

Parallel Numerical Algorithms

Chapter 1 – Parallel Computing

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Outline

- 1 Motivation
- 2 Architectures
 - Taxonomy
 - Memory Organization
- 3 Networks
 - Network Topologies
 - Graph Embedding
- 4 Communication
 - Message Routing
 - Communication Concurrency
 - Collective Communication



Why Parallel Computing?

Parallel computing

- provides cost-effective (often only) means of meeting enormous resource demands of large-scale simulations
- leverages existing resources or relatively inexpensive commodity parts
- offers alternative when individual processor speeds ultimately reach limits imposed by fundamental physical laws



Reasons for Caution

Parallel computing should be approached with caution

- unstable commercial market
- relative lack of available software
- immature computing environment
- challenging complexity of parallel programming
- physical constraints (power, cooling, packaging, etc.)

Nevertheless, insatiable appetite of computational scientists for ever greater computing capability has led them to embrace large-scale parallelism



Flynn's Taxonomy

Flynn's taxonomy: classification of computer systems by numbers of *instruction* streams and *data* streams:

- *SISD*: single instruction stream, single data stream
 - conventional serial computers
- *SIMD*: single instruction stream, multiple data streams
 - special purpose, “data parallel” computers
- *MISD*: multiple instruction streams, single data stream
 - not particularly useful, except perhaps in “pipelining”
- *MIMD*: multiple instruction streams, multiple data streams
 - general purpose parallel computers



SPMD Programming Style

SPMD (single program, multiple data): all processors execute same program, but each operates on different portion of problem data

- Easier to program than true MIMD, but more flexible than SIMD
- Although most parallel computers today are MIMD architecturally, they are usually programmed in SPMD style



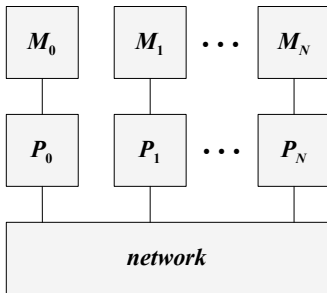
Architectural Issues

Major architectural issues for parallel computer systems include

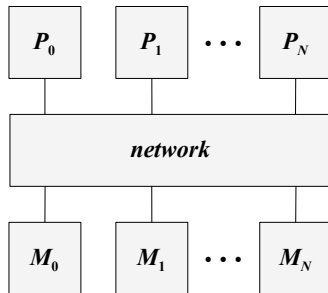
- *processor coordination*: synchronous or asynchronous?
- *memory organization*: distributed or shared?
- *address space*: local or global?
- *memory access*: uniform or nonuniform?
- *granularity*: coarse or fine?
- *scalability*: additional processors used efficiently?
- *interconnection network*: topology, switching, routing?



Distributed-Memory and Shared-Memory Systems



distributed-memory multicomputer



shared-memory multiprocessor



Distributed Memory vs. Shared Memory

	distributed memory	shared memory
scalability	easier	harder
data mapping	harder	easier
data integrity	easier	harder
performance optimization	easier	harder
incremental parallelization	harder	easier
automatic parallelization	harder	easier

Hybrid systems are common, with memory shared locally within SMP (symmetric multiprocessor) nodes but distributed globally across nodes



Network Topologies

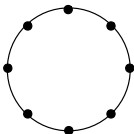
- Access to remote data requires communication
- Direct connections would require $\mathcal{O}(p^2)$ wires and communication ports, which is infeasible for large p
- Limited connectivity necessitates routing data through intermediate processors or switches
- Topology of network affects algorithm design, implementation, and performance



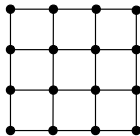
Some Common Network Topologies



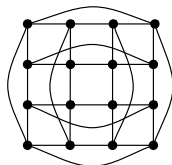
1-D mesh



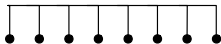
1-D torus (ring)



