Parallel Numerical Algorithms

Chapter 2 – Parallel Thinking
Section 2.3 – Parallel Performance

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Efficiency: effectiveness of parallel algorithm relative to its serial counterpart (more precise definition later)

Factors determining efficiency of parallel algorithm

- **Load balance**: distribution of work among processors
- **Concurrency**: processors working simultaneously
- **Overhead**: additional work not present in corresponding serial computation

Efficiency is maximized when load imbalance is minimized, concurrency is maximized, and overhead is minimized
Parallel Efficiency

(a) perfect load balance and concurrency
(b) good initial concurrency but poor load balance
(c) good load balance but poor concurrency
(d) good load balance and concurrency but additional overhead
Algorithm Attributes

- **Memory** ($M$) — overall memory footprint of the algorithm in words
- **Work** ($Q$) — total number of operations (e.g., flops) computed by algorithm, including loads and stores
- **Depth** ($D$) — longest sequence (chain) of dependent work operations
- **Time** ($T$) — elapsed wall-clock time (e.g., secs) from beginning to end of computation, expressed using
  - $\alpha$ — time to transfer a 0-byte message
  - $\beta$ — bandwidth cost (per-word)
  - $\gamma$ — time to perform one local operation (unit work)

Note that effective $\gamma$ is generally between the time to compute a floating point operation and the time to load/store a word, depending on local computation performed.
Scaling of Algorithm Attributes

- Subscript indicates number of processors used (e.g., $T_1$ is serial execution time, $Q_p$ is work using $p$ processors, etc.)

- We assume the *input size*, an attribute of the *problem* rather than the *algorithm*, is $M_1$

- Most algorithms we study will be *memory efficient*, meaning $M_p = M_1$ in which case we drop subscript and write just $M$

- If serial algorithm is optimal then $Q_p \geq Q_1$

- *Parallel work overhead*: $O_p := Q_p - Q_1$
Basic Definitions

- Amount of data often determines amount of computation, in which case we may write $Q(M)$ to indicate dependence of computational complexity on the input size.

- For example, when multiplying two full matrices of order $n$, $M = \Theta(n^2)$ and $Q = \Theta(n^3)$, so $Q(M) = \Theta(M^{3/2})$.

- In numerical algorithms, every data item is typically used in at least one operation, so we generally assume that work $Q$ grows at least linearly with the input size $M$. 
Execution Time and Cost

**Execution time** \( \geq \frac{\text{total work}}{\text{overall processor speed}} \)

- **Serial execution time:** \( T_1 = \gamma Q_1 \)
- **Parallel execution time:** \( T_p \geq \gamma Q_p / p \)

We can quantify \( T_p \) in terms of the critical path cost (sum of costs of longest chain of dependent subtasks)

\[
\text{Cost} := (L, W, F) := (\text{#messages}, \text{#words}, \text{#flops})
\]

\[
\max(\alpha L, \beta W, \gamma F) \leq T_p \leq \alpha L + \beta W + \gamma F
\]
Efficiency and Speedup

- **Speedup**:

  \[ S_p := \frac{\text{serial time}}{\text{parallel time}} = \frac{T_1}{T_p} \]

- **Efficiency**:

  \[ E_p := \frac{\text{speedup}}{\text{number of processors}} = \frac{S_p}{p} \]
Example: Summation

- Problem: compute sum of $n$ numbers

- Using $p$ processors, each processor first sums $n/p$ numbers

- Subtotals are then summed in tree-like fashion to obtain grand total
Example: Summation

Generally, $\alpha \gg \beta \gg \gamma$, which we use to simplify analysis.

**Serial**
- $M_1 = n$
- $Q_1 \approx n$
- $T_1 \approx \gamma n$

**Parallel**
- $M_p = n$
- $Q_p \approx n$
- $T_p \approx \alpha \log(p) + \gamma n/p$

$$S_p = \frac{T_1}{T_p} \approx \frac{\gamma n}{\alpha \log(p) + \gamma n/p} = \frac{p}{1 + (\alpha/\gamma)(p/n) \log p}$$

$$E_p = \frac{S_p}{p} \approx \frac{1}{1 + (\alpha/\gamma)(p/n) \log p}$$

To achieve a good speed-up want $\alpha/\gamma$ to be small and $n \gg p$
**Parallel Scalability**

- **Scalability**: relative effectiveness with which parallel algorithm can utilize additional processors

