CATEGORY: **VISUALIZATION - IN-SITU & SCIENTIFIC - VS04**

POSTER **P5200**

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GPU TECHNOLOGY CONFERENCE

G^{3}NA: A GPU Optimized Global Gene Network Alignment Tool.

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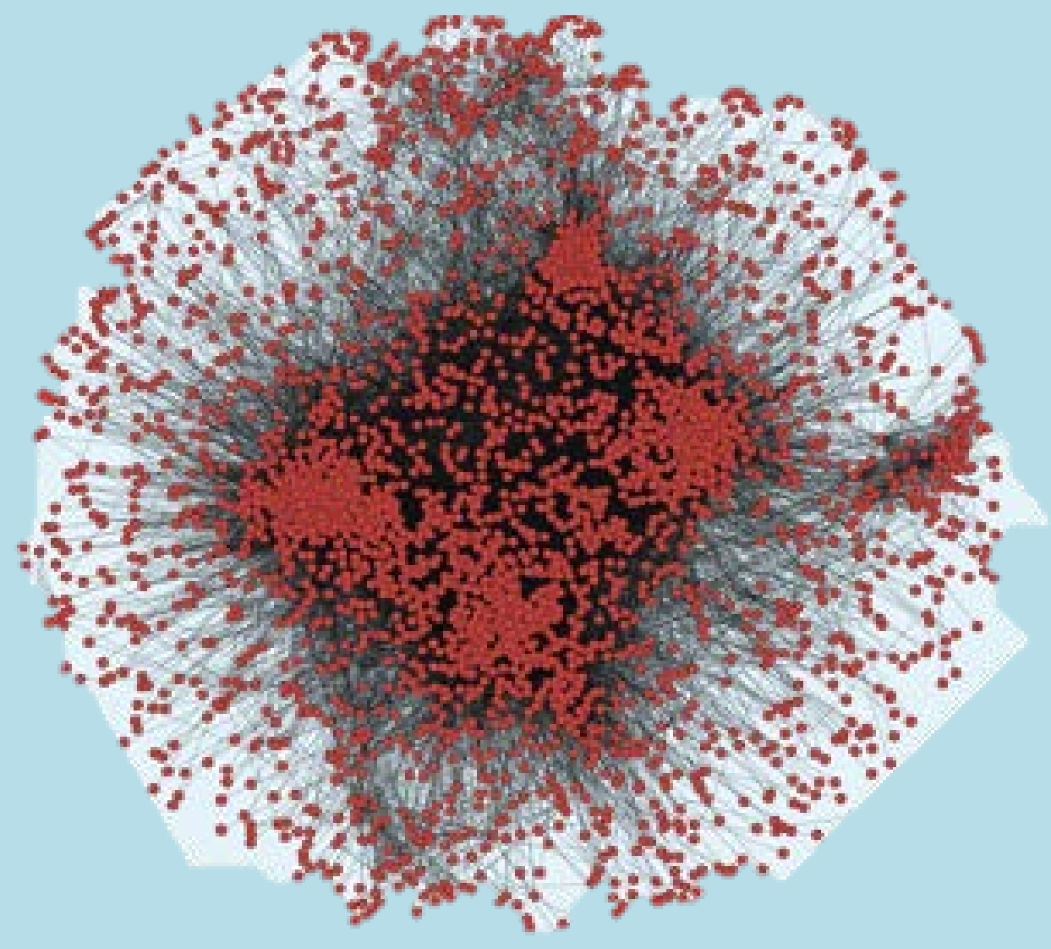
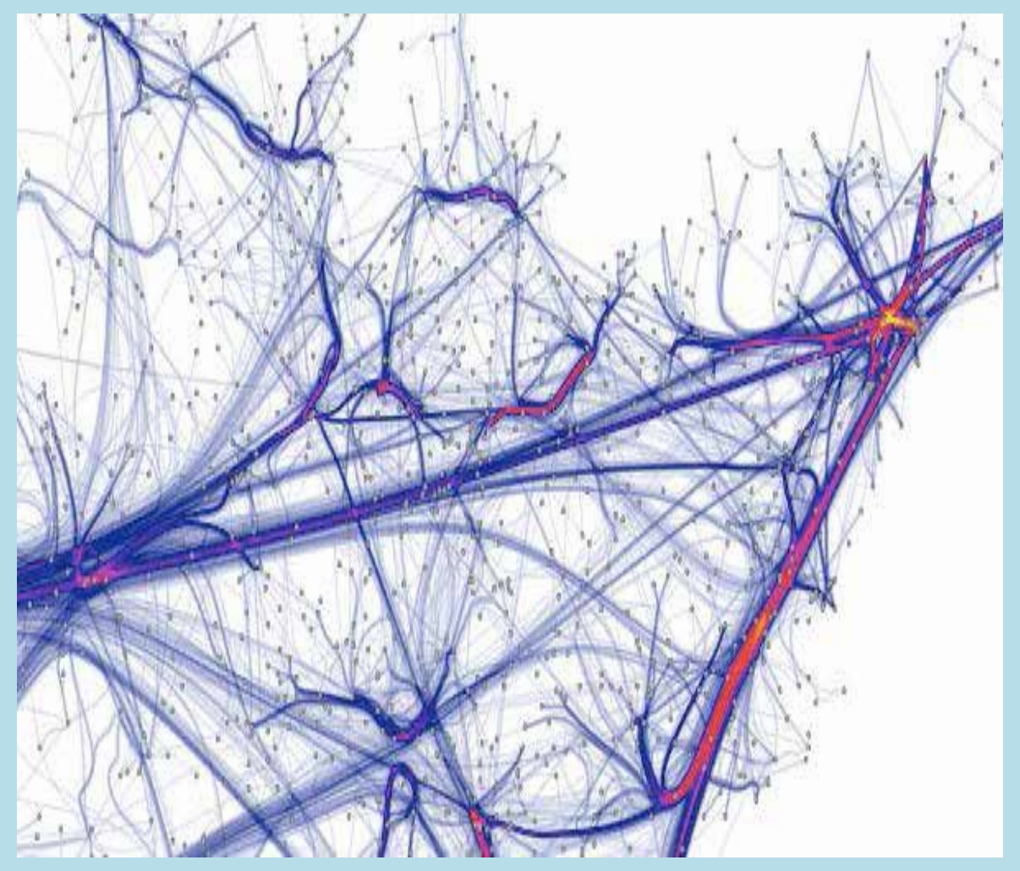
Abstract

