Porting OpenMP to GPGPU to accelerate Krylov space computations in coupled geodynamics simulator

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ABSTRACT

Understanding the causality between the events leading upto and post fault slip and the earthquake recording is important for seismic design and monitoring of underground structures, bridges and reinforced concrete buildings as well as climate mitigation projects like carbon sequestration and energy technologies like enhanced geothermal systems or oilfield wastewater disposal. While the events leading upto fault slip are typically governed by poroelastostatics, the events post fault slip can easily transition into poroelastodynamics territory due to runaway fault slip velocities. An understanding of expected fault slip velocities is critical apriori, as an algorithm which can seamlessly transition from time marching in poroelastostatics realm to poroelastodynamics realm and vice-versa is extremely difficult to achieve. That being said, every effort in the direction of accelerating the computations on the flow side are a necessary step forward in rendering a fast coupled geodynamics simulator. In this document, we present a framework in which we study the porting of the OpenMP parallelism of the flow simulator to a GPGPU

1 Introduction

The earthquake cycle, from slow deformation associated with interseismic behavior to rapid deformation associated with earthquake rupture, spans spatial scales ranging from fractions of a meter associated with the size of contact asperities on faults and individual grains to hundreds of kilometers associated with plate boundaries [1]. Similarly, temporal scales range from fractions of a second associated with slip at a point during earthquake rupture to hundreds of years of strain accumulation between earthquakes. In many cases, earthquakes are triggered after pore pressure perturbations activate critically stressed seismogenic faults [1], not just due to natural causes like earth tides [2], rainfall [3], snowfall [4], typhoons [5], but also due to human activity [6]. As faults slip, the induced stress field spawns seismic waves, which travel through and around the earth and can be recorded with seismometers. There are several different kinds of seismic waves, and they all move in different ways. The two main types of waves are body waves (P- and S-) and surface waves. Body waves can travel through the Earth's inner layers, but surface waves can only move along the surface of the planet like ripples on water. Understanding the causality between the events leading upto and post fault slip and the earthquake recording is important for seismic design and monitoring of underground structures [7], bridges [8] and reinforced concrete buildings [9] as well as climate mitigation projects like carbon sequestration [10] and energy technologies like enhanced geothermal systems [11] or oilfield wastewater disposal [12].

The complexity of the many physical processes operating over this vast range of scales leads most researchers to focus on a narrow space-time window to isolate just one or a few processes; the limited spatial and temporal coverage of observations also often justifies this narrow focus. For quasi-static simulations, the inertial term is ignored and time dependence only enters through the constitutive models and the loading conditions. As a result, a quasi-static simulation is the solution to a series of static problems with potentially time-varying physical properties and boundary conditions. In dynamic simulations, we shall include the inertial term to resolve the propagation of seismic waves, with an intended focus on applications for earthquake physics and ground-motion simulations. The only place where things can accelerate fast is on the fault and the only time it happens is when fault slips seismically (> 1 cm/sec). If the fault slip is aseismic or creeping (< 0.1 mm/sec), then accelerations are negligible and quasi-static and quasi-dynamic [13] approximations are valid. In our models, we know the fault is the location where things will happen, but we do not know a priori is whether it will be seismic, aseismic or in the transition region. While back-of-the-envelope estimations can be done from the strain energy accumulated in the rock surrounding the faults, the fault's friction properties, and the rock's elastic moduli, the more optimal and accurate option is to use the simulator to do this estimation by equipping it with the physics of elastodynamics.

Algorithm 1: Time-marching

```

/* Initialization */
1 while  $t < T$  do
    /* time marching till final time */
2     while Not converged do
        /* Staggered solution algorithm loop */
3         while Not converged do
            /* Flow loop */
4             Solve flow problem for pressures using GMRES; // Krylov subspace solver in OpenMP
                parallel flow simulator
5             Port information from flow to geodynamics;
6             Solve geodynamics problem for displacements using GMRES; // Krylov subspace solver
                in MPI parallel geodynamics simulator
7             Port information from geodynamics to flow;
8          $t \leftarrow t + \Delta t$ ;

```

The simulator is a mixed programming language hybrid MPI and OpenMP framework in which the open source geodynamics code [14, 15] written in Python and C++ is MPI-based and the in-house multiphase/multicomponent flow code written in C++ is OpenMP-based [16]. As shown in Algorithm 1, the framework follows the popular staggered solution algorithm which allows for different simulators written in separate languages with respective parallelism frameworks are coupled together to render a coupled simulator [16–26]. There are three layers in which the code framework operates out of separate directories

- ✓ The high-level Python code in the geodynamics module makes use of Pyre [27] to link the sub-modules together at runtime
- ✓ The low-level C++ code performs operations on matrices and vectors in parallel using the Standard Template Library [28]
- ✓ The SWIG [29] code with all the .i files, and SWIG-generated python code and MODULENAME_wrap.cxx which wraps the Python code around the C++ code to create python modules.

