### Efficient Direct-Connect Topologies for Collective Communications

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ACE Theme 3 To be presented at NSDI '25







- **Collective Communication**: a set of communication operations among a group of nodes in a parallel computing system, serving as building blocks for distributed computing.
  - e.g. broadcast, reduce, allgather, reduce-scatter, allreduce, all-to-all, etc.
- Originally a topic in HPC, it is now extensively used for gradient, parameter, and activation synchronization in distributed ML training and inferencing.

#### Allgather



## Collective Communication

- We focus on accelerating **allgather**, **reduce-scatter**, and **allreduce**, three widely used collective operations in distributed ML.
- Focus on Allgather: allgather can be transformed into reduce-scatter and allreduce.
  - reduce-scatter = reversed allgather
  - allreduce = reduce-scatter + allgather





#### Reduce-Scatter

An emerging approach is to use **optical circuit network**:

- Higher bandwidth at lower capital expenditure and energy cost.
- The network can be configured into any **direct-connect** topology.
- Exhibit high reconfiguration latency, requiring relatively fixed topologies.







The topology of an optical circuit network can be modeled as a **direct-connect network**:

- Nodes are **directly connected** without the use of packet switches. Pairs of unconnected nodes cannot communicate directly.
- The network can be unidirectional (directed graph) or bidirectional (undirected graph).
- The topology is typically *d*-regular and homogeneous.
- $\alpha$ - $\beta$  cost model: the time cost of sending a size-M message over a link is  $\alpha + M/b$ .



• Allreduce-Type Collectives (e.g., allgather, reduce-scatter, allreduce)

- All-to-All Communication
  - Because of bandwidth tax, point-to-point flows should be as short as possible.
  - All-to-all throughput also requires low-diameter topology.
- Workloads may require both low diameter and load-balanced allreduce.
  - e.g., expert-parallel training involving both allreduce and all-to-all.

Ideal Topology: low-diameter topology with load-balanced collective communication.

# Traditional HPC Topologies

Problem: For a given workload (e.g., ML or HPC), what is the most efficient topology?

- Traditional HPC topologies are limited to a few ring-based graphs.
  - e.g., ring, torus, multi-ring.
- Pros: load-balanced collective, high-throughput allreduce-type collective operations.
- **Cons:** high diameter, detrimental for all-to-all throughput and latency-sensitive small-data allreduce.



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- Low-diameter expander graphs from graph theory.
  - e.g., de Bruijn graph, Kautz graph.
- Pros: low diameter, ideal for all-to-all throughput and small-data allreduce.
- Cons: complex structure, lack of load-balanced allreduce-type schedules.



(a) de Bruijn Graph



Topology Type	Small-Data Allreduce Latensy-Sensitive	Large-Data Allreduce Throughput-Sensitive	<b>All-to-All</b> Throughput
Traditional HPC Topologies	—	$\checkmark$	—
Low-Diameter Expander Graphs	$\checkmark$	—	$\checkmark$

Topology Type	Small-Data Allreduce Latensy-Sensitive	Large-Data Allreduce Throughput-Sensitive	<b>All-to-All</b> Throughput	
Traditional HPC Topologies	×	$\checkmark$	×	
Low-Diameter Expander Graphs	$\checkmark$	—	$\checkmark$	

• Latency and all-to-all throughput are bounded by topology diameter.

Topology Type	Small-Data Allreduce Latensy-Sensitive	Large-Data Allreduce Throughput-Sensitive	All-to-All Throughput	
Traditional HPC Topologies	×	$\checkmark$	×	
Low-Diameter Expander Graphs	$\checkmark$	???	$\checkmark$	

- Latency and all-to-all throughput are bounded by topology diameter.
- Question: Can we have load-balanced allreduce schedules on low-diameter topologies?

Challenge: Optimizing communication schedule can be computationally intractable.

- **Data Dependency:** unlike point-to-point traffic, flow conservation is not sufficient to maintain data dependency in collective communication due to multicast/aggregation.
- Earlier works track data dependency in chunks, leading to NP-hard discrete optimization.
  - SCCL [PPoPP '21] uses satisfiability modulo theories (SMT).
  - TACCL [NSDI '23], TE-CCL [SIGCOMM '24] use mixed integer linear program (MILP).

