profs. W.P. Jones, R.P. Lindstedt, Drs. F. Marquis, **A. Morgans**, S. Navarro-Martinez, S. Rigopoulos, and G.Rein; Lancaster University: Prof. X. Jiang; Loughborough University: Profs. W. Malalasekara, J. McGuirk, and Dr. A Garmory; University College London: Prof. K.H. Luo; University of Durham: Prof. P. Gaskell; University of Leeds: Prof. D. Bradley and Dr. G. Sharpe; University of Manchester: Dr. R. Prosser; University of Southampton: Drs. E.S. Richardson, **K.K.J. Ranga Dinesh**, **and A. Aspden**;University of Ulster: Profs. M. Delichatsios and V.B. Novozhilov; Warwick University: Prof. J.X. Wen

World class and world leading scientific output: *ARCHER should enable high quality and world-leading science to be delivered. This should generate high impact outputs and outcomes that increase the UK's position in world science.*

- For the reporting period please provide a bullet pointed list of key research findings and any linked publications.
- For the reporting period please include a bullet pointed list of any relevant press announcements and other communications of significance to an international community.
- ***Since ARCHER came on line***, what are the top 5 scientific outcomes that have resulted from projects supported by the Consortium? This could be research that has been published in high impact journals, work that has been highly cited, or research that has had a significant impact on the consortium's community or strategic direction.

➢ Key research outcomes and linked publications

- **Improved physical understanding and modelling of multi-phase (i.e. spray and coal) combustion using high-fidelity simulations**

T. Brosh, D. Patel, D. Wacks, N. Chakraborty, "Numerical investigation of localised forced ignition of pulverised coal particle-laden mixtures: A Direct Numerical Simulation (DNS) analysis." Fuel , 145, 50-62, 2015.

T. Brosh, F. Marincola, D. Patel, D.H. Wacks, N. Chakraborty, "On conditions for self-sustained combustion of pulverised coal particle-laden mixtures following localised forced ignition: A Direct Numerical Simulation analysis", 25th International Colloquium on Dynamics of Explosions and Reactive Systems, Leeds University, Leeds, UK, 2nd -7th August, 2015.

E. Demosthenous, E. Mastorakos, R. S. Cant, "Direct Numerical Simulations of dual fuel non-premixed autoignition", Combust. Sci. Technol. (in press).

E. Demosthenous, G. Borghesi, E. Mastorakos, E., R.S. Cant, Direct Numerical Simulations of premixed methane flame initiation by pilot n-heptane spray autoignition. Combustion and Flame, 163, 122-137, 2016.

S Gallot Lavallèe, S. and Jones, W. P., Large Eddy Simulation of Spray Auto-ignition under EGR Conditions, Flow, Turbulence and Combustion. (in press).

W.P. Jones, A.J. Marquis, D. Noh, A stochastic modelling for LES of a two-phase combusting flow, ", 7th European Combustion Meeting (ECM2015), 30th March-2nd April, Budapest, 2015.

D.H. Wacks, N. Chakraborty, E. Mastorakos, Statistical analysis of turbulent flame-droplet interaction: A Direct Numerical Simulation Study, Flow, Turbulence and Combustion, DOI 10.1007/s10494-015-9652-y, 2015.

D.H. Wacks, N. Chakraborty, E. Mastorakos, "Statistical Analysis of the Reaction Progress Variable and Mixture Fraction Gradients in Flames Propagating into Droplet Mist: A DNS Analysis", 25th International Colloquium on Dynamics of Explosions and Reactive Systems, Leeds University, Leeds, UK, 2nd -7th August, 2015.

D.H. Wacks, N. Chakraborty, "Flame structure and topology in turbulent spray flames: A Direct Numerical Simulation analysis", Clean Air 2015, 5th-9th July, Lisbon, 2015.

D. Wacks, N. Chakraborty, "Flame structure and propagation in turbulent flame-droplet interaction: A Direct Numerical Simulation analysis", 9th Mediterranean Combustion Symposium, 7th-11th June, Rhodes Island, 2015.

D. Wacks, N. Chakraborty, "Effects of droplets on flame structure in premixed spray flames: A Direct Numerical Simulation analysis", 7th European Combustion Meeting (ECM2015), 30th March-2nd April, Budapest, 2015.

