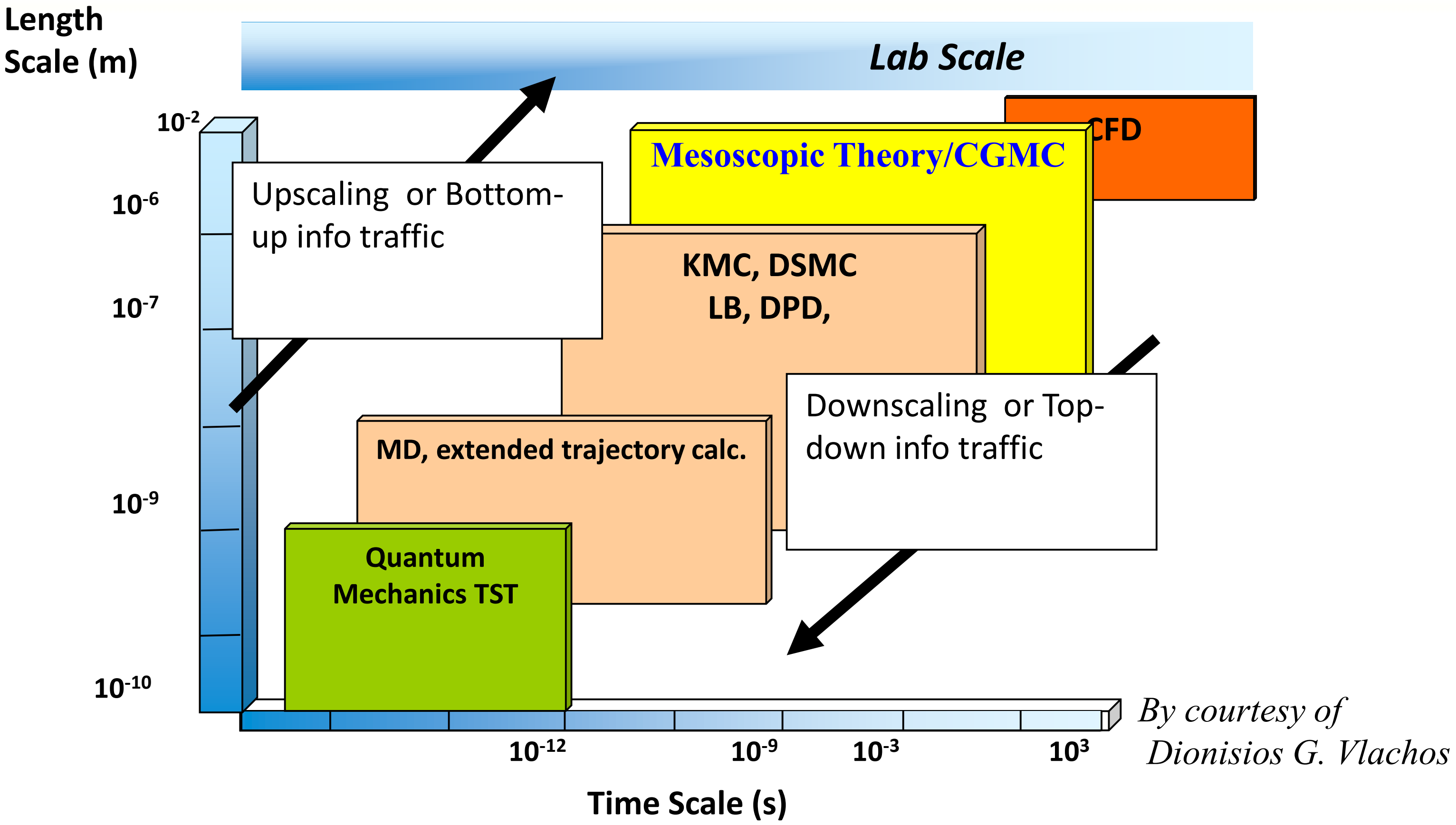
Parallelization of Tau-Leap Coarse-Grained Monte Carlo Simulations on GPUs

Lifan Xu, Michela Taufer,
Stuart Collins, Dionisios G. Vlachos

Global Computing Lab
University of Delaware

Multiscale Modeling: Challenges



Upscaling or Bottom-up info traffic

Downscaling or Top-down info traffic

By courtesy of Dionisios G. Vlachos

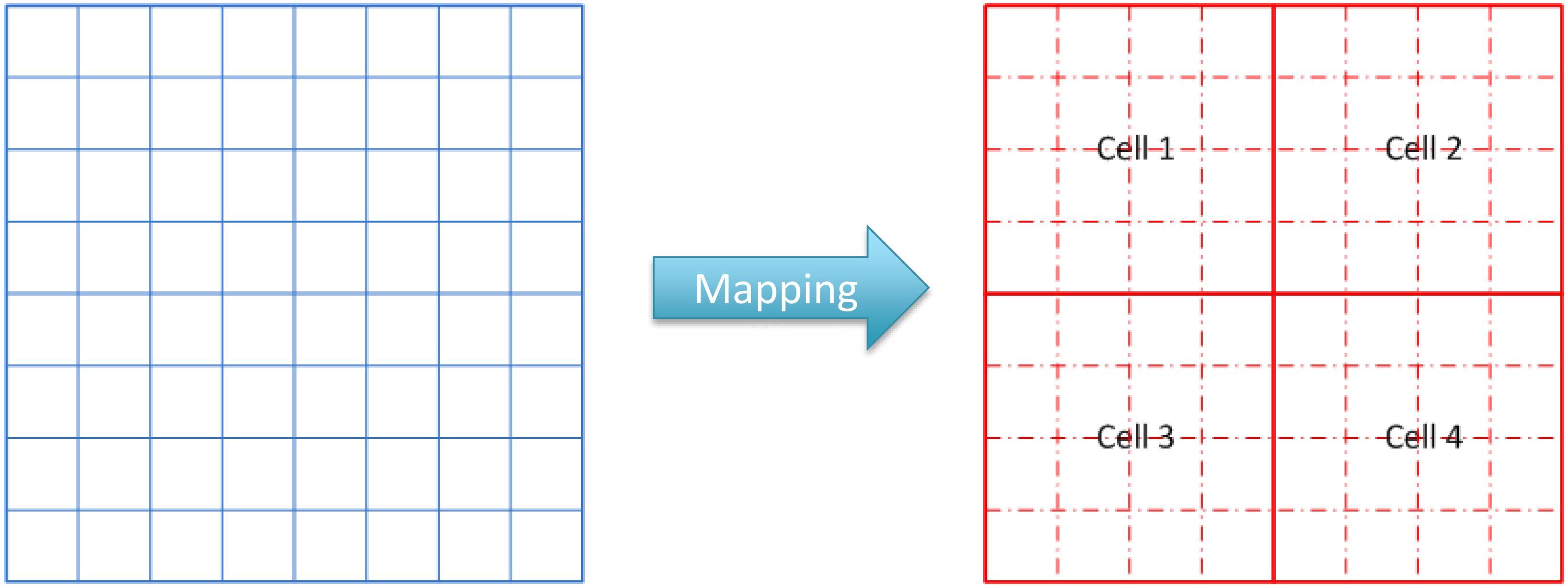
Our Goal: increase time and length scale for the CGMC by using GPUs

Outline

- Background
  - CGMC
  - GPU
- CGMC implementation on single GPU
  - Optimize memory use
  - Optimize algorithm
- CGMC implementation on multiple GPUs
  - Combine OpenMP and CUDA
- Accuracy
- Conclusions
- Future work

