Multi-Stage Builds

Reference to the documentation

One might want to install software that requires external libraries that are not available with the distribution or to recompile existing with different options. Usually, this will require installing common building tools and compilers that are not needed for running the executables...

Similar to Docker multi-stage builds, Singularity also offers a multi-stage builds that allows for copying files between stages (Singularity can copy only from previous to current stage). Below is an example definition file that compiles the ARPIP (Ancestral sequence Reconstruction under the Poisson Indel Process) tool. The recipe is following the local installation for the static binary build.

```
Bootstrap: docker
 2 From: ubuntu:20.04
3 Stage: devel
 4
 5 %post
 6
     export LC_ALL=C
     export DEBIAN_FRONTEND=noninteractive
 7
 8
9
      # Package cache in /tmp
10
      mkdir -p /tmp/apt20 && echo "Dir::Cache "/tmp/apt20";" >
11
    /etc/apt/apt.conf.d/singularity-cache.conf
12
13
      apt-get update && apt-get -y dist-upgrade && \
14
      apt-get install -y wget git cmake build-essential zlib1g-dev
15
16
      # Download
17
      export TMPD=/tmp/downloads && mkdir -p $TMPD
      mkdir -p /installs
18
19
20
      # bpp-core http://biopp.univ-montp2.fr/
21
      cd /installs
22
      git clone https://github.com/BioPP/bpp-core
23
      cd bpp-core
24
      git checkout tags/v2.4.1 -b v241
25
      mkdir build
      cd build
26
27
      cmake ..
28
      make -j 16 install
29
30
      # bpp-seq http://biopp.univ-montp2.fr/
```

```
31
     cd /installs
32
       git clone https://github.com/BioPP/bpp-seq
33
      cd bpp-seq
       git checkout tags/v2.4.1 -b v241
34
35
      mkdir build
      cd build
36
      cmake ..
37
38
      make -j 16 install
39
40
       # bpp-phyl http://biopp.univ-montp2.fr/
      cd /installs
41
       git clone https://github.com/BioPP/bpp-phyl
42
43
      cd bpp-phyl
44
      git checkout tags/v2.4.1 -b v241
45
      mkdir build
      cd build
46
47
      cmake ..
48
      make -j 16 install
49
50
      # boost - C++ Libraries http://www.boost.org/
51
      cd /installs
       wget -P $TMPD -c
52
    https://boostorg.jfrog.io/artifactory/main/release/1.79.0/source/bo
53
54
    ost_1_79_0.tar.gz
55
      tar xvf $TMPD/boost_1_79_0.tar.gz
56
      cd boost_1_79_0
57
      ./bootstrap.sh --prefix=/usr/
58
       ./b2
       ./b2 install
59
60
61
       # glog - Google Logging Library https://github.com/google/glog/
62
       cd /installs
       git clone -b v0.5.0 https://github.com/google/glog
63
64
      cd glog
      cmake -H. -Bbuild -G "Unix Makefiles"
65
       cmake --build build --target install
66
67
68
      # gtest - Google Test Library
69
    https://github.com/google/googletest/
70
      cd /installs
71
       git clone https://github.com/google/googletest.git -b release-
72
   1.11.0
73
      cd googletest
      mkdir build
74
75
      cd build
76
      cmake ..
      make -j 4 install
77
78
79
      # ARPIP
80
      cd /opt
81
       git clone https://github.com/acg-team/bpp-arpip/
82
       cd bpp-arpip
83
       cmake --target ARPIP -- -DCMAKE_BUILD_TYPE=Release-static
84
    CMakeLists.txt
```

```
85
       make - j 8
86
87
       clean
       cd / && rm -rf /installs
88
89
     90
91
92
     Bootstrap: docker
     From: ubuntu:20.04
93
     Stage: final
94
95
     %files from devel
96
97
     /opt/bpp-arpip
                                         /opt/
98
      /usr/local/lib/libbpp-core.so.4
                                        /usr/local/lib/libbpp-
99
    core.so.4
     /usr/local/lib/libbpp-seq.so.12
                                        /usr/local/lib/libbpp-
100
101
     seq.so.12
      /usr/local/lib/libbpp-phyl.so.12
102
                                       /usr/local/lib/libbpp-
103
     phyl.so.12
104
      /usr/local/lib/libglog.so.0
                                        /usr/local/lib/libglog.so.0
105
106
     %environment
107
     export LC_ALL=C
108
      export PYTHONNOUSERSITE=True
109
     %post
110
111
     export LC_ALL=C
112
      export PYTHONNOUSERSITE=True
113
       export DEBIAN_FRONTEND=noninteractive
       # Package cache in /tmp
       mkdir -p /tmp/apt20 && echo "Dir::Cache "/tmp/apt20";" >
     /etc/apt/apt.conf.d/singularity-cache.conf
       apt-get update && apt-get -y dist-upgrade && \
       apt-get install -y wget git libc6 libstdc++6 libgcc-s1
     %runscript
       /opt/bpp-arpip/ARPIP "$@"
```

Stage: devel lines 1-82 are compiling all the required libraries and tools to compile the ARPIP code. This stage can be used in a container that will run perfectly fine and with a bit more luck, if the final executable was fully static, one can even try to copy the file outside the container and run it as it is. Unfortunately, extracting the executable on Rackham shows these disappointing results.

Under Ubuntu 20.04 GLIBC... problems are resolved but libbpp-core.so.4, libbpp-seg.so.12, libbpp-seg.so.12, and libglog.so.0 we just compiled remain missing.

```
ldd ARPIP
./ARPIP: /lib64/libm.so.6: version `GLIBC_2.29' not found (required by
```

```
./ARPIP)
./ARPIP: /lib64/libstdc++.so.6: version `GLIBCXX_3.4.26' not found
(required by ./ARPIP)
./ARPIP: /lib64/libstdc++.so.6: version `CXXABI_1.3.9' not found
(required by ./ARPIP)
./ARPIP: /lib64/libstdc++.so.6: version `GLIBCXX_3.4.20' not found
(required by ./ARPIP)
./ARPIP: /lib64/libstdc++.so.6: version `GLIBCXX_3.4.21' not found
(required by ./ARPIP)
       linux-vdso.so.1 => (0x00007ffe9257f000)
       libbpp-core.so.4 => not found
       libbpp-seq.so.12 => not found
       libbpp-phyl.so.12 => not found
       libglog.so.0 => not found
        libpthread.so.0 => /lib64/libpthread.so.0 (0x00002b529980d000)
       libstdc++.so.6 => /lib64/libstdc++.so.6 (0x00002b5299a29000)
       libm.so.6 \Rightarrow /lib64/libm.so.6 (0x00002b5299d31000)
       libgcc_s.so.1 => /lib64/libgcc_s.so.1 (0x00002b529a033000)
       libc.so.6 => /lib64/libc.so.6 (0x00002b529a249000)
        /lib64/ld-linux-x86-64.so.2 (0x00002b52995e9000)
```

And that is what we are doing in Stage: final - we copy the compiled libraries from Stage: devel in to a minimum Ubuntu 20.04 (could be other flavor as well) (lines: 90-95). In this case we avoid "stuffing" the container with unnecessary packages needed for compiling - cmake build-essential zlib1g-dev. There are no shortcuts - one needs to check you have everything you need in the new container - in this case apt-get install -y libc6 libstdc++6 libgcc-s1 which will make sure we have the remaining libraries in /lib64/....