Parallel/GPU Computing and HPC Research: Past, Present and Future

Research Conclave 2025 Talk @ TCE

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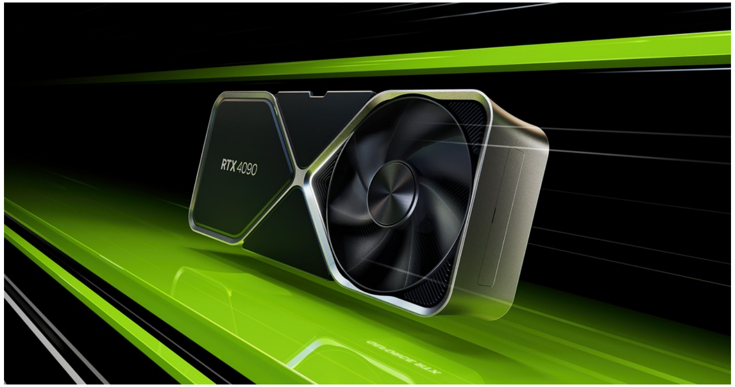
Outline

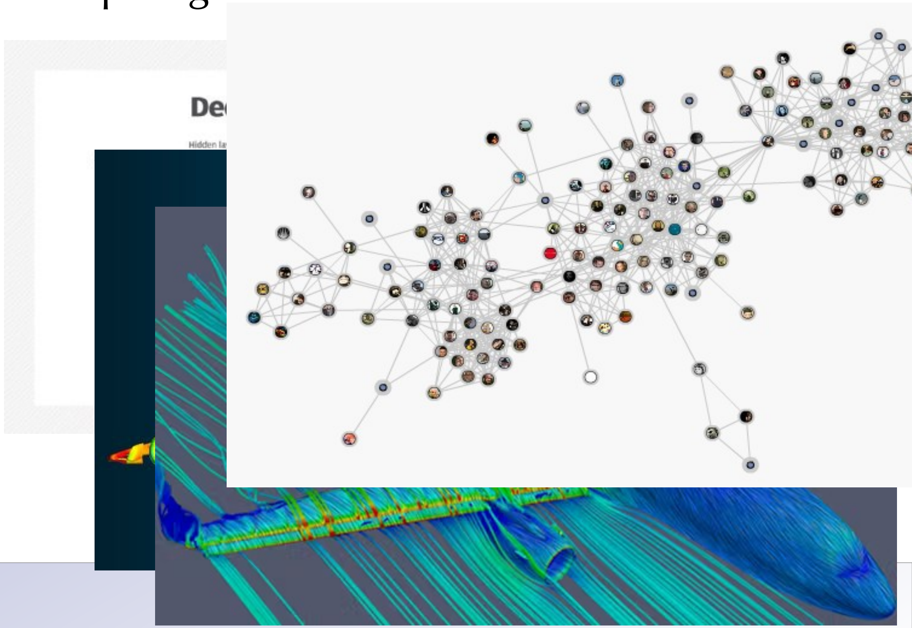
- Motivation
- Beginning of GPGPU era
  - It all started here in India/IIIT
- Present
  - Graph algorithms
  - AI/ML Training
- Future
- Summary



Motivation

- Graphics
  - 3D Games
  - Video rendering
  - 3D Graphics
  - Animations

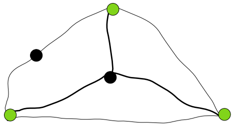
- Non-Graphics
  - Machine learning
  - Scientific simulations
  - HPC
  - Graph algorithms



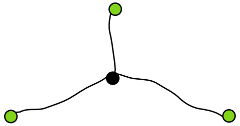
Sequential Computing

Input
Small -> less time
Large -> longer time

Input



Output

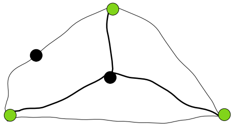


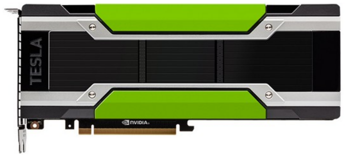
Graph

- Minimum Spanning Tree
- Single source shortest path

Parallel Computation

Input

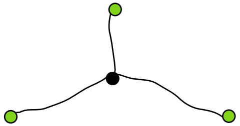


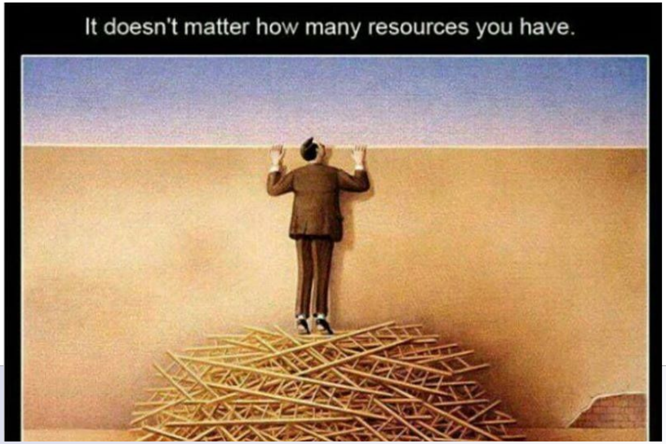


+

Efficient Algorithms

Output





Top 10 super computers. 7/10 GPUs
Checkout top500.org

2016. Joel Hruska 10 years ago, Geforce 8800 graphics card changed PC gaming, computing forever

Parallel Platforms

Software/Frameworks

CUDA

MPI

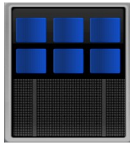
OpenMP

ROCm

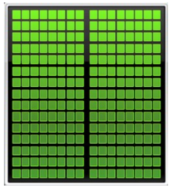
OpenACC

OpenCL

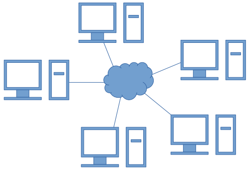
Underlying hardware for parallelization



CPU



GPU



Distributed

The beginning of GPGPU

Accelerating large graph algorithms on the GPU using CUDA

Pawan Harish and P. J. Narayanan

Center for Visual Information Technology
International Institute of Information Technology Hyderabad, INDIA
{harishpk@research., pjn@}iiit.ac.in

Abstract. Large graphs involving millions of vertices are common in many practical applications and are challenging to process. Practical-time implementations using high-end computers are reported but are accessible only to a few. Graphics Processing Units (GPUs) of today have high computation power and low price. They have a restrictive programming model and are tricky to use. The G80 line of Nvidia GPUs can be treated as a SIMD processor array using the CUDA programming model. We present a few fundamental algorithms – including breadth first search, single source shortest path, and all-pairs shortest path – using CUDA on large graphs. We can compute the single source shortest path on a 10 million vertex graph in 1.5 seconds using the Nvidia 8800GTX GPU costing $600. In some cases optimal sequential algorithm is not the fastest on the GPU architecture. GPUs have great potential as high-performance co-processors.

