# Arachne: An Open-Source Framework for Interactive Massive-Scale Graph Analytics



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 \$188M of research awards
- 300+ publications,  $\geq$  13,900 citations, h-index  $\geq$  66
- 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.





# Today's talk is dedicated to my uncle

Elliot Norman Ashrey

- B: 23 Sep 1931 in New York City, New York, USA
- D: 26 Apr 2024 in New York City, New York, USA



# 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'; 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

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**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.



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"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

"Wall Street Journal/College Pulse Ranks NJIT No. 2 Public University in the US" – 6 Sep 2023



# NJT INSTITUTE FOR DATA SCIENCE

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

Solving real-world challenges

- Urban sustainability
  Healthcare analytics
  Trustworthy, Free and Fair Elections
- Insider threat detection
- Utility infrastructure protection
- Cyberattack defense
- Disease outbreak and epidemic monitoring



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of Technology



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### Graph Data Science: Real-world challenges

### All involve exascale streaming graphs:

- Health care → disease spread, detection and prevention of epidemics/pandemics (e.g. SARS, Avian flu, H1N1 "swine" flu)
- Massive social networks → understanding communities, intentions, population dynamics, pandemic spread, transportation and evacuation
- Intelligence 
   business analytics, anomaly detection, security, knowledge discovery from massive data sets
- Systems Biology → understanding complex life systems, drug design, microbial research, unravel the mysteries of the HIV virus; understand life, disease,
- Electric Power Grid  $\rightarrow$  communication, transportation, energy, water, food supply
- **Modeling and Simulation** → Perform full-scale economic-social-political simulations

### **REQUIRES PREDICTING / INFLUENCE CHANGE IN REAL-TIME AT SCALE**



### Massive Data Analytics: Infrastructure

- The U.S. high-voltage transmission grid has >150,000 miles of line.
- Real-time detection of changes and anomalies in the grid is a large-scale problem.
- May mitigate impact of widespread blackouts due to equipment failure or intentional damage.

#### The New York Times

Thursday, September 4, 2008

#### Report on Blackout Is Said To Describe Failure to React

By MATTHEW L. WALD Published: November 12, 2003

A report on the Aug. 14 blackout identifies specific lapses by various parties, including FirstEnergy's failure to react properly to the loss of a transmission line, people who have seen drafts of it say.

A working group of experts from eight states and Canada will meet in private on Wednesday to evaluate the report, people involved in the investigation gold Tuesday. The report, which the Energy Department

$\bowtie$	E-MAIL
₿	PRINT
	SINGLE-PAGE
ē	REPRINTS
G,	SAVE
Ⴑ	SHARE



Network Analysis for Intelligence and Surveillance

- [Krebs '04] Post 9/11 Terrorist Network Analysis from public domain information
- Plot masterminds correctly identified from interaction patterns: centrality

- A global view of entities is often more insightful
- Detect anomalous activities by exact/approximate graph matching



Image Source: http://www.orgnet.com/hijackers.html



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### Massive Data Analytics: Public Health

- CDC/national-scale surveillance of public health
- Cancer genomics and drug design
  - Computed Betweenness Centrality of Human Proteome



# Mining Twitter for Social Good

#### **ICPP 2010**

#### Massive Social Network Analysis: Mining Twitter for Social Good

David Ediger Karl Jiang Jason Riedy David A. Bader Georgia Institute of Technology Atlanta, GA, USA

Courtney Corley Rob Farber William N. Reynolds Pacific Northwest National Lab. Least Squares Software, Inc. Albuquerque, NM, USA Richland, WA, USA

Abstract-Social networks produce an enormous quantity of data. Facebook consists of over 400 million ac- 120 'friendship' connections each and sharing 5 billion tive users sharing over 5 billion pieces of information each month. Analyzing this yast quantity of unstructured data presents challenges for software and hardware. We present GraphCT, a Graph Characterization Toolkit for massive graphs representing social network data. On a 128processor Cray XMT, GraphCT estimates the betweenness centrality of an artificially generated (R-MAT) 537 million vertex, 8.6 billion edge graph in 55 minutes and a realworld graph (Kwak, et al.) with 61.6 million vertices and 1.47 billion edges in 105 minutes. We use GraphCT to analyze public data from Twitter, a microblogging network. Twitter's message connections appear primarily tree-structured as a news dissemination system. Within the

involves over 400 million active users with an average of references to items each month [11].

