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Parallel numerical simulations of anisotropic and heterogeneous diffusion equations with GPGPU

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Abstract

The aim of this work is to show how the anisotropic and heterogeneous diffusion equations can be solved numerically through the GPU technologies obtaining a speed-up improvement. Particularly, we want provide a decision-making tool to choose the appropriate binomial algorithm-GPU memory region to get the best performance in terms of computational efficiency and reduction of calculation times. The numerical simulations have been performed using finite differences method for space discretization and Euler method for time discretization, the numerical schemes have been implemented using the NVIDIA CUDA GPU.

Heterogeneous and Anisotropic Diffusion Equations

Anisotropic diffusion equations have various fields of application, ranging from image processing and computer vision [1], [2] to tumor modeling [3]. Beside typical regularizing effects, the most important feature of such models is that different diffusion rates could produce strikingly nontrivial patterns. Therefore, the numerical solution often requires very long computational time, for the large amount of data to be traded in order to accurately capture the details of a physical phenomenon. Moreover, especially for clinical operators and applied scientists involved in setting up realistic experiments, the possibility of running fast comparative simulations using simple algorithms implemented into affordable processors is of a primary interest. In this context, parallel computing based on modern graphics processing units (GPUs) enjoys the advantages of a high performance system with relatively low cost, allowing for software development on general-purpose microprocessors even in personal computers. As a matter of fact, GPUs are revolutionizing scientific simulation by providing two or more orders of magnitude of increased computing capability inside a mass-market product, making these facilities economically attractive across subsets of industry domains.

Model and Numerical Methods

All models above can be rewritten as the following Cauchy-Dirichlet problem for anisotropic and heterogeneous diffusion equations. For the sake of simplicity we consider, 2D models defined as follow:

$$\begin{cases} \frac{\partial I}{\partial t} = \nabla \cdot (A \cdot \nabla I) \\ I(x, y, 0) = I_0 \\ I|_{\partial\Omega} = K \end{cases} \quad (1)$$

where $I = I(x, y, t)$, I_0 is the initial condition and $I|_{\partial\Omega} = K$ is the boundary condition over the frontier of the computational domain.

We consider the general case of anisotropic and heterogeneous diffusion with the matrix

$$A = \begin{bmatrix} a(x, y) & b(x, y) \\ b(x, y) & c(x, y) \end{bmatrix} \quad (2)$$

which is symmetric and the diffusion coefficients are constant in time, but spatially varying. Using the diffusion equation in (1) we can write

$$\frac{\partial I}{\partial t} = a \frac{\partial^2 I}{\partial x^2} + c \frac{\partial^2 I}{\partial y^2} + 2b \frac{\partial^2 I}{\partial x \partial y} \quad (3)$$

$$\frac{\partial I}{\partial x} \frac{\partial a}{\partial x} + \frac{\partial I}{\partial x} \frac{\partial b}{\partial x} + \frac{\partial I}{\partial y} \frac{\partial b}{\partial x} + \frac{\partial I}{\partial y} \frac{\partial c}{\partial y}$$

where the diffusion rates $a(x, y), b(x, y), c(x, y)$ are not constants.

Under fairly weak regularity assumptions on the rate functions in the diffusion matrix, the well-posedness of the Cauchy-Dirichlet problem and the continuous dependence on the initial data (ensuring stability with respect to perturbations typically originated in experimental measurements) proceed from the general theory of parabolic differential systems [4] (see also [5] for nonlinear problems). We remark that the procedures employed in this work are certainly adaptable to the case of nonlinear time-dependent diffusion equations [2], [5], but that framework will be explicitly discussed in a future work.

For numerical simulations we consider a 2D square domain with dimensions X_{dim} and Y_{dim} with spatial discretization constants $\Delta x = \frac{X_{dim}}{x_{grid}}$ and $\Delta y = \frac{Y_{dim}}{y_{grid}}$ where x_{grid} and y_{grid} are the number of elements of the discretization grid in the x and y directions. Finally we consider time step Δt constant and time $t_n = n \Delta t$, where $n \in N$. We discretize equation (3) with forward schemes for double derivatives in directions x and y whereas we use centered-centered scheme for terms with mixed derivatives xy and yx . In this case, we obtain the numerical scheme:

$$\begin{aligned} \frac{d}{dt} I_{i,j} = & \frac{1}{\Delta x} \left(a_{i+\frac{1}{2},j} \frac{I_{i+1,j} - I_{i,j}}{\Delta x} - a_{i-\frac{1}{2},j} \frac{I_{i,j} - I_{i-1,j}}{\Delta x} \right) \\ & + \frac{1}{2\Delta x} \left(b_{i+1,j} \frac{I_{i+1,j+1} - I_{i+1,j-1}}{2\Delta y} - b_{i-1,j} \frac{I_{i-1,j+1} - I_{i-1,j-1}}{2\Delta y} \right) \\ & + \frac{1}{2\Delta y} \left(b_{i,j+1} \frac{I_{i+1,j+1} - I_{i-1,j+1}}{2\Delta x} - b_{i,j-1} \frac{I_{i+1,j-1} - I_{i-1,j-1}}{2\Delta x} \right) \\ & + \frac{1}{\Delta y} \left(c_{i,j+\frac{1}{2}} \frac{I_{i,j+1} - I_{i,j}}{\Delta y} - c_{i,j-\frac{1}{2}} \frac{I_{i,j} - I_{i,j-1}}{\Delta y} \right) \end{aligned} \quad (4)$$

In this case, the follow stability condition holds:

$$\Delta t \leq \frac{\min(\Delta x^2, \Delta y^2)}{8 \max_{i,j} [a_{i,j}, c_{i,j}]} \quad (5)$$

Simulations and Results

For the numerical simulations we consider this function for the initial data:

$$I(x, y, 0) = \begin{cases} 150, & \text{if } (x, y) \in [0, 25] \times [0, 50] \\ 100, & \text{if } (x, y) \in [0, 80] \times [0, 100] \\ 50, & \text{elsewhere} \end{cases} \quad (6)$$

We work in a square domain $D = [0, x_{grid}] \times [0, y_{grid}]$ with x_{grid} from 128 to 2048, $x_{grid} = y_{grid}$ and grid dimensions $X_{dim} = x_{grid}$, $Y_{dim} = y_{grid}$, in this way we have $\Delta x = \Delta y = 1$. As regards to the matrix A four different areas has been considered with:

$$A = \begin{bmatrix} 0.5 & 0.025 \\ 0.025 & 0.3 \end{bmatrix} \quad (7)$$

for $0 \leq x < (\frac{x_{grid}}{2} - 1)$ and $(\frac{y_{grid}}{2} - 1) \leq y \leq (y_{grid} - 1)$;

$$A = \begin{bmatrix} 1.5 & 0.03 \\ 0.03 & 1.3 \end{bmatrix} \quad (8)$$

for $(\frac{x_{grid}}{2} - 1) \leq x < (x_{grid} - 1)$ and $(\frac{y_{grid}}{2} - 1) \leq y \leq (y_{grid} - 1)$;

$$A = \begin{bmatrix} 1.3 & 0.02 \\ 0.02 & 0.5 \end{bmatrix} \quad (9)$$

for $0 \leq x < (\frac{x_{grid}}{2} - 1)$ and $0 \leq y < (\frac{y_{grid}}{2} - 1)$;

$$A = \begin{bmatrix} 0.5 & 0.025 \\ 0.025 & 0.3 \end{bmatrix} \quad (10)$$

for $(\frac{x_{grid}}{2} - 1) \leq x < (x_{grid} - 1)$ and $0 \leq y < (\frac{y_{grid}}{2} - 1)$.

For these values of the elements on the matrix A , considering $x_{grid} = y_{grid}$ from 128 to 2048 and space step $\Delta x = \Delta y = 1$ the stability condition in (5) is satisfied for Δt equal to 0.02.

The choice of these values for matrix A has been carried out to model a stronger diffusion along a diagonal of the considered domain. These conditions can be found, for example in the tumor dynamics model in case we are performing a simulation close to an highly vascularized area and then near a tissue easily attacked by the cancer. In the next figures we report some graphs related to speed-up and efficiency obtained after 45000 iterations, with a time step Δt equal to 0.02, performing a tiling inside the GPU to get the best performance. We perform the tests using the differeny memory region inside the GPU such as Texture, Global and Shared memories and writing three different code for each memory region. We written all codes optimizing the memory usage and using NVIDIA CUDA 4.2/5.0 and C language. We report in the flowing graphs results related to the simulations performed using the three levels of memory (Texture, Global and Shared) of GPU NVIDIA CUDA for different case of analysis such as: Isotropic and Homogeneous Diffusion Equation, Isotropic and Heterogeneous Diffusion equation and finally Anisotropic and Heterogeneous Diffusion Equation. The first three graphs are related to CUDA Kernel execution time for the three different cases studies analyzed. In the last two graphs we report the results related to the study of speed-up and efficiency related to the dimensions tile used inside the CUDA code. We get the best performance for our algorithm optimizing the shared memory code with a maxium speed-up equal to 21.5 and max efficiency equal to 12% for the case of full anisotropic and heterogeneous diffusion equation. All numerical simulations were performed using an NVIDIA GTX 670 with 1344 CUDA cores and 4Gbyte of RAM installed on an HP DL585G7, AMD Opteron 6128 (2.0 GHz), 64 Gbytes of RAM, CentOS 5.5 on Rocks Cluster 5.4.3 OS, gcc compiler and NVIDIA CUDA 4.2/5.0 linux 64 bit.