HiPC'2007

Why GPU for graph processing?

- <u>GPU for General Purpose = GPGPU</u>

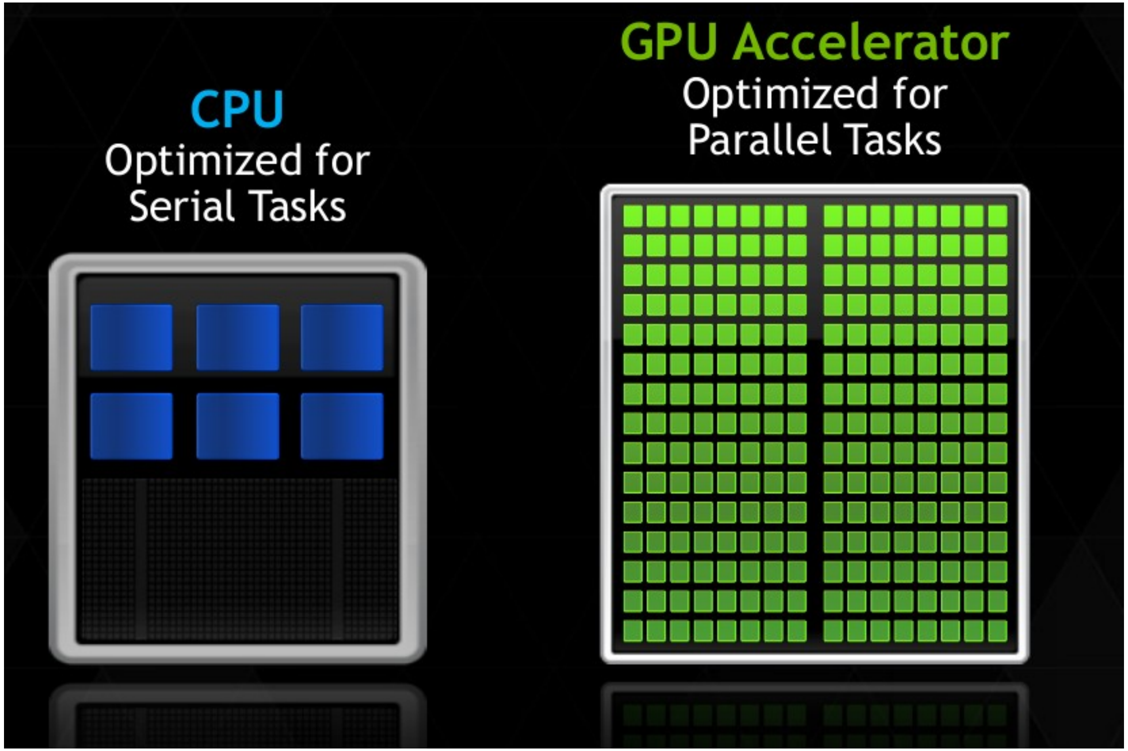
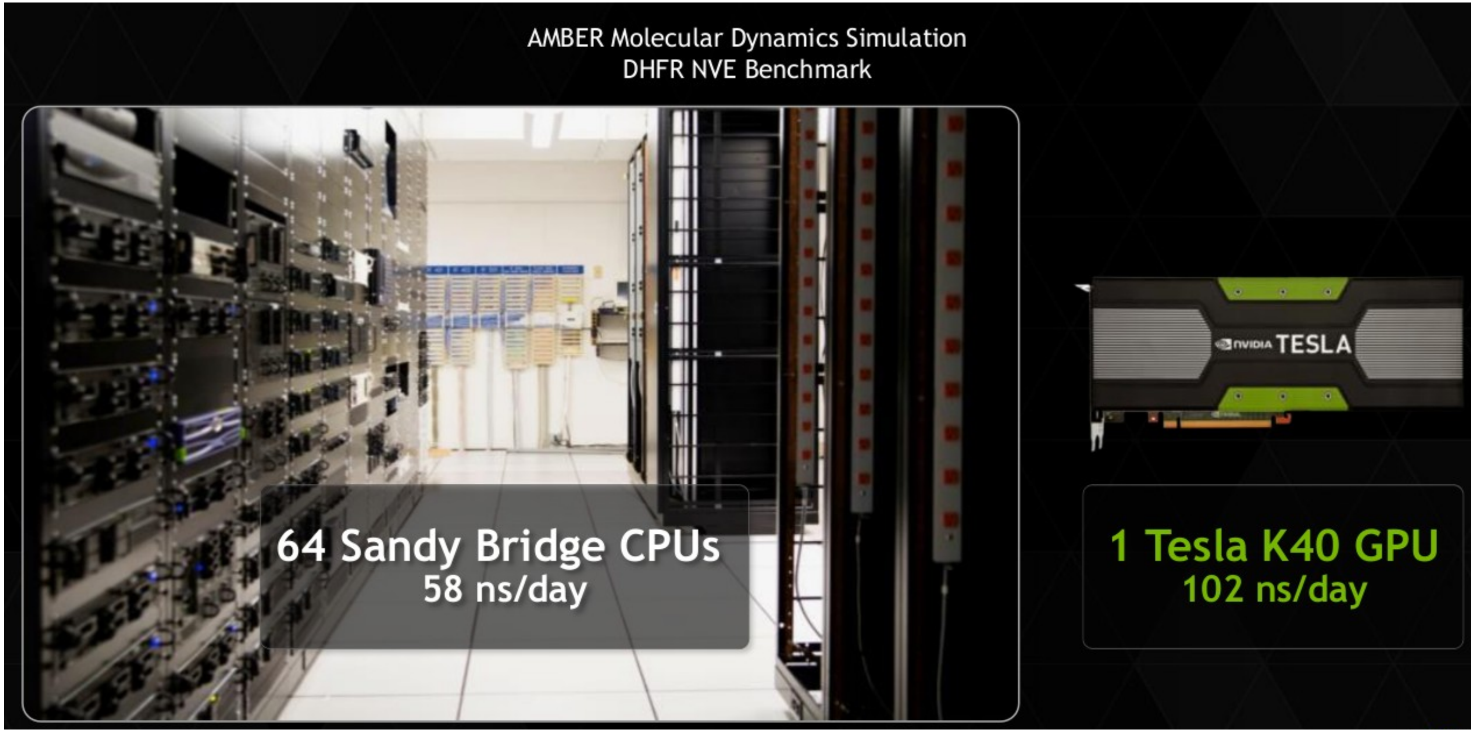


Image Source: GPU Technology Conference (GTC) 2014

Why GPU for graph processing?

