Tuning Deep Learning Training & Evaluation Performance on the OU Supercomputer

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Challenges

OU Supercomputer:

- Many CPU-only nodes; small number of nodes with Graphical Processing Units (GPUs)
  - GPU nodes are expensive!
- Large number of users -> compute resources are mostly in "use" at any given instant in time
- For deep learning, we have a great set of tools built into Tensorflow and Pytorch to map models onto one more more GPUs
  - If used properly, can achieve 10x - 100x speed up over CPU-only training
  - Must properly manage GPU allocation
  - And must ensure that the data flow into the GPUs can keep up

Goals for Today

Better understand:

- Effective GPU utilization with TensorFlow
- Management of data flow from spinning disk to GPUs (and CPUs)

CPU vs. GPU Processing

There are two types of computational devices we have access to:

CPU

- General purpose
- few (1-64) cores / parallel operations
- Must handle I/O tasks for data in RAM and
- Python code you write runs here

GPU

- Specialized
- Many (1000+) cores / parallel operations
- Can only operate on data in VRAM (GPU memory)
- TensorFlow code can run here

Using Python/DL with GPUs

- Tensorflow/PyTorch packages in Python provide an API for interfacing with GPUs
- By default, tensorflow-gpu will use all available memory on all GPU devices
- When multiple programs attempt to use the same GPU, they can interfere destructively with one-another
- Approach: in addition to reserving a node, also reserve one or more GPUs on this node

Reserving GPUs

Add to your batch file:

- Single GPU reservation:

```
#SBATCH --gres=gpu:1
```

- Two GPUs:

```
#SBATCH --gres=gpu:2
```

- During execution, your batch file environment variable $CUDA_VISIBLE_DEVICES will be set to a comma-separated string containing the integers of the physical GPUS that have been allocated

Using Reserved GPUs with Tensorflow

We want your Tensorflow code will only be able to see the allocated GPUs

```
    # Turn off GPUs: necessary for the current SLURM
    if not args.gpu or "CUDA_VISIBLE_DEVICES" not in os.environ.keys():
        tf.config.set_visible_devices([], 'GPU')
        print('NO VISIBLE DEVICES!!!!')

    # GPU check
    visible_devices = tf.config.get_visible_devices('GPU')
    n_visible_devices = len(visible_devices)

    print('GPUS:', visible_devices)
    if(n_visible_devices > 0):
        for device in visible_devices:
            tf.config.experimental.set_memory_growth(device, True)
        print('We have %d GPUs\n'%n_visible_devices)
    else:
        print('NO GPU')

# Do the work …
```

Using Multiple GPUs with Tensorflow

There are multiple options - the simple one is the Mirrored Strategy:

- Place a copy of the model onto each GPU
- Split the batch into N pieces, sending one piece to each GPU
- Each GPU performs a forward/backward pass with its batch
- The weight updates are summed & then shared back to each GPU
- Repeat

Using Multiple GPUs with Tensorflow

Using the Mirrored Strategy is Relatively Straight Forward:

```
strategy = tf.distribute.MirroredStrategy()

with strategy.scope():
    # build the model (in the scope)
    model = network_fn(**network_args)
    # Must instantiate the loss/metrics here
    model.compile(...)
   :
   :
history = model.fit(...)
```

Note: batch size should generally be scaled by number of GPUs

Monitoring CPU, Memory, GPU, and I/O Loads

- Identify the unique jobid:
  squeue -o "%i %.18A %j %P %u %T %M %R"
  ^^ unique jobid

- Open a bash shell on the node your job is running on:
  `srun --jobid=UNIQUE_JOBID --pty bash`

In that shell:

