Module 1 Part 3 Concurrency Opportunity Recognition - K-means Algorithm

Carnegie Mellon University
18-645

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What we discussed in Part 2:

- **Course Goal**
  - When your research/application needs to be fast, you will be able to:
    1. **F**eel comfortable hacking up a solution
    2. **L**everage existing software building blocks
    3. **I**ndicate which platform is the best one to use
    4. **R**eason about why a piece of existing code is slow
    5. **T**ake care of potential performance bottlenecks

- **Hardware Architectures:**
  - Multicore vs Manycore – instruction latency vs throughput optimization
  - Opportunities in ILP, SIMD, SMP
  - Metrics for memory hierarchy
  - Metrics for system granularity

Questions you should ask yourself…

- What is the difference between concurrency and parallelism?
- What are the four key elements of the human problem solving process?
- What are the characteristics of a current algorithm implementation?
- What levels of concurrency can be **exposed** in the k-mean algorithm?
- What levels of parallelism are available to be **exploited**?
- What mapping between concurrency and parallelism can be **explored**?
- How is this relevant to writing fast code?

How to Write Fast Code?

Fast Platforms + **Good Techniques**

- **Multicore platforms**
- **Manycore platforms**
- **Cloud platforms**

- **Data structures**
- **Algorithms**
- **Software Architecture**

- This Lecture: Recognizing levels of concurrency in an application
- Effective Mapping of concurrency in an application with parallelism of a platform

→ **Fast code**

Outline

- The Application Developer
- Application-level Concurrency
- The Problem Solving Process

A number of figures in todays lecture were selected from Andrew Moore's tutorials in Statistical Data Mining (http://www.cs.cmu.edu/~awm/tutorials)

Distinction: Concurrency vs. Parallelism

Concurrency	Parallelism
The property of **an application** that… ...allows for tasks to **have the potential** to be… ...**executed simultaneously**	The property of **a platform** that… ...allows for tasks to **have the potential** to be… ...**executed simultaneously**
The **application architecture** in which… ...**more than one task** is active and able to… ...**make progress** at one time	The **platform architecture** in which.. ...**more than one task** can be active and… ...**make progress** at same time
We **expose concurrency** in our applications.	We **exploit parallelism** in our platforms.

The Application Developer

- Writing fast code is a process coherent with

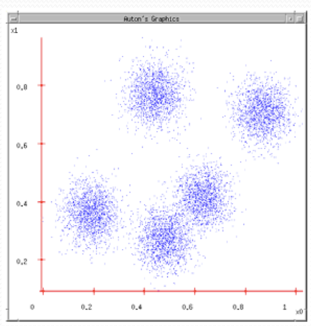
"general problem solving behavior"

- Newell and Simon, Human Problem Solving (1972), pp. 72-73

- The process of problem solving involves:
  1. Understand the **current state**
  2. Observe the **internal representation**
  3. **Search** among alternatives
  4. Select from a set of **choices**

k-means Problem

- Find *k* cluster centers that minimize the distance from each data point to a cluster center
- Important algorithm in machine learning:
  - Statistical data analysis
  - Vector quantization (Speech Recognition)
- NP-hard for arbitrary input
- ***k*-means algorithm** frequently finds a reasonable solutions quickly
- Issues:
  - Worst case running time is super-polynomial
  - Approximation can be arbitrarily bad



k-means Problem

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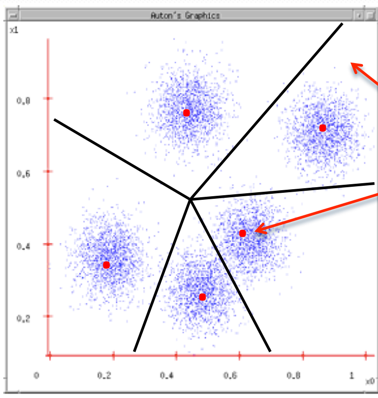

Cluster

Cluster center (centroid)

k: Number of clusters (defined a-priori)
Cluster: Assignment of data points to a class
Cluster Center: μ of data points in a cluster