- GPU for General Purpose = GPGPU
- Computation power



Source: GPU Technology Conference (GTC) 2014
Harvey et al. *Journal of Chemical Theory and Computation*, 2009

Why GPU for graph processing?

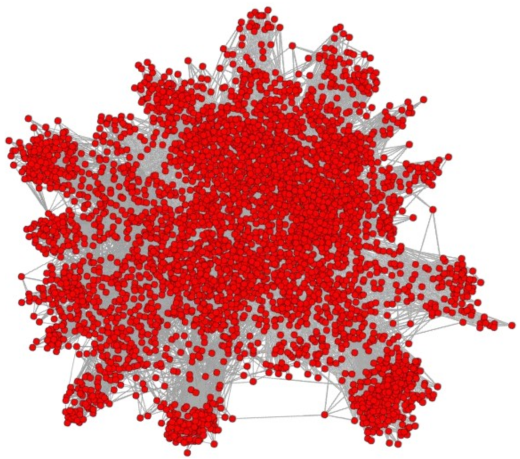
- GPU for General Purpose = GPGPU
- Computation power
- Lesser cost
- Energy efficient

  compared with CPUs

Image Source: GPU Technology Conference (GTC) 2014

Graphs are everywhere

- Networks: Road, Social, Biological, Wireless, and more.
- Such Graphs are extremely large.
- Faster computation is expected.



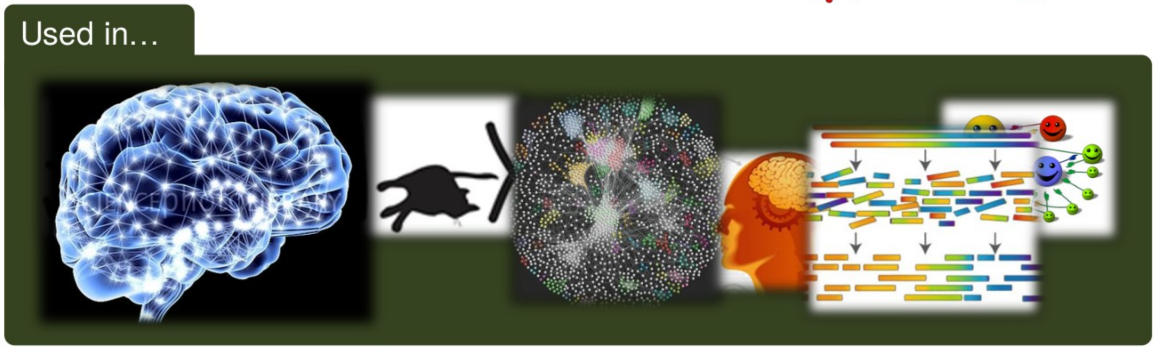
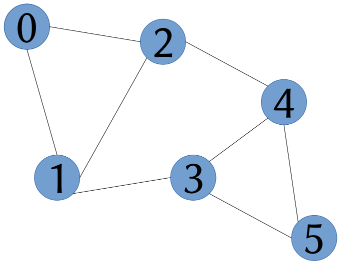


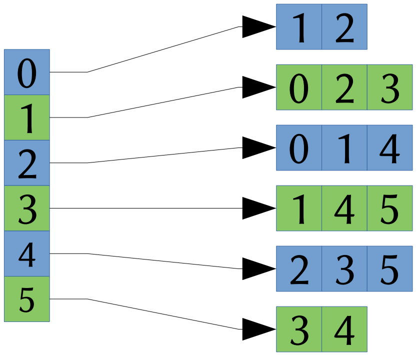
Image Source: https://spcl.inf.ethz.ch/Publications/.pdf/pushpull-slides.pdf

Graph Representation

- Adjacency Matrix
- Adjacency list



$$
\begin{array}{c}
0\\1\\2\\3\\4\\5\\ \\
\end{array}
\begin{array}{c}
\begin{pmatrix}
0 & 1 & 1 & 0 & 0 & 0\\
1 & 0 & 1 & 1 & 0 & 0\\
1 & 1 & 0 & 0 & 1 & 0\\
0 & 1 & 0 & 0 & 1 & 1\\
0 & 0 & 1 & 1 & 0 & 1\\
0 & 0 & 0 & 1 & 1 & 0
\end{pmatrix}\\
\begin{matrix} 0 & 1 & 2 & 3 & 4 & 5 \end{matrix}
\end{array}
$$



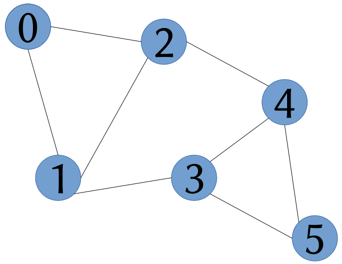
Graph Representation – EdgeList

- EdgeList / Coordinate Format (COO)
- Compressed Spare Row (CSR)

Reduce repetitions?

0	0	1	1	1	2	2	2	3	3	3	4	4	4	5	5

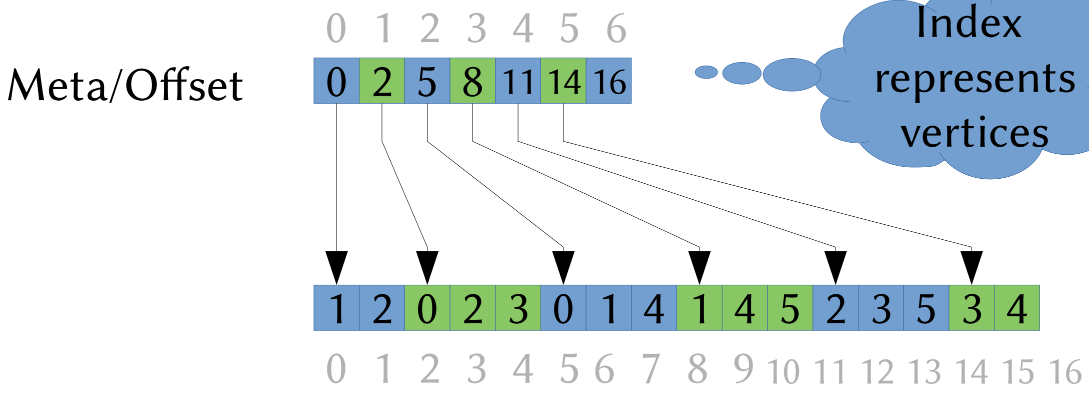
1	2	0	2	3	0	1	4	1	4	5	2	3	5	3	4



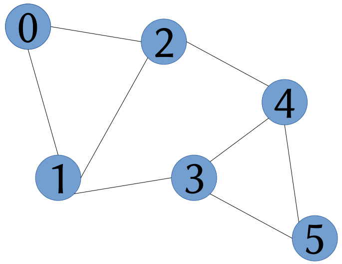
Two 2m-sized array

Graph Representation - CSR

- EdgeList / Coordinate Format (COO)
- Compressed Spare Row (CSR)



