### Massive Dataset Analysis in Arkouda



David A. Bader



http://www.cs.njit.edu/~bader



### David A. Bader

### Distinguished Professor and Director, Institute for Data Science

- IEEE Fellow, ACM Fellow, SIAM Fellow, AAAS Fellow
- IEEE Sidney Fernbach Award
- 2022 inductee into University of Maryland's Innovation Hall of Fame, A. James Clark School of Engineering
- Recent Service:
  - White House's National Strategic Computing Initiative (NSCI) panel
  - Computing Research Association Board
  - Chair, NSF Committee of Visitors for Office of Advanced Cyberinfrastructure
  - NSF Advisory Committee on Cyberinfrastructure
  - Council on Competitiveness HPC Advisory Committee
  - IEEE Computer Society Board of Governors
  - IEEE IPDPS Steering Committee
  - Editor-in-Chief, ACM Transactions on Parallel Computing
  - Editor-in-Chief, IEEE Transactions on Parallel and Distributed Systems
- Over \$186M of research awards
- 300+ publications,  $\geq$  13,000 citations, h-index  $\geq$  65
- National Science Foundation CAREER Award recipient
- Directed: Facebook AI Systems
- Directed: NVIDIA GPU Center of Excellence, NVIDIA AI Lab (NVAIL)
- Directed: Sony-Toshiba-IBM Center for the Cell/B.E. Processor
- Founder: Graph500 List benchmarking "Big Data" platforms
- Recognized as a "RockStar" of High Performance Computing by InsideHPC in 2012 and as HPCwire's People to Watch in 2012 and 2014.





### Dedication: Morris Bader (26 October 1932 – 21 April 2005)





Morris Bader, 72, of Bethlehem, died peacefully at home on April 21, 2005. He was the husband of Karen (Roberts) Bader. They were married for 45 years. Born in New York, he was the son of the late Louis and Esther (Saltzman) Bader. He was a graduate of Stuyvesant High School in New York City. He was a 1953 graduate of the City University of New York (formerly City College of New York) and earned his Ph.D. in physical chemistry at Indiana University, Bloomington, IN. He taught at New York University, Marietta College in Marietta, OH, and Moravian College. He was an emeritus professor of chemistry at Moravian College. He taught chemistry and computer science from 1962 until his retirement in 1995. He also taught physical chemistry, developed the initial computer science program, conceived and funded the SOAR program for funding student and faculty summer research, and collaborated and developed a plant growth hormone. He was a scientific glassblower, making much of his own equipment. He developed scientific programs and published five computer manuals and software which sold worldwide, the profits of which were donated to assist faculty research travel to conferences. He developed the course "Chemistry for the Non-Science Major" and his paper "A Systematic Approach to Standard Addition Methods in Instrumental Analysis" is highly-cited and used widely in practice. He holds two patents: one for a bicycle gearing system and one for a quartz infrared cell; both manufactured. He has published numerous articles in numerical scientific computation for chemical analysis, solution of hard differential equations, and improved accuracy and error analysis in numerical computing. His chemistry publications include various chemical experiments for use by educators, and guidelines and error estimates for the neglect of buoyancy in laboratory weighings. He has published in the Journal of Chemical Education and in American Laboratory of which he was a contributing editor. He was a championship chess player and the Moravian College Chess Club advisor. He supported the Moravian College Foreign Film Festival. His many volunteering activities included teaching swimming to toddlers at the 3rd St. Alliance (Easton), Rodale Theater, State Theatre (Easton), 21-year Musikfest volunteer, LVH-Muhlenberg Hospital, Financial Advisor to the Friendship Circle of the J.C.C., and Assistant Scoutmaster of Troops 304 and 346 in the Minsi Trails Council, Boy Scouts of America. Morris was a member of Congregation Beth Avraham (formerly Agudath Achim) of Bethlehem; Member of the Board and then President for 20 years. He read Torah services. was а and led he

SURVIVORS: Wife; Sons, William A. of Bethlehem, Joel S. and his wife Jennifer of Baltimore, MD, David A. and his wife Sara Gottlieb of Albuquerque, NM; daughter, Debra S. and her husband Eric Eisenstein of Ithaca, NY; sisters: Rose and husband Ralph Hittman, Marion Ashrey, all of New York City; and five grandchildren.