Coarse Grained Kinetic Monte Carlo (CGMC)

- Study phenomena such as catalysis, crystal growth, and surface diffusion
- Group neighboring microscopic sites (molecules) together into “coarse-grained” cells



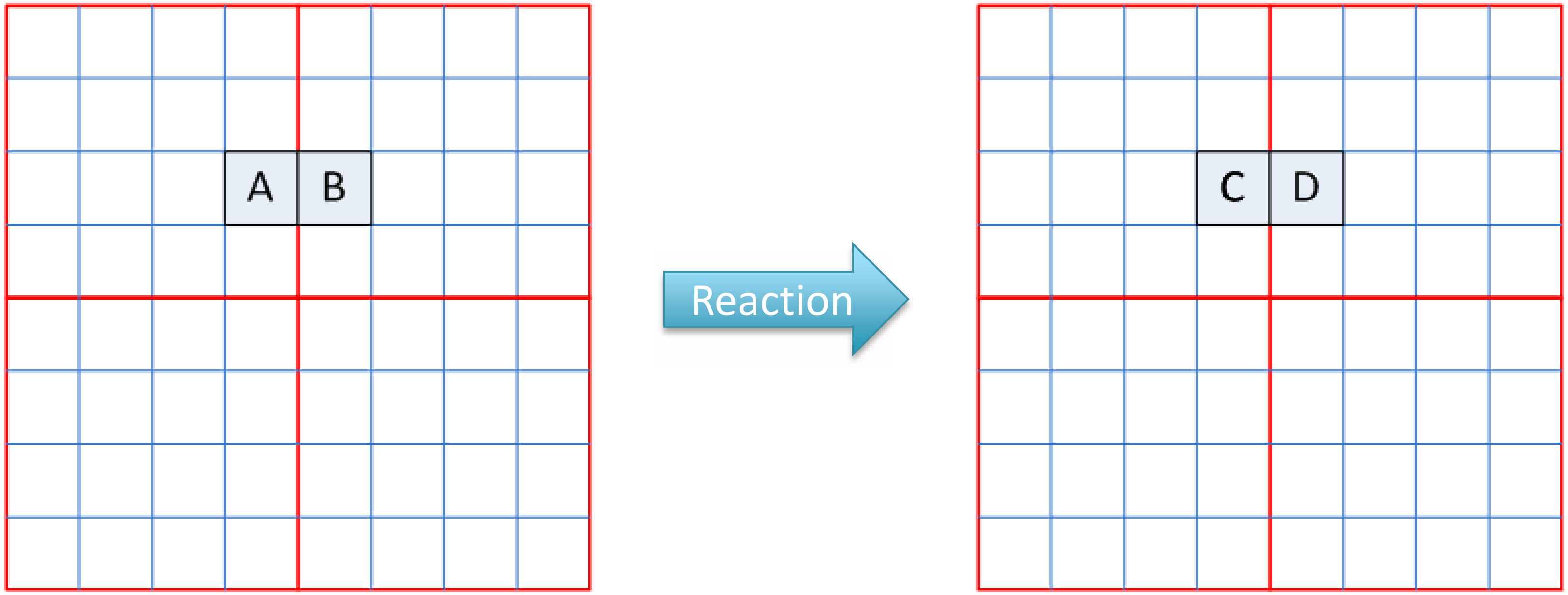
8 X 8 microscopic sites

2 X 2 cells

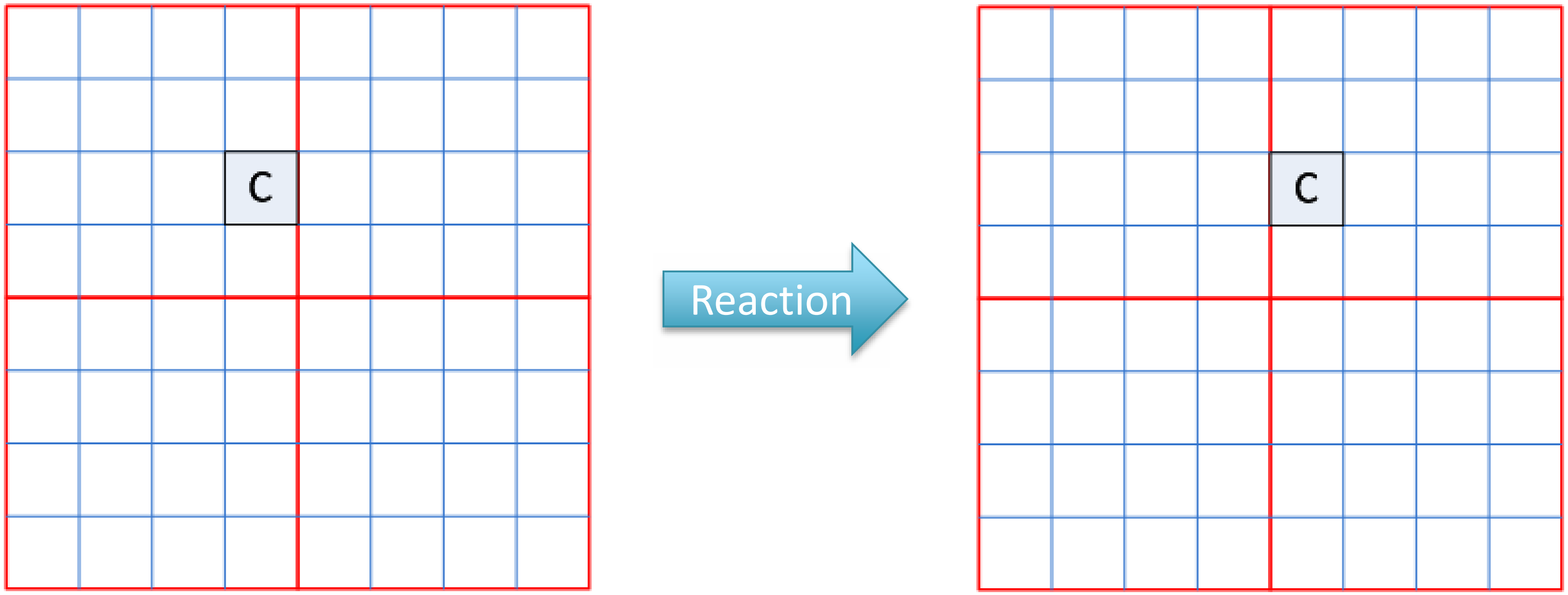
Terminology

- Coverage
  - A 2D matrix contains number of different species of molecules for each cell
- Events
  - Reaction
  - Diffusion
- Probability
  - A list of probabilities of all possible events on every cell
  - Probability is calculated based on neighboring cell's coverage
  - Probability has to be updated if the coverage of its neighbor changed
  - Events are selected based on probabilities