Execution Time Speed Up and Efficiency

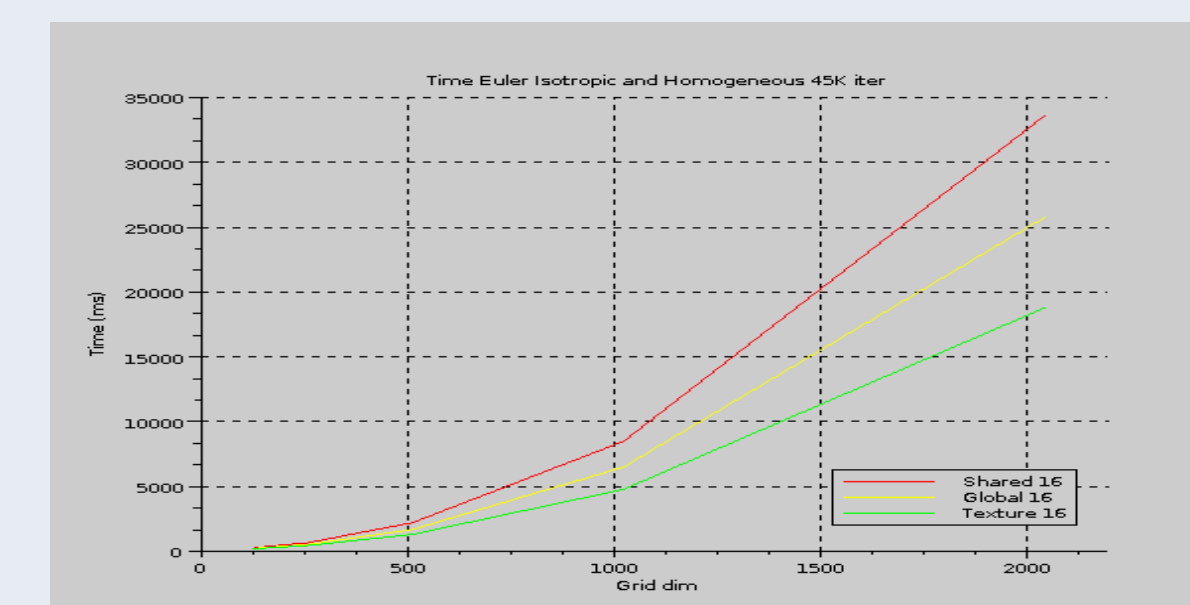