One analysis approach treats the interactions as graphs and applies tools from graph theory, social network analysis, and scale-free networks [29]. However, the volume of data that must be processed to apply these techniques overwhelms current computational capabilities. Even well-understood analytic methodologies require advances in both hardware and software to process the growing corpus of social media.

Social media provides staggering amounts of data. Acres from



#### TOP 15 USERS BY BETWEENNESS CENTRALITY

Rank	Data	Set
	H1N1	atlflood
1	@CDCFlu	@ajc
2	@addthis	@driveafastercar
3	<pre>@Official_PAX</pre>	@ATLCheap
4	@FluGov	@TWCi
5	Qnytimes	@HelloNorthGA
6	Otweetmeme	@11AliveNews
7	@mercola	@WSB_TV
8	0 CNN	@shaunking
9	@backstreetboys	@Carl
10	@EllieSmith_x	@SpaceyG
11	@TIME	@ATLINtownPaper
12	@CDCemergency	@TJsDJs
13	@CDC_eHealth	@ATLien
14	@perezhilton	@MarshallRamsey
15	@billmaher	@Kanye



Image credit: bioethicsinstitute.org





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# Arachne: Interactive Property Graph Analytics at Scale





Image Credit: Matias Del Carmen



### 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) \$2.2M 3/2021 - 6/2024 NSF CCF-2109988

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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 April 2024

Written by: Evan Koblentz

David A. Bader

### Arkouda: Dedication to Michael H. Merrill (June 2, 1964 ~ November 8, 2022)



"Mike was a dedicated civil servant. He was a Computer Scientist at the Department of Defense for 34 years and was recognized in 2022 with a Distinguished Civilian Service Medal. He loved computers and technology, especially high performance computing. Mike was a problem solver and innovative thinker; he was recognized for inspiring and leading numerous large projects over the course of his career. He loved to share his knowledge and mentored many colleagues over the years sometimes calling them his kids, sometimes his minions, but always calling them his friend."



# Productivity + Performance







### Connect with Chapel: the parallel programming language powering Arkouda

#### **ChapelCon – free virtual event**

- June 5<sup>th</sup> Tutorial Day
- June 6<sup>th</sup> Coding Day
- June 7<sup>th</sup> Conference Day

### Come code or chat with us!

- GitHub <u>https://github.com/chapel-lang/chapel</u>
- Gitter <u>https://gitter.im/chapel-lang/chapel</u>
- Discourse <u>https://chapel.discourse.group</u>
- StackOverflow <u>https://stackoverflow.com/questions/tagged/chapel</u>

### Follow us on social media

- LinkedIn <a href="https://www.linkedin.com/company/chapel-programming-language">https://www.linkedin.com/company/chapel-programming-language</a>
- YouTube <u>https://www.youtube.com/@ChapelLanguage</u>
- Twitter/X <u>https://x.com/ChapelLanguage</u>
- Facebook <u>https://www.facebook.com/ChapelLanguage</u>

#### **REGISTER FOR CHAPELCON**



#### TAKE THE CHAPEL COMMUNITY SURVEY



# Arkouda + Arachne Framework

### Arkouda

 an existing open-source Python framework that allows for array and dataframe operations on data that is terabytes in size but lacks graph processing operations.

### Arachne

 an open-source extension to Arkouda to convert massivescale dataframes to graphs with high-performance graph kernels and property graph capabilities while maintaining a NetworkXlike API for new Python users to easily transition to utilizing it.



# Arkouda + Arachne Framework

**Chapel Server** 



- This work extends Arachne to store massive-scale graphs.
- Arachne can be thought of as a wrapper that creates a logical graph.



# Karate Club Graph Example



# The Connectome Project





Drosophila Hemibrain Dataset, [Scheffer et al. 2020]



Drosophila Auditory Circuit [Baker et al. 2022] Video: Amy Sterling, FlyWire



Slide credit: Jakob Troidl, Hanspeter Pfister, Jeff Lichtman (Harvard University)

- Using Arkouda, we can covert connectome datasets with one hundred million rows of JSON objects to distributable HDF5 files in under two hours.
- Using Arachne, a graph of this size can be queried in seconds to create smaller subgraphs for deeper analysis.







# **Spatial Neighborhood Analysis**



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# Using Graph Analytics to Understand the Brain

### 1 mm<sup>3</sup> of brain tissue

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### Motifs are recurrent connectivity patterns of neurons in the brain.

