Lecture 7:
Performance Optimization Part II:
Locality, Communication, and Contention

Parallel Computer Architecture and Programming
CMU 15-418/15-618, Spring 2017

( how to be l33t )
The Lumineers
Ho Hey
(The Lumineers)

“Clearly, this was a song about data locality.”
- Wesley Schultz
Today: more parallel program optimization

- Last lecture: strategies for assigning work to workers (threads, processors, etc.)
  - Goal: achieving good workload balance while also minimizing overhead
  - Discussed tradeoffs between static and dynamic work assignment
  - Tip: keep it simple (implement, analyze, then tune/optimize if required)

- Today: strategies for minimizing communication costs
Let’s begin by talking about message passing, since it makes communication explicit
Recall the grid-based solver example

In previous lectures we expressed this parallel program using data parallel and SPMD programming abstractions

```c
int N;
float* A = allocate(n+2, n+2);

void solve(float* A) {
    bool done = false;
    float diff = 0.f;
    while (!done) {
        for_all (red cells (i,j)) {
            float prev = A[i,j];
                         A[i+1,j] + A[i,j+1]);
            reduceAdd(diff, abs(A[i,j] - prev));
        }
        if (diff/(N*N) < TOLERANCE)
            done = true;
    }
}
```
Let’s think about expressing a parallel grid solver with communication via messages

- Each thread has its own address space
  - No shared address space abstraction (i.e., no shared variables)
- Threads communicate and synchronize by sending/receiving messages

One possible message passing machine configuration: a cluster of two workstations (you could make this cluster yourself using the machines in the GHC labs)
Message passing model: each thread operates in its own address space

In this figure: four threads

The grid data is partitioned into four allocations, each residing in one of the four unique thread address spaces

(four per-thread private arrays)
Data replication is now required to correctly execute the program

"Ghost cells" are grid cells replicated from a remote address space. It's common to say that information in ghost cells is "owned" by other threads.

Example:
After red cell processing is complete, thread 1 and thread 3 send row of data to thread 2 (thread 2 requires up-to-date red cell information to update black cells in the next phase)

Thread 2 logic:
```c
float* local_data = allocate(N+2,rows_per_thread+2);
int tid = get_thread_id();
int bytes = sizeof(float) * (N+2);

// receive ghost row cells (white dots)
recv(&local_data[0,0], bytes, tid-1);
recv(&local_data[rows_per_thread+1,0], bytes, tid+1);

// Thread 2 now has data necessary to perform future computation
```
**Message passing solver**

Similar structure to shared address space solver, but now communication is explicit in message sends and receives

```c
int N;
int tid = get_thread_id();
int rows_per_thread = N / get_num_threads();
float* localA = allocate(rows_per_thread+2, N+2);

// assume localA is initialized with starting values
// assume MSG_ID_ROW, MSG_ID_DONE, MSG_ID_DIFF are constants used as msg ids

void solve()
{
    bool done = false;
    while (!done)
    {
        float my_diff = 0.0f;

        if (tid != 0)
            send(&localA[1,0], sizeof(float)*(N+2), tid-1, MSG_ID_ROW);
        if (tid != get_num_threads()-1)
            send(&localA[rows_per_thread,0], sizeof(float)*(N+2), tid+1, MSG_ID_ROW);

        if (tid != 0)
            recv(&localA[0,0], sizeof(float)*(N+2), tid-1, MSG_ID_ROW);
        if (tid != get_num_threads()-1)
            recv(&localA[rows_per_thread+1,0], sizeof(float)*(N+2), tid+1, MSG_ID_ROW);

        for (int i=1; i<rows_per_thread+1; i++)
            for (int j=1; j<n+1; j++)
            {
                float prev = localA[i,j];
                                    localA[i,j-1] + localA[i,j+1]);
                my_diff += fabs(localA[i,j] - prev);
            }

        if (tid != 0)
            send(&mydiff, sizeof(float), 0, MSG_ID_DIFF);
        recv(&done, sizeof(bool), 0, MSG_ID_DONE);
        else
        {
            float remote_diff;
            for (int i=1; i<get_num_threads()-1; i++)
                recv(&remote_diff, sizeof(float), i, MSG_ID_DIFF);
            my_diff += remote_diff;

            if (my_diff/(N*N) < TOLERANCE)
                done = true;
            for (int i=1; i<get_num_threads()-1; i++)
                send(&done, sizeof(bool), i, MSG_ID_DONE);
        }
    }
}
```

