Parallel design patterns
ARCHER course

Vectorisation and active messaging
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Finding Concurrency
• Task Decomposition, Data Decomposition, Group Tasks, Order Tasks, …

Algorithm Structure
• Tasks Parallelism, Divide and Conquer, Geometric Decomposition, Recursive Data, …

Supporting Structures
• SPMD, Master/Worker, Loop Parallelism, Fork/Join, …

Implementation Mechanisms
• UE Management, Synchronisation, Communication, …
Vectorisation: The Problem

- Vectorisation is an *Implementation Strategy*
- The Problem: Given a program whose run time is dominated by a set of calculations, how can this be translated into a parallel program?
- Also known as SIMD
Single Instruction Multiple Data

- Single stream of instructions operating on multiple data streams

- The problem is typically defined in terms of arrays that can be updated concurrently using the same instructions
- Create a single stream of instructions
  - Can have a mask to allow for some selection based on data
- Can work well when your problem is truly data parallel
int inputNumbers[1000];

int i, finalSum;

finalSum = 0;
for (i = 0; i <= 999; i++) {
    finalSum += inputNumbers[i];
}

int inputNumbers[1000];
int results[4];

int i, j, finalSum;

for (i = 0; i <= 3; i++) {
    results[i] = 0;
    for (j = 0; j <= 249; j++) {
        results[i] += inputNumbers[i + j*4];
    }
}

finalSum = 0;
for (i = 0; i <= 3; i++) {
    finalSum += results[i];
}
Streaming SIMD Extensions (SSE)

- SIMD instruction set added to Intel CPUs in 1999
  - SSE1 added eight 128 bit registers where data can be packed into and operated on concurrently with associated instructions

\[
\begin{align*}
\text{result.x} &= v1.x + v2.x; \\
\text{result.y} &= v1.y + v2.y; \\
\text{result.z} &= v1.z + v2.z; \\
\text{result.w} &= v1.w + v2.w;
\end{align*}
\]

```plaintext
movaps xmm0, [v1]
addps xmm0, [v2]
```

<table>
<thead>
<tr>
<th>v1.x</th>
<th>v1.y</th>
<th>v1.z</th>
<th>v1.w</th>
</tr>
</thead>
<tbody>
<tr>
<td>v1.x+v2.x</td>
<td>v1.y+v2.y</td>
<td>v1.z+v2.z</td>
<td>v1.w+v2.w</td>
</tr>
</tbody>
</table>
SIMD technologies

- **SSE**
  - 128 bit
  - 2 x DP
  - 4 x SP

- **AVX**
  - 256 bit
  - 4 x DP
  - 8 x SP

- **MIC**
  - 512 bit
  - 8 x DP

- **AVX-512**
  - 512 bit
  - 16 x SP
Automatic vectorisation

- Compilers will attempt to automatically vectorise your code when compiled with optimisation enabled (–O3 on GCC)
  - With GCC you can get feedback on this using the -ftree-vectorizer-verbose=n flag, where n is 1 to 6 (the higher = more information)

- For single and double precision floating point can instruct the compiler to do this via SSE
  - With gcc using the flags -msse2, -mfpmath=sse
  - Can involve lots of memory to register movements so work experimenting with this flag to see if it is worth it
Manual vectorisation through GCC

- Compiler intrinsics support SSE

```c
typedef int v4si __attribute__((vector_size(16)));

v4si v1, v2, result;

result = v1 + v2;
```

- The base type
- Vector is 16 bytes wide, which is 4 integers
- Each of these variables contains 4 integer elements
- Each element of v1 added to corresponding element of v2 and the result stored in result
```c
#include <emmintrin.h>
...
int inputNumbers[1000];

__m128i s, v = _mm_set_epi32(0,0,0,0);

int j, finalSum=0;

for (j=0; j<999; j+=4) {
    s = _mm_set_epi32(inputNumbers[j], inputNumbers[j+1], inputNumbers[j+2], inputNumbers[j+3]);
    v += s;
}

for (j=0; j<3; j++) {
    finalSum += ((int*) &v)[j];
}
```
OpenMP 4.0 SIMD

```c
int inputNumbers[1000];
int i, finalSum = 0;
#pragma omp simd reduction(+:finalSum)
for (i=0; i<=999; i++) {
    finalSum += inputNumbers[i];
}
```

- The SIMD directive means that iterations of the loop can be executed by the SIMD lanes available to the thread.

