Advanced Docker Course

Use Case: Comparing Aligners

We want to compare some short-read aligners (all of them are available via conda):

- BWA
- Bowtie2

We want to run those programs, and to store the results outside the container for a later analysis.

The data are stored here

Using the aligners

BWA

- bwa index lambda_virus.fa.gz to build the index
- bwa aln lambda_virus.fa.gz reads_1.fq.gz -f reads_1.fq.gz.sai
 to build the sai file

bwa samse lambda_virus.fa.gz reads_1.fq.gz.sai reads_1.fq.gz -f resul
to compute the alignments

Bowtie2

- the index is already built
- bowtie2 -x index/lambda_virus -U reads_1.fq.gz to compute the alignments

Use Case: Images for pipelines

Base

```
FROM ubuntu:18.04
LABEL author="Raoul Jean Pierre Bonnal"
LABEL maintainer="bonnal@ingm.org"
ENV TINI VERSION="v0.18.0"
ENV MINICONDA_VERSION="3-4.5.4"
ENV LANG=C.UTF-8 LC ALL=C.UTF-8
ENV PATH=/opt/conda/bin:$PATH
ENV DEBIAN_FRONTEND=noninteractive
RUN apt-get update -- fix-missing && \
    apt-get install -y \
            apt-utils \
            bzip2 \
            build-essential \
        ca-certificates \
        curl \
        qit \
        wget \
        procps \
        uuid-runtime
WORKDIR /opt
RUN wget --quiet https://repo.anaconda.com/miniconda/Miniconda${MINICONDA_VERSION}-Linux-x86_64.sh -0 miniconda.
    chmod ugo+x miniconda sh
```

Use Case: Images for pipelines

Base

```
FROM bionic-ingm-base:0.1
# How to build
# docker build -t inam-elixir:0.1 .
# docker tag ingm-elixir:0.1 localhost:5000/ingm-elixir:0.1
# docker push localhost:5000/ingm-elixir:0.1
LABEL software.iread="https://www.biorxiv.org/content/early/2017/10/04/135624www.libpls.net/iread"
ENV DEBIAN FRONTEND=noninteractive
#RUN apt-qet update && install apt-qet -y liblapack3 libboost1.62-dev gawk
RUN apt-get update && apt-get install -y piqz unzip libparallel-forkmanager-perl
# libparallel-forkmanager-perl required by iREAD 0.8.0
# argparse is requierd by iREAD 0.8.0
WORKDIR /opt
RUN conda create -n elixir python=2.7 &&\
    /bin/bash -c "source activate organoids && \
                  conda install -c bioconda \
                      samtools=1.8 \
                      bedops=2.4.35 \
                      argparse=1.4.0 \
                      fastoc=0 11 7 \
```