Latest Development of Gunrock: a Graph Processing Library on GPUs

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https://gunrock.github.io
What is the Gunrock Library?

A CUDA-based graph processing library, aims for:

- **Generality**
  covers a broad range of graph algorithms

- **Programmability**
  makes it easy to implement graph algorithms
  extends to multi-GPUs as simple as possible

- **Performance**
  maintains good performance

- **Scalability**
  fits in (very) limited GPU memory space
  performance scales when using more GPUs
Programming Model

A generic graph algorithm:

Data-centric abstraction
- Operations are defined on a group of vertices or edges \( \equiv \) a frontier
  => Operations = manipulations of frontiers

Bulk-synchronous programming
- Operations are done one by one, in order
- Within a single operation, computing on multiple elements can be done in parallel, without order
How to Write a Graph Primitive with Gunrock?

=> Section S8586, Writing Graph Primitives with Gunrock

Key items for a graph primitive / app:

- Problem: data used by the algorithm
- Enactor: operations on the data
- App: higher level routines
- Test: CPU reference and result verification
New APIs

External interfaces
- **app.**: callable from external
- **graph**: external data structures (e.g. GoAI)
- **operator**: calls external operators (e.g. GraphBLAS)

Test Driver
- **Problem = App. specific data**
- **Graph loader / generator**

1 Run = 1 set of parameters + 1 Enact()
1 Experiment = multiple runs with different parameters

Application
- **Iteration-loop**

Iteration
- **Frontier**
  - **Operator**
  - **Operator**

Graph

1 Run             = 1 set of parameters + 1 Enact()
1 Experiment     = multiple runs with different parameters
New APIs - oprtr::Advance

```
cudaError_t gunrock::oprtr::Advance
<FLAG> (          // type (V2V, V2E, etc.) and
  // option (Idempotence, Mark_Preds, ...)
  graph,            // graph representation
  input_frontier,   // input set of elements
  output_froniter,  // output set of elements
  oprtr_parameters, // operator parameters (stream, etc.)
  advance_op,       // per-element advance lambda
  filter_op)        // per-element filter lambda (optional)
```

- Only 7 parameters, down from 20+
- Interface independent of graph representations
  - App. implementation isolated from graph representations
  - Operator will select a suitable implementation based on the given graph representation(s)
- Advance and filter operator share the same interface
- Lambda operator signatures are fixed for advance and filter
- Merged Cond. and Apply functors in older API
New APIs - oprtr::Advance

Example: SSSP advance

```cpp
auto advance_op = [distances, weights, preds] __host__ __device__ (  
    const VertexT &src, VertexT &dest, const SizeT &edge_id,  
    const VertexT &input_item, const SizeT &input_pos, SizeT &output_pos) -> bool
{
    ValueT src_distance = Load<cub::LOAD_CG>(distances + src);
    ValueT edge_weight  = Load<cub::LOAD_CS>(weights + edge_id);
    ValueT new_distance = src_distance + edge_weight;
    if (new_distance >= atomicMin(distances + dest, new_distance))
        return false;
    Store(preds + dest, src);
    return true;
};

// Call the advance operator, using the advance operation
oprtr::Advance<oprtr::OprtrType_V2V>(
    graph.csr(), frontier.V_Q(), frontier.Next_V_Q(),
    oprtr_parameters, advance_op, filter_op);
```
New APIs - oprtr::Filter

```cpp
cudaError_t gunrock::oprtr::Filter
<FLAG> (          // type (V2V, V2E, etc.) and
    // option (Idempotence, Mark_Preds, ...)
graph,            // graph representation
input_frontier,   // input set of elements
output_froniter,  // output set of elements
oprtr_parameters, // operator parameters (stream, etc.)
advance_op,       // per-element advance lambda (optional)
filter_op)        // per-element filter lambda
```

Example: SSSP filter

```cpp
auto filter_op = __host__ __device__ ([labels, iteration] (const VertexT &src, VertexT &dest, const SizeT &edge_id,
    const VertexT &input_item, const SizeT &input_pos,
    SizeT &output_pos) -> bool
{
    if (!util::isValid(dest)) return false;
    if (labels[dest] == iteration) return false;
    labels[dest] = iteration;
    return true;
};
```

// Call the filter operator, using the filter operation
oprtr::Filter<oprtr::OprtrType_V2V>(
    graph.csr(), frontier.V_Q(), frontier.Next_V_Q(),
    oprtr_parameters, filter_op);

Filter:
select and reorganize
New APIs - Compute Operators

```cpp
cudaError_t gunrock::util::Array1D<...>::__ForEach__(
    compute_op,   // per-element computation lambda (w/o pos)
    num_elements, // number of elements
    target,      // where to perform the computation, CPU or GPU
    stream)      // cudaStream
```
New APIs - Graph Primitives / Apps

```cpp
template <typename GraphT, ..., ProblemFlag FLAG>
struct Problem : ProblemBase<GraphT, FLAG>
{
    Problem(util::Parameters &parameters,
             ProblemFlag flag = Problem_None);

cudaError_t Init(GraphT &graph,
                  util::Location target);

cudaError_t Reset(src, target);

cudaError_t Extract(distances, preds, target);

cudaError_t Release(target);
};

template <typename Problem, ...>
struct Enactor : public EnactorBase<...>
{
    Enactor();
    cudaError_t Init(Problem &problem, target);
    cudaError_t Reset(src, target);
    cudaError_t Enact(src, target);
    cudaError_t Release(target);
};
```

Template: data types & option switches
util::Parameters: running parameters
src, distances, preds: algorithm specific inputs
target: where to do the action
Init: initialization, only do once
Reset: data / status reset, do for each run
Enact: invoke the algorithm implementation
Extract: get back the results
Release: clean-up
New APIs - External Interfaces