- Monitor CPU, memory and I/O:
  `top`
- Monitor GPU load and memory use:
  `nvidia-smi`

top

```
top - 14:34:13 up 35 days, 18:44,  1 user,  load average: 0.94, 0.78, 0.75
Tasks: 400 total,   1 running, 399 sleeping,   0 stopped,   0 zombie
%Cpu(s):  6.3 us,  1.4 sy,  0.0 ni, 92.3 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
KiB Mem : 65710052 total, 52559580 free,  8746172 used,  4404300 buff/cache
KiB Swap:  8388604 total,  7595868 free,   792736 used. 53733932 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
29085 jroth     20   0   58.7g   6.6g 514280 S 187.0 10.5  68:19.11 python
 1884 telegraf  20   0 2263992  10636   3744 S   2.3  0.0 279:34.50 telegraf
29592 jroth     20   0  579224 106480  10308 S   1.3  0.2   1:58.88 jupyter-lab
30523 jroth     20   0 5235448 126764  14524 S   1.3  0.2   0:28.89 wandb-serv+
 1074 root      20   0       0      0      0 S   0.3  0.0   3:21.12 xfsaild/dm+
 1717 root      20   0       0      0      0 S   0.3  0.0   0:10.09 nv_queue
 1981 root      20   0  773304  16548   2412 S   0.3  0.0  25:05.59 salt-minion
 9951 fagg      20   0  172692   2588   1616 R   0.3  0.0   0:00.02 top
    1 root      20   0  194660   4716   2520 S   0.0  0.0   9:51.90 systemd
    2 root      20   0       0      0      0 S   0.0  0.0   0:04.33 kthreadd
    4 root       0 -20       0      0      0 S   0.0  0.0   0:00.00 kworker/0:+
    6 root      20   0       0      0      0 S   0.0  0.0   0:01.39 ksoftirqd/0
    7 root      rt   0       0      0      0 S   0.0  0.0   0:00.44 migration/0
    8 root      20   0       0      0      0 S   0.0  0.0   0:00.00 rcu_bh
    9 root      20   0       0      0      0 S   0.0  0.0  17:54.38 rcu_sched
   10 root       0 -20       0      0      0 S   0.0  0.0   0:00.00 lru-add-dr+
   11 root      rt   0       0      0      0 S   0.0  0.0   0:07.97 watchdog/0
```

Monitoring CPU, Memory and I/O Loads (with top)

- CPU: max use should stay within your reservation (--cpus_per_task)
  - For your process: ceiling(%CPU / 100) <= cpus_per_task
  - If load average > total number of threads available on the node, then someone is not behaving
- Memory: max use should stay within your reservation (--mem)
  - For your process: RES is the amount of RAM that your process is using
  - If free memory is low compared to total RAM, then someone is not behaving

nvidia-smi

```
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 515.57       Driver Version: 515.57       CUDA Version: 11.7     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-PCI...  On   | 00000000:3B:00.0 Off |                  Off |
| N/A   49C    P0    74W / 250W |  39751MiB / 40960MiB |     63%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-PCI...  On   | 00000000:5E:00.0 Off |                  Off |
| N/A   62C    P0   212W / 250W |  39751MiB / 40960MiB |     93%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A    236087      C   python                          39749MiB |
|    1   N/A  N/A    167230      C   python                          39749MiB |
+-----------------------------------------------------------------------------+
```

Monitoring GPU Utilization

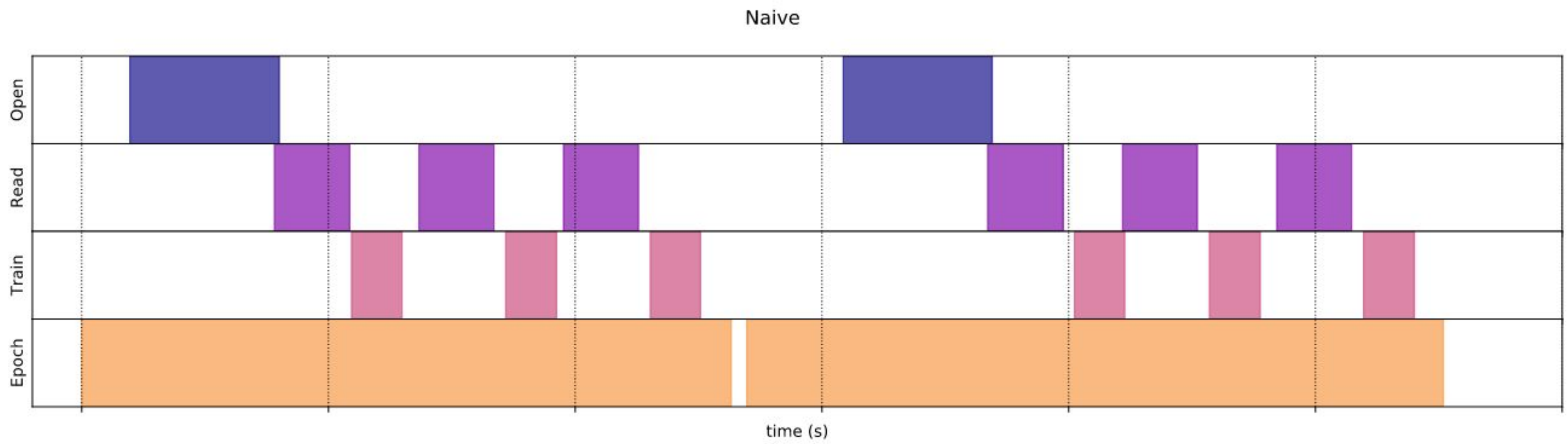
- GPU-Util: want this to be as close to 100% as possible. If it is not, you have various things you can try:
  - Increase batch size
  - Increase the number of threads available for your TF Datasets (more on this coming)
  - Cache your dataset closer to the GPU (more on this coming)