Currently, the code base is hybrid MPI and OpenMP, in which the geodynamics code is MPI-parallel and the flow code is OpenMP-parallel. This hybrid framework, although accurate, brings in efficiency issues for large size simulations. While the geodynamics elements are distributed among MPI processes with each process running the same tasks on a different sub-grids of the main grid, the

flow elements are all stacked together in the root process, and the tasks are distributed among threads in the root process. When the data structures port information from the geodynamics code to the flow code, they are assembled into the root process using the MPI_Gather command, and then transferred to the flow simulator. This porting can happen multiple times in each time step depending on the convergence requirements of the staggered solution algorithm, and this adds inefficiency to the overall computational run-time. The first option to increase efficiency is to port the OpenMP parallel functionality to MPI parallel [30] on the flow side, and the second option is to offload the OpenMP parallel computations onto a GPGPU [31].

The second option is definitely more engaging as it leverages the massive computational power of the GPGPU. That being said, the advent of new, massively parallel architectures [32] has greatly increased the penalty for suboptimal non-vectorized code while providing much more energy efficient performance. They also increase the imbalance between flop rate and memory bandwidth or latency, so that thousands of flops can be needed to cover outstanding memory references. GPUs in particular have very high memory latency coupled with a wide bus, making the memory access pattern critical for good performance. In addition, the size of fast cache memory per core has shrunk dramatically, so that it cannot easily be used to hide irregular memory access. We explore the second option in this document.

2 Governing equations

2.1 Solid subsystem

The governing equation for linear momentum balance of the solid system can be expressed as

$$\nabla \cdot \boldsymbol{\sigma} + \rho_b \mathbf{g} = \rho_b \ddot{\mathbf{u}} \quad (1)$$

where $\boldsymbol{\sigma}$ is the Cauchy total stress tensor, $\mathbf{g}$ is the gravity vector, and $\rho_b = \phi \sum_{\beta}^{n_{\text{phase}}} \rho_{\beta} S_{\beta} + (1 - \phi) \rho_s$ is the bulk density, ρ_{β} and S_{β} are the density and saturation of fluid phase β , ρ_s is the density of the solid phase, ϕ is the true (Eulerian) porosity, and n_{phase} is the number of fluid phases. In the quasi-static case, the inertial term $\rho_b \ddot{\mathbf{u}}$ is ignored. Note that, by definition, the sum of all fluid phase saturations satisfies $\sum_{\beta}^{n_{\text{phase}}} S_{\beta} \equiv 1$. Following [33], the poroelasticity equations can be written in incremental form as

$$\delta \boldsymbol{\sigma} = \mathbf{C}_{dr} : \delta \boldsymbol{\varepsilon} - b \delta \tilde{p} \mathbf{1} \equiv \mathbf{C}_{dr} : \delta \boldsymbol{\varepsilon} - \sum_{\beta} b_{\beta} p_{\beta} \mathbf{1}, \quad (2)$$

where $\tilde{p} = \sum_{\beta} S_{\beta} p_{\beta}$, and $b_{\beta} = b S_{\beta}$ are the Biot coefficients for individual phases such that $\sum_{\beta} b_{\beta} = b$, $\mathbf{C}_{dr}$ is the rank-4 drained elasticity tensor, $\mathbf{1}$ is the rank-2 identity tensor, b is the Biot coefficient of the saturated porous material, $\boldsymbol{\varepsilon}$ is the linearized strain tensor, defined as the symmetric gradient of the displacement vector $\mathbf{u}$,

$$\boldsymbol{\varepsilon} := \frac{1}{2} (\nabla \mathbf{u} + \nabla^T \mathbf{u}) \equiv \frac{1}{3} \varepsilon_v \mathbf{1} + \mathbf{e}, \quad (3)$$

where $\varepsilon_v = \text{tr}(\boldsymbol{\varepsilon})$ is the volumetric strain and $\mathbf{e}$ is the deviatoric strain tensor. The increment in mean total stress is given by

$$d\sigma_v = \frac{1}{3} \text{tr}(\delta \boldsymbol{\sigma}) = \frac{1}{3} \text{tr}(\mathbf{C}_{dr} : \delta \boldsymbol{\varepsilon} - b \delta \tilde{p} \mathbf{1}) = K_{dr} d\varepsilon_v - b \delta \tilde{p} \quad (4)$$

where K_{dr} is drained bulk modulus of porous medium. Eq. (4) can also be written as

$$d\varepsilon_v = \frac{d\sigma_v}{K_{dr}} + \frac{b d\tilde{p}}{K_{dr}} \quad (5)$$

