# Annual Report for EPSRC High End Computing Consortia

## Reporting Period: February 2016 - January 2017

### 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 3rd annual progress review meeting of the UKCTRF, and the meeting between the management team and the Impact Advisory Panel (IAP) members, took place on 15th -16th September 2016 in Collingwood College, University of Durham. There were 2 invited keynote lectures (45 min) and 16 contributed oral presentations (15 min each). The invited keynote lectures were delivered by Dr. G. Bulat from Siemens Plc. and Prof. Markus Klein, Universitat der Bundeswehr Munchen, Neubiberg, Germany. The next annual progress review meeting and the meeting between the management team and IAP members will take place in Southampton on the 7th -8th of September 2017. Three keynote speakers of significant international repute (Prof. C. Dopazo from University of Zaragoza, Prof. Andreas M. Kempf from University of Duisburg and Dr. I. Boxx from DLR, Germany) have already been invited. In order to showcase the diverse range of ongoing research within the consortium, the next two annual progress review meetings will be treated as international conferences with workshops on simulations 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. The management team is also considering a joint meeting with UKTC on the topic of turbulent mixing and scalar transport during the course of this 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 recent call on flagship software development call, a proposal entitled "Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows" has been submitted to EPSRC on behalf of UKCTRF. 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 will

enable 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. Hence AMR will offer a step-change in capability for the computational analysis of turbulent reacting flows, and will provide data having a degree of detailed physical information not currently available from simulations using existing CFD codes. We are currently waiting for the outcome of the research proposal.

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 (to be held in the summer of 2017) will be provided, at a rate of £500 per Research group.

### Issues and Problems

It took some time and the sustained effort of the management team before the level of utilisation of the allocated computational time by the UKCTRF users increases substantially. It 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 June-November 2016 allocation cycle was utilised, for the latest allocation cycle which started from December 2016, we have received requests for computer time for a total of 453181.6 kAUs within the application deadline decided by the UKCTRF management team, whereas we only had 127101 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 6000kAUs received only 6000kAUs) 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.

### 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 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**;City University, London: **Dr. K. Vogiatzaki**; Cranfield University: Dr. K.W. Jenkins ; Daresbury Laboratory: Prof. D. Emerson, Drs. C. Moulinec and X. Gu; University of Edinburgh: Prof. J. Torero, Dr. S. Welch, and **D. Hyuk Shin**; Imperial College, London: Profs. W.P. Jones, R.P. Lindstedt, Drs. F. Marquis, **A. Morgans**, S. Navarro-Martinez, S. Rigopoulos, and G.Rein; Lancaster University: Prof. X. Jiang; Loughborough University: Profs. W. Malalasekara, J. McGuirk, and Dr. A Garmory; University College London: Prof. K.H. Luo; University of Durham: Prof. P. Gaskell; University of Leeds: Prof. D. Bradley and Dr. G. Sharpe; University of Manchester: Dr. R. Prosser; University of Southampton: Drs. E.S. Richardson, **K.K.J. Ranga Dinesh**; University of Ulster: Profs. M. Delichatsios and V.B. Novozhilov; Warwick University: Prof. J.X. Wen

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

- 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 publications

- **Improved physical understanding and modelling of multi-phase combustion using high-fidelity simulations**

E. Demosthenous, E.Mastorakos, R.S. Cant, (2016) Direct Numerical Simulations of Dual-Fuel Non-Premixed Autoignition. Combust. Sci. Technol., 188(4-5), 542-555.

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

S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty (2016) Analysis of fuel mass fraction dissipation rate transport in turbulent flame-droplet interaction: A Direct Numerical Simulation study, ILASS2016, Brighton, UK, 4th -7th September, 2016.

S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty (2016) Analysis of the co-variance of fuel mass fraction and mixture fraction in turbulent flame-droplet interaction: A Direct Numerical Simulation study", Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.