- Can combine with the `for` directive to split iterations across threads and then across SIMD lanes

  - The schedule should be a multiple of the SIMD length

- [https://doc.itc.rwth-aachen.de/download/attachments/28344675/SIMD+Vectorization+with+OpenMP.PDF](https://doc.itc.rwth-aachen.de/download/attachments/28344675/SIMD+Vectorization+with+OpenMP.PDF)
GPUs as a big vector machine

CPU (few large cores) 
GPU (many simple cores)

Code (compute kernels) + data

Result data

- Use GPU for floating point intensive calculations
- Use CPU for everything else
- Single Instruction Multiple Thread (SIMT)
Kernels, Blocks, Warps and Threads

- 32 threads per warp which are mapped to SMs for execution
  - Each thread executes on a CUDA core which are themselves pipelined
- Each thread of the warp executing on a CUDA core must be doing the same instruction, just on different data
  - Keeps electronics simple, warps can be paused and interleaved
Key performance factors

1. How quickly you can transfer data to & from the GPU
   - Parallel overhead

2. The amount of time the CPU and/or GPU will be idle
   - Wasted resources/load imbalance

3. How well your code takes advantage of the GPU architecture
   - Keeping the floating point engine busy!

<table>
<thead>
<tr>
<th>Porting step</th>
<th>Million pairs/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial MPI+OpenMP</td>
<td>250</td>
</tr>
<tr>
<td>Initial OpenACC</td>
<td>37</td>
</tr>
<tr>
<td>Optimised data transfer</td>
<td>61</td>
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<td>Lattice data kept on GPU</td>
<td>839</td>
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<td>Memory access pattern optimised for GPU</td>
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<tr>
<td>Concurrency with streams</td>
<td>1270</td>
</tr>
<tr>
<td>Vectorised halo data movement</td>
<td>1812</td>
</tr>
</tbody>
</table>
Example: Modelling the atmosphere

- Data transfer is asynchronous
- Constants copied across only once on model initialisation
- Share data between GPU kernels
  - Wind in x,y,z is common to all

**CPU**
- Send required data to GPU

**Dynamics**
- Diffusion
- Viscosity
- Coriolis
- Buoyancy

**GPU**
- Advection

**Step fields combining CPU and GPU data**

**GPU source terms**

**CPU and GPU source terms**

**Wait for results from GPU**
Vectorisation - summary

• Parallelism at multiple levels
  - Instruction level, core level, processor level, node level
  - Significant performance improvements can be obtained by leveraging vectorisation correctly
  - Many compilers will do this automatically for you, but not all compilers are created equally!
  - Technologies such as OpenMP and OpenACC (for GPUs) make this look similar to loop parallelism

• Viewing GPUs as SIMD engines
  - Need to keep them feed with calculations to work on
  - They work best doing floating point arithmetic
  - Need to consider how to keep the CPU and GPU busy at the same time
Active messaging is an *Implementation Strategy*

The Problem: We want to run multiple tasks, which are driven by irregular interactions, on a UE. How can we best structure our code to support this?
Example problem

- I am running a code with lots of tasks per UE
  - There are lots of tasks (e.g. function calls) that I have available to run on the UE and-so don’t want to block for communications. However my communications are irregular and I need to work with values I receive.

  ```
a = receive(1);
calculate(a);
handle = nonblocking_receive(1);
while (!test(handle)) {
  Do some other work
}
calculate(a);
```

- This is OK but relies on being able to find some other work to do and carry lots of request handles around
  - Might not be possible, or with irregular & unpredictable communications might be difficult to structure code generally to support this
Active messaging

- The arrival of a message will activate some handling block of code on the target UE (also known as a *callback*):

  ```c
  send(data, target rank, unique identifier);
  register_recv(callback, source rank, unique identifier);
  ```

- The unique identifier (UUID) is used to match the message with a specific handler.
- The callback function will typically receive the data and metadata (such as amount of data, type etc.).
- Sending is either blocking or non-blocking.
- The receive call is non-blocking.

```c
send(data, 1, "hello");

UE 0

UE 1

register_recv(calculate, 0, "hello");

void calculate(data, metadata) {
    ........
}
```
Active messaging

• Called *active messaging* as messages explicitly activate the block of code which will handle them
  – Some or all of the code will be structured around these handlers
  – Callback handlers might persist (i.e. can be called for many different messages) or transitory (once called they are deregistered.)

