Developing a Genome Annotation Workflow Within Galaxy

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ABSTRACT

Current DNA sequencing technologies enable routine generation of microbial genomes. While automated annotation tools exist, they are subject to regular improvement, and the effort required to install, update, and execute these tools in a systematic way poses a barrier for many researchers. To facilitate rigorous and reproducible annotation, we demonstrate a Galaxy-driven genome annotation workflow. In the process, we documented proposed IT best practices for sustainable tool and workflow development within Galaxy.

BACKGROUND

Routine generation of microbial genomes using next generation sequencing technologies places high demand on bioinformatics for whole-genome annotation. The emergence of annotation tools and automated pipelines coupled with their continual improvement and availability of new data makes rigorous annotation and re-annotation useful for genome analysis. However, the effort required to install and update these tools in a systematic way poses a barrier for many researchers, particularly while complying with information management and reproducibility standards and best practices. We aim to facilitate these efforts by leveraging Galaxy, an open web-based workflow platform, and developing workflows that tie in several existing annotation pipelines and tools.1,2

METHODOLOGY

We begin by enabling genome annotation software in Galaxy that is not currently available to the galaxy community. This involves developing the web-based user interface (wrappers) and creating tool-dependency packages to build and install the software. The tools are tied together into a galaxy-driven genome annotation workflow that: 1) heuristically and empirically annotates genes with Maker3, 2) identifies gene clusters with AntiSMASH 2,3, 3) identifies gene function using InterProScan 5, 4) locates microsatellites with MISA, 5) detects SNPs via Mauve6, and 6) designs flanking primers by leveraging Primer37 (Figure 1B). Our Galaxy-tailored systems development life cycle facilitates development efforts while ensuring a stable production environment through several checkpoints, as shown in Figure 1A.

IMPACT & DISCUSSION

The workflow leverages Galaxy’s ability to install and systematically execute annotation software on whole genomes, thereby ensuring minimal effort rigorous genome annotations. Furthermore, Galaxy permits simple updates, amendments, and drop-in replacement of tools in the workflow as required. The ability to make multiple tool versions available concurrently ensures annotation reproducibility by allowing the utilization of historical workflow and tool versions. In addition, we promote the Generic Feature Format (GFF) version 3 as the unified annotation file type, through developing format conversion tools, to simplify importing genomes and annotations into a genome browser for manual curation and publication. By combining the Tool Shed and SCM repositories during development, the developer easily pushes modifications to the Tool Shed for testing and utilize the SCM to revert or commit changes quickly and as needed. This results in the developer consistently testing the installation of the repository into Galaxy from the Tool Shed, which can be automated using the Galaxy API.

CONCLUSION & FUTURE WORK

The developed workflow permits rigorous genome annotations with minimal effort reproducibility within Galaxy. The outlined development flow promotes rapid tool development while maintaining best practices. We present these to the Galaxy community for discussion. The source code is available via GitHub (http://github.com/AAFC-MBB) and the workflow and wrappers will be made available to the community shortly.

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REFERENCES