SERVICES: graveside, were held Friday, April 22, Beth Avraham / Agudath Achim Cemetery, Fountain Hill. Arr. by Long Funeral Home, Bethlehem.

MEMORIALS: in Morris's memory made be made to Congregation Beth Avraham, 1555 Linwood Street, Bethlehem, PA, 18017; or to the Bader Memorial Scholarship Prize in Chemistry, Moravian College, 1200 Main St., Bethlehem, PA, 18018.



### 2021 IEEE Sidney Fernbach Award



David Bader cited for the development of Linux-based massively parallel production computers and for pioneering contributions to scalable discrete parallel algorithms for real-world applications.



2022 IEEE Computer Society President Bill Gropp presents David Bader with the Sidney Fernbach Award at SC21



### 1998: Bader Invents the Linux Supercomputer

#### DEPARTMENT EDITOR: Alex Magoun, annals-anecdotes@computer.org

#### ANECDOTES

#### Linux and Supercomputing: How My Passion for Building COTS Systems Led to an HPC Revolution

David A. Bader 🧕, Ying Wu College of Computing, New Jersey Institute of Technology, Newark, NJ, USA

Back in the early 1990s, when I was a graduate student in electrical and computer engineering at the University of Maryland, the term "supercomputer" meant Single Instruction, Multiple Data (SIMD) vector processor machines (the Cray-1) was the most popular), or massively parallel multiprocessor systems, such as the Thinking Machine CM-5. These systems were bulky—a Cray-1 occupied 2.7m × 2m of floor area and contained 60 miles of wires<sup>1</sup>; expensive, selling for several million dollars; and required significant expertise to program and operate. required a simultaneous development of scalable, high performance algorithms and services. Otherwise, application developers would be forced to develop algorithms from scratch every time vendors introduced a newer, faster, hardware platform.

By the late 1990s, the term "cluster computing" was common among computer science researchers and several of these systems had received significant publicity. One of the first cluster approaches to attract interest was Beowulf, which cost from a tenth to a third of the price of a traditional supercomputer. A typical setup





Source: UC San Diego https://ucsdnews.ucsd.edu/pressrelease/pioneering-scientist-and-innovator-larry-smarr-retires

### "This effort of yours has enormous historic resonance,"

– Larry Smarr, Distinguished Professor Emeritus, UC San Diego Founding Director of NCSA, Founding Director of Calit2



### Impact: Top500 Supercomputers Running Linux



Photo credit: Information Week, 2008

### 667

**L** oday, 100% of the Top 500 supercomputers in the

world are Linux HPC systems, based on Bader's technical contributions and leadership. This is one of the most significant technical foundations of HPC."

 Steve Wallach is a guest scientist for Los Alamos National Laboratory and 2008 IEEE CS Seymour Cray Computer Engineering Award recipient.



David A. Bader

# New Jersey Institute of Technology

# New Jersey Institute of Technology



"NJIT Climbs the Rankings of U.S. News & World Report, A Top 50 Public University" – 13 Sep 2021

"NJIT Named As One of Nation's 'Best Colleges' for 2022, The Princeton Review Says" - 6 Sep 2021





Launched in July 2019, with inaugural director David A. Bader (~40 faculty in current centers)

Solving real-world challenges Urban sustainability
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Disease outbreak and epidemic monitoring



New Jersey Institute

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#### Edited by DAVID A. BADER



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Michaleas, Lauren Milechin	Interactive Graph Analytics at Scale in Arkouda
Parallel Algorithms for Butterfly Computations	Zhihui Du, Oliver Alvarado Rodriguez, Joseph Patchett, and David A. Bader
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# Edge Computing

- Bring computations closer to the devices that are performing the data collection instead of transmitting it straight to the cloud.
- Consists of decentralized architectures with a high need for low latency and network connections to other edge nodes.





Image source: https://www.lanner-america.com/blog/4-edge-computing-technologies-enabling-iot-ready-network-infrastructure-2018/

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### To the Edge...