Slide credit: Jakob Troidl, Hanspeter Pfister 26 April 2024 H01 dataset, [Shapson-Coe et al. 2021]



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# Connectome: Requires Exascale Graph Analytics



5 orders of magnitude scale up within the past 10 years



# Connectome: H01 Dataset

- ~ 1.4 PB image data
- ~ 57,000 cells
- ~ 133 Million synapses

Slide credit: Jakob Troidl, Hanspeter Pfister 26 April 2024 New Jersey Institute of Technology



Image Credit: Wikipedia Slide credit: Jakob Troidl, Hanspeter Pfister









Image Credit: Wikipedia Slide credit: Jakob Troidl, Hanspeter Pfister



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26 April 2024

# Motif finding

- Large Networks. ~57,000 nodes and ~130 million edges.
- Expensive Computation. Verifying the existence of a motif in a larger network is NP-complete.
- **Complex 3D structure.** Neurons span long volumes and form complex branching patterns.
- Algorithms:
  - **Ullmann** (2010) which is a recursive backtracking algorithm for solving the subgraph isomorphism problem
  - **Cordella** (2004) another algorithm based on Ullmann's, VF2, which improves the refinement process using different heuristics and uses significantly less memory.

Slide modified from: Jakob Troidl, Hanspeter Pfister

Neuroscientists with to correlate motif connectivity to neuron morpholog



Image credit: Jakob Troidl, Hanspeter Pfister







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Slide credit: Jakob Troidl, Hanspeter Pfister

# Finding Patterns in Clinical Patient Records

- The adoption of electronic health record (EHR) systems has simultaneously changed clinical practice.
- In data from 2019 and 2021, 96% of general acute care hospitals had adopted EHR\*



\* Office of the National Coordinator for Health Information Technology. Adoption of Electronic Health Records by Hospital Service Type 2019-2021, Health IT Quick Stat #60. April 2022.

- Utilize community detection algorithms to identify groups of vertices.
- These communities may correspond to subpopulations of patients with similar clinical characteristics or disease trajectories.

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Data pre-processed by different tasks on multicore Arachne server

Vertex: Patient Edge: Shared clinical features


### Contact Tracing Networks (COVID, HIV, etc.)



# Population Health Data Analysis



•

•

# The Arkouda-Arachne Netflow Data Pipeline

IPV4_SRC_ADDR	L4_SRC_PORT	IPV4_DST_ADDR	L4_DST_PORT	PROTOCOL	L7_PROTO	IN_BYTES	OUT_BYTES	IN_PKTS	OUT_PKTS	TCP_FLAGS	FLOW_DU	IRATION_MS	Attack
192.168.100.6	52670	192.168.100.1	53	17	5.21	71	126	1	1	0	42	94966	Benign
192.168.100.6	49160	192.168.100.149	444	6	0	217753000	199100	4521	4049	24	41	76249	Theft
192.168.100.46	3456	192.168.100.5	80	17	0	8508021	8918372	9086	9086	0	41	75916	Benign
192.168.100.3	80	192.168.100.55	8080	6	7	8442138	9013406	9086	9086	0	41	75916	Benign
$\frown$	ak c	tick()											
			integer id gen			IPV4_SRC	IP	V4_SRC_id	IPV4_	DST	IPV4_DST	_id	
						192.168.100.6:5	2670	3473	192.168.2	100.1:53	3455		
			ak GroupBy()			192.168.100.6:4	9160	4234	192.168.10	0.149:444	3233		
IPV4 source addresses and ports together make up the source			orts e	ak.groupby.broadcast()								<b>Т 1</b>	-

vertex of the edge and respectively the same columns for the

destination vertex of the edge.

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To Arachne!

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# Back-End Storage and Querying

	SRC	DST	IND	SETS		INTS	REALS	•	Relationships	s are store	d in sets pe	redge.
sdi	0	1	0	{1}	ties	REF	REF		User specifie	s a query,	and we sea	rch the
nshi	0	2	1	{0}	ber	REF	REF		probing the s	sets in am	ortized cons	tant time.
atio	1	0	2	{1}	e Pro	REF	REF	•	Properties ar	e stored s	plit by type	and for
Rel	1	2	3	{0,2}	Edge	REF	REF		associative d	omain wh	ere we extra	act the data
	2	2	4	{0}		REF	REF		by simply doi	ing an acc	ess edge_pr	op[col_id].
	R-N	1AP	IND			1	2		COL-MAP	IND	ΤΥΡΕ	
	ber	nign	0		$\leq$	VAL	VAL		L7_PROTO	0	FLOAT	
	theft DDoS		1						IN_BYTES	1	INT	
			2		REAL	0		C	OUT_BYTES	2	INT	
						I VAL						

All searching is guaranteed to be O(m/p) since it only involves iterating over the edge set in parallel with each processor.