Related Problems and Algorithms

- ***k*-means++**: Maximize scattering on initial cluster centers
- **KD-trees**: Fast *k*-means - Pre-compute distance between data points
- ***x*-means**: *k*-means with efficient estimation of the number of classes
- Gaussian Mixture Models:
  - Probabilistic assignments to clusters
  - Multivariate Gaussian distributions instead of means
- Expectation Maximization algorithms (EM algorithms)
  - Find maximum likelihood estimates of parameters in a statistical model, where the model depends on unobserved latent variables.
- Expectation Maximization Algorithms for Conditional Likelihoods
  - Estimate parameters in a statistical model to optimize conditional likelihood (where the objective function is a rational function)

k-means Algorithm (*"Lloyd's algorithm"*)

- Given an initial set of k means $\mathbf{m}_1^{(1)},\ldots,\mathbf{m}_k^{(1)}$
- **Expectation Step:** Assign each observation to the cluster with the closest mean

$$S_i^{(t)} = \left\{\mathbf{x}_j : \left\|\mathbf{x}_j - \mathbf{m}_i^{(t)}\right\| \le \left\|\mathbf{x}_j - \mathbf{m}_{i^*}^{(t)}\right\| \text{ for all } i^* = 1,\ldots,k\right\}$$

- **Maximization Step:** Calculate the new means to be the centroid of the observations in the cluster.

$$\mathbf{m}_i^{(t+1)} = \frac{1}{|S_i^{(t)}|}\sum_{\mathbf{x}_j \in S_i^{(t)}} \mathbf{x}_j$$

- Iterate until convergence or stopping criteria met

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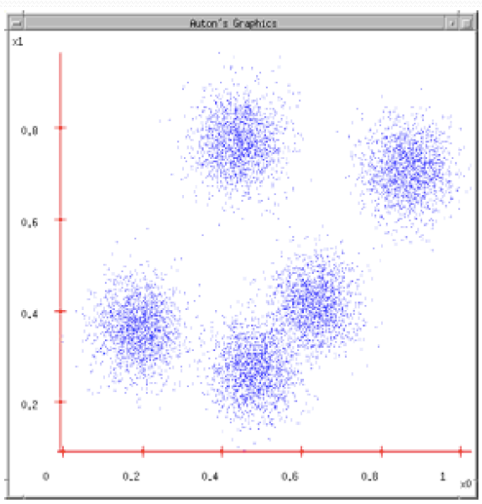
The Algorithm

Example:
k=5
Distance metric=euclidean
Dimensions=2

1. Randomly select k cluster Centers
2. Assign closest Center to each data point
3. Update Centers based on assignments from (2)
4. Re-iterate steps 2-3 until convergence or stopping criteria met



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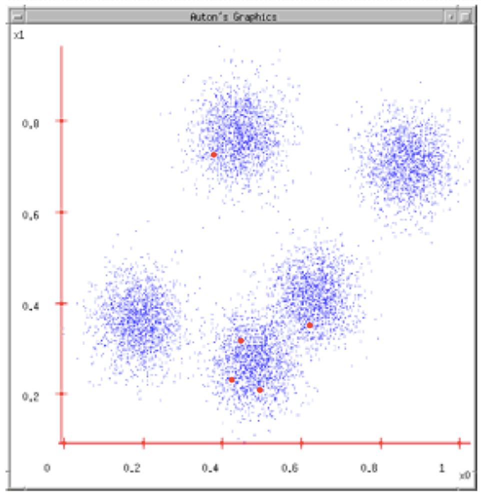

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The Algorithm

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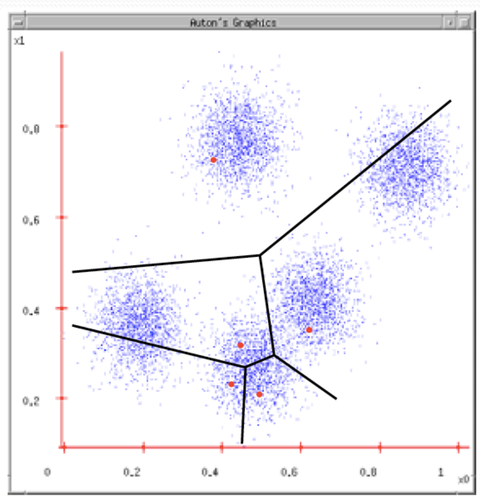

