Parallel Numerical Algorithms

Chapter 2 – Parallel Algorithm Design

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Outline

Computational Model

- *Task*: sequential program and its local storage
- *Parallel computation*: two or more tasks executing concurrently
- *Communication channel*: link between two tasks over which messages can be sent and received
  - *send* is *nonblocking*: sending task resumes execution immediately
  - *receive* is *blocking*: receiving task blocks execution until requested message is available

Example: Laplace Equation in 1-D

- Consider Laplace equation in 1-D

$$u''(t) = 0$$

on interval $a < t < b$ with BC

$$u(a) = \alpha, \qquad u(b) = \beta$$

- Seek approximate solution values $u_i \approx u(t_i)$ at mesh points $t_i = a + ih$, $i = 0, \ldots, n+1$, where $h = (b-a)/(n+1)$

Example: Laplace Equation in 1-D

- Finite difference approximation

$$u''(t_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

yields tridiagonal system of algebraic equations

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 0, \quad i = 1, \ldots, n,$$

for u_i, $i = 1, \ldots, n$, where $u_0 = \alpha$ and $u_{n+1} = \beta$

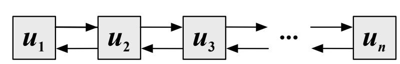
- Starting from initial guess $\boldsymbol{u}^{(0)}$, compute Jacobi iterates

$$u_i^{(k+1)} = \frac{u_{i-1}^{(k)} + u_{i+1}^{(k)}}{2}, \quad i = 1, \ldots, n,$$

for $k = 1, \ldots$ until convergence

Example: Laplace Equation in 1-D

- Define n tasks, one for each u_i, $i = 1, \ldots, n$
- Task i stores initial value of u_i and updates it at each iteration until convergence
- To update u_i, necessary values of u_{i-1} and u_{i+1} obtained from neighboring tasks $i-1$ and $i+1$



- Tasks 1 and n determine u_0 and u_{n+1} from BC

Example: Laplace Equation in 1-D

initialize u_i
for $k = 1, \ldots$
    if $i > 1$, send u_i to task $i-1$ { send to left neighbor }
    if $i < n$, send u_i to task $i+1$ { send to right neighbor }
    if $i < n$, recv u_{i+1} from task $i+1$ { receive from right neighbor }
    if $i > 1$, recv u_{i-1} from task $i-1$ { receive from left neighbor }
    wait for sends to complete
    $u_i = (u_{i-1} + u_{i+1})/2$ { update my value }
end

Mapping Tasks to Processors

- Tasks must be assigned to physical processors for execution
- Tasks can be mapped to processors in various ways, including multiple tasks per processor
- Semantics of program should not depend on number of processors or particular mapping of tasks to processors
- Performance usually sensitive to assignment of tasks to processors due to concurrency, workload balance, communication patterns, etc
- Computational model maps naturally onto distributed-memory multicomputer using message passing

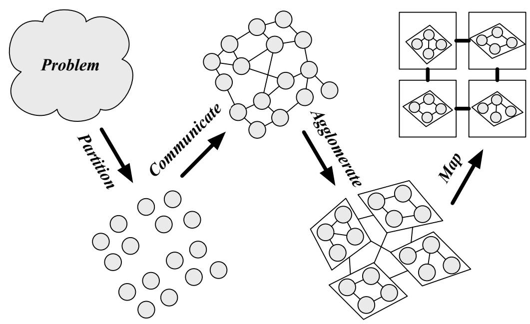
Other Models of Parallel Computation

- PRAM — Parallel Random Access Machine
- LogP — Latency/Overhead/Gap/Processors
- BSP — Bulk Synchronous Parallel
- CSP — Communicating Sequential Processes
- Linda — Tuple Space
- and many others

Four-Step Design Methodology

- *Partition*: Decompose problem into fine-grain tasks, maximizing number of tasks that can execute concurrently
- *Communicate*: Determine communication pattern among fine-grain tasks, yielding *task graph* with fine-grain tasks as nodes and communication channels as edges
- *Agglomerate*: Combine groups of fine-grain tasks to form fewer but larger coarse-grain tasks, thereby reducing communication requirements
- *Map*: Assign coarse-grain tasks to processors, subject to tradeoffs between communication costs and concurrency

Four-Step Design Methodology



Graph Embeddings

- Target network may be *virtual network topology*, with nodes usually called *processes* rather than processors
- Overall design methodology is composed of sequence of graph embeddings:
  - fine-grain task graph to coarse-grain task graph
  - coarse-grain task graph to virtual network graph
  - virtual network graph to physical network graph
- Depending on circumstances, one or more of these embeddings may be skipped
- Target system may automatically map processes of virtual network topology to processors of physical network