- **High-fidelity LES and modelling of turbulent premixed and stratified mixture combustion**

M.A. Abdel-Raheem, S.S. Ibrahim, W. Malalasekera, A.R. Masri, Large eddy simulation of hydrogen-air premixed flames in a small scale combustion chamber, International Journal of Hydrogen Energy, 40, 3098 -3109, 2015.

M.A. Abdel-Raheem, S.S. Ibrahim, W. Malalasekera and M. Bragin, Numerical Simulations of CNG, LPG & H2 Lean Premixed Deflagrating Flames, Paper presented at the 25th ECDERS Conference Leeds, August 2015.

N.J. Beavis, S.S. Ibrahim, W. Malalaskera and P. K. Manickam , Characteristics of GDI Engine Flow Structures, Merkmale der Strömungsstrukturen eines Benzinmotors mit Direkteinspritzung, paper presented at the Engine Combustion Processes Conference in Ludwigsburg, March 12th & 13th 2015.

D. Butz, Y. Gao, A.M. Kempf, N. Chakraborty, "Large Eddy Simulations of a turbulent premixed swirl flame using an algebraic Scalar Dissipation Rate closure." Combustion and Flame, 162, 3180-3196, 2015.

Z. Chen, S. Ruan and N. Swaminathan. Numerical simulation of lifted jet flames, The Fourth International Education Forum on Environment and Energy Science, 6-10 December, 2015, Maui Island, Hawaii, USA

Y. Gao, N. Chakraborty, "Modelling of Lewis Number dependence of Scalar dissipation rate transport for Large Eddy Simulations of turbulent premixed combustion." Numerical Heat Transfer A, DOI: 10.1080/10407782.2015.1125732.

Y.Gao, N. Chakraborty, N. Swaminathan, "Dynamic scalar dissipation rate closure for Large Eddy Simulations of turbulent premixed combustion: A Direct Numerical Simulations analysis." Flow Turbulence and Combustion, DOI 10.1007/s10494-015-9631-3.

Y.Gao, N. Chakraborty, M. Klein, "Assessment of sub-grid scalar flux modelling in premixed flames for Large Eddy Simulations: A-priori Direct Numerical Simulation." European Journal of Mechanics, Fluids-B , 52, 97-108, 2015.

Y.Gao, N. Chakraborty, N. Swaminathan "Scalar dissipation rate transport and its modelling for Large Eddy Simulations of turbulent premixed combustion." Combustion Science and Technology, 187(3), 362-383, 2015.

Y.Gao, N. Chakraborty, M. Klein, "Assessment of the performances of sub-grid scalar flux models for premixed flames with different global Lewis numbers: A Direct Numerical Simulation analysis", International Journal of Heat and Fluid Flow, 52, 28-39, 2015.

R.A.C. Griffiths, J.H. Chen, H., Kolla, R.S. Cant, W. Kollmann, Three-dimensional topology of turbulent premixed flame interaction. Proceedings of the Combustion Institute, 35(2), 1341-1348, 2015.

W.P. Jones, A.J. Marquis, F. Wang, Large eddy simulation of a premixed propane turbulent bluff body flame using the Eulerian stochastic field method, Fuel, 140, 514–525, 2015.

M. Klein, C. Kasten, Y. Gao, N. Chakraborty, "A-priori Direct Numerical Simulation assessment of sub-grid scale stress tensor closures for turbulent premixed combustion." Computers & Fluids, 122, 1-11, 2015.

M. Klein, N. Chakraborty, Y. Gao, "Scale similarity based models and their application to subgrid scale scalar flux modelling in the context of turbulent premixed flames." International Journal of Heat and Fluid Flow, 57,91-108, 2016.

I. Langella, N. Swaminathan, Y. Gao, N. Chakraborty, "Assessment of Dynamic Closure for Premixed Combustion LES." Combustion Theory and

