

OPTIMIZATION AND PARALLELIZATION OF DIFFUSION SOLVERS USING ALTERNATING DIRECTION IMPLICIT AND RANDOM WALK METHODS

Samuel Maloney

Department of Mathematics
ETH Zürich
Zürich, Switzerland

ABSTRACT

Optimized and parallelized code for numerical simulation of the diffusion equation is presented. Two different algorithms, Alternating Direction Implicit (ADI) and Random Walk (RW) are studied. The algorithms are implemented in C++ and verified against an analytic solution, and then scalar optimizations, AVX vectorization, and OpenMP parallelization are carried out. Benchmarking tests are conducted on the Piz Daint cluster to determine single-core performance and runtime improvements, as well as strong and weak scaling characteristics on multiple cores of a single node. Approximate performance gain of 5X for ADI, and runtime speedups of approximately 6X and 3000X for ADI and RW respectively are observed, along with acceptable OpenMP scaling.

1. BACKGROUND

Motivation. Diffusion is the process by which a quantity of interest spreads from regions of high density to regions of low density and are integral in the study of fluids. Diffusion terms arise in all numerical models of computational fluid dynamics, which are used for such problems as aerodynamic design, turbine flows, chemical reaction mixing, and many others. Efficient and accurate simulation codes for diffusion are thus of great importance in many fields.

In this study, two different algorithms to simulate the diffusion process, Alternating Direction Implicit (ADI) and Random Walk (RW), were implemented, optimized, and parallelized. The mathematical formulations for diffusion in general and for each of these two methods specifically are presented next.

Mathematical Formulation. The process of diffusion is driven by it's concentration gradient according to the diffusion equation:

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = D \Delta \rho(\mathbf{r}, t) \quad (1)$$

where $\rho(\mathbf{r}, t)$, with position \mathbf{r} at time t , is the quantity of interest and D is the diffusion constant and is a given value for

the system. For this study, homogeneous Dirichlet boundary conditions are used at all boundaries. The initial density distribution used for this study is:

$$\rho(x, y, 0) = \sin(\pi x) \sin(\pi y) \quad (2)$$

and it's corresponding analytic solution, which was used for verification, is:

$$\rho(x, y, t) = \sin(\pi x) \sin(\pi y) e^{-2D\pi^2 t} \quad (3)$$

The studied simulation domain is a unit square with x and y each ranging from 0 to 1, which is discretized using a uniform grid such that $\delta h = \delta x = \delta y$. A superscript n is used to denote the timestep $t_n = n\delta t$ and subscripts i and j to denote the indices of the nodes in the mesh $x_i = i\delta x$ and $y_j = j\delta y$ such that $\rho_{i,j}^n = \rho(x_i, y_j, t_n)$.

Alternating Direction Implicit. The ADI method is an operator splitting scheme based on finite difference discretizations of the derivatives. It works by splitting the each time step into two half time steps, in the first of which the time integration is carried out implicitly in the x -direction and explicitly in the y -direction, and in the second half time step the directions are switched such that the integration in the x -direction is explicit and in the y -direction is implicit.

Using a second order centered approximation for the spatial derivative in Eq. (1) means that each implicit integration step requires only the solution of a tridiagonal linear system, for which the Thomas Algorithm (for formulae see [1]) can be used to efficiently compute the result. These tridiagonal systems can be found by considering the discretization equations:

$$\rho_{i,j}^{n+\frac{1}{2}} = \rho_{i,j}^n + \frac{D\delta t}{d\delta x^2} (\rho_{i-1,j}^{n+\frac{1}{2}} - 2\rho_{i,j}^{n+\frac{1}{2}} + \rho_{i+1,j}^{n+\frac{1}{2}}) \quad (4)$$

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n+\frac{1}{2}} + \frac{D\delta t}{d\delta x^2} (\rho_{i,j-1}^{n+\frac{1}{2}} - 2\rho_{i,j}^{n+\frac{1}{2}} + \rho_{i,j+1}^{n+\frac{1}{2}}) \quad (5)$$

These can be rewritten in the form $\mathbf{A}\rho^* = \rho^{*-\frac{1}{2}}$ where \mathbf{A} is the tridiagonal matrix to be solved at each half timestep.

