Heat Equation Solution using alpaka

alpaka Team

HZDR

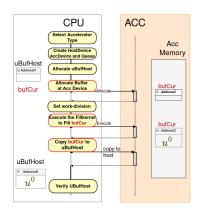
October 1, 2024

Overview

- 1 Steps filling a buffer in parallel
- 2 Memory Allocation and Passing to Kernel
- 3 Define InitilizeBuffer Kernel and Execute
- 4 Introduction for Heat Equation
- 5 Main Simulation Loop of Heat Eqn.
- 6 Heat Eqn. Domain and Stencil
- **7** Setting up the stage to run kernels
- 8 Optimization of Heat Eqn. Solution
- 9 Recap

Steps of Filling a Buffer in Parallel

- Select the accelerator
- Create host-device, acc-device and the queue
- 3 Allocate host and device memory
- 4 Decide how to parallelize: set work-division
- Decide where will the parallel and non-parallel parts of the code run
- 6 Create the kernel instance and execute kernel
- Copy the result from Acc (e.g GPU) back to the host buffer



Allocate memory at Host and at Device

Define number of dim and index type

```
using Dim = alpaka::DimInt<2u>; // Number of dim: 2 as a type
using Idx = std::size_t; // Index type of the threads and buffers
```

Define domain and halo extents

```
// alpaka::Vec is a static array similar to std::array.
// Dim is a compile-time constant, which is 2.
// Create a static array of size Dim.

constexpr alpaka::Vec < Dim, Idx > numNodes {64, 64};
constexpr alpaka::Vec < Dim, Idx > haloSize {2, 2};
constexpr alpaka::Vec < Dim, Idx > extent = numNodes + haloSize;
```

Allocate memories at host and accelerator

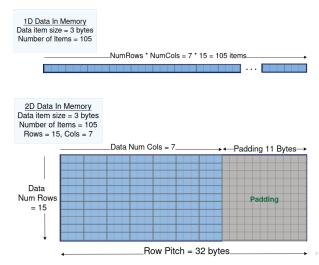
```
// Allocate memory for host-buffer
auto uBufHost = alpaka::allocBuf<double, Idx>(devHost, extent);

// Allocate memory for accelerator buffer
auto uBufAcc = alpaka::allocBuf<double, Idx>(devAcc, extent);
```

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Allocated area at the memory

Let's assume that 105 item with 3-byte each will be allocated to pass to the kernel. The pitch value (actually the row-pitch) depends on the GPU or CPU type.



Passing multi dimensional buffer to the kernel

■ Pass 3 variables for a buffer: pointer, row-pitch, and datasize

Multi-dimensional memory allocated in memory uses aligned rows. Hence, if a pointer of a 2D buffer is passed to the kernel as a pointer; 2 additional values **pitch** and item **data-size** should also be passed.

```
// Signature of function operator of the Kernel
template<typename TAcc, typename TDim, typename TIdx>
ALPAKA_FN_ACC auto operator()(

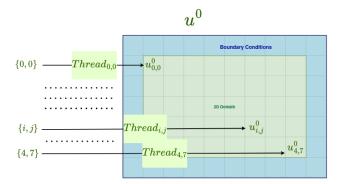
TAcc const& acc,
double* const bufData,
// 2 variables row—pitch and data—type size
alpaka::Vec<TDim, TIdx> const pitch,
double dx,
double dy) const -> void
```

■ Simple Alternative: Pass an alpaka mdspan object

```
template<typename TAcc, typename TDim, typename TIdx, typename TMdSpan>
ALPAKA_FN_ACC auto operator()(
TAcc const& acc,
TMdSpan uAccMdSpan
...) const -> void
```

The Kernel to Initialize Heat Values

Calculate and set initial heat values, the u^0 matrix, by running a grid of threads.



The Kernel to Initialize Heat Values

9 10 The InitializeBufferKernel fills the given buffer at the accelerator device (e.g GPU) Prepare kernel to set initial heat values

- Thread Index: Find thread index in the kernel to be used as index to set 2D buffer.
- Initial Condition at the point: Find analytically the heat value at the point which has coordinates equal to the 2D thread index.
- Memory Adress in Buffer: Calculate the corresponding memory adress in buffer using thread index. Take into account pitch and data-size
- Set Value at the Adress: Set the data at the memory position to the calculated initial condition.