Gene interaction graphs help genomics researchers discover gene expression patterns across multiple tissues and experimental conditions. Alignment of these graphs reveals conserved sub-graphs that show evolutionarily or condition conserved sets of genes controlling biological processes. However, alignment of medium sized graphs (2000+ nodes) is computationally expensive and visually overwhelming, and for large graphs alignment can become unrealistic without the use of advanced computing resources. Thus, we have developed a GPU based optimized framework to perform multi-genomic network alignment and in-situ based visualization using GPUs. We aligned two gene interaction networks from rice and maize (each ~2,000 nodes/~20,000 edges) on the Palmetto Supercomputer using NVIDIA K20 GPUs. Maize-rice alignment took 152 seconds compared to 8 hours with IsoRankN. For larger random network (8,000 nodes/60,000 edges), we observed a speed-up of 51.3x.We examine the results of alignment using a visualization tool. Furthermore, we provide visualization of these networks using OpenGL on Palmetto and WebGL on a web-browser.

MOTIVATION

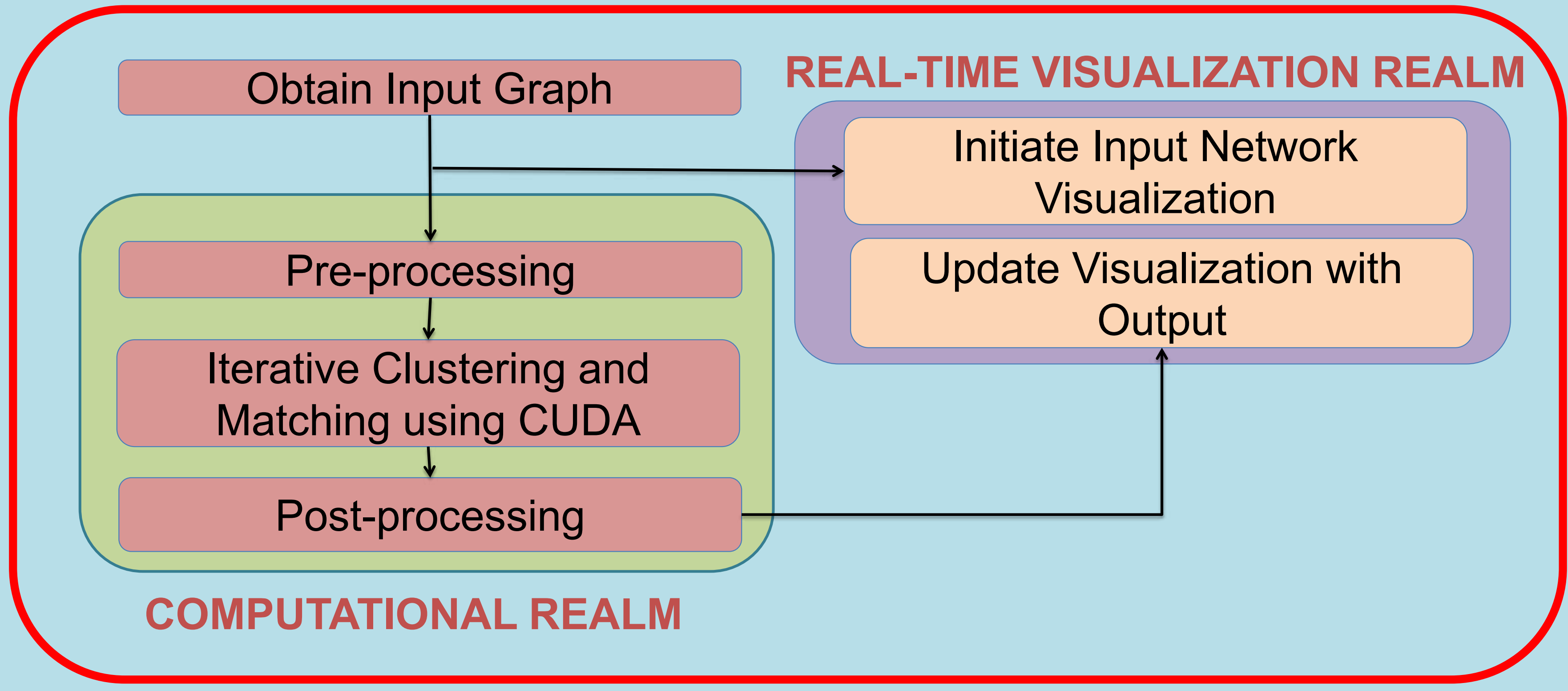




- **Medium Networks such as Rice and Maize go up to 2000 Nodes and 40,000 Edges**
- **Large Scale Networks such as for Humans can go up to 10,000 Nodes and 200,000 edges**
- **Analysis and Visualization of Large-scale Network**
- **Real-time In-situ visualization is tough with large-scale**
- **GPUs are really good at Computation and Visualization**
- **Existing Approaches do not utilize the GPU or all the resources on a node completely.**

OUR APPROACH

G3NA Workflow



REAL-TIME VISUALIZATION REALM

Obtain Input Graph

Initiate Input Network Visualization

Update Visualization with Output

Pre-processing

Iterative Clustering and Matching using CUDA

Post-processing

COMPUTATIONAL REALM

Input: {***Graph A***, ***GRAPH B***, ***Homology Graph A–B***}
Primary Output: {***Interaction Graph A-B***}
Secondary Output: {***Web-Browser based Visualization***, ***GPU Based Visualization***}

Computation Realm

- CUDA code performs the alignment of Graph A and Graph B on Palmetto using NVIDIA K20s
- Python scripts for Pre- and Post-Processing
- Can perform multi network-alignment using pair-wise alignment

Visualization Realm

- Real-time *OpenGL and CUDA based variation of* force-directed layout visualization on Palmetto using NVIDIA K20s
- Web-Browser based visualization using *WebGL*
- Interaction and attribute based layout in 2D and 3D

