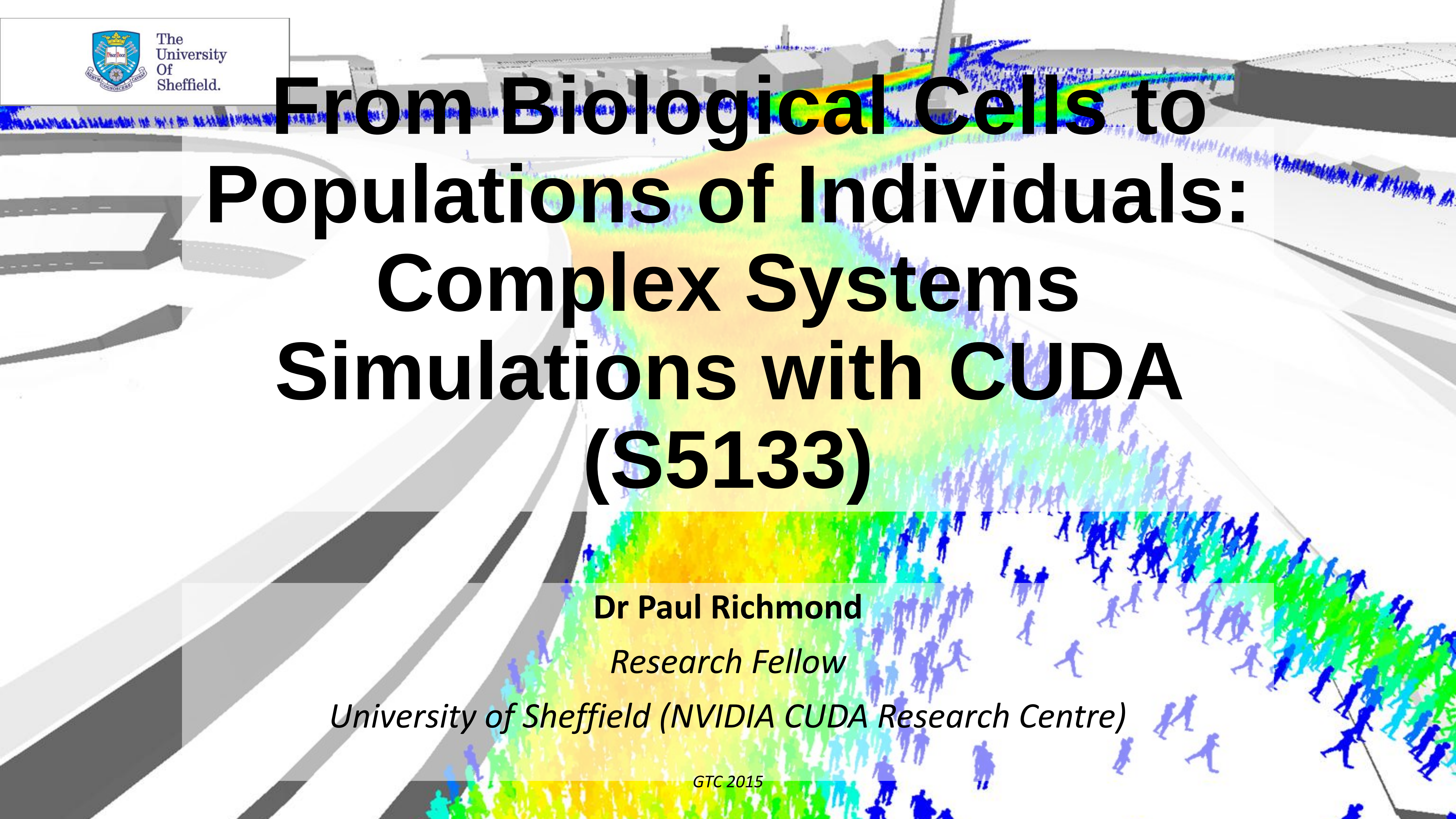

From Biological Cells to Populations of Individuals: Complex Systems Simulations with CUDA (S5133)

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GTC 2015

Overview

- Complex Systems
- A Framework for Modelling Agents
- Degrees of Parallelisation
- Agent Communication
- Putting it all together

Complex Systems

- Many **individuals**
- **Interact** and behave according to simple rules
- System level behaviour **emerges**

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Agent Based Modelling

- A method for specification and simulation of a complex system
  - Model is a set of autonomous communicating agents
- Simulation helps to understand complex systems
  - Interventions and prediction
- Presents a computational challenge!
  - Especially for real time or faster

Difficulties in Applying GPUs

- Agents are heterogeneous
  i.e. **They diverge**
- Agents are born and agents die
  Leads to **sparse populations** and non coalesced access
- Agents communicate
  No global mechanism for GPU thread communication
- Agents don't stay still
  Acceleration structures used for simulation need to be rebuilt