- Memory Usage:
  - Keep batch size small enough so that you are not maxing out available VRAM (get close, but don't exceed)
  - Exceeding -> memory allocation error, Out of Memory (OOM)

Large Data Sets

- Our data sets are often small enough to fit into RAM/GPU RAM
- For interesting data sets (e.g., where we have a large number of images), these data don't fit! Only a subset of data will fit in RAM at once
  - For Mel Wilson Reyes' Visibility data set, we have ~1.8M images
- We will swap parts of data set into RAM as they are needed … we call these batches
- Pipeline the process of loading, preparing, and computing gradients for different batches simultaneously
  - Perform I/O and Training at the same time to avoid bottleneck

Large Data Sets: Naive Approach

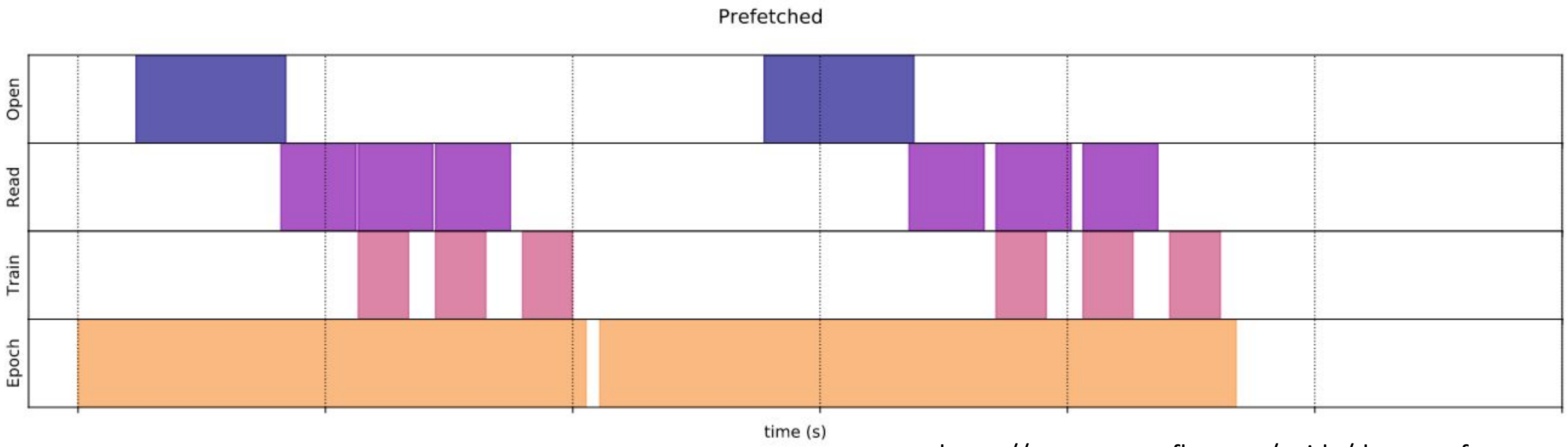


- Blue: Initializing fetch of data from spinning disk
- Purple: Loading/preparing data
- Pink: Training with the GPU

