MAKING CONTAINERS EASIER WITH HPC CONTAINER MAKER (HPCCM)

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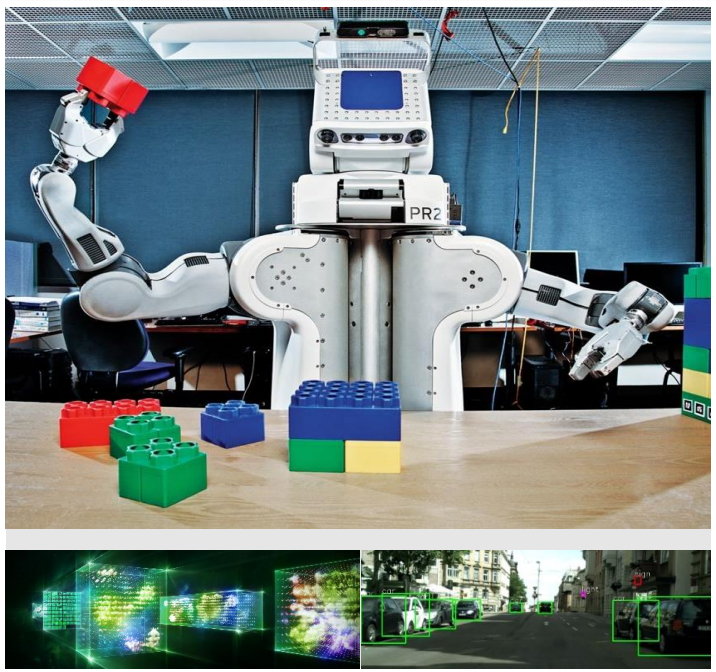
NVIDIA
“THE AI COMPUTING COMPANY”

GPU Computing

Computer Graphics

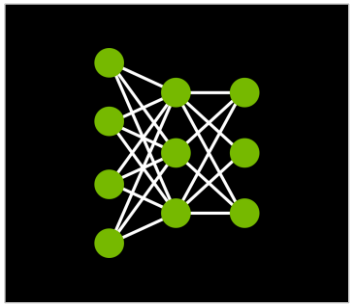


Artificial Intelligence

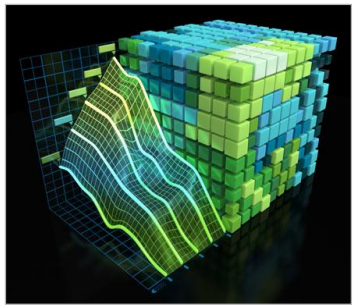
DEEP LEARNING INSTITUTE

Fundamentals and advanced hands-on training in key technologies and application domains

Caffe2 · Microsoft Cognitive Toolkit · mxnet · TensorFlow · PYTORCH · Keras · theano



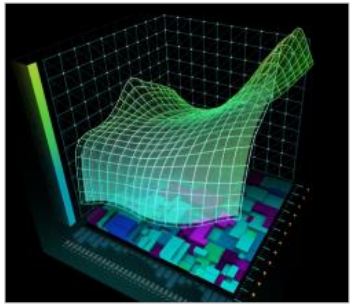
Deep Learning Fundamentals



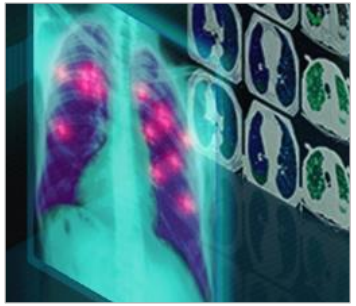
Accelerated Computing Fundamentals

AI for Autonomous Vehicles

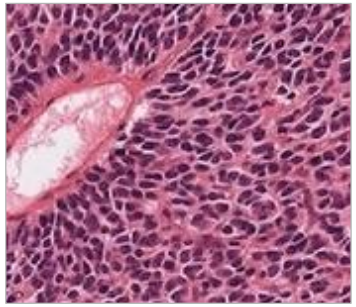
AI for Digital Content Creation and Game Development