Hands-On Session

Hands-on Session: Filling an accelerator buffer paralelly

The Heat Equation

■ The heat equation models the Heat Diffusion over time in a given medium.

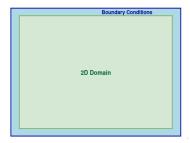
$$\frac{\partial u(x,y,t)}{\partial t} = \alpha \left(\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} \right)$$

Difference approximations for Time and Spatial Derivatives:

$$\left. \frac{\partial u(x,y,t)}{\partial t} \right|_{t=t^n} \approx \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} \qquad \left. \frac{\partial^2 u(x,y,t)}{\partial x^2} \right|_{x=x_j,y=y_i} \approx \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2}$$

Resulting difference equation:

$$u_{i,j}^{n+1} = u_{i,j}^n + \alpha \Delta t \left(\frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} \right)$$



The Heat Equation- Cont.

■ The difference equation:

$$u_{i,j}^{n+1} = u_{i,j}^n + \alpha \Delta t \left(\frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} \right)$$

• Substitute: $\alpha = 1$, $r_X = \frac{\Delta t}{\Delta x^2}$, $r_Y = \frac{\Delta t}{\Delta y^2}$

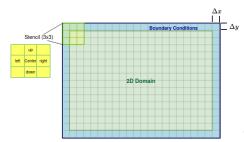
Then $u_{i,j}^{n+1}$ is:

$$u_{i,j}^{n+1} = u_{i,j}^{n} + r_{X} \left(u_{i+1,j}^{n} - 2u_{i,j}^{n} + u_{i-1,j}^{n} \right) + r_{Y} \left(u_{i,j+1}^{n} - 2u_{i,j}^{n} + u_{i,j-1}^{n} \right)$$

By regrouping the terms related to $u_{i,j}^n$, the equation can be rewritten as:

$$u_{i,j}^{n+1} = u_{i,j}^{n} \left(1 - 2r\chi - 2r\gamma\right) + r\chi \left(u_{i+1,j}^{n} + u_{i-1,j}^{n}\right) + r\gamma \left(u_{i,j+1}^{n} + u_{i,j-1}^{n}\right)$$

$$S = \begin{pmatrix} 0 & r_Y & 0 \\ r_X & 1 - 2r_X - 2r_Y & r_X \\ 0 & r_Y & 0 \end{pmatrix}$$



Main Simulation Loop: Leveraging Parallelism

Initialization:

- Define the "host device" and "accelerator device". The "Host" and "Device" in short.
- Set initial conditions and boundary conditions.
- Allocate data buffers to host and device.
- Copy data from host to device buffer to pass to the kernel.
- Define parallelisation strategy (determine block size).

Simulation Loop:

- Step 1: Execute StencilKernel to compute next values.
- Step 2: Apply boundary conditions using BoundaryKernel.
- **Step 3:** Swap buffers for the next iteration so that calculated $u_{i,i}^{n+1}$ becomes the $u_{i,i}^n$ for the next step.

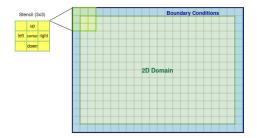
Parallel Efficiency:

- Subdomains are processed in parallel, with halos ensuring data consistency and correct boundary conditions.
- Optimization: Shared memory optimizes memory access within each block using chunks of data.

Validation

Parallel Heat Equation Solution

- Data Parallelism: Each point on the grid can be updated independently based on its neighbors, enabling parallel computation.
- Stencil Operations: Stencil is a core computational pattern in PDE solvers. Updates a grid point in time
 using its immediate neighbors (left, right, up, down) according to the difference equation. A 5-point stencil
 is needed.



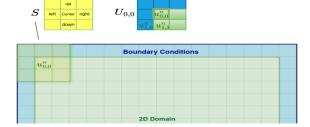
- Halo Region for BC: A layer of grid cells surrounding the problem domain for Boundary Conditions.
 - Facilitates stencil operations at the boundaries of subdomains.

