Annual Report for EPSRC High End Computing Consortia

Reporting Period: February 2017 - November 2018

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

Consortia Chair: Prof. Nilanjan Chakraborty

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.

Workshops and New Opportunities

The 4th annual progress review meeting of the UKCTRF, and the meeting between the management team and the Impact Advisory Panel (IAP) members, took place on 7th -8th September 2017 at the University of Southampton. It was organised as an international workshop on simulation and modelling of turbulent reacting flows. There were 3 invited keynote lectures (45 min) and 23 contributed oral presentations (15 min each). The invited keynote lectures were delivered by Profs. Cesar Dopazo (University of Zaragoza, Spain), A.M. Kempf (from University of Duisburg, Essen, Germany), and Dr. Isaac Boxx (DLR, German Aerospace Centre). In order to showcase the diverse range of ongoing research within the consortium and enable exchange of research ideas, the 5th annual meeting was organised as an international conference. This conference and the annual meeting between the management team and IAP members took place at Selwyn College, Cambridge on the 12th -13th of September 2018 where 4 invited keynote lectures (45 min) and 21 contributed oral presentations (15 min each) were delivered. Four combustion scientists of significant international repute (Prof. J.H. Chen, Sandia National Laboratory, USA; Prof. A. Kronenburg, University of Stuttgart, Germany; Prof. Suresh Menon, Georgia Institute of Technology, USA; Dr. Khawar Syed, Infosys Limited) delivered the keynote lectures. A special issue in the journal entitled Combustion Science and Technology based on the research took place under the umbrella of UKCTRF is currently under way and Profs. N. Chakraborty (Newcastle University), R.S. Cant (University of Cambridge), W.P. Jones, S. Navarro-Martinez (Imperial College, London) are acting as guest editors for this special issue. So far, 15 submissions have been received and they are currently under review. It is anticipated that the special issue will be ready for publication by March 2019. The next annual progress meeting and the meeting between the management team members and Impact Advisory Panel (IAP) members will take place in the University of Brighton in September 2019 . It is expected that the number of contributors will grow considerably for the next meeting because of the increasing number of users of ARCHER in the consortium. The UKCTRF consortium chair and the management team members of UKCTRF routinely take part in the CCP-12 meetings and activities.

In response to EPSRC's call on High-End Consortia call in summer 2017, a proposal entitled Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF) was submitted to EPSRC on behalf of UKCTRF. The reviewers' comments were extremely supportive of the research outlined in the proposal. We were invited for an interview at the EPSRC's headquarters Polaris House, Swindon on the 2nd of February, 2018

and our application turned out to be positive based on the outcome of this interview. In fact, the UKCTRF proposal was ranked 1st in the ranked-order panel list. The new expanded UK Consortium on Turbulent Reacting Flows (UKCTRF) will further utilise the developments of High-Performance Computing (HPC) to offer improved fundamental understanding and modelling of turbulent reacting flows, which are pivotal in the effective usage of energy resources, development of reliable fire safety measures, and manipulation of the combustion processes to ensure environmental friendliness. Over the next 4 years, the consortium's goals are to: (i) further utilise HPC resources to conduct world-leading turbulent reacting flow research involving, Reynolds Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS); (ii) extract fundamental physical insights from simulations to develop high-fidelity modelling methodologies to study turbulent reacting flows relevant to power production, transportation and fire safety engineering; and (iii) ensure a forward-looking software development strategy to develop computationally efficient algorithms, and effectively exploit current and future developments of HPC hardware.

The proposal on behalf of UKCTRF entitled Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows (EP/P022286/1) submitted to EPSRC in response to their call on flagship software development call in 2016 has been successful. This project focuses on the development, validation, and documentation of a next-generation fully parallelised computational fluid dynamics (CFD) code called HAMISH based on adaptive mesh refinement (AMR) which enables high-fidelity DNS of advanced turbulent reacting flows such as flame-wall interaction, localised ignition, and droplet combustion including atomisation processes. Such simulations cannot be achieved at present without limiting simplifications due to their prohibitive computational cost. Hence, AMR offers a step-change in capability for the computational analysis of turbulent reacting flows and provides data having a degree of detailed physical information not currently available from simulations using existing CFD codes.