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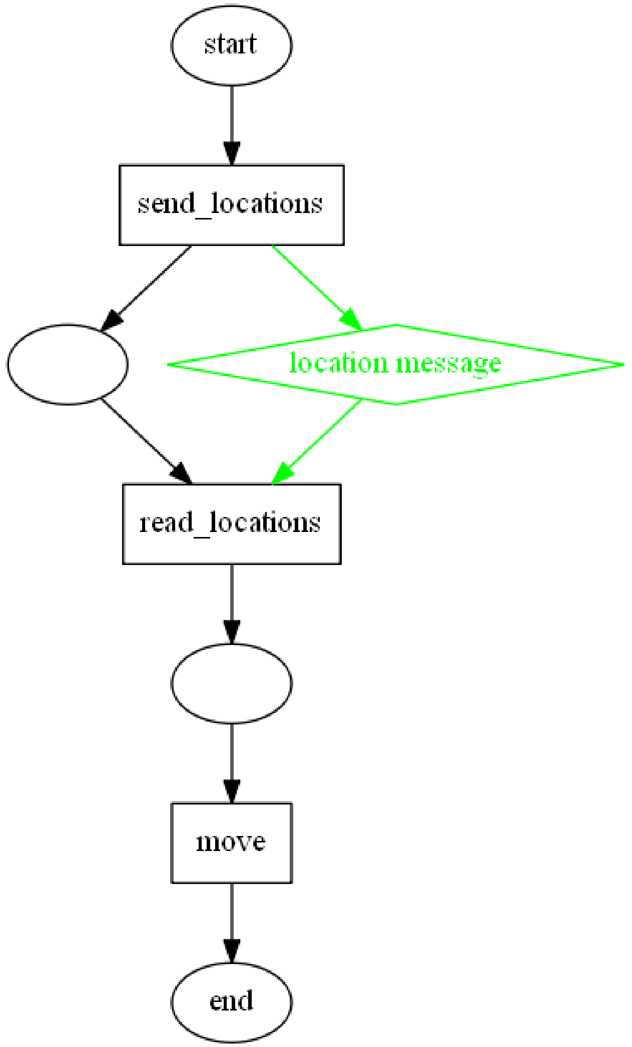
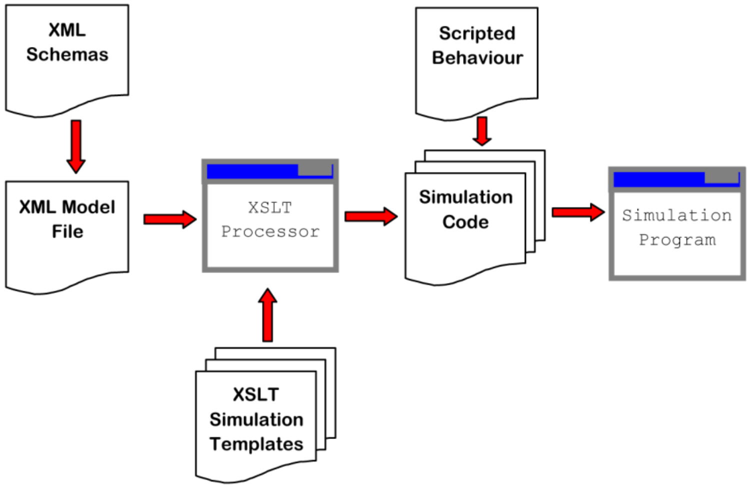
A Formal Model of an Agent

- Abstract the underlying architecture
  - Let modellers write models not parallel programs
- Describe agents as a form of state machine (X-Machine)
  - Minimises divergence
- Describe state transition functions (agent functions) using high level script
- Describe communication as message dependencies between agent functions
  - Results in Directed Acyclic Graph
  - Identifies synchronisation points for scheduling



FLAME GPU: A Code Generation Framework

- XML Model File
  - Describe Agents and Communication (messages) as a model in XML
- XSLT Templates
  - Code generate a simulation API from agent descriptions
- Scripted Behaviour
  - Scripted behaviour links with dynamic simulation API
- Simulation Program
  - Loads initial data and provides I/O or interactive visualisation



Code Generation using XSLT

- Powerful technique for code generation from Declarative XML model
  - Full functional programming language

```xml
<xagents>
    <gpu:xagent>
      <name>Circle</name>
      <memory>
        <gpu:variable>
          <type>int</type>
          <name>id</name>
        </gpu:variable>
        <gpu:variable>
          <type>float</type>
          <name>x</name>
        </gpu:variable>
        <gpu:variable>
          <type>float</type>
          <name>y</name>
        </gpu:variable>
        <gpu:variable>
          <type>float</type>
          <name>z</name>
        </gpu:variable>
        <gpu:variable>
          <type>float</type>
          <name>fx</name>
        </gpu:variable>
        <gpu:variable>
          <type>float</type>
          <name>fy</name>
        </gpu:variable>
      </memory>
...
```

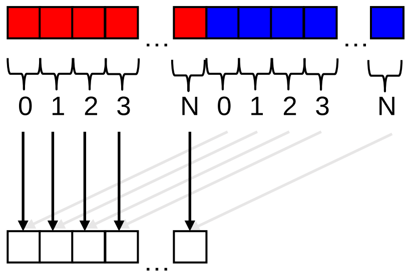
```xml
<xsl:for-each select="xagents/gpu:xagent">
struct __align__(16) xmachine_memory_<xsl:value-of select="name"/>
{<xsl:for-each select="memory/gpu:variable">
  <xsl:value-of select="type"/><xsl:text> </xsl:text><xsl:if test="arrayLength">*</xsl:if><xsl:value-of select="name"/>;
  </xsl:for-each>
};
</xsl:for-each>
```

```c
struct __align__(16) xmachine_memory_Circle
{
    int id;
    float x;
    float y;
    float z;
    float fx;
    float fy;
};
```

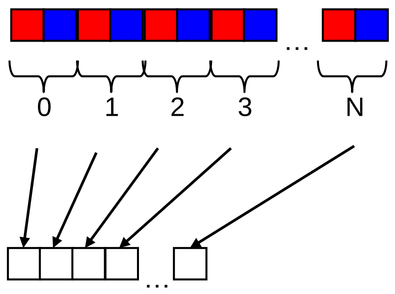
Mapping an Agent to the GPU

- Each agent function is corresponds to a single GPU kernel
  - Each CUDA thread represents a single agent instance
- Agent functions use a dynamically generated API
- Agent Data is transparently loaded from Structures of arrays

```
typedef struct agent_list{
  float x[N];
  float y[N];
} xm_memory_agent_list;
```




```
typedef struct agent{
  float x;
  float y;
} xm_memory_agent_list [N];
```




```
__FLAME_GPU_FUNC__ int read_locations(
  xmachine_memory_bird* xmemory,
  xmachine_message_location_list* location_messages)
{
  /* Get the first message */
  xmachine_message_location* location_message =
    get_first_location_message(location_messages);

  /* Repeat untill there are no more messages */
  while(location_message)
  {
    /* Process the message */
    if distance_check(xmemory, location_message)
    {
        updateSteerVelocity(xmemory, location_message);
    }

    /* Get the next message */
    location_message =
      get_next_location_message(location_message,
                                location_messages);
  }

  /* Update any other xmemory variables */
  xmemory->x += xmemory->vel_x*TIME_STEP;
  ...

  return 0;
}
```