https://www.tensorflow.org/guide/data_performance

Large Data Sets: Prefetching + Parallel Execution

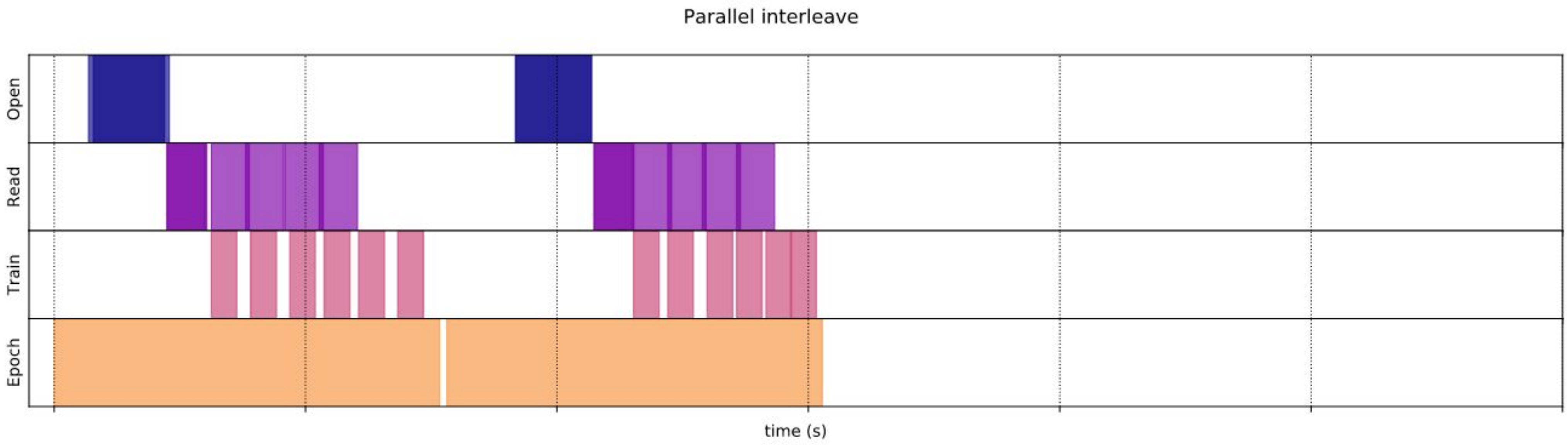
- Fetching new batch before training with the current batch completes
- Better utilization of the GPU



https://www.tensorflow.org/guide/data_performance

Large Data Sets: Prefetching Multiple Batches at Once

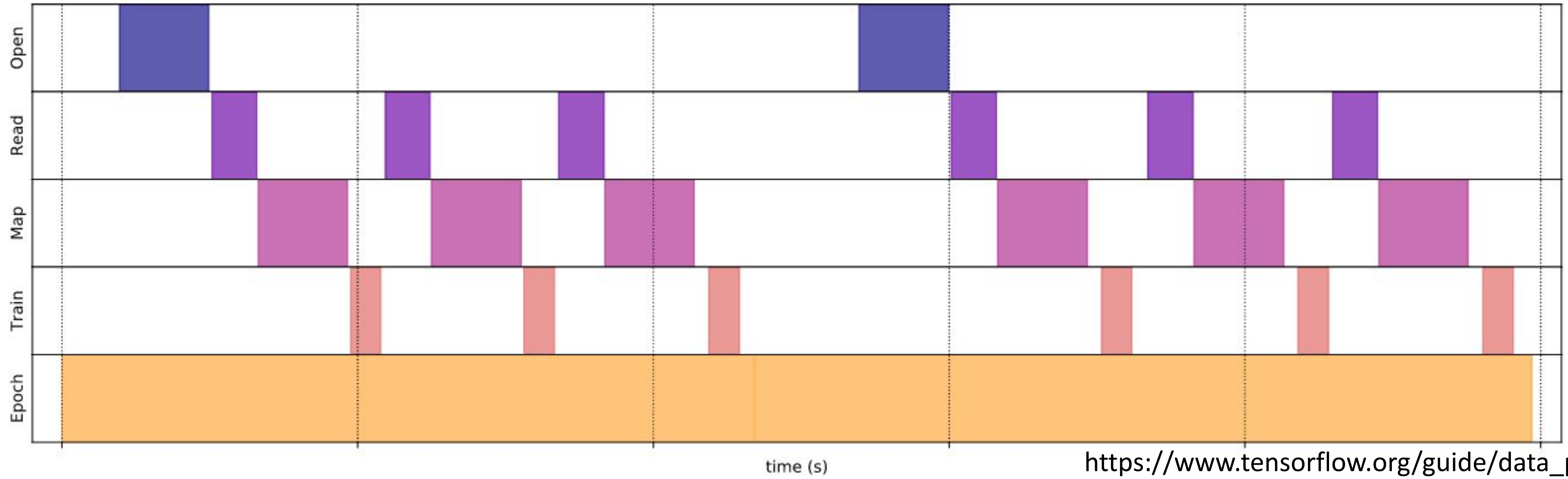
- Each batch is fetched using one or more threads