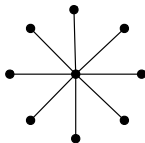
2-D mesh



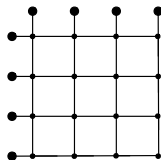
2-D torus



bus



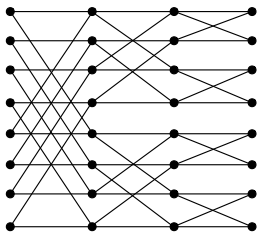
star



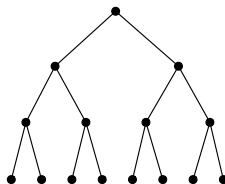
crossbar



Some Common Network Topologies



butterfly



binary tree



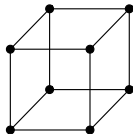
0-cube



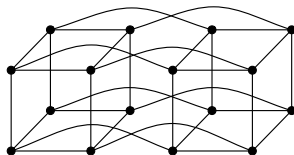
1-cube



2-cube



3-cube



4-cube

hypercubes



Graph Terminology

- **Graph**: pair (V, E) , where V is set of vertices or nodes connected by set E of edges
- **Complete graph**: graph in which any two nodes are connected by an edge
- **Path**: sequence of contiguous edges in graph
- **Connected graph**: graph in which any two nodes are connected by a path
- **Cycle**: path of length greater than one that connects a node to itself
- **Tree**: connected graph containing no cycles
- **Spanning tree**: subgraph that includes all nodes of given graph and is also a tree



Graph Models

- Graph model of network: nodes are processors (or switches or memory units), edges are communication links
- Graph model of computation: nodes are tasks, edges are data dependences between tasks
- Mapping task graph of computation to network graph of target computer is instance of *graph embedding*
- *Distance* between two nodes: number of edges (*hops*) in *shortest* path between them



Network Properties

Some network properties affecting its physical realization and potential performance

- *degree*: maximum number of edges incident on any node; determines number of communication ports per processor
- *diameter*: maximum distance between any pair of nodes; determines maximum communication delay between processors
- *bisection width*: smallest number of edges whose removal splits graph into two subgraphs of equal size; determines ability to support simultaneous global communication
- *edge length*: maximum physical length of any wire; may be constant or variable as number of processors varies



Network Properties

Network	Nodes	Deg.	Diam.	Bisect. W.	Edge L.
bus/star	$k + 1$	k	2	1	var
crossbar	$k^2 + 2k$	4	$2(k + 1)$	k	var
1-D mesh	k	2	$k - 1$	1	const
2-D mesh	k^2	4	$2(k - 1)$	k	const
3-D mesh	k^3	6	$3(k - 1)$	k^2	const
n-D mesh	k^n	$2n$	$n(k - 1)$	k^{n-1}	var
1-D torus	k	2	$k/2$	2	const
2-D torus	k^2	4	k	$2k$	const
3-D torus	k^3	6	$3k/2$	$2k^2$	const
n-D torus	k^n	$2n$	$nk/2$	$2k^{n-1}$	var
binary tree	$2^k - 1$	3	$2(k - 1)$	1	var
hypercube	2^k	k	k	2^{k-1}	var
butterfly	$(k + 1)2^k$	4	$2k$	2^k	var



Graph Embedding

Graph embedding: $\phi: V_s \rightarrow V_t$ maps nodes in source graph $G_s = (V_s, E_s)$ to nodes in target graph $G_t = (V_t, E_t)$

Edges in G_s mapped to paths in G_t

- **load:** maximum number of nodes in V_s mapped to same node in V_t
- **congestion:** maximum number of edges in E_s mapped to paths containing same edge in E_t
- **dilation:** maximum distance between any two nodes $\phi(u), \phi(v) \in V_t$ such that $(u, v) \in E_s$



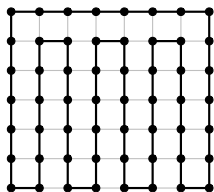
Graph Embedding

- Uniform load helps balance work across processors
- Minimizing congestion optimizes use of available bandwidth of network links
- Minimizing dilation keeps nearest-neighbor communications in source graph as short as possible in target graph
- Perfect embedding has load, congestion, and dilation 1, but not always possible
- Optimal embedding difficult to determine (NP-complete, in general), so heuristics used to determine good embedding