M.P. Sitte, E. Mastorakos (2016) Modelling of Spray Flames with Double Conditional Moment Closure. 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016.

D. Wacks, S.P. Malkeson, N. Chakraborty (2016) Statistical behaviour of fuel mass fraction variance transport in turbulent flame- droplet interaction: A Direct Numerical Simulation analysis, Numer. Heat Trans. A, 70, 1087-1100.

D.H. Wacks, N. Chakraborty (2016) Statistical Analysis of the Reaction Progress Variable and Mixture Fraction Gradients in Flames Propagating into Droplet Mist: A Direct Numerical Simulation Analysis, Combust. Sci. Technol., 188, 2149-2177.

D. Wacks, N. Chakraborty (2016) Flame structure and topology in turbulent spray flames: A Direct Numerical Simulation analysis, Fuel, 184,922-947.

D. Wacks, N. Chakraborty (2016) Flame structure and propagation in turbulent flame-droplet interaction: A Direct Numerical Simulation analysis, Flow Turb. Combust., 96, 1053-1081.

D. Wacks, N. Chakraborty, E. Mastorakos, "Statistical analysis of the effects of droplets on flame propagation: A Direct Numerical Simulation analysis" Flow Turb. Combust., 96, 573-607, 2016.

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

U. Allauddin, M. Pfitzner, M. Klein, N. Chakraborty (2016) 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., DOI: 10.1080/10407782.2016.1257309.

Z.Chen, S. Ruan, N. Swaminathan (2016) Large eddy simulation of flame edge evolution in a spark-ignited methane-air jet, Proc. Combust. Inst., 36, doi:10.1016/j.proci.2016.06.023, (2016)

Z. Chen, S. Ruan and N. Swaminathan (2016) Numerical study of transient evolution of lifted jet flames: partially premixed flame propagation and influence of physical dimensions, Combust. Theory Modelling, 20(4), 592-612.

A.L. Comer, T. Kipouros, R.S. Cant (2016). Multi-objective numerical investigation of a generic airblast injector design. Journal of Engineering for Gas Turbines and Power, 138(9).

Y.Gao, Y. Minamoto, M. Tanahashi, N. Chakraborty (2016) A priori assessment of scalar dissipation rate closure for Large Eddy Simulations of turbulent premixed combustion using a detailed chemistry Direct Numerical Simulation database." Combust. Sci. Technol., 188,1398-1423.

Y. Gao, N. Chakraborty (2016) Modelling of Lewis Number dependence of Scalar dissipation rate transport for Large Eddy Simulations of turbulent premixed combustion. Numer. Heat Trans. A, 69, 1201-1222.

M. Klein, N. Chakraborty, M. Pfitzner (2016) Analysis of the combined modelling of subgrid transport and filtered flame propagation for premixed turbulent combustion. Flow Turb. Combust., 96, 921-938.

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

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

J. Li, X. Han, Y. Xia & A. S. Morgans, Thermoacoustic analysis of combustors consisting of long flames using a low order network model approach, International Symposium on Thermoacoustic Instabilities in Gas Turbines and Rocket Engines: Industry Meets Academia, Munich, 2016.

C.Y. Lee, R.S. Cant (2016). Nonlinear hydrodynamics of a bluff-body stabilized turbulent premixed flame. In Proceedings of the ASME Turbo Expo 2016, paper no. GT2016-57492.

C.Y. Lee, L.K.B. Li, M.P. Juniper, R.S. Cant (2016). Nonlinear hydrodynamic and thermoacoustic oscillations of a bluff-body stabilised turbulent premixed flame. Combustion Theory and Modelling, 20(1), 131-153.

X. Yu, I. Duran,. A. S. Morgans, X. Han (2016) Dispersion of entropy waves propagating through combustion chambers, International Congress on Sound and Vibration, Athens.