Calculation of $u_{i,i}^{n+1}$ from $u_{i,i}^n$

- Each kernel execution by alpaka calculates $u_{i,j}^{n+1}$ using $u_{i,j}^{n}$
- Each heat point is separately calculated by a thread using Frobenious Inner Product
- The Frobenius inner product between matrix S and matrix $U_{i,j}$ is:

$$u_{i,j}^{n+1} = \langle S, U_{i,j}^n \rangle_F = \sum_{m=1}^M \sum_{n=1}^K s_{m,k} u_{m,k}$$

■ S and $U_{0,0}^n$ is used by a thread to calculate $u_{0,0}^{n+1}$



■ Another thread calculates $u_{0,1}^{n+1}$ using S and $U_{0,1}^n$

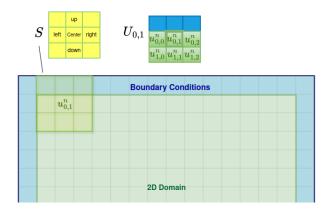
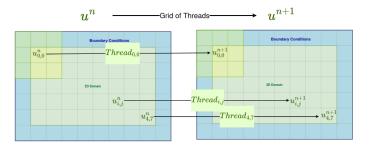


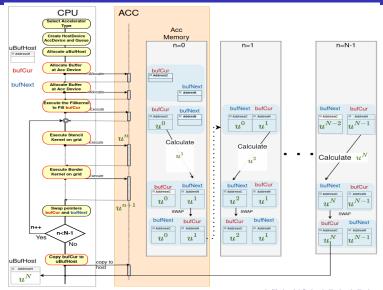
Figure: Second thread calculates $u_{0.1}^{n+1}$ using

Stencil Kernel Execution by a grid of threads



- Stencil kernel will update only core nodes not the border
- The workdiv for stencil kernel can be calculated by setting gridthread extent to nodes domain
- The workdiv for the borders kernel would need extended extents, because halo is going to updated as well
- Some threads other than the ones updating the border will do nothing when running Boundary kernel

Complete Heat Equation solution



The Stencil Kernel

What kind of parallelization needed to calculate $u_{i,j}^{n+1}$ using $u_{i,j}^{n}$

- StencilKernel needs a Work-division to work on domain of all nodes (without halo)
- Boundary kernel needs a Workdivision which covers nodes + halo region
- Boundary kernel will only use threads corresponding to halo region

Coding StencilKernel

- Input: Check the size of the input buffer, it should include halo region as well
- Thread Index: Find thread index in the kernel. This index will be used as the center of 3x3 stencil.
- Memory Adress in Buffer: Calculate the corresponding memory adress in buffer using thread index. Take into account pitch and data-size
- **Calculate new heat value:** Calculate $u_{i,i}^{n+1}$ using Frobenious Inner Product of 3x3 matrices
- Set Value at the Adress: Set the data at the memory adress.

Hands-On Session

Hands-on Session:Stencil Kernel

alpaka Basics

Setting up the stage to run kernels

- Selecting the accelerator and host devices
- 2 Allocating and setting host and accelerator device memory
- 3 Alpaka Vector, Buffer and View?
- Passing data to the accelarator
- 5 WorkDiv
- 6 Define Queue

Accelerator, Device and Host

Define number of dim and index type

```
using Dim = alpaka::DimInt<2u>; // Number of dim: 2 as a type
using Idx = std::size_t; // Index type of the threads and buffers
```

Define the accelerator

```
// AccGpuCudaRt, AccGpuHipRt, AccCpuThreads, AccCpuSerial,
// AccCpuOmp2Threads, AccCpuOmp2Blocks, AccCpuTbbBlocks
using Acc = alpaka::AccGpuHipRt < Dim, Idx >;
using DevAcc = alpaka::Dev < Acc >;
```

Select a device from platform of Acc

```
auto const platform = alpaka::Platform < Acc > {};
auto const devAcc = alpaka::getDevByIdx(platform, 0);
```

