Annual Report for EPSRC High End Computing Consortia

Reporting Period: November 2018 – October 2019

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 current incarnation of UK Consortium on Turbulent Reacting Flows (UKCTRF) was launched on the 8th of January 2019 upon the successful outcome of EP/R029369/1: Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (involving 15 UK institutions, 1 Principal Investigator and 34 Co-Investigators), which was submitted to the Engineering and Physical Sciences Research Council (EPSRC) in response to the High End Computing (HEC) call. The new expanded UK Consortium on Turbulent Reacting Flows 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. These challenges are multi-faceted and will require collaboration across a wide range of scientific areas. The UKCTRF brings together 43 experts (PI, 6 Co-Investigators, and 36 members) across 19 UK institutions, experienced in using HPC to enable concerted collaborative Computational Fluid Dynamics (CFD)-related fundamental and applied research on turbulent reacting flows to reduce duplication, and tackle challenges grander than individual attempts. Since its inception in 2014, the UKCTRF has achieved significant scientific and industrial impact with over 450 journal and conference papers which utilised ARCHER. The President of the Combustion Institute (PCI), Prof. J.F. Driscoll, has stated in his support letter that the publications of the UKCTRF members are among the best which help develop the minds of young researchers and the support letter from Rolls Royce states that as a result of the UKCTRF significant progress was made in the prediction of combustion phenomena with the help of HPC. 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 proposed research will build on the foundations of the previous incarnation of UKCTRF (EP/K025163/1, which ran between 2014-2019) and Flagship Software development (EP/P022286/1) grants and will address universal challenges of energy efficiency, sustainability and high-fidelity fire safety. The progress in HPC will enable this new incarnation of UKCTRF to reinforce existing strengths, but also address the following timely intellectual and industry-driven challenges: (i) simulation and modelling of multi-phase reacting flows (e.g. droplet and pulverised coal/biomass combustion); (ii) combustion analysis of biogas and low calorific fuels derived from coal gasification; (iii) flame-wall interaction; and (iv) combustion at elevated pressures, which have only recently become accessible due to the advancement of HPC.

Workshops and New Opportunities

The 1st annual progress review meeting of the most recent incarnation of UKCTRF, and the meeting between the management team and the Impact Advisory Panel (IAP) members, took place on 11th -12th September 2019 at Imperial College London (http://www.ukctrf.com/index.php/upcoming-events-2019/). There were 2 invited keynote lectures (45 min) and 16 contributed oral presentations (15 min each). Prizes were given to the early career researchers for the best technical content and audio-visual materials based on these presentations. The invited keynote lectures were delivered by Dr. N. Tonello from Renuda Ltd. and Prof. Peter Lindstedt, Imperial College, London. The next annual progress review meeting and the meeting between the management team and IAP members will take place in Daresbury Laboratory, Warrington sometime in early September in 2020. One keynote speaker from industry and another academic of significant international repute (Prof. B. Greenberg) have already been invited. In order to showcase the diverse range of ongoing research within the consortium, the annual progress review meetings in 2021 (to be held at Brunel University) and 2022 (to be held at Newcastle University) will be treated as international conferences with workshops on simulation and modelling of turbulent reacting flows. It is anticipated

that the number of contributors will grow considerably for the next meeting because of the increasing number of users of ARCHER in the consortium.