The biennial International Symposium on Combustion, Turbulent Heat and Mass Transfer and the Engineering Turbulence Modelling and Measurements are the premier conferences, which took place in 2018. Papers presented at these meetings are of the highest quality, and the interactions with peers during the symposium are intellectually stimulating. UKCTRF members in the past have been successful in getting papers accepted for special issues of journals like Combustion Science and Technology, Combustion Theory and Modelling, Flow, Turbulence and Combustion in a very competitive environment, especially as the publications in these journals carry high impact factors. To help members to maximise the impact of disseminating their results, partial funding is available for attending these conferences. Every named investigator's research group was eligible for a maximum of £2000 for disseminating their research at major international conferences in 2017. In 2018, every research group who had a paper accepted in the 37th International Symposium on Combustion received £1000 from the consortium and further £500 per named investigator's group was made available for disseminating research done under the umbrella of UKCTRF to other conferences (e.g. Turbulent Heat and Mass Transfer and the Engineering Turbulence Modelling and Measurement). The list of awards can be seen from: http://www.ukctrf.com/members-area/past-conference-funding/.

Issues and Problems

Currently the demand for computational time is much greater than the amount awarded to the consortium. Almost 100% of computational time for June-November 2017 allocation cycle was utilised, for December 2017-May 2018 allocation cycle we have received requests for computer time for a total of 289,105 kAUs within the application deadline decided by the UKCTRF management team, whereas we only had 130,446 kAUs to allocate. In order to allocate computational time to all applicants, the management team had to award severely reduced computational time to the applicants (e.g. anybody who requested more than 13,251kAUs received only 13,251kAUs) which adversely affected productivity. The utilisation of the computational time was 100% in the aforementioned allocation periods For the allocation cycle which started in June 2018, we received applications for 201,000kAUs (please note that demand did not go down but applicants tailored their requests based on the availability of the computational time), whereas we only had 168,503 kAUs to allocate. As a result, any applications, which requested more than 14,000 kAUs, received 14,000kAUs.Computational time usage is closely monitored by the management team of UKCTRF and if there is no significant usage within a period of two months, then that time is reallocated to other deserving users. The management team of the UKCTRF also ensures linear usage of time with a slope of unity during the allocation period.

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), A. Aspden; University of Brighton: Dr. K. Vogiatzaki; University of Brunel: Dr. J. Xia; University of Cambridge: Profs. R.S. Cant, E. Mastorakos, M. Kraft, and N. Swaminathan, and Dr. C. Armitage; University of Central Lancashire: Prof. G.M. Makhviladze, Drs. W. Liu, and J. Mai; Cranfield University: Dr. K.W. Jenkins; Daresbury Laboratory: Prof. D. Emerson, Drs. C. Moulinec and X. Gu; University of Edinburgh: Profs. **G. Jomaas**, J. Torero, Dr. S. Welch, and D. Hyuk Shin; Imperial College, London: Profs. **P. Aleiferis**, W.P. Jones, R.P. Lindstedt, Drs. **A.Guisti,** F. Marquis, A. Morgans, S. Navarro-Martinez, **G. Papadakis**, S. Rigopoulos, and G. Rein; Liverpool John Moore University: **Dr. S. P. Malkeson**; Loughborough University: Profs. W. Malalasekara, J. McGuirk, Drs. A Garmory, **I. Langella**; Northumbria University: **M. Jiangi**; Queen Mary London: Prof. X. Jiang; 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; University of Ulster: Profs. M. Delichatsios and V.B. Novozhilov, **Dr. J. Zhang**; 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.*

- If all the publications relating to the work of the Consortium for this reporting period have been added to ResearchFish / will be added to ResearchFish by the end of the ResearchFish reporting exercise, please indicate this below.
- If submission of a full list of publications to the Consortium record/s in ResearchFish has **not** been possible for this reporting period please provide a list of publications that have resulted from work performed on ARCHER by the Consortium during this reporting period (this can be included as a separate attachment).
- For the reporting period please provide a bullet pointed list of key / important research findings that has resulted from work performed on ARCHER by the Consortium. Please reference any related 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.

➢ **Key research outcomes and linked journal publications and book chapters**

Fundamental understanding and modelling of multi-phase combustion using high-fidelity simulations

U. Ahmed, C. Turquand-Auzay, M. Muto, N. Chakraborty, R. Kurose, Statistics of reaction progress variable and mixture fraction gradients of a pulverised coal jet flame using Direct Numerical Simulation data, Proc. Combust. Inst., 37, https://doi.org/10.1016/j.proci.2018.06.223.