- **Fundamental physical understanding and modelling of conventional turbulent combustion**

A. J. Aspden, M. S. Day, and J. B. Bell (2016) Three-Dimensional Direct Numerical Simulation of turbulent lean premixed methane Combustion with Detailed Kinetics, Combust. Flame, 166, 266-283, 2016 dx.doi.org/10.1016/j.combustflame.2016.01.027.

A. J. Aspden (2016) A Numerical Study of Diffusive Effects in Turbulent Lean Premixed Hydrogen Flames, Proc. Combust. Inst., 36, dx.doi.org/10.1016/j.proci.2016.07.053.

A. J. Aspden, J. B. Bell, M. S. Day, and F. N. Egolfopoulos (2016) Turbulence-flame interactions in lean premixed Dodecane flames, Proc. Combust. Inst., 36, dx.doi.org/10.1016/j.proci.2016.07.068.

L. Cifuentes, N. Chakraborty, C. Dopazo (2016) Kinetic energy and its dissipation rate budgets in statistically planar turbulent premixed flames at different Lewis numbers", Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.

N.A.K. Doan, N. Swaminathan, N. Chakraborty (2016) Multiscale analysis of turbulence-flame interaction in premixed flames. Proc. Combust. Inst. 36, doi:10.1016/j.proci.2016.07.111.

H.G. Im, M. Klein, C. Kasten, N. Chakraborty, P. Arias (2016) Modelling of turbulent scalar fluxes in the broken reaction zones regime, American Physical Society, Division of Fluid Dynamics Section conference, 21st November, 2016G.V. Nivarti, R.S. Cant (2016). Direct numerical simulation of the bending effect in turbulent premixed flames, Proc. Combust. Inst., 36, http://dx.doi.org/10.1016/j.proci.2016.07.076.

W. Liu, A. Alakalabi, T. Graham, X. Gu (2016) Large eddy simulations of heavy gas dispersion within building group, 9th International Conference on Computational Fluid Dynamics (ICCFD9), Istanbul, Turkey, July 11 – 15, 2016.

M. Klein, C. Kasten, N. Chakraborty, P.Aries, H.G. Im, "Turbulent scalar fluxes in detailed chemistry based premixed flame DNS simulations of h2-air flames in different regimes of combustion", Engineering Turbulence Modelling and Measurement 11, Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016.

M. Klein, N. Chakraborty, A comparison of strategies for direct numerical simulation of turbulence chemistry interaction in generic planar turbulent premixed flames, Engineering Turbulence Modelling and Measurement 11, Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016).

W. Liu (2016), A theory for steady and self-sustained premixed combustion waves, Cogent Engineering 3: 1205308.

J. Mai, A. Chamchine (2016) Transient Flame Translation from Within an Enclosure to Its Opening, ISFEH8, He Fei, China, April 2016.

V. Sabelnikov, A.N. Lipatnikov, N. Chakraborty, S. Nishiki, T. Hasagawa, "A balance equation for the mean rate of product creation in premixed turbulent flames." Proc. Combust. Inst. , 36, http://dx.doi.org/10.1016/j.proci.2016.08.018.

V. Sabelnikov, A. Lipatnikov, N. Chakraborty, S. Nishiki, T. Hasegawa (2016) A transport equation for reaction rate in turbulent flows, Phys. Fluids, 28, 081701.

D.H. Wacks, N. Chakraborty, M. Klein, P.G. Aries, H.G. Im (2016) Flow topologies in different regimes of premixed turbulent combustion: A direct numerical simulation analysis, Phys. Rev. F, 1, 083401.

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

N. A. K. Doan, N. Swaminathan, Y. Minamoto (2016) DNS of partially premixed MILD combustion: Preliminary investigation, Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.

N. A. K. Doan, N. Swaminathan, Y. Minamoto (2016) DNS of MILD combustion with inhomogeneous fuel distribution, The fifth international education forum on environment and energy science, Dec. 15 – 21, 2016 Maui, Hawaii.