In response to EPSRC's recent Collaborative Computational Project (CCP) Networks call, a proposal entitled "Collaborative Computational Project on Reacting Turbulent Flows (CCP-ReacT)" has been submitted to EPSRC on behalf of UKCTRF. CCP-ReacT will focus on retaining and expanding the international impact of the research undertaken by our community by creating a unique set of networking activities combined with ambitious software engineering and development activities. Training our researchers will be a key aspect of CCP-ReacT which will be achieved through regular events e.g. summer schools on turbulent reacting flow physics and modelling along with understanding how to exploit developments in High-Performance Computing to offer improved fundamental understanding of turbulent reacting flows. This will be pivotal for the purpose of building of expertise and training of early career researchers for the computational turbulent reacting flow community based in the UK so that a pool of highly trained UK-based personnel is readily available for conducting cutting-edge research on the effective usage of energy resources, development of reliable fire safety measures, and manipulation of the combustion processes to ensure environmental friendliness. These challenges are multi-faceted, and need collaboration spanning a wide range of scientific areas, and thus CCP-ReacT will work closely with the UK Consortium on Turbulent Reacting Flows to hold annual training sessions and user meetings for all major codes used by the turbulent reacting flow community in the UK. Furthermore, much of CCP-ReacT's activities and research (with the help of core computational science support from Computational Science Centre for Research Communities (CoSeC)) will focus upon supporting and expanding the functionality of the major codes used by the community. Over the next 5 years, our objectives are to: (i) expand the pool of highly-skilled personnel who will be trained to utilise HPC resources to conduct world-leading turbulent reacting flow research involving Reynolds Averaged Navier-Stokes simulations (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS); (ii) train users in the efficient use of our core codes, explain the latest developments, and share ideas for future developments; (iii) develop strategies to introduce computationally efficient algorithms, and (iv) ensure our software development strategy embraces developments in computationally efficient algorithms that will exploit current and future developments of HPC hardware. This project will build on the foundations of UKCTRF and recently completed Flagship Software development project (EP/P022286/1) and will address universal challenges of energy efficiency, sustainability and high-fidelity fire safety. The activities of CCP-ReacT will reinforce the UK's world-leading status in turbulent reacting flow research.

The biennial International colloquium on dynamics of explosions and reactive systems (ICDERS), the Society of Industrial and Applied Mathematics: Numerical Combustion conference (SIAMNC), and the Mediterranean Combustion Symposium (MCS) are the premier conferences in the field of combustion. 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 for attending one of the ICDERS, SIAMNC and MCS conferences has be provided, at a rate of £500 per Research group.

Issues and Problems

The consortium has now reached a level where the demand for computational time is much greater than the amount awarded to the consortium. Almost 100% of computational time for last three allocation period was utilised, for the latest allocation cycle which started from July 2019, we have received requests for computer time for a total of 459306.6 kAUs within the application deadline decided by the UKCTRF management team, whereas we only had 241051 kAUs to allocate. In order to allocate computational time to all applicants, the management team had to award reduced computational time to the applicants, which will adversely affect productivity. Computational time usage will be very closely monitored by the management team of UKCTRF, and if there is no significant usage within a period of two months, then that time will be reallocated to other deserving users. The planned downtime of ARCHER and RDF in 2020 will certainly adversely affect the research activities of our community.

Several countries (e.g., China, Japan, USA, Germany, France, etc.), including those which did not traditionally have a track record of computational research (e.g. China, India, Saudi Arabia), are investing heavily in high-performance computing infrastructure. In this scenario, the investment in ARCHER2 (which is expected place the UK around 15th position in the Top 500 list) is not only timely but also essential for maintaining the UK's world-leading status in turbulent reacting flow research. Furthermore, a vision for exascale computing capability based in the UK in the near future is urgently necessary for the UKCTRF community to remain globally competitive. Our recent input into UKRI's e-Infrastructure roadmap pushed for the UK to establish a clear strategy for exascale computing at the earliest opportunity. It is worth noting that the advancements in computational power will enable reactive flow simulations, which are typical of engineering applications and laboratory-scale experiments. Thus, one-off simulations in short term (or medium term) are expected to be routine in medium term (or long term). Furthermore, it will enable UK researchers to aim for multi-scale multi-physics simulations in the future, which are currently inaccessible because of computational limitations.

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, **U. Ahmed**; 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

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Fundamental physical understanding and modelling of conventional turbulent premixed, non-premixed and stratified mixture combustion

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

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I. Konstantinou, U. Ahmed, N. Chakraborty, Influence of fuel Lewis number on flame-wall interaction for impinging turbulent premixed flames, 27th International Colloquium on Dynamics of Explosions and Reactive Systems, Beijing, China, 28th July -2nd August, 2019.
I. Konstantinou, U. Ahmed, N. Chakraborty, Flame-wall interaction of impinging turbulent premixed flames at different pressure levels, High Pressure Turbulent Premixed Combustion Workshop, 19th -20th September, 2019.
I. Konstantinou, U. Ahmed, M. Klein, N. Chakraborty, Statistics of turbulence during head-on quenching of turbulent premixed combustion in boundary layers, International Workshop on "Clean Combustion: Principles and Applications", 25th -26th September, 2019.
P. Zhao, L. Wang, N. Chakraborty, Vectorial structure of the near-wall premixed flame, Phys. Rev. F, 4,063203, 2019.