Edge



Time	Data
0:00	jdkbfjksdbfbfasdkfb
0:15	???????????????????????????????????????
0:30	sdfjhsdjkfhjskalhdfjk
0:45	asjdhfkasdhfkasdhfkj
1:00	asdfhjasdhfsadhfahs
1:15	???????????????????????????????????????
1:30	djfhjsdkfhkjashdfjkha

Revealed unanticipated periodicity in the data!



### And back.





### Institute for Data Science Aims to Democratize Supercomputing With NSF Grant



New algorithms from at NJIT can make supercomputer power available to almost anyone

High Performance Algorithms for Interactive Data Science at Scale (PI: Bader) 3/2021 – 2/2023 NSF CCF-2109988

Ordinary people could soon have greater ability to analyze massive amounts of information, based on new algorithms and software tools being designed at NJIT, intended to simplify

### https://news.njit.edu/institute-data-science-aims-democratize-supercomputing-nsf-grant

26 October 2022

Written by: Evan Koblentz

David A. Bader



### The Arkouda Framework with Arachne



• Arachne is built as an add-on with Arkouda and is fully interoperable.

Image source: <a href="https://chapel-lang.org/CHIUW/2020/Reus.pdf">https://chapel-lang.org/CHIUW/2020/Reus.pdf</a>



### Major Contributions

- Arachne, a large-scale graph analysis framework, extends Arkouda for productive graph analysis. Arachne is built on a novel sparse graph data structure.
- Arachne leverages productivity through Python with high performance backed by Chapel.
- Arachne, Arkouda, Chapel are all open-source.
  - <u>https://github.com/Bears-R-Us/arkouda-njit</u>
  - <u>https://github.com/Bears-R-Us/arkouda</u>
  - <u>https://github.com/chapel-lang/chapel</u>
- Experimental results on real-world and synthetic graphs demonstrate that Arachne works for graphs with billions of edges.



### Arachne Double-Index (DI) Data Structure

[Alvarado Rodriguez, Du, Patchett, Li, Bader 2022]



### Advantages of DI over CSR:

- 1. O(1) time complexity:
  - locating a vertex from a given edge ID.
  - locating the adjacency list from a given vertex ID.
- 2. We can search from edge ID to vertex ID, this is not possible in CSR.
- 3. DI can support both edge-centric and vertex-centric algorithms whereas CSR can only support the latter.
- 4. DI can easily achieve load balancing with the edge array being distributed equally amongst many locales.



### Modules of Arachne



### Graph Algorithms in Arachne

- **Breadth-first search (BFS)** [Du, Alvarado Rodriguez, Bader 2021] Returns an array of size *n* with how many hops away some vertex *v* is from an initial vertex *u*.
- Connected components

Returns an array of size n where all vertices who belong to the same component have the same value x. The value of x is the label of the largest vertex in the component.

• Truss Analytics [Patchett, Du, Bader 2021]

<u>K-truss</u> returns every edge in the truss where each edge must be a part of k - 2 triangles that are made up of nodes in that truss. <u>Max truss</u> returns the maximum k. <u>Truss decomposition</u> returns the maximum k for each edge.

Jaccard Coefficients

Returns an array of size n with the Jaccard metric between some vertices u and v.

- **Triangle counting** [Du, Alvarado Rodriguez, Patchett, Bader 2021] Returns the number of triangles in a graph.
- Triangle centrality [Patchett, Du, Bader 2022]

Returns an array of size n with the proportion of triangles centered at a vertex v.



# Algorithmic Contributions

Algorithm	Novelty
Breadth-First Search	High-level algorithm based off Chapel's high-level distributed bag data structure outperforms low-level manual aggregation algorithm.
Connected Components	Fast-spreading algorithm that involves propagating the lowest vertex label of each component to all other vertices. It completes in $O(\log(d_{max}) + 1)$ iterations where $d_{max}$ is the diameter for the largest connected component.
Triangle Counting	Minimum search triangle counting can identify two smaller adjacency lists and employ fine- grained parallelism to achieve better performance by searching for a vertex to complete a triangle edge in the smaller adjacency list.
Triangle Centrality	Uses minimum search triangle counting to find (1) the sum of the number of triangles of the given vertex's adjacency list and itself, and (2) the sum of the number of triangles of the given vertex's neighbors that are connected by a triangle.
Truss Analytics	Uses minimum search triangle counting to speed up the triangle search process of truss edges.
Jaccard Coefficients	Edge-centric graph partitioning allows for high memory access locality.