J. Lai, N. Chakraborty, A. Lipatnikov, Vorticity and enstrophy transport in head-on quenching of turbulent premixed flames, Eur. J. Mech. Fluids/B., http://dx.doi.org/10.1016/j.euromechflu.2016.10.013.

J. Lai, M. Klein, N. Chakraborty, A priori direct numerical simulation assessment of algebraic flame surface density models for turbulent flame-wall interaction in the context of large eddy simulation, Engineering Turbulence Modelling and Measurement 11, Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016.

J. Lai, N. Chakraborty (2016) Modelling of Progress Variable Variance Transport in Head on Quenching of Turbulent Premixed Flames: A Direct Numerical Simulation Analysis, Combust. Sci. Technol., 188,1925-1950.

J. Lai, N. Chakraborty (2016) A-priori Direct Numerical Simulation modelling of Scalar Dissipation Rate transport in Head-on Quenching of Turbulent Premixed Flames Combust. Sci. Technol., 188,1440-1471.

J. Lai, N. Chakraborty (2016) Statistical behaviour of scalar dissipation rate for head on quenching of turbulent premixed flames: A Direct Numerical Simulation analysis. Combust. Sci. Technol., 188, 250-276.

J. Sellmann, J. Lai, N. Chakraborty, A.M. Kempf, Flame Surface Density based modelling of head-on quenching of turbulent premixed flames. Proc. Combust. Inst., 36, http://dx.doi.org/10.1016/j.proci.2016.07.114

J. Lai, N. Chakraborty (2016) Effects of Lewis Number on Head on Quenching of Turbulent Premixed Flame: A Direct Numerical Simulation analysis, Flow Turb. Combust., 96, 279-308.

- **Simulation and modelling of ignition, flame extinction and blowout**

E. Mastorakos (2016) Forced ignition of turbulent spray flames, Proc. Combust. Inst., 36, **http://dx.doi.org/10.1016/j.proci.2016.08.044**

D. Patel, N. Chakraborty (2016) Effects of fuel Lewis number on localised forced ignition of globally stoichiometric stratified mixtures: A numerical investigation. Flow Turb. Combust., 96, 1083-1105.

D. Patel, N. Chakraborty (2016) Effects of fuel Lewis number and the energy deposition characteristics on localized forced ignition of homogeneous mixture: A numerical investigation, Int. J. Spray Combust. Dyn. 8, 183-196.

D. Patel, N. Chakraborty (2016) Effects of mixture distribution on localised forced ignition of stratified mixtures: A Numerical Investigation, Combust. Sci. Technol., 188,1904-1924.

H. Zhang, E. Mastorakos (2016) Modelling Local Extinction in Sydney Swirling Non-premixed Flames with LES/CMC. Proc. Combust. Inst., 36, doi: 10.1016/j.proci.2016.07.051.

H. Zhang, A. Giusti, E. Mastorakos (2016) Modelling formation and initial propagation of flame kernels in turbulent non-premixed methane jets with LES/CMC. Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016.

- **Simulation and modelling of fire, deflagration to detonation transition**

I. Ahmed, T. Bengherbia, R. Zhvansky, G. Ferrara, J. X. Wen, N. G. Stocks (2016) Validation of geometry modelling approaches for offshore gas dispersion simulations, J of Loss Prevention in the Process Industry 2016. http://dx.doi.org/10.1016/j.jlp.2016.07.009.

M. Alam, J.X. Wen, S. Dembele (2016) Numerical prediction of liquid pool fire burning rate with a CFD approach, Proc. 14th Interflam Conference, 4-6 July 2016, Royal Holloway College, University of London, Windsor, UK.

L. A. Dombrovsky, S. Dembele, J. X. Wen (2016) A simplified model for the shielding of fire thermal radiation by water mists, Int. J. Heat and Mass Trans.,96, 199–209.