# of nodes	4	8	16	32	64
SCCL	0.59s	0.86s	21.4s	$> 10^4 s$	$> 10^4 s$
TACCL	0.50s	7.39s	1801s	1802s	n/a

Table: Generation Time on Hypercube

# of nodes	4	9	16	25	36
SCCL	0.61s	1.00s	60s	3286s	$> 10^4 s$
TACCL	0.45s	67.8s	1801s	1802s	n/a

Table: Generation Time on 2D Torus  $(n \times n)$ 







- Expansion Techniques: expand small-scale optimized topologies and schedules into large-scale ones.
  - Avoid intractable direct construction of large-scale topologies and schedules.
- Schedule Generation: generate optimal Breadth-First-Broadcast (BFB) schedule on large topologies.
  - Optimizing BFB schedule can be done with polynomial-time linear program.

Given a base topology and its associated communication schedule,

- We have graph transformations to expand the **base topology** into larger ones.
- The **base schedule** is also expanded to match the expanded topology.
- The expansion involves simple mapping of nodes, edges, and data send/recv.
- The sacrifice in overall performance is mathematically bounded during the process.

Line Graph Expansion:





Degree Expansion:





# Line Graph Expansion

We borrow the concept of **line graph** from graph theory:

- Edge (u, v) in base graph  $G \iff$  Node uv in the line graph L(G).
- For every uv, vw node pair in the line graph, there is an edge (uv, vw).
- $N_{L(G)} = N_G \cdot \deg G$ ;  $\deg L(G) = \deg G$ .







(b)  $L(K_{2,2})$  (N = 8, d = 2)

ac

cb

# Line Graph Expansion

The schedule can be mapped from base topology to the expanded topology:

- Any (shortest) path  $w_0 \rightarrow w_1 \rightarrow \cdots \rightarrow w_n$  in  $K_{2,2}$  can be mapped to a (shortest) path  $w_{-1}w_0 \rightarrow w_0w_1 \rightarrow \cdots \rightarrow w_{n-1}w_n \rightarrow w_nw_{n+1}$  in  $L(K_{2,2})$ , for any  $w_{-1}w_0 \neq w_nw_{n+1}$ .
- Data going from ca to bd in  $L(K_{2,2})$  can follow the corresponding path of a to b in  $K_{2,2}$ .



- Line graph expansion can be **applied repeatedly** to scale topology and schedule indefinitely.
  - Node degree is preserved, friendly to hardware constraints.
- The performance sacrifice is limited.
  - If the base is throughput-optimal with N nodes, then the expanded schedule is **at most**  $\frac{1}{(d-1)N}$  away from throughput optimality.
  - Expansion preserves low-diameter property. *N* increases *d*-fold while diameter increases by 1.



- G \* n makes n copies of G, and connect  $(a_i, b_j)$  for any (a, b) in G.
  - $\deg(G*n) = n \cdot \deg G$ ;  $N_{G*n} = n \cdot N_G$ .
- Degree expansion preserves throughput optimality.
  - Broadcast path in figure (a) is mapped to non-overlapping red and blue paths in (c).





(b) G \* 2 (N = 8, d = 2)



(c) Broadcasts w.r.t.  $a_1, a_2$ 

### Cartesian Product Expansion

- From graph theory, given graphs  $G_1, G_2, \ldots, G_n$ , we can construct a Cartesian product graph  $G_1 \square G_2 \square \ldots \square G_n$ .
  - $N_{G_1 \square G_2 \square \dots \square G_n} = \prod_i N_{G_i}; \quad \deg(G_1 \square G_2 \square \dots \square G_n) = \sum_i \deg(G_i).$
- $G_1 \square G_2 \square ... \square G_n$  is throughput-optimal if each  $G_i$  is throughput-optimal.
  - e.g., torus with arbitrary dimensions d<sub>1</sub> × d<sub>2</sub> × ··· × d<sub>n</sub>. Previously, only torus with equal dimensions (d<sub>1</sub> = d<sub>2</sub> = ··· = d<sub>n</sub>) has efficient schedules.
  - Use BFB schedule generation (to be introduced later).
  - Cartesian product greatly expands the set of throughput-optimal topologies we construct.



# **Topology Finder**

- Given a target topology size, the topology finder explores all known base topologies and potential combinations of expansion techniques.
- The resulting candidate topologies and schedules form a **Pareto-frontier**. The best one is then decided by hardware/workload specifications.
  - Pareto-frontier: low-diameter vs. load-balanced allreduce.
  - All-to-all performance is strongly related to graph diameter D(G).