Modelling, 19, 628-656.
I. Langella, N. Swaminathan. Unstrained and strained flamelets for LES of premixed combustion, submitted to Combust. Theory Modelling (Accepted).
Y. Minamoto, K. Aoki, M. Tanahashi, and N. Swaminathan DNS of swirling hydrogen-air premixed flames. International Journal of Hydrogen Energy, 40(39) 13604-13620, 2015.
I. A. Mulla, A. Dowlut, T. Hussain, S. R. Chakravarthy, N. Swaminathan, and R. Balachandran, Evolution of flame-kernel in laser-induced spark ignited mixtures: a parametric study. Combustion and Flame (Accepted).
I. A. Mulla, A. Dowlut, T. Hussain, Z. M. Nikolaou, S. R. Chakravarthy, N. Swaminathan, and R. Balachandran. Heat release rate estimation in laminar premixed flames using laser-induced fluorescence of CH2O and H-atom, Combustion and Flame (accepted).
G. V. Nivarti and R. S. Cant: DNS of High Turbulence Intensity Premixed Methane-Air Flames in a 3D Inflow-Outflow Configuration, 15th International Conference on Numerical Combustion, Avignon, France, April 2015.
G. V. Nivarti, R. S. Cant: Aerodynamic Quenching and Burning Velocity of Turbulent Premixed Methane-Air Flames, ASME Paper GT2015-43416, ASME Gas Turbine Technical Conference and Exhibition, Montreal, Canada, June 2015.
S. Ruan, N. Swaminathan, M. Isono, T. Saitoh, K. Saitoh, Simulation of premixed combustion with varying equivalence ratio in a gas turbine combustor. J. Propulsion and Power, 31(3), pp. 861-871, DOI: 10.2514/1.B35517, 2015.

- **Fundamental physical understanding and modelling of turbulent premixed flame-wall interaction**

J. Lai, N. Chakraborty, "Statistical behaviour of scalar dissipation rate for head on quenching of turbulent premixed flames: A Direct Numerical Simulation analysis". Combustion Science and Technology, DOI:10.1080/00102202.2015.1102903.
J. Lai, N. Chakraborty, "Effects of Lewis Number on Head on Quenching of Turbulent Premixed Flame: A Direct Numerical Simulation analysis", Flow, Turbulence and Combustion, DOI 10.1007/s10494-015-9629-x.
J. Lai, N. Chakraborty, "Modelling of Progress Variable Variance Transport in Head on Quenching of Turbulent Premixed Flames: A Direct Numerical Simulation Analysis", 25th International Colloquium on Dynamics of Explosions and Reactive Systems, Leeds University, Leeds, UK, 2nd -7th August, 2015.
J. Sellmann, J. Lai, A. M. Kempf, N. Chakraborty, "Statistical behaviour of Flame Surface Density transport in head on quenching of turbulent premixed flames: A Direct Numerical Simulation Analysis", Clean Air 2015, 5th-9th July, Lisbon, 2015.
J. Lai, N. Chakraborty, "Statistical behaviour of scalar dissipation rate for head on quenching of turbulent premixed flames: A Direct Numerical Simulation analysis", 9th Mediterranean Combustion Symposium, 7th-11th June, Rhodes Island, 2015.
J. Lai, N. Chakraborty, "Direct Numerical Simulation analysis of turbulent kinetic energy transport in head on quenching of turbulent premixed flames" 7th European Combustion Meeting (ECM2015), 30th March-2nd April, Budapest, 2015.

- **Implementation of Conditional Moment Closure (CMC) in the context of LES to account for flame extinction and blowout**

H. Zhang, A. Garmory, D.E. Cavaliere, E. Mastorakos, Large Eddy Simulation/Conditional Moment Closure modeling of swirl-stabilized non-premixed flames with local extinction. Proceedings of the Combustion Institute, 35. pp. 1167-1174, 2015.
A. Garmory, E. Mastorakos, Numerical simulation of oxy-fuel jet flames using unstructured LES-CMC. Proceedings of the Combustion Institute, 35. pp. 1207-1214, 2015.

➢ Relevant press announcements and other communications of significance

The image entitled "Music, order and chaos in a combustion chamber" by I. Langella (a PhD student of Prof. N. Swaminathan, University of Cambridge) received the 1st prize in ARCHER image competition. This image originated from the research carried out in this consortium and appeared in ARCHER 2016 calendar.