P. Huang, P. K. Li, H. Chen, Q. Wang, J.X. Wen, J. Sun (2016) Experimental and modeling analysis of thermal runaway propagation over the large format energy storage battery module with Li4Ti5O12 anode, Applied Energy, vol. 183: 659-673.

R. Khodadadi Azadboni, J.X. Wen, A. Heidari, S.P.R. Muppala, C.J. Wang (2016) Numerical Modelling of Deflagration to Detonation Transition in Inhomogeneous Hydrogen/Air Mixtures, accepted by the 11th International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosion (ISHPMIE) hosted in Dalian, China July 24-29 2016.

W. Rudy, A. Teodorczyk, J. Wen (2016) Self-ignition of hydrogen–nitrogen mixtures during high-pressure release into air, Int. J. Hydrogen Energy, http://dx.doi.org/10.1016/j.ijhydene.2016.06.051.Z.S. Saldi, J.X. Wen (2016) Modeling thermal response of polymer composite hydrogen cylinders subjected to external fires. Int. J. Hydrogen Energy, http://dx.doi.org/10.1016/j.ijhydene.2016.06.108.

I. Sikic, J.X. Wen, S. Dembele, An assessment of the weighted-sum-of-grey-gases approach in fire simulations, Poster presentation at the 14th Interflam Conference, 4-6 July 2016, Royal Holloway College, University of London, Windsor, UK.

C.J., Wang, J.X. Wen (2016) Numerical simulation of flame acceleration and deflagration-to-detonation transition in hydrogen-air mixtures with concentration gradients. Int. J. Hydrogen Energy, http://dx.doi.org/10.1016/j.ijhydene.2016.06.107.B. P. Xu, J.X. Wen (2016) Large eddy simulation of a mechanically ventilated compartment fire for nuclear applications, Proc. 8th International Symposium on Fire and Explosion Hazards, Hefei, China, April 25-29, 2016.

### ➢ Relevant press announcements and other communications of significance

- A paper by X. Yu, I. Duran, A. S. Morgans, X. Han, entitled 'Dispersion of entropy waves propagating through combustion chambers' presented at International Congress on Sound and Vibration, Athens, 2016 was nominated for Sir James Lighthill Best Student Paper Award.
- A paper by S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty, entitled 'Analysis of fuel mass fraction dissipation rate transport in turbulent flame-droplet interaction: A Direct Numerical Simulation study' ILASS2016, Brighton, UK, 4th -7th September, 2016 was selected for the Best Paper Award.

### ➢ Relevant grants and awards

- EPSRC Grant, CHAMBER: Combustor thermoacoustics for multi-burner low emissions gas turbines, £757k (2017-2020). PI: Dr. A. S. Morgans, Imperial College London
- CORNET: H2020/Clean Sky RIA project: £382k (2016-2019). Investigators: A. P. Dowling, N. Swaminathan, T. P. Hynes
- Grant from MHI, Japan: LES of Azimuthal instability in GT combustor, £352k (2016-2019). PI: Prof. N. Swaminathan
- Dr. K. Vogiatzaki from the City University, London was awarded the prestigious Hinshelwood Prize for 2006 by the British Section of Combustion Institute for his meritorious contribution to combustion science.
- Prof. N. Chakraborty (Newcastle University) received funding from the Ministry of Human Resources Development, India as a part of Global Initiative of Academic Network (GIAN) scheme to offer an invited course on "Computational Modelling of Turbulent Combustion" at Jadavpur University, Kolkata, India in December 2016
- 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)

## 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 and highly-detailed chemistry, as well as improvements made to time stepping and boundary conditions. Support regarding optimisation of an adaptive grid based DNS code (i.e. HAMISH) is being carried out in

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

In response to EPSRC's recent call on flagship software development, a proposal entitled "Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows" has been submitted to EPSRC on behalf of UKCTRF. 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 CIs of this proposal. This project focuses on the development, validation and documentation of a next-generation fully parallelised computational fluid dynamics (CFD) code HAMISH based on adaptive mesh refinement (AMR) which will enable 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 will offer 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 will offer a step-change in capability for the computational analysis of turbulent reacting flows, and will provide data with the degree of detailed physical information which is not currently available from simulations using existing CFD codes.

