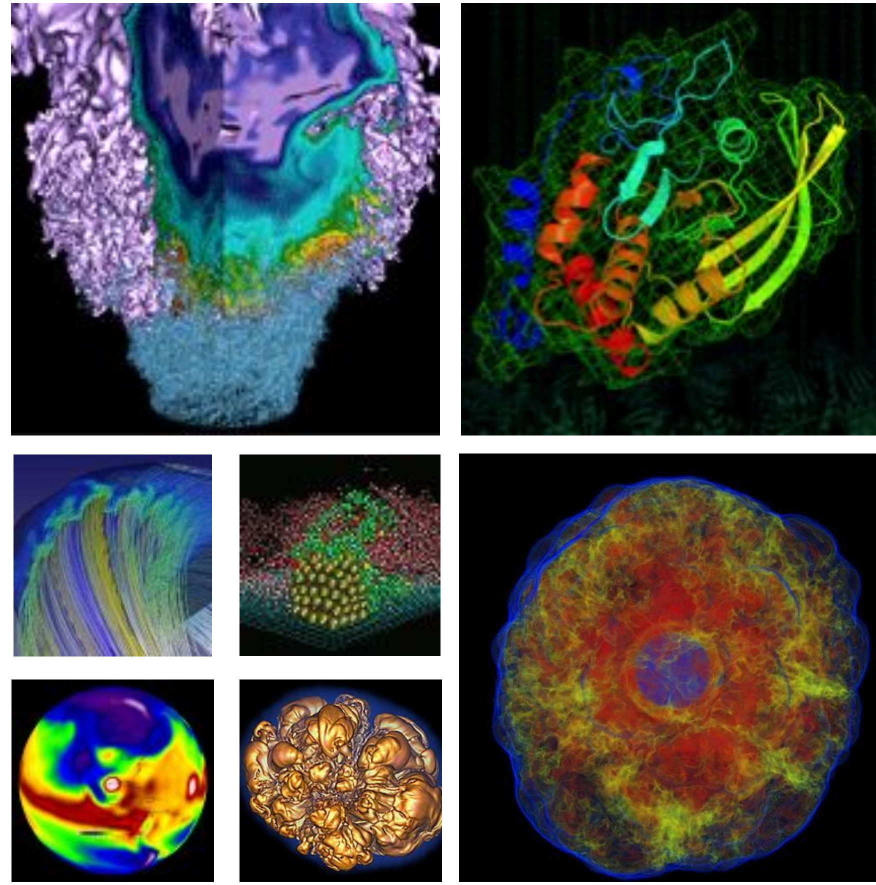
Overview of Deep Learning Stack



Wahid Bhimji, Prabhat,
Mustafa Mustafa, Steve Farrell

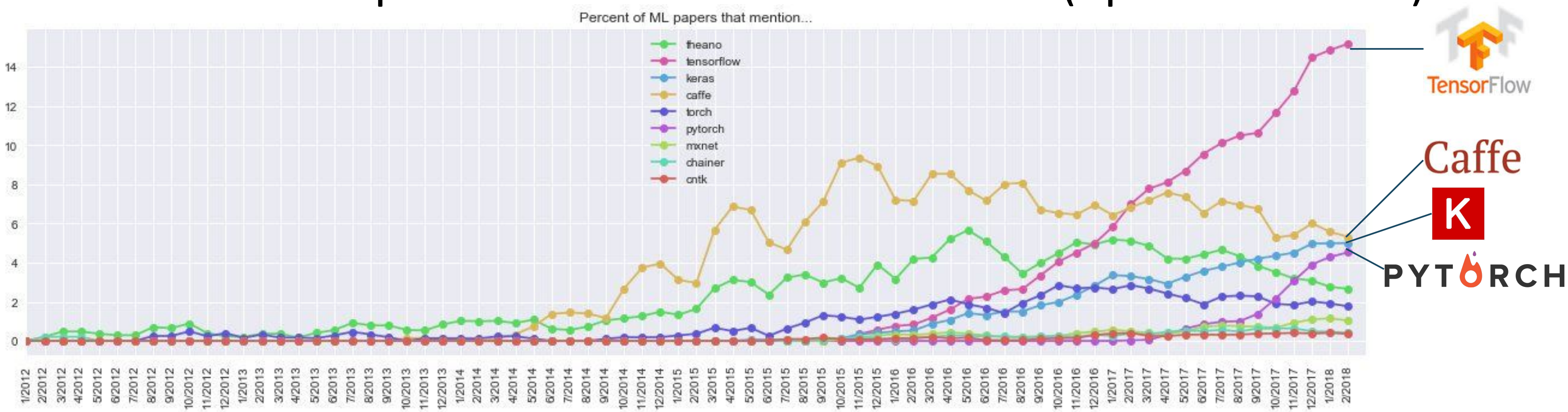
New User Training
June 21 2019

Deep Learning Stack on HPC

	Technologies
Deep Learning Frameworks	K, TensorFlow, PYTORCH, Caffe, Neon, CNTK, MXNet, …
Multi Node libraries	Cray ML PE Plugin, Horovod, MLSL, MPI, GRPC
Single Node libraries	MKL-DNN, CuDNN
Hardware	CPUs (KNL), GPUs, FPGAs, Accelerators

Software Frameworks

- Different frameworks popularity has evolved rapidly
- % of ML Papers that mention a framework (up to Mar 2018)



Source: https://twitter.com/karpathy/status/972295865187512320?lang=en

- Caffe and Theano most popular 3-4 years ago
- Then Google released TensorFlow which now dominates
- PyTorch is recently rising rapidly in popularity
- See also DL power scores (also rates Tensorflow top):
  https://towardsdatascience.com/deep-learning-framework-power-scores-2018-23607ddf297a

Subjective evaluation

- **TensorFlow:**
  - Reasonably easy to use directly within python (not as easy as with Keras)
  - Very nice tools for development like TensorBoard
  - Active development for features (e.g. dynamic graphs) and performance (e.g. for CPU/KNL) and ease of use

- **Keras:**
  - High-level framework sits on top of tensorflow (or theano) (and now part of TensorFlow)
  - Very easy to create standard and even advanced deep networks with a lot of templates/ examples

Subjective evaluation

- **PyTorch** PYTORCH
  - Relatively recent python adaption of ‘torch’ framework - heavily contributed to by Facebook
  - More pythonic than Tensorflow/Keras
  - Dynamic graphs from the start - very flexible
    - Popular with some ML researchers
  - Previously some undocumented quirks but Version 1.0 release added stability and performance
- **Caffe** Caffe
  - Optimised performance (still best for certain NN on CPUs)
  - Relatively difficult to develop new architectures
  - Caffe2 and PyTorch projects merged

Tensorflow and Keras @NERSC

- **Easiest is to use default anaconda python:**

```
module load python
python
>>> import tensorflow as tf
```

- **Active work by Intel to optimize for CPU:**
  - Available in anaconda. Modules on Cori:

```
module avail tensorflow  #Display versions
module load tensorflow
```

  - Loads the default (**intel-1.13.1-py36** as of Jun 2019)
- **Can also tune variables for performance (e.g. see intel blog)**
  - E.g Inter-op and Intra-op