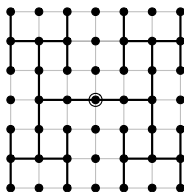


Examples: Graph Embedding

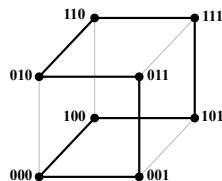
For some important cases, good or optimal embeddings are known, for example



ring in 2-D mesh
 dilation 1



binary tree in 2-D mesh
 dilation $\lceil (k-1)/2 \rceil$



ring in hypercube
 dilation 1



Gray Code

Gray code: ordering of integers 0 to $2^n - 1$ such that consecutive members differ in exactly one bit position

Example: binary reflected Gray code of length 16

0000 = 0	1100 = 12
0001 = 1	1101 = 13
0011 = 3	1111 = 15
0010 = 2	1110 = 14
0110 = 6	1010 = 10
0111 = 7	1011 = 11
0101 = 5	1001 = 9
0100 = 4	1000 = 8



Computing Binary Reflected Gray Code

```
/* Gray code */  
int gray(int i) {  
    return((i>>1)^i);}
```

```
/* inverse Gray code */  
int inv_gray(int i) {  
    int k; k=i;  
    while (k>0) {k>>=1; i^=k;}  
    return(i);}
```



Hypercube Embeddings

- Visiting nodes of hypercube in Gray code order gives *Hamiltonian cycle*, embedding ring in hypercube
- For mesh or torus of higher dimension, concatenating Gray codes for each dimension gives embedding in hypercube



Message Passing

Simple model for time required to send message (move data) between adjacent nodes:

$$T_{\text{msg}} = t_s + t_w L$$

- $t_s = \textit{startup time} = \textit{latency}$ (i.e., time to send message of length zero)
- $t_w = \textit{incremental transfer time per word}$ ($1/t_w = \textit{bandwidth}$ in words per unit time)
- $L = \textit{length}$ of message in words

For most real parallel systems, $t_s \gg t_w$



Message Routing

Messages sent between nodes that are not directly connected must be *routed* through intermediate nodes

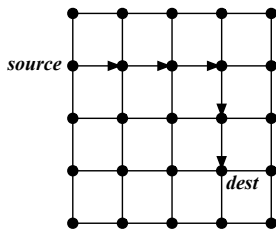
Message routing algorithms can be

- *minimal* or *nonminimal*, depending on whether shortest path is always taken
- *static* or *dynamic*, depending on whether same path is always taken
- *deterministic* or *randomized*, depending on whether path is chosen systematically or randomly
- *circuit switched* or *packet switched*, depending on whether entire message goes along reserved path or is transferred in segments that may not all take same path

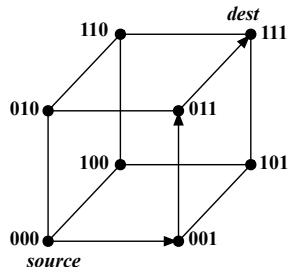


Message Routing

Most regular network topologies admit simple routing schemes that are static, deterministic, and minimal



2-D mesh



hypercube



Store-and-Forward vs. Cut-Through Routing

Store-and-forward routing: entire message is received and stored at each node before being forwarded to next node on path, so

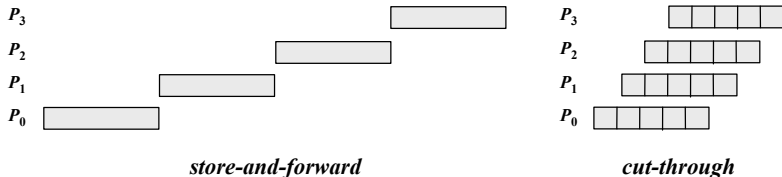
$$T_{\text{msg}} = (t_s + t_w L)D, \text{ where } D = \text{distance in hops}$$

