Data Reduction and Partitioning in an Extreme Scale GPU-Based Clustering Algorithm

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DRBSD-2 Workshop
November 17th 2017
Denver, CO
Our History with Scalable Reductions

MRNet was built as a scalable reduction framework for debuggers, performance tools, and applications. Scalability is achieved by a software defined tree based overlay network (TBON). [Roth 04]
Our History with Scalable Reductions

Debuggers

Performance Tools

Applications

MRNet

Stack Trace Analysis Tool
[Arnold 2007]

Live debugging of millions of processes (max run to date 6+ million procs at LLNL). MRNet provides the scaleable reduction of stack traces collected from processes.
Since STAT’s release, MRNet has been used as the reduction framework by a number of commercial debuggers.
Our History with Scalable Reductions

Debuggers

Performance Tools

Applications

MRNet

TAU

[2004 - 2017]

Performance monitoring framework. MRNet is used to scalable collect performance data from thousands of nodes.

MRNet

STAT

Cray

CCBD

Total

View

Cray

ATP

TAU

[Nataraj 2008]
Our History with Scalable Reductions

Commercial and open source tools have continued to use MRNet for scalable communication.
Our History with Scalable Reductions

Debuggers
- STAT
- Cray CCBD
- Total View
- Cray ATP

Performance Tools
- MRNet
- TAU
- CBTF
- Open Speed Shop
- CEPBA Toolkit

Applications
- Mean Shift [Arnold 2006]

Scalable method of identifying local maximums in a data set (mean shift algorithm).

Data Reduction and Partitioning in Mr. Scan
Our History with Scalable Reductions

_Debuggers_

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_Performance Tools_

- MRNet
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- Open Speed Shop
- CEPBA Toolkit

_Applications_

- Mean Shift
- Highly scalable density based clustering algorithm. First known implementation to scale to over thousands of nodes and to process billions of points
- Mr. Scan

[Welton 2014]

2004

Data Reduction and Partitioning in Mr. Scan
MRNet – Multicast / Reduction Network

General-purpose Tree Based Overlay Network (TBON)

- **Network**: user-defined topology
- **Stream**: logical data channel
  - to a set of back-ends
  - multicast, gather, and custom reduction
- **Packet**: collection of data
- **Filter**: stream data operator
  - User definable aggregation and reduction operations.
- Fully asynchronous across multiple streams.

Data Reduction and Partitioning in Mr. Scan
Introducing Mr. Scan

Mr. Scan is a scalable density-based clustering algorithm

Designed to cluster billions of data points.
Clustering Example (DBSCAN[1])

Goal: Find regions that meet minimum density and spatial distance characteristics

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\textsuperscript{[1]} M. Ester et. al., A density-based algorithm for discovering clusters in large spatial databases with noise, (1996)
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Clustering Example (DBSCAN$^1$)

$MinPts$: 3

The two parameters that determine if a point is in a cluster is $\text{Epsilon (Eps)}$ and $\text{MinPts}$. If the number of points in $\text{Eps}$ is greater than $\text{MinPts}$, the point is a core point.

For every discovered point, this same calculation is performed until the cluster is fully expanded.

Clustering Example (DBSCAN$^{[1]}$)

$\text{MinPts: 3}$

The two parameters that determine if a point is in a cluster is $\varepsilon$ ($\varepsilon$), and $\text{MinPts}$. If the number of points in $\varepsilon$ is $\gt \text{MinPts}$, the point is a core point.

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Intro to Mr. Scan

Mr. Scan Phases

Partition: Distributed

DBSCAN: GPU (on BE)

Merge: CPU (x #levels)

Sweep: CPU (x #levels)
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Data Reduction and Partitioning in Mr. Scan
Properties of a Scalable TBON App

Applications must have the following properties to be scalable in a TBON:

\[ F(x_1, \ldots, x_n) \]
Properties of a Scalable TBON App

Applications must have the following properties to be scalable in a TBON:

- Same amount of work across all nodes in the tree.

![Diagram of TBON architecture with nodes and functions labeled]

\[ F(x_1, \ldots, x_n) \]
Properties of a Scalable TBON App

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Mr. Scan must have these properties to scale.

Data Reduction and Partitioning in Mr. Scan
Challenges To Scaling DBSCAN

Workload Balance:
- DBSCAN requires that points near one another must be processed on the same node.

Size of data needed for merging:
- Simple merging methods require sending all points in all clusters to merge accurately
  - Sending billions of points in the merge phase is infeasible.
Our Solutions

Solve the balance and data size issues jointly with the following techniques:

- **Smart Partitioning**
  - Selectively performing redundant computation to reduce merge data size (using data duplicated at edge of each partition).
  - Use an estimate of partition density to identify hard to compute partitions.

- **Dense Box Algorithm**
  - Reduces the complexity of computation of extremely dense partitions.

- **Representative Points**
  - Leverage the redundant computation to create a merge method that requires only a small fixed subset of points.
Partition Phase
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The DBSCAN Density Problem

- Imbalances in point density can cause huge differences in runtimes between Thread Groups inside of a GPU (10-15x variance in time)
  - Issue is caused by the lookup operation for a points neighbors in the DBSCAN point expansion phase.

\[ \varepsilon \]

Higher density results in higher neighbor count which increases the number of comparison operations.
Dense Box

- **Dense Box** eliminates the need to perform neighbor lookups on points in dense regions by labeling points as a member of a cluster before DBSCAN is run.

1. Start with an $\epsilon$ region.
2. Divide the region of data into areas of size $\frac{\epsilon}{2\sqrt{2}}$ for dense area detection*.
3. For each $\frac{\epsilon}{2\sqrt{2}}$ area which has point count $\geq$ MinPts. Mark points as members of a cluster. Do not expand these points.

* $\frac{\epsilon}{2\sqrt{2}}$ chosen because it guarantees all points inside are within $\epsilon$ distance of each other.
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Merge Algorithm

- **Two phases in the merge operation**
  - 1. Select Representative points (Leaf Node)
  - 2. Merge operation (Internal Node)
Representative Points (Leaf Nodes)

- Large clusters are too expensive to move up the tree
- In border regions we select eight representative points to represent the cluster
- These points guarantee that any overlap of clusters detected on adjacent nodes
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Merge Operation (Internal Nodes)

- Merge overlapping clusters found on different DBSCAN leaf nodes
- Merge needs to have low overhead and must operate without the entire dataset (Representative Points + Non-Core points)

MinPts = 3

Data Reduction and Partitioning in Mr. Scan
Merge Operation (Internal Nodes)

Compare representative points sent by leaf nodes

- If an overlap in representative points exists between two nodes, those clusters merge.
- Otherwise, the clusters are complete and no further propagation of representative points occurs.

Cluster on Node 1 and 2 have overlapping representative points and are merged.
Merge Operation (Internal Nodes)

Compare representative points sent by leaf nodes

- If no overlap exists between clusters, finalize the clusters and do not propagate representative points.

No overlap in regions between Node 1 and 2. Clusters in both nodes are now final and no further propagation is needed.
Takeaway Lessons for Scalable Data Reduction

○ By selectively duplicating processing, we could use a less data intensive merging algorithm
○ We were able to equalize the workload between nodes by use of the dense box algorithm
○ Using these approaches, we were able to scale Mr. Scan up to 8192 nodes.
○ MRNet is a general scalability framework for data reductions
Questions?