Send and receive ghost rows to “neighbor threads”

Perform computation (just like in shared address space version of solver)

All threads send local my_diff to thread 0

Thread 0 computes global diff, evaluates termination predicate and sends result back to all other threads

Example pseudocode from: Culler, Singh, and Gupta
Notes on message passing example

- **Computation**
  - Array indexing is relative to local address space (not global grid coordinates)

- **Communication:**
  - Performed by sending and receiving messages
  - Bulk transfer: communicate entire rows at a time (not individual elements)

- **Synchronization:**
  - Performed by sending and receiving messages
  - Think of how to implement mutual exclusion, barriers, flags using messages

- For convenience, message passing libraries often include higher-level primitives (implemented via send and receive)

```c
reduce_add(0, &my_diff, sizeof(float)); // add up all my_diffs, return result to thread 0
if (pid == 0 && my_diff/(N*N) < TOLERANCE)
    done = true;
broadcast(0, &done, sizeof(bool), MSG_DONE); // thread 0 sends done to all threads
```
Synchronous (blocking) send and receive

- `send()`: call returns when sender receives acknowledgement that message data resides in address space of receiver.

- `recv()`: call returns when data from received message is copied into address space of receiver and acknowledgement sent back to sender.

Sender:

- Call `SEND(foo)`
- Copy data from buffer ‘foo’ in sender’s address space into network buffer
- Send message
- Receive ack
- `SEND()` returns

Receiver:

- Call `RECV(bar)`
- Receive message
- Copy data into buffer ‘bar’ in receiver’s address space
- Send ack
- `RECV()` returns
As implemented on the prior slide, there is a big problem with our message passing solver if it uses synchronous send/recv!

Why?

How can we fix it?
(while still using synchronous send/recv)
Message passing solver
(fixed to avoid deadlock)

Example pseudocode from: Culler, Singh, and Gupta
Non-blocking asynchronous send/recv

- **send():** call returns immediately
  - Buffer provided to send() cannot be modified by calling thread since message processing occurs concurrently with thread execution
  - Calling thread can perform other work while waiting for message to be sent

- **recv():** posts intent to receive in the future, returns immediately
  - Use checksend(), checkrecv() to determine actual status of send/receipt
  - Calling thread can perform other work while waiting for message to be received

**Sender:**

- Call SEND(foo)
- SEND returns handle h1
- Copy data from ‘foo’ into network buffer
- Send message
- Call CHECKSEND(h1) // if message sent, now safe for thread to modify ‘foo’

**Receiver:**

- Call RECV(bar)
- RECV(bar) returns handle h2
- Receive message
- Messaging library copies data into ‘bar’
- Call CHECKRECV(h2) // if received, now safe for thread // to access ‘bar’

RED TEXT = executes concurrently with application thread
Let’s talk about Pittsburgh...
Pittsburgh is now hot stuff!

36 Hours in Pittsburgh

Weekend Guide
By BRENDAN SPIEGEL, JULY 15, 2015

Beyond Pittsburgh’s pretty downtown, transformation and momentum reign, with former industrial areas giving way to art venues. By Fritzie Andrade, Louie Alfaro, Jessey Dearing, Andrew Hida and Aaron Wolfe on July 15, 2015. Watch in Times Video »
And so is Bay Area rent…

**The Median Rent for an SF Two-Bedroom Hits $5,000/Month**

Friday, October 9, 2015, by Tracy Elsen

It's that time of month again when rental website Zumper releases their **monthly rent report** and dashes San Franciscans' dreams of being able to move again. The new median rental price for a two-bedroom in the city is **$3,620**, up $90 in **just one month**. This is also up 13 percent over last year's mark. As Zumper points out, even bigger increase has been in two-bedroom rents, which hit a **$5,000** median for the first time this month and are up 19 percent **year over year**. San Francisco remains, of course, the most expensive city in the country for rents.