➢ Top 5 scientific outcomes from the UKCTRF community since ARCHER came on line

- **Significant advances in computational simulation and modelling of multi-phase multi-physics combustion (**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 and see the other high-quality publications listed above under the heading of **Improved physical understanding and modelling of multi-phase (i.e. spray and coal) combustion using high-fidelity simulations)**
- **Advances in LES and modelling of turbulent combustion (**see the high-quality publications listed above under the heading of **High-fidelity LES and modelling of turbulent premixed and stratified mixture combustion** and **Implementation of Conditional Moment Closure (CMC) in the context of LES to account for flame extinction +** W.P. Jones, A.J. Marquis, K. Vogiatzaki, Combustion and Flame, **161**(1):222-239, (2014); G. Bulat, W.P. Jones, and A.J. Marquis, Combustion and Flame, **161**(7) 1804-1825 (2014); W. P. Jones, M. Jurisch, and A.J. Marquis, Flow, Turbulence and Combustion. (2015) (DOI) 10.1007/s10494-015-9637-x**)**
- **Application of Direct Numerical Simulations to address the new physics (e.g. flame-wall interaction and MILD combustion) and gain improved physical understanding (**see the high-quality publications listed above under the heading of **Improved physical understanding and modelling of turbulent premixed flame-wall interaction+** Y. Minamoto and N. Swaminathan, Proceedings of the Combustion Institute, 35. pp. 3529-3536 (2015); Y. Minamoto and N. Swaminathan, R.S. Cant, T. Leung, Combustion Science and Technology, 186. pp. 1075-1096 (2014); Y. Minamoto, N. Swaminathan, Combustion and Flame, 161. pp. 1063-1075 (2014);Y. Minamoto and N. Swaminathan, R.S. Cant, T. Leung, Combustion and Flame, 161. pp. 2801-2814 (2014)**)**
- **Improved physical understanding of ignition and extinction processes and their modelling (**see the high-quality publications listed above under the heading of **Implementation of Conditional Moment Closure (CMC) in the context of LES to account for flame extinction +** L. Bates, D. Bradley, G. Paczko, N. Peters, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015 ; G. Borghesi, E. Mastorakos, Combustion and Flame, 162. pp. 2544-2560 (2015) ; D. Bradley; P.H. Gaskell, X.Gu, A. Palacios, Combustion and Flame (accepted); T. Brosh, N. Chakraborty, Energy & Fuels, 28(9), 6077-6088,2014; T. Brosh, D. Patel, D. Wacks, N. Chakraborty, *Fuel* , 145, 50-62, 2015; 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; Z. Chen, S. Ruan, N. Swaminathan, Combustion and Flame, 162. pp. 703-716 (2015); D. Patel, N. Chakraborty, Combust. Theo. Modell., 18,627-651, 2014; D. Patel, N. Chakraborty, International Journal of Spray and Combustion Dynamics, 7, 151-174, 2015; D. Patel, N. Chakraborty, International Journal of Spray and Combustion Dynamics (accepted); D. Patel, N. Chakraborty, Flow, Turbulence and Combustion; S. Ruan, N. Swaminathan and O. Darbyshire, Combustion Theory and Modelling, 18. pp. 295-

329 (2014); D. Patel, N. Chakraborty, , 9th Mediterranean Combustion Symposium, 8th -12th June, 2015D. Patel, N. Chakraborty, 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2nd -7th August, 2015; D. Patel, N. Chakraborty, Clean Air 2015, 5th-9th July, Lisbon, 2015; A.Tyliszczak, D.E. Cavaliere, E. Mastorakos, Flow, Turbulence and Combustion, 92. pp. 237-267 (2014))

Development of methods for new computational architecture (F. Sewerin, S. Rigopoulos, Combustion and Flame 162, 1375-1394 (2015); F. Sewerin, S. Rigopoulos, Proceedings MCS-9, Rhodes, Greece; F. Sewerin, S. Rigopoulos,15th International Conference on Numerical Combustion, Avignon, France (2015)**)**

Greater scientific productivity: *As well as speed increases, the optimisation of codes for the ARCHER machine will enable problems to be solved in less time using fewer compute resources.*

- For the reporting period please provide a brief update on progress of software development activities associated with the consortium and the impact this has had on consortium members and the broader research community.

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. It is worth noting that HAMISH is a new code which is under development and will be rolled out over the next 2-3 years. A dedicated postdoctoral researcher, Dr Jian Fang, joined Daresbury in November, 2014 is working with partners to develop the capabilities of HAMISH. Dr. J. Fang is making good progress with HAMISH and has already made significant advances in debugging the code. There is also a strong element of research into the algorithms that need careful attention in relation to the development of HAMISH, particularly the adaptive meshing for DNS. Moreover, new code and algorithm development evolve naturally and should not be considered as a routine task.