https://www.tensorflow.org/guide/data_performance

Large Data Sets: Data Transformation

- Typically storage format on the spinning disk is different than what we need for training
  - Disk: PNG format: pixel color is captured with 3 x 1-byte integers
  - Training: TF Tensor: pixel color is 3 x float32s or float16s
- Transformation process is referred to as “mapping”

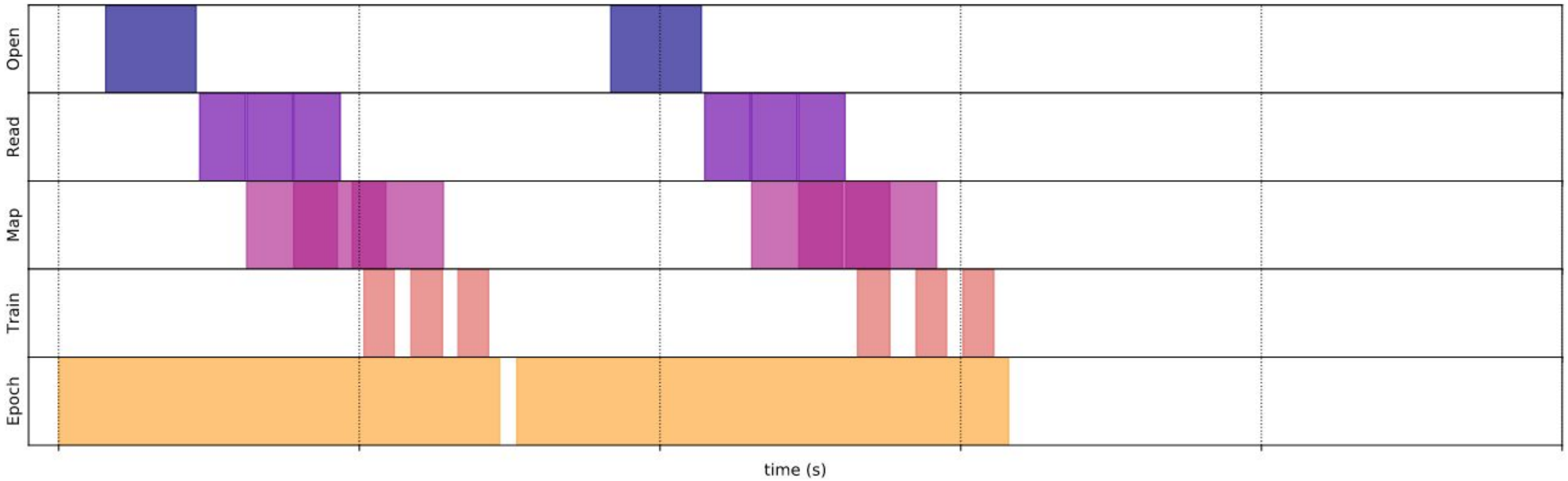


https://www.tensorflow.org/guide/data_performance

Large Data Sets: Parallel Fetching, Mapping and Training

- One or more threads dedicated to fetching and mapping

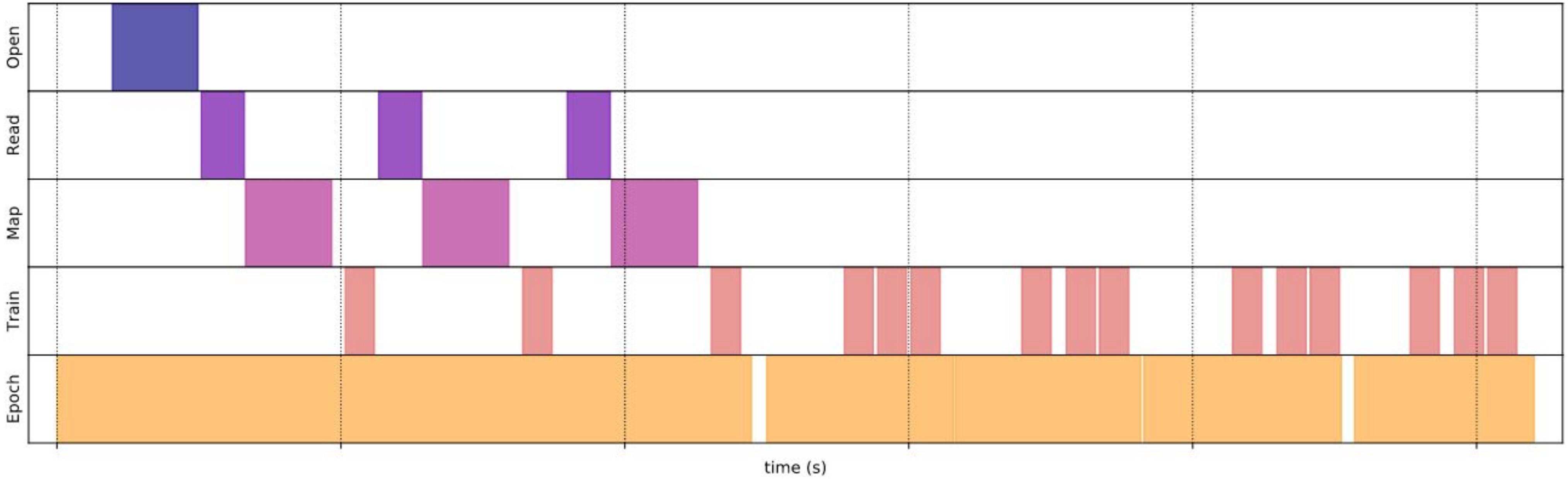
Parallel map



https://www.tensorflow.org/guide/data_performance

Large Data Sets: Caching