Random Walk. Diffusion can also be simulated by tracking the random motion of a set of M identical particles with no inertia. A probability $\lambda = D\delta t/\delta x^2$ is defined, such that at each time step, each particle has a $1 - 4\lambda$ probability of remaining in the same position. If it does not stay, it is then moved to one of the 4 neighbouring nodes, with an equal probability of moving in any direction. Clearly, one requires $\lambda < 1/2$ to maintain a positive probability of staying.

The initial condition for the number of particles at each grid point $m_{i,j}$ is given as:

$$m_{i,j}^0 = \left\lfloor \frac{M\rho(x_i, y_j, 0)}{\iint_{\Omega} \rho(x, y, 0) dx dy} \right\rfloor \quad (6)$$

And the approximate solution after a given timestep can then be calculated as:

$$\rho_{i,j}^n = \frac{m_{i,j}^n}{M} \iint_{\Omega} \rho(x, y, 0) dx dy \quad (7)$$

2. BASELINE IMPLEMENTATION

In this section, the basic implementation and verification of the described algorithms is presented. All code is based on the Diffusion2D class structure of the solution code provided with the course exercises. All code for each version of the class is contained within a single .cpp source file, and includes user defined header files *timer.hpp* and *tsc_x86.hpp* for measuring runtime in seconds and cycles respectively. The *timer.hpp* file is from the HPCSE I course exercises, and the *tsc_x86.hpp* file is from the exercises of the How to Write Fast Numerical Code course exercises.

The programs take arguments to set the diffusion constant D , size N of one dimension of the grid, timestep δt , number of repetitions n_{runs} to run the simulation, and the number of timesteps n_{steps} to run each simulation for. The RW codes also take a value for the number of particles M in the simulation. For all codes the values for n_{runs} and n_{steps} are optional, and default to $n_{runs} = 1$ and $n_{steps} = 0.1/\delta t$ respectively. The ordering of these input arguments can be displayed by running the program with no arguments.

For each simulation run, a new Diffusion2D class object is initialized, with one-time initialization routines happening outside of the timing structures. Once initialization is complete, the simulation is run to completion by a single call to the `run_simulation` function, and this call is the only part of the program which is timed and contains all code which will be optimized.

ADI. An order verification study (OVS) of the ADI code in both spatial and temporal dimensions was performed by comparing the simulation results to the analytic solution in Eq. (3). The results can be seen in Fig. 1 and show the implementation to be second order accurate in both space and time, as expected for this discretization scheme.

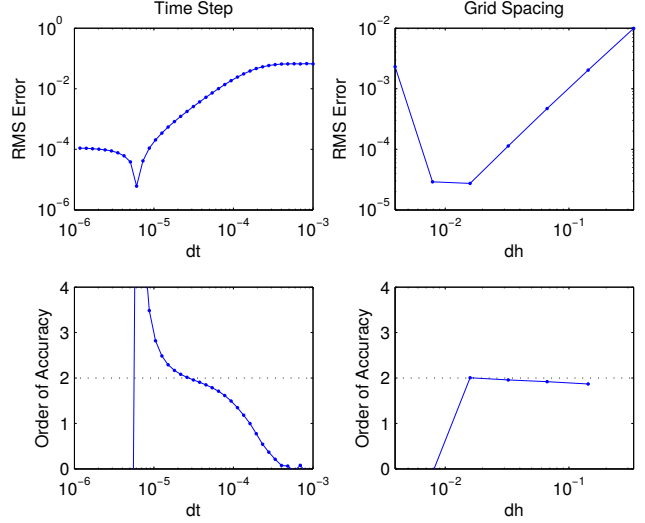


Fig. 1. Order Verification study of the ADI code.

The ADI algorithm complexity should be $O(N^2)$ as it does a constant number of operations for updating value at each point in the grid. Its runtime scaling (see 4.1, Fig. 6) is also found to agree with this expected complexity.