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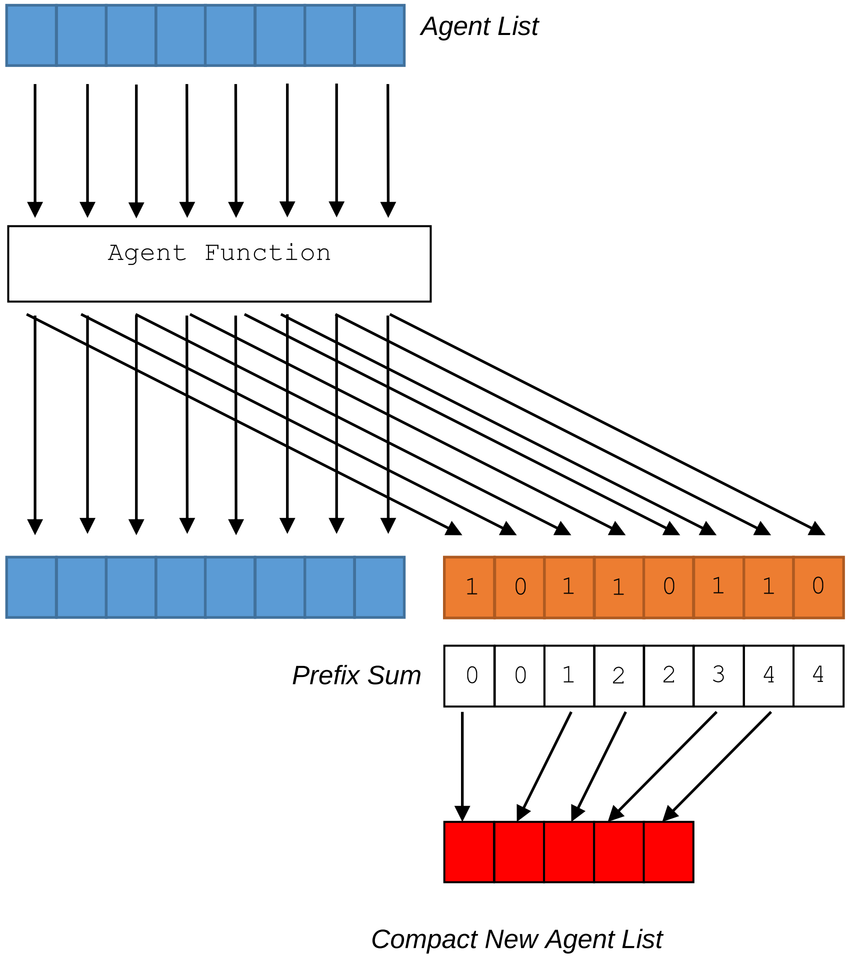
Agent Divergence and Sparsity

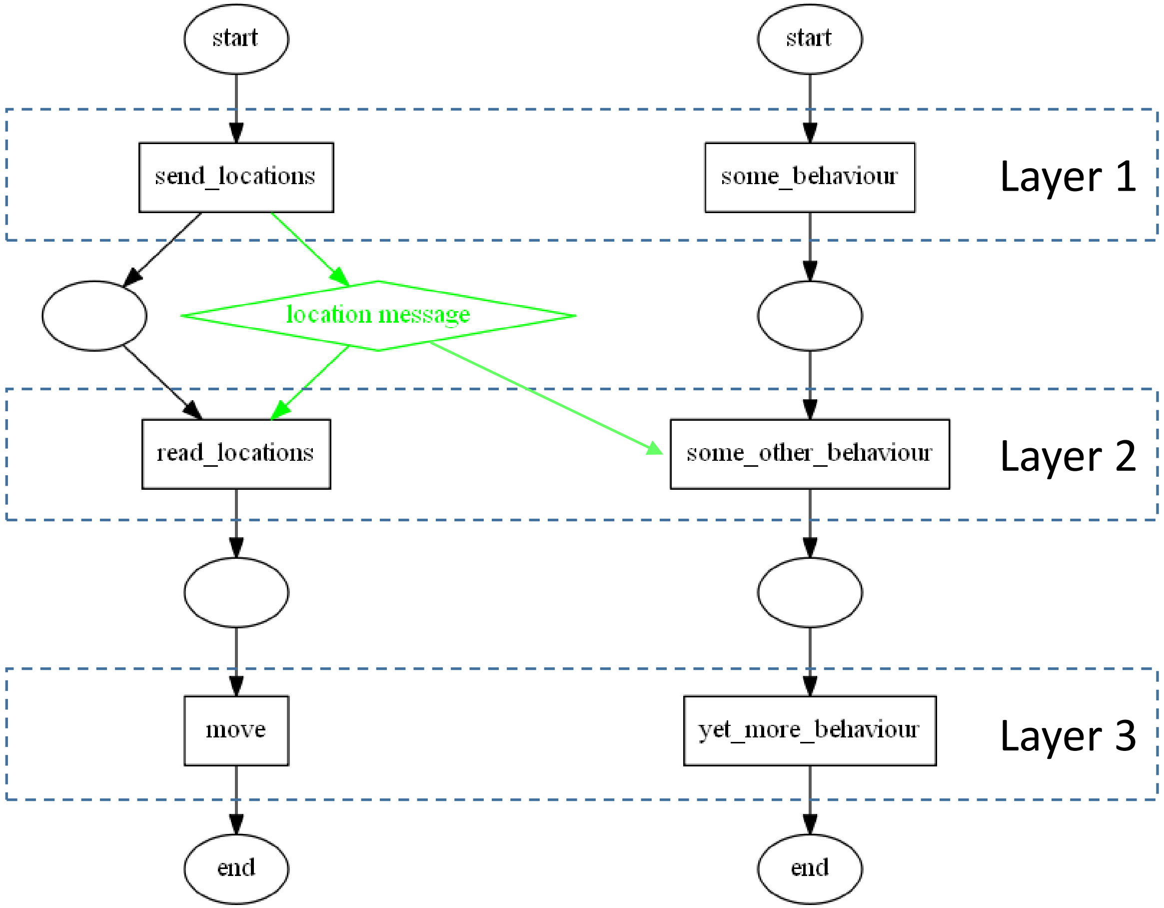
- **Divergence**: Must group agents (threads)
  - Good News: Agents are already grouped by state
  - Bad News: Agents change states so we are left with sparse lists