The development of a module for noise generation prediction in Code_Saturne is currently on-going in Daresbury Laboratory as a part of eCSE application and this activity is closely aligned with thermo-acoustic instability related research in this consortium.

Increasing the UK's CSE skills base (including graduate and post doctorate training and support): *This builds on the skills sets of trained people in HPC, both in terms of capacity and raising the overall skill level available to the sector.*

- For the reporting period please provide a bullet pointed list of training activities undertaken by the Consortium, providing information on the target audience and level of attendance.

Most users of the consortium are early career researchers (i.e. PhD students, Postdoctoral Research Associates). In the 2nd Annual Progress meeting of UKCTRF, early career researchers (ECRs) gave 16 oral presentations out of 18 oral presentations and about 30 ECRs attended the meeting. This substantiates the high level of involvement of ECRs in the consortium activities. The members of UKCTRF and their respective institutions have expertise and training facilities of parallel computation (i.e. MPI, OpenMP) and access to the training facilities organised by regional facilities (e.g. N8). For this reason, no special training on parallel computation is organised by the consortium. However, the training sessions, webinars organised by EPCC for ARCHER users, eCSE calls and the specialised training courses organised by Daresbury Laboratory (e.g. OpenFOAM training in November 2015) are publicised to the consortium members by the UKCTRF secretarial staff. The EPCC's consortium contact for ARCHER was invited to the 2nd Annual Progress review meeting of the UKCTRF to publicise and discuss about the training options and other facilities (e.g. effective file management and efficient usage of RDF) to the consortium users. The EPCC's consortium contact for ARCHER is also invited to join the Impact Advisory Panel (IAP) and is in close contact with MT to explore the possibility of having training sessions which might be beneficial for the consortium users.

The previous incarnations of UKCTRF (i.e. Consortium On Computational Combustion For Engineering Applications (COCCFEA)) had the option for summer schools on computational combustion. Under the new regulation of EPSRC, it was not possible to include the summer school in the proposal for UKCTRF. However, both academic experts and industrial members of IAP commented in the kick-off meeting that there is a need for a summer school at regular intervals. This issue was discussed in the meeting between the MT and IAP members in the presence of an EPSRC representative during the 2nd Annual progress meeting of UKCTRF and it was decided the demand for this training will be catered through the EPSRC funded Centre of Doctoral Training Centres (CDTs) based at the University of Leeds and Imperial College, London. Furthermore, the international Combustion Institute arranges training workshops for ECRs every year which also covers the cost of travel and accommodation of PhD students. It has been decided by the MT of the consortium that the availability of such facilities will be disseminated more extensively among the consortium members in the

future and they will be encouraged to take the available opportunities.

Increased impact and collaboration with industry: *ARCHER does not operate in isolation and the 'impact' of ARCHER's science is converted to economic growth through the interfaces with business and industry. In order to capture the impacts, which may be economic, social, environmental, scientific or political, various metrics may be utilised.*

- Please provide a brief update on any planned activities / collaborations / outcomes outlined in the original Pathways to Impact plan for the Consortium.
- For the reporting period please provide information on any Consortium projects that have been performed in collaboration with industry, this should include details of the company involved, a statement on the impact that the work has / is making and, if relevant, details of any in kind or in cash contributions that have been associated with this work.
- For the reporting period include a list of Consortium publications that have industrial co-authorship.
- For the reporting period please provide details of the any other activities involving industrial participation e.g. activities involving any Industrial Advisory panels, attendance / participation in workshops and Consortium based activities.

➢ Collaboration with industry as outlined in the original Pathways to Impact for the consortium

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., 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 (MMI Engineering Ltd., Renuda, Rolls Royce, Shell, 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 representatives of Shell Plc., Siemens Plc., Renuda Ltd. And Rolls Royce Plc.(i.e. Prof. R. Cracknell, Drs. G. Bulat, N. Tonello and M. Zedda) attended the 2nd Annual Progress meeting of the consortium and offered their valuable inputs. 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. 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.

➢ Projects that have been performed in collaboration with industry

- **Autoignition and Jet flame analysis in collaboration with Shell Research (PI: Prof. Derek Bradley,**

University of Leeds, UK): Combined experimental and computational investigation of turbulent jet flames and autoignition characteristics in automotive applications. Prof. D. Bradley acts as a consultant to Shell.