The proposed software will be 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 UKCTRF members. The newly developed code, HAMISH, will not only be ported to ARCHER, but also be 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. This user guide will be made available on a website for public download along with the open-source version of the code, and the associated documentation on code validation and user tutorials.

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 will allow 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 will also benefit 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.

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 £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.

**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 3rd Annual Progress meeting of UKCTRF, ECRs gave 13 oral presentations out of 17 oral presentations and about 30 ECRs attended the meeting. This substantiates the high level of involvement of ECRs in the consortium activities. UKCTRF members of 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 3rd Annual Progress review meeting of the UKCTRF to publicise and discuss about the training options and other facilities (e.g. effective file management and efficient usage of RDF) to the consortium users. The EPCC's consortium contact for ARCHER is also invited to join the Impact Advisory Panel (IAP) and is in close contact with the management team to explore the possibility of having training sessions which might be beneficial for the consortium users.

The previous incarnations of UKCTRF (i.e. Consortium On Computational Combustion For Engineering Applications (COCCFEA)) had the option for summer schools on computational combustion. Under 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 a 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.

**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 are actively involved in RANS and LES simulations of turbulent reacting flows in complex engineering configurations for the purpose of designing new generation energy-efficient and environment-friendly industrial combustion devices for automotive and gas turbine applications.

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

The representatives of Shell Plc., Siemens Plc., Renuda Ltd. And Rolls Royce Plc. (i.e. Prof. R. Cracknell, Drs. G. Bulat, N. Tonello and M. Zedda) attended the 2nd Annual Progress meeting of the consortium and offered their valuable inputs. The industrial colleagues of IAP identified that focused research is needed on explosions modelling, spray and soot modelling, bio-fuel combustion and thermo-acoustic interaction. This industrial view is consistent with the priority areas identified by the consortium. There is a possibility that the IAP members of Shell will be able to provide some experimental data on their explosions test cases and constant volume Diesel spray combustion. Rolls Royce and Siemens have offered to provide test cases with experimental data for validating RANS/LES simulations. Siemens is also willing to share some experimental data on thermo-acoustic interaction. It was felt by industrial colleagues and 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 identifying those methodologies which will be useful for pre-processing and post-processing of industrial simulations.

### ➢ Projects that have been performed in collaboration with industry

- **Autoignition and Jet flame analysis in collaboration with Shell Research (PI: Prof. Derek Bradley, University of Leeds, UK):** Combined experimental and computational investigation of turbulent jet flames and autoignition characteristics in automotive applications. Prof. D. Bradley acts as a consultant to Shell.
- **Firefoam development for industrial fire simulations in collaboration with FM Global (PI: Prof. Jennifer Wen, Warwick University, UK):** The Warwick group has been involved with continuous development of the FireFOAM code, the LES based fire simulation solver within OpenFOAM. 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**

- S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty, "Analysis of the co-variance of fuel mass fraction and mixture fraction in turbulent flame-droplet interaction: A Direct Numerical Simulation study", Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.
- S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty, "Analysis of fuel mass fraction dissipation rate transport in turbulent flame-droplet interaction: A Direct Numerical Simulation study", ILASS2016, Brighton, UK, 4th -7th September, 2016.
- D. Wacks, S.P. Malkeson, N. Chakraborty, "Statistical behaviour of fuel mass fraction variance transport in turbulent flame- droplet interaction: A Direct Numerical Simulation analysis." *Numer. Heat Trans. A*, 70, 1087-1100, 2016.

**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
- **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 Califoirnia 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.