Expansion Techniques	# of Nodes	Deg	Moore	BW
Line Graph Exp L <sup>n</sup> (G)	d"N	d	~	×
Degree Exp $G * n$	nN	nd	×	$\checkmark$
Cartesian Power $G^{\Box n}$	N <sup>n</sup>	nd	×	$\checkmark$
Cartesian Prod $G_1 \Box \dots \Box G_n$	$\prod_i N_i$	$\sum_{i} d_{i}$	×	$\checkmark$

Table: Summary of Expansion Techniques

Topology	$T_L$	T <sub>B</sub>	$2(T_L+T_B)$	D(G)	All-to-All
Π <sub>4,1024</sub>	$5\alpha$	1.332 <sup>M</sup> /в	323.5us	5	409.1us
$L^{3}(C(16, \{3, 4\}))$	$6\alpha$	1.020 <sup>M</sup> /B	291.0us	6	403.5us
$L^2(\text{Diamond}^{\square 2})$	8α	1.004 <sup>M</sup> /B	328.4us	8	446.6us
$L(DBJMod(2,4)^{\square 2})$	$11\alpha$	1.000 <sup>M</sup> /B	387.8us	9	529.9us
$(\text{UniRing}(1,4)\square\text{UniRing}(1,8))^{\square 2}$	$20\alpha$	0.999 <i>М/в</i>	567.6us	20	1174.4us
Baseline: 32x32 Torus	$62\alpha$	0.999 <i>M/B</i>	1407.6us	32	1342.2us
Theoretical Bound	<b>5</b> α	0.999 <i>M</i> / <i>B</i>	267.6us	5	382.3us

Table: Pareto-frontier for N = 1024, d = 4 with  $\alpha = 10 \mu s$  and M/B = 1MB/100Gbps.

#### **Observations:**

- Expansion techniques have huge gaps in the coverage of topology sizes.
  - Given a base topology with N = 4, d = 2, line graph expansion can only generate topologies of 8, 16, 32, ...  $(d^n N)$  number of nodes.
- There exist off-the-shelf low-diameter expander graphs from graph theory.

#### Question

Given a topology from graph theory, can we efficiently construct an efficient schedule for it?

Allgather: each node broadcasts a shard of data simultaneously.

- We perform a Breadth-First-Broadcast (BFB) from each node.
  - At time step t, from each source node, nodes at distance t 1 collectively broadcast the data shard to nodes at distance t.
- A linear program is used to balance workloads on links at each time step.
- Latency: data always follows the shortest paths, optimal for the given topology.
- Throughput: provably throughput-optimal for many types of graphs.









## BFB Example



## BFB Example





Nodes a and c each have a data shard to broadcast.









Broadcast data to neighbors.

Broadcast data to node *e*.

- Both *b*, *d* can provide shard *a*.
- Both *b*, *f* can provide shard *c*.

**Question:** How can data be sent while balancing the workload across links?



#### Perfect balance is achieved if

- d sends  $\frac{2}{3}$  of shard a.
- f sends  $\frac{2}{3}$  of shard c.
- b sends  $\frac{1}{3}$  of shard a and  $\frac{1}{3}$  of shard c.



#### Perfect balance is achieved if

- d sends  $\frac{2}{3}$  of shard a.
- f sends  $\frac{2}{3}$  of shard c.
- *b* sends  $\frac{1}{3}$  of shard *a* and  $\frac{1}{3}$  of shard *c*. Each link sends  $\frac{2}{3}$  of a shard in total.



### **BFB** Linear Program

For each node  $u \in V$  and time step  $t \in \{1, 2, \dots, D(G)\}$ ,

- Data shards from source nodes v at distance t to u should reach u at step t.
- $x_{v,(w,u),t}$  is the proportion of v's shard sent through link (w, u) at step t.
  - Only nodes w on the shortest paths from v to u can provide v's data shard; otherwise,  $x_{v,(w,u),t}$  is undefined.

minimize $U_{u,t}$ Minimize the max workload averagesubject to $\sum_{v,(w,u),t}^{v} \leq U_{u,t}, \quad \forall w \in N^-(u)$ Ensure  $U_{u,t}$  is the max workload $\sum_{v}^{v} x_{v,(w,u),t} = 1, \quad \forall v \in N_t^-(u)$ Ensure u receives all the data $0 \leq x_{v,(w,u),t} \leq 1.$  $\forall w, v$ minimize  $U_{\mu,t}$ 

Minimize the max workload across links Ensure  $U_{\mu,t}$  is the max workload

• Solve the linear program for each *u* and *t*.