- **Firefoam development for industrial fire simulations in collaboration with FM Global (PI: Prof. Jennifer Wen, Warwick University, UK):** The Warwick group has been involved with continuous development of the FireFOAM code, the LES based fire simulation solver within OpenFOAM. This work is benefitting from the financial contribution of FM Global (i.e. £87.5K) for a PhD student as well as their technical support including providing 6 weeks onsite training to the PhD student and continuous support over emails and phone. The work is part of their strategy to use numerical modelling with validated predictive tools to reduce the number of large scale expensive fire tests (typically $50k each) required for their business.

➢ Publications that have industrial co-authorship

- G. Bulat, W.P. Jones, A.J. Marquis, NO and CO formation in an industrial gas-turbine combustion chamber using LES with the Eulerian sub-grid PDF method., Combustion and Flame, 161(7),1804-1825, 2014.
- S. Ruan, N. Swaminathan, M. Isono, T. Saitoh, K. Saitoh, Simulation of premixed combustion with varying equivalence ratio in a gas turbine combustor. J. Propulsion and Power, 31(3), pp. 861-871, DOI: 10.2514/1.B35517,2015.

Strengthening of UK's international position: *The impacts of ARCHER's science extend beyond national borders and most science is delivered through partnerships on a national or international level.*

- For the reporting period please provide a bullet pointed list of projects that have involved international collaboration.
- For the reporting period please provide a list of consortium publications with international co-authorship.
- For the reporting period please detail any other international activities that the Consortium might be involved in (workshops, EU projects etc.).

➢ Projects involved international collaboration

- **Advanced numerical techniques for pulverized biomass combustion modelling (Investigator from UKCTRF: Prof. N. Chakraborty (Newcastle University)):** Collaboration involving Instituto Superiorio de Técnico (IST), Portugal, University of Duisburg, Germany
- **Analysis of jet flames (Investigator from UKCTRF: Prof. Derek Bradley (University of Leeds)):** Collaboration involving Universities of Barcelona, Puebla, and State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei, Anhui.
- **Autoignition in engines (Investigator from UKCTRF: Prof. Derek Bradley (University of Leeds)):** Collaboration involving Institute for Combustion Technology, RWTH Aachen, Germany, Institute for Combustion Technology, RWTH Aachen, Germany
- **Development of combustion models using DNS data and it's *a-posteriori* validation (Investigator from UKCTRF: Prof. N. Chakraborty (Newcastle University)):** Collaboration involving Chalmers University, Sweden, University of Duisburg, Germany; Universität der Bundeswehr München, Germany, ONERA, France
- **Fundamental understanding of premixed turbulent combustion using DNS data (Investigators from UKCTRF: Profs. N. Chakraborty (Newcastle University), R.S. Cant, N. Swaminathan (University of Cambridge)):** Collaboration involving Universität der Bundeswehr München, Germany (RSC and NC), Sandia National Laboratory (NC, RSC and NS), Shanghai Jiao'Tong University (NC), Tokyo Institute of Technology, Japan (NC and NS), University of Zaragoza (NC).
- **Flame acceleration and transition to detonation (Investigator from UKCTRF: Prof. J. Wen (Warwick University)):** Collaboration involving University of Science and Technology, China
- **Fully coupled fluid-solid simulation of upward flame spread and fire growth (Investigator from UKCTRF: Prof. J. Wen (Warwick University)):** Collaboration involving FM Global, USA
- **Integrated safety strategies for on hydrogen storage systems (Investigator from UKCTRF: Prof. J. Wen (Warwick University)):** Collaboration involving University of Ulster and University of Bath
- **Modelling radiative heat transfer in fires (Investigator from UKCTRF: Prof. J. Wen (Warwick University)):** Collaboration involving FM Global, USA
- **Numerical characterization and modelling of SYNGAS combustion (Investigators from UKCTRF: Profs. X.**

Jiang (Lancaster University); K.H. Luo (University College London), J. Wen (Warwick University), K.K.J. Ranga Dinesh (University of Southampton)): Collaboration involving University of Eindhoven, Netherlands.