C. Bilger, M. Aboukhedr, K. Vogiatzaki, R. S. Cant, Evaluation of two-phase flow solvers using Level Set and Volume of Fluid methods. J. Comput. Phys., 345, 665-686, 2017.

A. Giusti, E. Mastorakos, Detailed chemistry LES/CMC simulation of a swirling ethanol spray flame approaching blow-off, Proc. Combust. Inst., 36, 2652-2633, 2017.

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Modelling of conventional turbulent premixed, non-premixed and stratified mixture combustion

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I. Langella, N. Swaminathan, Y. Gao, N. Chakraborty, LES of premixed combustion using an algebraic closure involving scalar dissipation rate. Combust. Sci. Technol., 189, 43-77, 2017.

A.N. Lipatnikov, V. Sabelnikov, N. Chakraborty, S. Nishiki, T. Hasegawa, A DNS study of closure relations for convection flux term in transport equation for mean reaction rate in turbulent flow, Flow, Turb. Combust., https://doi.org/10.1007/s10494-017-9833-y (2017).

M. Klein, N. Chakraborty, A-priori analysis of an alternative wrinkling factor definition for Flame Surface Density based Large Eddy Simulation modelling of turbulent premixed combustion, Combust. Sci. Technol., DOI: 10.1080/00102202.2018.1452394.

M. Klein, C. Kasten, N. Chakraborty, A-priori direct numerical simulation assessment of models for generalized sub-grid scale turbulent kinetic energy in turbulent premixed flames, Computers & Fluids, 154, 123-131, 2017.

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Fundamental physical understanding of conventional combustion processes

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Fundamental physical understanding and modelling of unconventional combustion processes (e.g. flame-wall interaction and MILD combustion)

U. Ahmed, N.A. K. Doan, J. Lai, M. Klein, N. Chakraborty, N. Swaminathan, Multiscale analysis of head-on quenching premixed turbulent flames, Phys. Fluids, 30,105102, 2018.
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Advanced numerical techniques and simulation methodologies

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➢ Relevant grants and awards

- Prof. N. Chakraborty (Newcastle University) was awarded the Mercator Fellowship, Germany: Detailed analysis and modelling of turbulent stratified combustion using Large Eddy Simulations, Funded by DFG, Germany (total value 43,000 Euro)
- EPSRC research grant EP/R029369/1: Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF) (£501,644, PI: Prof. Nilanjan Chakraborty, Co-Is: Profs. R.S. Cant, W. P. Jones, E. Mastorakos, N. Swaminathan, Dr. S. Navarro-Matrinez)
- Prof. N. Chakraborty (Newcastle University) was awarded the short term Japanese Society of Promotion of Science (JSPS) fellowship for collaborative research on multi-phase turbulent reacting flows at the University of Kyoto in the summer of 2017 (Host: Prof. R. Kurose)

- EPSRC research grant EP/P022286/1: Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows (£475k, PI: Prof. Nilanjan Chakraborty, Co-Is: Profs. R.S. Cant, D. Emerson, Dr. C. Moullinec)
- UK-Gulf Institutional Links 2016 grant (2791341267): A combined experimental and numerical investigation of ignition probability of turbulent inhomogeneous biogas-air mixtures (£371k, PI: Prof. Nilanjan Chakraborty)
- ERC-Consolidator grant: Acoustic-flow interactions in the combustion chambers of aeroplane engines and power gas turbines (€1.98m, PI: A.Morgans)
- eCSE project: Integration of an implicit stiff ordinary differential equation solver into the Direct Numerical Simulation code SENGA2 for turbulent reacting flows PI: Prof. Nilanjan Chakraborty, Co-Is: Prof. R.S. Cant)

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 the 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. During the reporting period, the main workhorse of Work Package 1 of UKCTRF, SENGA2 (already ported on ARCHER) was updated, incorporating new functionality for droplets, coal/biomass particles and highly-detailed chemistry, as well as improvements made to time stepping and boundary conditions.

The proposal on behalf of UKCTRF entitled Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows submitted to EPSRC in response to their call on flagship software development in 2016 has been successful. Prof. N. Chakraborty (Newcastle University) is the PI and Profs. R.S. Cant (Cambridge),D. Emerson (Daresbury Laboratory) and Dr. C. Moulinec (Daresbury Laboratory) are the Co-Is of this proposal.