Although San Francisco's median rent for a one-bedroom is exceptionally high, there are actually only eight neighborhoods above that median. The **most expensive neighborhood is the Financial District**, with a **$4,270 per month median rent** for a one-bedroom, followed by Mission Bay/ Dogpatch at $3,900 and Pacific Heights at $3,850. South Beach, Russian Hill, Potrero Hill, SoMa, and the Mission also sit above the median. And while the NoMad and Flatiron neighborhoods in New York are still more expensive than any neighborhood in San Francisco, the Financial District now has the same median one-bedroom rent as Tribeca, which used to sit far above any San Francisco spot.
Hey, let’s move to Pittsburgh! (all the cool tech kids are doing it!)
Everyone wants to get to Pittsburgh!

(Latency vs. throughput review)

Assume only one car in a lane of the highway at once. When car on highway reaches Pittsburgh, the next car leaves San Francisco.

Distance: ~ 4,000 km

Latency of moving a person from San Francisco to Pittsburgh: 40 hours

Throughput: 1/40 person per hour (1 car every 40 hours)
Improving throughput

**Approach 1: drive faster!**
Throughput = 1/20 people per hour (1 car every 20 hours)

**Approach 2: build more lanes!**
Throughput: 1/10 people per hour (4 cars every 40 hours)
Using the highway more efficiently

Car’s velocity: 100 km/hr

Cars spaced out by 1 km

Throughput: 100 people/hr (1 car every 1/100th of hour)

Car’s velocity: 100 km/hr

Throughput: 400 people/hr (4 cars every 1/100th of hour)
Pipelining
Example: doing your laundry

Operation: do your laundry

1. Wash clothes
2. Dry clothes
3. Fold clothes

Latency of completing 1 load of laundry = 2 hours
Increasing laundry throughput
Goal: maximize throughput of many loads of laundry

One approach: duplicate execution resources:
use two washers, two dryers, and call a friend

Latency of completing 2 loads of laundry = 2 hours
Throughput increases by 2x: 1 load/hour
Number of resources increased by 2x: two washers, two dryers
Pipelining

Goal: maximize throughput of many loads of laundry

Latency: 1 load takes 2 hours
Throughput: 1 load/hour
Resources: one washer, one dryer
Another example: an instruction pipeline

Break execution of each instruction down into several smaller steps

Enables higher clock frequency (only a simple, short operation is done by each part of pipeline each clock)

time (clocks)

Latency: 1 instruction takes 4 cycles

Throughput: 1 instruction per cycle

(Yes, care must be taken to ensure program correctness when back-to-back instructions are dependent.)

Intel Core i7 pipeline is variable length (it depends on the instruction) ~15-20 stages

Four-stage instruction pipeline:

IF = instruction fetch
D = instruction decode + register read
EX = execute
WB = “write back” results to registers
Analogy to driving to Pittsburgh example

Task of driving from San Francisco to Pittsburgh is broken up into smaller subproblems that different cars can tackle in parallel (top: subproblem = drive 1 km, bottom: subproblem = drive 500m).

- **San Francisco**
  - **Car’s velocity:** 100 km/hr
  - **Throughput = 100 people per hour (1 car every 1/100 of an hour)**

- **Pittsburgh**

  **Cars spaced by 1 km on highway**

- **San Francisco**
  - **Car’s velocity:** 100 km/hr
  - **Cars now spaced by only 500m on highway**
  - **Throughput = 200 people per hour (1 car every 1/200 of an hour)**

  *Equivalent throughput to maintaining 1 km spacing of cars and driving at 200 km/hr*
Review: latency vs throughput

Latency

The amount of time needed for an operation to complete.
A memory load that misses the cache has a latency of 200 cycles.
A packet takes 20 ms to be sent from my computer to Google.
Asking a question on Piazza gets a response in 10 minutes.

Bandwidth

The rate at which operations are performed.
Memory can provide data to the processor at 25 GB/sec.
A communication link can send 10 million messages per second.
The TAs answer 50 questions per day on Piazza.
A simple model of non-pipelined communication

Example: sending a $n$-bit message

$$T(n) = T_0 + \frac{n}{B}$$

$T(n) =$ transfer time (overall latency of the operation)

$T_0 =$ start-up latency (e.g., time until first bit arrives at destination)

$n =$ bytes transferred in operation

$B =$ transfer rate (bandwidth of the link)

If processor only sends next message once previous message send completes...