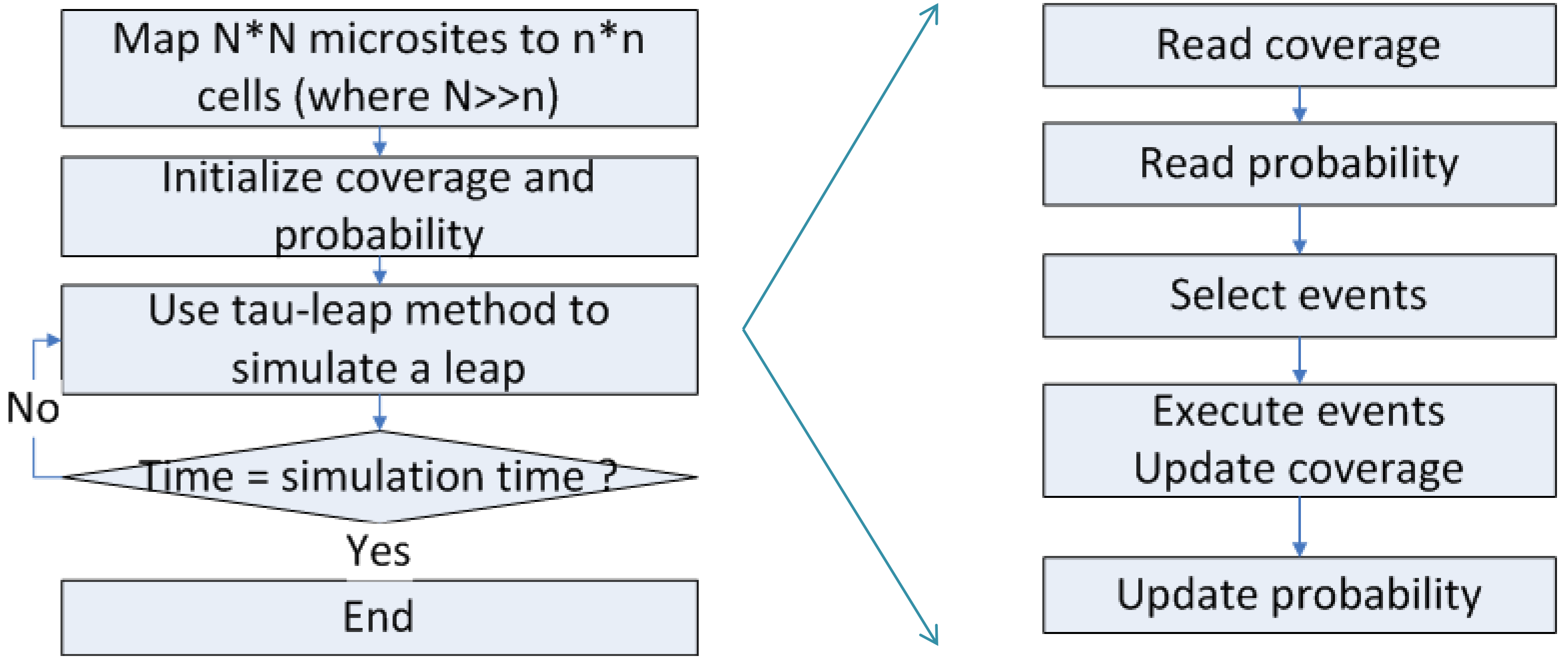
Reaction



Diffusion



CGMC Algorithm



Map N*N microsites to n*n cells (where N>>n)

Initialize coverage and probability

Use tau-leap method to simulate a leap

No

Time = simulation time ?

Yes

End

Read coverage

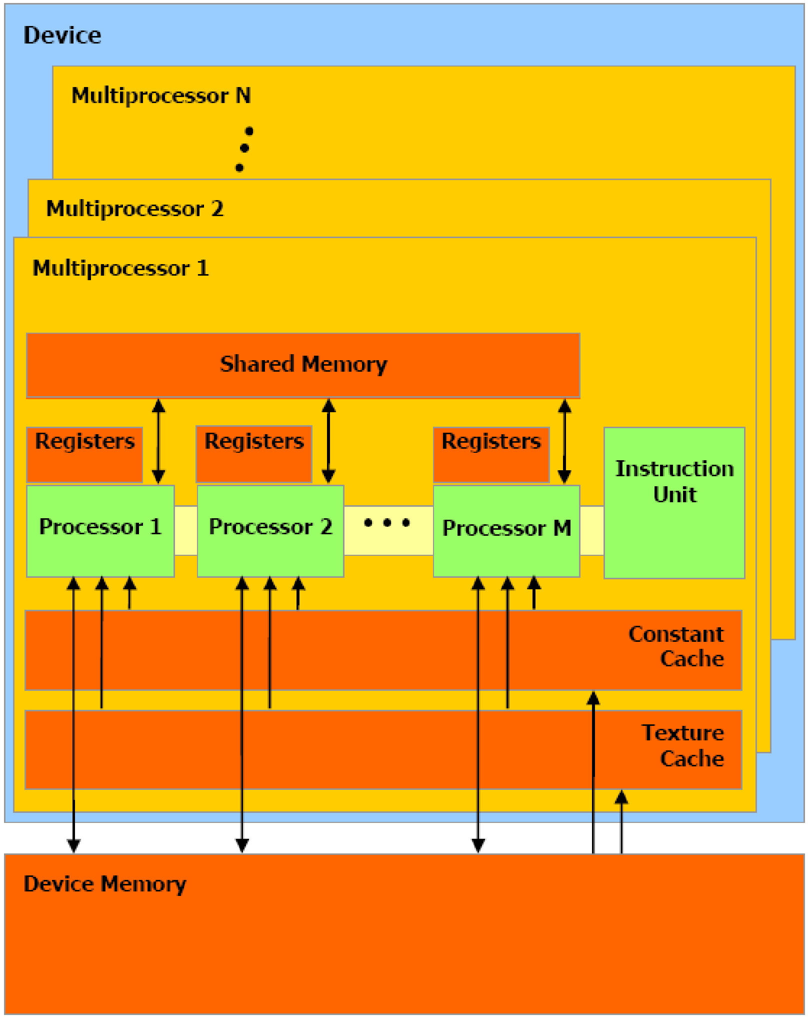
Read probability

Select events

Execute events
Update coverage

Update probability

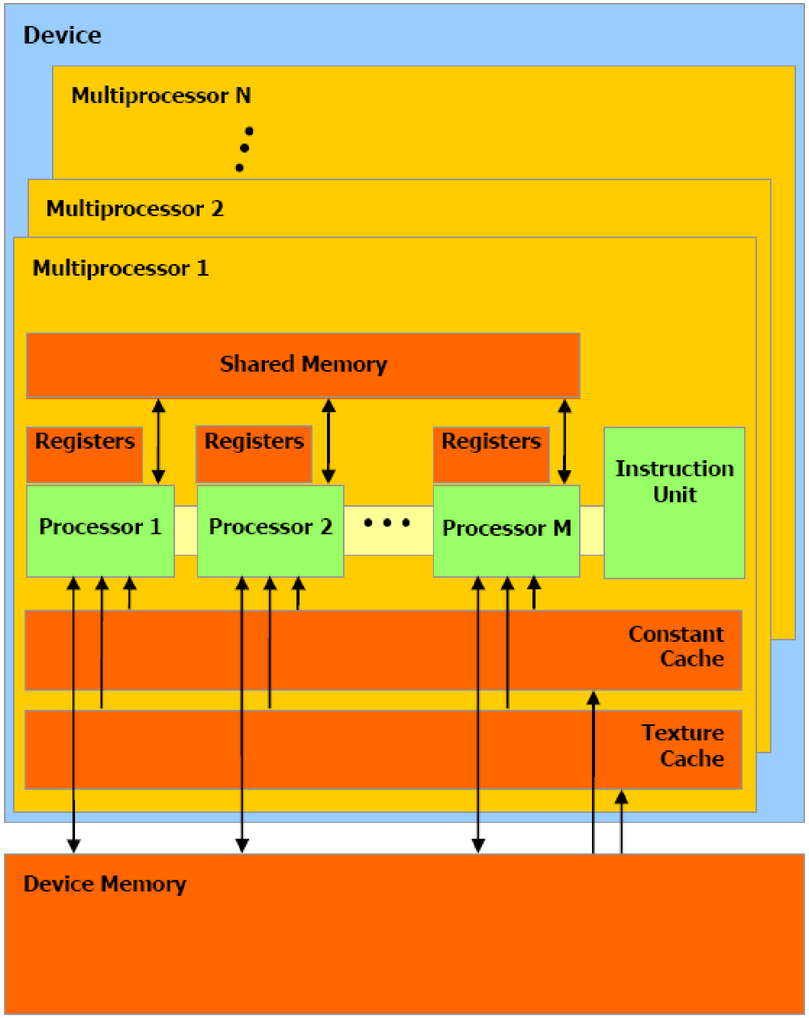
GPU Overview (I)