Simulation and modelling of fire, deflagration to detonation transition

R. K. Azadboni, A. Heidari, L.R. Boeck and J.X. Wen, The effect of concentration gradients on deflagration-to-detonation transition in a rectangular channel with and without obstructions – a numerical study, Int. J of Hydrogen Energy, Volume 44, 7032-7040, 2019
I. Sikic, S. Dembele and J. Wen, Non-grey radiative heat transfer modelling in LES-CFD simulated methanol pool fires, J. Quantitative Spectroscopy and Radiative Transfer, 234, 78-89, 2019
C.M.R. Vendra, J.X Wen, Numerical modelling of vented lean hydrogen deflagations in an ISO container, Int. J of Hydrogen Energy, 44, 8767-8779, 2019

➢ Relevant grants and awards

- S. Gkantonas (University of Cambridge) was awarded the British Flame and IOP Combustion Physics Group poster award at the IOP Early Career Researchers Meeting in University of Sheffield (19th Sep): Incompletely Stirred Reactor Network Modelling for Soot Emissions Prediction in Aero-Engine Combustors
- EPSRC Grant CHAMBER (Combustor thermoacoustics for multi-burner low emissions gas turbines), 2017-20, £757k
- ERC Consolidator Grant AFIRMATIVE (Acoustic-Flow Interaction Models for Advancing Thermoacoustic Instability prediction in Very low Emission combustors), 2018-23, €1.98M

- Lithium-ion battery safety in transport, storage and utilization, Innovate UK Faraday Challenge, led by Jaguar Land Rover (JLR), July 2019 ~ February 2021 (£397,398.21 of £5M).
- Characterisation of pressurised liquid hydrogen (LH2) releases (P-LH2), EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 September 2019 – 30 August 2021).
- Predicting flame acceleration and Deflagration to Detonation Transition in industrial scale explosions incorporating the Turbulence effects (TurbDDT) EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 March 2019 – 30 February 2021).
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)
- EPSRC network grant EP/S032134/1: A network for hydrogen-fuelled transportation (Network-H2) (£96,6316, Prof. N. Chakraborty, Co-I)
- EPSRC research grant EP/S025154/1: Numerical exploration and modelling of novel environmentally friendly combustion technique: droplet-laden MILD combustion (£791,000, PIs: Prof. Nilanjan Chakraborty, Newcastle University; Prof. N. Swaminathan, Cambridge University)

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 come to an end. Prof. N. Chakraborty (Newcastle University) was the PI and Profs. R.S. Cant (Cambridge), D. Emerson (Daresbury Laboratory) and Dr. C. Moulinec (Daresbury Laboratory) were the Co-Is of this project.

This project focussed 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. The newly developed code, HAMISH, is not only ported to ARCHER, but also is prepared for architectures supporting accelerators, thanks to OpenMP 4.5, which will support OpenACC, targeting a POWER8 cluster. The information on HAMISH and all the relevant documentation can be obtained from the following URL: http://www.ukctrf.com/index.php/flagship-software/ .

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 focussed 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 compuational science aspect of the software development and focuses principally on research into the algorithms, which need careful attention in relation to the development of HAMISH, particularly the adaptive meshing for DNS.

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 2018-19, HAMISH was improved in the following respects:
(a) Simulation of 1-D planar laminar premixed flames to demonstrate the capability of AMR in capturing the sharp gradients within the flame.
(b) 1-D head-on quenching of laminar premixed flames to demonstrate the capability of HAMISH in dealing with reacting flows in the presence of a wall.
(c) 2-D ignition problem, which demonstrates the capability of HAMISH to dynamically refine the mesh based on the position of the ignition front.
(d) 2-D laminar channel flow which shows that HAMISH is capable of refining the mesh in the boundary layer next to the wall.
(e) 3-D non-reacting Taylor-Green vortex which demonstrates HAMISH can deal with vortical motion typical of turbulent flows.
(f) 3-D premixed turbulent flame propagation under isotropic homogeneous decaying turbulence so that it can be shown that this code can be used for standard simulations for DNS of turbulent reacting flows in canonical configurations.

