UK Consortium on Turbulent Reacting Flows (UKCTRF): EP/R029369/1: Final Annual Meeting of current funding period

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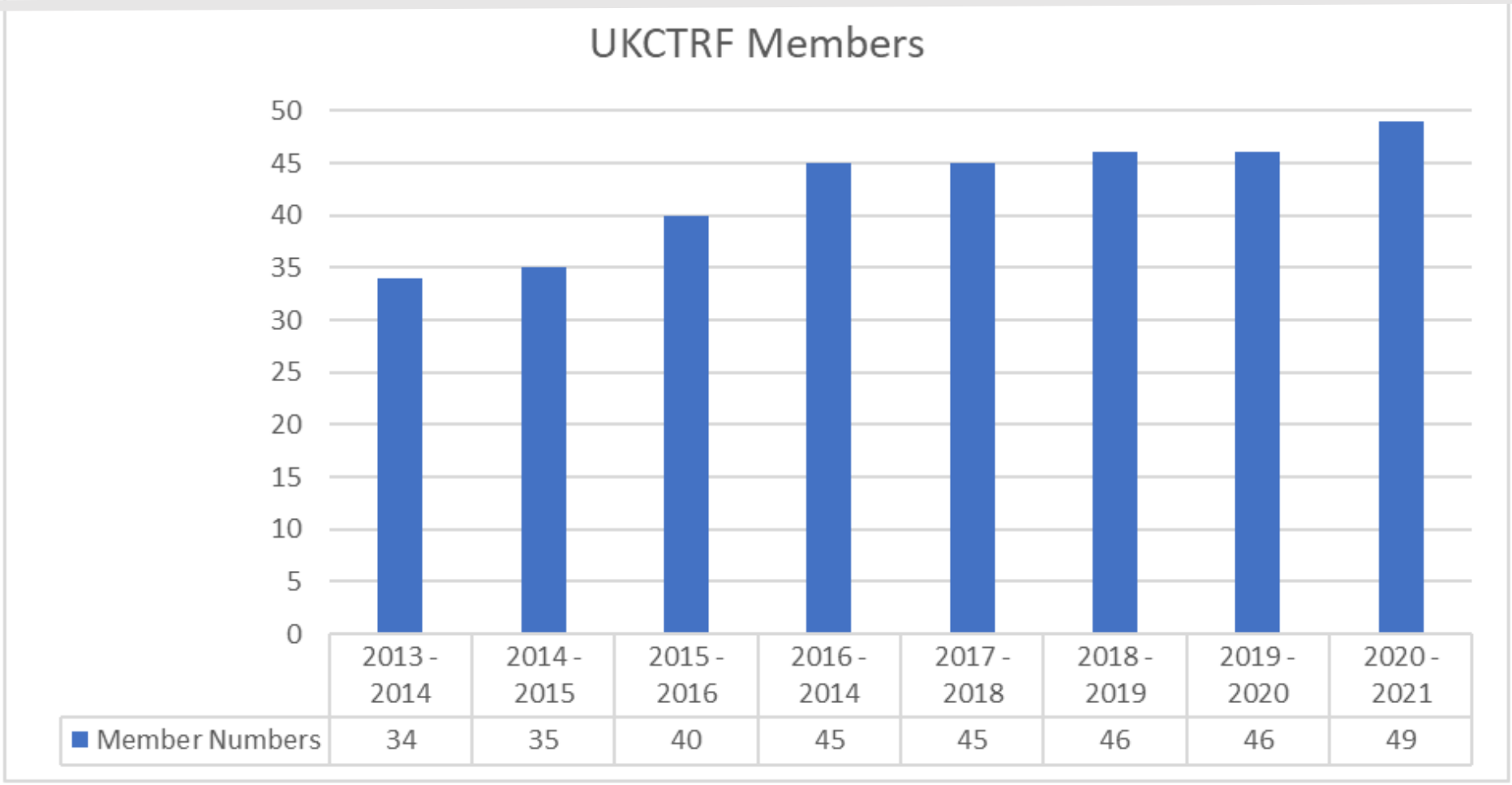
Outline

- Demands and availability of computational time
- Application for computational time allocation
- Feedback to applicants from the management team
- Current usage of computational time allocation
- Travel funding by consortium
- Annual progress report
- ExCALIBUR update
- UKCTRF updates
- Final comments