• Implementation choice between running handlers concurrently or sequentially
  – When a message arrives do we kick a UE off (i.e. a thread from a pool) which calls the handler
  – Or are messages queued up and processed one at a time?

• If you run handlers concurrently you will need to protect shared data shared between them (*shared data pattern.*)
Supports collective messaging too

The callback routine

Value on each process to use

Operation

Root

Unique ID

```
register_reduce(my_handler, my_value, "sum", 0, "my_reduction1");

void my_handler(data, metadata) {
    ........
}
```

- In this case each process issues a reduction, `my_handler` is then executed on process 0 with the resulting value
  - Callback is only executed on process 0 once every single process has issued this call and the reduction is completed.
  - The callback routine could be NULL on other processes.

- Crucially the UUIDs determine what collective messages match rather than the issue order
  - This provides greater flexibility for irregular applications where codes might issue collective messages in different orders.
Active messaging - implementation

- Have a map style structure where they key is a combination of the unique identifier and the source rank, the value is a pointer to the appropriate callback function.
- Behind the scenes you poll for a messages, from this extract the unique ID and use this in combination with the source rank to find the appropriate callback handler function to execute.
  - The rest of the message is then split up to extract the data and any other metadata.

```c
void fn1(data, metadata) {
    .......
}

void fn2(data, metadata) {
    .......
}
```
Active messaging - implementation

• Can build this on top of communication technologies like MPI
  - When sending package the data and metadata (unique ID etc) up and send as type MPI_BYTE
  - On the receiver side can probe for a messages and extract the message size (and source) from the status, allocate memory and then physical receive data (via MPI_Recv.)
    • Might be driven by a thread continually polling for incoming data

• Some implementation challenges
  - What if we have not yet registered a receive handler for a specific message but this message has arrived? – Need to store unmatched messages
  - When should we terminate? – when all UEs are idle, there is no data in flight and no messages are outstanding
Example: In-situ data analytics

Prognostics

Diagnostics
All of this on one core. But not very computationally intensive, so fine to have a thread pool and oversubscribe threads to the single core.
Active messaging technologies

- In other fields active messaging is fairly popular
  - Remote Procedure Call (RPC) is a concrete example of this such as Java’s Remote Method Invocation (RMI)
- Not so much in HPC but Charm++ is one example technology
  - Built on C++, the programmer expresses their program components as parallel objects called *chares*
  - The programmer can call methods on these *chares* held on other processes, which is effectively an active message to execute that method remotely with the provided arguments in a thread
  - As methods in a *chare* can share object data, by default only one method can be active at any one time (*one at a time concurrency protection – see shared data lecture.*)
  - NAMD, a popular molecular dynamics package is written in Charm++
Charm++ example

- Programmer must rewrite their code in C++ and this chares approach
  - An additional .ci file must be written that defines a proxy for each object and feeds into their compiler
- One at a time concurrently is limiting, can disable this but then is entirely up to the programmer to manage concurrency

Taken from http://charm.cs.illinois.edu/research/charm
Active messaging - Summary

• This way of structuring the communications can provide additional flexibility
  - Can be helpful when you have very many, asynchronous and different messages which you want to process in different ways
  - Using the unique identifier to match against handling logic means you can kick off lots of communications without worrying too much about the ordering in which they will arrive

• Structuring the code in this manner can help organise the concurrency
  - Especially if you allow for multiple handlers to execute concurrently
  - Each handler can be viewed as a task, driven by the arrival of data. But it gets more challenging when these handlers need to interact or work with some shared data
  - There are existing programming technologies, but none are mature