“Effective bandwidth” = $n / T(n)$

Effective bandwidth depends on transfer size (big transfers amortize startup latency)
A more general model of communication

Example: sending a n-bit message

Total communication time = overhead + occupancy + network delay

Send API call, copy message to network buffer

Send data over link 1 (slow link): $T_0 + \frac{n}{B_{\text{small}}}$

Send data over link 2 (fast link): $T_0 + \frac{n}{B_{\text{large}}}$

Copy message to receiver node’s network buffer:

- **Yellow** = Overhead (time spent on the communication by a processor)
- **Blue** = Occupancy (time for data to pass through slowest component of system)
- **Gray** = Network delay (everything else)

Example from: Culler, Singh, and Gupta
Pipelined communication

Assume network buffer can hold at most two messages (numbers indicate number of msgs in buffer after insert)

Sender emits burst of messages (faster than 1/occupancy)

Messages are buffered while link is busy

Occupancy determines communication rate!
(in steady state: msg/sec = 1/occupancy)

Example from: Culler, Singh, and Gupta
When I talk about communication, I’m not just referring to messages between machines in a cluster.

Examples:
Communication between cores on a chip
Communication between a core and its cache
Communication between a core and memory
Think of a parallel system as an extended memory hierarchy

I want you to think of “communication” very generally:
- Communication between a processor and its cache
- Communication between processor and memory (e.g., memory on same machine)
- Communication between processor and a remote memory
  (e.g., memory on another node in the cluster, accessed by sending a network message)

View from one processor

Accesses not satisfied in local memory cause communication with next level
So managing locality to reduce the amount of communication performed is important at all levels.
Two reasons for communication: inherent vs. artifactual communication
**Inherent communication**

Communication that **must** occur in a parallel algorithm. The communication is fundamental to the algorithm.

In our messaging passing example at the start of class, sending ghost rows was inherent communication.
Communication-to-computation ratio

\[
\text{amount of communication (e.g., bytes)} \quad \frac{\text{amount of computation (e.g., instructions)}}{}
\]

- If denominator is the execution time of computation, ratio gives average bandwidth requirement of code

- "Arithmetic intensity" = 1 / communication-to-computation ratio
  - I find arithmetic intensity a more intuitive quantity, since higher is better.
  - It also sounds cooler

- High arithmetic intensity (low communication-to-computation ratio) is required to efficiently utilize modern parallel processors since the ratio of compute capability to available bandwidth is high (recall element-wise vector multiple from lecture 2)
Reducing inherent communication

Good assignment decisions can reduce inherent communication (increase arithmetic intensity)

1D blocked assignment: N x N grid

- Elements computed (per processor) \( \approx \frac{N^2}{P} \)
- Elements communicated (per processor) \( \approx 2N \)

1D interleaved assignment: N x N grid

- Elements computed (per processor) \( \propto \frac{N}{P} \)
- Elements communicated = 1/2
Reducing inherent communication

2D blocked assignment: $N \times N$ grid

- $N^2$ elements
- $P$ processors
- Elements computed: $\frac{N^2}{P}$ (per processor)
- Elements communicated: $\propto \frac{N}{\sqrt{P}}$ (per processor)
- Arithmetic intensity: $\frac{N}{\sqrt{P}}$

Asymptotically better communication scaling than 1D blocked assignment

Communication costs increase sub-linearly with $P$

Assignment captures 2D locality of algorithm
Artifactual communication

- Inherent communication: information that fundamentally must be moved between processors to carry out the algorithm given the specified assignment (assumes unlimited capacity caches, minimum granularity transfers, etc.)

- Artifactual communication: all other communication (artifactual communication results from practical details of system implementation)
Artifactual communication examples

- System might have a minimum granularity of data transfer (result: system must communicate more data than what is needed)
  - Program loads one 4-byte float value but entire 64-byte cache line must be transferred from memory (16x more communication than necessary)

- System operation might result in unnecessary communication:
  - Program stores 16 consecutive 4-byte float values, so entire 64-byte cache line is loaded from memory, entirely overwritten, then subsequently stored to memory (2x overhead... load was unnecessary)

- Poor placement of data in distributed memories (data doesn’t reside near processor that accesses it most often)

- Finite replication capacity (same data communicated to processor multiple times because cache is too small to retain it between accesses)
Review of the three (now four) Cs
You are expected to know this from 15-213/513!

- **Cold miss**
  First time data touched. Unavoidable in a sequential program.