Utilisation of the computational time

- Our utilisation of computational time allocation is 91%, 93% and 73% on ARCHER2 in the last three allocation periods.
- The demand of the community was 3 times that of our available allocation on ARCHER. Our allocation on ARCHER2 has increased to 6 times the amount that we used to get on ARCHER. The community is currently getting used to it (i.e. the demand for usual application is currently 72% of the allocation) but this gives use some flexibility to fund flagship collaborative projects.
- Most of the computational time of the UKCTRF was used by SENGA+ users. It has given rise to 100+ high-quality journal publications in the last 4 years.
- SENGA+ is the leading computational fluid dynamics code on ARCHER2 in terms of its utilisation.
- There are some jobs on ARCHER2 which does not deserve the 25th fastest supercomputer in the world in terms of the number of processors used. In future, these jobs will be allocated to Tier-2 machines.

Evolution of member number of the UKCTRF



We are at the moment considering applications of 2 new applicants

Application for computational time allocation

- Application form is available on http://forms.ncl.ac.uk/view.php?id=5420
- Review process & review panel (UKCTRF management team)
- Queries are dealt within 48 hours
- Decision is made typically within 10 days
- We do not accept more than 2 applications from a particular named investigator's group
- Even though we have some flexibility, quality remains the primary criterion for awarding the computational time
- Any feedback to improve the process or make it better

Feedback to applicants from the management team

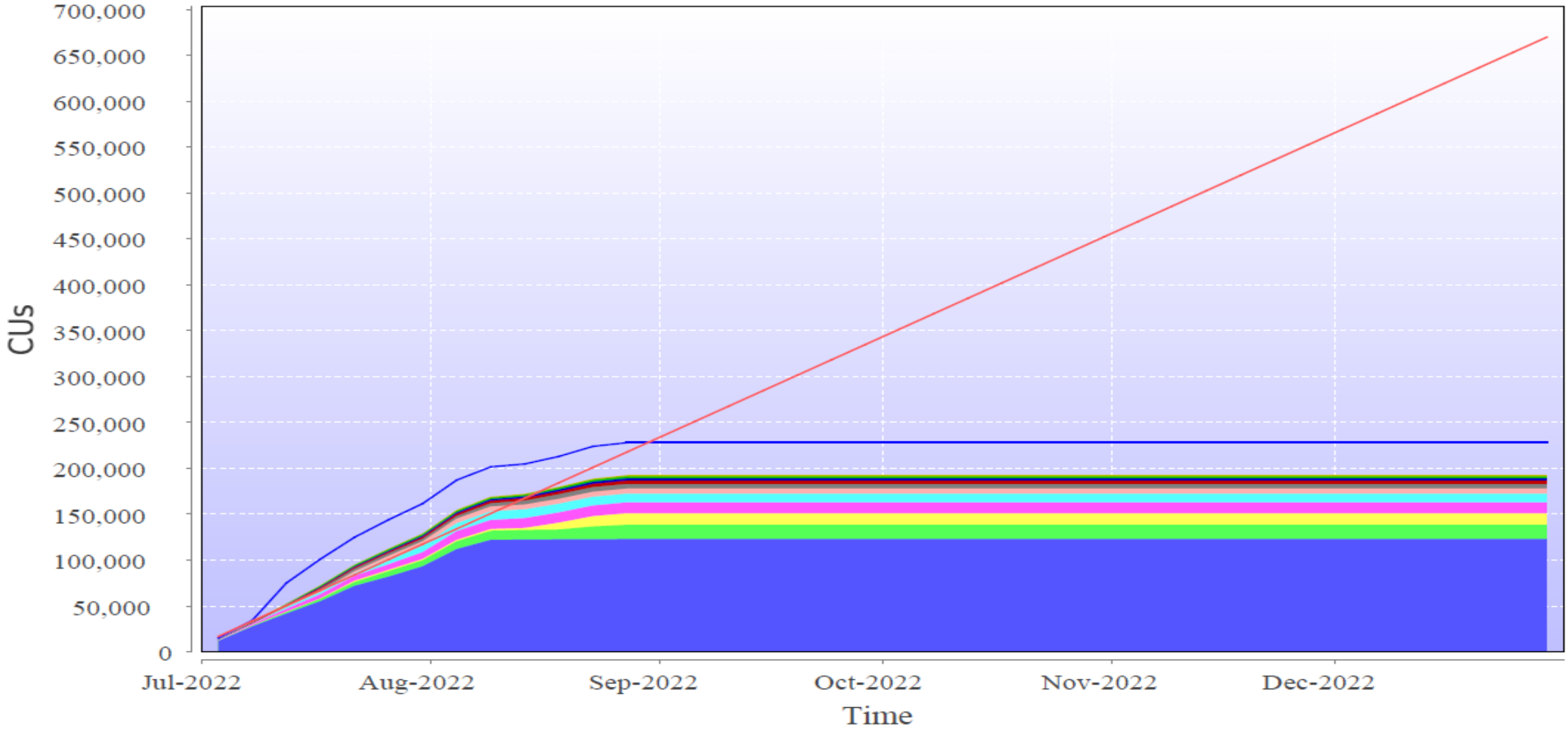
- The applicants need to justify their requests and they should not rely on the historical computational time allocations for their projects. This is especially important for the projects which fall in the periphery of the remit of this consortium.