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 cost $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 CCP Networks, a proposal entitled "Collaborative Computational Project on Reacting Turbulent Flows (CCP-ReacT)" 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. We, the UK-based computational turbulent reacting flow community, wish to undertake the Collaborative Computational Project on Reacting Turbulent flows (CCP-ReacT) for retaining and expanding the international impact of the research undertaken by our community by creating a unique set of networking activities combined with ambitious software engineering and development activities. Training our researchers will be a key aspect of CCP-ReacT which will be achieved through regular events e.g. summer schools on turbulent reacting flow physics and modelling along with understanding how to exploit developments in High-Performance Computing (HPC) to offer improved fundamental understanding of turbulent reacting flows. This will be pivotal for the purpose of building of expertise and training of early career researchers for the computational turbulent reacting flow community based in the UK so that a pool of highly trained UK-based personnel is readily available for conducting cutting-edge research on the effective usage of energy resources, development of reliable fire safety measures, and manipulation of the combustion processes to ensure environmental friendliness. These challenges are multi-faceted, and need collaboration spanning a wide range of scientific areas, and thus CCP-ReacT will work closely with the UK Consortium on Turbulent Reacting Flows to hold annual training sessions and user meetings for all major codes used by the turbulent reacting flow community in the UK. Furthermore, much of CCP-ReacT's activities and research (with the help of core computational science support from Computational Science Centre for Research Communities (CoSeC)) will focus upon supporting and expanding the functionality of the major codes used by the community. Over the next 5 years, our objectives are to: (i) expand the pool of highly-skilled personnel who will be trained to utilise HPC resources to conduct world-leading turbulent reacting flow research involving Reynolds Averaged Navier-Stokes simulations (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS); (ii) train users in the efficient use of our core codes, explain the latest developments, and share ideas for future developments; (iii) develop strategies to introduce computationally efficient algorithms, and (iv) ensure our software development strategy embraces developments in computationally efficient algorithms that will exploit current and future developments of HPC hardware. This project will build on the foundations of UKCTRF and recently completed Flagship Software development project

(EP/P022286/1) and will address universal challenges of energy efficiency, sustainability and high-fidelity fire safety. The activities of CCP-ReacT will maintain and reinforce the UK's world-leading status in turbulent reacting flow research

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 1st Annual Progress Review meeting of the new incarnation of UKCTRF (http://www.ukctrf.com/index.php/upcoming-events-2019/), ECRs gave 11 oral presentations out of 18 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 institutional and Tier-2 facilities. 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 training options and other facilities (e.g. effective file management and efficient usage of RDF) have been publicised to the consortium users in the Annual Progress Review meeting. 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 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/index.php/upcoming-events-2019/).

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 organised a weeklong course on combustion theory and modelling in 2019. Most ECRs associated with UKCTRF members benefit from this course. The management team of the UKCTRF hopes to re-establish annual summer school and annual software training session for ECRs if the CCP-ReacT application turns out to be successful.

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., and Renuda Ltd.), and international academic experts (Dr. W. Meier from Institute of Combustion Technology, DLR, Germany, Prof. D. Roekaerts, Technical University, Delft, Netherlands, and Prof. L. Vervisch, CORIA, Rouen, France). 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 Renuda Ltd., Rolls Royce Plc Shell Plc., and Siemens Plc. (i.e. Prof. R. Cracknell, Drs. M. Zedda, N. Tonello and S. Sadasivuni) attended the 1st 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. 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

