Lawrence Livermore National Laboratory

Science & Technology Facilities Council

NON-BINDING MEMORANDUM OF UNDERSTANDING

Between

LAWRENCE LIVERMORE NATIONAL SECURITY, LLC
and
SCIENCE & TECHNOLOGY FACILITIES COUNCIL

LLNL Case No. MO03062-0.0

Lawrence Livermore National Laboratory
Industrial Partnerships Office
P.O. Box 808, L-795, Livermore, CA 94551

29 August 2013

1 DESCRIPTION

This Memorandum of Understanding ("MOU") is between Lawrence Livermore National Security, LLC ("LLNS"), under its U.S. Department of Energy ("DOE") Contract No. DE-AC52-07NA27344, to manage and operate Lawrence Livermore National Laboratory ("LLNL"), and The Science and Technology Facilities Council ("STFC"), having one of its principal places of business at Sci-Tech Daresbury, Keckwick Lane, Daresbury, Warrington, WA4 4AD, United Kingdom. LLNS is a limited liability company organized in the State of Delaware, with its principal office at 2300 First Street, Suite 204, Livermore, California 94550-3153. LLNS and STFC are referred to jointly as "Participants," and each a "Participant." This MOU is subject to overriding obligations to the Federal Government pursuant to the provisions of LLNS' Contract No. DE-AC52-07NA27344 with the DOE for the operation of LLNL. The Participants understand that this MOU is not legally binding but reflects the spirit of cooperation between them.

2 PURPOSE

This MOU provides a vehicle for technical and business development strategy exchanges between LLNS and STFC towards the development and operation of high performance computing ("HPC") technologies and applications, and associated industrial outreach and partnership efforts as engaged in by the HPC Innovation Center ("HPCIC") at LLNL and the Hartree Centre ("HC") at STFC. The Participants acknowledge that the promises made herein are not intended to create legally enforceable obligations.

3 PARTICIPANTS

The HPCIC at LLNL opened in June 2011 as a public-private partnership initiative focused on broadening the industrial utilization of HPC by developing, proving, and deploying high-impact HPC-based solutions. By doing so, the HPCIC aims to substantively increase the competitiveness of US industries, accelerate the advancement of US science and technology, and help develop a future HPC-skilled workforce.

The HC was created in April 2012 as part of the UK's e-infrastructure initiative that commenced in 2011. The HC is dedicated to the development and demonstration of new software optimized to run on the latest and upcoming e-infrastructure hardware. The HC aims to add scalability and functionality for research and development work, and improve accessibility and usability to broaden and deepen the communities of users to include organizations that have no HPC specialists on the payroll. This objective, in particular, is aimed at generating positive economic impact from the HC's activities.

4 OBJECTIVES

The HPCIC and the HC share many goals. In particular, both centers:

- Aim at making HPC resources and expertise available to industrial and academic partners
- Seek to develop and deploy scalable solutions to solve customer problems
- Need to prove a return on investment to a sometimes skeptical audience
- Are focused on accelerating innovation to spur economic growth
- Share a partner in IBM, as well as base architecture (Blue Gene/Q) for their primary computational resource available for industrial partnerships

In light of the shared goals and purpose, the Participants seek to establish a collaboration with one another that explores the clear synergies for mutual benefit.

5 COLLABORATIVE ACTIVITIES

This MOU does not itself define specific collaboration projects but rather the general areas that are of interest for collaboration between HPCIC and HC and, in particular, the framework by which collaborative activities can be proposed, engaged in, and reviewed as necessary.

Potential collaborative activities of interest to HPCIC and HC can be grouped into three general categories: HPC Technology (Appendix 1), HPC Applications (Appendix 2), and Business Development (Appendix 3). This categorization is not intended to limit current or future areas of collaboration; as other areas or categories become apparent, they too may be covered under the scope of this MOU.

Specific collaborative projects are intended to be undertaken from time to time, each to have specific terms and conditions under which it is intended to be undertaken detailed within a separate, legally binding Joint Development Agreement ("JDA"). For the avoidance of doubt, no data or information that may be of specific use to the other Participant is to be exchanged under this MOU; all such exchanges are to take place within the specific collaborative projects and are to be governed by the relevant JDA.

6 ROLES AND RESPONSIBILITIES

To propose, evaluate, and manage ongoing collaborative activities, the Participants expect to form a Collaboration Executive Review Committee ("CERC") that intends to meet as often as mutually agreeable but not less than once per month. The Collaboration Executive Review Committee (see below) plans to maintain a portfolio of JDAs.