From the solid mass conservation equation, the incremental porosity update is given as [34, 35]

$$d\phi = \left(\frac{b - \phi}{K_{dr}} \right) (d\sigma_v + d\tilde{p}) \quad (6)$$

2.2 Fluid subsystem

Assuming that the fluids are immiscible, the mass-conservation equation for each phase α is

$$\frac{dm_\alpha}{dt} + \nabla \cdot \mathbf{w}_\alpha = \rho_\alpha f_\alpha, \quad (7)$$

where the accumulation term dm_α/dt describes the time variation of fluid mass relative to the motion of the solid skeleton, $\mathbf{w}_\alpha$ is the mass-flux of fluid phase α relative to the solid skeleton, and f_α is the volumetric source term for phase α that can model the effect of wells. In the deformed configuration, the mass of phase α per unit volume of porous medium is

$$m_\alpha = \rho_\alpha S_\alpha \phi J$$

where $J = 1 + \varepsilon_v$ is the Jacobian of deformation under infinitesimal deformation theory. The incremental fluid mass can be written as

$$\frac{dm_\alpha}{\rho_\alpha} = \phi J \frac{\partial S_\alpha}{\partial P_{\alpha\beta}} dP_{\alpha\beta} + \phi J S_\alpha c_\alpha dp_\alpha + \phi S_\alpha d\varepsilon_v + J S_\alpha d\phi, \quad (8)$$

where $c_\alpha = \frac{1}{\rho_\alpha} \frac{d\rho_\alpha}{dp_\alpha}$ is the compressibility of the fluid phase α , $P_{\alpha\beta} = p_\beta - p_\alpha$ is the capillary pressure and $\partial S_\alpha / \partial P_{\alpha\beta}$ is the inverse capillary pressure derivative which can be obtained from one of the $P_{\alpha\beta}$ vs. S_α models commonly used in flow simulations, e.g. the van Genuchten model. Substituting Eqs. (6) and (5) in Eq. (8) and assuming $\varepsilon_v \ll 1$ and noting that $b_\alpha = b S_\alpha$, we get

$$\frac{dm_\alpha}{\rho_\alpha} = \phi \frac{\partial S_\alpha}{\partial P_{\alpha\beta}} dP_{\alpha\beta} + \phi S_\alpha c_\alpha dp_\alpha + N S_\alpha \sum_\beta S_\beta \delta p_\beta + b^2 \frac{S_\alpha}{K_{dr}} \sum_\beta S_\beta \delta p_\beta + \frac{b_\alpha d\sigma_v}{K_{dr}}$$

where $N = (b - \phi)(1 - b)/K_{dr}$. Defining $N_{\alpha\beta}$ from the first three terms on the right hand side and substituting the above in Eq. (7), we obtain the multiphase flow equation for phase α in a poroelastic medium as:

$$\frac{\partial}{\partial t} \left(\rho_\alpha \sum_\beta \left(N_{\alpha\beta} + \frac{b_\alpha b_\beta}{K_{dr}} \right) p_\beta \right) + \frac{1}{K_{dr}} \frac{\partial}{\partial t} (\rho_\alpha b_\alpha \sigma_v) + \nabla \cdot \mathbf{w}_\alpha = \rho_\alpha f_\alpha \quad (9)$$

Because we assume that the fluids are immiscible, the mass-flux of phase α is $\mathbf{w}_\alpha = \rho_\alpha \mathbf{v}_\alpha$, where we adopt the traditional multiphase-flow extension of Darcy's law [36, 37]:

$$\mathbf{v}_\alpha = -\frac{\mathbf{k} k_\alpha^r}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha \mathbf{g}), \quad (10)$$

where μ_α and k_α^r are the dynamic viscosity and the relative permeability of phase α in presence of other fluid phases.

3 OpenMP to GPGPU

Data parallelism is a form of parallelization of computing across multiple processors in parallel computing environments. It mainly focuses on distributing the data across different parallel computing nodes. In a multiprocessor system executing a single set of instructions (SIMD), data parallelism is achieved when each processor performs the same task on different pieces of distributed data. In some situations, a single execution thread controls operations on all pieces of data. In others, different threads control the operation, but they execute the same code.