- After loading/mapping data, store in a cache so subsequent accesses are much faster
- In TensorFlow, can cache to RAM or to fast Disk (e.g., SSD)



Class: tensorflow.data.Dataset

- TF Datasets act like generators:
  - Implement a ‘next’ type method that produces the ‘next’ sequential element
  - Will signal if you have reached the end of the data set
  - model.fit() will iterate over each element of a Dataset for training purposes
    - model.evaluate(), model.predict(), too
  - Input side: some other sequence of items (often another Dataset)

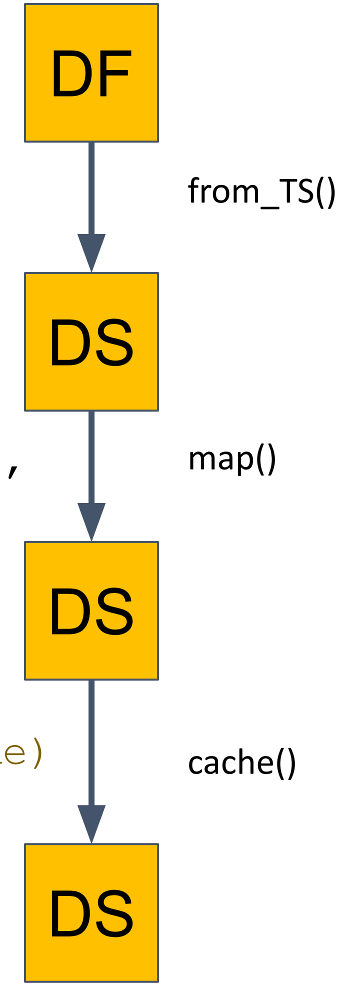
- Different TF Dataset methods for:
  - Mapping data
  - Buffering
  - Shuffling
  - Caching
  - Batching

