LA-UR-13-24118
Approved for public release; distribution is unlimited.

Title: CASL Institutional Computing Report, Calendar Year 2012

Author(s): Lee, Stephen R.

Intended for: Report

Issued: 2013-06-05

CASL Institutional Computing Report
Calendar Year 2012

Stephen Lee, CCS Division Leader (for Bruce Robinson, CNP-PO)

Introduction

CASL, the Consortium for Advanced Simulation of Light water reactors (or LWRs) is a multi-institutional, $22-25M per year, 5-year project lead by Oak Ridge National Laboratory. This project is one of DOE's Energy Innovation Hubs and started late in the last quarter of FY10. As part of this joint work with 10 different institutions, senior LANL management agreed to provide 10% of all Institutional Computing resources at Los Alamos to the project for the life of the project. This is part of an in-kind institutional contribution LANL is making to the CASL effort. Similar contributions have been made by all national laboratory partners in CASL (ORNL, LANL, INL, and SNL)[1].

CASL is a highly visible and extremely valuable project for Los Alamos, with line of sight visibility and attention from the Secretary of Energy and high-impact results delivered to the nuclear energy industry. It is considered to be a model for such large programs with multiple partners, as well as a model for future simulation hubs defined by DOE.

At the time of this writing, LANL leads three areas in the project. Thermal Hydraulics Methods (THM, Mark Christon, CCS-2), Materials Optimization and Performance (MPO, Chris Stanek, MST-8), and Validation and Uncertainty Quantification (VUQ, Brian Williams, CCS-6).

This report summarizes the use of Institutional Computing (IC) resources by the CASL project, for calendar year 2013.

Utilization of Institutional Computing Resources

A complete picture of CASL utilization can be obtained directly by those that manage the IC resources. Here, a quick summary of usage is provided. IC resources have been critical to the success of THM, and the successful completion of 5 CASL milestones (3 level 3, 1 level 2, and 1 level 1 milestone; level 1 and 2 milestones are DOE reportable). Conejo, Mapache, Pinto, and Mustang have been essential in this success. From 1/1/12 through 1/1/13, s11_casl used 18.58 million CPU hours, up from 3.35 million CPU hours during CY11. The table below summarizes the utilization by machine.

Table 1: CASL usage by machine

[1] There are 10 principle partners in CASL; national laboratories (ORNL, LANL, SNL, and INL), universities (NC State, U. Michigan, MIT), and industry (WEC, TVA, EPRI). There are many additional minor partners in the CASL project.

Machine	Hours Used	Percent Used
Conejo	3,464,213.7	1.7%
Mapache	617,213.2	9.1%
Pinto	957,456.4	4.9%
Mustang	13,544,498.6	17.2%

THM also makes use of the Titan computer at ORNL, and resources at SNL and INL, for computational cycles.

CASL utilization of Institutional Computing resources generally falls in the category of theory and modeling development for material science, numerical methods and code development for thermal hydraulics and neutronics, and integrated code development for fuels modeling and the virtual reactor tool that CASL is constructing.

At this point, no other partners are currently using LANL IC resources. This was expected to change during CY12, but it did not. There are active discussions in CASL as to how to manage computing resources at all partner sites in a more coherent manner. There are also active discussions with DOE NE as to computing needs for NE in general.

Materials Optimization and Performance

Transition metal spinel oxides are formed as corrosion products on stainless steels and during internal oxidation, especially in high temperature applications. One example of the importance of spinel corrosion products is the formation of so-called CRUD on the cladding surface of nuclear fuels, which is also the application that motivated the present study. CRUD is an acronym for Chalk River Unidentified Deposit and refers to corrosion products that deposit on internal light water reactor (LWR) components, specifically on the upper parts of fuel rods where sub-cooled nucleate boiling occurs. The major pressurized light water reactor (PWR) CRUD constituents are Ni and Fe oxides, which originate from corrosion of structures outside the pressure vessel such as steam generators. The structural materials used in steam generators are alloyed stainless steels with high concentration of Ni and Cr. In order to improve models of CRUD formation and growth, we have performed density functional theory (DFT) calculations on a number of Fe, Ni, Cr and Zn oxides relevant for either CRUD formation or corrosion processes. Specifically, the Fe3O4-NiFe2O4, Fe3O4-ZnFe2O4, Fe3O4-FeCr2O4, NiFe2O4-ZnFe2O4, NiFe2O4-NiCr2O4, NiCr2O4-FeCr2O4, ZnCr2O4-FeCr2O4 and ZnCr2O4-ZnFe2O4 pseudo-binary mixing energies were calculated. Intrinsic and extrinsic defect reactions and the formation of non-stoichiometric Fe, Ni, Cr and Zn spinel compounds were also investigated, which included excess or deficiency of A2+, B3+ and O2- ions. The calculated thermodynamic properties are compared to available experimental data. The results enable us to better understand both the formation of protective films on corrosion sources and the chemistry of the CRUD that is deposited on the fuel pins.