Index represents vertices



Well suited on GPUs

Two arrays:

Offset array : n+1

CSRList : 2m

https://networkrepository.com/mtx-matrix-market-format.html

Operator-formulation approach

```
Initialize(G,...);
do {

    Operator-Apply(G,...);
    // on set of nodes, edges
    // or property of G

} while (condition);
```

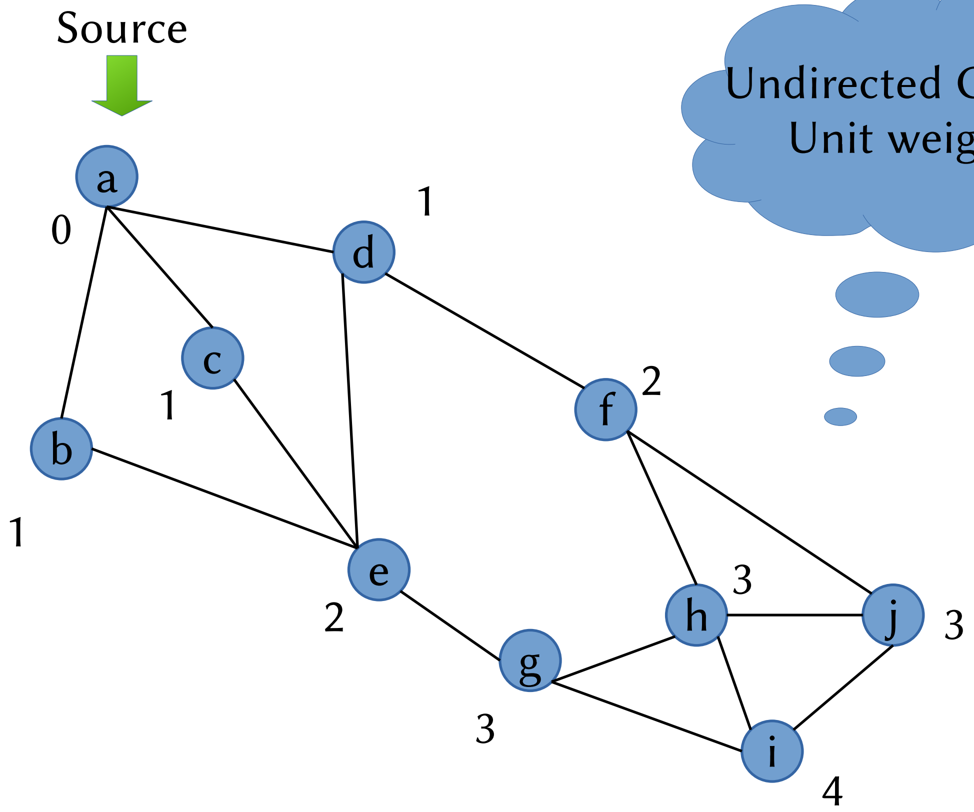
Parallel

Operator = GPU kernel

- BFS // Computing level information from source
- SSSP // Propagating distance from source

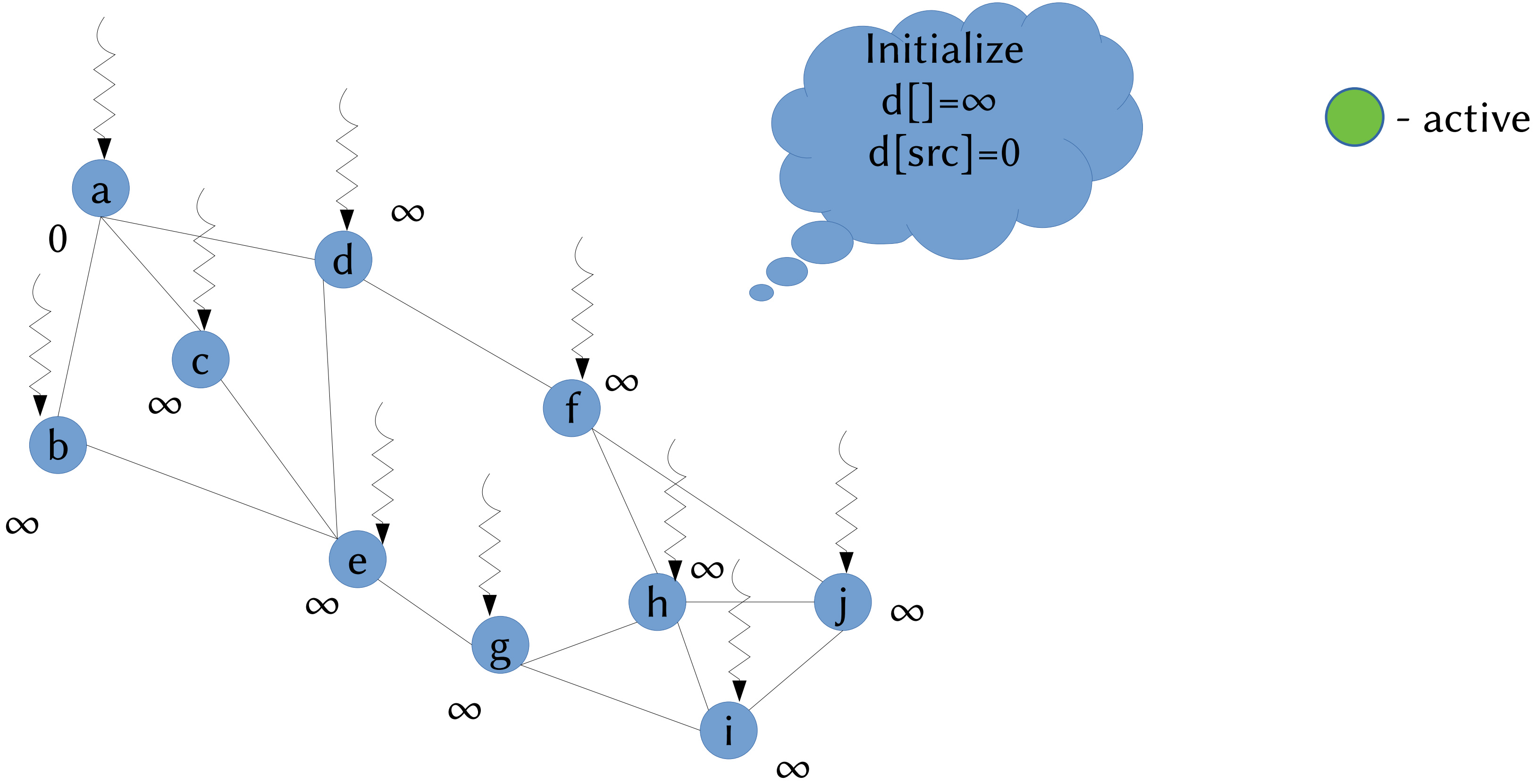
Pingali et. al. *The Tao of parallelism in algorithms.* **PLDI**, 2011