- All REFS point to arrays that are of the specified column type and that store the key-value pairs for column identifier to data.
- Query hits are returned in a Boolean array specified which edges matched. itute

# Code Example for Python Scripts & Jupyter

```
1. import arkouda as ak
2. import arachne as ar
3.
4. ## Get src and dst from input file.
5.graph = ar.PropGraph()
6.graph.add edges from(src,dst)
7.
8. ## Generate relationships df and edge properties df from input file.
9. graph.add edge relationships(relationships df)
10.graph.add edge properties(edge properties df)
11.
12.## User generates relationships to find and property query.
13.returned edges rel = graph.query relationships(relationships to find)
14. returned edges prop = graph.query edge properties("COLUMN", 67, ">")
15.
16.returned edges = ak.intersect1d(returned edges rel, returned edges prop)
17.subgraph src = returned edges[0]
18.subgraph dst = returned edges[1]
19.
20.subgraph = ar.Graph()
21.subgraph.add edges from(subgraph src, subgraph dst)
22.bfs = ar.bfs layers(subgraph)
23.cc = ar.connected components(subgraph)
24.tris = ar.triangles(subgraph)
25.squares = ar.squares(subgraph)
26.## And more!!!!!
```

- Line 6 input is generated from input files from types such as HDF5, CSV, Parquet, etc.
- Lines 9 and 10 input is generated from input files as well.
- Lines 13 and 14 relationships and properties to find are generated by the user.
- Lines 16-19 use Arkouda operations and slicing to get the edges that are returned by both queries.
- Lines 20 and 21 create a new Arachne simple graph with the returned edges of the queries.
- Lines 22-25 run some of the other algorithms available in Arachne!
- Arachne can also return arrays composing of the edges which can be converted to Python lists or NumPy arrays so they can be loaded into NetworkX for further analysist

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# Arachne DI Data Structure [Du et al. 2021]



- Allows for simple, compact, **distributable** storage of vertex and edge sets.
- Given an edge index, all vertices that make up that edge are found in **constant time**, avoiding a binary search into SRC (CSR offsets index equivalent).
- MAP allows explicitly storing original vertex labels, returning original graph involves creating arrays and place values of SRC[MAP] and DST[MAP] into new arrays.



# Property Graph Results







- Experiments conducted on a cluster where each compute node was composed of 128 cores (64 per AMD EPYC 7713 CPUs), 1TB DDR4 RAM, and an Infiniband HDR 200 GB/s node interconnect.
  - At time of results, some nodes had performance issues, hence the weird elbows.
  - Fifty random relationships were made and randomly assigned to edge indices meaning some edges could be picked more than once and some none at all.
- Querying involved searching for the edges that included three of the fifty relationships, each list performed a set and operation with the search space.

Takeaway: Building a graph of five billion edges takes under 60 seconds, running ETL to insert relationships takes under 4 minutes, and querying it under 10 seconds.



# 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.

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

<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.

- **Square counting** [Burkhardt, Harris 2023] Returns the number of four-cycles in the graph.
- Triangle centrality [Patchett, Du, Bader 2022][Patchett, 2022]
   Returns an array of size n with the proportion of triangles centered at a vertex v.
- **Subgraph isomorphism** [Dindoost, Bader, 2023, in progress] Finds instances of a pattern in a larger graph.



### Shared-Memory Parallel Breadth-First Search



### Distributed-Memory Parallel Breadth-First Search

Assume our edge list is split down the middle, then the neighborhood of some vertices will live on one compute node while the rest live on another compute node.