The Participants also expect to establish a joint working group ("JWG") to manage the overall HPCIC and HC plans development defined within this MOU. The JWG intends to meet regularly and to draw as needed on appropriate expertise from LLNS and STFC to complete individual plan elements.

The administration and adherence with the provisions of this MOU are the responsibility of the Director of the Hartree Centre at STFC and the Director of HPC Innovation Center at LLNL. Each plans to represent its respective organization or, if desired, formally appoint a representative to act as the point of contact ("POC") for routine administrative and operational elements of this MOU, and a POC for coordination of this arrangement with other programs being conducted by the respective Participants.

For STFC, the POC for the administrative and operational elements of this MOU should be the Director of the Hartree Centre.

For LLNS, the POC for the administrative and operational elements of this MOU should be the Industrial Partnerships Office (IPO) Business Development Executive.

Deliverables:

(1) A report on the establishment of the CERC and JWG, and other activities initiated and contemplated since the execution of the MOU. Due six months after commencement of the MOU (Month 6).
(2) A report on activities initiated, completed, and contemplated at each six month interval thereafter (Month 12, 18, etc.). Each such report ("Report") is expected to attach details, as a separate schedule, of the progress of activities under the active JDA during the period covered by the relevant Report. LLNS contemplates primary responsibility for producing the first Report required under paragraph 1 above, after which the Participants intend taking it in turn to have responsibility for the production of each six monthly Report. The Participant which does not have lead responsibility is expected to provide all assistance and information reasonably required by the producing Participant to complete the relevant Report.

7 FUNDING

This MOU should not be used to obligate or commit funds, or as the basis for a transfer of funds. All performance hereunder is subject to the availability of applicable funding of the Participant performing. Generally, each Participant is to bear all costs associated with its own efforts towards collaborative activities under this MOU. Otherwise, costs attributed to any JDA arising out of this MOU is to be apportioned by mutual consent of the Participants, with the Participants exchanging estimates of costs likely to be incurred before such items of expenditure arise, and agreeing on any proposed expenditure to be set out in each JDA.

8 TECHNICAL CONTACTS

The technical contacts for each Participant are as follows:

In the case of LLNS:

LAWRENCE LIVERMORE NATIONAL SECURITY, LLC
Lawrence Livermore National Laboratory
Industrial Partnerships Office
7000 East Avenue
P.O. Box 808, L-795
Livermore, CA 94551
U.S.A.

IPO Contact: Charity Follett
Tel: (925) 422-1817
Fax: (925) 423-8988
Email: follett2@llnl.gov

Technical Contact: Dr. Fred Streitz
Tel: (925) 423-3236
Fax: (925) 422-7819
Email: streitz1@llnl.gov

In the case of STFC:

SCIENCE & TECHNOLOGY FACILITIES COUNCIL
Keckwick Lane
Warrington
WA4 4AD
England

Commercial Contact: Michael Gleaves
Tel: +44 (0) 1925 603710
Email: michael.gleaves@stfc.ac.uk

Technical Contact: Dr. Mike Ashworth
Tel: +44 (0) 1925 603178
Email: mike.ashworth@stfc.ac.uk

9 TERM OF THE MOU

This MOU is effective upon the date of signature by the last signing Participant, and is to remain in effect for a period of three (3) years from the effective date of the MOU. This MOU may be modified at any time by mutual written consent of the Participants. The initiating Participant proposing modifications should provide the other Participant in writing with at least sixty (60) days' notice (unless waived by the other Participant) of a desired modification of the MOU. Either Participant may terminate this MOU by notice in writing at least sixty (60) days in advance of the desired termination.

10 MISCELLANEOUS

a. No provision of this MOU is intended to conflict with any law.

b. Should questions arise about the interpretation of this MOU, or issues arise in relation to this MOU, the Participants are expected to promptly consult with each other and work together to achieve a mutually acceptable solution.

c. The Participants acknowledge that any work performed hereunder by one Participant for the benefit of the other Participant is provided "as is" with all faults, defects and errors. The Participants make no warranty regarding their performance hereunder and disclaim any and all warranties, express or implied, relating to the work, including but not limited to the implied warranties of merchantability, fitness for a particular purpose, title, or non-infringement.

d. Each Participant is solely responsible for compliance with all applicable laws and regulations that may apply to this MOU, including, but not limited to, compliance with applicable export control requirements.

e. Nothing contained herein may be interpreted to conflict with LLNS' Contract No. DE-AC52-07NA27344 with the DOE, and to the extent that there is such a conflict, LLNS is to be deemed excused from performance hereunder.