- PhD studentship of Y. Xia, 2015-18, "Prediction of Thermoacoustic Instability in Gas Turbine Combustors", Imperial College London, co-funded By Siemens Lincoln, UK (supervised by Morgans and Jones)
- Integrated Safety Strategies for Onboard Hydrogen Storage Systems - SUPERGEN H2FC Challenge (Ulster led EPSRC Collaboration Agreement) EP/K021109/1, funded by: EPSRC "Understanding the likelihood and impact of UK wildfires", £450K within a £1M consortium, 15 Oct. 2013 - 14 Oct. 2018). There was an industrial advisory board.
- Improving Hydrogen Safety for Energy Applications (HySEA) through pre-normative research on vented deflagrations, EU Horizon 2020 (€450.4K within a €1.5M consortium, 1 Sep. 2015 to 31 Nov. 2018) - The project was co-ordinated by a SME in Norway. Three of the 5 partners were industrial organisations. There was an industrial advisory board.
- Lithium-ion battery safety in transport, storage and utilization, Innovate UK Faraday Challenge, is led by Jaguar Land Rover (JLR), July 2019 ~ February 2021 (£397,398.21 of £5M). The consortium includes 8 other industrial organisations.
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021) – there are 3 industrial partners in the consortium as well as an industrial advisory board.
- 'Mixing and Crystallisation' Workshop, Imperial College, 2019, organised by consortium members G. Papadakis and S. Rigopoulos. This consortium had significant participation from industry.

➢ Publications that have industrial co-authorship

- Y. Xia, D. Laera, A. S. Morgans, W. P. Jones, J. Rogerson, Thermoacoustic limit cycle predictions of a pressurised longitudinal gas turbine combustor, GT2018-75146, ASME Turbo Expo, 2018
- (Co-authored with Siemens)
- S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, E. Mastorakos, Comprehensive Soot Particle Size Distribution Modelling of a Model Rich-Quench-Lean Burner, in: MCS11, paper 133, Tenerife, Spain, 2019, doi:10.17863/CAM.43221
- S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, E. Mastorakos, Comprehensive Soot Particle Size Distribution Modelling of a Model Rich-Quench-Lean Burner, Submitted to Fuel,2019
- C.R.M Vendra, P. Sathiah and J X. Wen, Effects of congestion and confining walls on turbulent deflagrations in a hydrogen storage Facility-Part 2: Numerical Study, Int J of Hydrogen Energy,43(32): 15593-15621, June 2018.(Co-authored with Shell).
- T. Skjold, H. Hisken, L. Bernard, L. Mauri, G. Atanga, S. Lakshmipathy, M. Lucas, M. Carcassi, M. Schiavetti, C.R M Vendra, A. Sinha, J.X. Wen, I.C. Tolias, S. G. Giannissi, A.G. Venetsanos, J.R. Stewart, O.R. Hansen, C. Kumar, L. Krumenacker, F.

Laviron, R. Jambut, A. Huser, Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for inhomogeneous mixtures in 20-foot ISO containers, J of Loss Prevention in the Process Industries 61 220–236. 2019 (Co-authored with 3 industrial partners)

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

- The EPSRC Grant CHAMBER (2017-20) involves collaboration with NTNU in Norway
- Collaboration (via British Council/CSC funded PhD student visit) with Beihang University, China.
- Improving Hydrogen Safety for Energy Applications (HySEA) through pre-normative research on vented deflagrations, EU Horizon 2020 (€450.4K within a €1.5M consortium, 1 Sep. 2015 to 31 Nov. 2018) - The project was co-ordinated by a SME in Norway. Three of the 5 partners were industrial organisations. There was an industrial advisory board.
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)

➢ 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, 2821-2830,2019.

U. Ahmed, M. Klein, N. Chakraborty, On the stress-strain alignment in premixed turbulent flames, Scientific Reports, 9, 5092, 2019.

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A. Alquallaf, M. Klein, C. Dopazo, N. Chakraborty, Evolution of flame curvature in turbulent premixed Bunsen flames at different pressure levels, Flow Turb. Combust., https://doi.org/10.1007/s10494-019-00027-x, 2019.

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A.J. Aspden, M.S. Day J.B. Bell, Towards the distributed burning regime in turbulent premixed flames, J. Fluid Mech., 871, 1-21, 2019.

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(2), 2301-2609, 2019.