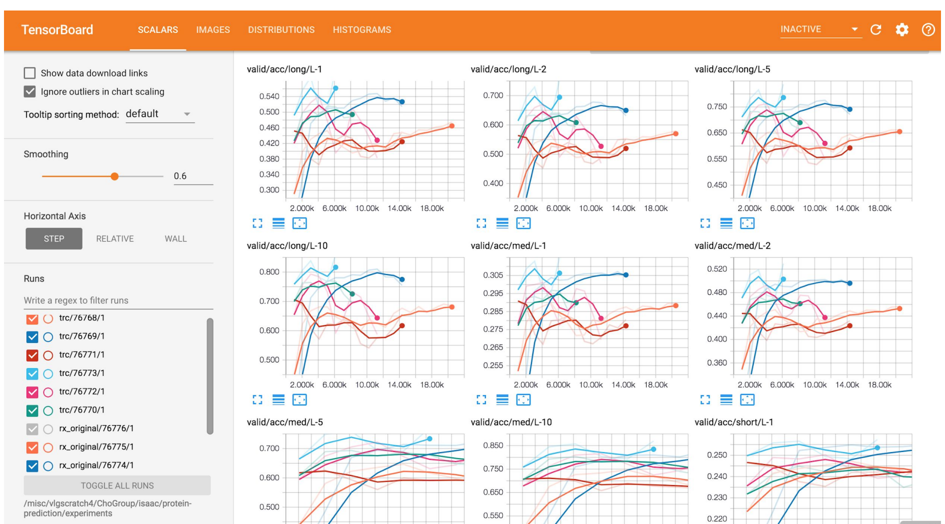
TensorBoard

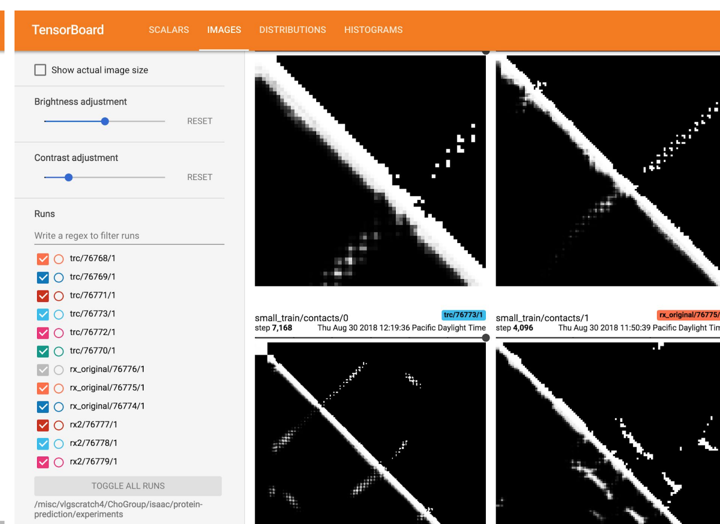
- **Easy, customisable, visualization of training in progress**
- **At NERSC run TensorBoard on login node; point to logs made by jobs on compute node (chose an unused port)**

```
cori05 > tensorboard --logdir=path/to/logs --port 9998
```

- **Use a ssh tunnel from your laptop to connect then open localhost:9998 in your browser (note: others will also be able to see your experiments if they connect to that port)**

```
YourLaptop > ssh -L 9998:localhost:9998 cori.nersc.gov
```





Figures: Isaac Henrion

PyTorch @NERSC

- **Again can use default anaconda python:**

```
module load python
python
>>> import torch
```

- **However the anaconda version isn't built with the [pytorch MPI] (for multi-node) - so we provide a build**
- **Again we are looped into intel optimizations**

- **Below has both those optimizations and MPI**

```
module load pytorch/v1.0.0-intel
```

Deep learning on Jupyter

Can use optimized modules by choosing kernels on jupyter.nersc.gov - e.g. :

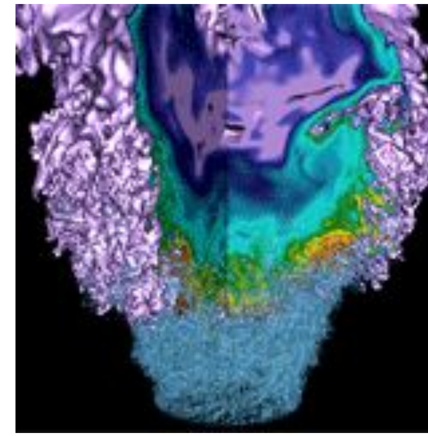
- tensorflow-intel(cpu)/1.13.1-py36
- pytorch-v1.1.0

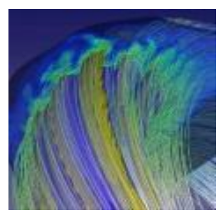
Running on NERSC jupyter hub is normally on a single shared node (so only for smaller models).