From: CUDA Programming Guide, NVIDIA

- NVIDIA Tesla C1060:
  - 30 Streaming Multiprocessor (1-N)
  - 8 Scalar Processors/SM (1-M)
  - 30, 8-way SIMD cores = 240 PEs
- Massively parallel multithreaded
  - Up to 30720 active threads handled by thread execution manager
- Processing power
  - 933 GigaFLOPS(single precision)
  - 78 GigaFLOPS(double precision)

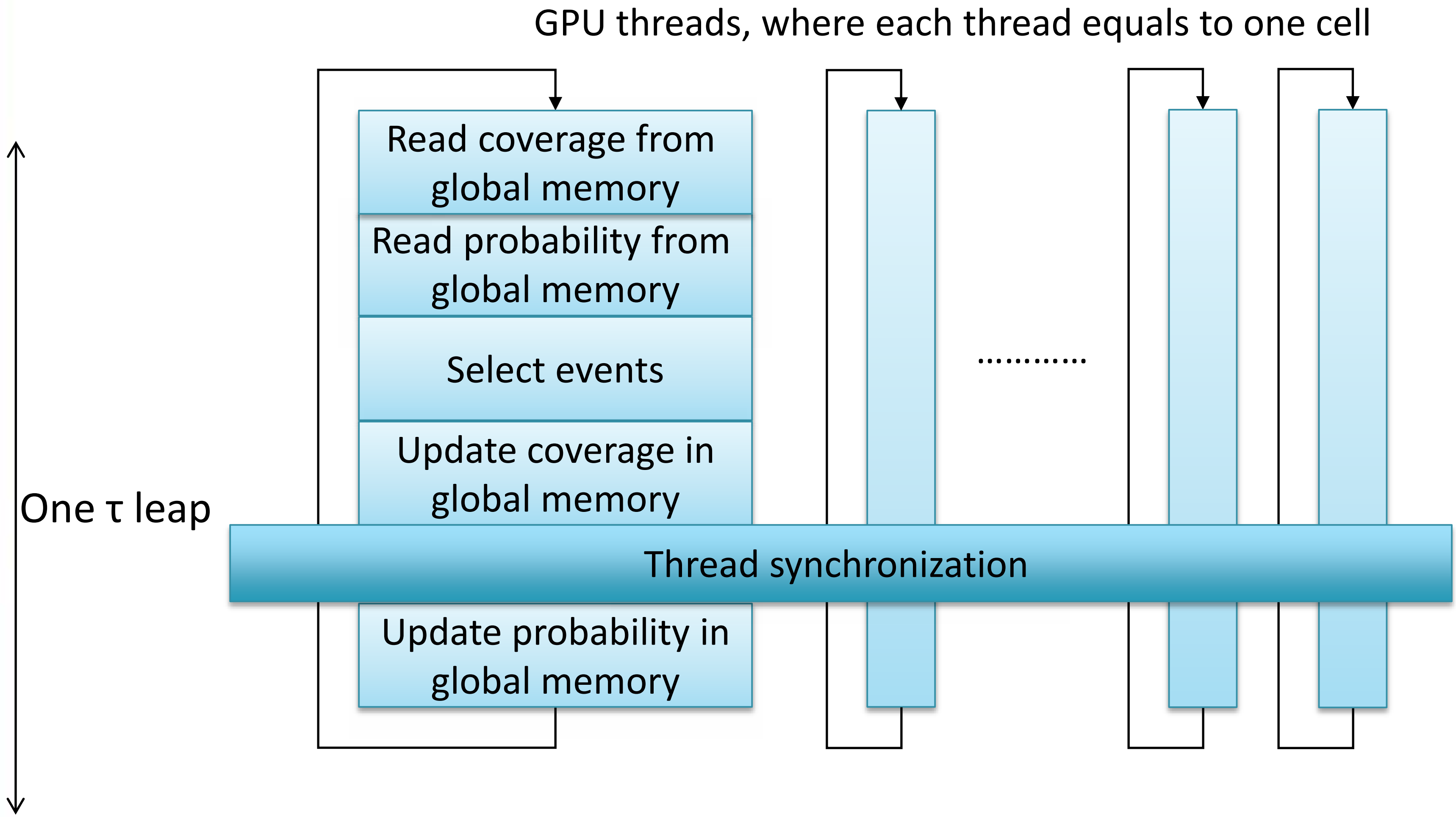
GPU Overview (II)