- Avoid Sparse Lists by using parallel compaction.
  - Thrust C++ library



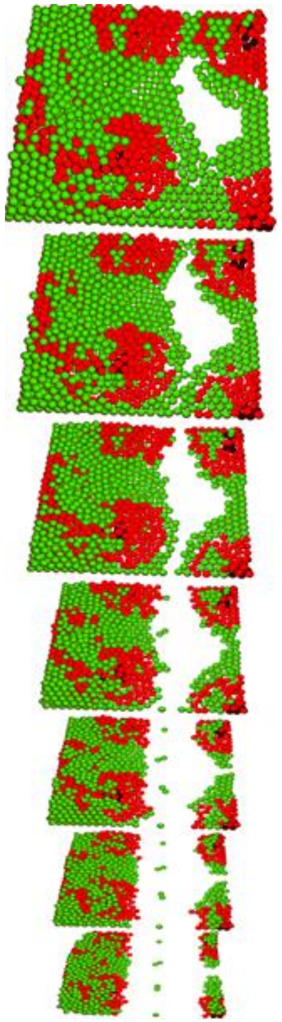
Parallelism within the model

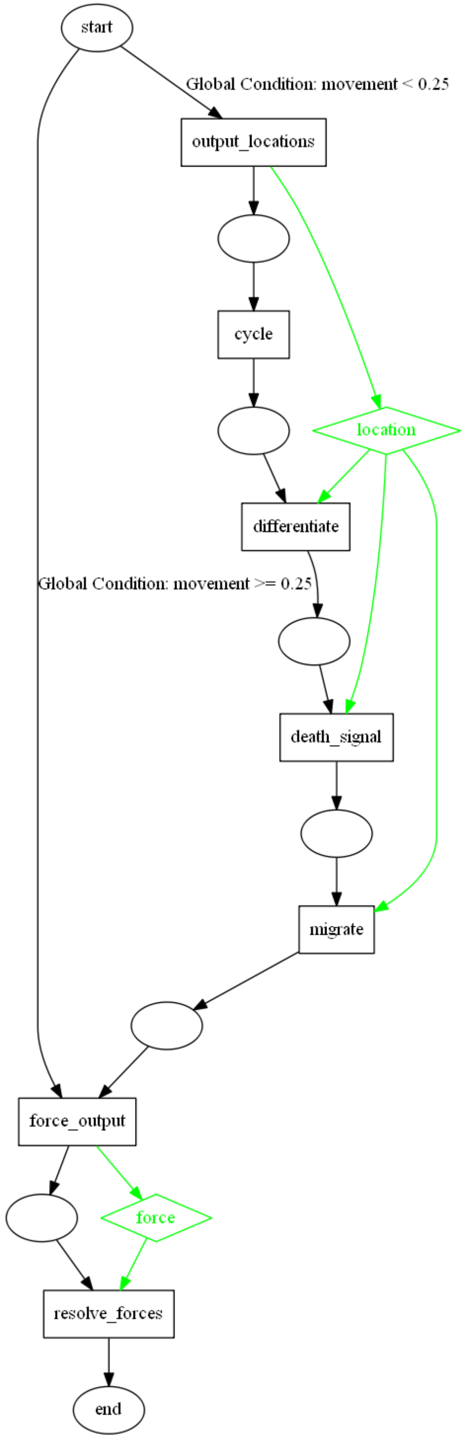
- Behaviour consists of function layers
  - Each layer is a synchronisation barrier
- Synchronisation between agents only required when a dependency exists (communication or agent memory)
- This creates parallelism within the function layers of the model
- **CUDA Streams can be used to execute independent functions**



High Divergence Example

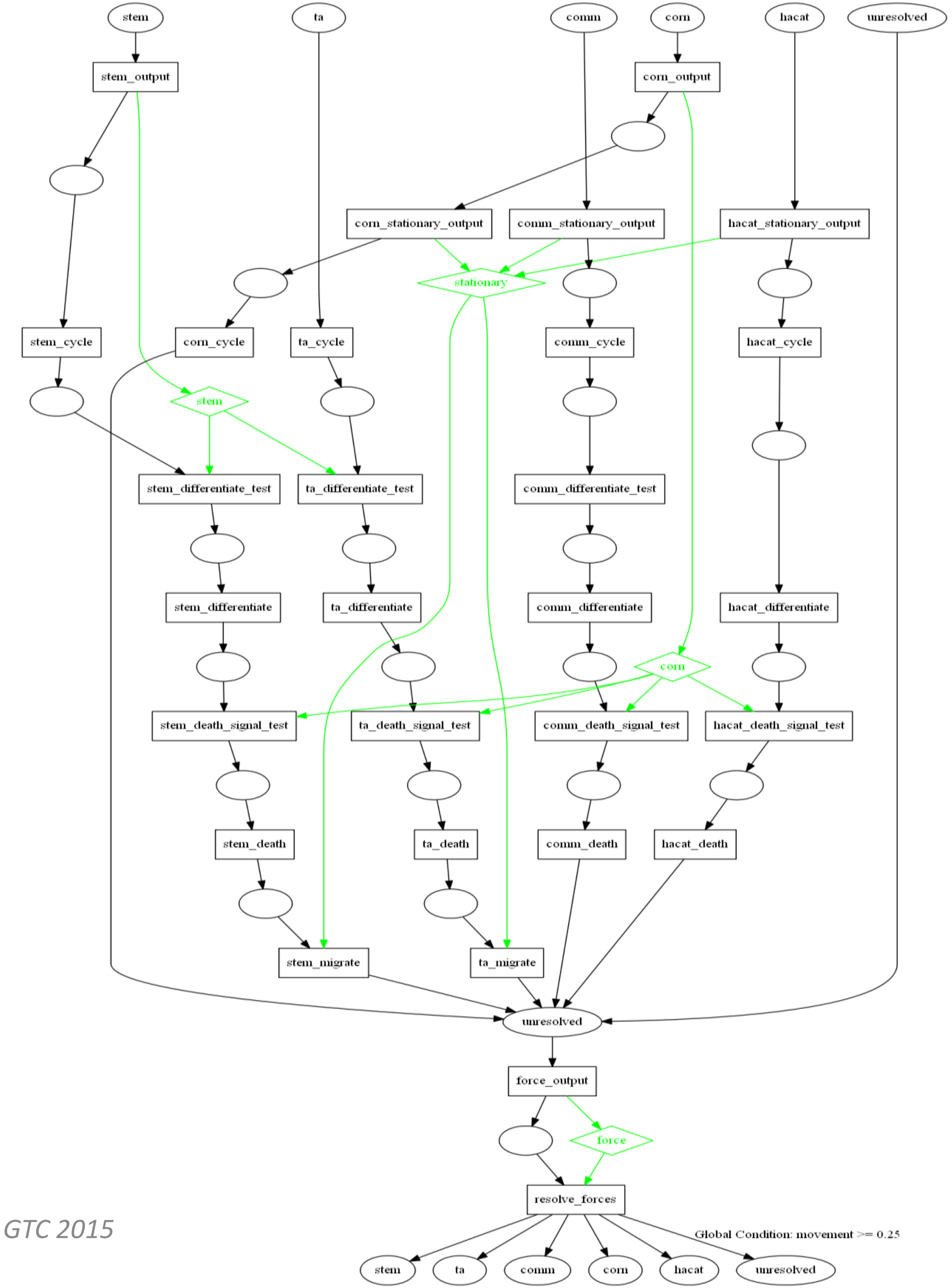
- Single agent ‘cell’ type
  - 5 types of cell within
  - Single message type
- Advantages
  - Large population counts (good utilisation)
  - Simple modelling (but complicated agent transition functions)
- Disadvantages
  - **Lots** of code divergence
  - Unnecessary message reading