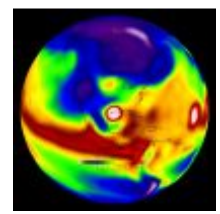
Users can deploy distributed deep learning workloads to Cori from Jupyter notebooks using IPyParallel.

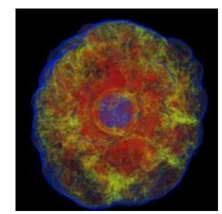
- Some examples for running multi-node training and distributed hyper-parameter optimization:
  - https://github.com/sparticlesteve/cori-intml-examples

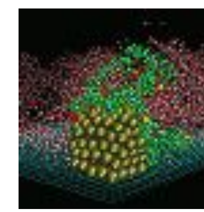
Easy Deep learning Example











Keras: MNIST CNN Classification

```python
import numpy as np
from tensorflow.keras.datasets import mnist
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout, Flatten
from tensorflow.keras.layers import Conv2D, MaxPooling2D
from tensorflow.keras import utils as k_utils

# Load MNIST data and add channel
(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train = np.expand_dims(x_train.astype('float32'), axis=-1)
x_test = np.expand_dims(x_test.astype('float32'), axis=-1)

# normalize data
x_train /= 255
x_test /= 255

num_classes=10

# convert class vectors to binary class matrices
y_train = k_utils.to_categorical(y_train, num_classes)
y_test = k_utils.to_categorical(y_test, num_classes)
```

Keras is TF's official high-level API

Example source: modified version of github.com/keras-team/keras/blob/master/examples/mnist_cnn.py

Keras: CNN Classification

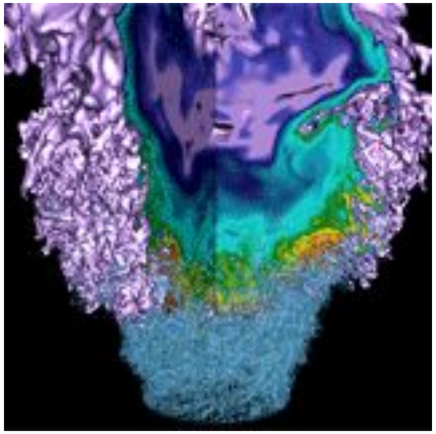
```
model = Sequential()
model.add(Conv2D(32, kernel_size=(3, 3),
                 activation='relu',
                 input_shape=[28, 28, 1]))
model.add(Conv2D(64, (3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Dropout(0.25))
model.add(Flatten())
model.add(Dense(128, activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(num_classes, activation='softmax'))
# compile model
model.compile(loss='categorical_crossentropy',
              optimizer='Adam',
              metrics=['accuracy'])
# check model architecture summary
model.summary()
batch_size=128
epochs=5
# train model
model.fit(x_train, y_train, batch_size=batch_size, epochs=epochs,
          verbose=1, validation_data=(x_test, y_test))
# evaluate model
score = model.evaluate(x_test, y_test, verbose=0)
print('Test loss:', score[0], 'Test accuracy:', score[1])
```

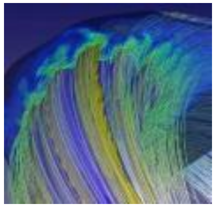
Layer (type)	Output Shape	Param #
conv2d_0 (Conv2D)	(None, 26, 26, 32)	320
conv2d_1 (Conv2D)	(None, 24, 24, 64)	18496
max_pooling2d_0 (MaxPooling2	(None, 12, 12, 64)	0
dropout_0 (Dropout)	(None, 12, 12, 64)	0
flatten_0 (Flatten)	(None, 9216)	0
dense_0 (Dense)	(None, 128)	1179776
dropout_1 (Dropout)	(None, 128)	0
dense_1 (Dense)	(None, 10)	1290