BFS/SSSP



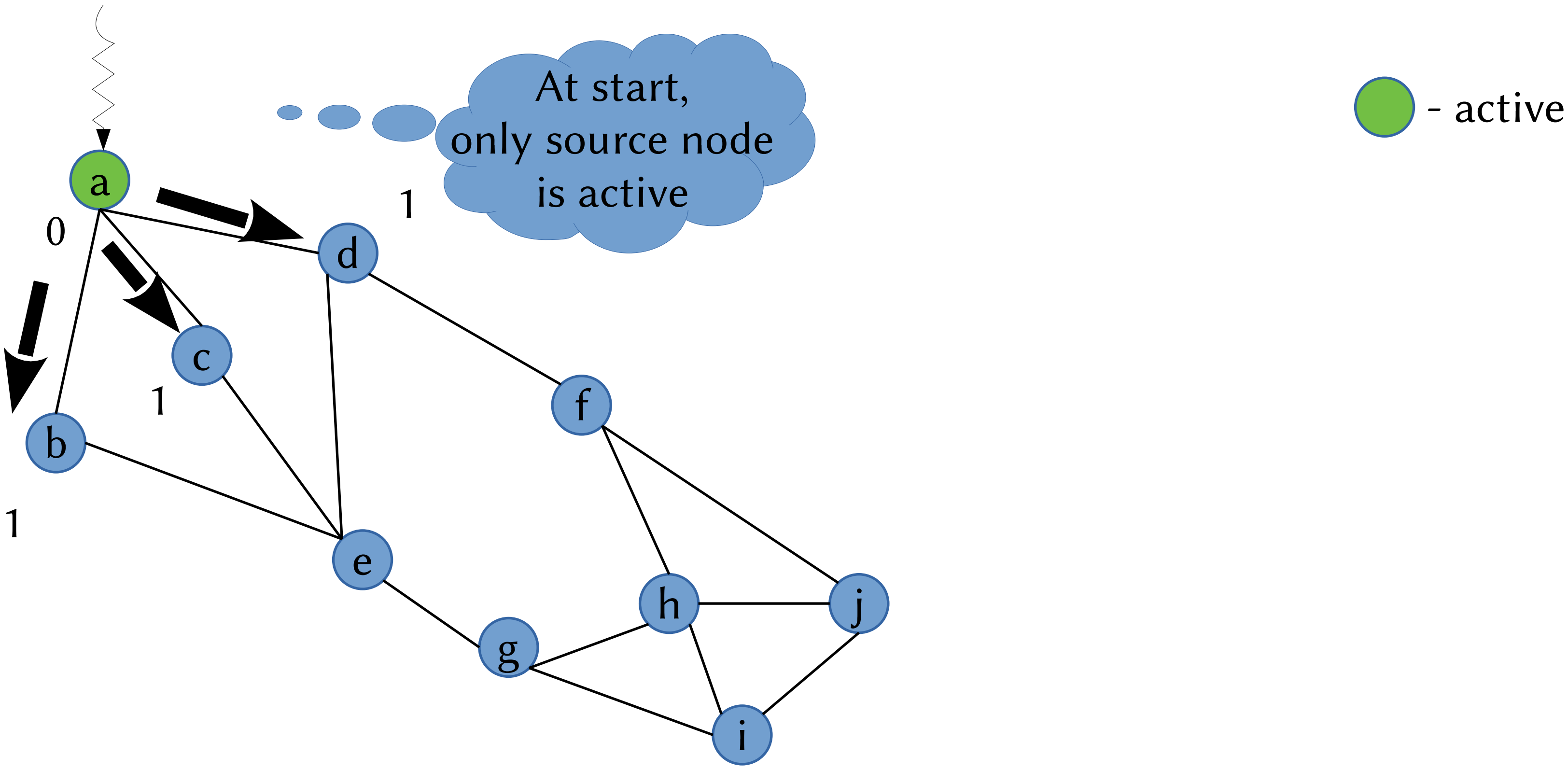
Undirected Graph.
Unit weights

SSSP: Single Source Shortest Path



Rupesh Nasre; Martin Burtscher; Keshav Pingali.
Data-Driven Versus Topology-driven Irregular Computations on GPUs, IPDPS 2013.