- A criterion: algorithm is *scalable* if its efficiency is bounded away from zero as number of processors grows without bound, or equivalently, \( E_p = \Theta(1) \) as \( p \to \infty \)

- Algorithm scalability in this sense is impractical unless we permit the input size to grow or bound the number of processors used
Parallel Scalability

Why use more processors?
- solve given problem in less time
- solve larger problem in same time
- obtain sufficient memory to solve given (or larger) problem
- solve ever larger problems regardless of execution time

Larger problems require more memory $M_1$ and work $Q_1$, e.g.,
- finer resolution or larger domain in atmospheric simulation
- more particles in molecular or galactic simulations
- additional physical effects or greater detail in modeling
Problem Scaling

The relative parallel scaling of different algorithms for a problem can be studied by fixing:

- input size: constant $M_1$
- input size per processor: constant $M_1/p$

The relative parallel scaling of different parallelizations of an algorithm can be studied by fixing:

- amount of work per processor: constant $Q_1/p$
- efficiency: constant $E_p$
- time: constant $T_p$

In all cases, we seek to quantify the relationship between parameters of the problem/algorithm with respect to the performance (time/efficiency)
**Strong Scaling**

*Strong scaling* – solving the same problem with a growing number of processors (constant input size)

- Ideal strong scaling to \( p \) processors requires \( T_p = T_1/p \)

- When problem is not embarrassingly parallel, the best we can hope for is \( T_p \approx T_1/p \) (i.e., \( E_p \approx 1 \)) up to some \( p \)

- We say an algorithm is *strongly scalable* to \( p_s \) processors if

\[
E_{p_s} = \Theta(1)
\]

i.e., we seek to asymptotically characterize the function \( p_s(Q_1) \) such that \( E_{p_s(Q_1)}(Q_1) = \text{const} \) for any \( Q_1 \)
Example: Summation

For summation example,

\[ E_p = \frac{1}{1 + (\alpha/\gamma)(p/n) \log p} \]

The binary tree summation algorithm is therefore strongly scalable to \( p_s = \Theta((\gamma/\alpha)n/\log((\gamma/\alpha)n)) \) processors.

The term \( \alpha/\gamma \) is constant for a given architecture, but can range from \( 10^3 \) to \( 10^6 \) on various machines.

Ignoring the dependence on this constant, the algorithm is strongly scalable to \( p_s = \Theta(n/\log(n)) \) processors.
Basic Bounds on Strong Scaling

- Since all processors have work to do only if $Q_p/p \geq 1$ for any $p$, the speed-up is bounded by
  \[ S_p \leq \frac{Q_1}{Q_p/p} \leq Q_1 \]

- It is possible but rare to achieve $S_p > M_1$ by using additional memory $M_p > M_1$, as otherwise some processors have no data to work on.
**Amdahl’s Law**

- **Amdahl’s law**: if a fraction $1/s$ of the computation is done sequentially, the achievable speed-up is at most $s$.
- Refers to most expensive unparallelized section of code.
- Recall that the depth ($D$) of an algorithm is the longest chain of dependent operations, i.e., this chain of operations is inherently sequential.
- Amdahl’s law implies that
  \[
  S_p = \frac{T_1}{T_p} \leq \frac{Q_1 \gamma}{D \gamma} = \frac{Q_1}{D}.
  \]
  In words, speedup $\leq$ work / depth.
- The law provides a basic strong scaling limit $p_s = O(Q/D)$, although communication cost often gives a tighter bound.
Weak Scaling

We refer to *weak scaling* as solving a problem with a fixed input size per processor \((M_1/p = \text{const})\).

- In literature, weak scaling often refers to fixed work per processor \(Q_1/p\), which is the same only if \(Q_1(M_1) = \Theta(M_1)\).
- This scaling mode \((M_1/p = \text{const})\) is natural when parallelism is being used to solve larger problems.
- An algorithm is *weakly scalable* to \(p_w\) processors if

\[
E_{p_w}(p_w M_0) = \Theta(1) \quad \Rightarrow \quad \frac{T_{p_w}(p_w M_0)}{T_1(M_0)} = \Theta \left( \frac{Q_1(p_w M_0)}{p_w Q_1(M_0)} \right)
\]

meaning when increasing \(p\) with constant \(M_1/p = M_0\), the time grows roughly as the work per processor until \(p > p_w\).