### What is Triangle Counting?





Triangle\_count = 5



24

### Minimum Search Triangle Counting (1/3) [Du, Alvarado Rodriguez, Patchett, Bader 2021]



Total time to search all triangles with a given edge:  $\max_{w \in Adj_l} \log_2(\min(|Adj_w|, |Adj_h|))$ vs. list intersection  $\log_2(|Adj_h|)$  where *h* is *u* or *v* with more adjacent vertices, *l* with less.



### Minimum Search Triangle Counting (2/3) [Du, Alvarado Rodriguez, Patchett, Bader 2021]

- 1. Given an edge (u, v) we assume that  $|Adj(u)| \leq |Adj(v)|$ .
- 2. Then, for  $\forall w \in Adj(u)$ we spawn |Adj(u)|parallel threads to check if we can form a complete triangle with (u, v, w).
- 3. If |Adj(w)| < |Adj(v)|we will check if  $v \in Adj(w)$ , else, we check if  $w \in Adj(w)$ .



Thread  $w_1$ : search for  $w_1$  in Adj(v), no match, kill.

Thread  $w_2$ : search for v in  $Adj(w_2)$ , no match, kill.

Thread  $w_3$ : search for v in  $Adj(w_3)$ , match! Increment count.



### Minimum Search Triangle Counting (3/3) [Du, Alvarado Rodriguez, Patchett, Bader 2021]

- Why does our minimum search method have less operations?
- If  $|Adj_l| = 4$ , and for every w in  $Adj_l$ ,  $|Adj_w| \le 8$ , and  $|Adj_h| = 1024$  then list intersection will use four parallel threads that amount to  $[\log_2 1024] = 10$  operations whereas our method yields  $[\log_2 8] = 3$  operations.
- List intersection requires analyzing the entire longer adjacency list (*h*) against the much shorter one (*l*). We avoid doing such a large, computationally intensive search every time.



### What are connected components?



- Connected subgraphs of a graph that is not part of a larger connected subgraph.
- If *u* is in connected component 1 and v is in connected component 2, there is so possible path  $u \rightarrow v$ .



# Fast-Spreading Connected Components (1/2)

Algorithm 2: Voltage-Mapping based Fast-Spreading Algorithm

1 FastSpreading(G)



Eventually L will make a graph that looks like this:







# Fast-Spreading Connected Components (2/2)



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# Using Arachne with Arkouda (1/3)

```
In [2]:
    ak.connect("d-6-15-4", 5555)
```

connected to arkouda server tcp://\*:5555

In [3]:

```
# Read in the graph.
filename = "/home/gridsan/oarodriguez/biggraph_shared/Adata/simple.txt"
ne = 13
nv = 10
G = ar.graph_file_read(ne, nv, 2, 0, filename, 1, 0, 0, 0, 1)
```

13 10 2 0 /home/gridsan/oarodriguez/biggraph\_shared/Adata/simple.txt 1 0 0 0 1

In [4]:

```
# Add the edges of the graph to a list of tuples.
src = ar.graph_query(G, "src")
dst = ar.graph_query(G, "dst")
edges = []
for (u, v) in zip(src.to_ndarray(), dst.to_ndarray()):
```

edges.append((u,v))

In [5]:

# Display the graph with NetworkX.
nxG = nx.Graph()
nxG.add\_edges\_from(edges)

pos = nx.spring\_layout(nxG, seed=225)
nx.draw\_networkx(nxG, pos, with\_labels=True)
plt.show()



### Using Arachne with Arkouda (2/3)



#### In [6]:

# Get value of the maximum degree. neighbour = ar.graph\_query(G, "neighbour") neighbourR = ar.graph\_query(G, "neighbourR") degrees = neighbour + neighbourR print("The value of the maximum degree is: {}".format(ak.max(degrees)))

The value of the maximum degree is: 4



### Using Arachne with Arkouda (3/3)

#### **Breadth-First Search**

In [7]: d = ar.graph\_bfs(G, int(ak.argmax(degrees)), 0) print(d)

[3 1 3 2 1 2 0 2 1 1]

In [8]:

# Get the size of each level of BFS.
d\_histogram = ak.histogram(d, bins=ak.max(d)+1)
print(d\_histogram)

(array([0. , 0.75, 1.5 , 2.25]), array([1 4 3 2]))





#### Graphs ca-GrOc ca-HepTh as-caida20071105

Graphs for Testing

facebook combined

loc-brightkite edges

ca-CondMat

email-Enron

soc-Epinions1

amazon0601

ca-AstroPh

ca-HepPh

Real-world

	com-Youtube	2987624	1134890	1	3056386	19	
	friendster	1806067135	65608366	1	4173724142	129	
				$\smile$			$\rightarrow$
	delaunayn20	3145686	1048576	1	2109090	4	
	delaunayn21	6291408	2097152	1	4218386	4	
Synthetic	delaunayn22	12582869	4194304	1	8436672	4	
-	delaunayn23	25165784	8388608	1	16873359	4	
	delaunayn24	50331601	16777216	1	33746670	4	

Edges

14484

25973

53381

88234

93439

118489

183831

198050

214078

405740

2443408

values found by our algorithms

Triangles

48260

28339

36365

1612010

173361

727044

3358499

1351441

494728

1624481

3986507

Max K

44 32

16

97

26

239

22

57

43

33

11

34

CCs

354

427

1

1

567

276

1065

289

547

2

7

Vertices

5242

9877

26475

4039

23133

12008

36692

18772

58228

75879

403394

Experiments were conducted on a highperformance server with 2 x Intel Xeon E5-2650 v3 @ 2.30GHz CPUs with 10 cores per CPU and a RAM capacity of 512GB.

few vertices, outperforms algorithms less some edges but more vertices.

delaunayn10 - delaunayn19

### Arachne Results – Real-World Graphs

[Alvarado Rodriguez, Du, Patchett, Li, Bader 2022]



#### **Key Points:**

- Graph construction is time consuming but once the graph is built into memory all the algorithms can use it in a highly efficient way.
- 2. The structural properties of graphs can significantly affect execution times even for the same algorithm.

35



### Arachne Results – Synthetic Graphs

[Alvarado Rodriguez, Du, Patchett, Li, Bader 2022]



#### **Key Points:**

- 1. Synthetic graphs demonstrate the scalability of our algorithms as the number of edges in a graph increase.
- 2. The memory requirements for each algorithm differ, hence the Jaccard coefficient algorithm encounters out of memory errors when the graph gets too big. Jaccard requires  $\frac{N \times N}{2}$  memory and  $\left(\frac{N}{P}\right)^2 \times \frac{M}{P}$  calculations.

36



### Conclusions & Further Work

- We can design and develop high performance graph analysis algorithms using Arkouda/Chapel quickly and efficiently.
- We plan to work on optimizing all current methods to work as efficiently as possible in single locale and multi locale environments.
- We plan to implement new novel algorithms such as stringology, a communication-efficient triangle counting, large-scale community detection, and machine learning.



### Publications

- Oliver Alvarado Rodriguez, Zhihui Du, Joseph Patchett, Fuhuan Li, David Bader (2022). Arachne: An Arkouda Package for Large-Scale Graph Analytics. IEEE HPEC.
- Joseph Patchett, Zhihui Du, Fuhuan Li, David Bader (2022). Triangle Centrality in Arkouda. IEEE HPEC.
- Zhihui Du, Oliver Alvarado Rodriguez, David Bader (2021). Large Scale String Analytics In Arkouda. IEEE HPEC.
- Zhihui Du, Oliver Alvarado Rodriguez, David Bader (2021). Enabling Exploratory Large Scale Graph Analytics through Arkouda. IEEE HPEC.
- Joseph Patchett, Zhihui Du, David Bader (2021). K-Truss Implementation in Arkouda (Extended Abstract). IEEE HPEC.
- Zhihui Du, Oliver Alvarado Rodriguez, Joseph Patchett, David Bader (2021). Interactive Graph Stream Analytics in Arkouda. Algorithms.
- Zhihui Du, Oliver Alvarado Rodriguez, David A. Bader, Michael Merrill, William Reus (2021). Exploratory Large Scale Graph Analytics in Arkouda. CHIUW.



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