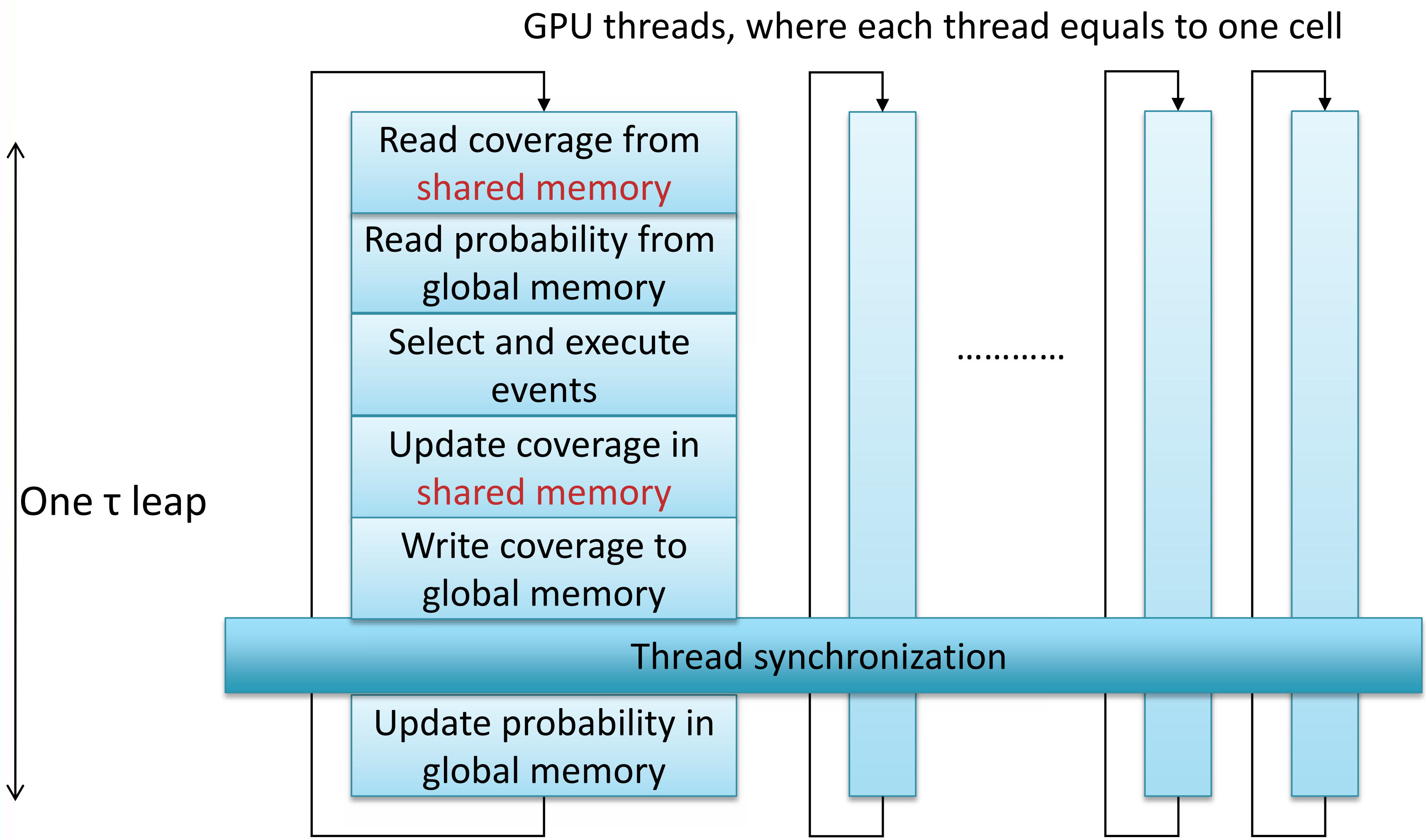
From CUDA Programming Guide, NVIDIA

- Memory types:
  - Read/write per thread
    - Registers
    - Local memory
  - Read/write per block
    - Shared memory
  - Read/write per grid
    - Global memory
  - Read-only per grid
    - Constant memory
    - Texture memory
- Communication among devices and with CPU
  - Through PCI Express bus

Multi-thread Approach


GPU threads, where each thread equals to one cell
Read coverage from global memory
Read probability from global memory
Select events
Update coverage in global memory
Thread synchronization
Update probability in global memory
…………
One τ leap

Memory Optimization



GPU threads, where each thread equals to one cell

One τ leap

Read coverage from shared memory

Read probability from global memory

Select and execute events

Update coverage in shared memory

Write coverage to global memory

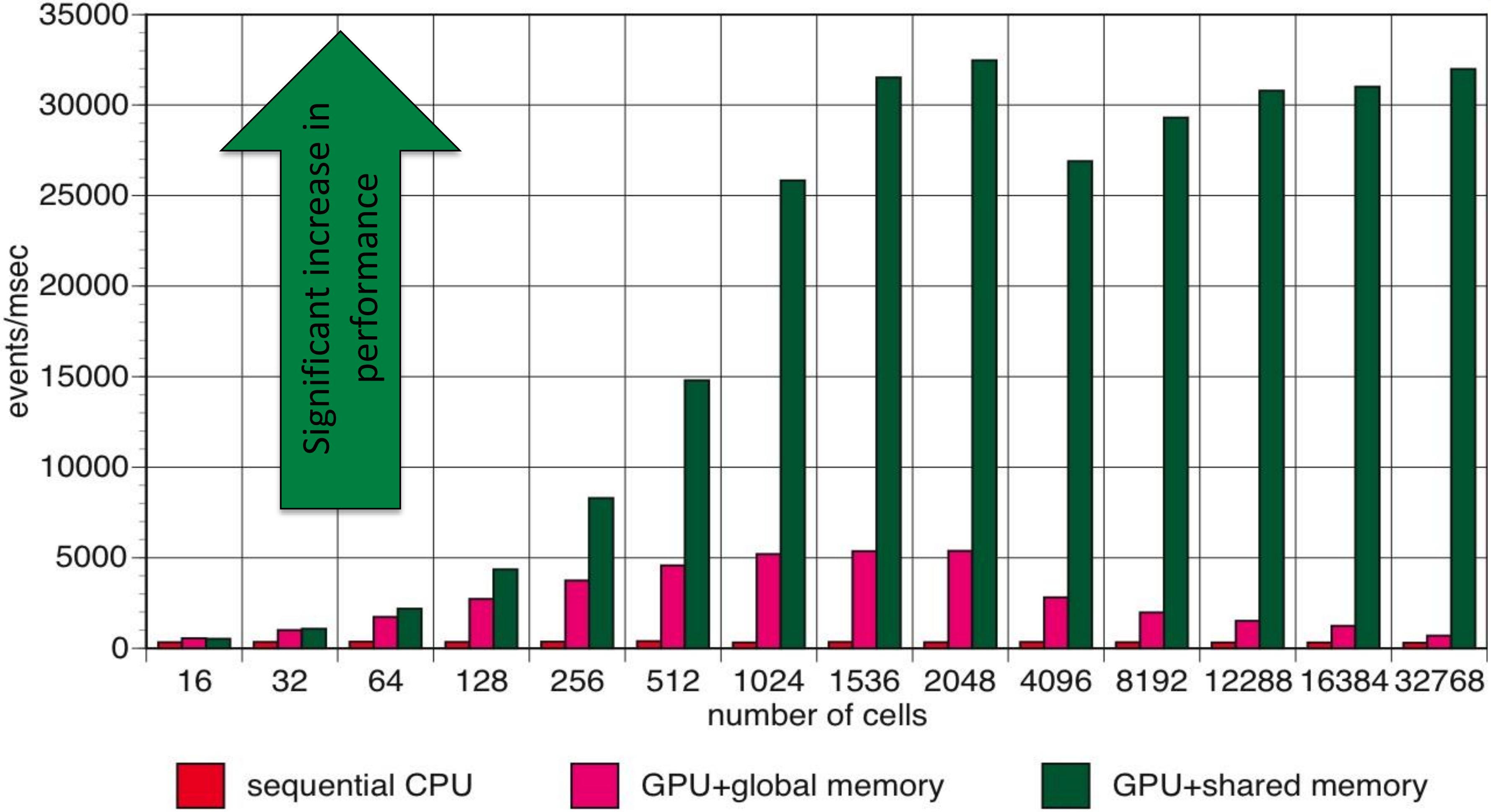
Thread synchronization

Update probability in global memory

Performance

Platforms			
GPU –Tesla C1060		Intel(R) Xeon(R) CPU X5450(CPU)	
Number of cores	240	Number of cores	4
Global memory	4GB	Memory	4GB
Clock rate	1.44 GHz	Clock rate	3 GHz

Performance



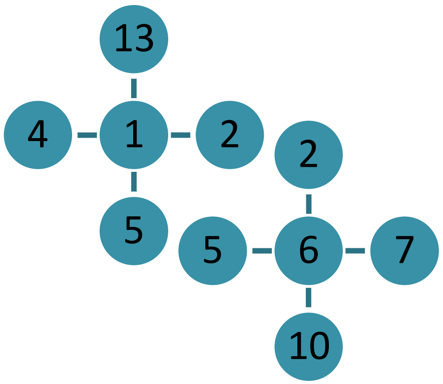
Time scale: CGMC simulations can be 100X faster than a CPU implementation

Rethinking the CGMC Algorithm for GPUs

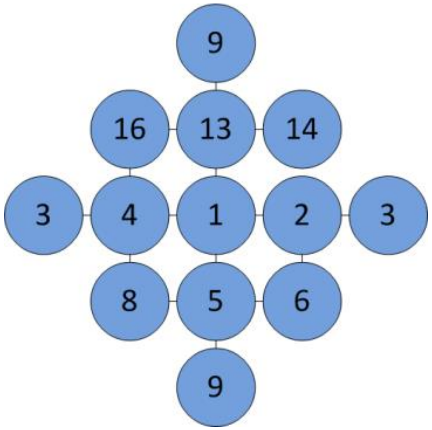
- Redesign of cell structures:
  - Macro-cell = set of cells
  - Number of cells per macro-cell is flexible
- Redesign of event execution:
  - One thread per macro-cell (coarse-grained parallelism) or one block per macro-cell (fine-grained parallelism)
  - Events replicated across macro-cells