- If \(Q_1(M)\) is linear with \(M\) then the right side is \(\Theta(1)\).
Example: Summation

If considering the binary tree summation where $M_1 = n$ and $Q_1(M_1) = M_1$, weak scalability to $p_w$ processors requires

$$\frac{T_{p_w}(p_wn)}{T_1(n)} = \Theta(1)$$

$$\frac{T_{p_w}(p_wn)}{T_1(n)} \approx \frac{\alpha \log(p_w) + \gamma n}{\gamma n} = 1 + (\alpha/\gamma) \log(p_w)/n$$

Therefore, the algorithm is weakly scalable up to $p_w = \Theta(2^{n\gamma/\alpha})$. We can conclude the following about the scalability of the binary tree algorithm with respect to $n$:

- it is strongly scalable to $p_s = \Theta(n/\log(n))$ processors
- it is weakly scalable to $p_w = \Theta(2^n)$ processors
Fixed Execution Time

- Maintaining fixed execution time is applicable when computation must be completed within strict time limit (e.g., real-time constraints) or when user wishes to maintain given turn-around time.

- Since $T_p \geq Q_1/p$, $Q_1/p$ must be constant or decreasing.

- If $Q_1$ grows faster than linearly with input size $M_1$, then $M_1$ must grow sublinearly with $p$ to maintain constant $T_p$.

- To achieve perfect execution time scalability, all cost components $(L, W, F)$ of the algorithm must stay constant when $Q_p$ and $p$ grow by the same factor.

- Easier to achieve than strong scaling, but harder than weak scaling, where $Q_p$ can increase as $p$ and $M_1$ grow.
Fixed Accuracy

For some problems, desired accuracy of solution determines amount of memory and work required.

It is pointless to increase input size beyond that necessary to achieve desired accuracy.

Choice of resolution can affect serial work $Q_1$ in subtle and complex ways:

- conditioning of problem
- convergence rate for iterative method
- length of time step for time-dependent problem
Fixed Efficiency

- Previous scaling invariants determined rate of growth in problem size, and then we analyzed resulting efficiency to determine scalability.

- An alternative approach is to use efficiency itself as scaling invariant, i.e., we determine minimum growth rate in work required to maintain constant efficiency.

- If this is possible, then algorithm is scalable, but it may still be impractical if required growth rate in work is excessive, leading to unacceptably large execution time.

- Thus, resulting growth rate in work determines degree to which algorithm is scalable.
**Isoefficiency Function**

*Isoefficiency function* $\tilde{Q}(p)$ is the amount of work required to maintain given constant efficiency $E_p$

- The scaling with input size associated with the isoefficiency function, $\tilde{M}(p)$ is defined by solving for $M_1$ in $Q_1(M_1) = \tilde{Q}(p)$, i.e., $\tilde{M}(p) = Q_1^{-1}(\tilde{Q}(p))$

- So more precisely, we want to find $\tilde{Q}(p) = Q_1(\tilde{M}(p))$ so

  $$E_p(\tilde{M}(p)) = \text{const.} \quad \text{for increasing } p$$

- In practice we are only concerned with the asymptotic scaling of $\tilde{Q}(p)$
Example: Isoefficiency

To get the isoefﬁciency function for the binary tree sum:

1. Find $\tilde{M}(p)$ so $E_p(\tilde{M}(p)) = \Theta(1)$, which for the binary tree is

$$E_p(\tilde{M}(p)) \approx \frac{1}{1 + (\alpha/\gamma)(p/\tilde{M}(p)) \log p} = \Theta(1)$$

$$(\alpha/\gamma)(p/\tilde{M}(p)) \log p = \Theta(1)$$

$$\tilde{M}(p) = \Theta((\alpha/\gamma)p \log(p))$$

2. Determine $\tilde{Q}(p) = Q_1(\tilde{M}(p))$, which for the binary tree is just $\tilde{Q}(p) = \tilde{M}(p)$

So, for the binary tree, constant efﬁciency is maintained so long as the work scales as $Q_1 = n = \Theta(p \log(p))$.

However, in this scaling mode, the time $T_p$ and memory footprint per processor $\tilde{M}(p)/p$ grow with $\log p$
If we scale with constant efficiency, $T_p = \Theta(\tilde{Q}(p)/p)$ stays constant if isoefficiency function is $\tilde{Q}(p) = \Theta(p)$, but otherwise $T_p$ grows with $p$.

Growth rate of $T_p$ or $\tilde{M}(p)/p$ may not be acceptable.

Isoefficiency function of $\Theta(p)$ is desirable, but for many problems is not attainable.

