MSc in HPC Project Proposal

Hugh Delaney

June 18, 2021

Project Supervisor: Kirk Soodhalter
Secondary Supervisor: Jose Refojo
Research Area: Computational Graph Theory

Project Brief

Let A to be the adjacency matrix of an undirected graph, G.

The matrix exponential is defined as:

$$e^{\beta A} = \sum_{k=1}^{N} \frac{\beta^k}{k!} A^k$$

$[e^{\beta A}]_{ij}$ gives us a good measure of the communicability of nodes i, j in a graph. This is due to the fact that $[A^k]_{ij}$ tells us the number of walks of length k between nodes i,j.

The graph exponential therefore gives us a weighted sum of walks of all lengths across our graph, where the weight is determined by $\beta > 0$, an inverse temperature parameter which can increase or decrease the importance of long walks between nodes i, j. Note that when A is hermitian, $e^{\beta A}$ is also hermitian.

In my project I will endeavour to compute the action of $\exp(A)$ on a vector v such that $\|v\| = 1$. The default choice will be the vector of ones, scaled by $\sqrt{n}$. The graph exponential is almost never computed explicitly, but rather by approximation, using Krylov methods. The Lanczos algorithm with some preconditioning is usually applied for such procedures. Parallel Lanczos methods to compute the exponential are not common in academic literature, which may be a challenge. See (1) and (2)

Implementation Details

I will aim to compute $\exp(A)v$, $\|v\| = 1$ using a parallel Lanczos-based algorithm. The implementation will use both MPI and CUDA.

A brief outline of steps in the project:

Primary Goals

- Writing a parallel Lanczos algorithm to compute $\exp(A)v$ on a sparse graph, using the METIS graph partitioning library to split the graph among processes.
  - In parallel using MPI
  - In parallel using MPI and CUDA
- Modifying the code to accomodate increasingly irregular graphs, with partitions among processes becoming increasingly involved being those outputted by METIS. The levels of complexity involved are as followed:
  - Graphs which can be neatly partitioned among processes without overlapping edges between processes (this is equivalent to a master-slave serial algorithm).
  - Graphs with more and more edges overlapping between processes (with edge cuts approximately minimized by METIS).

Secondary Goals

- Writing a serial graph-partitioning algorithm in the same vein as the METIS graph partitioning library, which is suitable for scale-free graphs, or graphs whose nodes' degrees follow a power law distribution, making the graphs highly irregular.
- Making the Lanczos algorithm run using the graph partitions found from self-written graph partitioning algorithm. Comparing the results with the results from METIS partition.

Partial Completion

The project will aim to complete all of the Primary Goals, and will only go on to the Secondary Goals once all Primary Goals have been accomplished. In the event that the Primary Goals take longer than anticipated, the project will terminate at a reasonable date, with as many Secondary Goals completed as possible (potentially none). The order in which Secondary goals are attacked is liable to change from the sequential order listed here.

References

1. Jasper vanden Eshof and Marlis Hochbruck. *Preconditioning lanczos approximations to the matrix exponential.* SIAM J. Sci. Comput., 27:1438–1457, November 2005.
2. Lorenzo Orecchia, Sushant Sachdeva, Nisheeth K. Vishnoi. *Approximating the Exponential, the Lanczos Method and an O(m)-Time Spectral Algorithm for Balanced Separator*