Select a host and hostype to allocate memory for data

```
// Get the host device for allocating memory on the host.
auto const platformHost = alpaka::PlatformCpu{};
auto const devHost = alpaka::getDevByIdx(platformHost, 0);
// Host device type is needed, still not known
using DevHost = alpaka::DevCpu;
```

What is Accelerator

Accelerator hides hardware specifics behind alpaka's abstract API

- On Host: Accelerator is a type. A Meta-parameter for choosing correct physical device and dependent types
- using Acc = acc::AccGpuHipRt < Dim, Idx>;
- Inside Kernel: Accelerator is a variable. Contains thread state, provides access to alpaka's device-side API
 - The Accelerator provides the means to access to the indices

```
// get thread index on the grid
auto gridThreadIdx = alpaka::getIdx<Grid, Threads>(acc);
// get block index on the grid
auto gridBlockIdx = alpaka::getIdx<Grid, Blocks>(acc);
```

 The Accelerator gives access to alpaka's shared memory (for threads inside the same block)

Enables synchronization on the block level

```
// synchronize all threads within the block
alpaka::syncBlockThreads(acc);
```

What is alpaka Buffer, Vector and View

- alpaka::Buf is multi-dimensional dynamic (runtime sized) container.
 - Contains memory adress, extent, datatype and the device that memory belongs to!
 - Since buffer already knows the it's device and extent; device to device copy is easy in alpaka
 - Supports [] operator but not [][].

```
// Allocate buffers
auto bufCpu = alpaka::allocBuf<float, Idx>(devCpu, extent);
auto bufCpu = alpaka::allocBuf<float, Idx>(devGpu, extent);
....
// Copy buffer from CPU to GPU - destination comes first
alpaka::memcopy(gpuQueue, bufGpu, bufCpu);
// cuda way: cudaMemcpy(b_d, b_host, sizeof(float)*N, cudaMemcpyHostToDevice)
```

alpaka::Vec is a static 1D array.

```
alpaka::Vec<SizeOfArrayAsType,DataT> myVec;
```

alpaka::View is a non-owning view to an already allocated memory, so that it can be used in alpaka::memcpy

What is alpaka::Queue

- alpaka::Queue is "a queue of tasks".
- Used for sycnhronization of tasks like memcpy or kernel-execution
- Queue is always FIFO, everything is sequential (in-order) inside the alpaka::queue
- If there is a second queue, queue feature "blocking" and "non-blocking" becomes important
- Different queues can run in parallel for many devices
- Within a single queue accelerator back-ends can be mixed (used in interleaves)

```
using QueueProperty = alpaka::NonBlocking;
// Create queue
using QueueAcc = alpaka::Queue<Acc, QueueProperty>;

QueueAcc computeQueue{devAcc};

// Copy host -> device, use the queue
alpaka::memcpy(computeQueue, uCurrBufAcc, uBufHost);
alpaka::wait(computeQueue); // Not needed we have single queue
// Create kernel instance
StencilKernel
stencilKernel
// Execute kernel using queue
alpaka::exec
// Execute kernel using queue
alpaka::exec
// Execute kernel using queue
// Execute kernel u
```

Queue Operations

Queues are used for synchronization

```
// block caller until all operations have completed
alpaka::wait(myQueue);
// block myQueue until myEvent has been reached
alpaka::wait(myQueue, myEvent);
// block myQueue until otherQueue has completed
alpaka::wait(myQueue, otherQueue);
```

Queues can be checked for completion of all tasks

```
bool done = alpaka::empty(myQueue);
```

Tasks and Events

- Device-side related operations (kernels, memory operations) can be wrapped in tasks.
- Tasks are executed by enqueue() function.
- Tasks on the same queue are executed in order (FIFO principle)

```
alpaka::enqueue(queueA, task1);
alpaka::enqueue(queueA, task2);
// task2 starts after task1 has finished, even if queueA is non-
blocking
```

Order of tasks in different queues is unspecified

```
alpaka::enqueue(queueA, task1);
alpaka::enqueue(queueB, task2);
// task2 starts before, after or in parallel to task1 if queueA is non blocking
```