More achievable isoefficiency function is $\Theta(p \log p)$ or $\Theta(p\sqrt{p})$, for which $T_p$ grows relatively slowly, like $\log p$ or $\sqrt{p}$, respectively, which may be acceptable.

Algorithm with isoefficiency function $\Theta(p^2)$ or higher has poor scalability, since $T_p$ grows at least linearly with $p$. 

Example: Atmospheric Flow Model

Let's now analyze a simplified version of the previously mentioned iterative method for the atmospheric flow model:

- 3-D \( n_x \times n_y \times n_z \) grid with \( n_z \ll n_x, n_y \)
- 5-point stencil on \( x, y \) (horizontal) planes
- Implicit solves along \( z \) (vertical) fibers

Assuming we can solve for each \( z \)-fiber with \( \Theta(n_z) \) work,

- Sequential work is \( Q_1 = \Theta(n_x n_y n_z) \) per iteration
- Depth \( D = \Theta(n_z) \) per iteration assuming each implicit solve is nonparallelizable
1-D Agglomeration Strategy

- **Partition**: assign one grid point per fine-grain task
- **Communicate**: near-neighbor communication for 5-point horizontal stencil, all-to-all vertical communication for vertical solve
- **Agglomerate**: First, consider 1-D agglomeration along one horizontal dimension of 3-D grid, with subgrid of size $n_x \times (n_y/p) \times n_z$ assigned to each coarse-grain task
Cost Analysis: 3-D Grid, 1-D Agglomeration

We would like to find the costs \((L, W, F)\) that will model the execution time as 
\[
T \approx \alpha L + \beta W + \gamma F
\]

- Since the parallel algorithm subdivides the mesh in a \textit{load balanced} way and works in a \textit{fully concurrent} manner,
  \[
  F = Q_p/p = Q_1/p = \Theta(n_x n_y n_z/p)
  \]

- Each task exchanges \(2n_x n_z\) grid points with each of its two neighbors, so 
  \[
  W = 2n_x n_z \quad \text{and} \quad L = 2
  \]

- Thus
  \[
  T_p = \alpha 2 + \beta 2n_x n_z + \Theta(\gamma n_x n_y n_z/p) = \alpha 2 + \beta 2n_x n_z + T_1/p
  \]
Efficiency Analysis: 3-D Grid, 1-D Agglomeration

**Efficiency:**

\[
E_p = \frac{S_p}{p} = \frac{T_1}{pT_p} = \frac{T_1}{p(\alpha 2 + \beta 2n_x n_z + T_1/p)}
\]

\[
= \frac{1}{1 + \frac{\alpha 2p/T_1 + \beta 2n_x n_z p/T_1}{T_1}} = \frac{1}{1 + \frac{\alpha 2p}{\gamma n_x n_y n_z} + \frac{\beta 2p}{\gamma n_y} }
\]

**Strong Scaling:**

1-D agglomeration is strongly scalable \((E_{ps} = \Theta(1))\)

\[
p_s = \Theta(\min[(\gamma/\alpha)n_x n_y n_z, (\gamma/\beta)n_y])
\]

processors, for a given machine configuration \(p_s = \Theta(n_y)\)

Amdahl’s law gives us a lower bound,

\[
S_{ps} \leq Q_1/D = \Theta(n_x n_y n_z/n_z) = \Theta(n_x n_y), \text{ so we observe that } 1\text{-D agglomeration may not be optimal}
\]
Weak Scalability: 3-D Grid, 1-D Agglomeration

We have \( E_p(n_x, n_y, n_z) = \frac{1}{1 + \frac{\alpha}{\gamma} \frac{2p}{n_x n_y n_z} + \frac{\beta}{\gamma} \frac{2p}{n_y}} \)

**Weak Scaling:**

- To reason about weak scaling, we need a notion of *increasing* input size for this problem
  - can increase \( n_x, n_y, n_z \) proportionally
  - can increase \( n_x, n_y \) while keeping \( n_z \) constant

- Assuming the latter, the weak scalability is characterized by constant

\[
E_{pw} \left( p_{w}^{1/2} n_x, p_{w}^{1/2} n_y, n_z \right) = \frac{1}{1 + \frac{\alpha}{\gamma} \frac{2}{n_x n_y n_z} + \frac{\beta}{\gamma} \frac{2\sqrt{p_{w}}}{n_y}}
\]