P. Brearley, U. Ahmed, N. Chakraborty, A.N. Lipatnikov, Statistical behaviours of conditioned two-point second-order structure functions in turbulent premixed flames in different combustion regimes, Phys. Fluids (accepted).

Z.X. Chen, I. Langella, N. Swaminathan, M. Stöhr, W. Meier, H. Kolla, Large Eddy Simulation of a dual swirl gas turbine combustor: Flame/flow structures and stabilisation under thermoacoustically stable and unstable conditions. Combust. Flame, 203, 279-300, 2019.

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D. Dasgupta, W. Sun, M.S. Day, A.J. Aspden, T. Lieuwen ,Analysis of chemical pathways and flame structure for n-dodecane/air turbulent premixed flames. Combust. Flame, 207, 36-50, 2019.

S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, E. Mastorakos, Comprehensive Soot Particle Size Distribution Modelling of a Model Rich-Quench-Lean Burner, in: MCS11, paper 133, Tenerife, Spain, 2019.

C. Kasten, N. Chakraborty, M. Klein, Modelling turbulent scalar fluxes in high pressure turbulent premixed combustion LESC, High Pressure Turbulent Premixed Combustion Workshop, 19th -20th September, 2019.

F.B. Keil, M. Klein, N. Chakraborty, Sub-grid reaction progress variable variance closure in turbulent premixed flames, 11th Mediterranean Combustion Symposium, Tenerife, Spain, 16th-20th June, 2019.

F.B. Keil, M. Klein, N. Chakraborty, Analysis of the closure of sub-grid scale variance of reaction progress variable at different pressure levels, High Pressure Turbulent Premixed Combustion Workshop, 19th -20th September, 2019.

M. Klein, A. Herbert, H. Kosaka, B. Böhm, A. Dreizler, N. Chakraborty, V. Papapostolou, H. G. Im, J. Hasslberger, Evaluation of flame area based on detailed chemistry DNS of premixed turbulent hydrogen-air flames in different regimes of combustion, Flow Turb. Combust. , https://doi.org/10.1007/s10494-019-00068-2, 2019.

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, 2019.

M. Klein, N. Chakraborty, A. Alquallaf, "The signature of flame instabilities on the transport of curvature in turbulent premixed flames", 17th International conference on numerical combustion, Aachen, Germany, 6th -8th May, 2019

I. Konstantinou, U. Ahmed, M. Klein, N. Chakraborty, "Near-wall behaviour of turbulence in flame-wall interaction of premixed turbulent combustion in boundary layers", 9th European Combustion Meeting, Lisboa, Portugal, 14th -17th April, 2019.

I. Konstantinou, U. Ahmed, N. Chakraborty, Influence of fuel Lewis number on flame-wall interaction for impinging turbulent premixed flames, 27th International Colloquium on Dynamics of Explosions and Reactive Systems, Beijing, China, 28th July -2nd August, 2019.

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M. Pfitzner, M. Klein, N. Chakraborty, Flame curvature distribution in high pressure turbulent Bunsen premixed flames, 17th International conference on numerical combustion, Aachen, Germany, 6th -8th May, 2019.

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R. Rasool, M. Klein, L. Seilnacht, N. Chakraborty, Algebraic Flame Surface Density modelling of high pressure turbulent premixed Bunsen flames, 11th Mediterranean Combustion Symposium, Tenerife, Spain, 16th-20th June, 2019.

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C. Tuquand-d'Auzay, U. Ahmed, A. Pillai, N. Chakraborty, R. Kurose, Statistics of progress variable and mixture fraction gradients in an open turbulent jet spray flame, Fuel , 247, 198-208, 2019.

C. Tuquand d'Auzay, V. Papapostolou, S. F. Ahmed, N. Chakraborty, Effects of turbulence intensity and biogas composition on thelocalised forced ignition of turbulent mixing layers, Combust. Sci. Technol., 191, 868-897, 2019.

C. Turquand d'Auzay, V. Papapostolou, S. F. Ahmed, N. Chakraborty, On the minimum ignition energy and its transition in the localised forced ignition of turbulent homogeneous mixtures, Combust. Flame, 201, 104-117, 2019.

