During Summer Student Program 2014 at JINR:

1. I've taken part in the tutorial on "Parallel programming technologies on hybrid architectures" 7-21 July 2014;
2. I've been involved in the project "Heterogeneous computing" at the LIT JINR;
3. I've developed parallel computational algorithm with the use of CUDA-technology for propagation of acoustic waves in homogeneous geologic media, which will be presented at the "MPAMCS 2014" conference in Dubna, 25-29 August 2014.
4. I've been testing the new heterogeneous cluster in LIT JINR by launching my parallel algorithm on it.

Numerical Modeling of 3D Seismic Problems in Homogeneous Media Using CUDA-technology

A.E. Tarkhov[1], N.I. Khokhlov[2], S.Yu. Nikitin[3]

Lomonosov Moscow State University, Department of General Physics and Wave Processes

I. Introduction

Parallel computational algorithm with the use of CUDA-technology for propagation of acoustic waves in homogeneous geologic media is being developed. Characteristic scales of 3D seismic problems are extremely large; for example, spatial scales may reach hundreds of kilometers and time scales could take from minutes to hours. The usage of graphical processors could provide large computational rate for prediction of earthquakes and tsunami in real time regime.

Correct modeling of these problems requires methods that are highly accurate in space and time. We apply grid-characteristic [1] and finite volume [9] methods to solving system of equation of solid mechanics. These methods allow using of higher order monotonic difference scheme [2, 5].

Complexity of 3D seismic problems requires parallelization of computational algorithm. Data parallelism of the problem has been taken into account during the development of the algorithm.

II. Mathematical model

Nonstationary theory of elasticity describes mathematical model of 3D seismic problem in homogeneous medium by the closed system of equations [3], using tensorial representation it can be written as:

$$\rho \frac{\partial v_i}{\partial t} = \nabla_j \sigma_{ij}, \qquad (1)$$

$$\frac{\partial \sigma_{ij}}{\partial t} = q_{ijkl} \frac{\partial \varepsilon_{kl}}{\partial t}, \qquad (2)$$

[1] Lomonosov Moscow State University, Department of General Physics and Wave Processes, Vorobievy Gory 1, Moscow, 119992, Russia, e-mail: tarkhov.andrey@gmail.com

[2] Moscow Institute of Physics and Technology, Institutskii per. 9, Dolgoprudny, Moscow Region, 141700, Russia, e-mail: k_h@inbox.ru

[3] Lomonosov Moscow State University, Department of General Physics and Wave Processes, Vorobievy Gory 1, Moscow, 119992, Russia, e-mail: sergeynikitin007@yandex.ru

where ρ – density of the medium, v_i – components of velocity vector, $\sigma_{ij}, \varepsilon_{ij}$ – components of stress and strain tensors, ∇_k – covariant derivative along k-axis. Tensor q_{ijkl} is defined by the rheology of the medium. In approximation of small deformations (isotropic linear elastic body) [3] it is given by:

$$q_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \quad (3)$$

where δ_{ij} – Kronecker's delta, λ and μ – Lame parameters.

In three dimensions we get:

$$\frac{\partial v_i}{\partial t} - \frac{1}{\rho}\nabla_j \sigma_{ij} = 0, \quad (4)$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda\delta_{ij}\frac{\partial \varepsilon_{kk}}{\partial t} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\frac{\partial \varepsilon_{kl}}{\partial t}, \quad (5)$$

$$\frac{\partial \varepsilon_{ij}}{\partial t} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}), \quad (6)$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda\delta_{ij}\frac{\partial v_k}{\partial x_k} + \mu(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}), \quad (7)$$