For performance analysis, the cost of the ADI code is defined as the number of floating point operations (FLOPs) including additions, multiplications, and, for the baseline implementation only, divisions. Moreover, the data movement in bytes between various levels of cache was measured using the Hardware Performance Counter (HWPC) functionality in CrayPat to quantify the operational intensity.

The results of a roofline analysis are shown in Fig. ?? for the baseline code. Three data series are presented, which use the same performance data but compute the operational intensity with respect to different levels of the cache hierarchy. The implementation appears compute bound with respect to memory transfers with RAM, but for large N it becomes clearly memory bound at higher levels of the cache, albeit with still significant room to improve towards the memory bandwidth rooflines. Maximum performance of 0.734 FLOPs/cycle, or 18% of peak scalar performance is observed. On the test machine, with an Intel Haswell central processing unit (CPU), the peak performance is calculated by considering the maximum throughput of 2 fused multiply add (FMA) instructions per cycle, giving 4 total FLOPs per cycle. Data for the cache bandwidths used in this (and subsequent) roofline plots was obtained from [3] and [4].

RW. Lorem Ipsum dolor sit amet.

Scaling for the RW method depends on which version is being considered. The baseline implementation should scale as $O(M)$, where M is the number of particles in the simulation. This is because a random number must be generated for each particle in the simulation to determine its

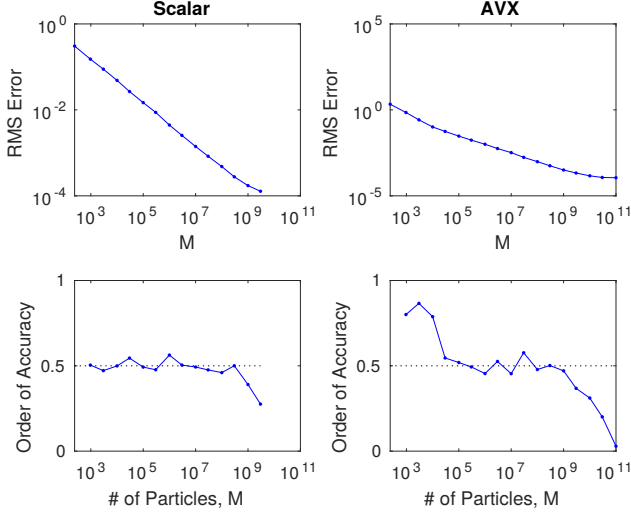


Fig. 2. Order Verification study of the RW code.

movement for a given timestep, independent of how many grid points there are in the simulation. The later versions that use a binomial random variable (see 3.2) to simulate particle movement scale as $O(N^2)$ because exactly four such random variables must be evaluated for each grid point, independent of the number of particles in the simulation.

3. OPTIMIZATION METHOD

In this section we explain the main optimizations that were undertaken. We discuss the optimizations of the ADI and RW methods in separate subsections.

3.1. ADI

We divide the optimizations in 4 sets called *revisions*.

Scalar. This revision consists mainly of

AVX. In this revision we used

OpenMP. This revision was targeted at

3.2. RW

The RW optimizations can be similarly broken down into revisions, similarly to those for the assembly.

Scalar. This is a direct implementation

AVX. Vectorization of the code was done by leveraging Intel fused-multiply-add (FMA) and advanced vector extension (AVX) intrinsics.

OpenMP. stuff...

4. OPTIMIZATION RESULTS

In this section the results of numerical benchmarks of the code at various stages are presented. Runtime, performance,

and roofline analyses were performed where applicable.

Experimental setup. All data was collected using a single XC50 node of Piz Daint, which has a 12 core Intel Xeon E5-2690 v3 running at 2.6 GHz [2]. Each physical processor core has a 64 KB L1 cache split equally into two 32 KB data and instruction caches, and a 256 KB unified L2 cache [5]. The 30 MB L3 cache is shared between all cores [6], and there is 24.9 GB/s bandwidth to main memory [3]. The Intel C++ Compiler v17.0.1 was used with `"-O3 -std=c++11 -DNDEBUG -march=core-avx2 -fno-alias -qopenmp -mkl"` flags. The Intel time stamp counter (TSC) was used for runtime measurements and CrayPat was used for cache miss measurements.