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

- 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.* , DOI: 10.1080/10407782.2016.1257309.
- L. Cifuentes, N. Chakraborty, C. Dopazo, "Kinetic energy and its dissipation rate budgets in statistically planar turbulent premixed flames at different Lewis numbers", Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.
- N. A. K. Doan, N. Swaminathan, Y. Minamoto, "DNS of MILD combustion with inhomogeneous fuel distribution", Presentation at the fifth international education forum on environment and energy science, Dec. 15 – 21, 2016 Maui, Hawaii.
- Y.Gao, Y. Minamoto, M. Tanahashi, N. Chakraborty, "A priori assessment of scalar dissipation rate closure for Large Eddy Simulations of turbulent premixed combustion using a detailed chemistry Direct Numerical Simulation database." *Combust. Sci. Technol.*, 188,1398-1423, 2016.
- H.G. Im, M. Klein, C. Kasten, N. Chakraborty, P. Arias, "Modelling of turbulent scalar fluxes in the broken reaction zones regime, American Physical Society, Division of Fluid Dynamics Section conference, 21st November, 2016.
- M. Klein, N. Chakraborty, M. Pfitzner, "Analysis of the combined modelling of subgrid transport and filtered flame propagation for premixed turbulent combustion". *Flow Turb. Combust.*, 96, 921-938, 2016.
- M. Klein, N. Chakraborty, Y. Gao, "Scale similarity based models and their application to subgrid scale scalar flux modelling in the context of turbulent premixed flames." *Int. J. Heat Fluid Flow*, 57, 91-108, 2016.
- M. Klein, C. Kasten, N. Chakraborty, P.Aries, H.G. Im, "Turbulent scalar fluxes in detailed chemistry based premixed flame DNS simulations of h2-air flames in different regimes of combustion", Engineering Turbulence Modelling and Measurement 11 ( Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016).
- M. Klein, N. Chakraborty, "A comparison of strategies for direct numerical simulation of turbulence chemistry interaction in generic planar turbulent premixed flames", Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016.
- J. Lai, N. Chakraborty, A. Lipatnikov, "Vorticity and enstrophy transport in head-on quenching of turbulent premixed flames." Eur. J. Mech. Fluids/B., http://dx.doi.org/10.1016/j.euromechflu.2016.10.013.
- J. Lai, M. Klein, N. Chakraborty, "A priori direct numerical simulation assessment of algebraic flame surface density models for turbulent flame-wall interaction in the context of large eddy simulation", Engineering Turbulence Modelling and Measurement 11 (Proceedings of the 11th ERCOFTAC Symposium on Engineering, Turbulence, Modelling and Measurements, Palermo, 21-23 September 2016)
- V. Sabelnikov, A.N. Lipatnikov, N. Chakraborty, S. Nishiki, T. Hasagawa, "A balance equation for the mean rate of product creation in premixed turbulent flames." Proc. Combust. Inst., 36, http://dx.doi.org/10.1016/j.proci.2016.08.018.
- V. Sabelnikov, A. Lipatnikov, N. Chakraborty, S. Nishiki, T. Hasegawa, "A transport equation for reaction rate in turbulent flows." *Phys. Fluids*, 28, 081701, 2016.
- J. Sellmann, J. Lai, N. Chakraborty, A.M. Kempf, "Flame Surface Density based modelling of head-on quenching of turbulent premixed flames." *Proc. Combust. Inst*., 36, http://dx.doi.org/10.1016/j.proci.2016.07.114
- D.H. Wacks, N. Chakraborty, M. Klein, P.G. Aries, H.G. Im, "Flow topologies in different regimes of premixed turbulent combustion: A direct numerical simulation analysis." *Phys. Rev. F*, 1, 083401 (2016).