### Breadth-First Search Communication Volume Results

delaunayn20		get		put				
locale	di	di-norev	di-agg-ls	di	di-norev	di-agg-ls		
0	15672640	7873842	639827	5629422	2749193	138070		
1	15834332	7939017	687156	1952226	1016946	127936		
2	15715554	7722659	226754	1942839	962031	45217		
3	15817879	7723971	226880	1951313	962201	45060		
4	15964559	7724880	226691	1961552	962199	51217		
5	15739226	7726504	230024	1940688	962439	52714		
6	15569450	7727678	229096	1925536	962680	51977		
7	15341933	7736094	225083	1904757	963418	48413		

di: 84 seconds di-agg-ls: 3.36 seconmds

delaunayn20 is a graph with 3 million edges and a large diameter

**Takeaway:** Aggregating writes drastically reduces communication volumes, improving performance, all done easily through Chapel by adapting aggregators for different uses.

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#### Minimum Search Triangle Counting

- 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)| - 1parallel 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<sub>2</sub>: 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 Operation Count Comparison

- Assume  $|Adj_u| < |Adj_v|$  and we spawn threads for every  $w \in |Adj_u|$ 
  - Minimum search:  $\max_{w \in Adj_{u}} \log_2(\min(|Adj_w|, |Adj_v|))$
  - List Intersection:  $\log_2(|Adj_v|)$
- Say we have the following information for our vertices:
  - $|Adj_u| = 4$  and  $|Adj_v| = 1024$
  - For every w in  $Adj_u$ ,  $|Adj_w| \le 8$

• List intersection: 4 threads amounting to  $\lceil \log_2 1024 \rceil = 10$  operations each.

• Minimum search: 4 threads amounting to  $\lceil \log_2 8 \rceil = 3$  operations each.



# Triangle Counting Results



 Our method outperforms with the Conte method with a highest speedup of 385.8 and an average speedup of 128.

**Takeaway:** Truss decomposition with minimum search triangle counting outperforms a C++ method coded with OpenMP, with SSE-Acceleration, binary searching on adjacency list, and no atomic operations.

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Graphs used were a variety of real-world graphs available for view in paper.



# 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.



### Publications

- Oliver Alvarado Rodriguez, Zhihui Du, Joseph Patchett, Fuhuan Li, David Bader (2022). Arachne: An Arkouda Package for Large-Scale Graph Analytics. IEEE HPEC.
- Oliver Alvarado Rodriguez, Fernando Vera Buschmann, Zhihui Du, David Bader (2023). Property Graphs in Arachne. IEEE HPEC.
- Soroush Vahidi, Baruch Schieber, Zhihui Du, David Bader (2023). Parallel Longest Common SubSequence Analysis In Chapel. 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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# 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.



DATA SCIENCE SERIES

#### MASSIVE GRAPH ANALYTICS



Edited by DAVID A. BADER



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### Chapters

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Algorithms: Search and Paths	Models
A Work-Efficient Parallel Breadth-First Search Algorithm (or How to Cope With	Recent Advances in Scalable Network Generation
the Nondeterminism of Reducers	Manuel Penschuck, Ulrik Brandes, Michael Hamann, Sebastian Lamm, Ulrich
Charles E. Leiserson and Tao B. Schardl	Meyer, Ilya Safro, Peter Sanders, and Christian Schulz
Multi-Objective Shortest Paths	Computational Models for Cascades in Massive Graphs: How to Spread a
Stephan Erb, Moritz Kobitzsch, Lawrence Mandow , and Peter Sanders	Rumor in Parallel
	Ajitesh Srivastava, Charalampos Chelmis, Viktor K. Prasanna
Algorithms: Structure	Executing Dynamic Data-Graph Computations Deterministically Using
Multicore Algorithms for Graph Connectivity Problems	Chromatic Scheduling
George M. Slota, Sivasankaran Rajamanickam, and Kamesh Madduri	Tim Kaler, William Hasenplaugh, Tao B. Schardl, and Charles E. Leiserson
Distributed Memory Parallel Algorithms for Massive Graphs	
Maksudul Alam, Shaikh Arifuzzaman, Hasanuzzaman Bhuiyan, Maleq Khan, V.S.	Frameworks and Software
Anil Kumar, and Madhav Marathe	Graph Data Science Using Neo4j
Efficient Multi-core Algorithms for Computing Spanning Forests and Connected	Amy E. Hodler, Mark Needham
Components	The Parallel Boost Graph Library 2.0
Fredrik Manne, Md. Mostofa Ali Patwary	Nicholas Edmonds and Andrew Lumsdaine
Massive-Scale Distributed Triangle Computation and Applications	RAPIDS cuGraph
Geoffrey Sanders, Roger Pearce, Benjamin W. Priest, Trevor Steil	Alex Fender, Bradley Rees, Joe Eaton
	A Cloud-based approach to Big Graphs
Algorithms and Applications	Paul Burkhardt and Christopher A. Waring
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Eugenio Angriman, Patrick Bisenius, Elisabetta Bergamini, Henning Meyerhenke	Jeremy Kepner, Peter Aaltonen, David Bader, Aydin Buluc, Franz Franchetti, John
Ordering Heuristics for Parallel Graph Coloring	Gilbert, Dylan Hutchinson, Manoj Kumar, Andrew Lumsdaine, Henning
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Partitioning Trillion Edge Graphs	Zalewski, and Timotny G. Mattson
George M. Slota, Karen Devine, Sivasankaran Rajamanickam, Kamesh Madduri	Graphuro: Linear Algebra Graph Kernels
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Jeremy Kepner, Kenjiro Cho, KC Claffy, Vijay Gadepally, Sarah McGuire, Peter	Interactive Graph Analytics at Scale in Arkouda
Michaleas, Lauren Milechin	Thibui Du Oliver Algerade Podriguez, Joseph Datchett, and David A. Pader
Parallel Algorithms for Butterfly Computations	zinnur Du, Onver Alvuruub Kourryuez, Joseph Patchett, und Davia A. Bader
Jessica Shi and Julian Shun	