SSSP: Data-driven



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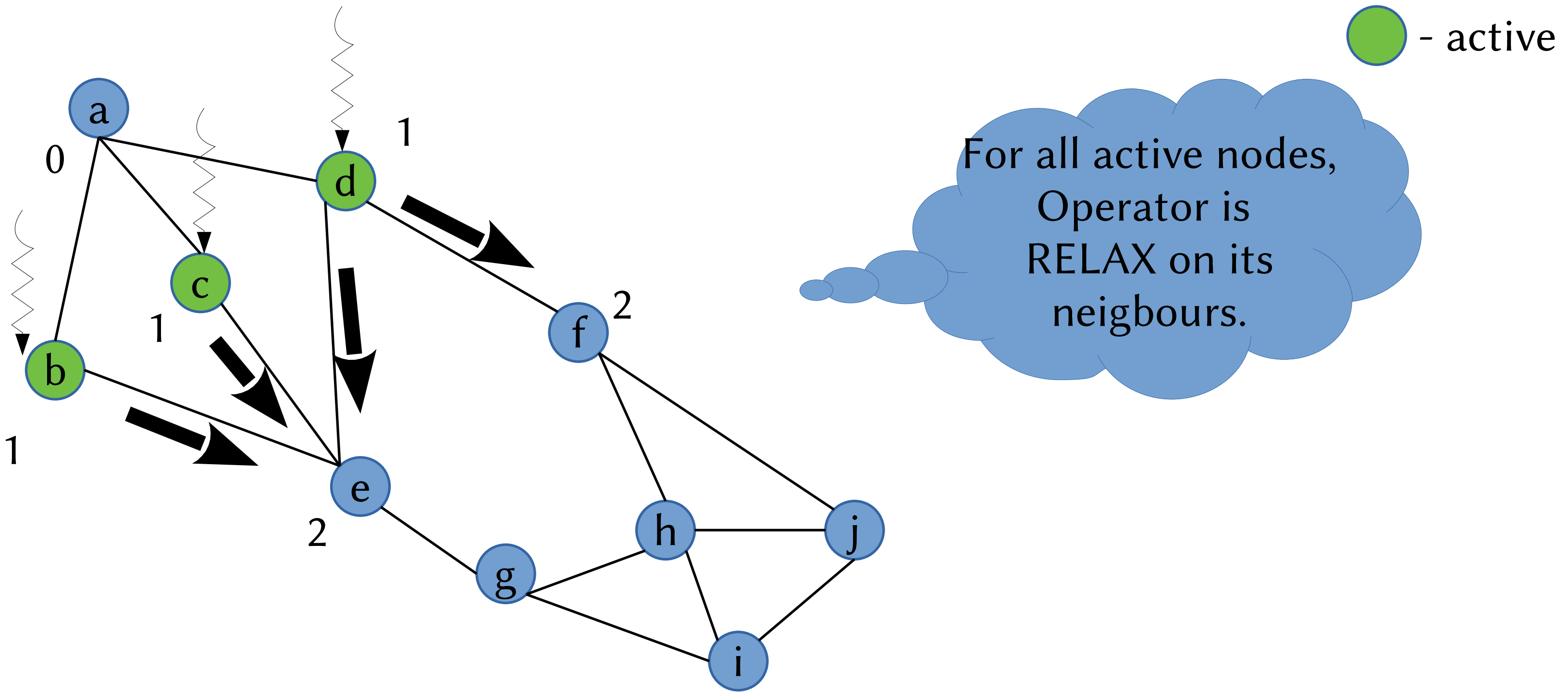

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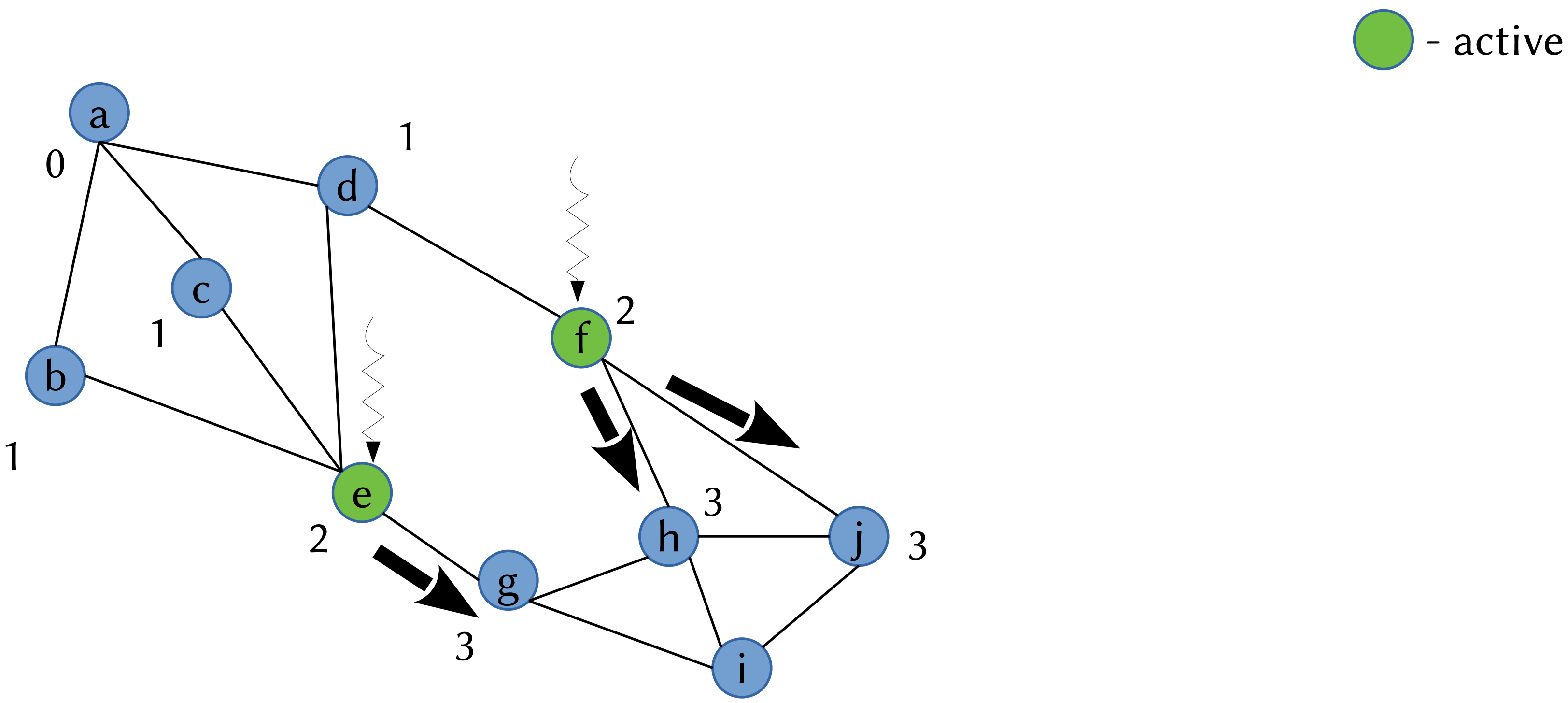
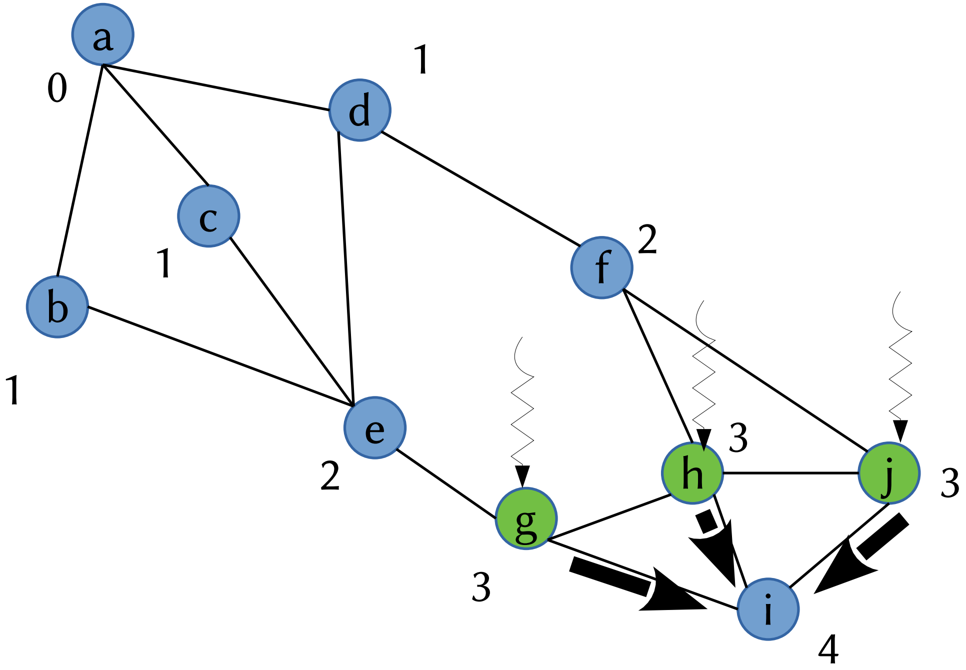