➢ Consortium publications with international co-authors for the reporting period

- A. Bagdanaviciusa, P. J. Bowen, D. Bradley, M. Lawes, M. S. Mansour, "Stretch rate effects and flame surface densities in premixed turbulent combustion up to 1.25 MPa", Combustion and Flame, 162 4158–4166, 2015.
- L. Bates, D. Bradley, G. Paczko, N. Peters, "Engine Hot Spots: Decay, Deflagration, Auto-Ignitive Propagation, or Detonation" 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, Leeds, 2015.
- D. Bradley, P.H. Gaskell, X. Gu, A. Palacios, "Jet flame heights, lift-off distances, and mean flame surface density for extensive ranges of fuels and flow rates" Combustion and Flame (in press).
- D. Butz, Y. Gao, A.M. Kempf, N. Chakraborty, "Large Eddy Simulations of a turbulent premixed swirl flame using an algebraic Scalar Dissipation Rate closure" Combustion and Flame, 162, 3180-3196, 2015.
- N. Chakraborty, I. Konstantinou, A. Lipatnikov, "Effects of Lewis number on vorticity and enstrophy transport in turbulent premixed flames" Physics of Fluids (in press).
- C. Dopazo, L. Cifuentes, N. Chakraborty, "Enstrophy evolution in turbulent premixed combusting flows", JJ70, Salamanca, Spain, 3rd -4th September, 2015.
- M. Fischer, X. Jiang, "Numerical optimisation for model evaluation in combustion kinetics", Applied Energy , 156: 793-803, 2015.
- M. Fischer, X. Jiang, "An investigation of the chemical kinetics of biogas combustion", Fuel, 150, 711-720, 2015.
- Y.Gao, N. Chakraborty, M. Klein, "Assessment of sub-grid scalar flux modelling in premixed flames for Large Eddy Simulations: A-priori Direct Numerical Simulation." European Journal of Mechanics, Fluids-B , 52, 97-108, 2015.
- Y. Gao, N. Chakraborty, M. Klein, "Assessment of the performances of sub-grid scalar flux models for premixed flames with different global Lewis numbers: A Direct Numerical Simulation analysis", International Journal of Heat and Fluid Flow, 52, 28-39, 2015.
- R.A.C. Griffiths, J.H. Chen, H., Kolla, R.S. Cant, W. Kollmann, Three-dimensional topology of turbulent premixed flame interaction. Proceedings of the Combustion Institute, 35(2), 1341-1348, 2015.
- M. Klein, N. Chakraborty, Y. Gao, "Scale similarity based models and their application to subgrid scale scalar flux modelling in the context of turbulent premixed flames." International Journal of Heat and Fluid Flow, 57,91-108, 2016.
- M. Klein, C. Kasten, Y. Gao, N. Chakraborty, "A-priori Direct Numerical Simulation assessment of sub-grid scale stress tensor closures for turbulent premixed combustion." Computers & Fluids, 122, 1-11, 2015.
- M. Klein, N. Chakraborty, Y. Gao, " Applications of scale similarity based models to subgrid scale scalar flux modelling in the context of turbulent premixed flames", 9th International Symposium on Turbulence and Shear Flow Phenomena (TSFP-9), Melbourne, Australia, 30th June -3rd July, 2015.
- M. Klein, C. Kasten, Y. Gao, N. Chakraborty, M. Pfitzner, "Analysis of the combined modelling of subgrid transport and filtered flame propagation for premixed turbulent combustion", 9th Mediterranean Combustion Symposium, 7th-11th June, Rhodes Island, 2015.
- M. Klein, C. Kasten, Y. Gao, N. Chakraborty, "A-priori assessment of sub-grid scale stress tensor closures for turbulent premixed combustion", 7th European Combustion Meeting (ECM2015), 30th March-2nd April, Budapest, 2015.
- A, Lipatnikov, V. Sabel'nikov, S. Nishiki, T. Hasegawa, N. Chakraborty, "DNS assessment of a simple model for evaluating velocity conditioned to unburned gas in premixed turbulent flames." Flow Turbulence and Combustion, 94, 513-526, 2015.
- Y. Minamoto, K. Aoki, M. Tanahashi, and N. Swaminathan DNS of swirling hydrogen-air premixed flames. Accepted in J. Hydrogen Energy, 40(39) 13604-13620, 2015.
- K.K. J. Ranga Dinesh, J.A. van Oijen, K. H. Luo, X. Jiang, "Nitric oxide pollutant formation in high hydrogen content (HHC) syngas flames" International Journal of Hydrogen Energy 40: 13621-1363, 2015.
- J. Sellmann, J. Lai, A. M. Kempf, N. Chakraborty, "Statistical behaviour of Flame Surface Density transport in head on quenching of turbulent premixed flames: A Direct Numerical Simulation Analysis", Clean Air

2015, 5th-9th July, Lisbon, 2015.