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

Cells in a 4x4 system

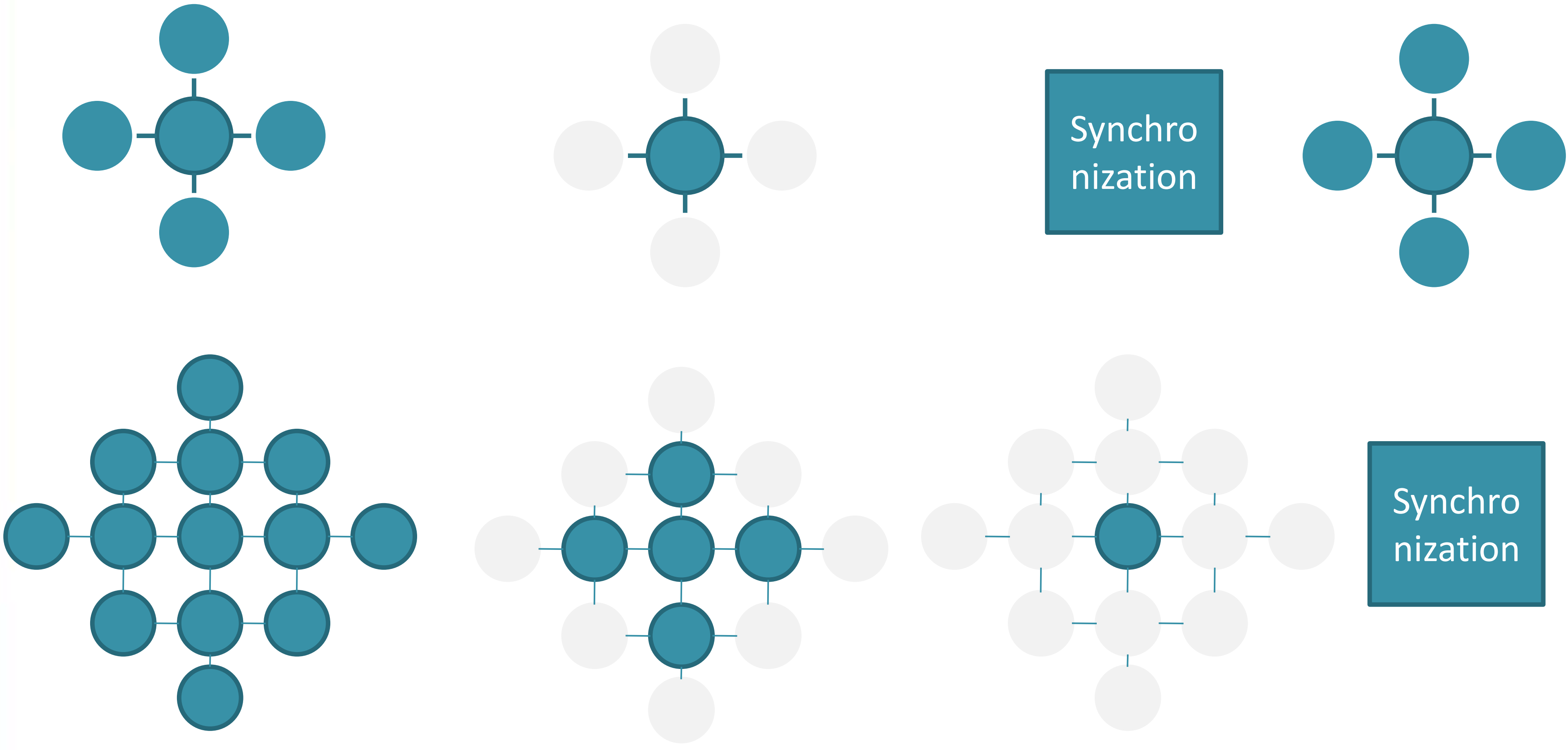


2-layer macro-cells



3-layer macro-cell

Synchronization Frequency



Synchronization

Synchronization

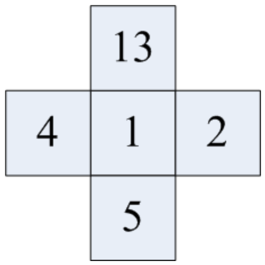
Leap 1

Leap 2

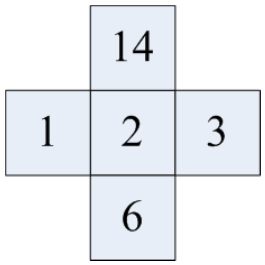
Leap 3

Leap 4

Event Replication



Macro-cell 1



Macro-cell 2

E1: A[cell 1] -> A[cell 2]