LLNS and STFC have signed this MOU by their respective officers, on the date stated below.

SCIENCE & TECHNOLOGY FACILITIES COUNCIL	LAWRENCE LIVERMORE NATIONAL SECURITY, LLC FOR LAWRENCE LIVERMORE NATIONAL LABORATORY
By: _____ (Signature)	By: _____ (Signature)
Name: Prof. John Womersley	Name: Penrose C. Albright
Title: Chief Executive Officer	Title: Director
Date signed: August 29, 2013	**Date signed:** August 29, 2013

APPENDIX 1 — HPC Technology

HPC Technology refers to the hardware and system software technologies and infrastructure, as well as operational policies, procedures, and best practices necessary to meet the requirements of partner's large-scale computing needs.

- *Data analytics.* Both HPCIC and HC are keenly interested in developing and deploying data analytics architectures. In particular, the HC is currently completing a Blue Gene Active Storage ("BGAS") system, the first in the world. HPCIC is leading the development and deployment of large-scale Hadoop clusters over parallel file systems.
- *Operational best practices.* Operating large-scale computing or supercomputer centers is a complex endeavor. Both HPCIC and HC are keenly interested in sharing best practices that may lead to more efficient and effective operations of these centers.
- *Massively parallel processing.* In preparation for exascale processing, the HPCIC and HC may collaborate to create a demonstration of a key software code across several Blue Gene systems around the world, hopefully reaching a total processing power of hundreds of petaflops.

APPENDIX 2 — HPC Applications

HPC Applications refers to specific software codes designed to model, simulate and/or analyze in a particular application area.

- *Engineering*. Computational Fluid Dynamics ("CFD") is a key technology in engineering, especially in the automotive and aerospace industries. HPCIC and HC contemplate collaborating on adding functionality and on integration of CFD codes with other codes such as finite element analysis (FEA) and materials codes to provide a full "software-zoom" facility. This is intended to help enable engineers to bring material properties and fluid flows together into single integrated models.
- *Materials properties under extreme conditions.* This work would be aimed at developing codes and models able to predict the behaviors, and especially lifetimes, of materials in conditions such as those expected in nuclear reactors (e.g. power stations) or in emergencies (e.g. fires and explosions). Experiments of this sort in the real world are, at the least, expensive, dangerous, impossible or unethical. *In-silico* experiments suffer none of these drawbacks yet can lead to greater understanding of the processes involved, longevity of components in such conditions, and safety for operators, the public, and the environment.
- *Meso-scale modeling.* This includes adapted dissipative particle dynamics ("DPD") codes such as DL_MESO, an HC code under development for use in the prediction of the behavior of mixtures. This can greatly speed up the innovation process for many chemicals-based industries, for example personal hygiene products, coatings, adhesives, smart textiles, organic electronics, energy storage materials, and long-term disinfection (e.g. surfaces in hospitals).
- *Biomedical modeling*. This includes modeling the heart and other major organs and processes in bodies.
- *Agent-based modeling*. This is intended to include modeling of processes and procedures in the health sector, for example in A&E departments of hospitals.
- *Bioinformatics*. This is intended to include development of new software tools for extracting information from medical and other records and databases, an aspect of Big Data research.
- *Smart Materials*. This includes modeling of materials with advanced, valuable properties such as anti-microbial activity, adhesion promotion, barrier formation and/or protective coatings.

APPENDIX 3 — Business Development

Business Development refers to those activities of the Participants aimed at recruiting collaborators, clients, funding, and resources in order to deliver the objectives of the MOU via a series of specific Projects and Programs to be initiated from time-to-time during the course of the MOU, and thereafter if required and appropriate.

- *Developing "industry-friendly" HPC opportunities.* HPCIC and HC contemplate engaging in discussions with organizations to help advance HPC opportunities that are attractive to industrial partners and encourage increased industrial utilization of HPC resources. Such opportunities may be beneficial to the respective nations through enhanced US and UK economic impact resulting from HPCIC and HC industrial engagements.
- *Target opportunities.* Identify and target a group of companies active in research and development in both the US and UK that could benefit from the use of HPC in their businesses and create a strategy to recruit these, or a subset of these, into a series of collaborative development programs aimed at optimizing application codes for their requirements and demonstrating, on the large machines in both sites, the benefits that can be delivered by such improved software.
- *Enhance usability of HPC systems.* Liaise with identified companies to develop bespoke and generic "on-ramp" user interfaces designed for use by non-HPC specialists in order to facilitate the widespread uptake of HPC by users and industries with little or no access to HPC specific expertise.