This project focuses on the development, validation and documentation of a next-generation fully parallelised computational fluid dynamics (CFD) code called HAMISH, based on adaptive mesh refinement (AMR) which enables high-fidelity Direct Numerical Simulations (DNS) of advanced turbulent reacting flows such as flame-wall interaction, localised ignition, and droplet combustion including atomisation processes.

Such simulations cannot be achieved at present without limiting simplifications due to their prohibitive computational cost. AMR for large-scale highly-parallel simulations of compressible turbulent reacting flows is a significant new functionality, which offers major benefits in terms of computational economy for problems involving thin fluid-mechanical structures, e.g. resolution of both the flame and the boundary layer in flame-wall interaction, droplet surfaces in atomisation in spray combustion, shock waves in localised forced ignition, etc. Such structures have either been ignored or simplified severely in previous work due to the prohibitive computational cost of fixed global meshes, thus limiting the usefulness of the simulations. Hence AMR offers a step-change in capability for the computational analysis of turbulent reacting flows and provides data with the degree of detailed physical information which is not currently available from simulations using existing CFD codes. The software is validated with respect to the results obtained from the well-proven uniform-mesh DNS code SENGA2, which has already been ported to ARCHER and is currently widely used by members of the UK Consortium on Turbulent Reacting Flows (UKCTRF). The newly developed code, HAMISH, is not only be ported to ARCHER, but also is prepared for architectures supporting accelerators, thanks to OpenMP 4.5, which will support OpenACC, targeting a POWER8 cluster. As a part of this project, a detailed user guide will be produced at each new release of the code.

The project started in July 2017 and Drs. U. Ahmed and G. Nivarti joined as Research Associates at Newcastle and Cambridge groups. A dedicated postdoctoral researcher, Dr Jian Fang, joined Daresbury in November 2014, and has been working with Newcastle and Cambridge groups to develop the capabilities of HAMISH. The Cambridge group is focussing on developing multi-phase capabilities in HAMISH, whereas the Newcastle group is involved in validation of HAMISH mainly based on single phase problems. Daresbury group is responsible for the computer science aspect of the software development and focuses principally into research into the algorithms, which need careful attention in relation to the development of HAMISH, particularly the adaptive meshing for DNS.

A significant progress has been made in the development of HAMISH with active support from the University of Cambridge, Newcastle University and Daresbury Laboratories. HAMISH was initially developed at Cambridge University as the next generation CFD solver based on adaptive mesh refinement (AMR) using Morton code and Octree algorithms. This technique is very efficient in capturing fine small-scale motions in reactive flows (such as droplets, flame/wall interaction), as it requires much less computing resources than classical methods because it is using dynamic mesh refinement. This code allows for new simulations in areas previously inaccessible due to high computational cost. The specific areas include flame-wall interaction,

two-phase flow and droplet combustion, but the development of this code also benefits the wider Combustion community with respect to DNS/LES-based research. During 2016, HAMISH was improved in the following respects:

1. Improvement of the basic N-S solver by successfully removing the existing grid-grid wiggle problem.
2. Testing the code for 3-D Taylor-Green Vortex cases up to 10,000 processors and profiling the code for the non-AMR mode.
3. Fixing some critical issues in terms of AMR-related algorithms.
4. Successfully running the code in the AMR code and testing the AMR solver for 1D/2D/3D flame diffusion cases in sequential mode.
5. Fixing some issues in terms of parallel-AMR-related algorithms.
6. Presenting the progress in the development of HAMISH code at the UKCTRF annual meeting in Durham.
7. Simulation of freely propagating premixed turbulent flames and head-on quenching of premixed flames by isothermal inert walls.

The team members feel that they are very close to the goal of running HAMISH with its full capacity (parallel and AMR on). There are also plans in place for adding more functionality to the code to support the wider research interests of the community.

Recent research carried out by UKCTRF members has also had a major impact on industry and policy. The development of an improved CFD model by the research group at the University of Warwick has been adopted by the sponsor FM Global and used by their engineers in numerical simulations to reduce the number of large scale fire tests, which typically costs $50K USD per test. The findings from a recently completed KTP project at Warwick have been adopted in the consulting practices at DNV GL, the world's leading classification society and a recognized advisor for the maritime industry. The outcome has resulted in a £400K increase in the annual sales turnover and is expected to lead to £2M increase in annual sales turnover in three years' time.