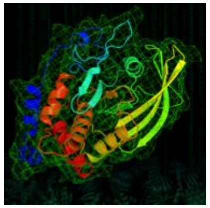
Total params: 1,199,882
Trainable params: 1,199,882
Non-trainable params: 0

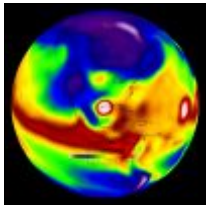
Test loss: 0.029
Test accuracy: 0.99

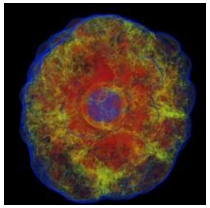
CPU Optimizations and Multi-node training

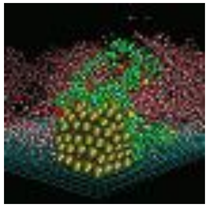






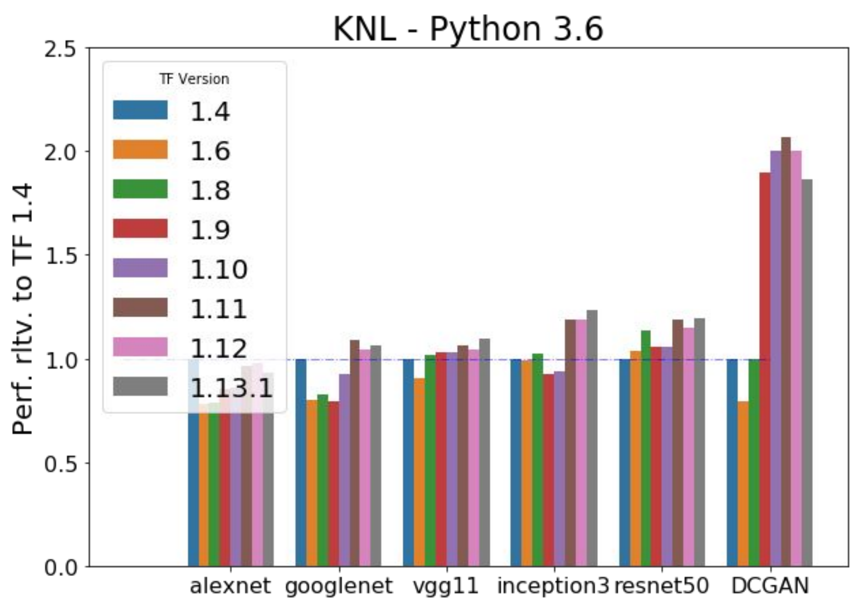






Tensorflow MKL Optimizations

- **Python frameworks rely on optimized backends to perform**
- **For CPU like Cori KNL this is Intel Math Kernel Library (MKL) (e.g. MKL-DNN) - all recent versions have optimizations**
- **Blog posts on Intel optimisations:**
  https://software.intel.com/en-us/articles/tensorflow-optimizations-on-modern-intel-architecture
  https://ai.intel.com/tensorflow-optimizations-intel-xeon-scalable-processor/
  https://software.intel.com/en-us/articles/using-intel-xeon-processors-for-multi-node-scaling-of-tensorflow-with-horovod