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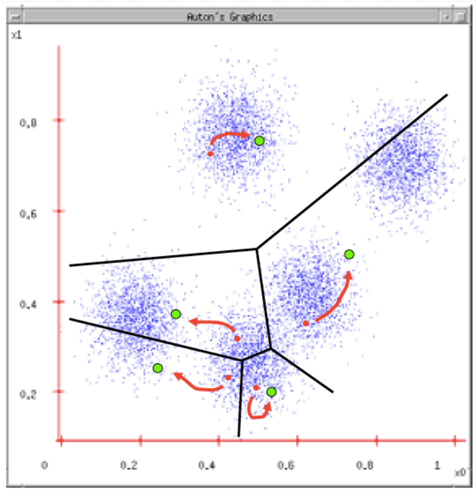

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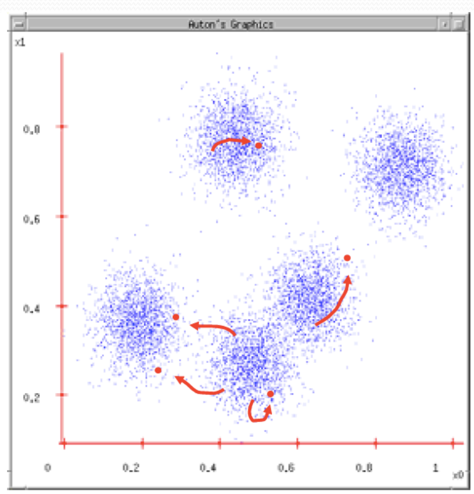

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The Phases

1. **Initialization:** Randomly select *k* cluster centers
   - Select *k* samples from data as initial centers [Forgy Partition]
2. **Expectation:** Assign each data point go closest center
   - Compare each data point (*N*) to each cluster center (*k*)
   - Distance Metric: Euclidean distance (*D* dimensions)
3. **Maximization:** Update centers based on assignments
   - For each cluster (*k*) compute mean (D dimensions) from data points assigned to that cluster
4. **Evaluate:** Re-iterate steps 2-3 until convergence or stopping criteria met
   - Percentage of data points re-assigned
   - Number of iterations (2-3)

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A Fast Implementation of *k*-means

- Following the process of problem solving with *k*-means:
  1. Understand the **current state**
     - Running on a platform
     - Using a specific set of resources
     - Achieving a specific performance
     - Meeting a specific criteria/requirement
  2. Observe the **internal representation**
  3. **Search** among alternatives
  4. Select from a set of **choices**

Assumption:
Starting from a functionally correct reference implementation

Implication:
Must observe the *current state* and *implementation requirements* before starting to solve a problem

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Understanding the Current State

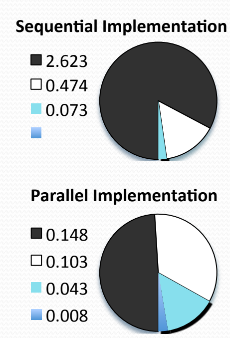
- **Running on a platform**
  - *Platform: Linux + GCC on x86 multicore processor*
- **Using a specific set of resources (ghcXX)**
  - *Computation: 2 to 8 cores, 2 to 8 way SIMD*
  - *Data: 32KB L1, 256KB L2, shared L3 cache, 2 to 16GB DRAM*
  - *Synchronization: on-chip shared-memory abstraction*
- **Achieving a specific performance**
  - *As measured in Homework 1*
- **Meeting a specific criteria/requirement**
  - *Matrix-Multiply: 5x performance on largest size test set*
  - *k-means: 1.5x performance on largest set*

What to Measure for Performance?