C. Turquand-d'Auzay, V. Papapostolou, S.F. Ahmed, N. Chakraborty, Effects of biogas composition on the edge flame propagation in igniting turbulent mixing layers, 11th Mediterranean Combustion Symposium, Tenerife, Spain, 16th-20th June, 2019.

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S. Trivedi, R.A.C. Griffiths, J.H. Chen, H. Kolla, R.S. Cant, Topology of pocket formation in turbulent premixed flames, Proc. Combust. Inst., 37, 2619-2626, 2019.

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➢ Involvement in international activities

- Characterisation of pressurised liquid hydrogen (LH2) releases (P-LH2), EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 September 2019 – 30 August 2021).
- Predicting flame acceleration and Deflagration to Detonation Transition in industrial scale explosions incorporating the Turbulence effects (TurbDDT) EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 March 2019 – 30 February 2021).
  Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)
- Developing computationally efficient approaches for modelling radiative heat transfer of soot and evaporating water droplets in FireFOAM, funded by FM Global (PhD studentship, March 2014 – September 2018) - the sponsor is based in the USA.

➢ Invited lectures by consortium members

- Prof. N. Chakraborty, Shanghai Jiao Tong University, Shanghai, China, 2019: Advanced simulations of turbulent reacting flows using High Performance Computing in the workshop on Advanced Marine Engineering
- Prof. A. Morgans Keynote at 2019 Parallel CFD Conference.
- Prof. J X. Wen, Achievement in the Pre-LibRIS project, 1st International Symposium on Lithium Battery Fire Safety, Hefei, China, 18-20 July 2019.
- Dr. E.S Richardson, 2nd High Performance Computing Combustion Workshop, HPCCOMB2019, Barcelona, Spain; Title: Turbulent Reacting Flow Modelling: Learning from Big Data
- Dr. S. Rigopoulos, Rouen, France, 2019: Modelling of turbulent reacting flows with particle formation

➢ Scientific committee of international conferences

- Prof. N. Chakraborty is a steering group member of Computational Science Centre for Research Communities (CoSeC).
- Prof. N. Chakraborty recently served as an editor of the Engineering and Material Science chapter for the science case for Exascale computing commissioned by EPSRC.

- Profs. N. Chakraborty, R.S. Cant, W.P. Jones and S. Havarro-Martinez edited a special issue for the journal entitled Combustion Science and Technology based on UKCTRF Workshop 2018.
- Prof. N. Chakraborty was the co-organizer of the ERCOFTAC sponsored Workshop on High Pressure Turbulent Premixed Combustion held in Munich between the 19th and 20th of September 2019.
- Prof. N. Chakraborty was one of the chairs of the turbulent combustion colloquium in the 11th Mediterranean Combustion Symposium (16th -20th June,2019). He also chaired a session on turbulent combustion modelling in this conference.
- Prof. DR Emerson is Member of the Scientific and Organising Committee for the annual Parallel CFD conference.
- Prof. A. Morgans is a member of PRACE Scientific Steering Committee and UK's CoSeC.
- Prof. J X. Wen is Member of the Scientific and Organising Committees, 15th International Conference on Combustion and Energy Utilization (15th ICCEU) will be held on April 2020 in Chengdu, China.
- Prof. J X. Wen is Member of the Scientific Committee and Session Chair, 3rd (2009), 4th (2011), 5th (2013), 6th (2015), 7th (2017) and 8th (2019) International Conference on Hydrogen Safety.
- Prof. J X. Wen is Member of the Programme Committee, 27th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), July 28, 2019 - August 02, 2019.
- Prof. J X. Wen is Co-chairs of the Awards Committee and member of the IAFSS 2020 Symposium Planning Committee for the 13th International Symposium on Fire Safety Science will be held between April 27 – May 1, 2020 at the University of Waterloo in Waterloo, ON Canada.
- Prof. J X. Wen is Organising committee member, 4th International Conference on "Battery and Fuel Cell Technology", September 05-06, 2019 Berlin, Germany.
- Prof. J X. Wen is Member of the Scientific Committee, 3rd European Symposium on Fire Safety Science, September 12-14, 2018 at the University of Lorraine, Nancy, France.
- Prof. J X. Wen is Member of the Scientific Committee and Co-Chair of the organising committee for the 2018 International Symposium on Hydrogen Fire, Explosion and Safety Standard (ISHFESS2018), July 6-8, 2018 in Hefei, China.