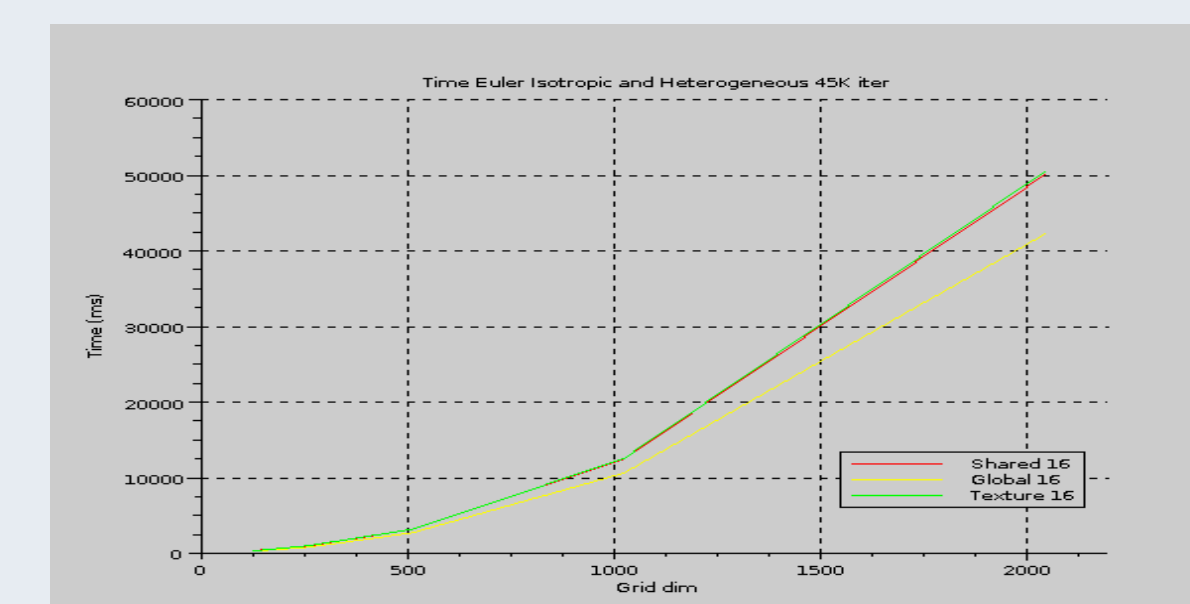
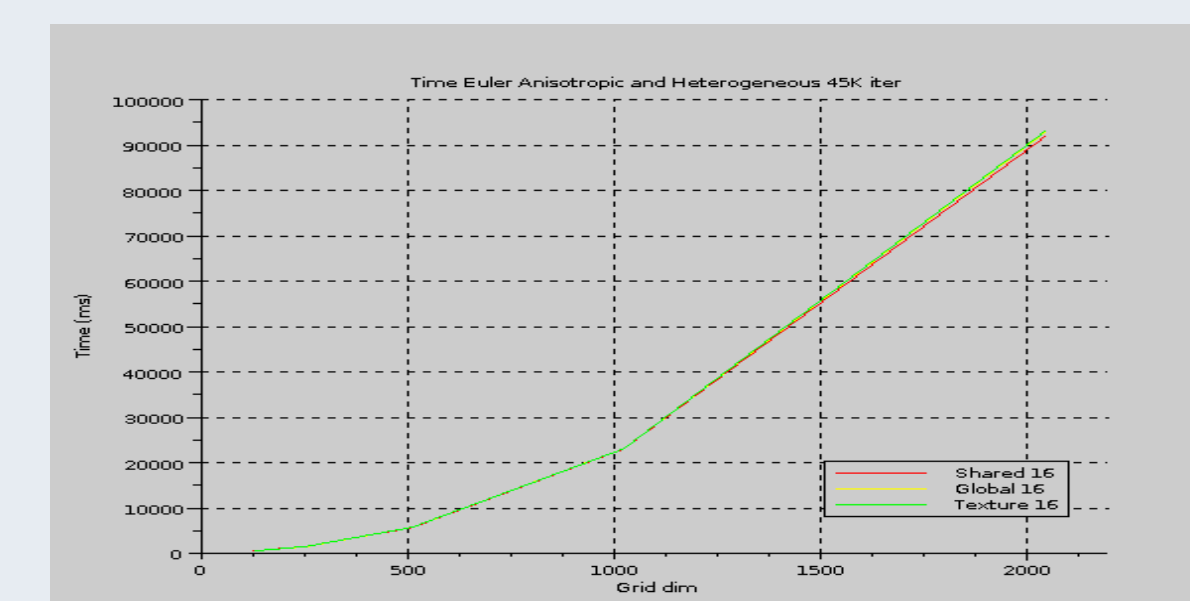