- Lecture coming up:

  Module 2 Part 3- **Performance Analysis: Roofline Model**

- Before that, a few simple techniques:
  - Observe the phases of execution
  - Characterize the execution time break downs
  - Reason about why a piece of code is slow
  - Identify performance bottlenecks



RTF: Real Time Factor (Proc Time / Real Time)
Phase 1 | Phase 3
Phase 2 | Seq. Overhead

Kisun You, Jike Chong, Youngmin Yi, Ekaterina Gonina, Christopher Hughes, Yen-Kuang Chen, Wonyong Sung, Kurt Keutzer, "Parallel Scalability in Speech Recognition: Inference engine in large vocabulary continuous speech recognition", IEEE Signal Processing Magazine, vol. 26, no. 6, pp. 124-135, November 2009.

Current state: *k*-means algorithm

- 4 Phases (Initialization, Expectation, Maximization, Evaluate)
  - Majority of time spent on Expectation and Maximization phases
- Entire data set can fit in memory on a single machine
- Number of samples (*N*) and feature dimensions (*D*) vary significantly
- Evaluation for any number of clusters ($2 \geq k \leq 300$)
- Example Data Sets:
  - *ionosphere_scale*: 351 Samples, 34 Dimensions
  - *svmguide*: 7089 Samples, 4 Dimensions
  - *cod-rna*: 59535 Samples, 8 Dimensions
  - *ljcnn1*: 191681 Samples, 22 Dimensions

Grade for mini-project1 base

A Fast Implementation of *k*-means

- Following the process of problem solving with *k*-means:
  1. Understand the **current state**
  2. Observe the **internal representation**
     - Application structure
       - Identified four phases of execution
     - Implementation concerns
       - Task considerations
       - Data representations
       - Concurrency opportunities
  3. **Search** among alternatives
  4. Select from a set of **choices**

Example Code (Initialize)

kmeans/seq_kmeans.c
lines: 116-119

```
....
    /* pick first numClusters elements of objects[] as initial cluster centers*/
    for (i=0; i<numClusters; i++)
        for (j=0; j<numCoords; j++)
            clusters[i][j] = objects[i][j];
....

__inline static float euclid_dist_2(int numdims, float *coord1, float *coord2)
{
  int i;
  float ans=0.0;
  for (i=0; i<numdims; i++)
    ans += (coord1[i]-coord2[i]) * (coord1[i]-coord2[i]);
  return(ans);
}
```

Define distance metric (Euclidian)

kmeans/seq_kmeans.c
lines: 51-63

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Example Code (Initialize)

kmeans/seq_kmeans.c
lines: 116-119

....
ers*/

Active Data Structures

objects: N x D clusters: k x D

...

__inline static float euclid_dist_2(int numdims, float *coord1, float *coord2)
{

Active Data Structures

coord1: 1 x D
coord2: 1 x D
ans: 1

}

Define distance metric (Euclidian)

kmeans/seq_kmeans.c
lines: 51-63

Possible concurrencies:
D (sum reduction) ← euclid_dist_2()

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Example Code (Expectation)

kmeans/seq_kmeans.c
lines: 136-147

```
....
    delta = 0.0;
    for (i=0; i<numObjs; i++) {
      /* find the array index of nestest cluster center */
      index = find_nearest_cluster(numClusters, numCoords, objects[i], clusters);

            ...

      /* if membership changes, increase delta by 1 */
      if (membership[i] != index) delta += 1.0;

      /* assign the membership to object i */
      membership[i] = index;
...
```

Evaluate distance to each cluster centroid and select closest

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Example Code (Expectation)

kmeans/seq_kmeans.c
lines: 136-147

```
....
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      index = find_nearest_cluster(numClusters, numCoords, objects[i], clusters);
```

Active Data Structures

objects: N x D clusters: k x D → membership: N x 1

```
      membership[i] = index;
...
```

Possible Concurrencies:
- N (independent)
- D (sum reduction) ← euclid_dist_2()
- k (min reduction)