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MASSIVE GRAPH ANALYTICS

DATA SCIENCE SERIES



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# **Community Detection**

- In complex networks, nodes cluster and form relatively dense groups – often called communities.
- Community detection is a fundamental graph algorithm with practical applications like *fraud detection* in Fintech and *identity and access management* in social networks



Vertices are Facebook users and edges represent Facebook friendships. Communities, represented by different colors.

Image credit: Fortunato, S., Newman, M.E.J. 20 years of network community detection. *Nat. Phys.* **18**, 848–850 (2022).



Open-Source Massive-Scale (Property) Graph Analytics in Python with Arachne+Arkouda powered by Chapel



**OPEN SOURCE:** <u>https://github.com/Bears-R-Us/arkouda-njit</u> **PUBLICATIONS:** <u>https://davidbader.net/publication/</u> filter with "Arkouda" or "Arachne"



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David A. Bader

### Modules of Arachne



#### Graphs ca-GrOc ca-HepTh

Graphs for Testing

as-caida20071105

ca-CondMat

ca-HepPh

facebook\_combined

Real-world

eal-world	email-Enron	183831	36692	1065	727044	22	
	ca-AstroPh	198050	18772	289	1351441	57	
	loc-brightkite_edges	214078	58228	547	494728	43	
	soc-Epinions1	405740	75879	2	1624481	33	
	amazon0601	2443408	403394	7	3986507	11	
	com-Youtube	2987624	1134890	1	3056386	19	
	friendster	1806067135	65608366	1	4173724142	129	
L L							delaunayn10 - delaunayn19
ſ	delaunayn20	3145686	1048576	1	2109090	4	delaunayn10 - delaunayn19
	delaunayn20 delaunayn21	3145686 6291408	1048576 2097152	1 1	2109090 4218386	<u> </u>	delaunayn10 - delaunayn19
Synthetic	delaunayn20 delaunayn21 delaunayn22	3145686 6291408 12582869	1048576 2097152 4194304	1 1 1	2109090 4218386 8436672	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	delaunayn10 - delaunayn19
Synthetic	delaunayn20 delaunayn21 delaunayn22 delaunayn23	3145686 6291408 12582869 25165784	1048576 2097152 4194304 8388608	1 1 1 1	2109090 4218386 8436672 16873359	$\begin{array}{c} & \\ & 4 \\ \hline & 4 \\ \hline & 4 \\ \hline & 4 \\ \hline \end{array}$	delaunayn10 - delaunayn19
Synthetic -	delaunayn20 delaunayn21 delaunayn22 delaunayn23 delaunayn24	3145686 6291408 12582869 25165784 50331601	1048576 2097152 4194304 8388608 16777216	1 1 1 1 1 1	2109090 4218386 8436672 16873359 33746670	$\begin{array}{c} \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \end{array}$	delaunayn10 - delaunayn19

CCs

354

427

567

276

1

1

Vertices

5242

9877

26475

23133

12008

4039

Edges

14484

25973

53381

88234

93439

118489

values found by our algorithms

Triangles

48260

28339

36365

1612010

173361

3358499

Max K

44 32

16

97

26

239

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 some less edges but more vertices.