For easier synchronization, alpaka Events can be inserted before, after or between Tasks:

```
auto myEvent = alpaka::Event < alpaka::Queue > (myDev);
alpaka::enqueue(queueA, myEvent);
alpaka::wait(queueB, myEvent);
// queueB will only resume after queueA reached myEvent
```

Execute the Kernel and copy data back to host

First create the queue

```
// Create queue,
// queue is needed for kernel execution and copies to/from accelerator
alpaka::Queue<Acc, alpaka::NonBlocking> queue{devAcc};
```

■ Execute the kernel using the queue, the workdiv and kernel arguments:

```
alpaka::exec<Acc>(queue, workDiv, initBufferKernel, uBufAcc.data(),
    pitchCurrAcc, dx, dy);
```

Copy the filled buffer back to the host

```
// Copy device -> host
// Since buffers know their corresponding devices (host or acc) memcopy does
not need any device variable
alpaka::memcpy(queue, uBufHost, uBufAcc);
alpaka::wait(queue);
```

Determine WorkDiv

Let alpaka calculate work division for you:

```
// All kernel inputs are needed because work-division depends on the kernel
// Create kernel instance
InitializeBufferKernel initBufferKernel;
// Elements per thread needed to determine work-div
constexpr alpaka::VecObim, Idx> elemPerThread{1, 1};
// Bundle the extent and elements per thread
alpaka::KernelCfg<Acc> const kernelCfg = {extent, elemPerThread};
// Kernel input row-pitch and data-type-size
auto const pitchCurrAcc(alpaka::getPitchesInBytes(uBufAcc));
// Determine the work-div
auto workDiv = alpaka::getValidWorkDiv(kernelCfg, devAcc, initBufferKernel,
uBufAcc,data(), pitchCurrAcc, dx, dv);
```

Determine the work-division manually

```
// Set Dim and Index type
using Dim1D = alpaka::DimInt<1u>; // 1 as a type
using Idx = uint32_t;
// M blocks each has 4 threads, each level is 1D
alpaka::WorkDivMembers<Dim1D, Idx> workdiv1D{M, 4, 1};
// Set Dim2D and use same index type
using Dim2D = alpaka::DimInt<2u>; // 2 as a type
alpaka::Vec<Dim2D, Idx> gridBlockExtent{M,N}; // 2D grid
alpaka::Vec<Dim2D, Idx> blockThreadExtent{32,32}; // 2D block
alpaka::Vec<Dim2D, Idx> elementExtentPerThread{1,1};
// MxN blocks each has 32x32 threads, each level is 2D
alpaka::WorkDivMembers<Dim2D, Idx> workdiv2D{gridBlockExtent,
blockThreadExtent, elementExtentPerThread}:
```

```
using DimlD = alpaka::Dimlnt<l>;//Set number of dims to 1
using VeclD = alpaka::Vec<DimlD, Idx>;//Define alias
auto workDivlD = alpaka::VorkDivMembers(VeclD{M}, VeclD{Au}, VeclD{1u});
// alternatively
using Dim3D = alpaka::Dimlnt<l>;//Set number of dims to 3
using Vec3D = alpaka::Vec<Dim3D, Idx>; //Define alias
auto workDiv3D = alpaka::Vec<Dim3D, Idx>; //Define alias
auto workDiv3D = alpaka::Vec<Dim3D, Idx>; //Define alias
```

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Optimization and usability

alpaka Usability and Optimization Features

- Use alpaka mdspan to set,get, pass buffers easily
- Use Domain Decomposition: Divide the domain in chunks
- Use 2 asynch queues for performance increase
- 4 Use **shared memory** for performance increase

alpaka::experimental::mdspan

Mdspan a multi-dimensional and non-owning view

- Part of C++23 standard. Can be used with C++17.
- Consists Data Pointer, Data Pitch and Data item size
- Has member functions to get/set data and to get extents

Mdspan Installation

- Set alpaka_USE_MDSPAN cmake variable to FETCH while installing alpaka
- Alternatively, set alpaka_USE_MDSPAN cmake variable to FETCH while configuring example if it is not already set while installation

```
// in build directory
cmake -Dalpaka_USE_MDSPAN=FETCH ..
```