Using matrix notation $\mathbf{u} = (v_x, v_y, v_z, \sigma_{xx}, \sigma_{xy}, \sigma_{xz}, \sigma_{yy}, \sigma_{yz}, \sigma_{zz})^T$ we get:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A_x}\frac{\partial \mathbf{u}}{\partial x} + \mathbf{A_y}\frac{\partial \mathbf{u}}{\partial y} + \mathbf{A_z}\frac{\partial \mathbf{u}}{\partial z} = 0, \quad (8)$$

where $\mathbf{A_x}, \mathbf{A_y}, \mathbf{A_z}$ - matrices of size 9×9, their explicit expression is not written here for the sake of brevity. These matrices can be made diagonal by transformation:

$$\mathbf{A_\alpha} = \mathbf{\Omega_\alpha \Lambda_\alpha \Omega_\alpha^{-1}}, \quad (9)$$

where $\alpha = x, y, z$ spatial index, matrices $\mathbf{\Lambda_\alpha} = diag(0,0,0,-c_s,-c_s,c_s,c_s,-c_p,c_p)$ have the same value for all spatial coordinates, and notation of velocities is introduced: $c_s = \sqrt{\mu/\rho}$ – velocity of transverse waves in the medium, $c_p = \sqrt{(\lambda + 2\mu)/\rho}$ – velocity of longitudinal waves in the medium. Columns of matrices $\mathbf{\Omega_\alpha}$ are eigenvectors of matrices $\mathbf{A_\alpha}$.

After splitting by spatial coordinates we get three one dimensional systems of equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A_\alpha}\frac{\partial \mathbf{u}}{\partial x_\alpha} = 0, \text{ where } \alpha = x, y, z. \quad (10)$$

We can transform each system to the diagonal form in new variables by multiplying it by corresponding matrix $\mathbf{\Omega_\alpha}$ on the left:

$$\mathbf{w_\alpha} = \mathbf{\Omega_\alpha^{-1} u}, \quad (11)$$

$$\frac{\partial \mathbf{w_\alpha}}{\partial t} + \mathbf{\Lambda_\alpha}\frac{\partial \mathbf{w_\alpha}}{\partial x_\alpha} = 0, \quad (12)$$

where $\alpha = x, y, z$ is spatial index.

Inverse transformation to the variables $\mathbf{u}$ is made by:

$$\mathbf{u} = \mathbf{\Omega_\alpha w_\alpha}. \quad (13)$$

Diagonal form of matrices $\mathbf{\Lambda_\alpha}$ leads to the splitting of system (12) into 9 independent scalar equations.

As the result, at each step of the algorithm, problem solving scheme after splitting by statial coordinates (10) (scheme described below should be repeated three times for each spatial coordinate) consists of three steps:

1. Transition to new variables $\mathbf{w}_{\boldsymbol{\alpha}}$ (11);
2. Solving system of independent scalar equations (12) with respect to the components of the vector $\mathbf{w}_{\boldsymbol{\alpha}}$; (14)
3. Transition to previous variables $\mathbf{u}$ (13).

III. Numerical scheme

For each of these independent scalar equations of the diagonalized system (12) we apply MUSCL ("Monotonic Upstream-Centered Scheme for Conservation Laws", introduced by van Leer [4]) with flux limiters (TVD conception – "Total Variation Diminishing", introduced by Harten [5]). Monotony of this scheme allows to get rid of nonphysical oscillations of solution. It is important to get rid of such oscillations for solving 3D seismic problems, which study wave processes close to the discontinuities. Godunov's theory [6] claims that linear monotonic scheme can be at most the first-order accurate, but usage of nonlinear flux limiter, for example, SuperBee limiter [7],

$$\phi_{sb}(r) = \max[0, \min(2r, 1), \min(r, 2)], \tag{15}$$

allows to reach the second-order accuracy for spatial coordinates preserving the property of monotony [5].

To calculate values of the component of the vector $\mathbf{w}_{\boldsymbol{\alpha}}$ at the next time step after transition to the new variables (11) we use difference scheme described below. Splitting by spatial coordinates (10) leads to the need of triple realization of the scheme for each value of spatial index $\alpha = x, y, z$. For the sake of brevity, we describe scheme one time for spatial coordinate *x*, omitting spatial index. We use uniform three-dimensional rectangular grid. Denoting one of the components of the vector $w = \mathbf{w}_{\mathbf{x},l}$, where $l \in 1 \dots 9$, we write solving scheme for the system of equations (12) (Harten, [5]):

$$w_{i,j,k}^{n+1} = F_{TVD}\left(w_{i-2,j,k}^{n}, w_{i-1,j,k}^{n}, w_{i,j,k}^{n}, w_{i+1,j,k}^{n}\right), \tag{16}$$