PERFORMANCE RESULTS

GPU versus Serial Implementation

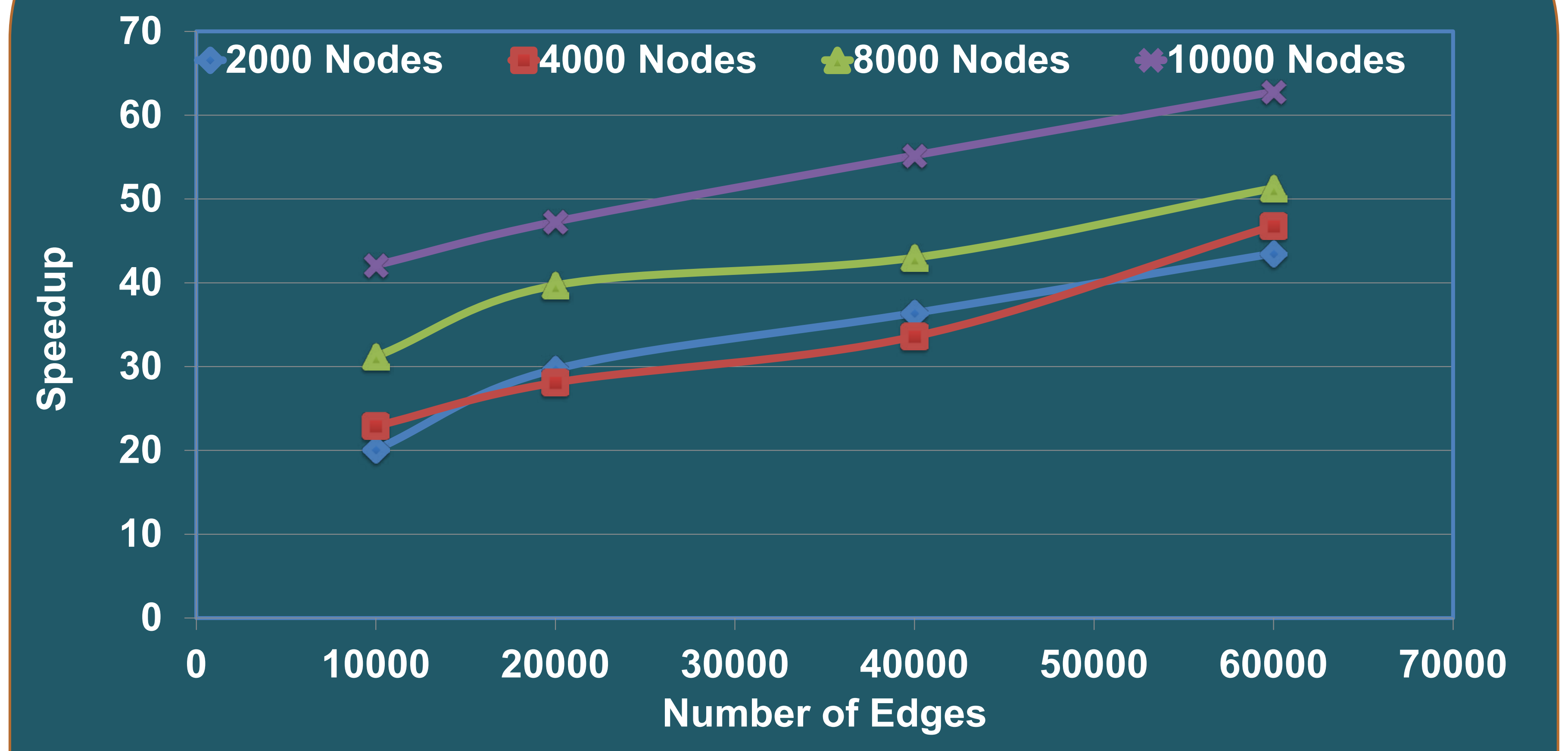


Figure 1. Speedup *for varying of nodes and edges in each of the two input graphs.*

