

kiwiPy: Robust, high-volume, messaging for big-data and computational science workflows

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Summary

The computational sciences have seen a huge increase in the use of high-throughput, automated, workflows over the course of the last two decades or so. Focusing on just our domain of computational materials science, there have been several large scale initiatives to provide high-quality results from standardised calculations (Curtarolo et al., 2012; Draxl & Scheffler, 2019; Jain et al., 2013; Landis et al., 2012; Saal, Kirklin, Aykol, Meredig, & Wolverton, 2013; Talirz et al., 2020). Almost all of these repositories are populated using results from high-throughput quantum mechanical calculations that rely on workflow frameworks (Jain et al., 2015; Mortensen, Gjerding, & Thygesen, 2020), including our own [AiiDA](#) (Huber et al., 2020; Pizzi, Cepellotti, Sabatini, Marzari, & Kozinsky, 2016) which powers the [Materials Cloud](#). One of the many challenges for such frameworks is maximising fault-tolerance whilst simultaneously maintaining high-throughput, often across several systems (typically the client launching the tasks, the supercomputer carrying out the computations, and the server hosting the database).

On the software level, these problems are perhaps best addressed by using messaging brokers that take responsibility for guaranteeing the durability (or persistence) and atomicity of messages and often enable event-based communication. Indeed, solutions such as [RabbitMQ](#), see widespread adoption in industry. However, adoption in academia has been more limited, with home-made queue data structures, race condition susceptible locks and polling based solutions being commonplace. This is likely due to message brokers typically having complex APIs (which reflect the non-trivial nature of the underlying protocol) as well as the lack of familiarity with event-based programming in general within the community. [KiwiPy](#) was designed specifically to address both these issues, by providing a tool that enables building robust, event-based systems with an interface that is as simple as possible.

In [kiwiPy](#), all messages are saved to disk by [RabbitMQ](#), meaning that any or all systems involved in a workflow, including the broker, can be shut down (abruptly or gracefully), and the previous state can be recreated allowing the workflow to continue when the necessary resources are brought back online. This is especially important for long-running HPC jobs that may take days or weeks. This feature differentiates [kiwiPy](#) from protocols such as [MPI](#), [ZeroMQ](#) or libraries such as [Dask](#), which do not persist their state.

A number of libraries for interacting directly with message brokers exist, including [Pika](#), [aiopika](#), [py-amqp](#), [kombu](#) and others. These tend to be rather low-level and focus on channels, exchanges, routing, sockets and so on. A comparison of the difference in focus between [Pika](#) and [kiwiPy](#) can be found in the [documentation](#). At the other end of the spectrum are libraries such as [Celery](#), [RQ](#) and [others](#) that provide task queues and libraries such as [RPyC](#),

[Spyne](#), [Python-JRPC](#) and [others](#) that enable remote procedure calls. In contrast, kiwiPy brings together three commonly used message types (task queues, Remote Procedure Calls (RPCs), and, broadcasts) in a single interface.

All messaging in kiwiPy is done in the `Communicator` class, which can be trivially constructed by providing a URI string pointing to the RabbitMQ server. By default, kiwiPy creates a separate communication thread that the user never sees, allowing them to interact with the communicator using familiar Python syntax, without the need to be familiar with either coroutines or multithreading. This has the additional advantage that kiwiPy will maintain heartbeats (a periodic check to make sure the connection is still alive) with the server whilst the user code can be doing other things. Heartbeats are an essential part of RabbitMQ's fault tolerance; two missed checks will automatically trigger the message to be requeued to be picked up by another client.

To demonstrate some of the possible usage scenarios, we briefly outline the way kiwiPy is used in AiiDA. AiiDA, amongst other things, manages the execution of complex workflows made up of processes that may have checkpoints.

Task queues

As is common for high-throughput workflow engines, AiiDA maintains a task queue to which processes are submitted (typically from the user's workstation). These tasks are then consumed by multiple daemon processes (which may also be on the user's workstation or remote) and will only be removed from the task queue once they have been acknowledged to be completed by the consumer. The daemon can be gracefully or abruptly shut down and no task will be lost, since the task will simply be requeued by the broker once it notices that the consumer has died. Furthermore, there are no worries about race conditions between multiple daemon processes, since the task queue is guaranteed to only distribute each task to, at most, one consumer at a time.

Remote Procedure Calls

These are used to control live processes. Each process has a unique identifier and can be sent a `pause`, `play`, or `kill` message, the response to which is optionally sent back to the initiator to indicate success or something else.

Broadcasts

These currently serve two purposes: sending `pause`, `play`, or `kill` messages to all processes at once by broadcasting the relevant message, and controlling the flow between processes. If a parent process is waiting for a child to complete, it will be informed of this via a broadcast message from the child saying that its execution has terminated. This enables decoupling, as the child need not know about the existence of the parent.

Together these three message types allow AiiDA to implement a highly-decoupled, distributed, yet, reactive system that has proven to be scalable from individual laptops to workstations, driving simulations on high-performance supercomputers with workflows consisting of varying durations, ranging from milliseconds up to multiple days or weeks.

It is our hope that by lowering the barriers to adoption, kiwiPy will bring the benefits of industry grade message brokers to academia and beyond, ultimately making robust scientific software easier to write and maintain.

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References

- Curtarolo, S., Setyawan, W., Hart, G. L. W., Jahnatek, M., Chepulskii, R. V., Taylor, R. H., Wang, S., et al. (2012). AFLOW: An automatic framework for high-throughput materials discovery. *Computational Materials Science*, 58, 218–226. doi:[10.1016/j.commatsci.2012.02.005](https://doi.org/10.1016/j.commatsci.2012.02.005)
- Draxl, C., & Scheffler, M. (2019). The NOMAD laboratory: from data sharing to artificial intelligence. *Journal of Physics: Materials*, 2(3), 036001. doi:[10.1088/2515-7639/ab13bb](https://doi.org/10.1088/2515-7639/ab13bb)
- Huber, S. P., Zoupanos, S., Uhrin, M., Talirz, L., Kahle, L., Häuselmann, R., Gresch, D., et al. (2020). AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Retrieved from <http://arxiv.org/abs/2003.12476>
- Jain, A., Ong, S. P., Chen, W., Medasani, B., Qu, X., Kocher, M., Brafman, M., et al. (2015). FireWorks: a dynamic workflow system designed for high-throughput applications. *Concurrency and Computation: Practice and Experience*, 27(17), 5037–5059. doi:[10.1002/cpe.3505](https://doi.org/10.1002/cpe.3505)
- Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., et al. (2013). The Materials Project: A materials genome approach to accelerating materials innovation. *APL Materials*, 1(1), 011002. doi:[10.1063/1.4812323](https://doi.org/10.1063/1.4812323)
- Landis, D. D., Hummelshoj, J. S., Nestorov, S., Greeley, J., Dulak, M., Bligaard, T., Norskov, J. K., et al. (2012). The Computational Materials Repository. *Computing in Science & Engineering*, 14(6), 51–57. doi:[10.1109/MCSE.2012.16](https://doi.org/10.1109/MCSE.2012.16)
- Mortensen, J., Gjerding, M., & Thygesen, K. (2020). MyQueue: Task and workflow scheduling system. *Journal of Open Source Software*, 5(45), 1844. doi:[10.21105/joss.01844](https://doi.org/10.21105/joss.01844)
- Pizzi, G., Cepellotti, A., Sabatini, R., Marzari, N., & Kozinsky, B. (2016). AiiDA: automated interactive infrastructure and database for computational science. *Computational Materials Science*, 111, 218–230. doi:[10.1016/j.commatsci.2015.09.013](https://doi.org/10.1016/j.commatsci.2015.09.013)
- Saal, J. E., Kirklin, S., Aykol, M., Meredig, B., & Wolverton, C. (2013). Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). *JOM*, 65(11), 1501–1509. doi:[10.1007/s11837-013-0755-4](https://doi.org/10.1007/s11837-013-0755-4)
- Talirz, L., Kumbhar, S., Passaro, E., Yakutovich, A. V., Granata, V., Gargiulo, F., Borelli, M., et al. (2020). Materials Cloud, a platform for open computational science, 1–22. Retrieved from <http://arxiv.org/abs/2003.12510>