Representing Metadata with Pandas Dataframes

Dataframe: 2D table

- Rows: single examples
- Columns: different properties for the examples
  - Image file path
  - Class
  - Other information (e.g., timestamp, location)
- Pandas Dataframe implements a lot of database-like operations that make it easy to organize data in many different ways
  - Select all daytime rows
  - Select all rows for a given class, example type…
  - Shuffle the rows

Example: DF Describes Images -> Dataset




```
# Convert DF with a file name and a class label to a dataset
ds = tf.data.Dataset.from_tensor_slices(df[[“filename”, “class”]].to_numpy())
```

(2,) (Strings)

```
# For each DF row, create a TF Tensor pair: rows x cols x 3  AND class
ds = ds.map(lambda x: tf.py_function(func=prepare_single_example, inp=[base_dir, x],
                                      Tout=(tf.float32, tf.int8)),
                              num_parallel_calls=4)
```

(128, 128, 3) AND (1,)

```
# Cache the data set (cache_location = path to local SSD; dataset_name = unique name)
ds = ds.cache('%s/cache_%s'%(cache_location, dataset_name))
```

(128, 128, 3) AND (1,)

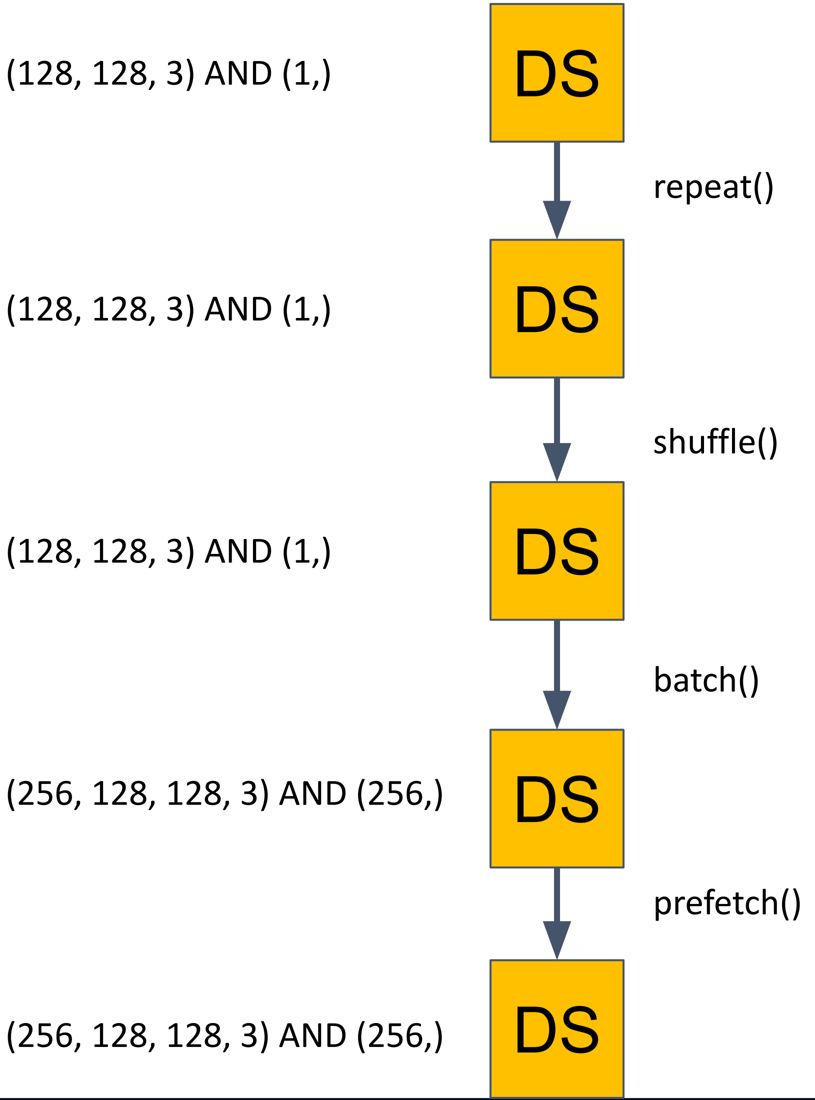
Example Continued

```
# Optionally repeat the data set indefinitely.  Use with caution!
if repeat:
    ds = ds.repeat()

# Pseudo shuffle the dataset (buffer size = 100)
ds = ds.shuffle(100)

# Batch individual examples into groups of 256
ds = ds.batch(256)

# Prefetch batches so we can be ready for requests
ds = ds.prefetch(2)
```