Visualization

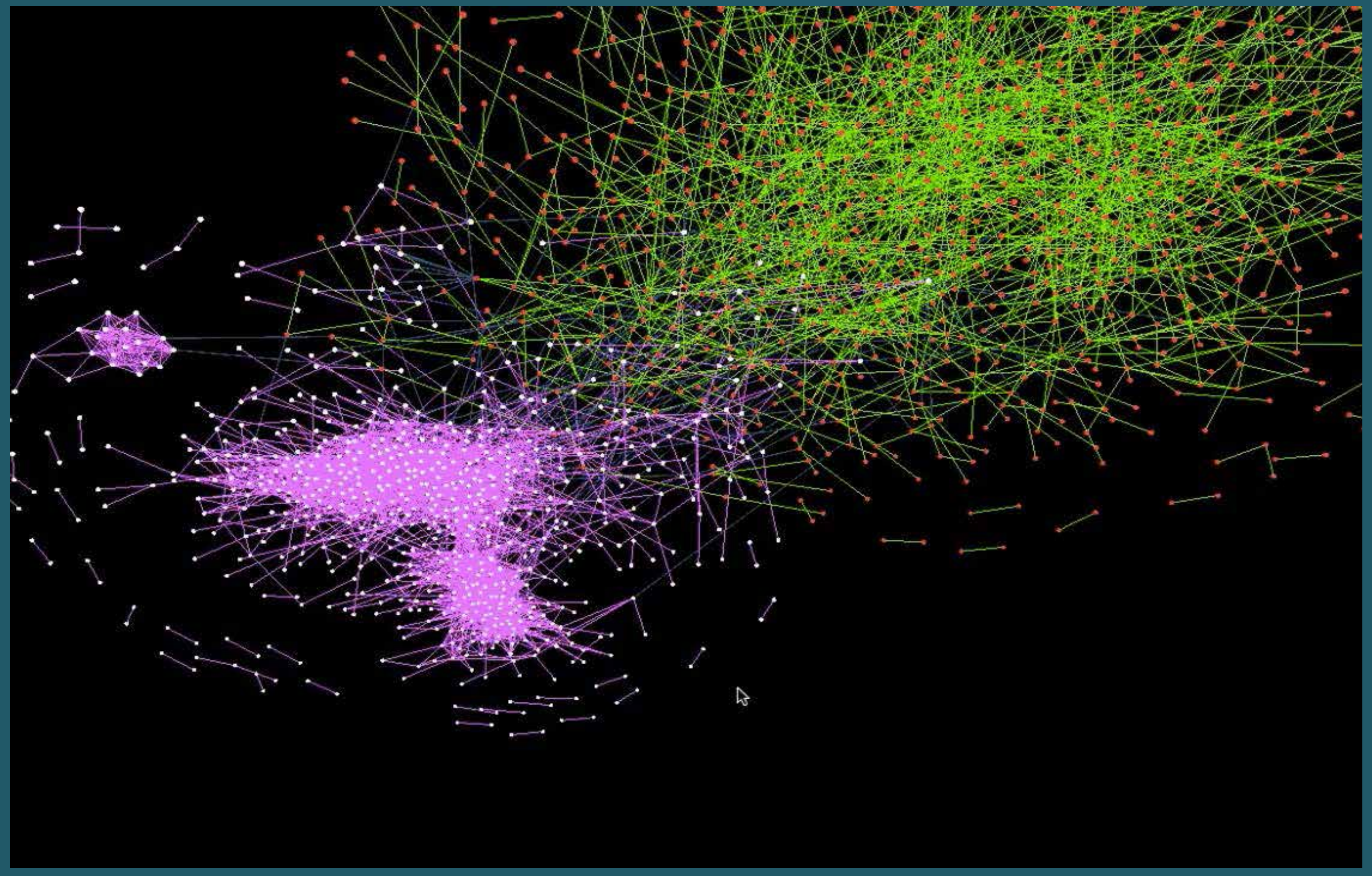


Figure 2. Palmetto based Network Alignment visualization using CUDA and OpenGL.