Cut-through (or *wormhole*) routing: message broken into segments that are pipelined through network, with each segment forwarded as soon as it is received, so

$$T_{\text{msg}} = t_s + t_w L + t_h D, \text{ where } t_h = \text{incremental time per hop}$$



Store-and-Forward vs. Cut-Through Routing



Cut-through routing greatly reduces distance effect, but aggregate bandwidth may still be significant constraint

Communication Concurrency

For given communication system, it may or may not be possible for each node to

- send message while receiving another simultaneously on *same* communication link
- send message on one link while receiving simultaneously on *different* link
- send or receive, or both, simultaneously on *multiple* links

Depending on concurrency supported, time required for each step of communication algorithm is effectively multiplied by appropriate factor (e.g., degree of network graph)



Communication Concurrency

- When multiple messages contend for network bandwidth, time required to send message modeled by

$$T_{\text{msg}} = t_s + t_w S L$$

where S is number of messages sent concurrently over same communication link

- In effect, each message uses $1/S$ of available bandwidth



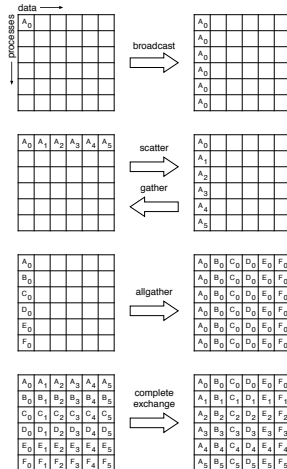
Collective Communication

Collective communication: multiple nodes communicating simultaneously in systematic pattern, such as

- *broadcast*: one-to-all
- *reduction*: all-to-one
- *multinode broadcast*: all-to-all
- *scatter/gather*: one-to-all/all-to-one
- *total or complete exchange*: personalized all-to-all
- *scan* or *prefix*
- *circular shift*
- *barrier*



Collective Communication



Broadcast

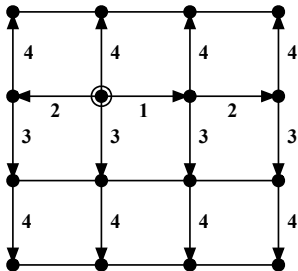
Broadcast: *source* node sends same message to each of $p - 1$ other nodes

Generic broadcast algorithm generates *spanning tree* with source node as root

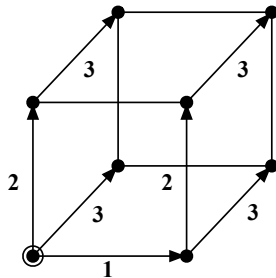
```
if source  $\neq$  me then  
    receive message  
end  
for each neighbor  
    if neighbor has not already received message then  
        send message to neighbor  
    end  
end
```



Broadcast



2-D mesh



hypercube



Broadcast

Cost of broadcast depends on network, for example

- 1-D mesh: $T = (p - 1) (t_s + t_w L)$
- 2-D mesh: $T = 2(\sqrt{p} - 1) (t_s + t_w L)$
- hypercube: $T = \log p (t_s + t_w L)$

For long messages, bandwidth utilization may be enhanced by breaking message into segments and either

- *pipeline* segments along *single* spanning tree, or
- send each segment along *different* spanning tree having *same* root

For example, hypercube with 2^k nodes has k *edge-disjoint* spanning trees for any given root node



Reduction

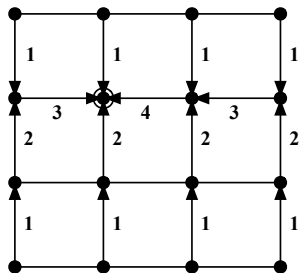
Reduction: data from all p nodes are combined by applying specified associative operation \oplus (e.g., sum, product, max, min, logical OR, logical AND) to produce overall result

Generic reduction algorithm uses spanning tree, but with data flow in opposite direction, from leaves to root

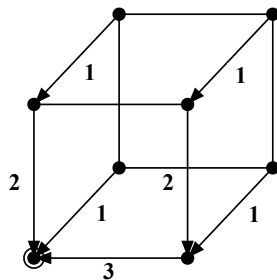
```
for each child of mine in spanning tree
    receive value from child
    my_value = my_value  $\oplus$  value
end
if root  $\neq$  me then
    send my_value to parent
end
```



