

Shallow Water: Initial Report

Group Number: 2

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Optimizations used or attempted:

Restructuring and annotation to enable greater vectorization, informed by results from profiling
Parallelization with OpenMP

More details:

1. Vectorization
 - a. Used compiler directives such as '#pragma ivdep' to encourage the compiler to vectorize loops and ignore possible dependencies that did not actually exist.
 - b. Attempted to restructure the code to make better use of memory locality and vectorization.
2. Parallelization
 - a. Use OpenMP to allow this code to be parallelized.
 - b. Split the simulation grid into rectangular blocks based on the number of threads available.
 - i. For an a-by-b grid with p threads, we set the block size to $\text{floor}(a/\sqrt{p})$ -by- $\text{floor}(b/\sqrt{p})$, based on the assumption that the grid is roughly square (so the threads should be distributed equally in the horizontal and vertical directions). If the grid is not square, or if p is not square, there may be more blocks than the number of processors, due to small rectangular blocks on the fringes of the grid. In this case, we assign multiple blocks to each processor sequentially in row-major order (e.g. processor 0 gets the blocks in position [0,0] and [0,1]). Although the extra blocks assigned to each processor can only be computed sequentially, each processor will usually have 3 or fewer blocks, so this should not affect performance too much.
 - ii. We will also have 2k layers of ghost cells for each block, so that each thread can compute k time steps before communication is necessary. k is a parameter that we will vary to figure out which value gives the best performance.
 1. We anticipate that we will use an even value of k, so we do not have to deal with the grid being offset (as it is after an odd number of steps).
 2. As per Professor Bindel's Piazza post, each thread will need to write its updates into two additional ghost cells per additional step in the batch.

Vectorization Results:

When we initially ran the `amplxe-cl` profiling tool on the original code and default `dam_break` test case, we found that by far the bottleneck was the `limited_derivs` function.

amplxe: Executing actions 50 % Generating a report	Function	Module	CPU Time	Spin Time	Overhead Time
-----	-----	-----	-----	-----	-----
Central2D<Shallow2D, MinMod<float>>>::limited_derivs	shallow		1.148s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::compute_step	shallow		0.659s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::compute_fg_speeds	shallow		0.230s	0s	0s
[Outside any known module]	[Unknown]		0.021s	0s	0s
_IO_file_xsputn	libc-2.12.so		0.015s	0s	0s
_IO_fwrite	libc-2.12.so		0.010s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::solution_check	shallow		0.004s	0s	0s
SimViz<Central2D<Shallow2D, MinMod<float>>>::write_frame	shallow		0.004s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::Central2D	shallow		0.003s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::run	shallow		0.001s	0s	0s
std::array<float, (unsigned long)3>::operator[]	shallow		0.001s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::offset	shallow		0.001s	0s	0s
do_lookup_x	ld-2.12.so		0.001s	0s	0s

After we made some changes to improve vectorization, we were able to speed up the `compute_step` and `compute_fg_speeds` functions slightly:

amplxe: Executing actions 50 % Generating a report	Function	Module	CPU Time	Spin Time	Overhead Time
-----	-----	-----	-----	-----	-----
Central2D<Shallow2D, MinMod<float>>>::limited_derivs	shallow		1.149s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::compute_step	shallow		0.548s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::compute_fg_speeds	shallow		0.130s	0s	0s
[Outside any known module]	[Unknown]		0.017s	0s	0s
_IO_file_xsputn	libc-2.12.so		0.012s	0s	0s
_IO_fwrite	libc-2.12.so		0.010s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::solution_check	shallow		0.005s	0s	0s
SimViz<Central2D<Shallow2D, MinMod<float>>>::write_frame	shallow		0.005s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::Central2D	shallow		0.002s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::run	shallow		0.002s	0s	0s
std::array<float, (unsigned long)3>::operator[]	shallow		0.002s	0s	0s
Central2D<Shallow2D, MinMod<float>>>::offset	shallow		0.001s	0s	0s
do_lookup_x	ld-2.12.so		0.001s	0s	0s

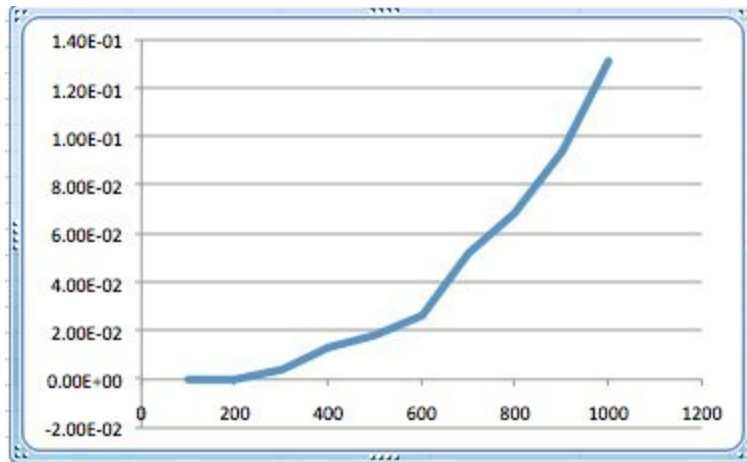
As can be seen, both the `compute_step` and `compute_fg_speeds` functions take about 0.1 seconds less time after vectorization is used. These numbers were not just coincidences or artifacts, but held up after repeated trials.

Table of overall speeds per frame vs. simulation grid size:

Grid size (dimension of one square side)	Average time per frame: with vectorization improvements (seconds)	Average time per frame: unoptimized original version (seconds)
100	5.17E-03	5.13E-03
200	3.55E-02	3.62E-02
300	1.21E-01	1.26E-01
400	2.79E-01	2.92E-01
500	5.92E-01	6.10E-01
600	1.10E+00	1.13E+00

700	1.52E+00	1.57E+00
800	2.30E+00	2.37E+00
900	3.20E+00	3.30E+00
1000	4.41E+00	4.54E+00

Chart of average speedup per frame in new code vs. simulation grid size:



The `#pragma ivdep` directive was helpful in loops where vectorization was only being held back by the compiler's prior inability to assume that the memory locations being modified and the memory locations being read did not overlap. However, in many cases, such as the `limited_derivs` function, the loops still did not vectorize, because they would actually have become slower than the serial version due to memory access patterns that disrupted cache locality. Therefore, it would be necessary to change the structure of the code to enable access patterns making use of cache locality. For instance, instead of using vectors of 'vecs' for `u`, `f`, `g`, and so on, we could instead store all this data in a flattened (single-dimensional) data structure and change our 'offset' function to convert three input numbers into an offset within this array, similar to what Professor Bindel did in his C code. We may use `valarrays` for this purpose.

The code with vectorization improvements is simply in `central2d.h`.

Parallelization results:

For the purposes of this submission, we opted to have one member work on figuring out the OpenMP parallelization scheme, and meanwhile simultaneously another team member would work on getting the C++ code properly vectorized.

We have implemented parallelization with OpenMP, but there still seem to be some bugs to work out with regards to the way we split up the grid into blocks and process these blocks in parallel. Thus, we do not have timing results to show for this part yet.

The code for the parallelization attempts so far is in `central2d_omp.h`.

Future steps:

We will finish restructuring the C++ code to attempt to get it close to the performance of the C code. We will finish implementing the grid parallelization scheme, and will tune parameters to find out the optimal number of layers of ghost cells per block.