AI for Finance



AI for Healthcare Image Analysis



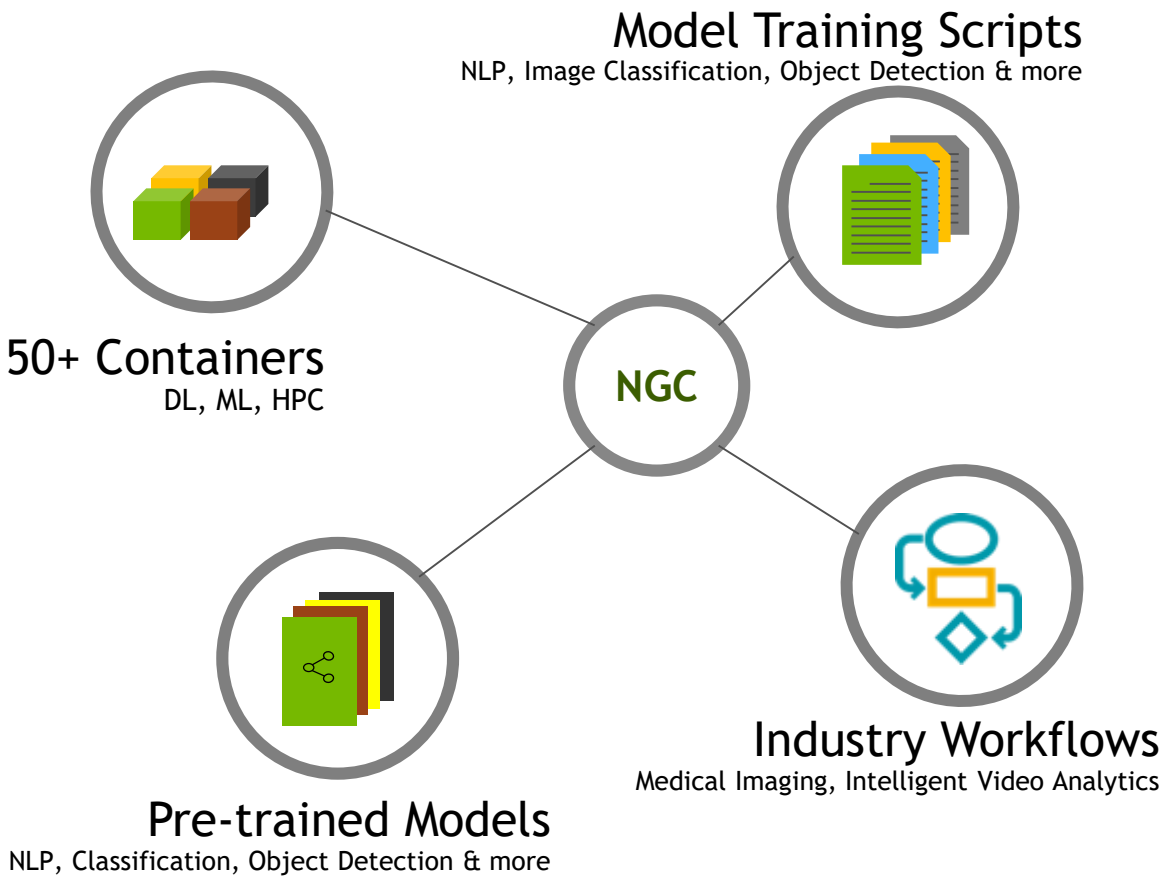
AI for Healthcare Image Analysis

AI for Intelligent Video Analytics

AI for Robotics

NVIDIA GPU CLOUD (NGC)

GPU-optimized Software Hub. Simplifying DL, ML and HPC Workflows



Simplify Deployments

Innovate Faster

Deploy Anywhere

WHAT IF A CONTAINER IMAGE IS NOT AVAILABLE FROM NGC?

BARE METAL VS. CONTAINER WORKFLOWS

Login to system (e.g., CentOS 7 with Mellanox OFED 3.4)

$ module load PrgEnv/GCC+OpenMPI

$ module load cuda/9.0

$ module load gcc

$ module load openmpi/1.10.7

Steps to build application

Result: application binary suitable for that particular bare metal system

```
FROM nvidia/cuda:9.0-devel-centos7
```

OPENMPI DOCKERFILE VARIANTS

Real examples – which one should you use?

A

```
RUN apt-get update \
  && apt-get install -y --no-install-recommends \
    libopenmpi-dev \
    openmpi-bin \
    openmpi-common \
  && rm -rf /var/lib/apt/lists/*
ENV LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/lib/openmpi/lib
```

B

```
RUN OPENMPI_VERSION=3.0.0 && \
    wget -q -O - https://www.open-
mpi.org/software/ompi/v3.0/downloads/openmpi-
${OPENMPI_VERSION}.tar.gz | tar -xzf - && \
    cd openmpi-${OPENMPI_VERSION} && \
    ./configure --enable-orterun-prefix-by-default --with-cuda --
with-verbs \
                --prefix=/usr/local/mpi --disable-getpwuid && \
    make -j"$(nproc)" install && \
    cd .. && rm -rf openmpi-${OPENMPI_VERSION} && \
    echo "/usr/local/mpi/lib" >> /etc/ld.so.conf.d/openmpi.conf &&
ldconfig
ENV PATH /usr/local/mpi/bin:$PATH
```

C

```
COPY openmpi /usr/local/openmpi
WORKDIR /usr/local/openmpi
RUN /bin/bash -c "source /opt/pgi/LICENSE.txt && CC=pgcc CXX=pgc++
F77=pgf77 FC=pgf90 ./configure --with-cuda --
prefix=/usr/local/openmpi”
RUN /bin/bash -c "source /opt/pgi/LICENSE.txt && make all install"
```

D

```
RUN mkdir /logs
RUN wget -nv https://www.open-
mpi.org/software/ompi/v1.10/downloads/openmpi-1.10.7.tar.gz && \
    tar -xzf openmpi-1.10.7.tar.gz && \
    cd openmpi-*&& ./configure --with-cuda=/usr/local/cuda \
    --enable-mpi-cxx --prefix=/usr 2>&1 | tee /logs/openmpi_config
&& \
    make -j 32 2>&1 | tee /logs/openmpi_make && make install 2>&1
| tee /logs/openmpi_install && cd /tmp \
    && rm -rf openmpi-*
```

