nf-core/proteinfold

A bioinformatics best-practice pipeline for protein 3D structure prediction

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Motivation

The advances in deep learning frameworks have revolutionised protein studies and contributed to unprecedented accurate predictions of protein structures. The release of AlphaFold2 has materialised this major breakthrough. AlphaFold2 has also paved the way towards the development of a new generation of publicly available prediction tools whose combination constitutes a powerful toolkit for the systematic study of unknown proteomes. Despite their obvious usefulness, the large-scale deployment of these new methods across the research community remains hampered by technical hurdles mainly due to the dependency onto a wealth of external software and sequence databases.

Overview

Here we present nf-core/proteinfold, a Nextflow pipeline developed according to nf-core guidelines that enables the prediction of 3D conformations from amino acid sequences using state of the art techniques in protein structure modelling.

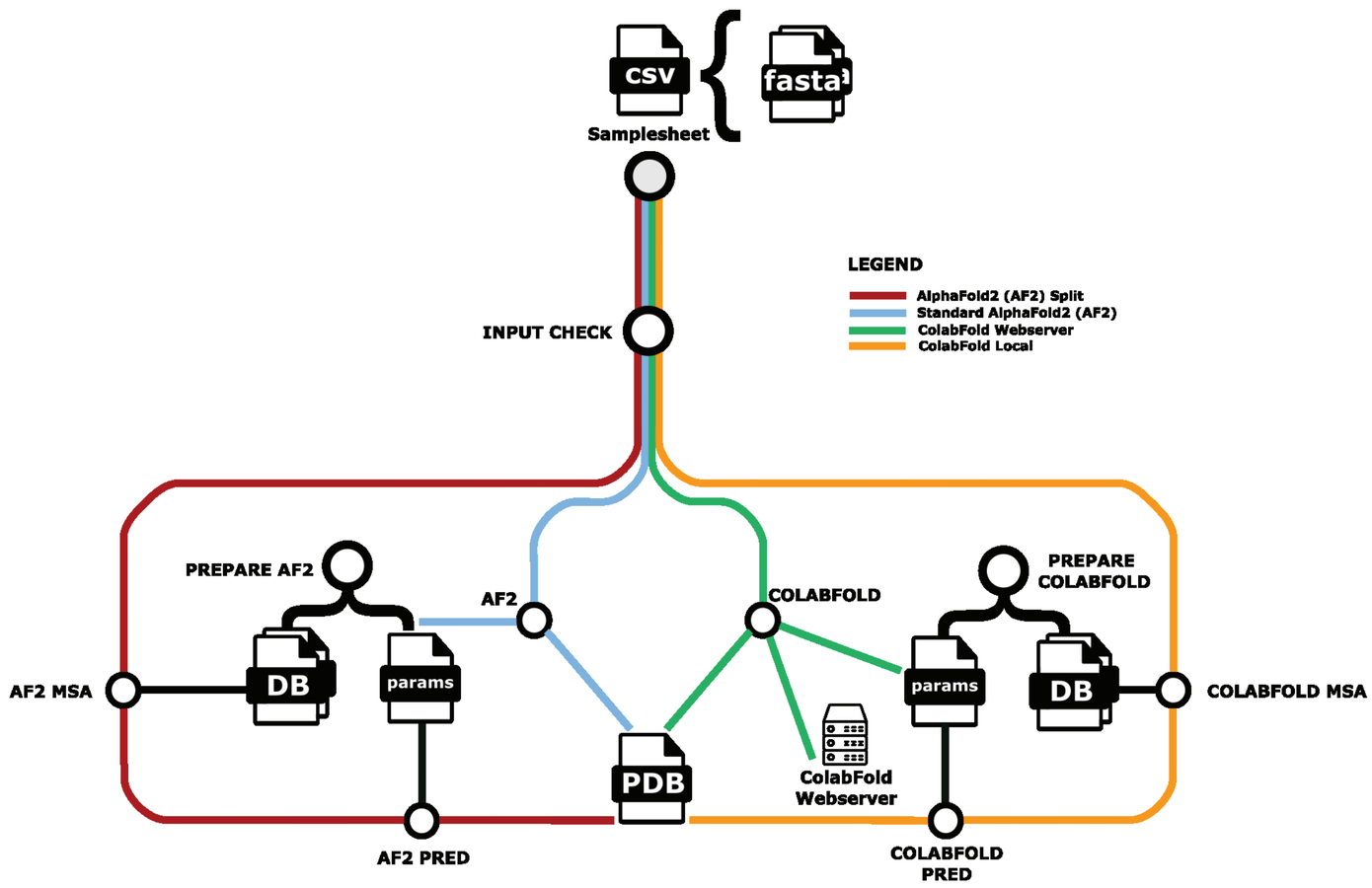
Workflow schematics and characteristics

Reproducibility

docker

Parallelisation

nextflow



Scalability and portability

slurm workload manager
GRID ENGINE
aws

Future plans

Create the first release of the pipeline

Add more open-source protein structure prediction tools such as OpenFold

Incorporate more advanced software for protein-protein interactions

Features

Open-source

Community developed

Extensive documentation

Contribute

nf-co.re/join

nf-core/proteinfold

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