Development of thermodynamic models of the Fe-Ni-Cr-Zn-O system also benefit from the DFT data presented in this work.

We have also investigated the thermal conductivity of CRUD. Since the spinel oxides have a significantly lower thermal conductivity than the fuel cladding (which is typically a Zr-based alloy), it is important to understand how the presence of CRUD will impact fuel rod surface temperatures. From an industrial perspective, the ability to accurately predict fuel surface temperature allows for determination of margin to potential cladding failure due to crud induced localized corrosion (CILC). However, despite its industrial importance, to date no thermal conductivity data exists for NiFe2O4. Experimental data of NiFe2O4 thermal conductivity will also facilitate development of compositionally aware software tools aimed at better understanding the formation and growth of CRUD, as well as its impact on nuclear fuel performance. In order to understand the easured thermal conductivity of NiFe2O4 DFT calculations were performed to qualitatively estimate the change in carrier concentration due to magnetic or structural disorder.

During CY12, two level 3 milestones were achieved that made use of IC resources.

THM
This area in CASL involves significant code development and use of IC resources in a more traditional sense: the creation of an integrated, multiphysics, simulation tool that will ultimately be part of the virtual reactor integration tool set being created by CASL. This is a new capability under development at LANL, funded by CASL and enabled by IC resources. This is not only important for the CASL project, but positions LANL well for future competition in other areas requiring thermo-mechanical modeling (everything from small modular reactors to wind turbine simulations).

This work progressed extremely well during 2012, with demonstrated scaling using hybrid meshes up to 100 million elements using implicit large eddy simulation (ILES). Milestones achieved directly address grid-to-rod fretting, an ongoing issue in light water reactors that affects the life of the nuclear fuel.

IC resources contributed to LANL successfully completing 5 milestones in THM during 2012.

VUQ
LANL recently assumed co-leadership of this focus area, and during 2012 significant milestone support was provided in the area of validation for Hydra-TH (a LANL code), Denovo (an ORNL transport code), and VERA in the form of calibration methodology (VERA is the integrated simulation code ORNL is building, which ultimately incorporates multiple other codes, including Hydra-TH, Denovo, and so on). We anticipate this sort of work increasing in the future, putting additional strain on IC resources.

Observations and Concerns

HPC staff has been very helpful resolving issues on IC resources. There remain some unresolved file system issues that affect restarts on Pinto.

Better ParaView support is needed on IC resources. The large scale problems run with Hydra-TH require ParaView. Anticipated work in VUQ will also drive this requirement. There are outstanding conflicts with gcc and ParaView modules, and newer versions of the ParaView server are needed. At present, the CASL team must build their own versions of ParaView which does not leverage expertise in HPC Division.

Publications List

"Mixing and non-stoichiometry in Fe-Ni-Cr-Zn-O spinel compounds: Density functional theory calculations", D. A. Anddersson, C.R. Stanek, under review in Physical Chemistry Chemical Physics (2013).

"Thermal Conductivity of $NiFe_2O_4$", D. A. Andersson, A. T. Nelson, J. A. Aguiar, K. J. McClellan, D. D. Byler, and C. R. Stanek, to be submitted (2013).

"Integration of Hydra-TH in VERA (L2 Milestone)," M. A. Christon, J. Bakosi, N. Barnett, M. M. Francois, R. B. Lowrie, R. Sankaran, LA-UR-12-22403.

"Hydra-TH User's Manual," M. A. Christon, J. Baksoi, and R. B. Lowrie, LA-UR-12-23181.

"Solution Algorithms for Multi-Fluid-Flow Averaged Equations," R. R. Nourgaliev, M. A. Christon, INL/EXT-12-27187.

"Hydra-TH Verification," Validation and Thermal-Hydraulics Benchmark Problems, J. Bakosi, M. A. Christon, L. Pritchett-Sheats, H. Luo, T. Xia and R. Nourgaliev, LA-UR-13-22017.

"Large-Scale Turbulent Simulations of Grid-to-Rod Fretting," J. Bakosi, N. Barnett, M. A. Christon, M. M. Francois, and R. B. Lowrie, CFD4NRS-4 conference, LA-UR-12-20281.

"Large-Eddy Simulations of Turbulent Flow for Grid-to-Rod Fretting in Nuclear Reactors," J. Bakosi, M. A. Christon, R. B. Lowrie, L. A. Pritchett-Sheats, R. R. Nourgaliev, submitted to Nuclear Engineering and Design, LA-UR-12-26572.

"Hydra-TH: A Thermal-Hydraulics Code for Nuclear Reactor Applications, R. R. "Nourgaliev, M. A. Christon, J. Bakosi, R. B. Lowrie, L. A. Pritchett-Sheats, NURETH-15, Pisa Italy, May 12 - 17, 2013.