The inputs are the number of grid points in domain discretization, the timestep between iterations, and the number of timesteps computed. We used grids of various sizes, up to $N \times N = 7680 \times 7680$. The diffusion constant $D = 1$ is used for all simulations, and for RW simulations $M = 1000N^2$ particles were used. For ADI, 1000 iterations were performed, and for RW 50 iterations were performed to achieve a reasonable runtime for measurements. Each simulation was repeated 10 times, with the minimum cycle count used for the runtime and the average cache misses used for the memory transfer (the average is used only because it would have prohibitively time-consuming to measure minimum values with CrayPat).

All experiments were performed with warm cache. This is largely to simulate real world usage scenarios, where the simulation would most likely be performed immediately after initialization while the data is still potentially in cache, exactly as in these experiments. It is noted, however, that the initial cache state should have little effect on the results in either case, as the effects will be amortized over the number of iterations performed, and should become negligible for the relatively large number of iterations used.

4.1. ADI

Roofline, runtime, and scaling experiments were conducted on the ADI code.

Results. The runtime plots of various revisions of the ADI code (see 3.1) are shown in Fig. ???. Each consecutive revision of the code resulted in a speedup.

4.2. RW

Benchmarking experiments were conducted on the RW code

Results. Results of the roofline, performance, and runtime analyses of the RW code will now be presented.

5. CONCLUSION

Conclude things

ADI Roofline, All Versions

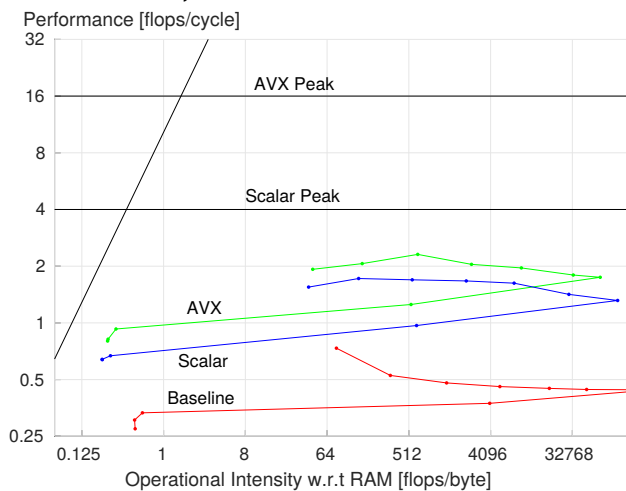


Fig. 3. Roofline analysis of the ADI code.

ADI Roofline, Scalar

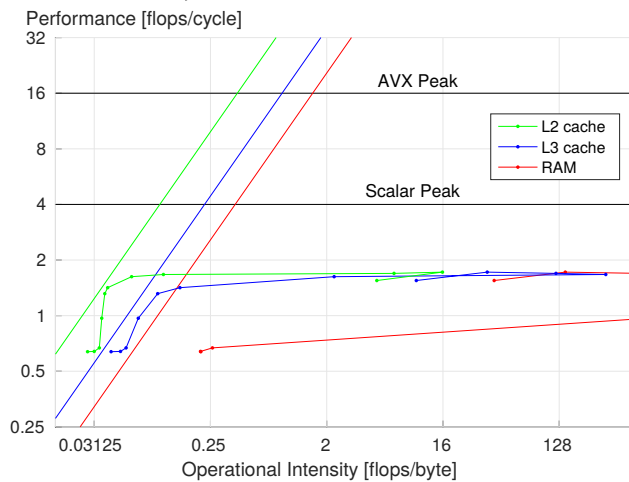


Fig. 5. Roofline analysis of the ADI scalar code.

ADI Roofline, AVX

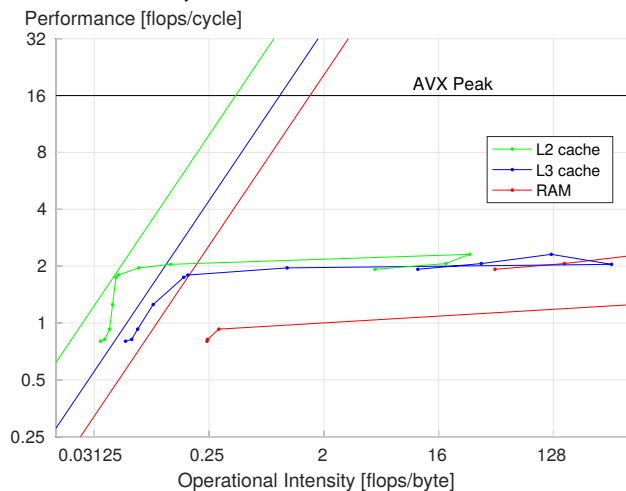


Fig. 4. Roofline analysis of the ADI AVX code.

ADI on Single Core

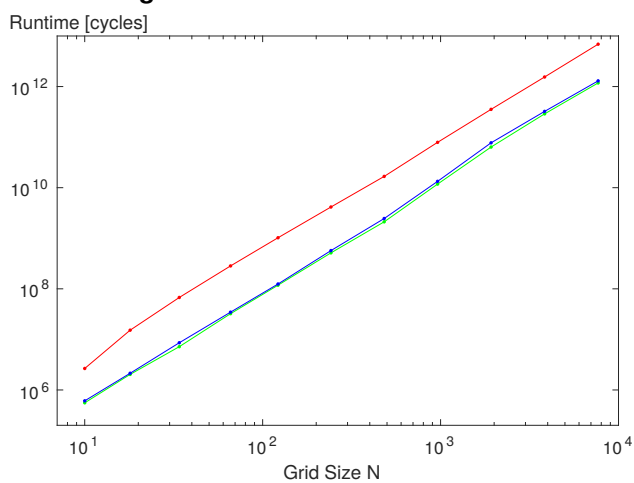


Fig. 6. Runtime analysis of the ADI code.

ADI Strong Scaling, N = 7680

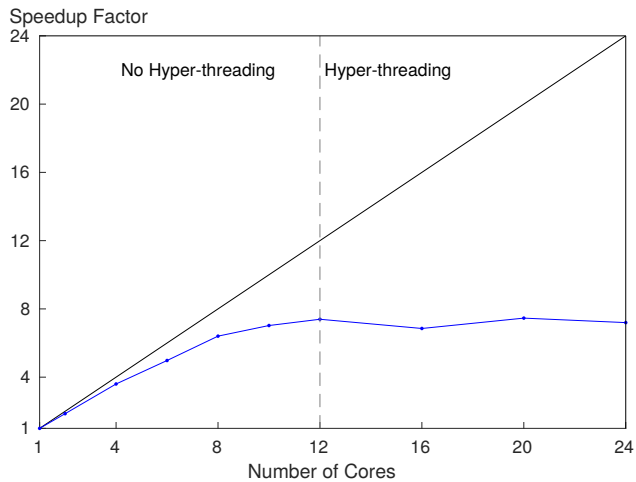


Fig. 7. Strong Scaling analysis of the ADI OpenMP code.

RW on Single Core

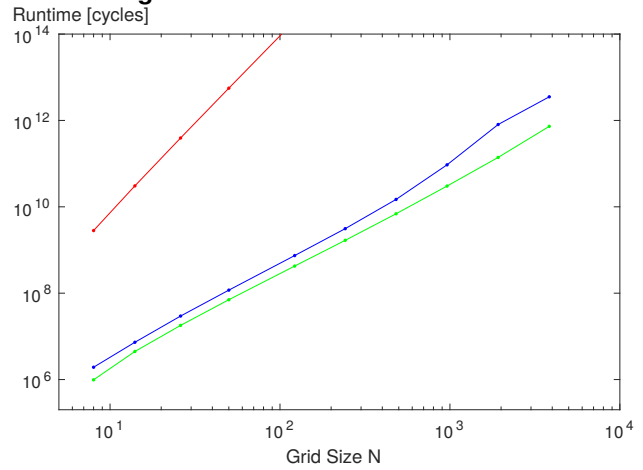


Fig. 9. Runtime analysis of the RW code.