- **Capacity miss**
  Working set is larger than cache. Can be avoided/reduced by increasing cache size.

- **Conflict miss**
  Miss induced by cache management policy. Can be avoided/reduced by changing cache associativity, or data access pattern in application.

- **Communication miss (new)**
  Due to inherent or artifactual communication in parallel system
Communication: working set perspective

This diagram holds true at any level of the memory hierarchy in a parallel system.

Question: how much capacity should an architect build for this workload?
Does the graph on the previous slide look familiar?
Techniques for reducing communication
Assume row-major grid layout.
Assume cache line is 4 grid elements.
Cache capacity is 24 grid elements (6 lines)

Recall grid solver application.
Blue elements show data in cache after update to red element.
Assume row-major grid layout.
Assume cache line is 4 grid elements.
Cache capacity is 24 grid elements (6 lines)

Blue elements show data in cache at end of processing first row.
Problem with row-major traversal: long time between accesses to same data

Assume row-major grid layout.
Assume cache line is 4 grid elements.
Cache capacity is 24 grid elements (6 lines)

Although elements (0,2) and (1,1) had been accessed previously, they are no longer present in cache at start of processing row 2

(What type of miss is this?)

This program loads three lines for every four elements.
Improving temporal locality by changing grid traversal order

Assume row-major grid layout.
Assume cache line is 4 grid elements.
Cache capacity is 24 grid elements (6 lines)

“Blocked” iteration order.
(recall cache lab in 15-213/513)

Now three lines for every eight elements.
Improving temporal locality by fusing loops

```c
void add(int n, float* A, float* B, float* C) {
  for (int i=0; i<n; i++)
    C[i] = A[i] + B[i];
}

void mul(int n, float* A, float* B, float* C) {
  for (int i=0; i<n; i++)
    C[i] = A[i] * B[i];
}


// assume arrays are allocated here

// compute E = D + ((A + B) * C)
add(n, A, B, tmp1);
mul(n, tmp1, C, tmp2);
add(n, tmp2, D, E);

void fused(int n, float* A, float* B, float* C, float* D, float* E) {
  for (int i=0; i<n; i++)
    E[i] = D[i] + (A[i] + B[i]) * C[i];
}

// compute E = D + (A + B) * C
fused(n, A, B, C, D, E);
```

**Two loads, one store per math op (arithmetic intensity = 1/3)**

**Two loads, one store per math op (arithmetic intensity = 1/3)**

**Overall arithmetic intensity = 1/3**

**Four loads, one store per 3 math ops (arithmetic intensity = 3/5)**

Code on top is more modular (e.g, array-based math library like numarray/numPy in Python)
Code on bottom performs much better. Why?
Improve arithmetic intensity by sharing data

- Exploit sharing: co-locate tasks that operate on the same data
  - Schedule threads working on the same data structure at the same time on the same processor
  - Reduces inherent communication

- Example: CUDA thread block
  - Abstraction used to localize related processing in a CUDA program
  - Threads in block often cooperate to perform an operation (leverage fast access to / synchronization via CUDA shared memory)
  - So GPU implementations always schedule threads from the same thread block on the same GPU core
Exploiting spatial locality

- Granularity of communication can be important because it may introduce artifactual communication
  - Granularity of communication / data transfer
  - Granularity of cache coherence (will discuss in future lecture)
Artifactual communication due to comm. granularity

2D blocked assignment of data to processors as described previously. Assume: communication granularity is a cache line, and a cache line contains four elements.

- Good spatial locality for non-local accesses to top-bottom rows.
- Poor spatial locality for non-local accesses to left-right columns.

Inherently need one element from left and right neighbor, but system must communicate four.

Implication: artifactual communication increases with cache line size!

= required elements assigned to other processors
Artifactual communication due to cache line communication granularity

Data partitioned in half by column. Partitions assigned to threads running on P1 and P2

Threads access their assigned elements (no inherent communication exists)

But data access on real machine triggers (artifactual) communication due to the cache line being written to by both processors *

* further detail in the upcoming cache coherence lectures
Reducing artifactual comm: blocked data layout

(Blue lines indicate consecutive memory addresses)

2D, row-major array layout

4D array layout (block-major)

Consecutive addresses straddle partition boundary

Consecutive addresses remain within single partition

Note: don’t confuse blocked assignment of work to threads (true in both cases above) with blocked data layout in the address space (only at right)
Contention
Example: office hours from 3-3:20pm (no appointments)