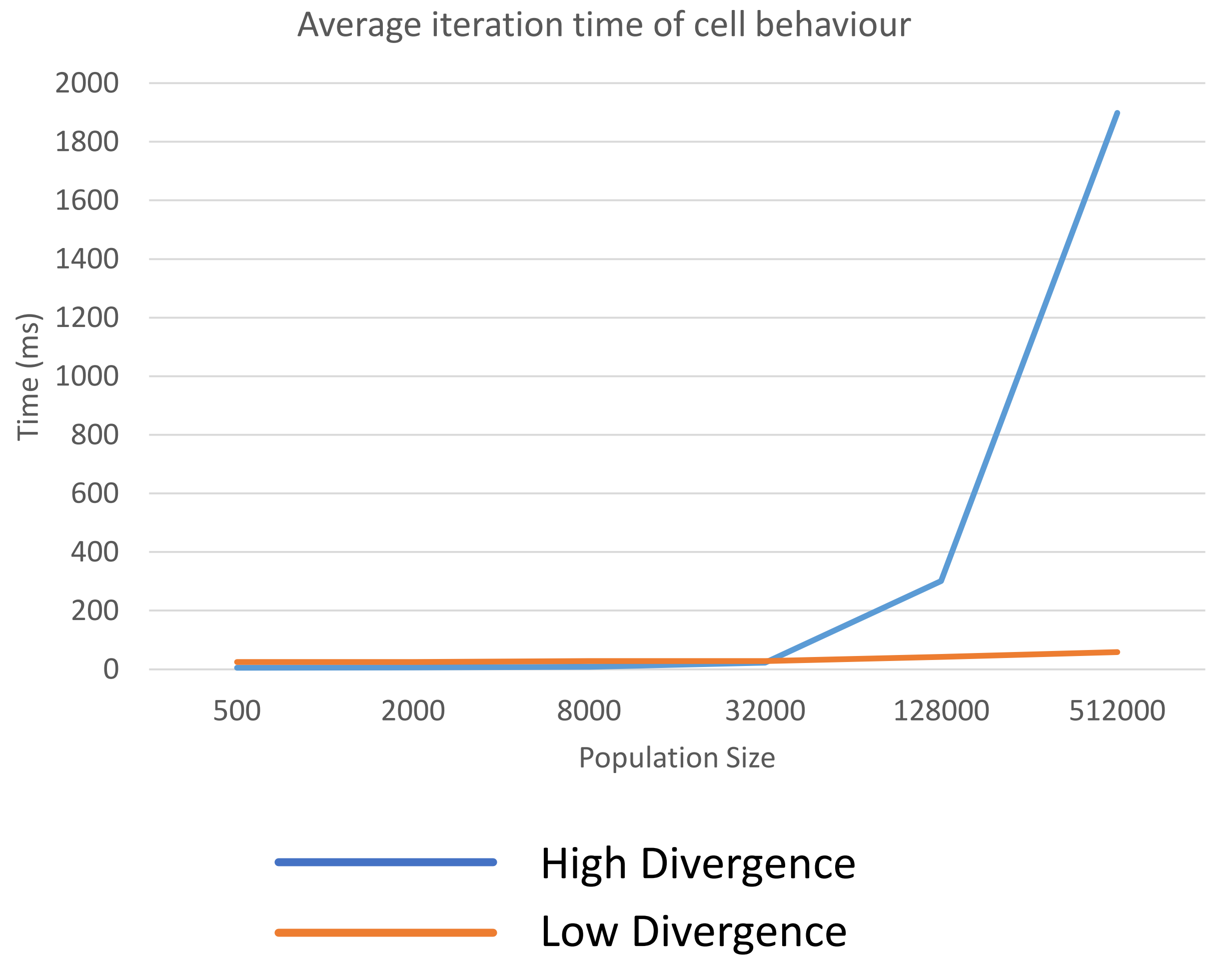


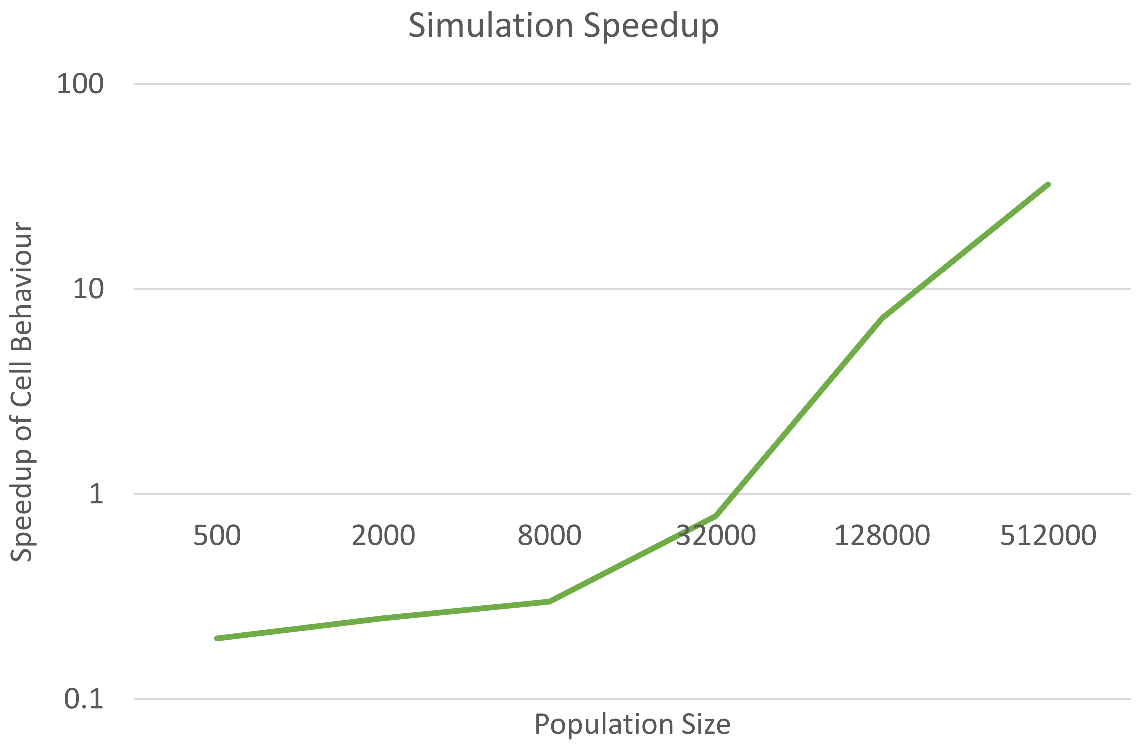
Low Divergence Example

- Multiple agent types
  - Different agent type for each cell type
  - Distinction between message
- Advantages
  - Less divergent code
  - More parallelism within the model
  - Less message reading
- Disadvantages
  - Complex dependencies
  - More complex (looking) model
  - **Smaller population sizes**



Parallelism within the model - performance





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Agent Communication

- Brute Force Messaging (N-Body problem)
  - Tile Messages into shared memory
- Spatially Distributed Agents
  - Build data structure to bin agents
  - CUDA Particles
  - **Use counting sort to improve performance**
- Discrete Space Limited Range (Cellular Automaton)
  - Cache results via texture cache (good locality)

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Spatially Distributed Communication

Radix Sorting

Hash Message

Sort using Thrust (Sort by Key)

