# High Performance Computing for Science and Engineering I

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## Set 2 - Diffusion and Multithreading

Issued: October 3, 2014 Hand in: October 10, 2014, 8:00am

#### Question 1: Diffusion in 2D

Heat flow in a medium can be described by the diffusion equation of the form

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = D\nabla^2 \rho(\mathbf{r}, t) \tag{1}$$

where  $\rho(\mathbf{r},\mathbf{t})$  is a measure for the amount of heat at position r and time t and the diffusion coefficient D is constant. Lets define the domain  $\Omega$  in two dimensions as  $x,y\in[-1,1]$ . We will use Dirichlet boundary conditions

$$\rho(-1, y, t) = \rho(x, -1, t) = \rho(1, y, t) = \rho(x, 1, t) = 0 \quad \forall \ t \ge 0$$
 (2)

and an initial density distribution

$$\rho(x, y, 0) = \begin{cases} 1 & |x, y| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$
 (3)

a) Discretize equation (1) using forward Euler in time and central differences in space and write a serial code to model the time evolution of  $\rho(x, y, t)$ .

Hint: To run the code use the example parameters in Table 1.

Discretizing equation (1) using forward Euler yields

$$\frac{\rho_{i,j}^{(n+1)} - \rho_{i,j}^{(n)}}{\Delta t} = D \left( \frac{\rho_{i+1,j}^{(n)} - 2\rho_{i,j}^{(n)} + \rho_{i-1,j}^{(n)}}{\Delta x^2} + \frac{\rho_{i,j+1}^{(n)} - 2\rho_{i,j}^{(n)} + \rho_{i,j-1}^{(n)}}{\Delta y^2} \right), \tag{4}$$

where n is the index of the time slice  $t = n \cdot \Delta t$  and i, j are the indices of the discretized spatial points  $x_i = i \cdot \Delta x$ ,  $y_i = j \cdot \Delta y$ .

Serial code: diffusion2d\_serial.cpp

b) Parallelize your code using manual C++ threads. Check that the parallel code produces the same result as the serial code and report your timings for n = 1, 6, 12 threads.

Hint: To run the code use the example parameters in Table 1.

A straightforward way to parallelize equation (4) on shared memory is to split the real-space domain into chunks and distribute them between different threads. For an out-of-place time step we store two copies of the density  $\rho$  and exchange their content after the synchronization point.

Parallel code: diffusion2d\_threaded.cpp

Table 1: Example parameters.

|       | D | Ω                | $\Delta t$ |
|-------|---|------------------|------------|
| Set 1 | 1 | $128\times128$   | 0.00001    |
| Set 2 | 1 | $256\times256$   | 0.000001   |
| Set 3 | 1 | $1024\times1024$ | 0.00000001 |

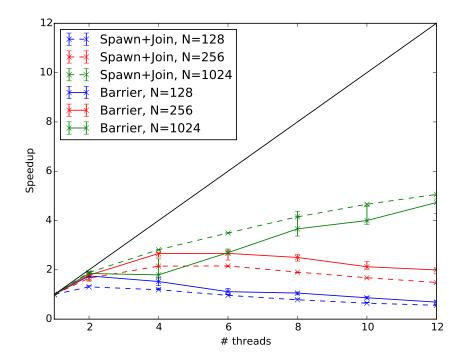


Figure 1: Strong scaling. Measured for 10'000 time-steps. Compiled with GCC.

c) Make a 2D density plot of  $\rho(x, y, t)$  at t = 0, 0.5, 1, 2.

The real-space Laplacian in equation (1) pushes the cloud away from the center and smoothens the edges of the initial density at t=0 fig. 2.

### Question 2: Barrier - Synchronization with threading

A barrier is a synchronization point between multiple execution units. In this exercise want to implement a barrier class using C++11 manual threading which fulfills the following syntax.

```
barrier b(nthreads);
// ... spawn 'nthreads' threads ...
// inside each thread:
b.wait()
```

The b.wait() statement returns only when all nthreads called that function.

a) Implement the barrier class and provide a small test for it.

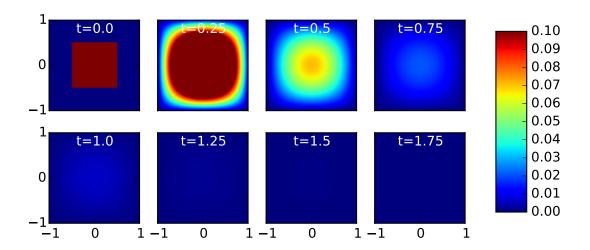


Figure 2: Density for a grid  $256 \times 256$ .

Code available in barrier.hpp, test program barrier\_test.cpp.

In the test we synchronize 500 times all threads and we repeat the check for all possible number of threads on our system.

b) Use the barrier in the diffusion code of Question 1 such that threads are kept alive and do not respawn on each iteration. Compare the timings with your previous implementation.

In Figure 1 we plot the timings of both versions. For small grids N=128 and N=256 we notice that the barrier shows a slightly better scaling, whereas for larger grid the two codes are similar.

The overhead of continuously spawning and joining threads is noticeable only on the small grids, where the parallel computation is much shorter.

Code: diffusion2d\_barrier.cpp.

## Summary

Summarize your answers, results and plots into a PDF document. Furthermore, elucidate the main structure of the code and report possible code details that are relevant in terms of accuracy or performance. Send the PDF document and source code to your assigned teaching assistant.