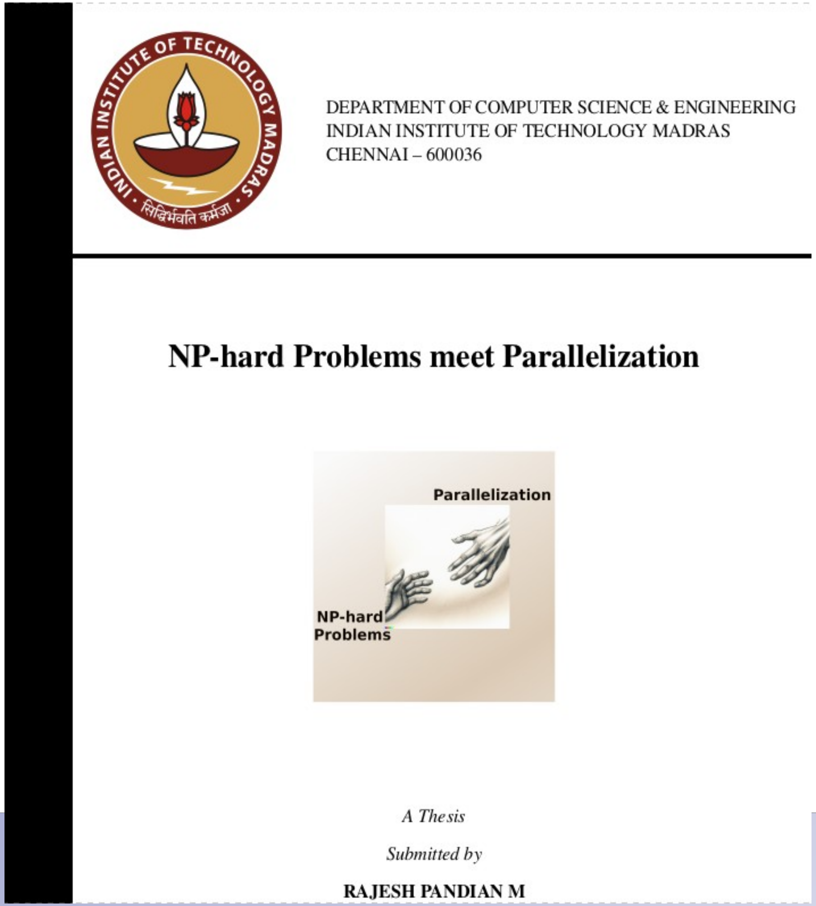
SSSP: Data-driven



- active

- Stop condition = No active node
- This Algorithm is Poly-time

PhD Thesis


DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY MADRAS
CHENNAI – 600036

NP-hard Problems meet Parallelization

A Thesis

Submitted by

RAJESH PANDIAN M

Steiner Tree Problem
Generalization of Min Spanning Tree

Vehicle Routing
Generalization of Travelling Salesman

Best sequential Algorithm → Parallelize → Run on GPU/Parallel HW

Our Philosophy

... take a **fresh look** at some of the classic graph algorithms and devise **faster** and more parallel GPU and CPU implementations.

- Fallin et al.

+

NP-hard

=

Our Philosophy

A High-Performance MST Implementation for GPUs

Alex Fallin, Dept. of Computer Science, Texas State University, San Marcos, Texas, USA, waf13@txstate.edu

Andres Gonzalez, Dept. of Computer Science, Texas State University, San Marcos, Texas, USA, ag1548@txstate.edu

Jarim Seo, Dept. of Computer Science, Texas State University, San Marcos, Texas, USA, j_s1195@txstate.edu

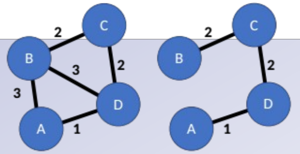
Martin Burtscher, Dept. of Computer Science, Texas State University, San Marcos, Texas, USA, burtscher@txstate.edu

SC'23

ABSTRACT

Finding a minimum spanning tree (MST) is a fundamental graph algorithm with applications in many fields. This paper presents ECL-MST, a fast MST implementation designed specifically for GPUs. ECL-MST is based on a parallelization approach that unifies Kruskal's and Borůvka's algorithm and incorporates new and existing optimizations from the literature, including implicit path compression and edge-centric operation. On two test systems, it outperforms leading GPU and CPU codes from the literature on all of our 17 input graphs from various domains. On a Titan V GPU,

lines. In this example, the cheapest distribution grid that allows everyone to deliver or receive electricity is the MST shown.