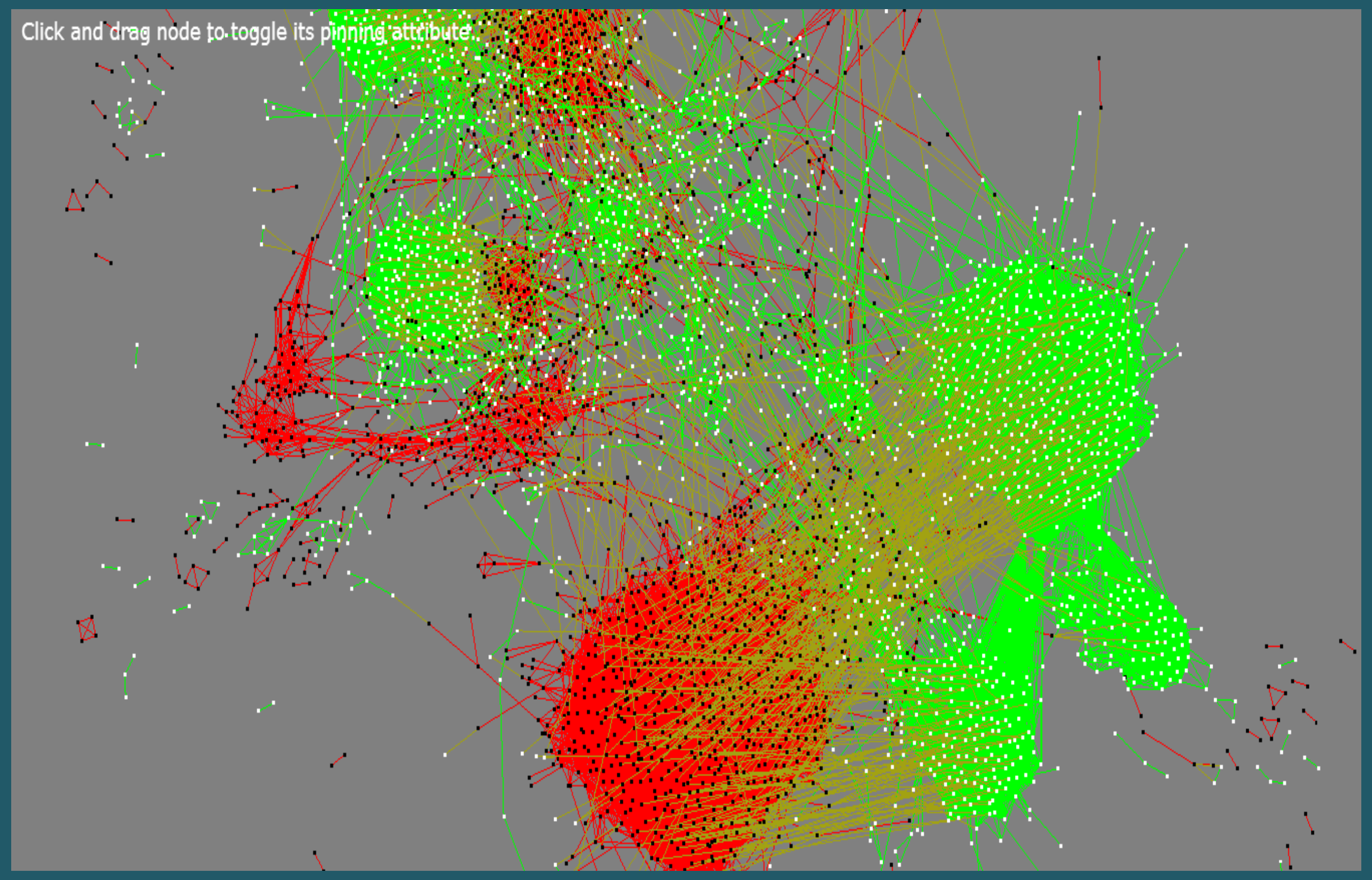


Figure 3. Web-Browser based Network Alignment visualization using WebGL and VivaGraphJS.

CONCLUSION

- We developed a framework that makes the node as a self-contained entity by perform GPU based alignment and visualize multiple gene interaction networks on the Palmetto Supercomputer on an NVIDIA K20s in real-time.
- Both Maize and Rice Network are ~2,000 nodes networks with ~20,000 edges in the network. The alignment of Maize and Rice network takes 152 seconds compared to 8 hours of IsoRankN [Liao et al. 2009] and obtain 32.1x speed-up compared to a serial version for the maize and rice network. For larger random network containing 8,000 nodes and 60,000 edges, we observed a speed-up of 51.3x.
- We have developed a web-interface for submission of alignment jobs for external research community.