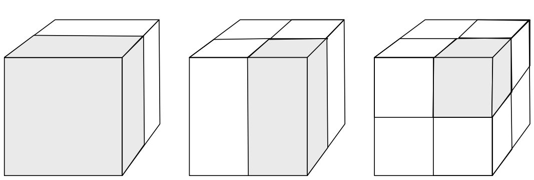
Partitioning Strategies

- *Domain decomposition*: subdivide geometric domain into subdomains
- *Functional decomposition*: subdivide system into multiple components
- *Independent tasks*: subdivide computation into tasks that do not depend on each other (*embarrassingly parallel*)
- *Array parallelism*: simultaneous operations on entries of vectors, matrices, or other arrays
- *Divide-and-conquer*: recursively divide problem into tree-like hierarchy of subproblems
- *Pipelining*: break problem into sequence of stages for each of sequence of objects

Desirable Properties of Partitioning

- Maximum possible concurrency in executing resulting tasks
- Many more tasks than processors
- Number of tasks, rather than size of each task, grows as overall problem size increases
- Tasks reasonably uniform in size
- Redundant computation or storage avoided

Example: Domain Decomposition



3-D domain partitioned along one (left), two (center), or all three (right) of its dimensions

With 1-D or 2-D partitioning, minimum task size grows with problem size, but not with 3-D partitioning

Communication Patterns

- Communication pattern determined by data dependences among tasks: because storage is local to each task, any data stored or produced by one task and needed by another must be communicated between them
- Communication pattern may be
  - local or global
  - structured or random
  - persistent or dynamically changing
  - synchronous or sporadic

Desirable Properties of Communication

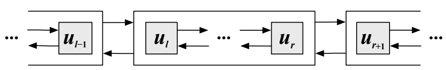
- Frequency and volume minimized
- Highly localized (between neighboring tasks)
- Reasonably uniform across channels
- Network resources used concurrently
- Does not inhibit concurrency of tasks
- Overlapped with computation as much as possible

Agglomeration

- Increasing task sizes can reduce communication but also reduces potential concurrency
- Subtasks that can't be executed concurrently anyway are obvious candidates for combining into single task
- Maintaining balanced workload still important
- Replicating computation can eliminate communication and is advantageous if result is cheaper to compute than to communicate

Example: Laplace Equation in 1-D

- Combine groups of consecutive mesh points t_i and corresponding solution values u_i into coarse-grain tasks, yielding p tasks, each with n/p of u_i values



- Communication is greatly reduced, but u_i values within each coarse-grain task must be updated sequentially

Example: Laplace Equation in 1-D

initialize $u_l, \ldots, u_r$
for $k = 1, \ldots$
  if $j > 1$, send u_l to task $j-1$ { send to left neighbor }
  if $j < p$, send u_r to task $j+1$ { send to right neighbor }
  if $j < p$, recv u_{r+1} from task $j+1$ { receive from right neighbor }
  if $j > 1$, recv u_{l-1} from task $j-1$ { receive from left neighbor }
  for $i = l$ **to** r
    $\bar{u}_i = (u_{i-1} + u_{i+1})/2$ { update local values }
  end
  wait for sends to complete
  $\boldsymbol{u} = \bar{\boldsymbol{u}}$
end

Overlapping Communication and Computation

- Updating of solution values u_i is done only after all communication has been completed, but only two of those values actually depend on awaited data
- Since communication is often *much* slower than computation, initiate communication by sending all messages first, then update all "interior" values while awaiting values from neighboring tasks
- Much (possibly *all*) of updating can be done while task would otherwise be idle awaiting messages
- Performance can often be enhanced by overlapping communication and computation in this manner

Example: Laplace Equation in 1-D

initialize $u_l, \ldots, u_r$
for $k = 1, \ldots$
  if $j > 1$, send u_l to task $j-1$ { send to left neighbor }
  if $j < p$, send u_r to task $j+1$ { send to right neighbor }
  for $i = l+1$ **to** $r-1$
    $\bar{u}_i = (u_{i-1} + u_{i+1})/2$ { update local values }
  end
  if $j < p$, recv u_{r+1} from task $j+1$ { receive from right neighbor }
  $\bar{u}_r = (u_{r-1} + u_{r+1})/2$ { update local value }
  if $j > 1$, recv u_{l-1} from task $j-1$ { receive from left neighbor }
  $\bar{u}_l = (u_{l-1} + u_{l+1})/2$ { update local value }
  wait for sends to complete
  $\boldsymbol{u} = \bar{\boldsymbol{u}}$
end

Surface-to-Volume Effect

- For domain decomposition,
  - *computation* is proportional to *volume* of subdomain
  - *communication* is (roughly) proportional to *surface area* of subdomain
- Higher-dimensional decompositions have more favorable surface-to-volume ratio
- Partitioning across more dimensions yields more neighboring subdomains but smaller total volume of communication than partitioning across fewer dimensions