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Example Code (Maximization)

kmeans/seq_kmeans.c
lines: 148-162

```
....
  /* update new cluster centers : sum of objects located within */
     newClusterSize[index]++;
     for (j=0; j<numCoords; j++)
        newClusters[index][j] += objects[i][j];
   }

   /* average the sum and replace old cluster centers with newClusters */
   for (i=0; i<numClusters; i++) {
      for (j=0; j<numCoords; j++) {
         if (newClusterSize[i] > 0)
            clusters[i][j] = newClusters[i][j] / newClusterSize[i];
         newClusters[i][j] = 0.0;   /* set back to 0 */
      }
      newClusterSize[i] = 0;      /* set back to 0 */
   }
...
```

prepare for next iteration

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Example Code (Maximization)

kmeans/seq_kmeans.c
lines: 148-162

```
....
  /* update new cluster centers : sum of objects located within */
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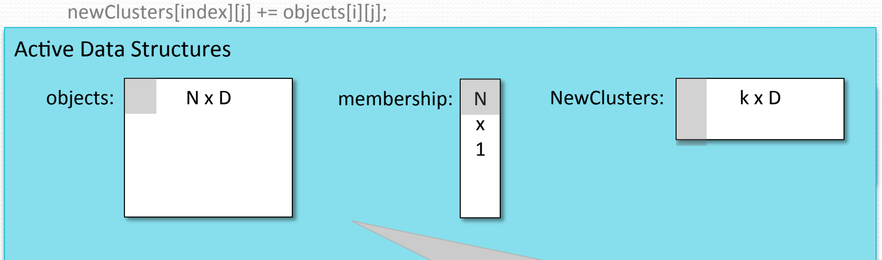


```
      }
      newClusterSize[i] = 0;      /* set bac
   }
...
```

Possible Concurrencies:
D (independent)
N (Histogram computation into k bins

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Example Code (Evaluate)

kmeans/seq_kmeans.c
lines: 164-165