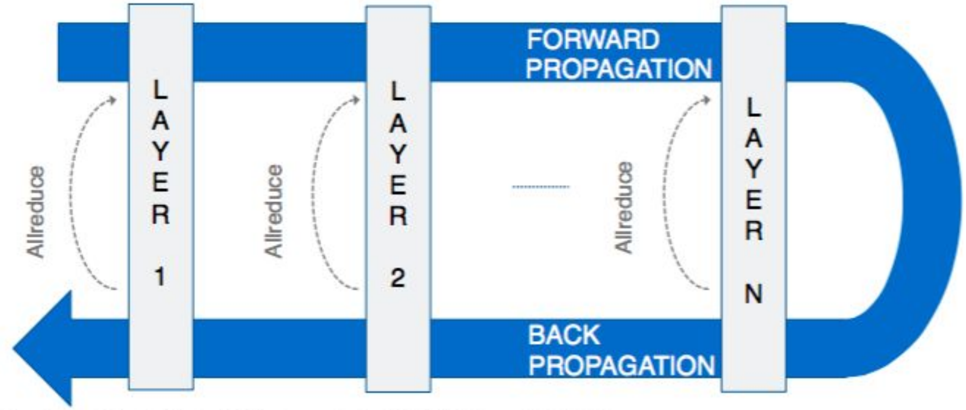


We track performance via benchmarks. More details at:
https://docs.nersc.gov/analytics/machinelearning/benchmarks/

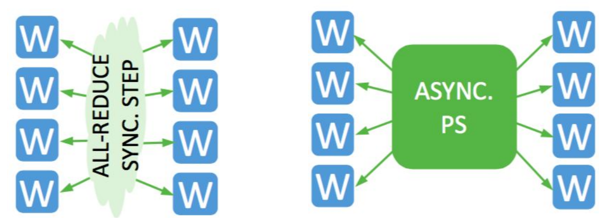
Multi-node training

- **Data parallel training for gradient descent**
  - Each node processes data independently then a global update
  - Synchronous; Asynchronous;hybrid gradient lag approaches

- **Challenges to HPC scaling have included convergence and performant libraries**

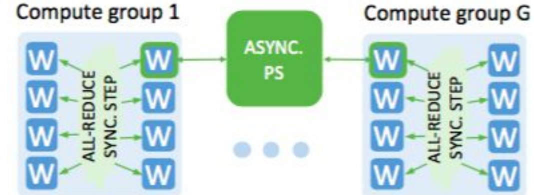


From Pradeep Dubey, "Scaling to Meet the Growing Needs of Artificial Intelligence (AI), IDF 2016
https://software.intel.com/en-us/articles/scaling-to-meet-the-growing-needs-of-ai



SYNCHRONOUS

ASYNCHRONOUS



HYBRID

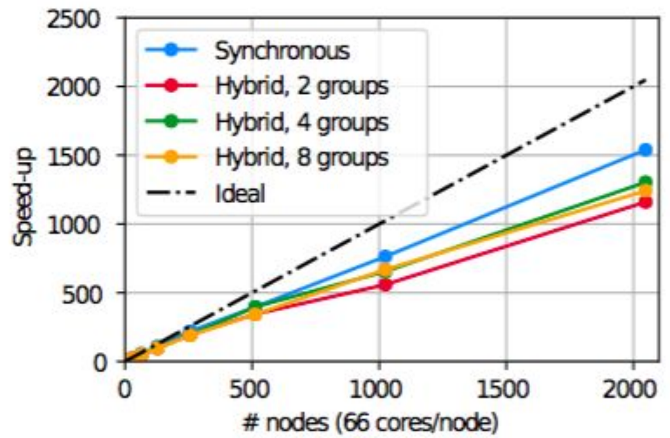
From Kurth et al. SC17 [arXiv:1708.05256](https://arxiv.org/abs/1708.05256)