sort keys

Reorder

scatter messages

build partition matrix

Count Sort

Hash Message

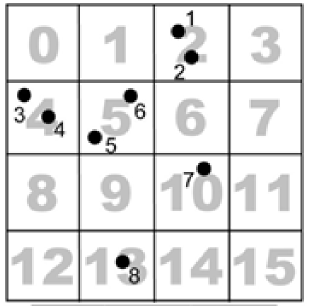
atomic add to bin

Prefix Sum

global index of bins

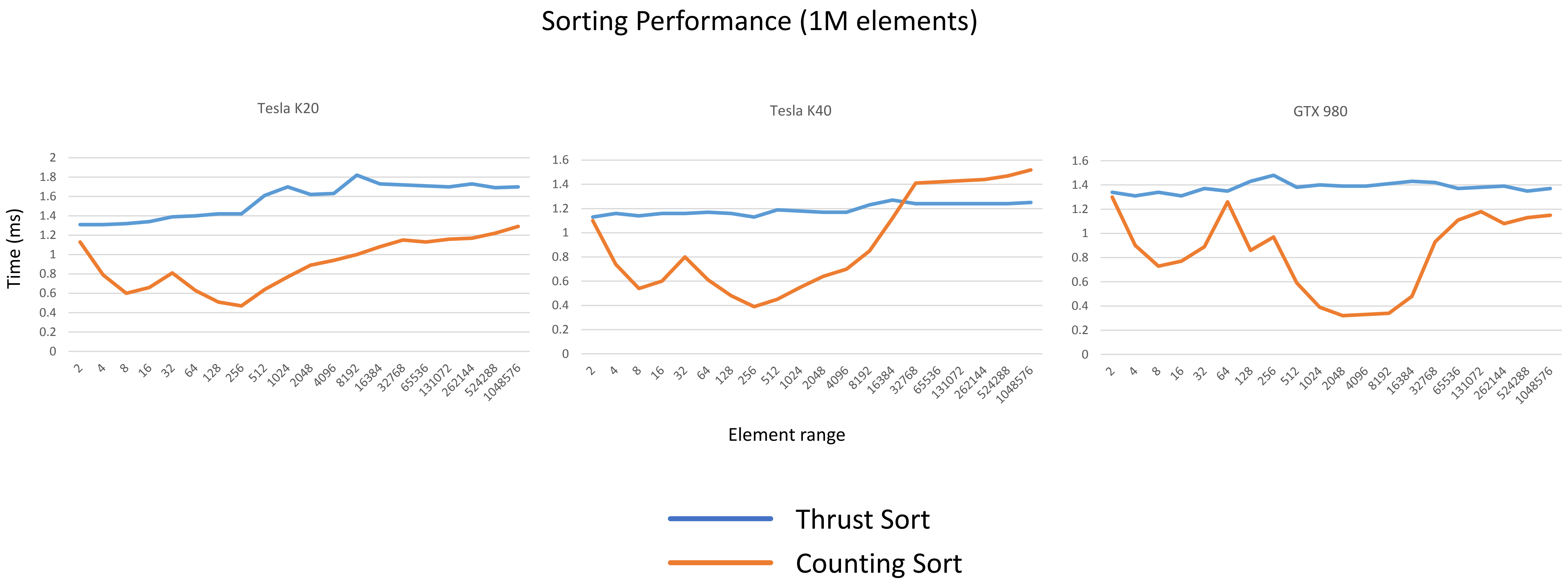
Reorder

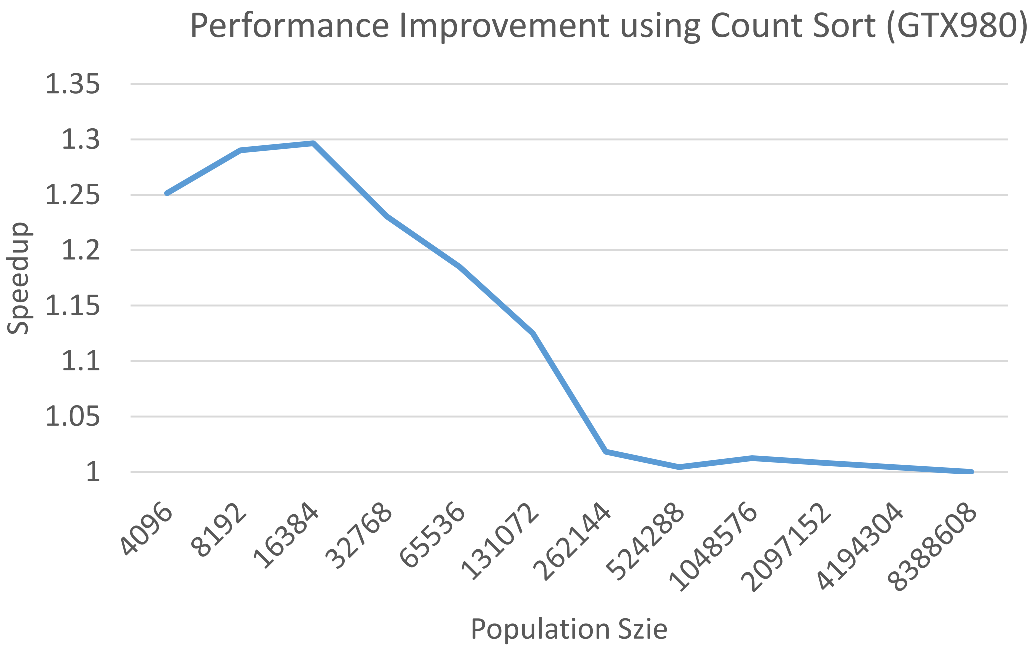
scatter messages

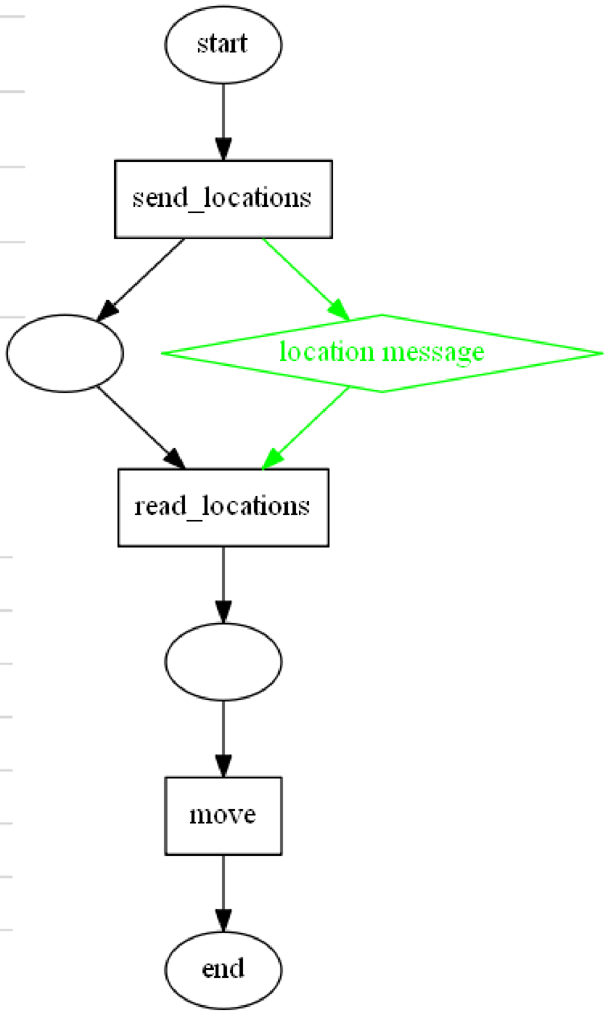


Partition	First agent	Last agent
0		
1		
2	1	2
3		
4	3	4
5	5	6
6		
7		
8		
9		
10	7	7
11		
12		
13	8	8
14		
15		

