HPAT Documentation

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Intel

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QUICK INTRODUCTION TO HPAT

High Performance Analytics Toolkit (HPAT) is a big data analytics and machine learning framework that provides Python's ease of use but is extremely fast.

HPAT scales analytics programs in python to cluster/cloud environments automatically, requiring only minimal code changes. Here is a logistic regression program using HPAT:

```
@hpat.jit
def logistic_regression(iterations):
    f = h5py.File("lr.hdf5", "r")
    X = f['points'][:]
    Y = f['responses'][:]
    D = X.shape[1]
    w = np.random.ranf(D)
    t1 = time.time()
    for i in range(iterations):
        z = ((1.0 / (1.0 + np.exp(-Y * np.dot(X, w))) - 1.0) * Y)
        w -= np.dot(z, X)
    return w
```

This code runs on cluster and cloud environments using a simple command like:

```
mpiexec -n 1024 python logistic_regression.py
```

HPAT compiles the source code to efficient native parallel code (with MPI). This is in contrast to other frameworks such as Apache Spark which are master-executor libraries. Hence, HPAT is typically 100x or more faster. HPAT is built on top of Numba and LLVM compilers.

CHAPTER

TWO

GETTING STARTED WITH HPAT

HPAT automatically parallelizes a subset of Python that is commonly used for data analytics and machine learning. This section describes this subset and how parallelization is performed.

HPAT compiles and parallelizes the functions annotated with the @hpat.jit() decorator. The decorated functions are replaced with generated parallel binaries that run on bare metal. The supported data structures for large datasets are Numpy arrays and Pandas dataframes.

2.1 How to install HPAT?

Todo: HPAT installing instructions

HPAT can be installed in Anaconda environment easily. On Linux/Mac/Windows:

```
conda create -n HPAT -c ehsantn -c anaconda -c conda-forge hpat
```

You can use the following step if master of Numba is needed for latest hpat package:

```
conda create -n HPAT -c ehsantn -c numba/label/dev -c anaconda -c conda-forge hpat
```

2.1.1 Building from Source on Linux

We use Anaconda distribution of Python for setting up HPAT.

Miniconda3 is required for build:

It is possible to build HPAT via conda-build or setuptools. Follow one of the cases below to install HPAT and its dependencies such as Numba on Ubuntu Linux.

Build with conda-build:

Build with setuptools:

```
conda create -n HPAT -q -y numpy scipy pandas boost cmake python=<3.6 or 3.7>
source activate HPAT
conda install -c numba/label/dev numba
conda install mpich mpi -c conda-forge
conda install pyarrow
conda install pyarrow
conda install h5py -c ehsantn
conda install gcc_linux-64 gxx_linux-64 gfortran_linux-64
git clone https://github.com/IntelPython/hpat
cd hpat
# build HPAT
HDF5_DIR=$CONDA_PREFIX python setup.py develop
```

Running example using HPAT:

A command line for running the Pi example on 4 cores:

```
mpiexec -n 4 python examples/pi.py
```

Running unit tests:

```
conda install pyspark
python hpat/tests/gen_test_data.py
python -m unittest
```

In case of issues, reinstalling in a new conda environment is recommended. Also, a common issue is hdf5 package reverting to default instead of the parallel version installed from ehsantn channel. Use conda list to check the channel of hdf5 package.

2.1.2 Building from Source on Windows

Building HPAT on Windows requires Build Tools for Visual Studio 2017 (14.0):

- Install Build Tools for Visual Studio 2017 (14.0).
- Install Miniconda for Windows.
- Start 'Anaconda prompt'
- Setup the Conda environment in Anaconda Prompt

It is possible to build HPAT via conda-build or setuptools. Follow one of the cases below to install HPAT and its dependencies on Windows.