### ➢ Involvement in international activities

- **EU and International projects**
  - "AMEL"- CleanSky 2 SAGE project (EU-Horizon 2020 grant, Investigator from UKCTRF: Profs. R.S. Cant, E. Mastorakos, N. Swaminathan (University of Cambridge), Start date: 1st December 2014; End date: 30th November 2016)
  - Clean Sky DREAMCODE (EU-Horizon 2020 grant, Investigator from UKCTRF: Profs. W. Jones, P. Lindstedt, Dr. S. Rigopoulos (Imperial College, London), Start date: 1st November 2013; End date: 31st December 2016)
  - "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**

- Prof. N. Chakraborty (Newcastle University): Plenary lecture: Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.
  Prof. E. Mastorakos (University of Cambridge): Topical review on forced ignition of turbulent spray flames in the 36th International Combustion Symposium.
  Prof. N Swaminathan (University of Cambridge): Invited lecture: 'A Perspective on Turbulent Combustion Physics' at NORDITA, Stockholm, Sweden, 9th September 2016.

- **Scientific committee of international conferences**

- Prof. E. Mastorakos (University of Cambridge): Colloquium chair for turbulent combustion colloquium in the 36th International Combustion Symposium; Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016.
- Prof. N. Swaminathan (University of Cambridge): Responsible for co-organising a month long workshop on "Turbulent combustion physics" at NORDITA Stockholm and a summer school on this topic at KTH Stockholm; also organised an Industry Day at KTH, Stockholm (day long workshop to bring out the current challenges in Gas Turbine and Automobile Engine combustion); Joint meeting of British, Spanish, and Portuguese Sections of The Combustion Institute, Fitzwilliam College, Cambridge, UK, April 12-13, 2016; International Advisory Committee at the Sixth International Congress on Computational Mechanics and Simulation, 27th June-1st July 2016.

- **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**

Profs. N. Chakraborty and N. Swaminathan (Guest Editors for the special issue on "Advances in turbulent premixed combustion" in Combustion Science and Technology)
Prof. E. Mastorakos (Associate editor of Combustion and Flame, Editorial board member of Combustion Theory and Modelling, Flow, Turbulence and Combustion, Guest Editor for the special issue on the 9th Mediterranean Combustion symposium in Flow Turbulence and Combustion; Co-chair of Turbulent Combustion colloquium of the 36th International Combustion Symposium)

**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 press announcements and other communications of significance**

- A paper by X. Yu, I. Duran, A. S. Morgans, X. Han, entitled 'Dispersion of entropy waves propagating through combustion chambers' presented at International Congress on Sound and Vibration, Athens, 2016 was nominated for Sir James Lighthill Best Student Paper Award.
- A paper by S.P. Malkeson, D.H. Wacks, L. Yi, N. Chakraborty, entitled 'Analysis of fuel mass fraction dissipation rate transport in turbulent flame-droplet interaction: A Direct Numerical Simulation study' ILASS2016, Brighton, UK, 4th -7th September, 2016 was selected for the Best Paper Award.

➢ **Relevant grants and awards**

- EPSRC Grant, CHAMBER: Combustor thermoacoustics for multi-burner low emissions gas turbines, £757k (2017-2020). PI: A. S. Morgans, Imperial College London
- Dr. K. Vogiatzaki from the City University, London was awarded the prestigious Hinshelwood Prize for 2006 by the British Section of Combustion Institute for his meritorious contribution to combustion science.
- Prof. N. Chakraborty (Newcastle University) received funding from the Ministry of Human Resources Development, India as a part of Global Initiative of Academic Network (GIAN) scheme to offer an invited course on "Computational Modelling of Turbulent Combustion" at Jadavpur University, Kolkata, India in December 2016.
- 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)

**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 todays and future HPC hardware.
- A platform to collaborate and share expertise within community 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, website development 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 a 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) Some funding for networking with related consortia (e.g. UKTC) will be useful for the next incarnation of the HEC consortia.

(iii) The job of annual reporting and handling other 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 (~10%) of secretarial support, so a provision for a part of a Research Associate's (RA's) time for

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| 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.