➢ Involvement in international activities

- **EU and International projects**
  - "AMEL"- CleanSky 2 SAGE project (EU-Horizon 2020 grant, Investigator from UKCTRF: Profs. R.S. Cant, E. Mastorakos, N. Swaminathan (University of Cambridge), Start date: 18th February 2015; Current status: On-going)
  - Clean Sky DREAMCODE (EU-Horizon 2020 grant, Investigator from UKCTRF: Profs. W. Jones, P. Lindstedt, Dr. S. Rigopoulos (Imperial College, London), Start date: 1st November 2013; Current status: On-going)
  - "HPC4E (High Performance Computing for Energy)" (EU-Horizon 2020 grant for multi-national EU-Brazil Collaborative project, Investigator from UKCTRF: Prof. X.Jiang (Lancaster University), Start date: 1st December 2015; Current status: On-going)
  - "Improving Hydrogen Safety for Energy Applications (HySEA) through pre-normative research on vented deflagrations" (EU-Horizon 2020 grant, Investigator from UKCTRF: Prof. J. Wen (Warwick University), Start date: 1st September 2015; Current status: On-going)
  - "Advanced numerical techniques for pulverized biomass combustion modelling" (Portuguese Foundation of Science grant, Investigator: Prof. N. Chakraborty (Newcastle University), Start date: 4th January 2016)
  - "NUMOXYCOAL: Advanced Numerical Models for Oxy-Coal Combustion" (European Research Council, HORIZON 2020: Research Fund for Coal and Steel Call: RFCS-2015 Topic: RFCS-01-2015, Investigators from UKCTRF: Profs. N. Chakraborty (Newcastle University), S. Navarro-Martinez, S. Rigopoulos (Imperial College, London) Current status: under review)
- **Invited lectures by consortium members**

  Prof. N. Chakraborty (Newcastle University): Keynote lecture: 29th Israeli Combustion Symposium, 10th December, Tel-Aviv,2015

  Prof. W.P. Jones (Imperial College, London): Plenary lecture, Clean Air 2015, 5th-9th July, Lisbon, 2015);

  Prof. E. Mastorakos (University of Cambridge): Plenary lecture, 7th European Combustion Meeting (ECM2015), 30th March-2nd April, Budapest, 2015

  Prof. N. Swaminathan (University of Cambridge): 2nd National Propulsion Conference and Combustion Workshop, 23rd -25th February, 2015, Indian Institute of Technology-Bombay, India
- **Scientific committee of international conferences**

  Prof. N. Chakraborty (Newcastle University): One of the coordinators of 1st International Workshop on Coal and Biomass Conversion 21st April, Avignon, France; Clean Air 2015, 5th-9th July, Lisbon, 2015; Workshop of turbulent premixed combustion, Cambridge, UK, 26th June, UK

  Prof. E. Mastorakos: University of Cambridge): 9th Mediterranean Combustion Symposium

  Prof. N. Swaminathan: Workshop of turbulent premixed combustion, Cambridge, UK, 26th June, UK; International Forum on Multidisciplinary Education, Hawaii - Dec. 2015

  Dr. J. Xia: International workshop on multiphase flows and phenomena, 7th-8th September, 2015, Brunel, UK.
- **Editorships**

  Prof. E. Mastorakos (Associate editor of Combustion and Flame, Editorial board member of Combustion Theory and Modelling, Flow, Turbulence and Combustion, Guest Editor for the special issue on the 9th Mediterranean Combustion symposium in Flow Turbulence and Combustion; Co-chair of Turbulent Combustion colloquium of the 36th International Combustion Symposium)

  Profs. N. Chakraborty and N. Swaminathan (Guest Editors for the special issue on "Advances in turbulent premixed combustion" in Combustion Science and Technology)

Future Vision: How do you see the Consortium strategy evolving and changing in the future? In the next 5 years, what new science questions will members of your Consortium be seeking to address? Why are these important?

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 in the next 5 years 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 models in the context of Probability Density Function (PDF) and Conditional Moment Closure (CMC) methodologies. Some of these methodologies (e.g. the stochastic field, and 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 and applications involving biofuels. A number of collaborative works is under way in the consortium on hydrogen blended hydrocarbon and biofuel 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.