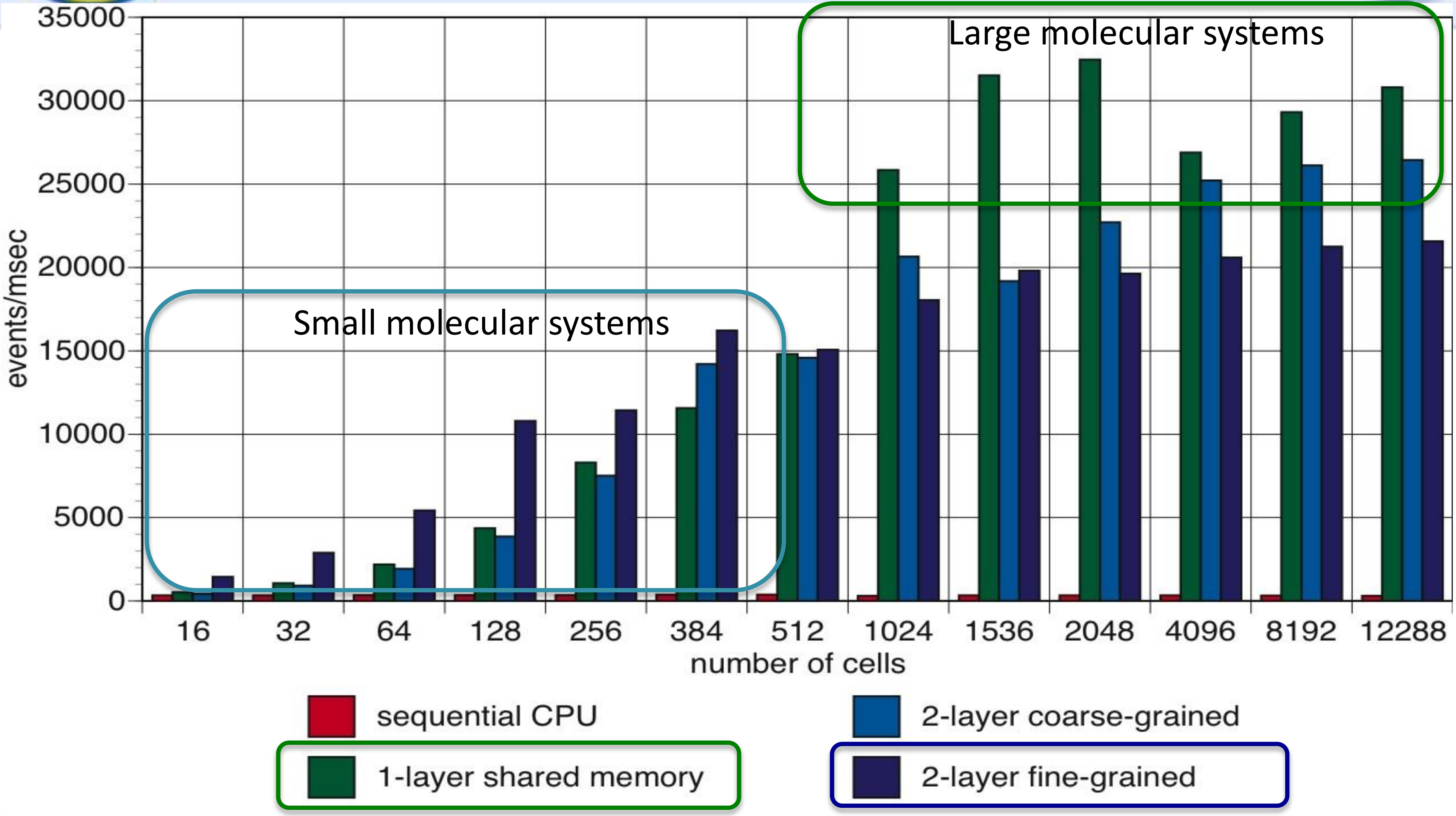
A is a molecule specie

	Macro-cell 1 (block 0)			**Macro-cell 2 (block 1)**			
	Cell 1 (thread 0)	Cell 2 (thread 1)	…	**Cell 2 (thread 5)**	Cell 1 (thread 6)	Cell 3 (thread 7)	…
Leap 1	E1(A--)	E1(A++)		E1(A++)	E1(A--)		
	E1(A--)	E1(A++)		E1(A++)	E1(A--)		
Leap 2	E1(A--)			E1(A++)			

Coarse-Grained vs. Fine-Grained

- 2-layer coarse-grained
  - Each thread is in charge of one macro-cell
  - Each thread simulates five cells in every first leap, one central cell in every second leap
- 2-layer fine-grained
  - Each block is in charge of one macro-cell
  - Each block has five threads
  - Each thread simulates one cell in every first leap
  - Five thread simulate the central cell together in every second leap

Performance



Time scale: CGMC simulations can be 100X faster than a CPU implementation

Multi-GPU Implementation

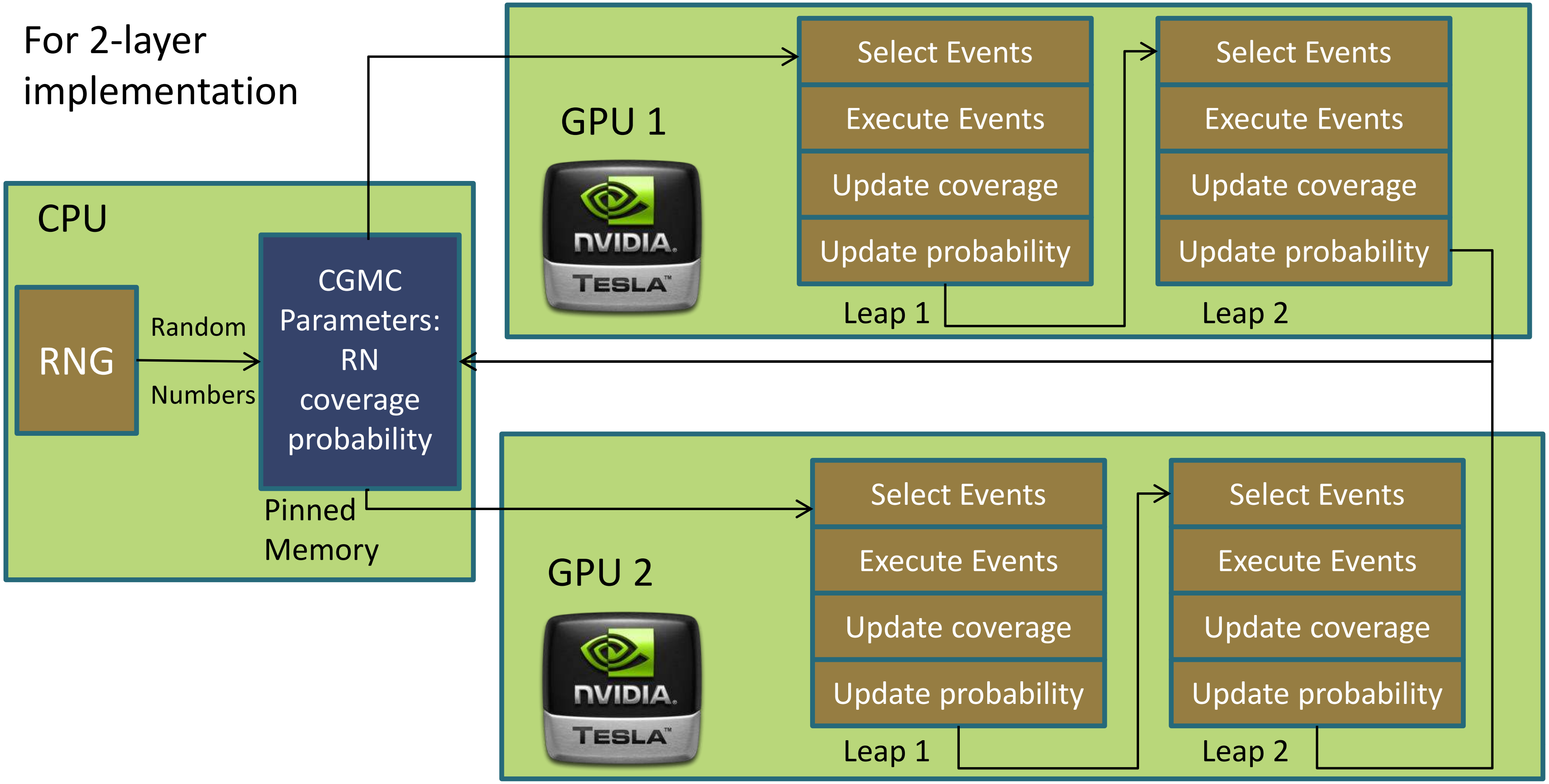
- Limit in number of cells for a single GPU implementation
  - Use multiple GPUs
- Synchronization between multiple GPUs is costly
  - Take advantage of 2-layer fine-grained parallelism
- Combine OpenMP with CUDA for multi-GPU programming:
  - Use portable pinned memory for communication between CPU threads
  - Use mapped pinned memory for data copy between CPU and GPU(zero copy)
  - Use write-combined memory for fast data access