where i, j, k – spatial grid index $i \in 2 \dots N_x - 2$, $j \in 0 \dots N_y - 1$, $k \in 0 \dots N_z - 1$, border conditions $w_{i,j,k}^{n+1}$ for $i = 0,1$ и $i = N_x - 2$, $N_x - 1$ are equal to $w_{2,j,k}^{n+1}$ and $w_{N_x-3,j,k}^{n+1}$ respectively. It assumes what process is localized far enough from the borders of the area and won't manage to reach them, n – time step number, $n \in 1 \dots N_t$. In formula (16) calculations of nodes with indices (*n*,*i*) are independent for different pairs (*j*,*k*); it effectively reduces dimension of the problem to two-dimensional and allows to parallelize calculations for different sets (*j*,*k*). For the sake of brevity we omit indices *n*, *j*, *k*, because they are constant in the expressions below. Function F_{TVD} (Harten, [5]) is given by:

$$F_{TVD}(w_{i-2}, w_{i-1}, w_i, w_{i+1}) = w_i - \alpha\left(g_{i+\frac{1}{2}} - g_{i-\frac{1}{2}}\right), \text{ where} \tag{17}$$

$$g_{i+\frac{1}{2}} = \frac{1}{2}\phi_{sb}\left(\frac{w_i - w_{i-1}}{w_{i+1} - w_i}\right)(1-\alpha)(w_{i+1} - w_i) + w_i, \tag{18}$$

$$g_{i-\frac{1}{2}} = \frac{1}{2}\phi_{sb}\left(\frac{w_{i-1}-w_{i-2}}{w_i-w_{i-1}}\right)(1-\alpha)(w_i - w_{i-1}) + w_{i-1}, \quad (19)$$

wherein $\alpha = \frac{\Lambda_l \tau}{h}$ – Courant's number for uniform grid with time step τ and spatial step h_x, Λ_l – eigenvalue of matrix $\mathbf{A_x}$, and $\phi_{sb}(r)$ – SuperBee flux limiter (14) [7]. After calculations of $\mathbf{w}_{\mathbf{x},l}$ for each $l \in 1 \dots 9$ we make inverse transition to variables $\mathbf{u}$ (13), then similar calculations should be made for two remaining axes, i.e. for $\alpha = y, z$.

IV. Parallelization

Splitting by spatial coordinates (10) and independence of these calculations for different pairs (j,k) (16) lead to the possibility to parallelize calculations by these pairs. On the example of the scheme (16) parallel computing thread with coordinates (j_m, k_m) gets data with indices j, k from interval $j \in j_m \dots j_{m+1} - 1$, $k \in k_m \dots k_{m+1} - 1$.

We use double precision numbers. Launch of parallel program was made on the NVIDIA Tesla M2070 graphics card, and serial program was launched on the MacBook Pro notebook with Intel Core i7 2GHz processor.

The difference between the results of calculations of parallel and serial programs for test problem (for grid size 64^3, initial condition – spherical perturbation of unit amplitude in the center of the domain with radius 10 spatial steps, for 200 time steps) does not exceed the value of machine epsilon for the numbers of double precision.

Test calculations were made for spherical and plane longitudinal, and plane transverse waves. We get qualitative agreement of results of calculations with their expected behavior, and quantitative agreement between propagation velocities for both types of waves.

Achievable rate of calculations is limited by the operations of memory access, that is why the way of data storage is important. Our algorithm arranges the components of the vector $\mathbf{u}$ in memory in series. We have reached increase of calculation rate by 20 times (for single-precision numbers) and by 7 times (for double-precision numbers) for grid's sizes 64^3, 128^3, 256^3.

V. Summary

The developed parallel algorithm using CUDA-technology for solving 3D seismic problem in homogeneous geological medium is consistent with serial algorithm with the accuracy of machine epsilon for double-precision numbers. Qualitative agreement with expected behavior of solution and quantitative agreement for longitudinal and transverse waves' velocities was achieved.

The work was performed as part of the Summer Student Program 2014 at LIT JINR [10].

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