ADI Weak Scaling, N = 7680

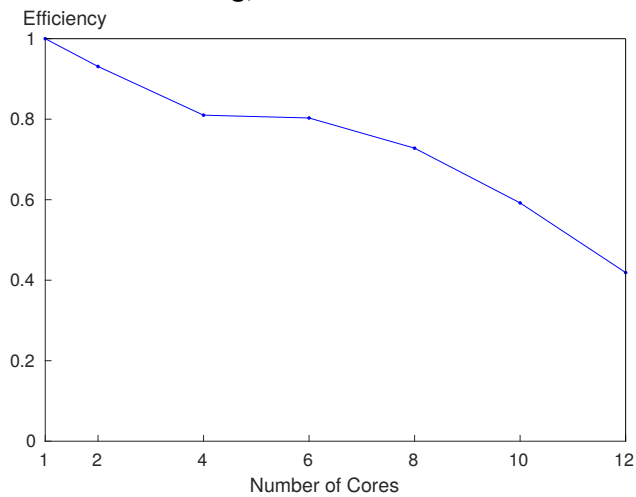


Fig. 8. Weak Scaling analysis of the ADI OpenMP code.

RW Strong Scaling, N = 7682

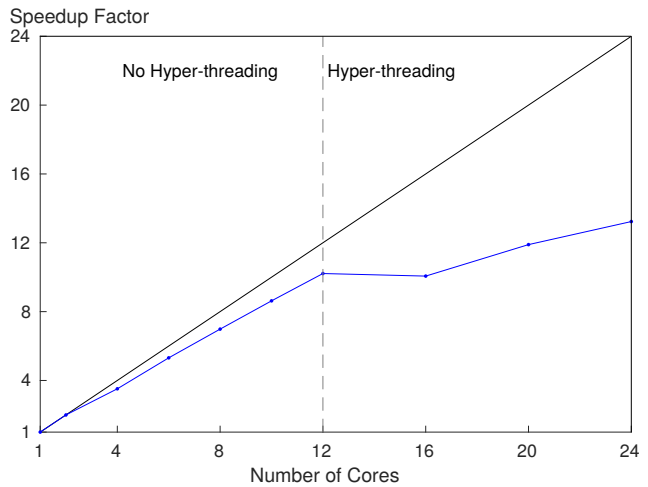


Fig. 10. Strong Scaling analysis of the RW OpenMP code.

RW Weak Scaling, N = 7682

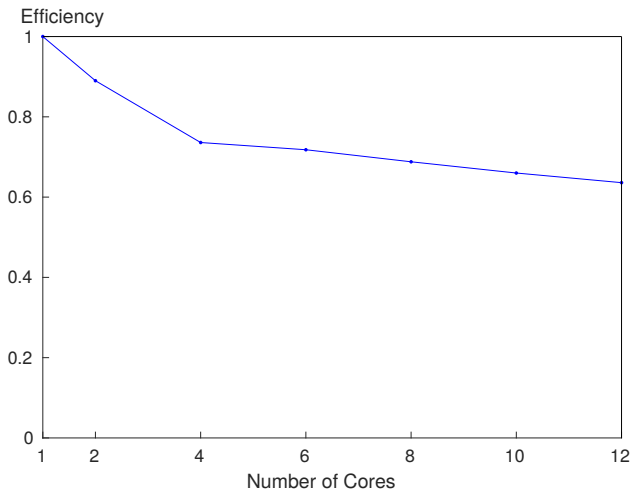


Fig. 11. Weak Scaling analysis of the RW OpenMP code.

6. REFERENCES

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