Create an mdspan view of a buffer, then pass to the kernel

```
// Host code: Allocate device memory
auto bufDevA = alpaka::allocBuf <DataType, Idx>(devAcc, extentA);
// Create mdspan views for device buffers using alpaka::experimental::getMdSpan
auto mdDevA = alpaka::experimental::getMdSpan(bufDevA);
// Execute the kernel
alpaka::exec<Acc>(queue, workDiv, kernel, mdDevA, mdDevB, mdDevC);
```

Kernel using mdspan instead of data buffer pointer and pitch

Example usage to access/set multi-dim data at host or in kernel

```
struct StencilKernel
{
   template < typename TAcc, typename TDim, typename TIdx, typename TMdSpan >
   ALPAKA_FN_ACC auto operator()(
    TAcc const& acc,
   TMdSpan uCurrBuf,
   TMdSpan uNextBuf,
   alpaka::Vec<TDim, TIdx > const chunkSize,
   double const dx,
   double const dy,
   double const dt) const -> void
   { . . . .
   } };
```

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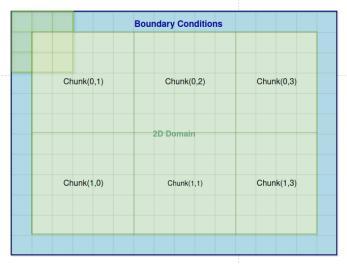
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Hands-On Session

Hands-on Session: Use mdspan for the kernel using shared memory

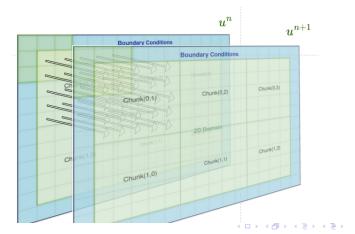
Chunk Definition

Chunk: Subdomains needed for latency management of block level parallelisation



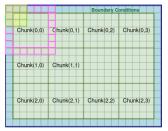
Calculation by a block of grids of stencil kernel

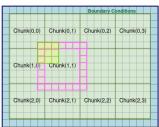
- Chunking is a domain decomposition method
- A block of threads update a chunk of heat data
- A grid of threads updates the whole domain



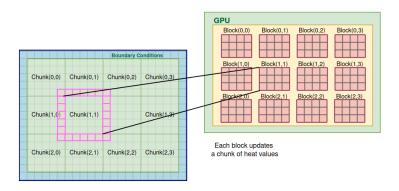
Chunks in Parallel Grid Computations

- Halo Region around chunk: A layer of grid cells surrounding the subdomains. In order to use the heat value beside the current chunk
- Halo Size: Typically 1 for a 5-point stencil.
- Chunks might include more than one blocks depending on the blocksize





Chunks in Parallel Grid Computations



Determine WorkDiv for Chunked Solution

Set work division fields directly:

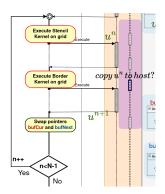
```
// Define a workdiv for the shared memory based heat eqn solution
    constexpr alpaka::Vec < Dim , Idx > elemPerThread {1, 1};
    // Get max threads that can be run in a block for this kernel
    auto const kernelFunctionAttributes = alpaka::getFunctionAttributes<Acc>(
        devAcc.
        stencilKernel,
        uCurrBufAcc.data(), uNextBufAcc.data(),
        chunkSize.
        pitchCurrAcc, pitchNextAcc,
9
        dx, dy, dt);
    auto const maxThreadsPerBlock = kernelFunctionAttributes.maxThreadsPerBlock:
    auto const threadsPerBlock
        = maxThreadsPerBlock < chunkSize.prod() ? alpaka::Vec < Dim , Idx > {
             maxThreadsPerBlock, 1} : chunkSize:
    alpaka::WorkDivMembers < Dim, Idx > workDiv_manual { numChunks, threadsPerBlock,
14
         elemPerThreadl:
```