Pinned Memory

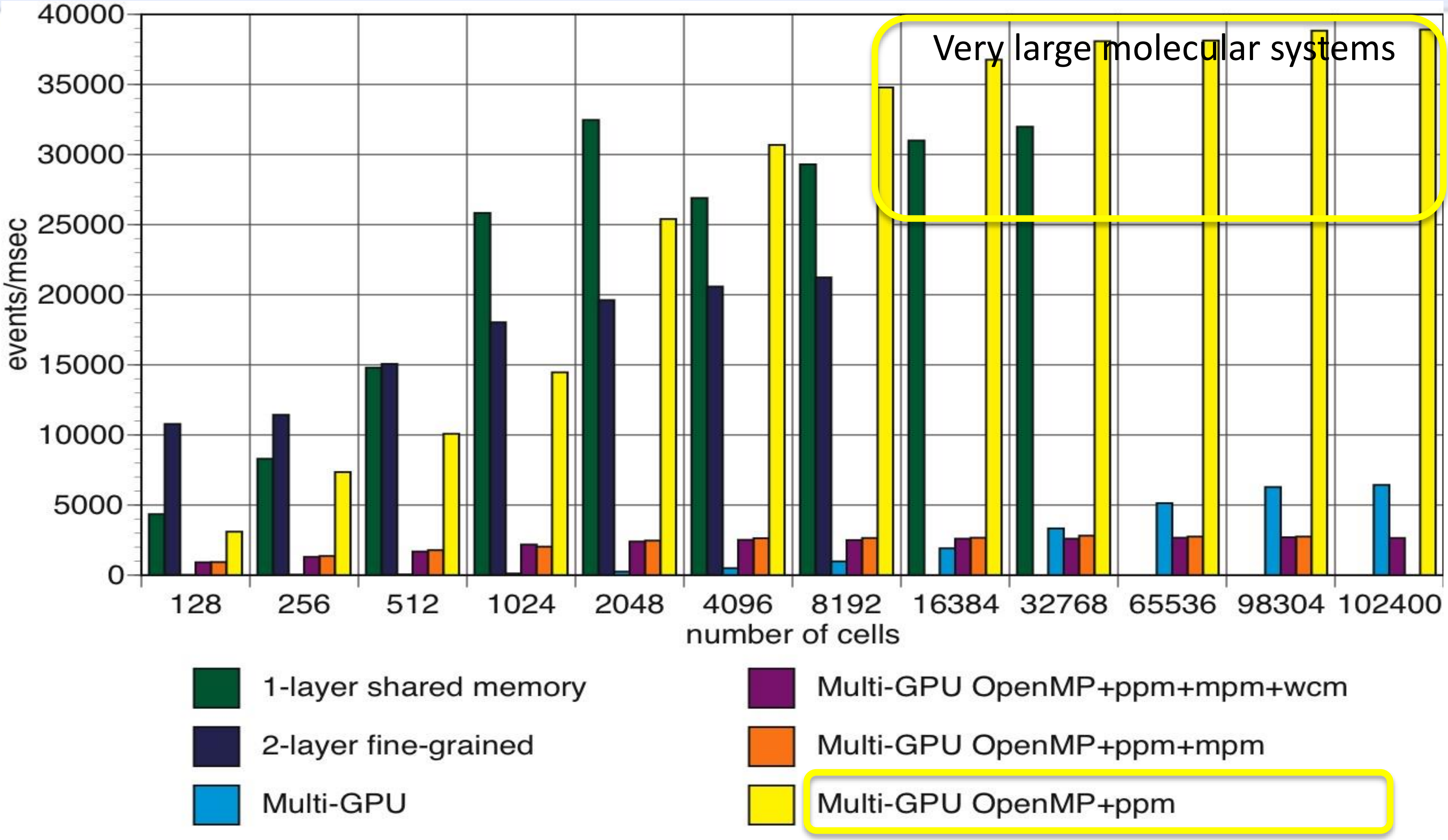
- Portable pinned memory(PPM)
  - Available for all host threads
  - Can be freed by any host thread
- Mapped pinned memory(MPM)
  - Allocate memory on host side
  - Memory can be mapped to device's address space
  - Two addresses: one in host memory and one in device memory
  - No explicit memory copy between CPU and GPU
- Write-combined pinned memory(WCM)
  - Transfers across the PCI Express bus,
  - Buffer is not snooped
  - High transfer performance but no data coherency guarantee

Multi-GPU Implementation

For 2-layer implementation



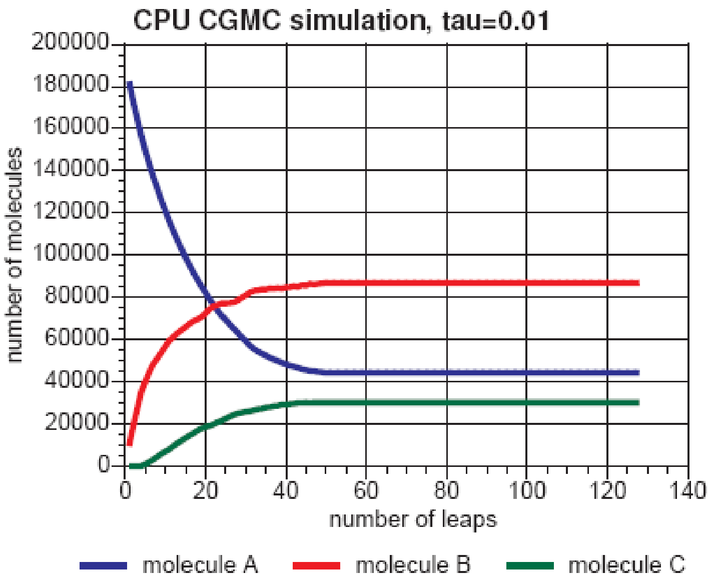
Performance

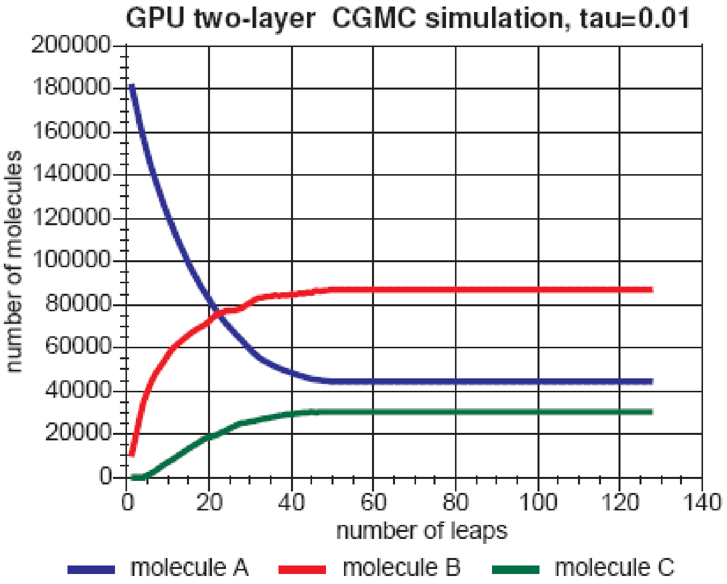


Length scale: 120X faster with molecular systems larger than 13,000 cells

Accuracy

- Simulations of three different species of molecules, A, B, and C
  - A change to B and vice-versa
  - 2 B molecules change to C and vice-versa
  - A, B, and C can diffuse
- Number of molecules in system reaching the equilibrium and in equilibrium





Conclusion

- We present a parallel implementation of the tau-leap method for CGMC simulations on single and multi-GPUs
- We identify the most efficient parallelism granularity for the simulations given a molecular system with a certain size
  - 42X speedup for small systems using 2-layer fine-grained thread parallelism
  - 100X speedup for average systems using 1-layer parallelism
  - 120X speedup for large systems using 2-layer fine-grained thread parallelism across multiple GPUs
- We increase both time scale (up to 120 times) and length scale (up to 100,000)

Future work

- Study molecular systems with heterogeneous distributions
- Identify the most efficient level of parallelism for a given system for:
  - Different system sizes
  - Different site distributions
- Combine MPI, OpenMP, and CUDA to use multiple GPUS across different machines
- Link phenomena and models across scales i.e., from QM to MD and to CGMC

Acknowledgements

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More questions: xulifan@udel.edu

Sponsors: