

---

**UK Consortium on Turbulent Reacting Flows  
(UKCTRF): EP/K025163/1  
5<sup>th</sup> Annual Review Meeting**

**Nilanjan Chakraborty**

School of Engineering

Newcastle University, Claremont Road, Newcastle-Upon-Tyne, NE1 7RU



Selwyn College, Cambridge University, 12<sup>th</sup> September 2018

---

# Updates

---

- Outcome of EPSRC's High End Computing (HEC) consortia call
  - Workplan of the running grant and current status
  - Demand and availability of computational time
  - Application process for computational time allocation
  - Travel funding by consortium
  - Consortium website
  - Annual progress report
  - Combustion Science and Technology special issue
  - Current financial status
  - Any Other Business (AOB) and matters arising from earlier meeting
-

# Outcome of EPSRC's HEC consortia call (1)

- In September 2017, a proposal entitled **“Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF)”** was submitted to EPSRC
- **PI:** Prof. N. Chakraborty, **Co-Is:** Profs. R.S. Cant, D. Emerson, W.P., Jones, E. Mastorakos, N. Swaminathan, Dr. S. Navarro-Martinez
- We received 4 reviews in November 2017 (6/6, 6/6,6/6, 6/6) and we were invited to an interview with the panel in early February 2018

Rank	Grant Reference	Principal Investigator	Holding Organisation	Grant Title	Value (£)
1.	<a href="#">EP/R029369/1</a>	Chakraborty, Professor N	Newcastle University	Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (UKCTRF)	501,644
2.	<a href="#">EP/R029407/1</a>	Khalid, Professor S	University of Southampton	The UK High-End Computing Consortium for Biomolecular Simulation	321,432
3.	<a href="#">EP/R029431/1</a>	Woodley, Dr SM	UCL	HIGH END COMPUTING MATERIALS CHEMISTRY CONSORTIUM	489,316
4.	<a href="#">EP/R029342/1</a>	Tennyson, Professor J	UCL	UK Atomic, Molecular and Optical physics R-matrix consortium (UK AMOR)	368,071
5.	<a href="#">EP/R029326/1</a>	Laizet, Dr S	Imperial College London	UK Turbulence Consortium	693,229
6.	<a href="#">EP/R029148/1</a>	Arber, Professor T	University of Warwick	Plasma Physics HEC Consortium	227,262
7.	<a href="#">EP/R029598/1</a>	Luo, Professor KH	UCL	UK Consortium on Mesoscale Engineering Sciences (UKCOMES)	331,316

# Outcome of EPSRC's HEC consortia call (2)

- New grant will start from the **8<sup>th</sup> of January 2019** and run until the **7<sup>th</sup> of January 2023**
- Prof. N. Chakraborty (PI) Profs. R.S. Cant, D. Emerson, W.P., Jones, E. Mastorakos, N. Swaminathan and Dr. S. Navarro-Martinez (Co-Is) will form the Management Team on the next incarnation of UKCTRF
- We have **£501,644** and **1888,323 kAUs** and SLA allocation **0.5 FTE** over **4 years**
- New UKCTRF will also have an Impact Advisory Panel (IAP) and the members of IAP are:
  - Academic members:** Profs. J. Driscoll, D. Roekaerts, L. Vervisch and Dr. W. Meier
  - Industrial partners:** Rendua, Rolls-Royce, Shell, Siemens
- Most current procedures will continue for the next incarnation of UKCTRF. However, we may reserve a part of the computational time and invite applications for flagship simulations in the future years.

# Workplan of EP/K025163/1 and current status (1)

Phases \ Quarter	1 1	1 2	1 3	1 4	2 1	2 2	2 3	2 4	3 1	3 2	3 3	3 4	4 1	4 2	4 3	4 4	5 1	5 2	5 3	5 4	Milestones/ Deliverable	
I. Orientation of new HPC users and initial allocation for HPC time				◀ M1																	⇒ M1 (Year 1 report)	
II. Code development and initial validation for WP1 and WP2																						
III. Production level runs for WP1 and WP2 using HPC facilities																					⇒ M2 (Year 2 report)	
IV. Architecture development for future platforms and post-processing tools																						
IV. Technology development from the findings of WP1 and WP2																					◀ M3	⇒ M3 (Year 3 report)
V. Website development and maintenance																						
VI. Dissemination																				◀ M4	⇒ M4 (Year 4 report)	
Progress markers	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>							<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	
	R1 Kick-off meeting (Year 1)		R2 Annual progress meeting (Year 1)			R3 Annual progress meeting (Year 2)				WS1: Workshop1 + R4 Annual progress meeting (Year 3)							R5 Annual progress meeting (Year 4)				WS2+ Final meeting (Year 5)	
	Initial planning of the utilization of computational time.		Year 1 Interim Report			Year 2 Interim Report				Year 3 Interim Report							Year 4 Interim Report				Final report	⇒ Deliverable

Jan 14

Jan 15

Jan 16

Jan 17

Jan 18

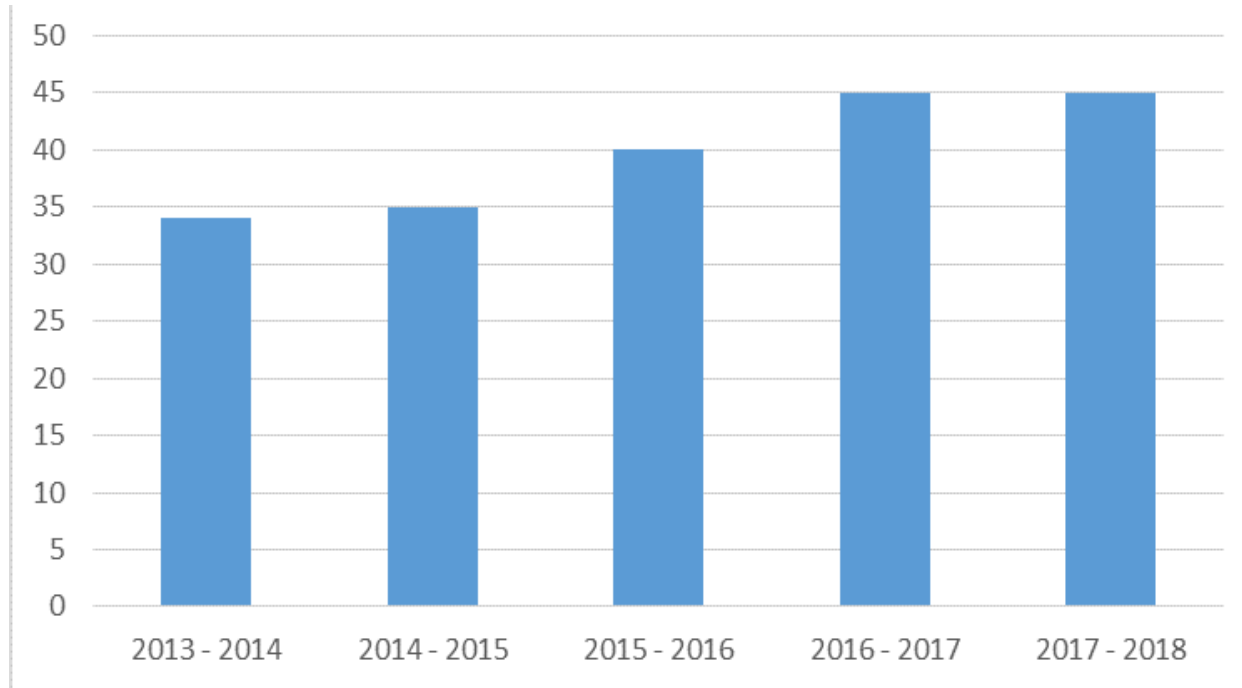
Jan 19



We are here

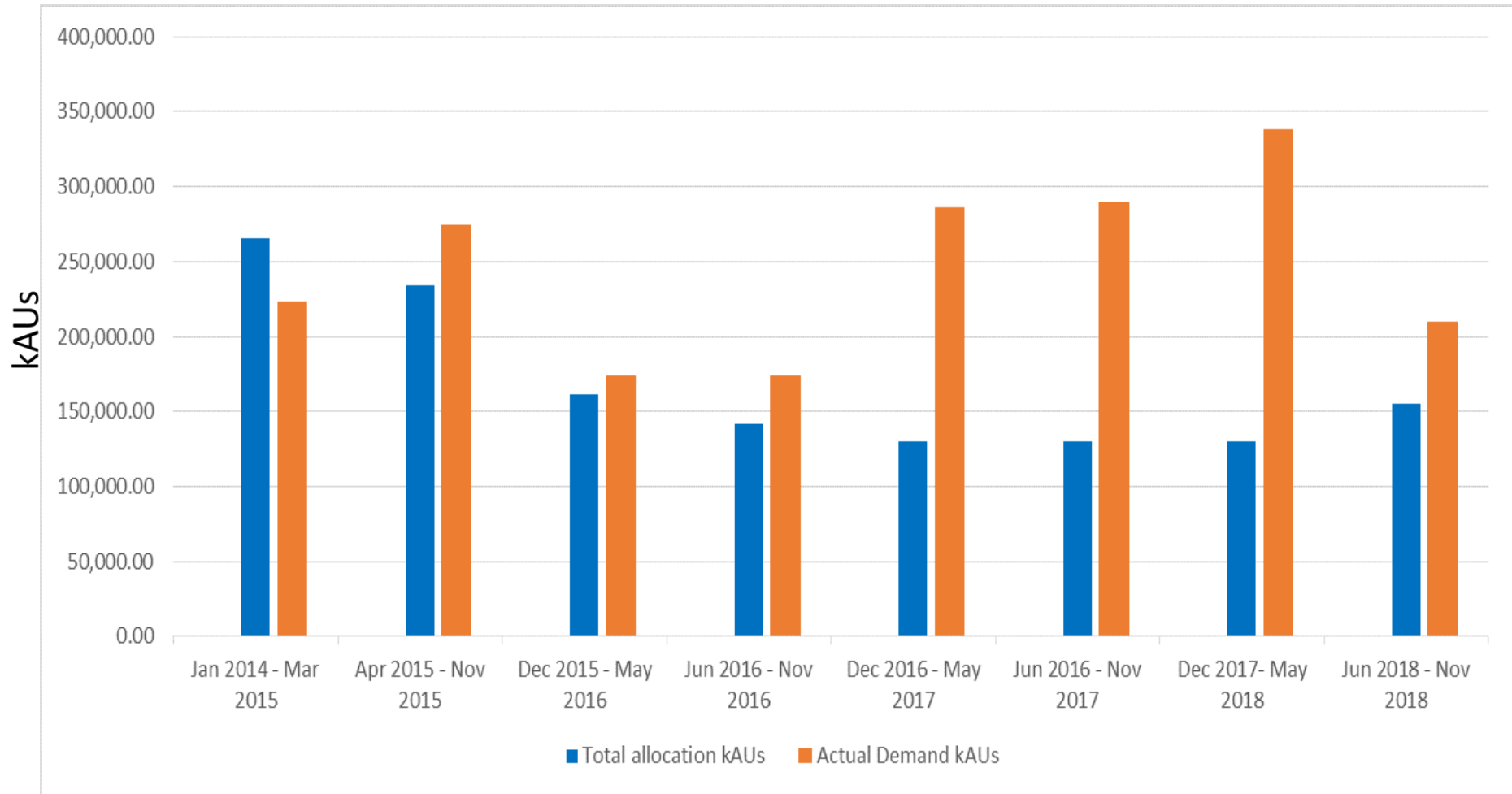
# Workplan of EP/K025163/1 and current status (2)

- The evolution of consortium member number during its lifetime is shown below:

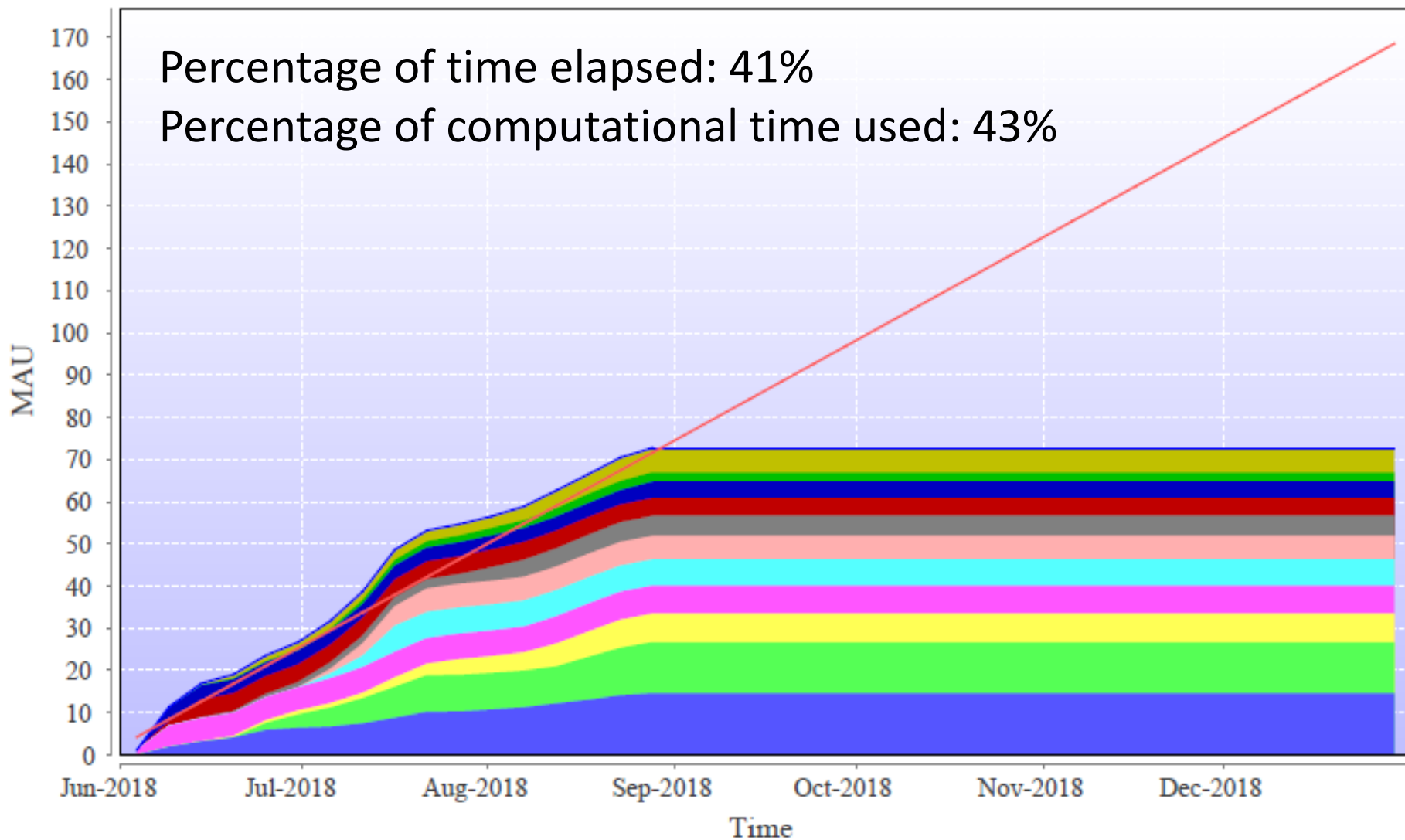


- Since its inception in 2014, the UKCTRF has achieved significant scientific and industrial impact with **over 400 publications**, **£10M research council funding**, **£10M industrial funding** which utilised ARCHER.
- More than **70 PhD students** and **30 Research Associates** benefited by UKCTRF and about **20** of them are in academic and industrial employment.

# Demand and availability of computational time



# Current usage of computational time allocation





# Computational time allocation: Current status

Group	Allocation	Remaining	After Change
1	6,053.10	456.5	456.5
2	9,907.20	9,816.80	9,816.80
3	2,000.00	1,629.70	1,629.70
4	3,600.00	3,600.00	3,600.00
5	13,803.10	13,304.20	13,304.20
6	1,050.00	246.7	246.7
7	2,000.00	1,995.50	1,995.50
8	2,000.00	2,000.00	2,000.00
9	8,000.00	3,791.80	3,791.80
10	14,053.10	6,677.20	6,677.20
11	4,500.00	2,844.00	2,844.00
12	1,058.30	0	0
13	6,161.40	3,974.10	3,974.10
14	7,891.70	3,361.00	3,361.00
15	14,053.10	9,148.80	9,148.80
16	21,994.80	6,248.40	6,248.40
17	14,053.10	483.7	483.7
18	6,171.00	6,171.00	6,171.00
19	9,526.50	1,959.40	1,959.40
20	4,526.60	4,526.60	4,526.60
21	3,100.00	3,100.00	3,100.00
22	5,000.00	4,311.80	4,311.80
23	2,000.00	389.8	389.8
24	6,000.00	-203.7	-203.7