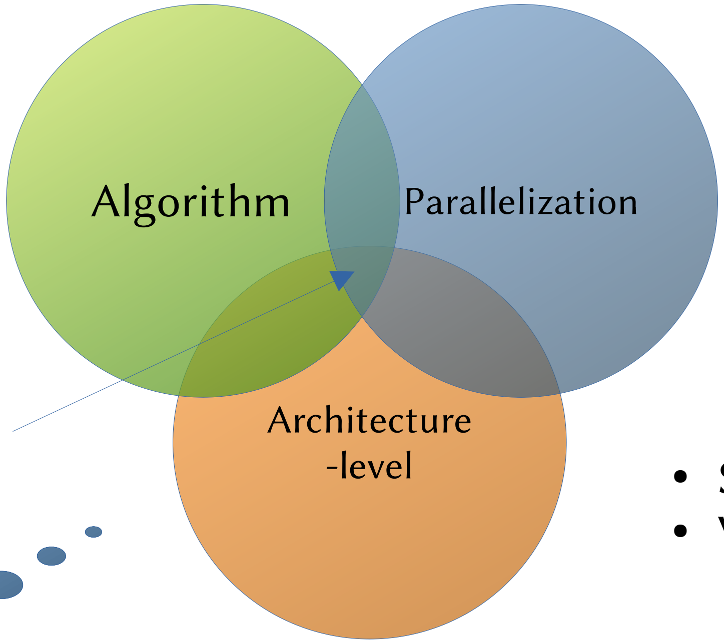
Optimizing for peak performance

OPTIMIZATIONS

- Input Characteristics
- Properties of substeps

- Vertex-/Edge- centric
- Data-/Topology-driven
- Push-/Pull-based

…



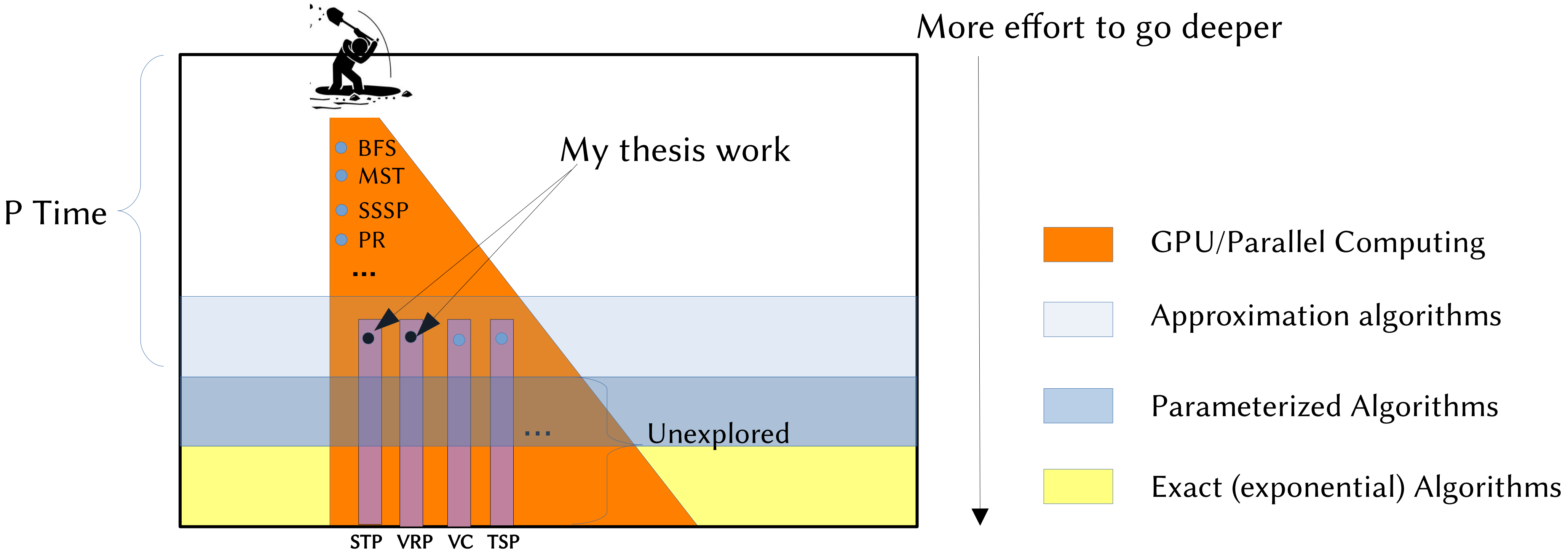
Even more

Peak performance

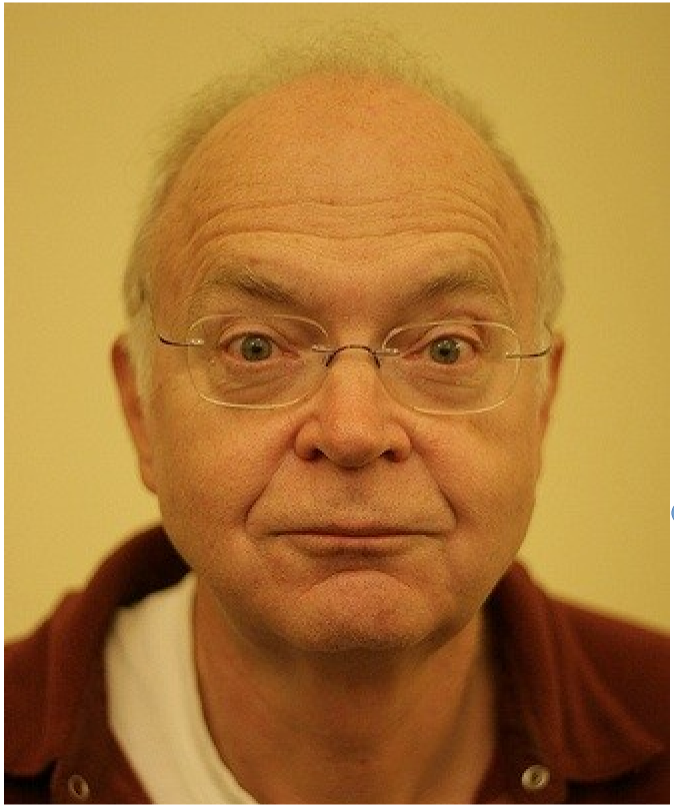
- Shared memory
- Warp-Intrincics

Is that all?

Landscape of Parallelization



Communicating Research



"Of equal importance to **solving a problem** is the **communication** of that **solution to others**."
- Donald Knuth

Summary

- Parallel Computing is here to stay forever
- Make your program to run in parallel
- Innovative ideas are more valued than tiny delta ideas
- Efficient algorithms and optimizations make faster parallel programs
- GPUs are everywhere, use it wisely.
- Efficiency $\propto$ Sustainability.

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https://mrprajesh.co.in/pages/research.html

https://bit.ly/hpc-research-talk

Thank you.