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• Solve the linear program for each *u* and *t*.

**Question:** Why is BFB able to use a polynomial-time linear program rather than NP-hard discrete optimizations?

Answer: BFB eliminates the need to track data dependencies using discrete data chunks. What specific data are the  $\frac{2}{3}$  shard sent by d and  $\frac{1}{3}$  shard sent by b?



What specific data are the  $\frac{2}{3}$  shard sent by *d* and  $\frac{1}{3}$  shard sent by *b*?

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- In BFB, they can be **any parts** of shard *a*, as long as the union is the whole shard.
  - e.g.,  $\{1,2\}$  and  $\{3\}$ , or  $\{1,3\}$  and  $\{2\}$ .



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- Only the amount of data to be sent needs to be decided, not the specific data chunks, enabling a **continuous optimization**.



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- Only the amount of data to be sent needs to be decided, not the specific data chunks, enabling a **continuous optimization**.
- BFB ensures that *b*, *d* receive the entire shard before forwarding it to *e*, a guarantee not provided by all scheduling methods.



Question: How does BFB achieve polynomial-time schedule generation?



Zhao et al. (UW, BBN, MIT)

arXiv:2202.03356 (NSDI '25)

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- Finding efficient schedules starting from the whole schedule space is NP-hard.
- BFB schedules are a subset of the schedule space.
- Finding efficient schedules within BFB schedule space is polynomial-time.



BFB linear program gives the optimal BFB schedule. **Question:** the optimal BFB schedule = the globally optimal schedule?



BFB linear program gives the optimal BFB schedule.

**Question:** the optimal BFB schedule = the globally optimal schedule?

- Case 1: the optimal BFB schedule is the globally optimal schedule.
  - **Topologies with certain symmetry properties,** e.g., torus with arbitrary dimensions, twisted torus used by TPU v4, circulant graph, distance-regular graph.
  - Cartesian product of graphs with globally optimal BFB schedules.



BFB linear program gives the optimal BFB schedule.

**Question:** the optimal BFB schedule = the globally optimal schedule?

- Case 2: the optimal BFB schedule is efficient but not the globally optimal schedule.
  - The optimal BFB schedule is **close to** throughput optimality, e.g., generalized Kautz Graphs.



BFB linear program gives the optimal BFB schedule.

**Question:** the optimal BFB schedule = the globally optimal schedule?

- Case 3: the optimal BFB schedule is not efficient at all.
  - Random topologies without any symmetry properties.
  - Throughput optimality in all cases—see follow-up work ForestColl (arXiv:2402.06787).



# **BFB** Efficient Topologies

Throughput-optimal topologies with BFB:

#### • Torus with arbitrary dimensions

- Cartesian product of rings, which have globally optimal BFB schedules.
- Previous schedules are only efficient on torus with equal dimensions (e.g.,  $n \times n$ ,  $n \times n \times n$ )

#### • Twisted Torus used by Google TPU v4

• Computationally verified for at least  $N \le 10^4$ .



(a) 3x4 2D Torus



(b) 4x2 Twisted Torus

# **BFB** Efficient Topologies

- Circulant Graph: throughput-optimal with BFB.
  - Can be constructed for any N and even-value d.
  - Significant improvement over ring in latency if throughput optimality is required.
    - d = 4: total-hop latency  $\approx \frac{\sqrt{2N}}{2}$  instead of N 1.
- Generalized Kautz Graph: diameter is at most one hop away from Moore Bound.
  - Can be constructed for any N and d.
  - Close to throughput optimality:



### BFB vs Existing Schedule Generations

- BFB schedule generation is orders of magnitude faster than previous methods.
- BFB schedule is always theoretically optimal on hypercube and 2D torus.

