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

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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 \cite{1}, combating opioid addiction \cite{2}, or simulating the decay of a neutron \cite{3}. While the increase in computational power has allowed scientists to better evaluate the underlying model, the size of these computational projects has 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 mapping (ORM) data management framework implemented in Python and based on the Django web framework. EspressoDB was developed to streamline data management, centralize and promote data integrity, while providing domain flexibility and ease of use. It is designed to directly integrate in utilized software to allow dynamical access to vast amount of relational data at runtime. Compared to existing ORM frameworks like SQLAlchemy or Django itself, EspressoDB lowers the barrier of access by simplifying the project setup and provides further features to satisfy uniqueness and consistency over multiple data dependencies. In contrast to software like DVC, VisTrails, or Taverna \cite{4}, which describe the workflow of computations, EspressoDB rather interacts with data itself and thus can be used in a complementary spirit.

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 ORM interface and web hosting component. The object oriented approach allows the whole team to determine table architectures without knowing SQL. Once tables have been implemented by users familiar with the details of the EspressoDB project, additional users can access data without detailed knowledge of the project itself. 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, contains 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 [5, 6]. 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 [7, 8].

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.**
2. **Dependent task generation and data processing;**

Using lattice QCD as a specific example, the computations can be organized as a directed multigraph: a single calculation requires tens-of-thousands to millions of independent MPI tasks to be completed. These tasks, while running independently, have nested and chained interdependencies (the output of some tasks are part of the input for other tasks). Several such complete computations must be performed to extract final answers. As a specific example, CalLat creates petabytes of temporary files that are written to the scratch file system, used for subsequent computations and ultimately processed down to hundreds of terabytes that are saved for analysis. It is essential to track the status of these files in real-time to identify corrupt, missing, or purgeable files.

\(^1\)Depending on the configuration, it is possible to provide selected access for multiple users on different levels.
Understandably, LCFs prohibit the submission of millions of small tasks to their supercomputers (clogged queues, overtaxed service nodes, etc.). It is therefore 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; To keep the nodes from going idle, the jobs must be backfilled while running with the next set of available tasks (item 1). Members of CalLat are addressing the task bundling through the creation of job management software, METAQ [9], and MPI_JM [3, 10], while LatteDB is designed to address the dependent task generation. A future feature of LatteDB is integration with MPI_JM.

For the second item, keeping track of the tasks, optimizing the order of tasks and ensuring no work is repeated requires a task manager that understands all these dependencies and the uniqueness of each task. Software to track and manage such a computational model at runtime, which does not require in-depth knowledge of, e.g., managing databases, does not currently exist, which motivated the creation of EspressoDB and LatteDB.

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References

[1] T. Kurth, S. Treichler, J. Romero, M. Mudigonda, N. Luehr, E. Phillips, A. Mahesh, M. Matheson, J. Deslippe, M. Fatica, Pfahler, and M. Houston, “Exascale deep learning for climate analytics,” *SC18: International Conference for High Performance Computing, Networking, Storage and Analysis*, Nov 2018.

[2] W. Joubert, D. Weighill, D. Kainer, S. Climer, A. Justice, K. Fagnan, and D. Jacobson, “Attacking the opioid epidemic: Determining the epistatic and pleiotropic genetic architectures for chronic pain and opioid addiction,” in *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis*, SC ’18, (Piscataway, NJ, USA), pp. 57:1–57:14, IEEE Press, 2018.

[3] E. Berkowitz, M. A. Clark, A. Gambhir, K. McElvain, A. Nicholson, E. Rinaldi, P. Vranas, A. Walker-Loud, C. C. Chang, B. Joó, T. Kurth, and K. Orginos, “Simulating the weak death of the neutron in a femtoscale universe with near-exascale computing,” in *SC18: International Conference for High Performance Computing, Networking, Storage and Analysis*, pp. 697–705, Nov 2018.

[4] K. Wolstencroft, R. Haines, D. Fellows, A. Williams, D. Withers, S. Owen, S. Soiland-Reyes, I. Dunlop, A. Nenadic, P. Fisher, J. Bhagat, K. Belhajjane, F. Bacall, A. Hardisty, A. Nieva de la Hidalga, M. P. Balcazar Vargas, S. Sufi, and C. Goble, “The Taverna workflow suite: designing and executing workflows of Web Services on
the desktop, web or in the cloud,” *Nucleic Acids Research*, vol. 41, pp. W557–W561, 05 2013.

[5] A. Walker-Loud, E. Berkowitz, C. Bouchard, D. A. Brantley, C. C. Chang, K. Clark, A. Gambhir, N. Garron, T. Kurth, C. Monahan, H. Monge-Camacho, A. Nicholson, and E. Rinaldi, “The proton’s structure and the search for new physics.” http://www.doeleadershipcomputing.org/wp-content/uploads/2019/03/2019INCITEFactSheets.pdf, 2019.