Build with conda-build:

```
conda create -n HPAT python=<3.7 or 3.6>
activate HPAT
conda install vc vs2015_runtime vs2015_win-64
git clone https://github.com/IntelPython/hpat.git
conda build --python <3.6 or 3.7> -c numba -c conda-forge -c defaults -c intel hpat/

-buildscripts/hpat-conda-recipe/
```

Build with setuptools:

```
conda create -n HPAT -c ehsantn -c numba/label/dev -c anaconda -c conda-forge -c_
intel python=<3.6 or 3.7> pandas pyarrow h5py numba scipy boost libboost tbb-devel_
impi-devel impi-devel impi_rt
activate HPAT
conda install vc vs2015_runtime vs2015_win-64
git clone https://github.com/IntelPython/hpat.git
cd hpat
set INCLUDE=%INCLUDE%;%CONDA_PREFIX%\Library\include
set LIB=%LIB%;%CONDA_PREFIX%\Library\lib
%CONDA_PREFIX%\Library\bin\mpivars.bat quiet
set HDF5_DIR=%CONDA_PREFIX%\Library
python setup.py develop
```

Troubleshooting Windows Build

- If the cl compiler throws the error fatal error LNK1158: cannot run 'rc.exe', add Windows Kits to your PATH (e.g. C:\Program Files (x86)\Windows Kits\8.0\bin\x86).
- Some errors can be mitigated by set DISTUTILS_USE_SDK=1.
- For setting up Visual Studio, one might need go to registry at HKEY_LOCAL_MACHINE\SOFTWARE\WOW6432Node\Microsoft\VisualStudio\SxS\VS7, and add a string value named 14.0 whose data is C:\Program Files (x86)\Microsoft Visual Studio 14.0\.

2.1.3 AWS Setup

This page describes a simple setup process for HPAT on Amazon EC2 instances. You need to have an account on Amazon Web Services (AWS) and be familiar with the general AWS EC2 instance launch interface. The process below is for demonstration purposes only and is not recommended for production usage due to security, performance and other considerations.

1. Launch instances:

- a. Select a Linux instance type (e.g. Ubuntu Server 18.04, c5n types for high network bandwidth).
- b. Select number of instances (e.g. 4).
- c. Select placement group option for better network performance (check "add instance to placement group").
- d. Enable all ports in security group configuration to simplify MPI setup (add a new rule with "All traffic" Type and "Anywhere" Source).

2. Setup password-less ssh between instances:

a. Copy your key from your client to all instances. For example, on a Linux clients run this for all instances (find public host names from AWS portal):

```
scp -i "user.pem" user.pem ubuntu@ec2-11-111-11-111.us-east-2.compute.

→amazonaws.com:~/.ssh/id_rsa
```

b. Disable ssh host key check by running this command on all instances:

```
echo -e "Host *\n StrictHostKeyChecking no" > .ssh/config
```

c. Create a host file with list of private hostnames of instances on home directory of all instances:

```
echo -e "ip-11-11-11.us-east-2.compute.internal\nip-11-11-11-12.us-

→east-2.compute.internal\n" > hosts
```

3. Install Anaconda Python distribution and HPAT on all instances:

```
wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh -O_
→miniconda.sh
chmod +x miniconda.sh
./miniconda.sh -b
export PATH=$HOME/miniconda3/bin:$PATH
conda create -n HPAT -c ehsantn -c anaconda -c conda-forge hpat
source activate HPAT
```

4. Copy the Pi example to a file called pi.py in the home directory of all instances and run it with and without MPI and see execution times. You should see speed up when running on more cores ("-n 2" and "-n 4" cases):

```
python pi.py # Execution time: 2.119
mpiexec -f hosts -n 2 python pi.py # Execution time: 1.0569
mpiexec -f hosts -n 4 python pi.py # Execution time: 0.5286
```

Possible next experiments from here are running a more complex example like the logistic regression example. Furthermore, attaching a shared EFS storage volume and experimenting with parallel I/O in HPAT is recommended.

2.2 How HPAT can improve my code?

Todo: Short paragraph for features overview should be written here.