- The members are not expected to request computational times for the same project from more than one consortia, but it needs to be declared if there is a good justification for doing so.

- It is very important that disk space is properly managed. Please delete the old files which are not used. Serial offenders might not be allowed to run jobs on ARCHER2.

Percentage of allocation used: 29%

Percentage of time elapsed: 32%



Travel funding by consortium

- Each named investigator's group £500 was allocated for each named member's group for orally presenting a paper originating from the UKCTRF research at other conferences other than combustion symposium. 14 groups have benefited from it so far. This will be revisited later today in the management team meeting.
- The management team decided to contribute £2500 to the cost of each named member's research group for orally presenting a paper at the 39th International Symposium on Combustion based on the UKCTRF funded research. This offer was also extended to all the management team members. We received 7 applications (9 separate papers) from the members for contributions to the cost of registration/travel to the 39th International Symposium on Combustion resulted from the UKCTRF activities. We also funded 2 management team members for strategic reasons.
- All those who have made applications are requested to send the invoice to Ms. Anna Cuninghame (anna.cuninghame@newcastle.ac.uk) as soon as possible if it is not done already.
- The papers for which travel funding will be provided will need to meet the following requirements:
  - **It needs to deal with reacting flows. If the paper is on laminar flows, it must have some relevance to turbulent reacting flow modelling**
  - **It needs to explicitly acknowledge ARCHER2 and consortium grant (EP/R029369/1)**

Consortium website (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/index.php/reimbursement/,http://www.ukctrf.com/index.php/travel-funding/ , http://www.ukctrf.com/index.php/computer-time-allocation/)

- List of the travel grants for PhD students and RAs

(http://www.ukctrf.com/index.php/conference-funding/)

- List of presentations given in earlier meetings, annual reports and case studies are available on the website (http://www.ukctrf.com/index.php/events/)
- Information on the flagship codes of the UKCTRF can be obtained from:(https://www.ukctrf.com/index.php/senga/,https://www.ukctrf.com/index.php/hamish/)

Annual progress report & Impact capture

- We ran a survey on UKCTRF participation after the last annual meeting and are currently in the process of analysing the results in preparation for the renewal.

- EPSRC expects an extensive report and a minimum of 3 case studies based on our annual activities. We will need volunteers for these case studies. The annual reports and case studies can be found on:
  https://www.ukctrf.com/index.php/impact/

- We will need list of publications, list of grants and prizes and case studies from the consortium members for the next annual progress report and future Researchfish submissions. Please provide the necessary information within the deadline.

ExCALIBUR (https://excalibur.ac.uk/excalibur)

- ExCALIBUR stands for **Exascale Computing ALgorithms and Infrastructures Benefitting UK Research**
- £45.7M initiative from the UK government's **Strategic Priorities Fund** (SPF)
- Led by the **Met Office**, **UK Research and Innovation** (UKRI) with the **UK Atomic Energy Authority** (UKAEA)
- The UK's Exascale Programme for 5 years (started November 2019)
- Focus on software and algorithms
- Funding breakdown: EPSRC - £22.8M, Met Office / UKAEA - £17.0M, Hardware and Enabling Software (H&ES) - £4.5M
- The intended outcomes are Knowledge integration; High priority use cases; Emerging requirements for HPC algorithms; Cross-cutting research; Proof-of-concept hardware (H&ES)

ExCALIBUR: UKCTRF updates

- A multi-institutional (involving Cambridge, Newcastle, Imperial, Southampton, Warwick, Daresbury Laboratory) EPSRC bid totalling £3M has turned out to be successful in response to ExCALIBUR Phase 1b call. This project will bring together (for the first time) communities representing two of the seven UK HEC Consortia, the UK Turbulence Consortium (UKTC) and the UK Consortium on Turbulent Reacting Flows (UKCRF) , to re-engineer or extend the capabilities of four of their production and research flow solvers for Exascale computing: Xcompact3d, OpenSBLI, uDALES and SENGA+.

