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e-Science in high energy density science research

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Abstract

We present three achievements related to e-Science in high energy density science research. We have developed a test module of new data base system for nation-wide users of the high power lasers at Osaka University with web technology, flexible control system and XML-database, which provide efficient, accurate and flexible R&D processing. We also constructed a EUV-GRID portal system for integrated computer simulations of laser produced plasma–extreme ultraviolet (LPP–EUV) light source development, which provides flexible framework for automatic sequencing of workflow for the integrated simulations. A dynamical domain decomposition method in molecular dynamic (MD) simulations is required to obtain a good adaptive load balancing for heterogeneous computing environments such as grid. We have developed a new algorithm of the dynamical domain decomposition. We successfully performed large scale MD-message passing interface (MPI) simulations on cluster computers connected through Super-SINET using the National Research Grid Initiative (NAREGI GRID) grid middleware and the new algorithm.

Keywords: e-Science; Grid computing; XML; Database; High energy density science; Laser produced plasma; Laser fusion; EUV; Lithography

1. Introduction

The term e-Science is here used to describe computational intensive science that is carried out in highly distributed network environments, science that uses immense data sets that require grid computing, and technologies that enable distributed collaboration. High power laser systems at the Institute of Laser Engineering (ILE), Osaka University, became officially national joint-use facilities for high energy density science research from 2006. We perform many national and international collaboration researches using the high power laser systems. The high energy density states are realized by irradiating high power laser onto a target. The high energy density science consists of the following inter-correlated three fields: (1) warm dense matter physics (condensed matter physics at extreme high pressure) that is related to exploring new materials and planetary science, (2) plasma radiation hydrodynamics that is related to laser astrophysics, radiation plasma physics and its applications, (3) relativistic plasma and high field science that are related to researches on laser–plasma interactions, fast ignition laser fusion, and laser acceleration. One peta watt, 10 kJ laser system, "LFEX-laser" is under construction for the exploration of the high energy density science. LFEX-laser is originally designed as a heating laser at 10 ps operation to achieve the ignition temperature of fuel compressed by Gekko XII laser (30 kJ) in fast ignition scheme of laser fusion [1]. It will be also the highest power laser in the world in short pulse duration of sub-picosecond.

We have developed a test module of a new database system for nation-wide users to analyze experimental and simulation data with web technology and Extensible Markup Language (XML) database based on R&D Chain Management (RCM) system by Quatre-*i* Science [2]. XML-database is superior to relational-database (RDB) in flexibility and changeability of data structure. Trace and search of data with XML-database become much easier in R&D processes than those with RDB.

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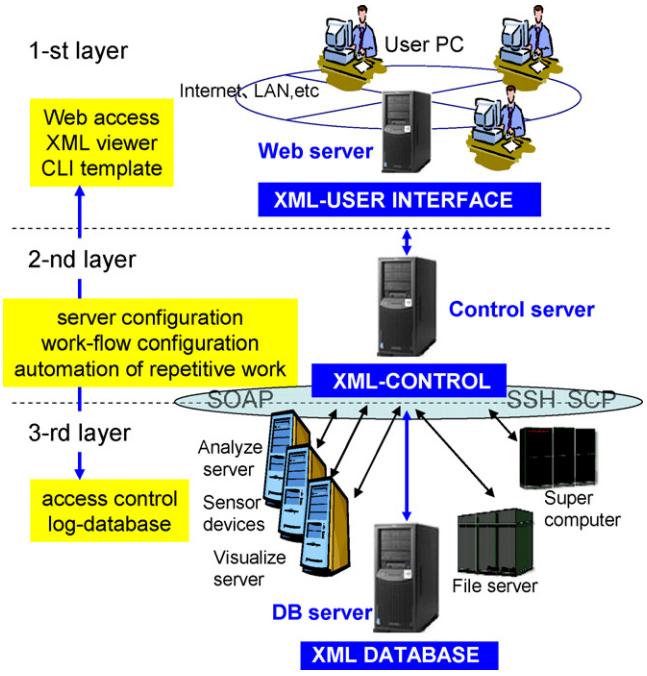

Fig. 1. Concept of the RCM system.

