ETH zürich

High Performance Computing for Science and Engineering I

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Set 3 - Diffusion and OpenMP

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Question 1: Diffusion in 2D

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

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

where $\rho(\boldsymbol{r},t)$ is a measure for the amount of heat at position $\boldsymbol{r}$ and time t and the diffusion coefficient D is constant.

Lets define the domain Ω in two dimensions as $\{x,y\} \in [-1,1]^2$. Equation 1 then becomes

$$\frac{\partial \rho(x,y,t)}{\partial t} = D\left(\frac{\partial^2 \rho(x,y,t)}{\partial x^2} + \frac{\partial^2 \rho(x,y,t)}{\partial y^2}\right). \tag{2}$$

Equation 2 is discretized with a central finite difference scheme in space and explicit Euler in time:

$$\frac{\rho_{i,j}^{n+1} - \rho_{i,j}^{n}}{\delta t} = D\left(\frac{\rho_{i-1,j}^{n} - 2\rho_{i,j}^{n} + \rho_{i+1,j}^{n}}{\delta x^2} + \frac{\rho_{i,j-1}^{n} - 2\rho_{i,j}^{n} + \rho_{i,j-1}^{n}}{\delta y^2}\right) \tag{3}$$

where $\rho_{i,j}^n = \rho(-1+i\delta x, -1+j\delta y, n\delta t)$ and $\delta x = \frac{2}{N}$, $\delta y = \frac{2}{M}$ for a domain discretized with $N \times M$ gridpoints.

We will use Dirichlet boundary conditions

$$\rho(-1,y,t) = \rho(x,-1,t) = \rho(1,y,t) = \rho(x,1,t) = 0 \quad \forall\, t \geq 0 \tag{4}$$

and an initial heat distribution

$$\rho(x,y,0) = \begin{cases} 1 & |x,y| < 1/2 \\ 0 & \text{otherwise} \end{cases}. \tag{5}$$

a) Analyze the stability of the scheme given in Equation 3 using the von Neumann stability analysis.

   To analyze the stability of the method, we substitute in Equation 3 the assumption made in the von Neumann stability analysis about the solution,

$$\rho_{r,s}^{(n)} = \zeta^n e^{i(k_x x_r + k_y y_s)} = \zeta^n e^{ik_x x_r} e^{ik_y y_s}, \tag{6}$$

so that we obtain the following:

$$\begin{aligned}\zeta^{n+1}e^{ik_x x_r}e^{ik_y y_s} = \zeta^n e^{ik_x x_r}e^{ik_y y_s} &+ \zeta^n \delta t D\frac{e^{ik_x x_{r-1}}e^{ik_y y_s} - 2e^{ik_x x_r}e^{ik_y y_s} + e^{ik_x x_{r+1}}e^{ik_y y_s}}{\delta x^2}\\ &+ \zeta^n \delta t D\frac{e^{ik_x x_r}e^{ik_y y_{s-1}} - 2e^{ik_x x_r}e^{ik_y y_s} + e^{ik_x x_r}e^{ik_y y_{s+1}}}{\delta y^2}.\end{aligned}$$

Note that in this case ρ is used to indicate the heat and thus we use ζ for the amplitude term in the assumption. We also changed the index notation from $\{i, j\}$ to $\{r, s\}$ to avoid any confusion with the imaginary unit i.

For stability we require

$$|\zeta| \leq 1 \tag{7}$$

otherwise the solution will grow and diverge.

Taking the above equation and substituting $x_{r\pm1} = x_r \pm \delta x$ and $y_{s\pm1} = y_s \pm \delta y$ and dividing the whole by $\zeta^n e^{ik_x x_r}e^{ik_y y_s}$ we get:

$$\zeta = 1 - D\delta t\left(\frac{e^{ik_x\delta x} - 2 + e^{-ik_x\delta x}}{\delta x^2} + \frac{e^{ik_y\delta y} - 2 + e^{-ik_y\delta y}}{\delta y^2}\right). \tag{8}$$

Using the trigonometric properties $\frac{e^{i\theta}+e^{-i\theta}}{2} = \cos\theta$ first and $\frac{1-\cos\theta}{2} = \sin\frac{\theta}{2}$ we get

$$\begin{aligned}\zeta &= 1 - \frac{D\delta t}{\delta x^2}\left((2\cos(k_x\delta x) - 2\right) + \frac{D\delta t}{\delta y^2}\left(2\cos(k_y\delta y) - 2\right) &(9)\\ &= 1 + 4\frac{D\delta t}{\delta x^2}\sin^2\left(\frac{k_x\delta x}{2}\right) + 4\frac{D\delta t}{\delta y^2}\sin^2\left(\frac{k_y\delta y}{2}\right), &(10)\end{aligned}$$

which together with Equation 7 and the worst case scenario for the trigonometric functions $(\sin(k_y\delta y/2) = \pm 1)$ leads to the stability condition

$$4\frac{D\delta t}{\delta x^2} + 4\frac{D\delta t}{\delta y^2} \leq 2\,. \tag{11}$$

The time step should therefore satisfy

$$\delta t \leq \frac{1}{2D}\frac{\delta x^2\delta y^2}{(\delta x^2 + \delta y^2)}\,. \tag{12}$$

For equal spacing in x and y direction $\delta x = \delta y$ this simplifies to

$$\delta t \leq \frac{\delta x^2}{4D}\,. \tag{13}$$

b) Parallelize your code from Exercise 1a using OpenMP and make both strong and weak scaling plots up to 24 cores. Define the problem size as the number of grid points in the discretization of Ω. Try different problem sizes for the scaling plots, do they affect the scaling? Try using both the gcc OpenMP and the Intel OpenMP libraries. Can you see a difference?

To parallelize our code with OpenMP, we add a `#pragma omp parallel for collapse(2)` in front of the main loop in space in the method `advance()`:

```
value_type advance()
{
    // Dirichlet boundaries
    // central differences in space, forward Euler in time
#pragma omp parallel for collapse(2)
    for(size_type i = 0; i < N_; ++i) {
        for(size_type j = 0; j < N_; ++j) {
            rho_tmp[i*N_ + j] = rho_[i*N_ + j] +
            fac_
            *
            (
             (j == N_-1 ? 0. : rho_[i*N_ + (j+1)])
             +
             (j == 0    ? 0. : rho_[i*N_ + (j-1)])
             +
             (i == N_-1 ? 0. : rho_[(i+1)*N_ + j])
             +
             (i == 0    ? 0. : rho_[(i-1)*N_ + j])
             -
             4.*rho_[i*N_ + j]
             );
        }
    }
```

In the same manner we parallelize the loop that sets the initial conditions. Note that this is needed on Non-Uniform Memory Architecture (NUMA) nodes such as Euler's[1], where the access time to a NUMA node from another is different than the access time within the same NUMA node. Parallelizing the data initialization as mentioned above, is a simple — but quite effective — way to make the code "NUMA-aware": each thread creates the data it will work on in its own physical memory so that we reduce the need for threads to fetch data that others have. The principle of initializing the data owned by the thread is called "first-touch" policy.

Additionally, on Euler, to get good and stable performance using all 24 cores of a node we have to set the environment variable `OMP_PROC_BIND` so that each thread is mapped on a single core.

Figures 1 and 2 show the strong scaling obtained with the parallelized code for two different problem sizes. In all cases, we ran the code with and without setting `OMP_PROC_BIND` with Intel icpc and g++ and the `-O3` optimization flag. The results shown are averaged over 10 samples of 10000 time steps each. We observe how g++ is strongly influenced by the environment variable when using 24 threads, whereas icpc is much less affected. In general however, if we use a smaller number of threads this setting has a negative impact on the overall performance of the code and the effect is much stronger on codes compiled with icpc.

From the plots we can also see the effect of problem size on scaling: larger problem sizes tend to scale much better than smaller ones. This is a common behavior and is explained

[1]The 24 core Euler nodes have 2 NUMA nodes.

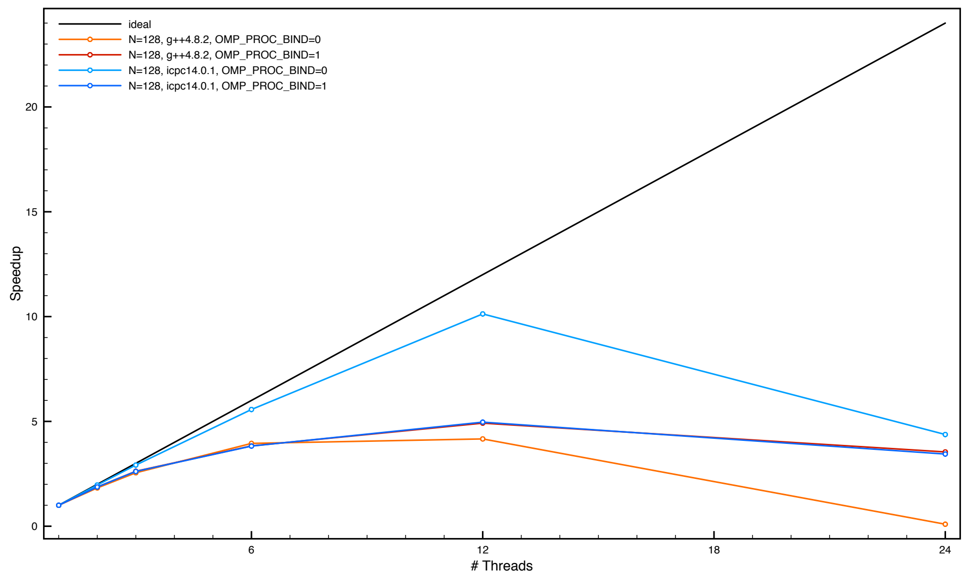


Figure 1: Strong scaling measured by averaging 10 samples of 10000 time steps for a problem size of N=128.

by the amount of work that each thread has to perform: for smaller problem sizes, the workload is also small and overheads tend to dominate as well as possible loads imbalances. This suggests that for a given problem size, we might not want to just use all the computing resources we have at our disposal as we would just waste them.

The plots show how not only the code has an impact on the performance but the compiler, the knowledge of the hardware and the problem size as well.

In the case of the larger problem, we obtained a speedup of 17.85x over 24 threads and we can obtain an almost perfect speedup for up to 12 threads. A factor that has an important influence on these results is the amount of memory bandwidth available, as an increase of the number of threads corresponds to a linear increase in computational performance but not in memory bandwidth. We will later see how memory bandwidth is a constraint that is more important than computational capacity in many scientific applications.

In the weak scaling plot (Figure 3 we can observe a similar behavior as for the strong scaling with respect to the `OMP_PROC_BIND`. Using all cores in the compute node drops the efficiency dramatically and only by setting `OMP_PROC_BIND` we get much better results. We observe that with the Intel compiler we get constantly better results and even with 24 threads we keep the efficiency around 85%.

Parallel code: `diffusion2d_openmp.cpp`

The total amount of heat in the system $N(t)$ and the second moment of the cloud $\mu^2(t)$ at a time t can be computed as

$$N(t) = \int_\Omega dx\, dy\, \rho(x, y, t), \qquad \mu^2(t) = \int_\Omega dx\, dy\, \rho(x, y, t)(x^2 + y^2). \tag{14}$$

c) Make a plot of the time evolution of $N(t)$ and $\mu^2(t)$ for $D = 1, 2, 5$ and $t \in [0, 10]$. What is the effect of the boundary? What is the effect of D?

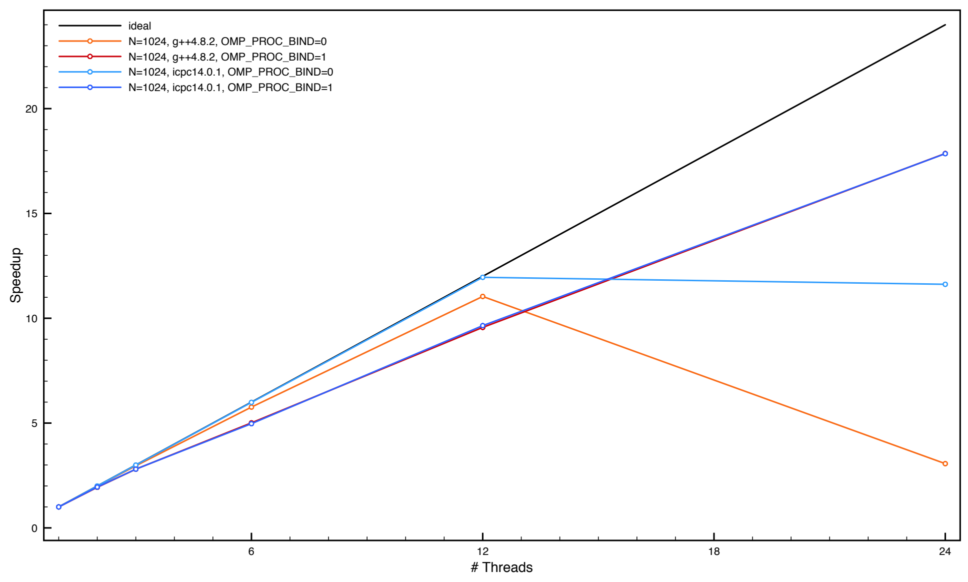


Figure 2: Strong scaling measured by averaging 10 samples of 10000 time steps for a problem size of N=1024.

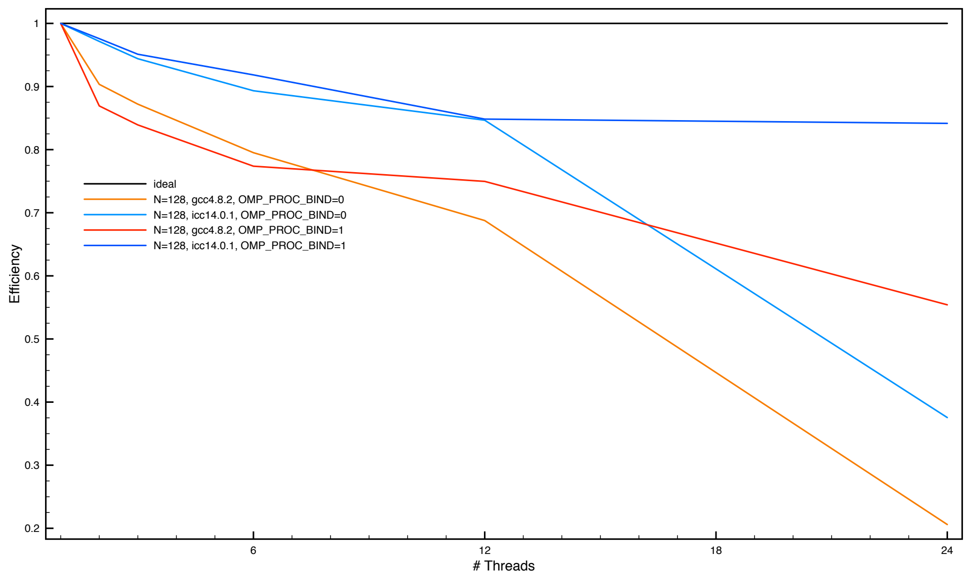
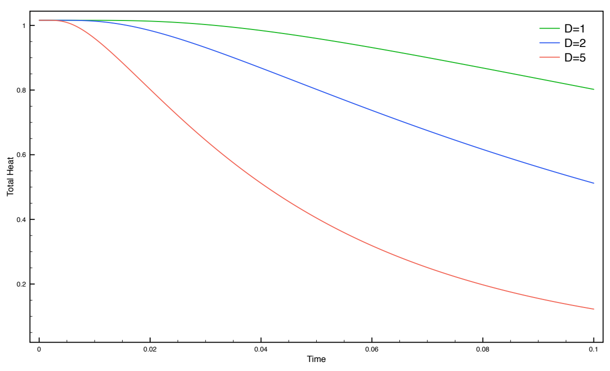
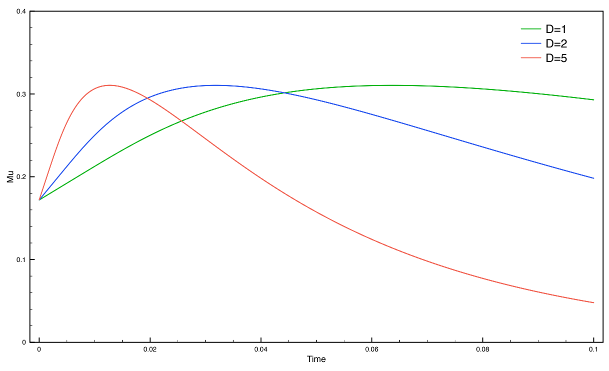


Figure 3: Weak scaling. Measured for 100 time-steps. Compiled with gcc



(a) Total heat



(b) $\mu^2(t)$

Figure 4: Total heat $N(t)$ and second moment $\mu^2(t)$. Domain size $\Omega = 128 \times 128$

Figure 4a shows that after a certain amount of time, the system starts losing heat, depending on D. This is caused by the Dirichlet boundary condition that absorbs the "heat" that reaches the boundary and thus removes it from the system. As heat diffuses away from the initial position the second moment μ^2, which measures the spread of the cloud, increases and reaches a maximum when a significant amount of heat has escaped from the system (see Figure 4b).

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.