Performant Multi-Node Libraries

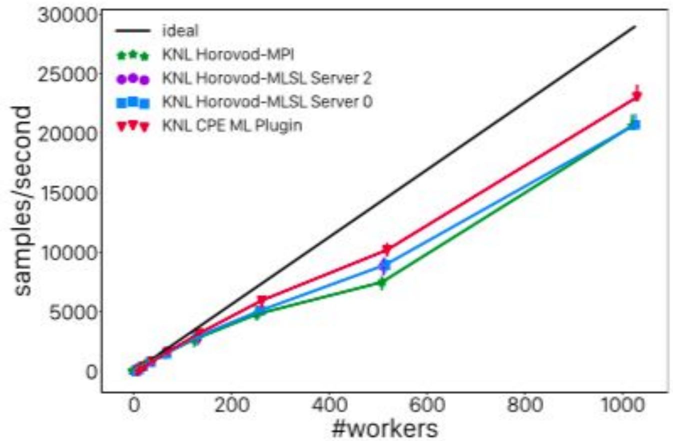
- **Initial scaling on NERSC involved a lot of work**
  – e.g. with Intel-Caffe and Intel-MLSL
- **Default TensorFlow uses gRPC for communication - non-ideal for Cori high-speed network**
  – See e.g. Mathuriya et. al (arXiv:1712.09388)

- **Fortunately now libraries based on MPI with Horovod and Cray PE ML Plugin**

Kurth et al. SC17 **arXiv:1708.05256**



Kurth et al. Concurrency Computat Pract Exper. 2018;e4989



Horovod Keras Simple Snippets

Available in default NERSC tensorflow modules

- **When building model:**

```
from keras import models
import horovod.keras as hvd
model = models.Model(inputs, outputs)
hvd.init()
model.compile(optimizer=hvd.DistributedOptimizer(optimizers.Adam),...
```

- **When training model:**

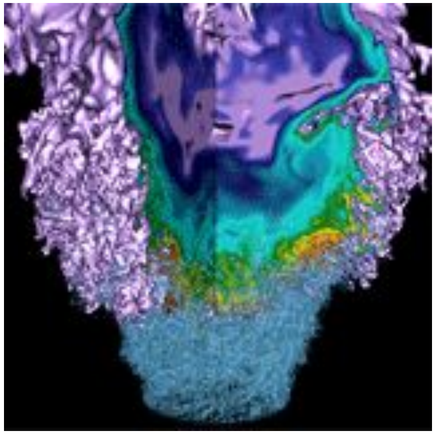
```
model.fit(callbacks=[hvd.callbacks.BroadcastGlobalVariablesCallback(0),...
```

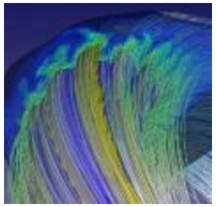
Guidelines for DL at scale

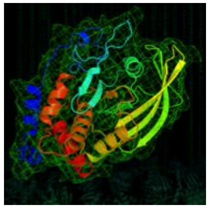
Convergence at scale is an active area of research. Some current experiences from multiple projects:

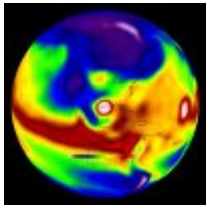
- **If strong scaling (small node count): decrease per-node batch size with increasing synchronous node count**
- **Experiment with increasing learning rate sub-linearly to linearly with number of workers:**
  - Warmup period starting at initial learning rate
  - Reduce learning rate if learning plateaus
- **Advanced Layer-wise adaptive (LARS/LARC) strategies**
- **Be careful with batch normalization for multi-node performance, consider Ghost Batch Normalization**
- **With 'global shuffle' of training examples, use of Burst Buffer can help with I/O at NERSC**

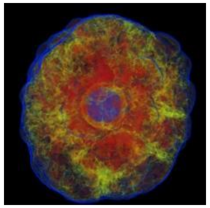
Support

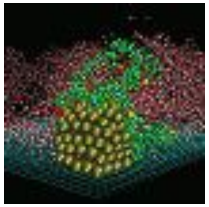












Contact us

https://docs.nersc.gov/analytics/machinelearning/overview/

General help with deep learning modules;

and running DL at NERSC open tickets via:

consult@nersc.gov

For collaborations contact ML-Engineers at NERSC:

Mustafa Mustafa: mmustafa@lbl.gov

Steve Farrell: SFarrell@lbl.gov

Wahid Bhimji: wbhimji@lbl.gov