- These open-source, well-established, community flow solvers are based on finite-difference methods on structured meshes. We consider it to be the best strategy to achieve performance at scale (no meshing issues, no load balancing issues, possibilities to limit data movement & global communications, wide range of options to optimise bandwidth and memory usage, such as memory tiling and near-neighbour communications). A key aim of this project is to leverage the well-established Domain Specific Language (DLS) framework OPS and the 2DECOMP&FFT library to allow Xcompact3d, OpenSBLI, uDALES and SENGA+ to run on large-scale heterogeneous computers.

UKCTRF updates & Renewal

- UKCTRF members are strongly encouraged to take part in the knowledge exchange activities of the ExCALIBUR programme. It will provide future opportunities of collaborative research involving software development for future Exascale machines and hybrid infrastructure.
- An ARCHER2 pioneer project on large-scale DNS of Flame-Wall Interaction of Hydrogen-air flames in turbulent boundary layer was successful in 2020. This project is now in full swing on ARCHER2.
- We have received mostly positive feedback based on UKCTRF's outline proposal in response to EPSRC's call for High End Computing consortia renewal. The full proposal will be submitted at the end of September 2022. This proposal is led by Dr. S. Navarro-Martinez (Imperial College) and the co-investigators are Profs. N. Chakraborty (Newcastle University), N. Swaminathan (University of Cambridge), J. Wen (Warwick University), Drs. K. Vogiatzaki (Oxford) and J. Xia (Brunel University).

Workplan & Current Stage

:(Proposed activity at the desired level); : : (Proposed activity for reduced resource); :Activity in Flagship Software grant (EP/P022286/1)

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	Milestones/ Deliverablee
I. initial allocation for HPC time and continuation of UKCTRF activities in WP1 & WP2					◄ M1												➲ M1 (Year 1 report)
II. Code development and initial validation for new capabilities WP1 and WP2								◄M2									
III. Production level runs for WP1 and WP2 using HPC facilities																	➲ M2 (Year 2 report)
IV. Algorithm and architecture development for future platforms in WP 3c + WP 3d																	
V. Validation & documentation of SENGA+ and HAMISH and new release of SENGA+ (WP3a &3b)												◄M3					➲ M3 (Year 3 report)
VI. Website development and maintenance																	
VII. Dissemination																◄M4	➲ M4 (Year 4 report)
Progress markers	☑		☑		☑		☑		☑		☑		☑		☑		
	R1 Kick-off meeting (Year 1)		R2 Annual progress meeting (Year 1)				WS1:Workshop1 + R3 Annual progress meeting (Year 2)				R4 Annual progress meeting (Year 3)				WS2:Workshop 2+ R5 Final Meeting (Year 4)		
	Initial planning of utilisation of computational time		Year 1 Interim Report				Year 2 Interim Report				Year 3 Interim Report				Year 4 Final Report		➲ Deliverable

Jan 19 Jan 20 Jan 21 Jan 22 Jan 23

We are here

Final comments

- There will be a special issue in Flow, Turbulence and Combustion based on the UKCTRF activities after this meeting. All the members of the UKCTRF and impact advisory panel members are invited to submit to this special issue.
- Profs. N. Chakraborty, N. Swaminathan and Dr. S. Navarro-Martinez will form the guest editorial board of this special issue. The title of the special issue is: '**Special issue on UKCTRF workshop 2022'**. The deadline for final submission will be on the **30th of January 2023**. The special issue editorial team will decide on the list of invited papers by the 30th of September 2022. In addition, any member who wants to submit a paper to the special issue should communicate this to Prof. Nilanjan Chakraborty (nilanjan.chakraborty@ncl.ac.uk) by the 30th of September 2022 with a provisional title. The formal invitations will be sent out on the 15th of October 2022 with a response deadline on the 30th of October 2022.
- We would like to thank all the Impact Advisory Panel members for devoting their valuable time. Special thanks are due to the plenary lecture speakers for their time and effort.
- I am also grateful to the session chairs for their support.
- I would like to thank Ms. Caroline Armstrong, Anna Cuninghame, Susan Earley, Joanne Emery, Debbie Wilde, Jo Redshaw, Jennifer Richmond, Georgina Swan, Drs. Malasree Home, Sarah Whalley for their administrative help during the lifetime of this consortium.