Mapping Function Example

```
def prepare_single_example(base_dir: str, example: np.array) -> [tf.Tensor]:
    # example[0]: string file name
    # example[1]: string class index: "d" where d is a digit
    fname = example[0]

    # Extract Class number
    cl = example[1]
    cl = tf.strings.to_number(cl, out_type=tf.int8)

    # Load image from file system
    img = load_single_png_image(base_dir, fname)

    return img, cl
```

Mapping Function Example

```
def load_single_image(base_dir: str, fname: str) -> tf.Tensor:
    # Implementation uses all TF operators -> can be mapped to GPU

    # Load raw data from file
    image_string = tf.io.read_file(base_dir + "/" + fname)

    # Interpret it as a PNG file
    image = tf.image.decode_png(image_string, channels=3)

    # Convert to standard TF Tensor format
    image = tf.image.convert_image_dtype(image, tf.float32)

    return image
```

Cache Behavior

The Dataset.cache() object:

- As the underlying data are read in and converted, the data are all stored in a single cache file (+ an index file) - on the `$LSCRATCH` SSD
- What you get:
  - Your first pass through your entire dataset still requires all of the data to be fetched from spinning disk (and across network)
  - In subsequent passes through the data set, the data will be taken from the cache file on the SSD instead of over the network

Notes on Caching

- `$LSCRATCH` is allocated to your job – just for its lifetime
- Each node has a different size SSD
- The space available on your `$LSCRATCH` is proportional to the fraction of threads that you reserve on the node
    - #SBATCH --cpus-per-task=20
    - Different nodes also have different numbers of threads available

Advanced TF Datasets

- Combining multiple Datasets
  - sample_from_datasets(): sample based on a probability distribution from the child Datasets
    - Can use to oversample classes with a small number of examples
  - choose_from_datasets(): iterate through each child Dataset, taking one sample

- Models that take as input multiple images:
  - batch() or choose_from_datasets() to put together the K images into a single example input

- Repeating Datasets: tread carefully here
  - model.fit(): must set steps_per_epoch to something other than None (the default)

Advanced TF Datasets

- Storing a datasets to a file:
  - ds.save(path)
  - Saves dataset to a small number of files in the specified directory

- Loading the dataset back in:
  - tf.Dataset.load(path)
  - The smaller number of files makes for faster reading

Summary: TF Datasets

- Not static objects
- Instead:
  - Constantly producing “next” items
  - Backfilling with their input Dataset (or other sequence of items)
- Serve as inputs directly into Keras Model objects:
  - model.fit()
  - model.predict()
  - model.evaluate()

Tuning to Maximize GPU Utilization

- Batch size tuning
  - Increase the size of the batches until you fill the GPU memory
- Caching
  - Cache to the directory given by SLURM environment variable `$LSCRATCH`
  - `Coming soon on Sooner: Burst Buffer (large SSD)`
- Prefetching
- tune number of threads for operations with tf.data.AUTOTUNE:
  - .prefetch(tf.data.AUTOTUNE)
  - .map(..., num_parallel_calls=tf.data.AUTOTUNE)
  - .batch(..., num_parallel_calls=tf.data.AUTOTUNE)
  - Tread carefully with AUTOTUNE - there are some bugs…

Why Do All These Things?

One example: image classification task

- 160K images: shape: 128x128x3
- 10 Classes
- CPU vs tuned multi-GPU implementation
    - CPU-only requires 50-100x more wall clock time