Science needs to rethink how it interacts with big data: Five principles for effective scientific big data systems

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Abstract

We should be in a golden age of scientific discovery, given that we have more data and more compute power available than ever before. But paradoxically, in many data-driven fields, the eureka moments are becoming more and more rare. Scientists, and the software tools they use, are struggling to keep pace with the explosion in the volume and complexity of scientific data. We describe here, five architectural principles we believe are essential in order to create effective, robust, and flexible platforms that make us of the best of emerging technology.

Thousands of climate scientists are eagerly awaiting the data from the sixth iteration of the Climate Model Intercomparison Project, which will be available online imminently¹. The data, at a volume that may exceed 20 Petabytes, represent the most detailed predictions ever made about the future of our planet. Buried among the ones and zeros are answers to urgent societal questions, like which regions should expect more droughts or whether we can expect hurricanes to become more damaging. Yet once the data are released, the waiting is not over. Scientists will keep waiting...waiting for data to download, waiting for analysis scripts to churn through the files, waiting for that eureka moment when a beautiful figure finally appears on their computer screen.

We should be in a golden age of scientific discovery, given that we have more data and more compute power available than ever before. But paradoxically, in many data-driven fields, the eureka moments are becoming more and more rare. Scientists, and the software tools they use, are struggling to keep pace with the explosion in the volume and complexity of scientific data. The “big data
revolution”, which has had a major impact within the private sector, is failing to similarly empower scientific analysis, which is often more varied, iterative, multidimensional, and interactive than enterprise data science. For today’s scientists, the problem goes beyond the obvious inefficiencies of working with inadequate tools. We argue that the inability to freely explore large datasets creates an insidious pressure to look for “safe”, expected results - the antithesis of innovative science.

It’s clear that downloading Petabytes of data is impractical; Big Data platforms therefore tend to provide both the data and a computing framework for analyzing it. Numerous such big-data science gateways have been developed using both open-source and proprietary technologies\(^2,3\), and major progress has been made in processing large scientific data volumes\(^4-9\). However, all-in-one systems can’t hope to anticipate completely what operations scientists will want to perform. And IT departments can’t hope to support an ever-growing suite of tools in one single platform. We need systems which are: powerful, allowing scientists to apply bespoke analyses to very large amounts of data; flexible, accommodating a wide range of different use cases; and cost efficient, only only incurring charges whilst computations are being performed. Such systems are only now becoming possible thanks to a set of emerging technologies, such as cloud computing, container orchestration, automatic parallelism, and thin-client interfaces.

To this end, we created Pangeo (http://pangeo.io/) which tackles these problems by combining tried and tested professional technology design tenets with open source tooling, and an understanding of the needs of scientists. It was inspired by the acute challenges faced by climate scientists, in particular, how to best use the large multidimensional, gridded datasets produced by satellites and climate models. Pangeo is, however, being adopted in varied fields from astronomy to neuroscience to economics. Here we endeavor to spare the technical details of Pangeo, and instead share the principles that we think are important for effective interactions with scientific data and which serve as a strong foundation future scientific research platforms.

**Move data as little as possible**

As our data grows in volume, it becomes harder to move - sometimes referred to as “data inertia”. For instance, pulling data from an archive to a local desktop for analysis is rapidly becoming impractical. Instead we need to move our computations closer to the stored data, that is to dedicated compute which is efficiently coupled to the data store. This design has proved very effective in systems used by enterprise; for example the widely-used data science platform Hadoop\(^10\), which offers a suite of opinionated data processing operations suitable for oft-repeated analyses. However, these systems have only been of limited use for scientific analysis\(^9\), largely due to the nature of scientific data processing, which is typically more highly dimensional, more ad hoc, and more complex. Put another way, science does not need a train, it needs an all terrain vehicle.

For instance, Pangeo makes use of Jupyter Notebooks\(^11\) which have been an
Figure 1: (top) traditional remote data access, where storage is remote and
scientist access data through by downloading/copying the archive. (bottom)
emerging data proximate paradigm, where analysis, computing and data are
collocated.
effective platform for providing a common interface to a broad range of local and remote computing systems. Scientists interact with Jupyter Notebooks in their web browser, which sends commands and queries via the internet to compute resources which are co-located with data. This means scientists’ workstations can now be minimally powerful - a so called “thin-client” approach.

**Separate concerns and specialize late**

It is almost impossible to say what a scientist is going to want to do with their data. Analyses are hand crafted to answer complex questions, and they often need to utilize the latest domain-specific data analysis techniques. Similarly, the technologies that a system comprises are being rapidly developed, with new potentially useful functionality appearing regularly. As such, any scientific data platform should be readily adaptable, both in terms of the tools available to the end user, and the technologies used in the system.

Pangeo achieves this by coupling together a series of unitary components which do one (and only one thing) well - so called “separation of concerns”. For instance, in our system we have a user interface (Jupyter Notebooks), a data model (Xarray), a parallel job distribution system (Dask), a system for managing resources (Kubernetes), and a storage system (object store, e.g. AWS S3). This makes it practically possible to adapt the way individual components work, as long as they still fulfill the same purpose. Importantly, individual components can be readily exchanged.

For this to be truly effective, it is important that domain specific design decisions affect as few components as possible - a principle which we term “specializing late”. For instance, if the data store component needlessly assumes that data will be stored in a geospatial data forms, it prohibits the system from being used later for astrophysics.