Counting Sort Performance Study

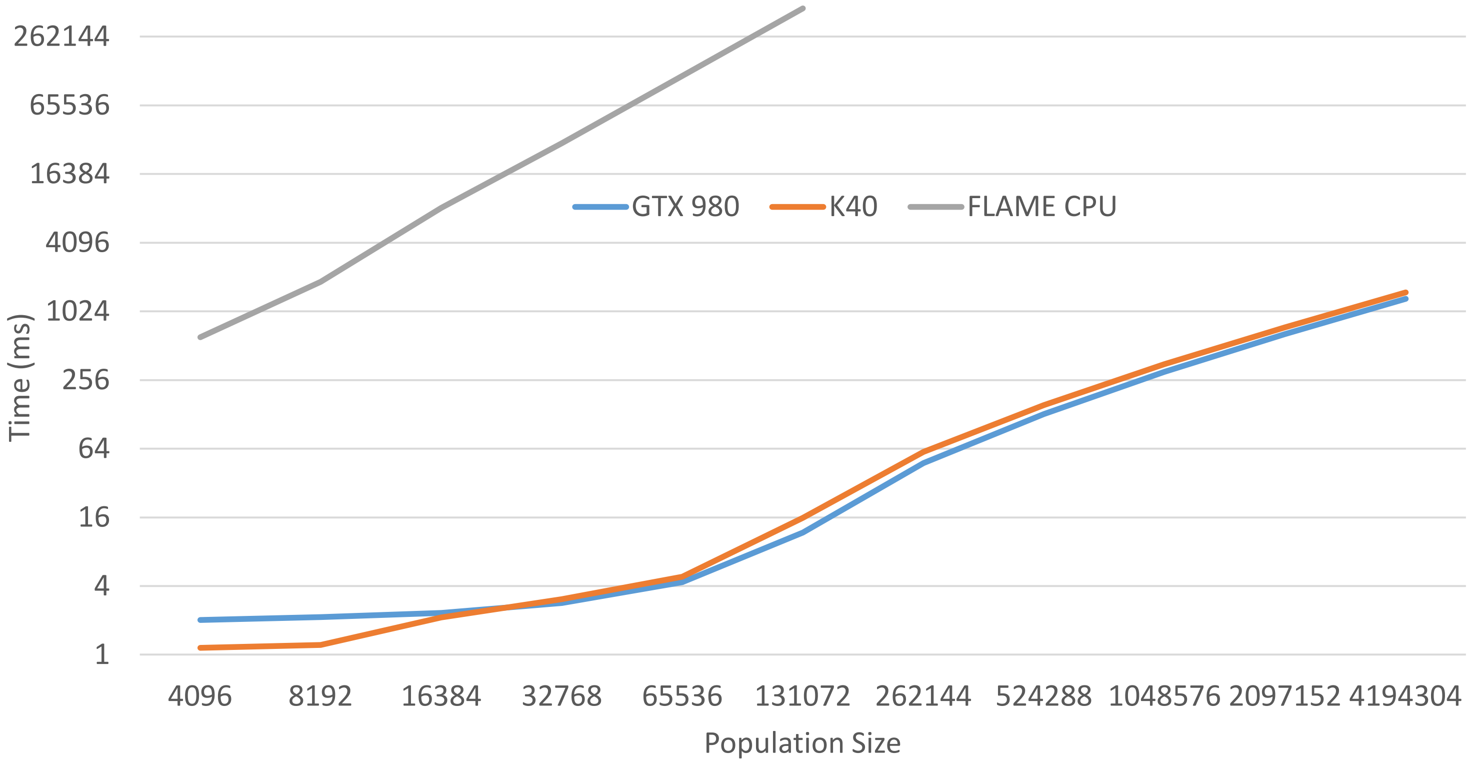






- Counting sort best suited to smaller population sizes
- Message reading is the bottleneck

Spatially Distributed Communication Benchmark



27k faster than FLAME on CPU with 50k agents (*apples != oranges*)
700x faster than FLAME II with 50k agents on 16 cores (using MPI, vector splitting)

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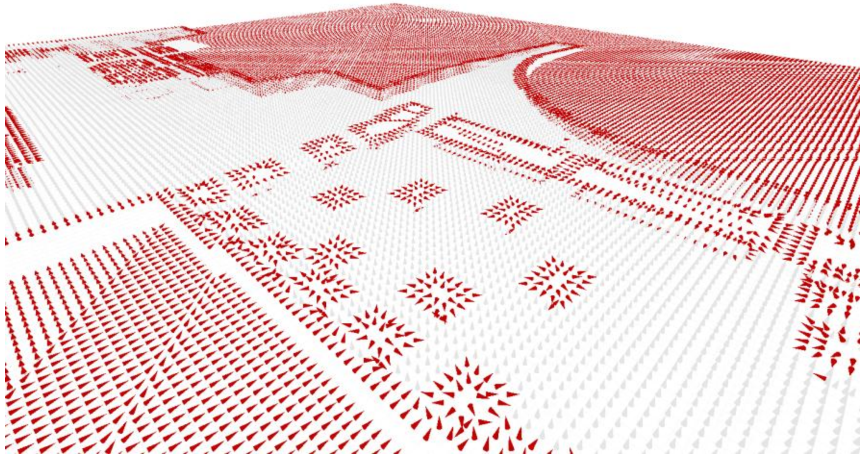
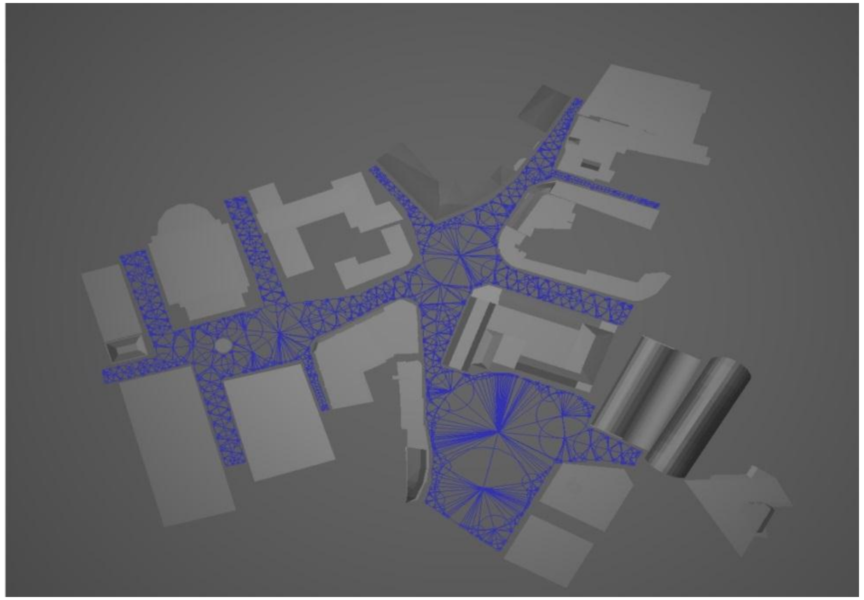
Pedestrian Dynamics

- Pedestrian agents
  - Social Repulsion (Social Forces)
  - Reynolds steering forces
  - Reciprocal Velocity Obstacles
- Navigation agents
  - Global Vector Field
  - Navigation Graph
  - Environment and Goals are calculated as a weighted influence
- An extension: Navigation graphs





Conclusions

- Agent based modelling can be used to represent complex systems at differing biological scales
- FLAME GPU is a framework for model description and CUDA code generation
- Using state based representation avoids divergence and allows parallelism within a model to be exploited
- Counting sort helpful for highly divergent population
- Visualisation is extremely cheap

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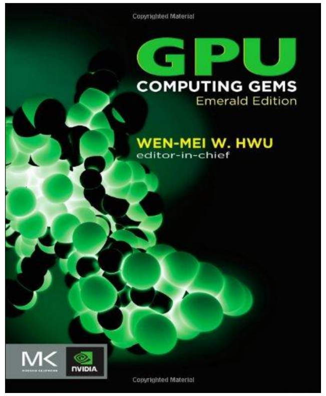
Thank You

Get the code for free from:

http://www.flamegpu.com

www.github.com/FLAMEGPU



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