UKCTRF members based at Warwick have also started a new EU project (HySEA) with the support of international companies Air Products, Air Liquide, Shell, FIKE and FM Global to conduct research that will result in recommendation to update both the International and European Standards concerning protection of hydrogen energy applications through explosion venting.

In response to EPSRC's call on High End Computing consortia, a proposal entitled Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF) has been submitted to EPSRC on behalf of UKCTRF. Prof. N. Chakraborty (Newcastle University) is the PI, and Profs. R.S. Cant (Cambridge), E. Mastorakos (Cambridge), N. Swaminathan (Cambridge), W.P. Jones (Imperial College), D. Emerson (Daresbury Laboratory) and Dr. S. Navarro-Martinez (Imperial College) are the Co-Is of this proposal. This grant application turned out to be successful. The focus of the proposed activity in the new incarnation of the consortium will be on providing highly-skilled technical support to the consortium and the development and maintenance of our core software, SENGA+ and HAMISH, to ensure efficient utilisation of the HPC resources. In recent years, the complex hierarchical memory structure of modern hardware (e.g. heterogeneous multicore) has created significant challenges for delivering performance. Extracting this new level of concurrency from these hardware platforms represents a major technical challenge. For example, emerging platforms now involve floating point accelerators provided by Graphical Processing Units (GPUs) or Intel's Xeon Phi. WP3 enables our core codes to successfully adapt to the evolving hardware and take advantage of future high-end computing. This activity is relevant for ARCHER/ARCHER2 and Tier 0 facilities available through PRACE and international collaborations. In particular, the proposed research will focus on: (a) Non-intrusive language directives (OpenMP 4.5+ and OpenACC) and vectorisation to exploit multicore, manycore and GPU-based accelerators for discretisation techniques; (b) Improvement of I/O performance for petascale execution, which is key factor for the overall performance on large core counts (> 100,000 cores); (c) Development of AMR-based Weighed Essentially Non-Oscillatory (WENO) schemes in HAMISH to give it the ability of capturing discontinuities to deliver high-fidelity solutions that retain robustness whilst resolving challenging flow physics; and (d) Adaptation of HAMISH to problems with complex geometries with the implementation of the immersed boundary method together with the AMR solver.

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 information on the number of PhDs and Post-Docs that have been trained in the use of ARCHER as a result of work relating to the Consortium.
- 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 ((ECRs) i.e. PhD students, Postdoctoral Research Associates). In the 4th Annual Progress meeting of UKCTRF (http://www.ukctrf.com/ukctrf-events/future-events/), ECRs gave 20 oral presentations out of 26 oral presentations and about 40 ECRs attended the meeting. This substantiates the high level of

involvement of ECRs in the consortium activities. UKCTRF members 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 are publicised to consortium members by the UKCTRF administration. The EPCC's consortium contact for ARCHER was invited to the 4th Annual Progress review meeting of the UKCTRF to publicise and discuss 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 the management team to explore the possibility of having training sessions which might be beneficial for the consortium users. We also scheduled an advanced MPI training course just ahead of the 4th Annual Progress meeting of UKCTRF at the same venue in collaboration with EPCC staff members. We also used the fund for workshop organisation to award first and second prizes for the best oral presentation and best image/videos to the ECRs based on the feedback of the attendees and Impact Advisory Panel (IAP) members (http://www.ukctrf.com/news/).

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 new regulations 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 such training activities at regular intervals. It was decided by the management team that 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 UKCTRF Management team that the availability of such facilities will be disseminated more extensively among the consortium members in the future and they will be encouraged to make use of all available opportunities. Most UKCTRF members are also the members of the British Section of the Combustion Institute (BSCI) and BSCI has plans to organise a weeklong course on combustion theory and modelling in the near future. The ECRs associated with UKCTRF members will benefit from this course.

The consortium has a strong link to the UK Fluids Network through its Combustion Science and Technology and Droplets and Sprays Special Interests Group, where the PI of the UKCTRF is involved as the co-leader and this link is utilised to broaden the UKCTRF user base, interaction and exchange of ideas with experimentalists, training activities of ECRs and also for the outreach purpose.

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.*

- For the reporting period please provide where possible information on Consortium projects that have been performed in collaboration with industry, this should include:
  - Details of the companies involved.
  - Information on the part ARCHER and the Consortium played.
  - A statement on the impact that the work has / is making.
  - If relevant, details of any in kind or 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 is 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 UKCTRF members alike 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 identify 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. 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 required for their business. The development of an improved CFD model by the research group at the University of Warwick has been adopted FM Global, and used by their engineers in numerical simulations to reduce the number of large scale fire tests, which typically costs $50K USD per test.