Hands-On Session

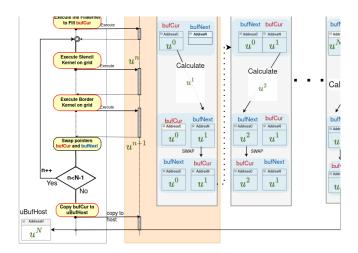
Hands-on Session: Optimized Heat Eqn. solution by Domain Decomposition

Running 2 parallel queues: Additional queue to dump temporary results

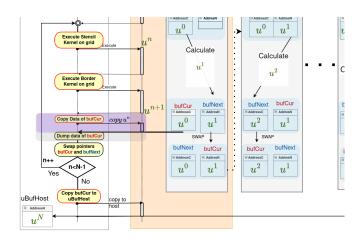
- Create an additional alpaka::queue instance at accelerator to run parallely
- The temporary heat result uⁿ will be copied to host from accelerator at the end of each iteration
- Copying can start while the stencil and boundary kernels are running
- In order to run 2 queues paralelly they should be a NonBlocking queues
- The copied heat data will be used to create an animation of images



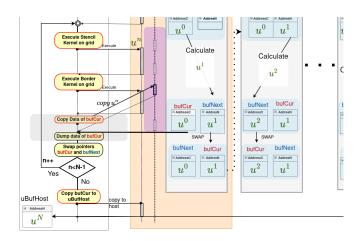
Current Loop



Copy u^n back at each iteration sequentially



Copy u^n back at each iteration in parallel



Hands-On Session

Running 2 parallel queues

Efficient Stencil Application with Shared Memory

Shared Memory at GPUs

- A fast, limited-size memory accessible by all threads within a block.
- Used to store data locally in Compute Unit(or SM), reducing the need to access slower global memory.
- Shared Memory allocation can be static or dynamic
 - Static (compile time determined extent)
 - Dynamic (runtime determined extent)
- Filling shared memory is done by the same kernel calculating the stencil
- Threads in a block must synchronize to ensure all data is loaded into shared memory before computation begins.

Benefits:

Reduces memory latency by storing the working set of data (halo + core) in shared memory.

Shared memory data: chunk with halo

- Halo Region around chunk: A layer of grid cells surrounding the subdomains. In order to use the heat value beside the current chunk
- Halo Size: Typically 1 for a 5-point stencil.
- Chunks might include more than one blocks depending on the blocksize
- Kernel will install the data to shared memory then use the data from shared memory





Steps of Stencil Kernel using shared memory

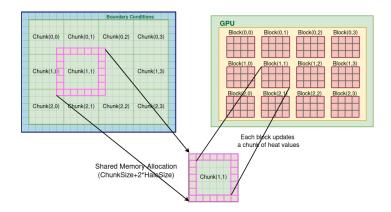
Allocate shared memory inside kernel

- Calculate thread index
- Fill the shared memory by block of threads
- Wait for shared memory to be filled by all block threads

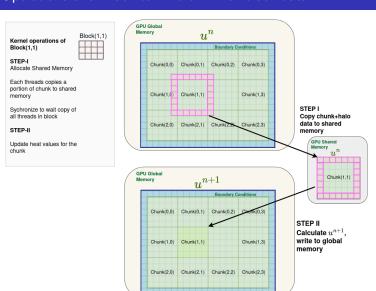
```
1 alpaka::syncBlockThreads(acc);
```

- Calculate new heat value using the data from the shared memory
- Set the new heat value

Updating chunks using shared memory



Kernel Operations of a Block to Find u^{n+1} for block data



Hands-On Session

Hands-on Session: Optimized Heat Eqn. solution by using shared memory

Conclusion: Parallel Techniques For Solving Heat Equation

Kernel Definition

- Kernel to fill a buffer in parallel
- Stencil Kernel for calculating the next set of heat values
- Boundary Kernel

Work division

- Getting a valid work division according to accelerator
- Setting work-division manually

Allocating and Setting Memory at Host and Accelerator

- Using alpaka::buffer
- Using alpaka::memcpy

Alpaka Structures

Accelerator, Device, Queue, Task

Optimizations and Usability

- Using alpaka Mdspan
- Domain Decomposition
- Using Multiple Async Queues
- Using GPU's Shared Memory

Questions?