- **Operation to perform:** Professor Kayvon helps a student with a question

- **Execution resource:** Professor Kayvon

- **Steps in operation:**
  1. Student walks from Gates Cafe to Kayvon’s office (5 minutes)
  2. Student waits in line (if necessary)
  3. Student gets question answered with insightful answer (5 minutes)
Example: office hours from 3-3:20pm (no appointments)

- **Student 1**: 2:55pm - 3:05pm = Walk to Kayvon's office (5 minutes)
- **Student 2**: 3pm - 3:15pm = Wait in line
- **Student 3**: 3:05pm - 3:20pm = Get question answered
- **Student 4**: 2:55pm - 3:10pm = Walk to Kayvon's office (5 minutes)
- **Student 5**: 3:10pm - 3:20pm = Wait in line

**Time cost to student:**
- **Student 1**: 10 minutes
- **Student 2**: 23 minutes

**Problem:** contention for shared resource results in longer overall operation times (and likely higher cost to students)
Example: two students make appointments to talk to me about course material (at 3pm and at 4:30pm)

Student 1 (appt @ 3pm)

Time:
- 2:55pm
- 3pm
- 3:05pm

Time cost to student: 10 minutes

Student 2 (appt @ 4pm)

Time:
- 4:25pm
- 4:30pm
- 4:35pm

Time cost to student: 10 minutes
Contestation

- A resource can perform operations at a given throughput (number of transactions per unit time)
  - Memory, communication links, servers, TAs at office hours, etc.

- Contention occurs when many requests to a resource are made within a small window of time (the resource is a “hot spot”)

Example: updating a shared variable

Flat communication:
potential for high contention
(but low latency if no contention)

Tree structured communication:
reduces contention
(but higher latency under no contention)
Example: distributed work queues reduce contention (contention in access to single shared work queue)

Subproblems (a.k.a. “tasks”, “work to do”)

Set of work queues (In general, one per worker thread)

Worker threads:
Pull data from OWN work queue
Push new work to OWN work queue
(no contention when all processors have work to do)

When local work queue is empty...
STEAL work from random work queue
(synchronization okay since processor would have sat idle anyway)
Example: memory system contention in CUDA

```c
#define THREADS_PER_BLK 128

__global__ void my_cuda_program(int N, float* input, float* output)
{
    __shared__ float local_data[THREADS_PER_BLK];
    int index = blockIdx.x * blockDim.x + threadIdx.x;

    // COOPERATIVELY LOAD DATA HERE
    local_data[threadIdx.x] = input[index];

    // WAIT FOR ALL LOADS TO COMPLETE
    __syncthreads();

    // DO WORK HERE ..
    //
}
```

All threads in block access memory here

Threads blocked waiting for other threads here.

Uh oh, there no threads to run since all threads are either accessing memory or blocked at barrier. (no latency hiding ability!)

In general, a good rule of thumb when CUDA programming is to make sure you size your thread blocks so that the GPU can fit a couple of thread blocks worth of work per core of the GPU.

(This allows threads from one thread block to cover latencies from threads in another block assigned to the same core in a cooperative load situation like the one above.)
Multi-bank shared memory

32 SIMD ALUs

Crossbar

Shared memory SRAM (32 banks)
Example: Accessing NVIDIA GTX 480 shared memory

- Shared memory implementation
  - On-chip storage, physically partitioned into 32 SRAM banks
  - Address X is stored in bank B, where B = X % 32
  - Each bank can provide one word of data to warp per clock

- Figure shows memory addresses requested from each bank as a result of a shared memory load instruction (keep in mind this instruction is executed by all 32 threads in a warp)

```c
__shared__ float A[512];
int index = threadIdx.x;
float x2 = A[index]; // single cycle
float x3 = A[3*index]; // single cycle
float x4 = A[16 * index]; // 16 cycles
```
Example: create grid of particles data structure on large parallel machine (e.g., a GPU)

- Problem: place 1M point particles in a 16-cell uniform grid based on 2D position
  - Parallel data structure manipulation problem: build a 2D array of lists

- Recall: Up to 2048 CUDA threads per SM core on a GTX 1080 GPU (20 SM cores)
Common use of this structure: N-body problems