➢ Publications that have industrial co-authorship

- Z. Chen, S. Ruan, N. Swaminathan, Large Eddy Simulation of flame edge evolution in a spark-ignited methane-air jet, Proc. Combust. Inst., 36, 1645-1652, 2017.
- Z. Chen, N. Swaminathan, M. Stöhr, W. Meier, Interaction between self-excited oscillations and fuel-air mixing in a dual swirl combustor.Proc. Combust. Inst. ISSN 1540-7489 (2018).
- I. Langella, Z. Chen, N. Swaminathan, S.K. Sadasivuni, Large-eddy simulation of reacting flows in industrial gas turbine combustor. J. Propulsion and Power, 34. pp. 1269-1284, 2018.
- S.P. Malkeson, D.H. Wacks, N. Chakraborty, Modelling of Variance and Co-variance in Turbulent Flame–Droplet Interaction: A Direct Numerical Simulation Analysis, Droplets and Sprays, (Eds. S. Basu, A. Mukhopadhyay), 1st Edition, Springer, 2017.
- W.C. Ullrich, Y. Mahmoudi, K. Lackhove, A. Fischer, C. Hirsch, T. Sattelmayer, A.P. Dowling, N. Swaminathan, A. Sadiki, M. Staufer, Prediction of Combustion Noise in a Model Combustor Using a Network Model and a LNSE Approach. J. Engineering for Gas Turbines and Power, 140. ISSN 0742-4795, 2018.

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 each example please provide a brief summary of the part that ARCHER and the Consortium have played.
- 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

- **UK-Gulf Institutional Links 2016 grant (2791341267): A combined experimental and numerical investigation of ignition probability of turbulent inhomogeneous biogas-air mixtures (Investigator from UKCTRF: Prof. N. Chakraborty (Newcastle University)):** Collaboration involving Qatar University, Qatar
- **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), King Abdullah University of Science and Technology, Saudi Arabia (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 and California Institute of Technology
- **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
- **Modelling radiative heat transfer in fires (Investigator from UKCTRF: Prof. J. Wen (Warwick University)):** Collaboration involving FM Global, USA
- **EPSRC funded project Integrated safety strategies for onboard hydrogen storage systems (Investigator from UKCTRF: Prof. J Wen (University of Warwick)):** This project is supported by an Advisory Board involving over a dozen international experts from industry, research laboratories and universities.
- DFG funded **Mercator Fellowship for Prof. N. Chakraborty (Newcastle University)** linked with the project on Detailed analysis and modelling of turbulent stratified combustion using Large Eddy Simulations, Funded by DFG, Germany (total value 43,000 Euro)

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

- U. Ahmed, C. Turquand-Auzay, M. Muto, N. Chakraborty, R. Kurose, Statistics of reaction progress variable and mixture fraction gradients of a pulverised coal jet flame using Direct Numerical Simulation data, Proc. Combust. Inst., 37, https://doi.org/10.1016/j.proci.2018.06.223 (2018).
- U. Ahmed, N.A. K. Doan, J. Lai, M. Klein, N. Chakraborty, N. Swaminathan, Multiscale analysis of head-on quenching premixed turbulent flames, Phys. Fluids, 30,105102, 2018.
- U. Allauddin, M. Pfitzner, M. Klein, N. Chakraborty, A-priori and a-posteriori analysis of algebraic flame surface density modelling in the context of large eddy simulation of turbulent premixed combustion. Numer. Heat Trans. A., 71, 153-171, 2017.
- A.J. Aspden, J.B. Bell, M.S. Day, F.N. Egolfopoulos, Turbulence-flame interactions in lean premixed dodecane flames, Proc. Combust. Inst., 36, 2005-2016, 2017.
- A.J. Aspden, N. Zettervall, C. Fureby, An a priori analysis of a DNS database of turbulent lean premixed methane flames for LES with finite-rate chemistry, Proc. Combust. Inst., 37, 10.1016/j.proci.2018.05.017 (2018).
- N. Chakraborty, L. Wang. I. Konstantinou, M. Klein, Vorticity statistics based on velocity and density-weighted velocity in premixed reactive turbulence, J. Turb., 18, 9, 2017.
- N. Chakraborty, M. Klein, D. Alwazzan, H. G. Im, Surface Density Function statistics in Hydrogen-air flames for different turbulent premixed combustion regimes, Combust. Sci. Technol., https://doi.org/10.1080/00102202.2018.1523152 (2018).
- N. Chakraborty, D.H. Wacks, S. Ketterl, M. Klein, H. G. Im, Scalar dissipation rate transport conditional on flow topologies in different regimes of premixed turbulent combustion, Proc. Combust. Inst., 37, https://doi.org/10.1016/j.proci.2018.06.092 (2018).
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➢ Involvement in international activities

