Advanced Docker Course

Use Case: Comparing Aligners

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

- BWA
- Bowtie2
- Gmap
- STAR

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

Using the aligners

Gmap
- `bwa index data/lambda_virus.fa.gz` to build the index
- `bwa mem data/lambda_virus.fa.gz data/reads_1.fq.gz` to compute the alignments

STAR
- the index is already built
- `bowtie2 -x data/index/lambda_virus -U data/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 \
        git \
        wget \
        procps \
        uuid-runtime

WORKDIR /opt

RUN wget --quiet https://repo.anaconda.com/miniconda/Miniconda${MINICONDA_VERSION}-Linux-x86_64.sh -O miniconda.s
    chmod ugo+x miniconda.sh
```

Use Case: Images for pipelines

Base

```
FROM   bionic-ingm-base:0.1

#
# How to build
# docker build -t ingm-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-get update && install apt-get -y liblapack3 libboost1.62-dev gawk
RUN apt-get update && apt-get install -y pigz 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 \
                       fastqc=0.11.7 \
```