// @brief Entry of gunrock_sssp function
// @tparam GraphT Type of the graph
// @tparam ValueT Type of the distances
// @param[in] parameters Execution parameters
// @param[in] graph Input graph
// @param[out] distances Shortest distances from source
// @param[out] preds Predecessors of each vertex
// \return double Accumulated elapsed times

template <
    typename GraphT,
    typename ValueT = typename GraphT::ValueT>

double gunrock_sssp(
    gunrock::util::Parameters &parameters,
    GraphT &graph,
    ValueT **distances,
    typename GraphT::VertexT **preds = NULL)
{
    ...
}

<= Using gunrock data types
Using raw data pointers =>

Able to take in graphs in GPU
/ CPU memory

Able to take in different graph representations

=> GoAI and other libraries

<= Using gunrock data types
Using raw data pointers =>

Able to take in graphs in GPU
/ CPU memory

Able to take in different graph representations

=> GoAI and other libraries
New Features - Graph Representations

- Graph representation is isolated from most parts of Gunrock
  - Only operator implementations, graph generators & converters need to know the representation
  - Application level implementations does NOT need to know
    - External graph inputs (e.g. GoAI)
    - New graph representations (e.g. mutable graphs)

- Current status:
  - 3 basic representations: CSR, CSC, COO
  - SSSP on CSR, PR on COO
New Primitives - Random Walks

Find x random paths of given length y

- **Algorithm**
  
  \( Q_0 \leftarrow \{x \text{ randomly select source vertices}\} \)
  
  Do y iterations:
  
  \( Q_1 \leftarrow \{\} \)
  
  For each vertex v in \( Q_0 \):
  
  Randomly select a neighbor u of v

  Put u in \( Q_1 \)

  \( Q_0 \leftarrow Q_1 \)

Running time of GPU random walk
New Primitives - Graph Coloring

Find the minimum number of vertex sets (i.e. colors), such that no edge has endpoints in the same set

- **Algorithm**
  
  Assign each vertex a random number
  Do until no more independent sets are found:
  
  Assign vertices with the minimum and the maximum number among neighbors to two sets, respectively

- **Optimizations**
  
  ○ use more colors per iteration,
    
    => makes the problem simpler, but loses accuracy in terms of amount of colors.
New Primitives - Subgraph Matching

Find the occurrences of a small graph in a large graph a.k.a. graph isomorphism, more info => poster P8290

- Design a BFS-based algorithm, to leverage Gunrock’s high performance operators
- Use $k$-look-ahead, neighborhood encoding, and node equivalence, to generate fewer intermediate results

The algorithm =>

<= Speed-up of Enron dataset, compared to Tran et al.
New Primitives - Triangle Counting

Find the number of triangles in a graph

- Four implementations
  - Batch set-intersection
  - Batch set-intersection + filtered edge list
  - Subgraph matching
  - Matrix-matrix multiplication and element-wise multiplication

Execution-time speedup for our four GPU implementations vs. others

Leyuan Wang, Yangzihao Wang, Carl Yang, and John D. Owens. “A Comparative Study on Exact Triangle Counting Algorithms on the GPU”, HPGP `16
Better Scaling

Scales beyond 1-node multiple GPUs

● **Approach 1:**
  ○ use 1-node multiple GPU framework*
  ○ differentiate local and remote peer GPUs
  ○ use MPI for communications between remote peers

● **Tried with PageRank**
  => workable
  => but can’t scale to large number of GPUs

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*Yuechao Pan, Yangzihao Wang, Yuduo Wu, Carl Yang, and John D. Owens. “Multi-GPU Graph Analytics”, IPDPS `17.
Better Scaling

Scales beyond 1-node multiple GPUs

- **Approach 2:**
  * Separate high and low degree vertices
  * Use (I)AllReduce for high-d vertices
  * Use p2p Isend / Irecv for low-d vertices
  * Use bit-masks for high-d vertices
  * Use different computation kernels for different edge types

- **Tried with (DO)BFS**
  => works well
  => bit-masks only works for BFS, other apps will have higher communication costs

(DO)BFS weak scaling with a scale-26 RMAT graph per P100; 2x 100 Gbps + 4 P100s per node.
Upcoming - NeighborReduce

cudaError_t gunrock::oprtr::NeighborReduce
<FLAG> (          // type (V2V, V2E, etc.) and
   // option (Idempotence, Mark_Preds, ...)
graph,            // graph representation
input_frontier,   // input set of elements
output_froniter,  // output set of elements
oprtr_parameters, // operator parameters (stream, etc.)
advance_op,       // per-element advance lambda
reduce_op)        // neighborhood reduction lambda

auto reduce_op = [] __host__ __device__ (const VertexT &src, VertexT &dest, const SizeT &edge_id, const VertexT &input_item, const SizeT &input_pos, ValueT &val1, ValueT &val2, double probability) -> ValueT
{
  // return reduce(val1, val2);
}
Upcoming - More Graph Apps

- Clustering / Partitioning
- Abnormality Detections
- Asynchronous Graph Algorithms
- Cooperate with Machine Learning
- Mutable Graphs
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Q & A

Q: How can I find Gunrock?
A: https://gunrock.github.io/

Q: Papers, slides, etc.?

Q: Requirements?
A: CUDA ≥ 8.0, GPU compute capability ≥ 3.0, Linux || Mac OS

Q: Language?
A: C/C++, with a simple wrapper to connect to Python

Q: Is it free and open?
A: Absolutely (under Apache License v2.0)

Q: … (continue)