# Application for computational time allocation

---

- Application form is available on <http://forms.ncl.ac.uk/view.php?id=5420>
  - Review process & review panel (NC,RSC,DE,WPJ,EM,SNM,NS)
  - Queries are dealt within 48 hours
  - Decision is made typically within 10 days
  - Demand is higher than availability and EPSRC wants us to be more discerning before awarding the computational time
  - The track-record of the applicant in terms of conforming to the consortium requirements will be considered.
  - The members who do not supply required information for annual report and case study on a timely basis might get a reduced allocation or no allocation
-

# Travel funding by consortium

- We contributed £1000 per research group towards the cost of attending the International Combustion Symposium for those who had accepted papers for oral presentation (14 in total)
- Research carried out in this consortium gave rise to 27 symposium papers in the 37<sup>th</sup> International Combustion Symposium
- In 2017-2018 academic year 100+ journal and 120+ conference papers arose from this consortium
- The management team has decided to contribute £500 per group towards cost of the international conference other than the International Combustion Symposium (so far we approved travel costs for 11 research groups) (<http://www.ukctrf.com/members-area/travel-funding-4/>) : **The claims need to be received by the end of October 2018**

Please do not forget to acknowledge the consortium and ARCHER

# Consortium website ([www.ukctrf.com](http://www.ukctrf.com))

Please be familiar with the consortium website:

- Application forms for reimbursement, travel funding and computational time application are available (<http://www.ukctrf.com/members-area/reimbursement/>, <http://www.ukctrf.com/members-area/travel-funding-4/> <http://www.ukctrf.com/members-area/computer-time-allocation/> )
- List of sample publications by the consortium members (<http://www.ukctrf.com/impact/sample-publications/> )
- List of the travel grants for PhD students and RAs (<http://www.ukctrf.com/members-area/past-conference-funding/> )
- List of presentations given in earlier meetings, annual reports and case studies are available on the website (<http://www.ukctrf.com/ukctrf-events/> )
- Materials for the website and annual report will be requested soon.  
**Next annual report is due on the 30<sup>th</sup> of November**

# Annual progress report

---

- EPSRC needs an extensive report and a minimum of 3 case studies based on our year 4 activities
  - The Management Team (MT) prepared a provisional report and submitted 4 case studies (1 on soot formation from Imperial College, 1 on spray response to acoustic forcing from Loughborough University, 1 on sub- and super-critical injection dynamics from Brighton University and 1 on advanced ignition technology from Southampton University)
  - We will need list of publications, list of grants and prizes and case studies from the consortium members for the next annual progress report (due on the 30<sup>th</sup> of November 2018).
-

# Combustion Science and Technology special issue

---

- There will be a special issue of Combustion Science and Technology entitled **“Special issue on UKCTRF workshop 2018.”**
  - All the keynote speakers, Impact Advisory Panel and UKCTRF members are invited to submit papers to this special issue
  - The deadline for submission to this special issue is the 30<sup>th</sup> of September 2018
  - Please submit the paper using <https://mc.manuscriptcentral.com/gcst> and follow usual author guidelines. Please opt for Special issue on UKCTRF workshop 2018” while submission
  - The papers submitted to the special issue will go through the usual review process and the papers will be handled by the special issue editors (Profs. R.S. Cant, N. Chakraborty, W. Jones and Dr. S. Navarro-Martinez)
-

# Current financial status

	Budget	Actual	Commitment	Available
➤ UKCTRF Meetings	£20,491.00	£8,757.06	£ -	£11,733.94
➤ UKCTRF Dissemination	£100,407.00	£88,411.48	£ -	£11,995.52
➤ UKCTRF School Specific	£14,193.00	£13,246.80	£946.20	£0.00
➤ UKCTRF FEC Contribution	£34,388.00	£32,095.28	£2,292.72	£0.00
	<b>£169,479.00</b>	<b>£142,510.62</b>	<b>£3,238.92</b>	<b>£23,729.46</b>
➤ Estimated cost of 2018 Annual Meeting	£11,000.00			

# Any Other Business (AOB)

---

- Date of next annual progress review meeting  
(Tentative Plan: Brighton University, September 2019)
  - I would like to thank Ms. Joanne Emery, Caroline Armstrong, Debbie Wilde, Susan Earley, Georgina Swan, Drs. Malasree Home, Sarah Whalley for their administrative help during the lifetime of this consortium.
  - Thanks for attending this meeting and giving your valuable feedback.
-