[6] A. Walker-Loud, C. Morningstar, A. Nicholson, J. Bulava, K. Clark, E. Berkowitz, C. Bouchard, C. C. Chang, A. Gambhir, B. Hörz, D. Howarth, C. Körber, K. McElvain, H. Monge-Camacho, E. Rinaldi, and A. Hanlon, “The structure and interactions of nucleons from the standard model.” http://www.doeleadershipcomputing.org/wp-content/uploads/2020INCITEFactSheets.pdf, 2020.

[7] A. Nicholson, E. Berkowitz, H. Monge-Camacho, D. A. Brantley, N. Garron, C. C. Chang, E. Rinaldi, M. Clark, B. Joó, T. Kurth, B. Tiburzi, P. Vranas, and A. Walker-Loud, “Heavy physics contributions to neutrinoless double beta decay from QCD,” *Phys. Rev. Lett.*, vol. 121, p. 172501, 2018.

[8] C. C. Chang, A. Nicholson, E. Rinaldi, E. Berkowitz, N. Garron, D. A. Brantley, H. Monge-Camacho, C. J. Monahan, C. Bouchard, M. Clark, B. Joó, T. Kurth, K. Orginos, P. Vranas, and A. Walker-Loud, “A per-cent-level determination of the nucleon axial coupling from standard model,” *Nature*, vol. 558, no. 7708, pp. 91–94, 2018.

[9] E. Berkowitz, “METAQ: Bundle Supercomputing Tasks,” 2017.

[10] E. Berkowitz, G. R. Jansen, K. McElvain, and A. Walker-Loud, “Job Management and Task Bundling,” *EPJ Web Conf.*, vol. 175, p. 09007, 2018.

[11] C. Drischler, W. Haxton, K. McElvain, E. Mereghetti, A. Nicholson, P. Vranas, and A. Walker-Loud, “Towards grounding nuclear physics in QCD,” 2019.

[12] J. D. Bratt, R. G. Edwards, M. Engelhardt, P. Hagler, H.-W. Lin, M.-F. Lin, H. Meyer, B. Musch, J. W. Negele, K. Orginos, A. V. Pochinsky, M. Procura, D. G. Richards, W. Schroers, and S. N. Syritsyn, “Nucleon structure from mixed action calculations using $2+1$ flavors of asqtad sea and domain wall valence fermions,” *Phys. Rev.*, vol. D82, p. 094502, 2010.

## Supplemental Information

### Django overview

**EspressoDB** utilizes Python’s **Django** Object-Relational Mapping (ORM) framework. Tables correspond to Python classes, rows correspond to instances and columns correspond to attributes of the instances. One can filter instances by their attributes or generate summary tables (**pandas.DataFrame**) within one line of code. Furthermore, using an ORM allows one to have the same interface independent of the backend. It is possible to store data in a file based **SQLite** solution, or use more scalable options like **MySQL** or **Postgresql**. **Django** is part of many open-source projects and thus comes with extensive documentation. Additionally, **Django** is scalable, comes with reliable tests and vast community support which manifests in the fact that it is commonly used in large scale projects (BitBucket, Instagram, Mozilla, NASA and many more). One guiding principle of **EspressoDB** is to not “re-invent the wheel” but instead leverage the support coming from **Django**. As
a result, one can easily incorporate many of Django’s extensions and find solutions to technical questions online.

**Lattice QCD use case**

LQCD is an inherently a stochastic method of simulating quantum chromodynamics (QCD) the fundamental theory of nuclear strong interactions, which is responsible for confining quarks into protons and neutrons and ultimately, for binding these nucleons into the atomic nuclei we observe in nature. The application of LQCD to forefront research applications in nuclear physics is necessary to build a quantitative connection between our understanding of nuclei and QCD. This is important as nuclei serve as laboratories and/or detectors for many experiments aiming to test the limits of the Standard Model of particle physics in our quest to understand questions such as: Why is the universe composed of matter and not anti-matter? Does dark matter interact with regular matter other than gravitationally? What is the nature of the neutrino and is it related to the observed excess of matter over anti-matter? See Ref. [11] for a recent review of the interface of LQCD with our understanding of nuclear physics.

The application of LQCD to nuclear physics is an exascale challenge. One of the main reasons these calculations are so expensive is that when LQCD is applied to systems of one or more nucleons, an exponentially bad signal-to-noise problem must be overcome. While the optimal strategy for overcoming this challenge is not yet known, one thing common to all methods is the need for an exponentially large amount of statistics. As such, these LQCD computations require the completion of millions of independent sub-calculations (or tasks), with chained dependencies, in order to complete a single calculation. These chained tasks write large amounts of temporary files to the scratch file system which are used as input for subsequent files, often with multiple input files required for the later computations. Several such calculations must be performed in order to extrapolate the results to the physical point, defined as the limit of zero discretization (the continuum limit), the infinite volume limit and the limit of physical quark masses which are a priori unknown and so must be determined through this extrapolation/interpolation procedure. These requirements lead to a very complex set of computations that must be carried out with great care and a significant amount of human time and effort to ensure the computing cycles are used as efficiently as possible.

Compounding these challenges, the new computer Summit, is disruptively fast compared to previous generations of leadership class computers. Full machine-to-machine, Summit is approximately 15 times faster than Titan when applied to LQCD applications such as those carried out by CalLat [3]. While this is great for scientific throughput, it also means the management of the computational jobs has become unwieldy with the management models typically used for such computations: Summit churns through the computations so fast, and produces so much data, it is not possible to keep up with the data processing and management with our older management tools.

As a concrete example, we consider the nucleon elastic form factor project being carried out by CalLat [5, 6]. For each ensemble of gauge configurations used (one choice of input parameters) the computation requires the following dependent steps:

1. For each gauge configuration (of O(1000)) in an ensemble (of O(20)), make several quark sources (grouped in batches of 8);
2. For each source, create a quark propagator;
3. For each quark propagator:
   1. Create a proton correlation function to determine the proton mass;
   2. Create O(10) proton sequential sinks at different separation times (times 8 for different spin, flavor and parity combination);
4. For each time-separation, group the 8 sequential sinks from the 8 propagators into a single coherent sequential sink [12];
5. For each time-separation, Solve a sequential propagator from the coherent sequential sink;
6. For each time-separation, spin, flavor and parity, tie each of the original 8 propagators with the sequential propagator to construct a 4-dimensional (4D) formfactor correlation function;
7. Process the data to prepare it for analysis and the extraction of physics.
8. Repeat for multiple source sets (of 8) if more statistics are required.

Each of the steps above leads to the generation of many large (multi-gigabyte) data files, most of which are not saved. LatteDB is used to track the status of these data files to know if they need to be created or if the next step can proceed. The final data production step, 6, leads to our final data file that need further processing prior to our final analysis and saving of the files.

Inheriting the functionality of EspressoDB, LatteDB has the flexibility to faithfully reproduce a one-to-one mapping between the above computational workflow to database tables. For example, in step 1, the table of gauge configurations is defined such that every row in the table specifies a single gauge configuration. This reflects how on disk, we have thousands of files, each containing a snapshot of the QCD vacuum, and as such, every file, and every subsequent file as a result of the gauge configuration (e.g. propagators or correlation functions in steps 2 through 6) can also be tracked individually. However, at the end of the calculation, an observable is only well defined with an ensemble of gauge configurations. LatteDB allows one to define an ensemble table, with a Django ManyToMany data type which may be interpreted as a single column containing a list of references (foreign keys) to the table of gauge configurations. In SQL, a list of foreign keys is not a fundamental data type that is supported, and is only made possible with Django. However, even with Django, unique constraints can not be implemented on such a column. With LatteDB, we make it possible to define a unique constraint, which for this example, prohibits the user from inserting the exact same list of gauge configurations in the ensemble table more than once. Users are encouraged to consult the documentation of EspressoDB and examples in LatteDB for more information.

Additionally, LatteDB is also tremendously useful for managing the data processing steps (step 7) which proceed as:

7. Data processing:
   (a) For each configuration, for each time separation, for each of the 8 sources, time slice the 4D data formfactor files to only the time slices containing relevant data;
   (b) For each configuration, for each time separation, for each source set, average the 8 formfactor_tslised files to a source averaged file;
   (c) When all configurations are complete, concatenate these files together;
   (d) As needed, Fourier Transform these files to project the formfactors onto definite momentum transfers;
   (e) Analyze the correlation functions to extract the relevant physics.

In Figure 1, we show an example LatteDB Table from step 7b. The user is able to filter on each column to very quickly assess the production status (green means the tsliced_source_averaged file exists, red means it is missing) and decide what configurations in what ensembles need to be managed in production.

More importantly, our production scripts interact with LatteDB, therefore even without the visualization, the scripts will only generate work that LatteDB records as missing.
This interaction with LatteDB significantly reduces the amount of human time required to manage the computations. We are actively constructing routines to also store the final data files to tape, the status of which is stored in a related LatteDB table. Thus, the user can query the database instead of the file system for the existence of data files, significantly reducing the load on the file system as well. Examples of interacting with LatteDB can be found in our management repository for these INCITE projects https://github.com/callat-qcd/nucleon_elastic_FF. The scripts for interacting with LatteDB are in the scripts folder and contain lattedb in the name. Other examples can be found in the notebooks folder in LatteDB. These scripts will be updated regularly to encompass more and more utilities from EspressoDB providing a complete working example.

Other features that can be implemented is the storing of the data files in LatteDB as well as storing the analysis of the data files. This allows for communal data analysis within a collaboration with a centralized location for results, making it easier to combine results from different members and reduce redundant work. Depending upon the success and popularity of EspressoDB, it may be worth exploring whether OLCF (or other LCF) would be willing to allow users to host databases locally on the machines such that the compute nodes could interact with the database allowing users to minimize the number of small input files that are typically written to the file system as well. In our case, each separate task requires an input file and typically generates two or three small output files, rapidly polluting the file system with millions of small files. EspressoDB will minimally allow users to clean up these small files and store the relevant log and output information in the database.