

This website is free and open to all users and there is no login requirement. The code for this webserver, and all third party software used, are available under the open-source Apache 2.0, BSD 3-clause, or similar licenses.

The website is available at <https://lfz.corefacility.ca/superphy/spfy/>. Spfy’s code is provided at <https://github.com/superphy/backend> and documentation at <https://superphy.readthedocs.io/en/latest/>.

Our proposal covers an update to Superphy whiteside2016superphy, an online predictive genomics platform targeting *Escherichia coli*. The update, called Spfy, uses graph data structures to store and retrieve results for computational workflows. We demonstrate the ability of graph data structures to manage the 60,000 whole-genome sequences of *E. coli* accumulated so far, and show the ability to scale to X genomes. Current comparative computational workflows chain different analysis software, but lack storage and retrieval methods for generated results. By making the storage and retrieval of results part of the platform, with data effectively linked to the organisms of interest through a standardized ontology, we can mitigate the recomputing of analyses. Within Spfy, we store the output from all analyses, and link them together in the context of a genome graph. This graph also stores metadata for each genome, facilitating inquiries ranging from population genomics to epidemiological investigations. Integrated data storage will be necessary as whole genome sequencing data for bacterial pathogens have accumulated in public databases in the tens of thousands, with hundreds of thousands set to be available within the next few years.

Spfy was tested with 59,5323 public *E. coli* assembled genomes, 5,353 genomes from GenBank and 54,181 genomes are the GenBank genomes not included in the Enterobase set? from Enterobase (596 GB), storing every sequence and results for all included analysis modules. Spfy provides real-time subtyping, and the results are immediately displayed to the user following their completion. Subtyping options include O-antigen, H-antigen, Shiga-toxin 1 (Stx1), Shiga-toxin 2 (Stx2), and Intimin typing. Reference-lab tests include virulence factor and anti-microbial resistance annotation. All genomes are analyzed within the pan-genome framework of *E. coli*, and results from all analyses are automatically associated with the source genome. The resulting database had XYZ million nodes and XYZ million edges, with XYZ object properties, which worked out to X TB of data stored.

Existing scientific workflow technologies such as Galaxy [1], and pipelines such as the Bacterium Analysis Pipeline (BAP) [2] and the Integrated Rapid Infectious Disease Analysis (IRIDA) platform <http://www.irida.ca/> help automate the use of WGS data for public-health surveillance. Like IRIDA and BAP, Spfy automates workflows for users, and like Galaxy, Spfy uses task queues to distribute selected analysis. File uploads begin through the ReactJS-based website, where user-defined analyses options are selected. To these concepts, we add the use of Docker containerization for task queue workers, thus allowing analysis software to safely run in parallel. For result storage, existing workflow technologies use

relational tables [1], or store resulting files to disk [2]. Because output from these programs is user-specific or transitory, results from identical comparisons are often recomputed. Additionally, output from different analyses are structured using distinct terminology and formats, which must be converted before they can be compared. Without a unified structure, these conversions quickly become impractical for broad usage. Graph-based storage of all results solves these problems. To avoid proliferating ontologies, and to allow Spfy to integrate with existing ones, annotations from the GenEpiO griffiths2017context, FALDO bolleman2016faldo, and TypOn vaz2014typon ontologies are used to describe biological data. The entire platform is packaged using Docker-Compose, and can be recreated with a simple command.

Superphy has been up since early 2016 and the Spfy update has been up since May 2017. The server accepts assembled *E. coli* genomes with the *.fasta* or *.fna* extensions. Submissions are checked against a reference set of *E. coli* gene sequences before running analyses. Outputs are displayed on the website in tables and can be downloaded as *.csv* files.

Keywords: Bioinformatics, Graph database, Real-time analysis