```
....
   delta /= numObjs;
   } while (delta > threshold && loop++ < 500);
...
```

Two stopping criteria defined

- Two stopping criteria:
  - Percentage of data points that change class < *threshold*
  - Max 500 iterations (Assign and Update)

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The phases - concurrency

1. <u>Initialization:</u> Randomly select *k* cluster centers
2. **<u>Expectation:</u>** Assign closest center to each data point
   - *N* (independent)
   - *k* (min reduction)
   - *D* (sum reduction)
3. **<u>Maximization:</u>** Update centers based on assignments
   - *D* (independent)
   - *N* (Histogram computation into k bins)
4. <u>Evaluate:</u> Re-iterate steps 2-3 until convergence

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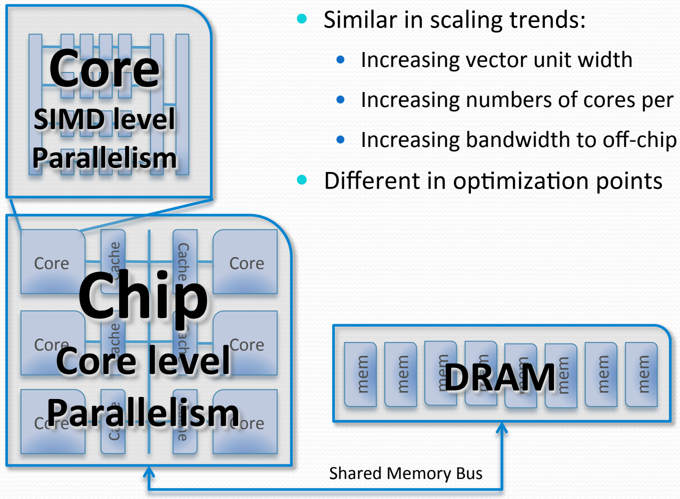
A Fast Implementation of *k*-means

- Following the process of problem solving with *k*-means:
  1. Understand the **current state**
  2. Observe the **internal representation**
  3. **Search** among alternatives
  4. Select from a set of **choices**

Search Among Alternatives

- Given the observed internal representations and the concurrency opportunities…
- What are the implementation **alternatives**?
  - Different mapping of **application concurrency** to **platform parallelism**
- The **search** process
  - More complex than one **application concurrency** to one **platform parallelism**
  - May want to sequentialize some operations:
    - Some parallel operations are as **"work-efficient"** as sequential operations
    - Reduction – sequential: O(N), Parallel: O(N logN)
  - One level of concurrency could map to multiple levels of parallelism

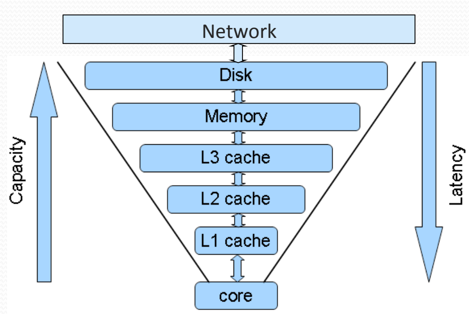
Multicore and Manycore Parallelism



- Similar in scaling trends:
  - Increasing vector unit width
  - Increasing numbers of cores per die
  - Increasing bandwidth to off-chip memory
- Different in optimization points

Memory Hierarchy

- **Cache**:
  - A piece of fast memory close to the compute modules in a microprocessor
  - Allows faster access to a limited amount of data
  - Physical properties of wires and transistors determines trade-off between **cache capacity** and **access throughput/latency**



(Capacity), (throughput), (latency)
Exa-Bytes, 0.1 GB/s, ~1-10B cycles
3TB, 6 GB/s, ~1M cycles
16GB, 34.08 GB/s, ~200 cycles
8 MB, 108.8 GB/s, 26-31 cycles
256 KB, 108.8 GB/s, 12 cycles
32 KB Data Cache, 163.2 GB/s, 4-6 cycles
Intel Core2 – 2600k @ 3.4GHz
(viewed from one core)

Mapping Concurrency to Parallelism

- How does it map to the platform?
  - SIMD level parallelism
  - Core level parallelism
- How does it map to the cache hierarchy?
  - What data is required for each concurrent operation?
  - What are the synchronization points in the algorithm?
- Expectation & Maximization Phases
  - SIMD & core-level parallelism across data-points (N)
    - Update membership for each data point sequentially
      - Compute distance to each cluster center and select index with min. distance
    - Histogram computation (summation / assignment count for new clusters)
  - Other possible concurrency mappings?

A Fast Implementation of *k*-means

- Following the process of problem solving with *k*-means:
  1. Understand the **current state**
  2. Observe the **internal representation**
  3. **Search** among alternatives
  4. Select from a set of **choices**
     - Does solution met required criteria
     - How to evaluate a mapping?
       - Efficiency: Runs quickly, makes good use of computational resources
       - Simplicity: Easy to understand code is easier to develop, debug, verify and modify
       - Portability: Should run on widest range of parallel computers
       - Scalability: Should be effective on a wide range of processing elements
     - Other considerations: Practicality, Hardware, Engineering cost

Evaluate Choice

- Expectation & Maximization Phases
  - SIMD & core-level parallelism across data-points (N)
    - Update membership for each data point sequentially
    - Histogram computation (summation / assignment count for new clusters)

  → OpenMP

- How we can evaluate the choice and make a decision
  - Efficiency
  - Simplicity / Maintainability
  - Portability
  - Scalability

How to write fast code

- **Expose** concurrencies in applications and algorithms
  - **Module 1 Part 3:** "Concurrency Opportunity Recognition"
  - Mini-Projects (1-3) & Term Project
- **Exploit** parallelisms on application platform
  - **Module 1 Part 2:** "Advanced Parallel Hardware Architectures"
  - Mini-Projects (1-3) & Term Project
- **Explore** mapping between concurrency and parallelism
  - The rest of the semester….
  - Abstractions to support mapping of concurrencies to parallelisms
    - OpenMP [**Module 2**]
    - CUDA [**Module 3**]
    - Hadoop [**Module 4**]