# of nodes	4	8	16	32	64	1024
SCCL	0.59s	0.86s	21.4s	$> 10^4 s$	$> 10^4 s$	$> 10^4 s$
TACCL	0.50s	7.39s	1801s	1802s	n/a	n/a
BFB	<0.01s	<0.01s	<0.01s	0.03s	0.17s	52.7s

Table: Generation Time on Hypercube

# of nodes	4	9	16	25	36	2500
SCCL	0.61s	1.00s	60s	3286s	$> 10^{4} s$	$> 10^{4} s$
TACCL	0.45s	67.8s	1801s	1802s	n/a	n/a
BFB	<0.01s	<0.01s	<0.01s	0.01s	0.03s	61.1s

Table: Generation Time on 2D Torus  $(n \times n)$ 



Figure: Theoretical Performance of Schedules

# BFB vs Existing Schedule Generations

- Unlike previous methods, BFB does not require parameter sweeps.
- Previous methods require specifying # of chunks for data dependency tracking and heuristic parameters to speedup.

Λ/	SCCL				TAC	TACCL w/o Symmetry			TACCL w/ Symmetry			RER	
74	c = 1	c=2	c=3	c=4	c=1	c=2	c=3	c=4	c=1	c=2	c=3	c=4	БГБ
Hypercube													
4	0.59	0.64	0.68	0.72	0.89	0.50	0.83	0.75	0.62	0.51	0.71	0.60	< 0.01
8	0.86	1.22	1.86	2.48	96.9	807	63.2	1800	7.97	645	7.39	1801	$<\!\!0.01$
16	21.4	48.4	130	573	1801	1801	1801	1802	1801	n/a	n/a	n/a	$<\!\!0.01$
32	>104	$> 10^{4}$	$> 10^{4}$	$>10^{4}$	1802	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.03
64	>104	$> 10^{4}$	$> 10^{4}$	$>10^{4}$	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.17
1024	>104	$> 10^{4}$	$> 10^{4}$	>104	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	52.7
					2	D Toru	$s(n \times r)$	i)					
4	0.61	0.63	0.67	0.76	0.68	0.50	0.82	0.72	0.45	0.51	0.76	0.64	< 0.01
9	1.00	1.51	2.22	3.44	1801	189	67.8	262	88.6	71.1	67.8	105	< 0.01
16	17.5	60	131	603	1801	1801	1801	1802	1801	1801	1801	n/a	< 0.01
25	3286	5641	>104	>104	1802	1802	1803	n/a	1802	n/a	n/a	n/a	0.01
36	>10 <sup>4</sup>	>104	>104	>10 <sup>4</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.03
2500	>104	>104	>104	>10 <sup>4</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	61.1







#### **Direct-Connect Optical Testbed**



(a) A100 Servers

(b) Optical Patch Panel

- 12 servers, each with an NVIDIA A100 GPU.
- 100 Gbps HP NIC, configured as 4x25Gbps breakout interfaces.
- Topology is reconfigurable via a *Telescent* optical patch panel.

### Allreduce Evaluation

- Generate our best bidirectional topologies for N = 5 to 12.
- Compare allreduce performance with shifted rings and double binary trees at data sizes 1KB, 1MB, and 1GB.
- **Result:** our topologies consistently outperform baselines across all topology sizes *N* and allreduce data sizes *M*.



### Data-Parallel DNN Training Evaluation





(b) 12-node GPT-2 Training.

Frontera Supercomputer at the Texas Advanced Computing Center (TACC)

- Intel Xeon CPU nodes in a torus topology with 25 Gbps per link.
- **Result:** BFB torus schedules outperform all other schedules and remain efficient for tori with unequal dimensions.



#### Simulated Expert-Parallel Training

- Expert-parallel training involves both allreduce and all-to-all communications.
  - While allreduce can be overlapped, all-to-all remains on the critical path.
- At 1024-node training of 1.6T MoE model, our topology outperforms torus by 40%+.
  - Torus spends 58% of the time on all-to-all, while our topology only spends 30%.
- Our topologies remain within 5% of the theoretical lower bound all the time.



(a) Simulated Training of Switch Transformers.

(b) Training Timeline.

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- In this work, we introduce
  - **Expansion techniques** to expand small-scale optimized topologies and schedules into large-scale ones.
  - **Breadth-First-Broadcast** method to generate efficient communication schedules for large-scale topologies in polynomial time.

Together, we enable efficient collective communications with direct-connect topologies.

• In evaluation, we demonstrate significant improvements over existing direct-connect topologies in collective communications and ML training performance.

Efficient Direct-Connect Topologies for Collective Communications arXiv: https://arxiv.org/abs/2202.03356 To be presented at NSDI '25