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# 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.



# 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.



# Breadth-First Search Improvements

Graph	num_vertices	num_edges	di (original)	di-norev	speedup
as-caida	26,475	53,381	2.22	1.22	1.82
delaunayn10	2,048	3,056	0.11	0.05	2.11
delaunayn20	1,058,576	3,145,686	90.49	47.61	1.90

Execution time in seconds on eight locales with 512GB memory and twenty processing units each.



- About 50% improvement in number of PUTs and GETs with di-norev by including full neighborhoods of each vertex contiguously in one array instead of maintaining reversed edges.
- No change in storage volume, 2m edges still stored.
- Similar changes could optimize the rest of our graph kernels.



#### STING Initiative: Focusing on Globally Significant Grand Challenges

- Many globally-significant grand challenges can be modeled by Spatio-Temporal Interaction Networks and Graphs (or "STING").
- Emerging real-world graph problems include:
  - Detecting community structure in large social networks
  - Defending the nation against cyber-based attacks
  - Discovering insider threats (e.g. Ft. Hood shooter, WikiLeaks)
  - Improving the resilience of the electric power grid
  - Detecting and preventing disease in human populations.
- Unlike traditional applications in computational science and engineering, solving these problems at scale often raises new research challenges due to:
  - Sparsity and the lack of locality in the massive data
  - Design of parallel algorithms for massive, streaming data analytics
  - The need for new exascale supercomputers that are energy-efficient, resilient, and easy-to-program



### STINGER – Time Frame



# Hornet (GPU only) – Time Frame



### STING Extensible Representation (STINGER) Design goals

- Enable algorithm designers to implement dynamic graph algorithms with ease.
- Portable semantics for various platforms
- Good performance for all types of graph problems and algorithms

   static and dynamic.
- Assumes globally addressable memory access
- Support multiple, parallel readers and a single writer
  - One server manages the graph data structures
  - Multiple analytics run in background with read-only permissions

### STING Extensible Representation (STINGER)

- Semi-dense edge list blocks with free space
- Compactly stores timestamps, types, weights
- Maps from application IDs to storage IDs
- Deletion by negating IDs, separate compaction



### STING: High-level architecture



- ▲ Server: Graph storage, kernel orchestration
- ▲ OpenMP + sufficiently POSIX-ish
- ▲ Multiple processes for resilience



### STINGER as an analysis package http://www.stingergraph.com/

# Anything that a static graph package can do (and a whole lot more):

#### Parallel agglomerative clustering:

Find clusters that are optimized for a userdefined edge scoring function.

#### **K-core Extraction:**

Extract additional communities and filter noisy high-degree vertices.

#### **Classic breadth-first search:**

Performs a parallel breadth-first search of the graph starting at a given source vertex to find shortest paths.

#### Parallel connected components:

Finds the connected components in a static network.



#### Streaming edge insertions and deletions:

New edge insertions, updates, and deletions in batches or individually. Optimized to update at rates of over 3 million edges per second on graphs of one billion edges.

#### Streaming clustering coefficients:

Tracks the local and global clustering coefficients of a graph.

#### Streaming connected components:

Real time tracking of the connected components.

#### **Streaming Betweenness Centrality:**

Find the key points within information flows and structural vulnerabilities.

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#### Streaming community detection:

Track and update the community structures within the graph as they change.


# Why not existing technologies?

- Traditional SQL databases
  - Not structured to do any meaningful graph queries with any level of efficiency or timeliness
- Graph databases mostly on-disk
  - Distributed disk can keep up with storing / indexing, but is simply too slow at random graph access to process on as the graph updates
- Hadoop and HDFS-based projects
  - Not really the right programming model for many structural queries over the entire graph, random access performance is poor
- Smaller graph libraries, processing tools
  - Can't scale, can't process dynamic graphs, frequently leads to impossible visualization attempts

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### AI Lab (NVAIL) 2019, PI: Bader Building the Future of Graph Analytics with RAPIDS

"Prof. David Bader and his lab ... are leaders in high performance computing algorithms, with a focus on both static and dynamic graph algorithms. With Prof. Bader and his lab, we will work on the design and implementation of scalable graph algorithms and graph primitives for integrating into cuGRAPH, leveraging their Hornet framework." – Sandra Skaff, NVIDIA, April 2019







