Hierarchical Partitioning for GPU-Based HPC Platforms

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Scalable Partitioning on GPUs
Motivation for our ongoing work

Overall Goal: Scalable partitioning for Multi-GPU platforms

Why? Representative of modern HPC architectures
▶ We consider hierarchical CPU+multi GPU systems.
▶ We consider large-scale scientific computing applications.

General challenges:
▶ Memory-constraints with efficient GPU memory usage.
▶ Extremely high parallel concurrency within node and across a distributed system.
▶ Hierarchical considerations for task placement, optimization criteria, etc. for both partitioning and target applications.
Prior Work: Porting XtraPuLP for GPUs

Challenges: Modifying CPU-only XtraPuLP for GPUs

- For distributed CPU processing, XtraPuLP demonstrated scaling to trillion-edge networks on thousands of MPI ranks. Porting to GPU at this kind of scale presents several common issues.
- Issue: Higher concurrency of GPU threading negatively impacts balancing phase. Part size and quality can wildly oscillate.
- Issue: Mitigating balance issue impacts scalability and speed.
- However: Refinement phase can still run quite efficiently.

Relative cut quality (left) and time (right) of GPU-XtraPuLP (G-XP) vs. XtraPuLP (XP) from 2–16 nodes/parts on a Sandia Labs application mesh. To achieve similar quality values on GPUs, we must restrict our allowable vertex→part movements over a larger number of iterations, reducing time to solution. In the plots, bigger is better.
Our Ongoing Work
And the topic of today’s talk (below in bold)

Observations:

▶ Modern spectral partitioners can give fast and high quality cuts on multiple GPUs (Acer et al., 2021).
▶ Efficient graph coarsening can also be performed on GPU (Gilbert et al., 2021).

Our current approach:

▶ We instead consider an initial balanced partitioning via a fast k-way spectral cut using Sphynx/Multi-Jagged in Trilinos.
▶ To mitigate memory overheads, we developed a constant memory representation for an arbitrary number of coarsening levels. We can extract the graph at any level.
▶ For coarsening, we are developing a parallel spectrum preserving method with nice theoretical guarantees.
▶ For refinement, we can use XtraPuLP to give us a fast, scalable, and relatively high quality final partition.
Constant memory coarsening

- Want to perform multilevel coarsening on a graph $G = (V, E)$ with constant memory overhead.
- We can do this using an array of size $2(n + m)$, where $n = |V|$ and $m = |E|$.
  
  a. Start with an adjacency list with $2m$ entries.
  
  b. For each node $v$ add an entry $nr + u$. $r$ is the level of coarsening that $v$ absorbed a node and $u$ is the node that was absorbed by $v$.
  
  c. For each node $v$ add an entry $nk + u$. $k$ is the level of coarsening that $v$ was absorbed and $u$ is the node that absorbed $v$.
  
  d. The first value acts as a pointer to continue the node adjacency of subsuming nodes. The other determines what node edges point to in the $k^{th}$ level of coarsening. We see this holding true in practice.
Constant memory coarsening

- Using this data structure we perform operations on the coarsened graph by checking our pointers.
- for instance...
  a. Can find the last node in a subsumption chain in $O(k)$ operations, where $k$ is the level of coarsening.
  b. Can determine the first node in our subsumption chain in $O(\log_2(k))$ operations.
  c. Can determine the nodes at the $k^{th}$ level of coarsening in $O(n)$ operations.
  d. Can recover the $k^{th}$ level graph in $O(n) + O(m\log_2(k))$ operations.
Spectral partitioning

We would like to be able to partition a given graph $G = (V, E)$ into equally weighted portions. A powerful tool for this is spectral partitioning as it provides us with useful global information and guarantees on cut quality.

- Requires $O(n^3)$ operations in the dense case.
- Requires $O(m)$ operations in the sparse case, with limited room for parallelism, and possible convergence issues.

Is there a way to coarsen a graph while closely preserving this information? Yes! However, they tend to be slow!

A spectral bound

A useful result (Jin. Loukas 2020) states the following...
If Λ and ̂Λ sorted vectors containing the eigenvalues of \( G \) and \( \hat{G} \) respectively. Then if we merge two nodes \( u, v \in V \) such that
\[
\| \frac{w_u}{d_u} - \frac{w_v}{d_v} \|_1 \leq \epsilon,
\]
we have,
\[
\| \Lambda - \hat{\Lambda} \|_\infty \leq \epsilon
\]
Explicit greedy method

Algorithm 1 Multilevel Graph Coarsening (MGC)

1: **Input:** Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$ and target size of the coarse graph $n$.
2: $s \leftarrow \mathcal{N}$
3: while $s > n$ do
4:   for $v_i \in \mathcal{V}_s$ do
5:     for $v_j \in \mathcal{N}_i$ do
6:       $d_s(i, j) = \left\| \frac{w(i)}{d(i)} - \frac{w(j)}{d(j)} \right\|_1$
7:     $i_{\min}, j_{\min} = \arg \min_{i, j} d_s(i, j)$
8:     $s \leftarrow s - 1$
9:     Merge nodes $v_{i_{\min}}$ and $v_{j_{\min}}$ to form the coarse graph $\mathcal{G}_s$.
10: return $\mathcal{G}_n = (\mathcal{V}_n, \mathcal{E}_n, \mathcal{W}_n)$
It’s too slow!

