EspressoDB: A scientific database for managing high-performance computing workflows

Chia Cheng Chang[1, 2, 3], **Christopher Körber**[2, 3], **and André~Walker-Loud**[3, 2]

1 iTHEMS RIKEN, Wako, Saitama 351-0198 **2** Department of Physics, University of California, Berkeley, California 94720 **3** Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

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Software

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Summary

Leadership computing facilities around the world support cutting-edge scientific research across a broad spectrum of disciplines including understanding climate change (Kurth et al., 2018), combating opioid addiction (Joubert et al., 2018), or simulating the decay of a neutron (Berkowitz, Clark, et al., 2018). While the increase in computational power has allowed scientists to better evaluate the underlying model, the size of these computational projects have grown to a point where a framework is desired to facilitate managing the workflow. A typical scientific computing workflow includes:

1. Defining all input parameters for every step of the computation;
2. Defining dependencies of computational tasks;
3. Storing some of the output data;
4. Post-processing these data files;
5. Performing data analysis on output.

`EspressoDB` is a programmatic object-relational data management framework implemented in Python and based on the `Django web framework`. `EspressoDB` was developed to streamline data management workflows, centralize and guarantee data integrity, while providing domain flexibility and ease of use.

The framework provided by `EspressoDB` aims to support the ever increasing complexity of workflows of scientific computing at leadership computing facilities (LCFs), with the goal of reducing the amount of human time required to manage the jobs, thus giving scientists more time to focus on science.

Features

Data integrity is important to scientific projects and becomes more challenging the larger the project. In general, a `SQL` framework type-checks data before writing to the database and controls dependencies and relations between different tables to ensure internal consistency. `EspressoDB` allows additional user-defined constraints not supported by `SQL` (*e.g.* unique constraints using information across related tables). Once the user has specified a set of conditions that entries have to fulfill for each table, `EspressoDB` runs these cross checks for new data before inserting them in the database.

`EspressoDB` also supports collaborative and open-data oriented projects by leveraging and extending `Django`'s web hosting component. In addition to providing a centralized data platform, it is possible to spawn customized web pages which can be hosted locally or on the world wide web[1]. EspressoDB simplifies creating projects by providing default Django configurations that set up for example, connections to the database and webpages to view associated tables. For example, with the default setting, EspressoDB spawns:

- Documentation views of implemented tables;
- A project wide notification system;
- Project specific Python interface guidelines which help writing scripts to populate the database;
- Admin pages for interacting with data in a GUI.

Further views can be implemented to interact with data and use existing Python libraries for summarizing and visualizing information. This allows users to create visual progress updates on the fly and to integrate the database information to the data-processing workflow, significantly reducing the human overhead required due to improved automation.

More details, usage instructions and examples are documented at espressodb.readthedocs.io.

Use case

LatteDB, an application of EspressoDB that is specialized to contain table definitions for lattice quantum chromodynamics (LQCD) calculations and analysis. LatteDB is currently being used by the CalLat Collaboration in their computations on Summit at the Oak Ridge Leadership Computing Facility (OLCF) through DOE INCITE Allocations (Walker-Loud et al., 2019, 2020). The website generated by LatteDB used by CalLat can be found at https://ithems.lbl.gov/lattedb/. A precursor to EspressoDB and LatteDB was used to support a series of LQCD projects (Chang et al., 2018; Nicholson et al., 2018).

Summit at OLCF is disruptively fast compared to previous generations of leadership class computers. There are two challenges which are both critical to address for near-exascale computers such as Summit, which will become more important in the exascale era:

1. *Efficient bundling and management of independent tasks*: LCFs prohibit the submission of millions of small tasks to their supercomputers (clogged queues, overtaxed service nodes etc.). It is imperative to have a task manager capable of bundling many tasks into large jobs while distributing the work to various components of the heterogeneous nodes;

2. *Dependent task generation and data processing*: As an example, CalLat creates peta-bytes of temporary files that are written to the scratch file system, used for subsequent computations and ultimately processed down to hundred of tera-bytes that are saved for analysis. It is essential to track the status of these files in real-time (identify corrupt, missing, or purgeable files).

Members of CalLat are addressing issue 1 through the creation of job management software, METAQ (Berkowitz, 2017) and MPI_JM (Berkowitz, Clark, et al., 2018; Berkowitz et al., 2018). LatteDB is designed to address the second issue. A future feature of LatteDB is integration with MPI_JM.

[1] Depending on the configuration, it is possible to provide selected access for multiple users on different levels.

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