- **EU and International projects**
  - A combined experimental and numerical investigation of ignition probability of turbulent inhomogeneous biogas-air mixtures (UK-Gulf Institutional Links 2016 grant, Investigator from UKCTRF: Prof. N. Chakraborty (Newcastle University), Start date: 10th July 2017, 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 Science Foundation grant): Investigator from UKCTRF: Prof. N. Chakraborty (Newcastle University), Start date: 1st February 2016; Current status: On-going)
  - CORNET - H2020/Clean Sky RIA project (Investigator from UKCTRF: N. Swaminathan (Cambridge University), Start date: 1st March 2016; Current status: On-going)
  - LES of Azimuthal instability in GT combustor (Grant from MHI, Japan): Investigator from UKCTRF: Prof. N. Swaminathan (Cambridge University), Start date: 1st July 2016; Current status: On-going)

- **Invited lectures by consortium members**

- JAXA (Japanese State Aerospace Laboratory), Tokyo, Japan; Title: Relevance and modelling of scalar dissipation rate in the context premixed turbulent combustion by Prof. N. Chakraborty (Newcastle University)
- Kyushu University Mechanical Engineering Department, Hakata, Japan; Title: Lewis number effects on turbulent premixed combustion and modelling implications: A Direct Numerical Simulation perspective by Prof. N. Chakraborty (Newcastle University)
- Osaka University Mechanical Engineering Department, Hakata, Japan; Title: Distributions of flow topology and enstrophy in different regimes of premixed turbulent combustion: A Direct Numerical Simulation investigation by Prof. N. Chakraborty (Newcastle University)
- UKTC annual meeting 2018, London, UK: Influences of heat release on turbulent fluid motion in premixed combustion by Prof. N. Chakraborty (Newcastle University)
- Duisburg University Mechanical Engineering Department, Duisburg, Germany: A Direct Numerical Simulation analysis of turbulent spherically expanding flames in droplet-laden mixtures by Prof. N. Chakraborty (Newcastle University)

- **Scientific committee of international conferences**
  - Prof. E. Mastorakos (University of Cambridge): Colloquium chair for turbulent combustion colloquium in the 37th International Combustion Symposium.
  - Prof. N. Chakraborty (Newcastle University): Colloquium chair for turbulent combustion colloquium in the 11th Mediterranean Combustion Symposium.

- **Invited courses**

  Prof. N. Chakraborty (Newcastle University): An invited course on Computational Modelling of Turbulent Combustion at Jadavpur University, Kolkata, India in December 2016. The course was funded by the Ministry of Human Resources Development, India as a part of Global Initiative of Academic Network (GIAN) scheme.

- **Editorships**

  Prof. E. Mastorakos (Associate editor of Combustion and Flame, Editorial board member of Combustion Theory and Modelling, Flow, Turbulence and Combustion; Co-chair of Turbulent Combustion colloquium of the 37th International Combustion Symposium)

  Profs. N. Chakraborty, R.S. Cant, W. P. Jones and Dr. S. Navarro-Martinez are the editors for the special issue of Combustion Science and Technology based on the 5th workshop of UKCTRF in 2018.

Other Highlights for the Current Reporting Period: Please provide details of any other significant highlights from the reporting period that are not captured elsewhere in the report.

➢ **Relevant achievements and impacts**

- Altogether 450+ publications over last 4 years and 25% of these publications involve international collaboration.
- A total £10M research council funding (EPSRC, ERC, EU and Newton grants) by the consortium members. A similar amount of industrial funding (estimated because all amounts are not disclosed) has been secured by the consortium members during this period.
- Altogether 50 PhD students and 30 Research Associates directly benefitted from the consortium activities
- A total of 15 Early Career Researchers who got benefitted by consortium activities are now in permanent academic and industrial jobs.