These architectural principles of “separation of concerns” and “specializing late” seem to be regularly disregarded. Sometimes, this is simply because of the rush to implement a system “that works”. Often it is in the pursuit of optimization: the temptation is to finely tune a system to do all the things that an end consumer could possibly want to do...only to have a consumer want it to do something else. Because the system has been over-engineered to optimize the performance of the initially conceived of functionality, it is often impossible to extend the system. These kind of finely tuned but brittle systems can prove useful for non-research data analyses, where use cases are relatively predictable and performance is of the utmost importance. However, we maintain that scientific use case is inherently variable and necessitates an adaptable system.

Keeping components of the systems as generic as possible future proofs them, allowing the thin layer of domain specific functionality built on top of them to be adapted to new use cases. For instance, in Pangeo, analysts interact with objects which represent earth science data (Xarray or Iris), and these systems invoke more generic operations in other components. This is why we have been able to easily repurpose Pangeo to work with other kinds of data, such as genomics.
and astronomy observations.

**Scale compute elastically**

Big data analyses are often optimized by dividing them into chunks which are evaluated simultaneously: “parallelization.” In order to perform analyses on interactive timescales, we need a cost-efficient way to run highly parallelized analyses. Institutions often maintain specialized parallel compute clusters, which are shared between multiple users. Analyses are queued to smooth out demand, ensuring compute resources are used efficiently. However, inefficiency is then merely transferred to the scientist, who has to wait for their analysis to run. In contrast, our system is “elastic”, in that it is capable of rapidly scaling its resources in response to demand on the system. Commercial “Cloud computing” providers such as Amazon Web Services (AWS), Microsoft Azure, and Google Cloud Platform (GCP), let customers rent various resources from very large centralized compute facilities. These providers broker these resources between their customers, whose applications include banking, website services, media streaming et cetera.

Sharing such huge resources between so many disparate users allows cloud computing providers to absorb individual consumer’s volatility while still making relatively efficient use of their resources. Resources are priced per unit of time, meaning that it costs the same to use one computer for 1000 minutes as it does to use 1000 computers for one minute. This is fundamentally different than the status quo - scientists can now run analyses faster for no extra cost.

When a user executes an analysis, a Pangeo compute cluster can automatically scale to several thousand compute nodes and distribute the work before relinquishing the compute nodes. The user doesn’t have to explicitly make this happen - they can execute the same high-level geoscience analysis they’re used to, but they get their answer faster. Working this way facilitates a more interactive relationship with data, leading to more creativity and new discoveries.

**Analyze data lazily**

We can also make sure that our system gets answers faster (and cheaper) by doing the minimal amount of analysis possible - so called “lazy evaluation”. Until now, expensive analyses are often performed once before being stored so users can inspect the data. However this approach comes with multiple downsides. It is often cost inefficient, as storage can be more expensive than re-computation, especially in the case of sparsely accessed data. It obscures the provenance of the data. Finally, it is a brittle process, as it is hard to change the nature of the analysis. Instead, we promote maintaining canonical, base-level datasets alongside “lazy” derived datasets, which access and process the canonical dataset on-demand. This was previously impractical as processing times were too long for on-demand data products, however, it becomes a practical proposition with elastic scaling of computing.
For instance, calculating the difference between historical spatially resolved surface temperature and satellite observations is an inexpensive calculation which results in a large data set. Pangeo allows users to subtract these two fields to create a “lazy” data object. This operation produces an object that represents the resultant field, but which encapsulates the latent calculation, executing it only when the data itself is accessed. For instance, if the user then chooses to look at the values over London, only that data is pulled from the data store, and only that calculation is performed.

**Federate data platforms**

Data generators are increasingly obliged to make their data available and useful to third parties, so they can extract domain specific value. For instance, reinsurane companies may want to perform bespoke analysis of climate projection data to design their policies. Currently, data is often made available by providing systems which allow consumers to request a subset of data, which they then download, a step which severely limits comprehensive analysis of large datasets. Consumers increasingly need co-located data analysis platforms in order to get full value from data. However, this leads to a tension: How can the data providers empower third parties to create bespoke analyses, while recuperating costs incurred?

Users can create ad hoc versions of Pangeo by implementing an automated recipe which defines the entire interconnected system - a technique known as Infrastructure as Code (IaC). The same recipe can be automatically deployed with any major cloud computing provider. In addition, it can also be deployed in-house on traditional compute cluster or HPC resources.

This confers an important property: It allows data generators to gracefully reassign the cost of different parts of the data processing pipeline. That is, they could choose to pay for storing data while empowering a third party consumer to create data products on their own cloud computing account, thereby shouldering the associated cost. As such, this gives us the option to shift cost away from the data generator to downstream organizations who should recoup costs from revenue from the derived data products. This is a practical way to disseminate big scientific datasets to businesses who can then harness the latent economic value. It can be particularly useful for datasets funded by public money, which can now add value to the economy, without the taxpayer effectively subsidizing private industry.

**Conclusion**

The principles described here, which frame modern technology architecture concepts in terms of the scientific use case, facilitate the construction of robust data analysis pipelines which are scalable and adaptable. Now that such systems help us cope with the volume of data, we can start to turn our focus towards more effective user/data interfaces and visualizations, as well as more powerful algorithms to extract more information from these datasets. In all, this can move
scientists away from the drudgery of exploring their big data, and back to inte-
tuitive and productive workflows, thereby accelerating scientific progress and
providing answers to our important societal questions.

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