E

```
WORKDIR /tmp
ADD http://www.open-
mpi.org//software/ompi/v1.10/downloads/openmpi-1.10.7.tar.gz /tmp
RUN tar -xzf openmpi-1.10.7.tar.gz && \
    cd openmpi-*&& ./configure --with-cuda=/usr/local/cuda \
    --enable-mpi-cxx --prefix=/usr && \
    make -j 32 && make install && cd /tmp \
    && rm -rf openmpi-*
```

F

```
RUN wget -q -O - https://www.open-
mpi.org/software/ompi/v3.0/downloads/openmpi-3.0.0.tar.bz2 | tar -
xjf - && \
    cd openmpi-3.0.0 && \
    CXX=pgc++ CC=pgcc FC=pgfortran F77=pgfortran ./configure --
prefix=/usr/local/openmpi --with-cuda=/usr/local/cuda --with-verbs
--disable-getpwuid && \
    make -j4 install && \
    rm -rf /openmpi-3.0.0
```

HPC CONTAINER MAKER

- Tool for creating HPC application Dockerfiles and Singularity definition files
- Makes it easier to create HPC application containers by encapsulating HPC & container best practices into building blocks
- Experimental support for ARM and Power containers
- Open source (Apache 2.0)
  https://github.com/NVIDIA/hpc-container-maker
- `pip install hpccm`

BUILDING BLOCKS TO CONTAINER RECIPES

```
Stage0 += openmpi()
```

hpccm  Generate corresponding Dockerfile instructions for the HPCCM building block

```
# OpenMPI version 3.1.2
RUN yum install -y \
        bzip2 file hwloc make numactl-devel openssh-clients perl tar wget && \
    rm -rf /var/cache/yum/*
RUN mkdir -p /var/tmp && wget -q -nc --no-check-certificate -P /var/tmp https://www.open-
mpi.org/software/ompi/v3.1/downloads/openmpi-3.1.2.tar.bz2 && \
    mkdir -p /var/tmp && tar -x -f /var/tmp/openmpi-3.1.2.tar.bz2 -C /var/tmp -j && \
    cd /var/tmp/openmpi-3.1.2 &&  CC=gcc CXX=g++ F77=gfortran F90=gfortran FC=gfortran ./configure --
prefix=/usr/local/openmpi --disable-getpwuid --enable-orterun-prefix-by-default --with-cuda=/usr/local/cuda --with-verbs
&& \
    make -j4 && \
    make -j4 install && \
    rm -rf /var/tmp/openmpi-3.1.2.tar.bz2 /var/tmp/openmpi-3.1.2
ENV LD_LIBRARY_PATH=/usr/local/openmpi/lib:$LD_LIBRARY_PATH \
    PATH=/usr/local/openmpi/bin:$PATH
```

HIGHER LEVEL ABSTRACTION

Building blocks to encapsulate best practices, avoid duplication, separation of concerns

```
openmpi(check=False,                                    # run “make check”?
        configure_opts=['--disable-getpwuid', …],       # configure command line options
        cuda=True,                                      # enable CUDA?
        directory='',                                   # path to source in build context
        infiniband=True,                                # enable InfiniBand?
        ospackages=['bzip2', 'file', 'hwloc', …],       # Linux distribution prerequisites
        prefix='/usr/local/openmpi',                    # install location
        toolchain=toolchain(),                          # compiler to use
        ucx=False,                                      # enable UCX?
        version='3.1.2')                                # version to download
```

Examples:

```
openmpi(prefix='/opt/openmpi', version='1.10.7’)
openmpi(infiniband=False, toolchain=pgi.toolchain)
```

Full building block documentation can be found on GitHub

EQUIVALENT HPCCM WORKFLOW

python

Login to system (e.g., CentOS 7 with Mellanox OFED 3.4)

```
$ module load PrgEnv/GCC+OpenMPI

$ module load cuda/9.0

$ module load gcc

$ module load openmpi/1.10.7
```

Steps to build application

Result: application binary suitable for that particular bare metal system

```
Stage0 += baseimage(image='nvidia/cuda:9.0-devel-centos7')
Stage0 += mlnx_ofed(version='3.4-1.0.0.0')

Stage0 += gnu()

Stage0 += openmpi(version='1.10.7')
```

Steps to build application

Result: portable application container capable of running on any system

DEMO

SUMMARY

- HPC Container Maker simplifies creating a container specification file
  - Best practices used by default
  - Building blocks included for many popular HPC components
  - Flexibility and power of Python
  - Supports Docker (and other frameworks that use Dockerfiles) and Singularity
  - Experimental support for ARM and Power containers
- DLI Course : High Performance Computing with Containers ($30)
- Open source: https://github.com/NVIDIA/hpc-container-maker
- `pip install hpccm`


Merci!
NVIDIA