- A common operation is to compute interactions with neighboring particles
- Example: given particle, find all particles within radius $R$
  - Create grid with cells of size $R$
  - Only need to inspect particles in surrounding grid cells
Solution 1: parallelize over cells

- One possible answer is to decompose work by cells: for each cell, independently compute particles within it (eliminates contention because no synchronization is required)
  - Insufficient parallelism: only 16 parallel tasks, but need thousands of independent tasks to efficiently utilize GPU
  - Work inefficient: performs 16 times more particle-in-cell computations than sequential algorithm

```
list cell_lists[16];    // 2D array of lists

for each cell c          // in parallel
  for each particle p    // sequentially
    if (p is within c)   // sequentially
      append p to cell_lists[c]
```
Solution 2: parallelize over particles

- Another answer: assign one particle to each CUDA thread. Thread computes cell containing particle, then atomically updates list.
  - Massive contention: thousands of threads contending for access to update single shared data structure

```c
list cell_list[16];  // 2D array of lists
lock cell_list_lock;

for each particle p  // in parallel
  c = compute cell containing p
  lock(cell_list_lock)
  append p to cell_list[c]
  unlock(cell_list_lock)
```
Solution 3: use finer-granularity locks

- Alleviate contention for single global lock by using per-cell locks
  - Assuming uniform distribution of particles in 2D space... ~16x less contention than solution 2

```c
list cell_list[16]; // 2D array of lists
lock cell_list_lock[16];

for each particle p // in parallel
  c = compute cell containing p
  lock(cell_list_lock[c])
  append p to cell_list[c]
  unlock(cell_list_lock[c])
```
Solution 4: compute partial results + merge

- Yet another answer: generate N “partial” grids in parallel, then combine
  - Example: create N thread blocks (at least as many thread blocks as SM cores)
  - All threads in thread block update same grid
    - Enables faster synchronization: contention reduced by factor of N and cost of synchronization is lower because it is performed on block-local variables (in CUDA shared memory)
  - Requires extra work: merging the N grids at the end of the computation
  - Requires extra memory footprint: Store N grids of lists, rather than 1
Solution 5: data-parallel approach

Step 1: compute cell containing each particle (parallel over input particles)

- particle_index: 0 1 2 3 4 5
- grid_index: 9 6 6 4 6 4

Step 2: sort results by cell (particle index array permuted based on sort)

- particle_index: 3 5 1 2 4 0
- grid_index: 4 4 6 6 6 9

Step 3: find start/end of each cell (parallel over particle_index elements)

```plaintext
cell = grid_index[index]
if (index == 0)
    cell_starts[cell] = index;
else if (cell != grid_index[index-1]) {
    cell_starts[cell] = index;
    cell_ends[grid_index[index-1]] = index;
}
if (index == numParticles-1) // special case for last cell
    cell_ends[cell] = index+1;
```

- cell_starts
  - 0
  - 2
  - 5
  - ... (not inclusive)

- cell_ends
  - 2
  - 5
  - 6
  - ... (not inclusive)

This solution maintains a large amount of parallelism and removes the need for fine-grained synchronization... at cost of a sort and extra passes over the data (extra BW)

This code is run for each element of the particle_index array. (each innovation has a unique valid of 'index')
Summary: reducing communication costs

- Reduce overhead of communication to sender/receiver
  - Send fewer messages, make messages larger (amortize overhead)
  - Coalesce many small messages into large ones

- Reduce latency of communication
  - Application writer: restructure code to exploit locality
  - Hardware implementor: improve communication architecture

- Reduce contention
  - Replicate contended resources (e.g., local copies, fine-grained locks)
  - Stagger access to contended resources

- Increase communication/computation overlap
  - Application writer: use asynchronous communication (e.g., async messages)
  - HW implementor: pipelining, multi-threading, pre-fetching, out-of-order exec
  - Requires additional concurrency in application (more concurrency than number of execution units)
Summary

**Inherent vs. artifactual communication**
- Inherent communication is fundamental given how the problem is decomposed and how work is assigned
- Artifactual communication depends on machine implementation details (often as important to performance as inherent communication)

**Improving program performance**
- Identify and exploit locality: communicate less (increase arithmetic intensity)
- Reduce overhead (fewer, large messages)
- Reduce contention
- Maximize overlap of communication and processing (hide latency so as to not incur cost)