➢ **Relevant grants and awards**

- Prof. N. Chakraborty (Newcastle University) was awarded the Mercator Fellowship, Germany: Detailed analysis and modelling of turbulent stratified combustion using Large Eddy Simulations, Funded by DFG, Germany (total value 43,000 Euro)
- EPSRC research grant EP/R029369/1: Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF) (£501,644, PI: Prof. Nilanjan Chakraborty, Co-Is: Profs. R.S. Cant, W. P. Jones, E. Mastorakos, N. Swaminathan, Dr. S. Navarro-Matrinez)
- Prof. N. Chakraborty (Newcastle University) was awarded the short term Japanese Society of Promotion of Science (JSPS) fellowship for collaborative research on multi-phase turbulent reacting flows at the University of Kyoto in the summer of 2017 (Host: Prof. R. Kurose, Kyoto University)
- EPSRC research grant EP/P022286/1: Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows (£475k, PI: Prof. Nilanjan Chakraborty, Co-Is: Profs. R.S. Cant, D. Emerson, Dr. C. Moullinec)

- UK-Gulf Institutional Links 2016 grant: A combined experimental and numerical investigation of ignition probability of turbulent inhomogeneous biogas-air mixtures (£371k, PI: Prof. Nilanjan Chakraborty)
- eCSE project: Integration of an implicit stiff ordinary differential equation solver into the Direct Numerical Simulation code SENGA2 for turbulent reacting flows PI: Prof. Nilanjan Chakraborty, Co-Is: Prof. R.S. Cant)

HEC Consortia Model: Over the coming months EPSRC will be looking at the future of the HEC Consortia model and potential future funding. We would like to use this opportunity to ask the Consortia Chairs for input:

- What are the key benefits that your community have experienced through the existence of the HEC Consortia?
- What elements of the financial support provided by the HEC Consortium's grant have worked well and what could be improved in the future?

➢ **Key benefits for the community due to the existence of the UKCTRF**

The existence of this consortium enabled the community to achieve the following:

- Exploit HPC resources to perform leading-edge reacting flow simulations involving Reynolds Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS);
- Obtain fundamental physical information and develop high-fidelity modelling methodologies for analysing turbulent reacting flows with relevance to energy, gas turbine, automotive and fire safety engineering;
- Develop a forward-looking software development strategy to efficiently exploit today's and future HPC hardware;
- A platform to collaborate and share expertise within community to avoid duplication of research and remain internationally competitive;
- Supporting both externally funded (e.g. EU and industrial) and internal (e.g. university funded) projects, which do not have dedicated HPC support of their own;
- Development of highly skilled manpower in the form of early career researchers who have received an extensive training on the reacting flow physics and modelling, mathematical analysis, high-performance computing and software development.

➢ **Elements of the financial support provided by the HEC Consortium's grant have worked well and what could be improved in the future**

The funding for travel and subsistence, workshop/meeting arrangement and website development has worked well so far. The financial support could be improved by considering the provision for funding of the following aspects:

(i) 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 such training activities at regular intervals. It is recognised that EPSRC funded CDTs can offer some of these training activities, but does not meet all the requirements. Especially, some funding for courses on advanced parallelisation techniques in collaboration with EPCC will be particularly helpful.

(ii) The job of annual reporting and handling other activities related to administrative duties of the consortium is becoming increasingly time consuming for a single academic as the consortium chair, even with a small percentage (~15%) of secretarial support, so provision for part of a Research Associate's (RA's) time for the help in the aforementioned administrative activities will be useful for the next incarnation of the HEC consortia.

Web-Content Approval:

Please indicate which sections of the annual report could be used to produce content for the Consortia pages on the ARCHER website: https://www.archer.ac.uk/community/consortia/

Section Heading	Yes / No / Maybe	Comments
Membership	Yes	Happy to disseminate on the website
World class and world leading scientific output	Yes	Happy to disseminate on the website

Greater scientific productivity:	Yes	Happy to disseminate on the website
Increasing the UK's CSE skills base	Yes	Happy to disseminate on the website
Increased impact and collaboration with industry	Yes	Happy to disseminate on the website
Strengthening of UK's international position**:**	Yes	Happy to disseminate on the website
Other Highlights for the Current Reporting Period	Yes	Happy to disseminate on the website

To Note: New web-content generated from the annual reports will not be published without the approval of the relevant Consortium Chair.