- As \( p_{w} \) grows, the last term in the denominator grows, so 1-D agglomeration is weakly scalable to

\[
p_{w} = \Theta(((\gamma/\beta)n_y)^2) \quad \text{processors}
\]
Isoefficiency gives a relative growth rate $\tilde{n}(p) = n_x(p) = n_y(p)$ needed to maintain constant efficiency, i.e.,

$$E_p(\tilde{n}(p), \tilde{n}(p), n_z) = 1/\left(1 + \frac{\alpha}{\gamma} \frac{2p}{\tilde{n}(p)^2 n_z} + \frac{\beta}{\gamma} \frac{2p}{\tilde{n}(p)}\right) = \Theta(1)$$

The last term in the denominator implies we need $\tilde{n}(p) = \Theta(p)$

- The isoefficiency function is then $\tilde{Q}(p) = \Theta(p^2)$
- Memory footprint grows in the same fashion $\tilde{M}(p) = \Theta(p^2)$
- Further, we would have $T_p = \Theta(pT_1)$
- Both the memory footprint per processor and the execution time must grow linearly with the number of processors to maintain constant efficiency
Cost Analysis: 3-D Grid, 2-D Agglomeration

Next consider 2-D agglomeration along both horizontal dimensions of 3-D grid, with subgrid of size
\[
\left(\frac{n_x}{\sqrt{p}}\right) \times \left(\frac{n_y}{\sqrt{p}}\right) \times n_z
\]
as assigned to each coarse-grain task.

For simplicity, we assume \(n_x = n_y = n\), which is consistent with the scaling of input size of interest.

Each task exchanges a total of
\[
2n_x n_z / \sqrt{p} + 2n_y n_z / \sqrt{p} = 4nn_z / \sqrt{p}
\]
points with its four neighbors, so
\[
T_p = \alpha 4 + \beta 4nn_z / \sqrt{p} + \gamma n^2 n_z / p
\]
Efficiency Analysis: 3-D Grid, 2-D Agglomeration

2-D agglomeration gives $E_p(n, n_z) = 1/ \left( 1 + \frac{\alpha}{\gamma} \frac{4p}{n^2 n_z} + \frac{\beta}{\gamma} \frac{4\sqrt{p}}{n} \right)$

- Setting $E_{ps}(n, n_z) = \Theta(1)$ shows strong scalability to $p_s = \Theta(\min[(\gamma/\alpha)n^2 n_z, (\gamma/\beta)^2 n^2])$ processors

- Meaning 2-D agglomeration will strong scale until each processor owns a constant-sized subgrid of vertical fibers (where the constant depends on relative values of $\alpha, \beta, \gamma$)

- Observing $E_p(n\sqrt{p}, n_z) = \Theta(1)$ for any $p$, shows the algorithm is weakly scalable to an arbitrary number of processors!

- Since efficiency is maintained unconditionally when work increases at the same rate as the number of processors, the isoefficiency function is $\bar{Q}(p) = \Theta(p)$
We consider mapping 1-D and 2-D agglomeration onto ideal choices of mesh networks

- **1-D mesh, 1-D agglomeration**
  - For 1-D agglomeration, we can map blocks of agglomerated tasks onto each processor
  - Only neighboring processors communicate, so there is no network contention
  - Any network that can embed a 1-D mesh is as good

- **2-D mesh, 2-D agglomeration**
  - For 2-D agglomeration, we can map 2-D blocks of agglomerated tasks onto each processor
  - Again only neighboring processors communicate, so there is no network contention
  - Any network that can embed a 2-D mesh is as good
Network Topology Mapping with Contention

The effect of network contention is evident when trying to map 2-D agglomeration onto a 1-D mesh

1. Map block-columns of agglomerated tasks to each processor, effectively yielding 1-D agglomeration, and avoiding network contention

2. Map a 2-D block of agglomerated tasks to each processor
   - One dimension can be mapped continuously, preserving near-neighbor communication
   - The other dimension would correspond to communication between processors $\sqrt{p}$ hops away from each other, yielding $\Theta(\sqrt{p})$ slow-down due to network contention
   - Our execution time then becomes
     \[ T_p \approx \alpha 2\sqrt{p} + \beta 2nn_z + \gamma n^2n_z / p \]
     same bandwidth cost as 1-D agglomeration, but more msgs

A. Grama, A. Gupta, and V. Kumar, Isoefficiency: measuring the scalability of parallel algorithms and architectures, *IEEE Parallel Distrib. Tech.* 1(3):12-21, August 1993


References