Mapping

- As with agglomeration, mapping of coarse-grain tasks to processors should maximize concurrency, minimize communication, maintain good workload balance, etc
- But connectivity of coarse-grain task graph is inherited from that of fine-grain task graph, whereas connectivity of target interconnection network is independent of problem
- Communication channels between tasks may or may not correspond to physical connections in underlying interconnection network between processors

Mapping

- Two communicating tasks can be assigned to
  - one processor, avoiding interprocessor communication but sacrificing concurrency
  - two adjacent processors, so communication between the tasks is directly supported, or
  - two nonadjacent processors, so message routing is required
- In general, finding optimal solution to these tradeoffs is NP-complete, so heuristics are used to find effective compromise

Mapping

- For many problems, task graph has regular structure that can make mapping easier
- If communication is mainly global, then communication performance may not be sensitive to placement of tasks on processors, so random mapping may be as good as any
- Random mappings sometimes used deliberately to avoid communication *hot spots*, where some communication links are oversubscribed with message traffic

Mapping Strategies

- With tasks and processors consecutively numbered in some ordering,
  - *block mapping*: blocks of n/p consecutive tasks are assigned to successive processors
  - *cyclic mapping*: task i is assigned to processor $i \bmod p$
  - *reflection mapping*: like cyclic mapping except tasks are assigned in reverse order on alternate passes
  - *block-cyclic mapping* and *block-reflection mapping*: blocks of tasks assigned to processors as in cyclic or reflection
- For higher-dimensional grid, these mappings can be applied in each dimension

Examples of Mappings

block	0 1 2 3	4 5 6 7	8 9 10 11	12 13 14 15
cyclic	0 4 8 12	1 5 9 13	2 6 10 14	3 7 11 15
reflection	0 7 8 15	1 6 9 14	2 5 10 13	3 4 11 12
block-cyclic	0 1 8 9	2 3 10 11	4 5 12 13	6 7 14 15

Dynamic Mapping

- If task sizes vary *during* computation or can't be predicted in advance, tasks may need to be reassigned to processors dynamically to maintain reasonable workload balance throughout computation
- To be beneficial, gain in load balance must more than offset cost of communication required to move tasks and their data between processors
- Dynamic load balancing usually based on local exchanges of workload information (and tasks, if necessary), so work diffuses over time to be reasonably uniform across processors

Task Scheduling

- With multiple tasks per processor, execution of those tasks must be scheduled over time
- For shared-memory, any idle processor can simply select next ready task from common pool of tasks
- For distributed-memory, analogous approach is manager/worker paradigm, with manager dispatching tasks to workers
- Manager/worker scales poorly, as manager becomes bottleneck, so hierarchy of managers and workers becomes necessary, or more decentralized scheme

Task Scheduling

- For completely decentralized scheme, it can be difficult to determine when overall computation has been completed, so termination detection scheme is required
- With multithreading, task scheduling can conveniently be driven by availability of data: whenever executing task becomes idle awaiting data, another task is executed
- For problems with regular structure, it is often possible to determine mapping in advance that yields reasonable load balance and natural order of execution

Example: Atmospheric Flow Model

- Fluid dynamics of atmosphere modeled by system of partial differential equations
- 3-D problem domain discretized by $n_x \times n_y \times n_z$ mesh of points
- Vertical dimension (altitude) z, much smaller than horizontal dimensions (latitude and longitude) x and y, so $n_z \ll n_x, n_y$
- Derivatives in PDEs approximated by finite differences
- Simulation proceeds through successive discrete steps in time

Example: Atmospheric Flow Model

Partition:

- Each fine-grain task computes and stores data values (pressure, temperature, etc) for one mesh point
- Typical mesh size yields 10^5 to 10^7 fine-grain tasks

Communicate:

- Finite difference computations at each mesh point use 9-point horizontal stencil and 3-point vertical stencil
- Solar radiation computations require communication throughout each vertical column of mesh points
- Global communication to compute total mass of air over domain

Example: Atmospheric Flow Model

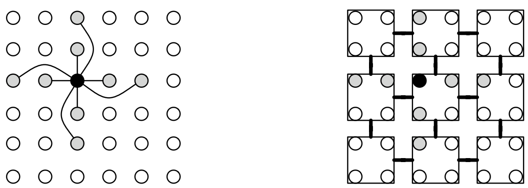
Agglomerate:

- Combine horizontal mesh points in blocks of four into coarse-grain tasks to reduce communication for finite differences to exchanges between adjacent nodes
- Combine each vertical column of mesh points into single task to eliminate communication for solar computations
- Yields $n_x \times n_y/4$ coarse-grain tasks, about 10^3 to 10^5 for typical mesh size

Map:

- Cyclic or random mapping reduces load imbalance due to solar computations

Example: Atmospheric Flow Model



Horizontal finite difference stencil for typical point (shaded black) in mesh for atmospheric flow model before (left) and after (right) agglomeration

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