Reduction



2-D mesh



hypercube



Reduction

Subsequent broadcast required if all nodes need result of reduction

Cost of reduction depends on network, for example

- 1-D mesh: $T = (p - 1) (t_s + (t_w + t_c) L)$
- 2-D mesh: $T = 2(\sqrt{p} - 1) (t_s + (t_w + t_c) L)$
- hypercube: $T = \log p (t_s + (t_w + t_c) L)$

where t_c = time per word for associative reduction operation

Often $t_c \ll t_w$, so t_c is sometimes omitted from performance analyses



Multinode Broadcast

Multinode broadcast: each of p nodes sends message to all other nodes (all-to-all)

- Logically equivalent to p broadcasts, one from each node, but efficiency can often be enhanced by overlapping broadcasts
- Total time for multinode broadcast depends strongly on concurrency supported by communication system
- Multinode broadcast need be no more costly than standard broadcast if aggressive overlapping of communication is supported



Multinode Broadcast

Implementation of multinode broadcast in specific networks

- 1-D torus (ring): initiate broadcast from each node simultaneously in same direction around ring; completes after $p - 1$ steps at same cost as single-node broadcast
- 2-D or 3-D torus: apply ring algorithm successively in each dimension
- hypercube: exchange messages pairwise in each of $\log p$ dimensions, with messages concatenated at each stage

Multinode broadcast implements reduction if messages are combined using associative operation instead of concatenation; avoids subsequent broadcast when result needed by all nodes



Multinode Reduction

Multinode reduction: each of p nodes is destination of reduction from all other nodes

Algorithms for multinode reduction are essentially reverse of corresponding algorithms for multinode broadcast



Personalized Collective Communication

Personalized collective communication: each node sends (or receives) *distinct* message to (or from) each other node

Examples

- *scatter*: analogous to broadcast, but root sends *different* message to each other node
- *gather*: analogous to reduction, but data received by root are concatenated rather than combined using associative operation
- *total exchange*: analogous to multinode broadcast, but each node exchanges *different* message with each other node



Scan or Prefix

Scan or *prefix*: given data values x_0, x_1, \dots, x_{p-1} , one per node, along with associative operation \oplus , compute sequence of partial results s_0, s_1, \dots, s_{p-1} , where

$$s_k = x_0 \oplus x_1 \oplus \dots \oplus x_k,$$

and s_k is to reside on node k , $k = 0, \dots, p - 1$

Scan can be implemented similarly to multinode broadcast, except intermediate results received by each node are selectively combined, depending on sending node's numbering, before being forwarded



Circular Shift

Circular k -shift: for $0 < k < p$, node i sends data to node $(i + k) \bmod p$

Circular shift implemented naturally in ring network, and by embedding ring in other networks



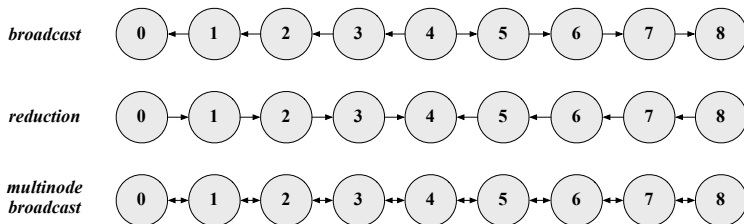
Barrier

Barrier: synchronization point that all processes must reach before any process is allowed to proceed beyond it

- For distributed-memory systems, barrier usually implemented by message passing, using algorithm similar to all-to-all
 - Some systems have special networks for fast barriers
- For shared-memory systems, barrier usually implemented using mechanism for enforcing *mutual exclusion*, such as test-and-set or semaphore, or with atomic memory operations



Graphical Depiction of Collective Communication



Arrows indicate general direction of data flow, but not necessarily specific implementation

May not be convenient (or possible) to indicate root, in which case two-headed arrows used



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