➢ Invited courses

- Dr. S. Rigopoulos hosted the ERCOFTAC course 'Best practice in CFD of turbulent combustion', Imperial College, 2018 and delivered lectures on soot formation and on machine learning in combustion.

➢ Editorships

- Profs. N. Chakraborty, R.S. Cant, W.P. Jones and S. Havarro-Martinez edited a special issue for the journal entitled Combustion Science and Technology based on UKCTRF Workshop 2018.
- Prof. N. Chakraborty to co-edit a special issue on high pressure turbulent premixed combustion for the journal entitled Combustion Science and Technology
- Prof. N. Chakraborty to co-edit a special issue on numerical modelling of reacting and non-reacting multi-phase flows for the journal Fluids.
- Prof. E. Mastorakos - Associate editor of *Combustion and Flame*, Editorial Board member of *Combustion Theory and Modelling*, and *Flow, Turbulence and Combustion*)
- Prof E. Mastorakos - Guest Editor in Topical Issue "Advances in Turbulence, Heat and Mass Transfer" in *Flow, Turbulence and Combustion*, 2019.

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

- A special issue of Combustion Science and Technology entitled "Special issue on UKCTRF workshop 2018" has been published (vol. 191, issues 5-6) based on the UKCTRF Workshop in 2018 (EP/K025163/1) is now online and can be found on: https://www.tandfonline.com/toc/gcst20/current). Altogether 16 papers were submitted and 13 were accepted for publication. All papers went through the usual review process (e.g. involving 2-3 reviews per paper) and some papers went through 2 rounds of revision.
- In 2018-2019 academic year 100+ journal and 120+ conference papers arose from this consortium Altogether 450+ publications over last 5 years and 30% of these publications involve international collaboration.
- The UKCTRF contributed £500 per research group towards the cost of attending the international conferences for those who had accepted papers for oral presentation (9 in total so far) (http://www.ukctrf.com/wp-content/uploads/2019/08/UKCTRF-Conference-Funding.pdf)

➢ Relevant grants and awards

- S. Gkantonas (University of Cambridge) was awarded the British Flame and IOP Combustion Physics Group poster award at the IOP Early Career Researchers Meeting in University of Sheffield (19th Sep): Incompletely Stirred Reactor Network Modelling for Soot Emissions Prediction in Aero-Engine Combustors
- EPSRC Grant CHAMBER (Combustor thermoacoustics for multi-burner low emissions gas turbines), 2017-20, £757k
- ERC Consolidator Grant AFIRMATIVE (Acoustic-Flow Interaction Models for Advancing Thermoacoustic Instability prediction in Very low Emission combustors), 2018-23, €1.98M
- Lithium-ion battery safety in transport, storage and utilization, Innovate UK Faraday Challenge, led by Jaguar Land Rover (JLR), July 2019 ~ February 2021 (£397,398.21 of £5M).
- Characterisation of pressurised liquid hydrogen (LH2) releases (P-LH2), EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 September 2019 – 30 August 2021).
- Predicting flame acceleration and Deflagration to Detonation Transition in industrial scale explosions incorporating the Turbulence effects (TurbDDT) EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 March 2019 – 30 February 2021).
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)
- EPSRC network grant EP/S032134/1: A network for hydrogen-fuelled transportation (Network-H2) (£96,6316, Prof. N. Chakraborty, Co-I)
- EPSRC research grant EP/S025154/1: Numerical exploration and modelling of novel environmentally friendly combustion technique: droplet-laden MILD combustion (£791,000, PIs: Prof. Nilanjan Chakraborty, Newcastle University; Prof. N. Swaminathan, Cambridge University)

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 the 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 annual progress review 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. Hopefully, a successful outcome of the CCP-ReacT proposal will enable us to establish annual summer schools and annual software training sessions.

(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.