## 2019 Facebook AI Systems Award: Scalable Graph Learning Algorithms

**Project Aim**: Develop scalable graph learning algorithms and implementations that open the door for learned graph models on massive graphs



Deep Learning (DL) has significantly impacted the tasks of speech recognition, image classification, object detection and recommendation

Complex tasks: self-driving, super-human image recognition, recommendation engines, machine natural language translation, content selection, learning patterns of life

Techniques used in DL: convolutional neural networks (CNNs)  $\rightarrow$  applicable for Euclidean data types and does not apply for Graphs

Solution: embedding graphs into a lower dimensional Euclidean space, generating a regular structure

- 1. developing a scalable high performance graph learning system based on GCNs algorithms, like GraphSage, by improving the workflow on shared-memory NUMA machines balancing computation between threads, optimizing data movement, and improving memory locality
- 2. investigate graph learning algorithm: specific decompositions and develop new strategies for graph learning that can inherently scale well while maintaining high accuracy
- Explore decomposition results from graph theory, for example forbidden graphs and the Embedding Lemma and determine how to apply such results into the field of graph learning
- Investigate whether these decompositions could assist in a dynamic graph setting

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Graphs are pervasive in large-scale data analysis

- Sources of massive data: peta- and exa-scale simulations, experimental devices, the Internet, scientific applications.
- New challenges for analysis: data sizes, heterogeneity, uncertainty, data quality.

Astrophysics Problem: Outlier detection. Challenges: massive datasets, temporal variations. Graph problems: clustering, matching.



Image sources: (1) <u>http://physics.nmt.edu/images/astro/hst\_starfield.jpg</u> (2,3) www.visualComplexity.com

Bioinformatics Problem: Identifying drug target proteins. <u>Challenges</u>: Data heterogeneity, quality. <u>Graph problems</u>: centrality, clustering.



#### Social Informatics Problem: Discover emergent communities, model spread of information. <u>Challenges:</u> new analytics routines, uncertainty in data. <u>Graph problems</u>: clustering, shortest paths, flows.



#### Characterizing Graph-theoretic computations



linear algebra (e.g., partitioning) or linear programming (e.g., matching) computations

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Streaming Analytics move us from reporting the news to predictive analytics

### **Traditional HPC**

- Great for "static" data sets.
- Massive scalability at the cost of programmability.
- Great for dense problems.
  - Sparse problems typically underutilize the system.



### **Streaming Analytics**

- Requires specialized analytics and data structures.
- Rapidly changing data.
- Low data re-usage.
  - Focused on memory operations and not FLOPS.



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## Graph Data Science

- Are there new graph techniques? Do they scale? Can the computational systems (algorithms, machines) handle massive networks with billions to trillions of items? Can the techniques tolerate noisy data, massive data, streaming data, etc. ...
- Communities may overlap, exhibit different properties and sizes, and be driven by different models
  - Detect communities (static or emerging)
  - Identify important individuals
  - Detect anomalous behavior
  - Given a community, find a representative member of the community
  - Given a set of individuals, find the best community that includes them
  - Find congestion, weak points, anomalies, surprises, ...



### Massive Streaming Graph Analytics



## Hierarchy of Interesting Analytics

### **Extend single-shot graph queries to include time.**

- Are there *s*-*t* paths between time  $T_1$  and  $T_2$ ?
- What are the important vertices at time *T*?

#### Use persistent queries to monitor properties.

- Does the path between s and t shorten drastically?
- Is some vertex suddenly very central?

### **Extend persistent queries to fully dynamic properties.**

- Does a small community stay independent rather than merge with larger groups?
- When does a vertex jump between communities?

### New types of queries, new challenges...



# Modeling Pandemic Spread

- The graph represents the contact patterns between individuals in a population.
- Various graph algorithms can be used to simulate the spread of a pandemic.
  - Centrality measures such as eigenvector centrality can identify the most important vertices in the network
  - Visualization of the spread of the pandemic can be created to check the effects of intervention and control strategies.
- The dataset can be a million or even a trillion vertices.



#### [Alguliyev, Aliguliyev, Yusifov, 2020]

R. Alguliyev, R. Alguliyev, and F. Yusifov, "Graph modelling for tracking the COVID-19 pandemic spread." Infectious disease modelling, 6, 2021: 112-122



# 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]))