As an industrial application of laser fusion research, we started a 5-year-long project, named as Leading Project, for development of laser produced plasma–extreme ultraviolet (LPP–EUV) light source for lithography in 2003. Moore's low requires implementing EUV lithography technology for production of next-generation microprocessors with node size less than 32 nm in manufacturing until 2011. EUV light of 13.5 nm wavelength from laser produced plasmas can be used as a light source, since Mo/Si multi-layer mirrors have high reflectivity at this wavelength [3]. The Leading Project aims at understanding physics and providing database and guideline for a practical use. One critical issue for realization of LPP–EUV light source is the conversion efficiency (CE) from incident laser power to EUV radiation of 13.5 nm wavelength within 2% bandwidth [4]. Development of an integrated numerical simulation code is indispensable for understanding physics of LPP and designing a high CE EUV light source. We constructed a EUV-GRID portal system for integrated simulations using many inter-correlated programs developed at different institutions. The GRID portal provides a flexible framework for automatic sequencing of workflow.

A large scale molecular dynamic (MD) simulation is indispensable for research of laser produced warm dense matter physics at extreme high pressure. A large scale MD simulation requires a large number of high performance computers. Grid computing allows us to use many computers connected through a net. A dynamical domain decomposition method is required to obtain a good adaptive load balancing for heterogeneous computing environments such as grid. We have developed a new algorithm of the dynamical domain decomposition [5] and tested on cluster computers connected between Osaka University and Tohoku University through Super-SINET with National Research Grid Initiative (NAREGI) grid middleware.

2. Database system based on web technology and XML-database

We have developed a portal system based on the RCM system that has three layers of web service for open network with high security as shown in Fig. 1. The RCM system itself has flexible

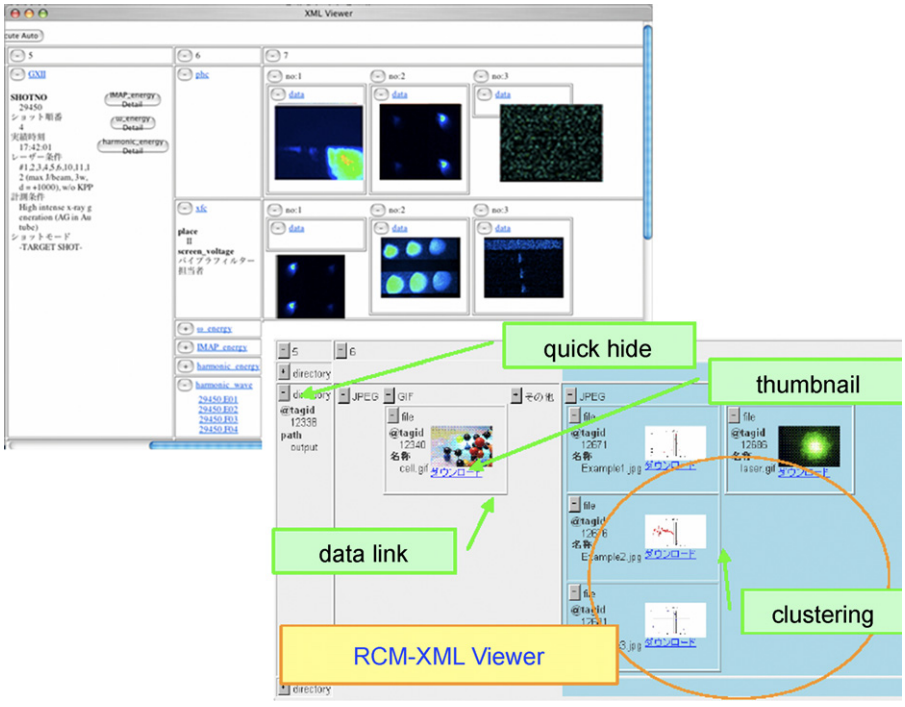

Fig. 2. Flexible data view with XML-Viewer.