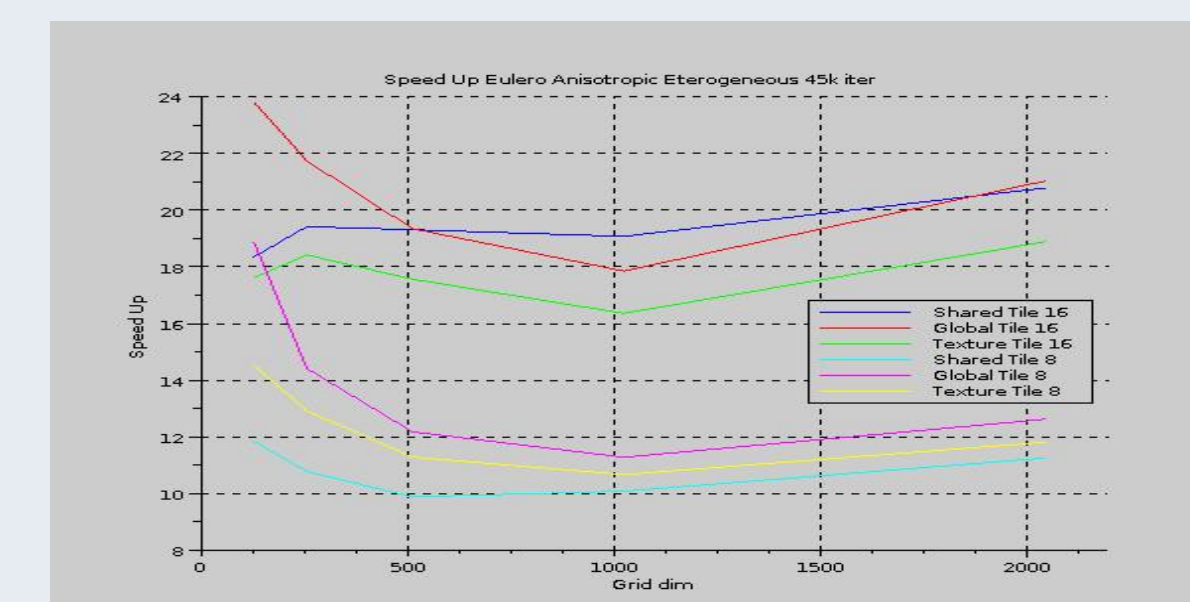
Figure: CUDA Kernel time execution Homogenous and Isotropic diffusion equation



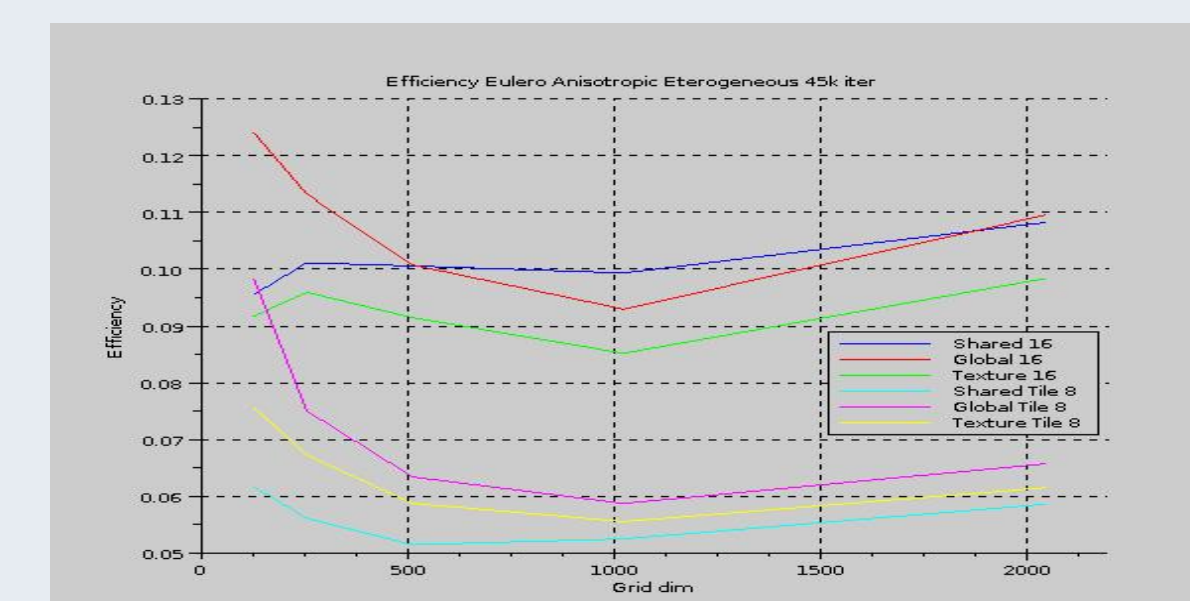
CUDA Kernel time execution Heterogenous and Isotropic diffusion equation



CUDA Kernel time execution Heterogenous and Anisotropic diffusion equation



Speed-Up for Heterogeneous and Anisotropic diffusion equation using CUDA



Efficiency for Heterogeneous and Anisotropic diffusion equation using CUDA

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