2.2.1 Automatic Parallelization

HPAT parallelizes programs automatically based on the *map-reduce* parallel pattern. Put simply, this means the compiler analyzes the program to determine whether each array should be distributed or not. This analysis uses the semantics of array operations as the program below demonstrates:

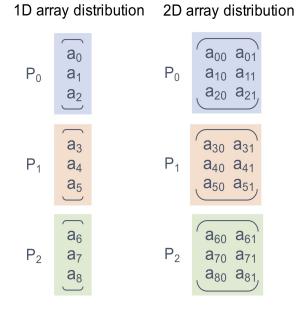
```
@hpat.jit
def example_1D(n):
    f = h5py.File("data.h5", "r")
    A = f['A'][:]
    return np.sum(A)
```

This program reads a one-dimensional array called A from file and sums its values. Array A is the output of an I/O operation and is input to np.sum. Based on semantics of I/O and np.sum, HPAT determines that A can be distributed since I/O can output a distributed array and np.sum can take a distributed array as input. In map-reduce terminology, A is output of a map operator and is input to a reduce operator. Hence, HPAT distributes A and all operations associated with A (i.e. I/O and np.sum) and generates a parallel binary. This binary replaces the $example_ID$ function in the Python program.

HPAT can only analyze and parallelize the supported data-parallel operations of Numpy and Pandas (listed below). Hence, only the supported operations can be used for distributed datasets and computations. The sequential computation on small data can be any code that Numba supports.

2.2.2 Array Distribution

Arrays are distributed in one-dimensional block (*1D_Block*) manner among processors. This means that processors own equal chunks of each distributed array, except possibly the last processor. Multi-dimensional arrays are distributed along their first dimension by default. For example, chunks of rows are distributed for a 2D matrix. The figure below illustrates the distribution of a 9-element one-dimensional Numpy array, as well as a 9 by 2 array, on three processors:



HPAT replicates the arrays that are not distributed. This is called *REP* distribution for consistency.

2.2.3 Argument and Return Variables

HPAT assumes argument and return variables to jitted functions are replicated. However, the user can annotate these variables to indicate distributed data. In this case, the user is responsible for handling of the distributed data chunks outside the HPAT scope. For example, the data can come from other jitted functions:

```
@hpat.jit(distributed={'A'})
def example_return(n):
    A = np.arange(n)
    return A

@hpat.jit(distributed={'B'})
def example_arg(B):
    return B.sum()
```

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```
n = 100
A = example_return(n)
s = example_arg(A)
```

2.2.4 Distribution Report

The distributions found by HPAT can be printed using the hpat.utils.distribution_report() function. The distribution report for the above example code is as follows:

This report suggests that the function has an array that is distributed in 1D_Block fashion. The variable name is renamed from A to \$A.23 through the optimization passes. The report also suggests that there is a parfor (data-parallel for loop) that is 1D_Block distributed.

2.2.5 Numpy dot() Parallelization

The np.dot function has different distribution rules based on the number of dimensions and the distributions of its input arrays. The example below demonstrates two cases:

```
@hpat.jit
def example_dot(N, D):
    X = np.random.ranf((N, D))
    Y = np.random.ranf(N)
    w = np.dot(Y, X)
    z = np.dot(X, w)
    return z.sum()

example_dot(1024, 10)
hpat.distribution_report()
```

Here is the output of *hpat.distribution_report()*:

The first dot has a 1D array with ID_Block distribution as first input (Y), while the second input is a 2D array with ID_Block distribution (X). Hence, dot is a sum reduction across distributed datasets and therefore, the output (w) is on the reduce side and is assigned REP distribution.

The second *dot* has a 2D array with $1D_Block$ distribution (X) as the first input, while the second input is a REP array (w). Hence, the computation is data-parallel across rows of X, which implies a $1D_Block$ distribution for output (z).

Variable *z* does not exist in the distribution report since the compiler optimizations were able to eliminate it. Its values are generated and consumed on-the-fly, without memory load/store overheads.

2.2.6 Explicit Parallel Loops

Sometimes explicit parallel loops are required since a program cannot be written in terms of data-parallel operators easily. In this case, one can use HPAT's prange in place of range to specify that a loop can be parallelized. The user is required to make sure the loop does not have cross iteration dependencies except for supported reductions.

The example below demonstrates a parallel loop with a reduction:

```
from hpat import jit, prange
@jit
def prange_test(n):
    A = np.random.ranf(n)
    s = 0
    for i in prange(len(A)):
        s += A[i]
    return s
```

Currently, reductions using +=, *=, min, and max operators are supported.

2.2.7 File I/O

Currently, HPAT supports I/O for the HDF5 and Parquet formats. For HDF5, the syntax is the same as the h5py package. For example:

```
@hpat.jit
def example():
    f = h5py.File("lr.hdf5", "r")
    X = f['points'][:]
    Y = f['responses'][:]
```

For Parquet, the syntax is the same as pyarrow:

```
import pyarrow.parquet as pq
@hpat.jit
def kde():
    t = pq.read_table('kde.parquet')
    df = t.to_pandas()
    X = df['points'].values
```

HPAT automatically parallelizes I/O of different nodes in a distributed setting without any code changes.

HPAT needs to know the types of input arrays. If the file name is a constant string, HPAT tries to look at the file at compile time and recognize the types. Otherwise, the user is responsile for providing the types similar to Numba's typing syntax. For example:

```
@hpat.jit(locals={'X': hpat.float64[:,:], 'Y': hpat.float64[:]})
def example(file_name):
    f = h5py.File(file_name, "r")
    X = f['points'][:]
    Y = f['responses'][:]
```

2.2.8 **Print**

Using print () function is only supported for *REP* values. Print is called on one processor only since all processors have the same copy.

2.2.9 Strings

Currently, HPAT provides basic ASCII string support. Constant strings, equality comparison of strings (== and !=), split() function, extracting characters (e.g. s[1]), concatination, and convertion to *int* and *float* are supported. Here are some examples:

```
s = 'test_str'
flag = (s == 'test_str')
flag = (s != 'test_str')
s_list = s.split('_')
c = s[1]
s = s+'_test'
a = int('12')
b = float('1.2')
```

2.2.10 Dictionaries

HPAT supports basic integer dictionaries currently. DictIntInt is the type for dictionaries with 64-bit integer keys and values, while DictInt32Int32 is for 32-bit integer ones. Getting and setting values, pop() and get() operators, as well as min and max of keys is supported. For example:

```
d = DictIntInt()
d[2] = 3
a = d[2]
b = d.get(3, 0)
d.pop(2)
d[3] = 4
a = min(d.keys())
```

2.3 Supported Pandas Operations

Below is the list of the Pandas operators that HPAT supports. Optional arguments are not supported unless if specified. Since Numba doesn't support Pandas, only these operations can be used for both large and small datasets.

In addition:

- Accessing columns using both getitem (e.g. df ['A']) and attribute (e.g. df . A) is supported.
- · Using columns similar to Numpy arrays and performing data-parallel operations listed previously is supported.
- Filtering data frames using boolean arrays is supported (e.g. df [df.A > .5]).

2.3.1 Integer NaN Issue

DataFrame columns with integer data need special care. 'Pandas http://pandas.pydata.org/, '_ dynamically converts integer columns to floating point when NaN values are needed. This is because Numpy does not support NaN values for integers. HPAT does not perform this conversion unless enough information is available at compilation time. Hence, the user is responsible for manual conversion of integer data to floating point data if needed.

2.3.2 Input/Output

- pandas.read_csv()
 - Arguments filepath_or_buffer, sep, delimiter, names, usecols, dtype, and parse_dates are supported.
 - filepath_or_buffer, names and dtype arguments are required.
 - names, usecols, parse_dates should be constant lists.
 - dtype should be a constant dictionary of strings and types.
- pandas.read_parquet()
 - If filename is constant, HPAT finds the schema from file at compilation time. Otherwise, schema should be provided.

2.3.3 General functions

- pandas.merge()
 - Arguments left, right, as_of, how, on, left_on and right_on are supported.
 - on, left_on and right_on should be constant strings or constant list of strings.
- pandas.concat()
 - Input list or tuple of dataframes or series is supported.

2.3.4 Series

- pandas.Series
 - Argument data can be a list or array.

Attributes:

- pandas.Series.values
- pandas.Series.shape
- pandas.Series.ndim
- pandas.Series.size

Methods:

• pandas.Series.copy()

Indexing, iteration:

- pandas.Series.iat
- pandas.Series.iloc

Binary operator functions:

- pandas.Series.add()
- pandas.Series.sub()
- pandas.Series.mul()
- pandas.Series.div()

• pandas.Series.truediv() • pandas.Series.floordiv() • pandas.Series.mod() • pandas.Series.pow() • pandas.Series.combine() • pandas.Series.lt() • pandas.Series.gt() • pandas.Series.le() • pandas.Series.ge() • pandas.Series.ne() Function application, GroupBy & Window: • pandas.Series.apply() • pandas.Series.map() • pandas.Series.rolling() Computations / Descriptive Stats: • pandas.Series.abs() • pandas.Series.corr() • pandas.Series.count() • pandas.Series.cov() • pandas.Series.cumsum() • pandas. Series. describe () currently returns a string instead of Series object. • pandas.Series.max() • pandas.Series.mean() • pandas.Series.median() • pandas.Series.min() • pandas.Series.nlargest() • pandas.Series.nsmallest() • pandas.Series.pct_change() • pandas.Series.prod() • pandas.Series.quantile() • pandas.Series.std()

• pandas.Series.nunique() Reindexing/Selection/Label manipulation:

pandas.Series.sum()pandas.Series.var()pandas.Series.unique()

- pandas.Series.head()
- pandas.Series.idxmax()
- pandas.Series.idxmin()
- pandas.Series.take()

Missing data handling:

- pandas.Series.isna()
- pandas.Series.notna()
- pandas.Series.dropna()
- pandas.Series.fillna()

Reshaping, sorting:

- pandas.Series.argsort()
- pandas.Series.sort_values()
- pandas.Series.append()

Time series-related:

• pandas.Series.shift()

String handling:

- pandas.Series.str.contains()
- pandas.Series.str.len()

2.3.5 DataFrame

• pandas.DataFrame

Only data argument with a dictionary input is supported.

Attributes and underlying data:

• pandas.DataFrame.values

Indexing, iteration:

- pandas.DataFrame.head()
- pandas.DataFrame.iat
- pandas.DataFrame.iloc
- pandas.DataFrame.isin()
- pandas.DataFrame.reset_index()

Function application, GroupBy & Window:

- pandas.DataFrame.apply()
- pandas.DataFrame.groupby()
- pandas.DataFrame.rolling()

Computations / Descriptive Stats:

• pandas.DataFrame.describe()

- pandas.DataFrame.pct_change()
- pandas.DataFrame.mean()
- pandas.DataFrame.std()
- pandas.DataFrame.var()
- pandas.DataFrame.max()
- pandas.DataFrame.min()
- pandas.DataFrame.sum()
- pandas.DataFrame.prod()
- pandas.DataFrame.count()

Missing data handling:

- pandas.DataFrame.dropna()
- pandas.DataFrame.fillna()
- pandas.DataFrame.drop()

Reshaping, sorting, transposing

- pandas.DataFrame.pivot_table()
 - Arguments values, index, columns and aggfunc are supported.
 - Annotation of pivot values is required. For example, @hpat.jit(pivots={'pt': ['small', 'large']}) declares the output pivot table pt will have columns called small and large.
- pandas.DataFrame.sort_values() by argument should be constant string or constant list of strings.
- pandas.DataFrame.append()

2.3.6 DatetimeIndex

- pandas.DatetimeIndex.year
- pandas.DatetimeIndex.month
- pandas.DatetimeIndex.day
- pandas.DatetimeIndex.hour
- pandas.DatetimeIndex.minute
- pandas.DatetimeIndex.second
- pandas.DatetimeIndex.microsecond
- pandas.DatetimeIndex.nanosecond
- pandas.DatetimeIndex.date
- pandas.DatetimeIndex.min()
- pandas.DatetimeIndex.max()

2.3.7 TimedeltaIndex

- pandas.TimedeltaIndex.days
- pandas.TimedeltaIndex.seconds
- pandas.TimedeltaIndex.microseconds
- pandas.TimedeltaIndex.nanoseconds

2.3.8 Timestamp

- pandas.Timestamp.day
- pandas.Timestamp.hour
- pandas.Timestamp.microsecond
- pandas.Timestamp.month
- pandas.Timestamp.nanosecond
- pandas.Timestamp.second
- pandas.Timestamp.year
- pandas.Timestamp.date()

2.3.9 Window

- Rolling.count
- Rolling.sum
- Rolling.mean
- Rolling.median
- Rolling.var
- Rolling.std
- Rolling.min
- Rolling.max
- Rolling.corr
- Rolling.cov
- Rolling.apply

2.3.10 GroupBy

- Groupby.apply
- Groupby.count
- Groupby.max
- Groupby.mean
- Groupby.median

- Groupby.min
- Groupby.prod
- Groupby.std
- Groupby.sum
- Groupby.var

2.4 Why HPAT isn't working for my code?

HPAT statically compiles user codes to generate efficient parallel programs. Hence, the user code needs to be *statically compilable*. This means that HPAT should be able to infer all the variable types, and be able to analyze the computations.

2.4.1 Type Stability

To enable type inference, the program should be *type stable*, which means every variable should have a single type. The example below is not type stable since variable a can be both a float and an array of floats:

```
if flag:
    a = 1.0
else:
    a = np.ones(10)
```

The use of isinstance operator of Python often means type instabillity and is not supported.

Similarly, function calls should also be deterministic. The below example is not supported since function f is not known in advance:

```
if flag:
    f = np.zeros
else:
    f = np.random.ranf
A = f(10)
```

One can usually avoid these cases in numerical code without significant effort.

REFERENCES

HPAT implements Pandas and Numpy API as a DSL. Data structures are implemented as Numba extensions, and compiler stages are responsible for different levels of abstraction. For example, Series data type support and Series transformations implement the Pandas Series API. Follow the pipeline for a simple function like *Series.sum()* for initial understanding of the transformations.

3.1 HPAT Technology Overview

This slide deck provides an overview of HPAT technology and software architecture.

These papers provide deeper dive in technical ideas (might not be necessary for many developers):

- HPAT paper on automatic parallelization for distributed memory
- · HPAT paper on system architecture versus Spark
- HPAT Dataframe DSL approach
- ParallelAccelerator DSL approach

3.2 Numba

HPAT sits on top of Numba and is heavily tied to many of its features. Therefore, understanding Numba's internal details and being able to develop Numba extensions is necessary.

- Start with basic overview of Numba use and try the examples.
- User documentation is generally helpful for overview of features.
- ParallelAccelerator documentation provides overview of parallel analysis and transformations in Numba (also used in HPAT).
- Setting up Numba for development
- Numba architecture page is a good starting point for understanding the internals.
- Learning Numba IR is crucial for understanding transformations. See the IR classes. Setting NUMBA_DEBUG_ARRAY_OPT=1 shows the IR at different stages of ParallelAccelerator and HPAT transformations. Run a simple parallel example and make sure you understad the IR at different stages.
- Exending Numba page provides details on how to provide native implementations for data types and functions. The low-level API should be avoided as much as possible for ease of development and code readability. The unicode support in Numba is an example of a modern extension for Numba (documentation planned).

- A more complex extension is the new dictionary implementation in Numba (documentation planned). It has examples of calling into C code which is implemented as a C extension library. For a simpler example of calling into C library, see HPAT's I/O features like get_file_size.
- Developer reference manual provides more details if necessary.

CHAPTER

FOUR

DISTRIBUTED

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