Their algorithm requires $O(n^2 m)$ work with dense vector operations, or $O(n^2 \langle d^2 \rangle)$ work with sparse vectors. We propose a heuristic to reduce this to $O(n \langle d^2 \rangle)$ work where $\langle d^2 \rangle$ is the second moment of the degree distribution. Furthermore our method is parallelizable and can be performed in $O(n^2 \langle d^2 \rangle)$ parallel time.
An observation

Spectral error arising from merges only compounds when multiple merges overlap.

- This means our error is bounded relative to our largest merged subgraph, instead of all merges.
- In fact, if we only perform merges between nodes which are connected, the spectral error after all merges will be bounded above by $D\epsilon$, where $D$ is the diameter of the largest merged subgraph, and $\epsilon$ is the largest norm-difference between any two individual merged nodes.
An observation

This observation allows us to never have to recompute norm-differences!

- We can obtain a spectral approximation of our graph using only the norm-differences $\| \frac{w_u}{d_u} - \frac{w_v}{d_v} \|_1$ in the original graph.

- This avoids the outer-loop in their explicit greedy method, and reduces the complexity by a factor of $n$, giving us a $O(n \langle d^2 \rangle)$ work algorithm.
Our algorithm

**Input:** $G = (V, E)$, $r$, $p$

**Result:** coarsened graph $G_c$

$G_c \leftarrow G$

$\text{merge\_fitness} \leftarrow \emptyset$

$\{E_1, \cdots, E_p\} \leftarrow \text{edgePartition}(E, p)$

for $i=1$ to $p$ in parallel do
  for $j=1$ to $|E_i|$ do
    $u \leftarrow E_i[j][1]$
    $v \leftarrow E_i[j][2]$
    $\text{merge\_fitness} \leftarrow \text{merge\_fitness} \cup ( \| \frac{w_u}{d_u} - \frac{w}{d_v} \|_1, E_i[j])$
  end
end

ascendingSort( \text{merge\_fitness} )

for $i=1$ to $|V| - r$ do
  $G_c \leftarrow \text{merge}(G_c, \text{merge\_fitness}[i][0], \text{merge\_fitness}[i][2])$
end

return: $G_c$
Our algorithm

As mentioned, out algorithm without parallelization has serial time $O(n \langle d^2 \rangle)$, and with parallelization the edge-weight calculations are reduced to $O(\frac{n}{p} \langle d^2 \rangle)$.

- We then perform a sort that requires $O( m \log(m) )$ work. Can be parallelized to $O(\frac{m}{p} \log(m))$ time.
- The merges must be done sequentially, and require $O( n - r )$ work.

Overall for this leaves us with an $O(\frac{n}{p} \langle d^2 \rangle + \frac{m}{p} \log(m) + (n - r))$ parallel time algorithm.
Results

We present scaling results from three example graphs. Two meshes from the Stanford 3D scanning repository, the “Stanford Bunny” (35,947 nodes, 104,176 edges) and “Dragon” (437,645 nodes, 1,307,121 edges), as well as the small “ego-Facebook” (4,039 nodes, 88,234 edges) graph from the SNAP network repository.

We also present some spectral approximation results.

*All runs were on a single nVidia Quadro M5000
Scaling Results

Bunny mesh strong scaling

- double precision
- single precision
Scaling Results

Dragon mesh strong scaling

- double precision
- single precision

![Graph showing scaling results with double and single precision lines.](image-url)
Scaling Results

Facebook graph (small) strong scaling

- double precision
- single precision

![Graph showing scaling results for Facebook graph with strong scaling. The graph compares time (ms) vs. threads, with a trend line for double precision and single precision, showing a decrease in time as the number of threads increases.]
Spectrum Results

Facebook coarsened spectra

Value vs. eigenvalue index

- original
- coarsened
Spectrum Results

Bunny coarsened spectra

- original
- coarsened

value

0.00 0.25 0.50 0.75 1.00 1.25 1.50

0 5000 10000 15000 20000 25000 30000 35000
eigenvalue index
Future Work

- As mentioned, the merges currently have to be done serially. However, this isn't necessarily true. If we have disjoint merges they can be parallelized. Therefore, by weighting edges inversely to their fitness function and performing a maximal matching we can further speed up our algorithm via parallel merges.

- This method relies on storing several arrays in GPU memory. This quickly leads to spatial constraints. Large graphs will require distributing the structure over multiple GPUs.

- One of our primary avenues for ongoing and future work is full integration with Sphynx/Multi-Jagged and XtraPuLP in distributed memory.
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Summary and Thanks

▶ We implemented a constant-memory graph representation for graph coarsening.
▶ We developed a spectrum preserving coarsening algorithm.
▶ We observe constant memory utilization in practice and promising strong scaling results for our coarsener.
▶ TODO: extend our coarsening to distributed GPUs and integrate with other methods for full partitioning.

Thank you!

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