3.1 OpenMP programming and memory model

OpenMP is an implementation of multithreading, a method of parallelizing whereby a master thread (a series of instructions executed consecutively) forks a specified number of slave threads and the system divides a task among them. The threads then run concurrently, with the runtime environment allocating threads to different processors. The section of code that is meant to run in parallel is marked accordingly, with a preprocessor directive that will cause the threads to form before the section is executed. Each thread has an id attached to it which can be obtained using a function (called `omp_get_thread_num()`). The thread id is an integer, and the master thread has an id of 0. After the execution of the parallelized code, the threads join back into the master thread, which continues onward to the end of the program. By default, each thread executes the parallelized section of code independently. Work-sharing constructs can be used to divide a task among the threads so that each thread executes its allocated part of the code. Both task parallelism and data parallelism can be achieved using OpenMP in this way. The runtime environment allocates threads to processors depending on usage, machine load and other factors. The runtime environment can assign the number of threads based on environment variables, or the code can do so using functions. The OpenMP functions are included in a header file labeled `omp.h` in C/C++. One might expect to get an N times speedup when running a program parallelized using OpenMP on a N processor platform. However, this seldom occurs for these reasons:

- ✓ When a dependency exists, a process must wait until the data it depends on is computed.
- ✓ When multiple processes share a non-parallel proof resource (like a file to write in), their requests are executed sequentially. Therefore each thread must wait until the other thread releases the resource.
- ✓ A large part of the program may not be parallelized by OpenMP, which means that the theoretical upper limit of speedup is limited according to Amdahl's law.
- ✓ N processors in a symmetric multiprocessing (SMP) may have N times the computation power, but the memory bandwidth usually does not scale up N times. Quite often, the original memory path is shared by multiple processors and performance degradation may be observed when they compete for the shared memory bandwidth.

Many other common problems affecting the final speedup in parallel computing also apply to OpenMP, like load balancing and synchronization overhead.

3.2 CUDA programming and memory model

The CUDA programming model [38] is a general-purpose multi-threaded SIMD model for GPGPU programming. A GPU is viewed as a parallel computing coprocessor, which can execute a large number of threads concurrently. A CUDA program consists of a series of sequential and parallel execution phases. Sequential phases have little or no parallelism, and thus they are executed on the CPU as host code. Parallel phases that exhibit rich data parallelism are implemented as a set of kernel functions, which are executed on the GPU. Each kernel function specifies GPU code to be executed in an SIMD fashion, by a number of threads invoked for each parallel phase. In the CUDA programming model, a host CPU and a GPU device have separate address spaces. For a CPU to access GPU data, the CUDA model provides an API for explicit GPU memory management, including functions to transfer data between a CPU and a GPU.

The CUDA memory model has

- ✓ an off-chip global memory space, which is accessible by all threads,
- ✓ an off-chip local memory space, which is private to each thread,
- ✓ a fast on-chip shared memory space, which is shared only by threads in the same thread block,
- ✓ and registers, which are private to each thread
- ✓ constant memory with a dedicated small cache for read-only global data

- ✓ texture memory with a dedicated small cache for read-only array data accessed through built-in texture functions

The shared memory and the register bank in a multiprocessor are dynamically partitioned among the active thread blocks running on the multiprocessor. Therefore, register and shared memory usages per thread block can be a limiting factor preventing full utilization of execution resources.

3.3 OpenMP to CUDA

```

1 // Serial
2 for (i = 0; i < n; i++){
3     for (j = 0; j < n; j++){
4         sum = 0;
5         for (k = 0; k < n; k++) sum = sum + a[i][k] * b[k][j];
6         c[i][j] = sum;
7     }
8 }
9 // OpenMP parallel
10 #pragma omp parallel for schedule(dynamic, chunk)
11 private(i, j) shared(a, b, c)
12 for (i = 0; i < lines; i++){
13     for (j = 0; j < columns; j++){
14         int sum = 0;
15         #pragma omp parallel
16         private(k)
17         for (k = 0; k < N; k++) sum = sum + a[i][k] * b[k][j];
18         c[i][j] = sum;
19     }
20 }
21 // CUDA parallel
22 __global__ void gpuMM(float *a, float *b, float *c, int n) {
23     int row = blockIdx.y*blockDim.y + threadIdx.y;
24     int col = blockIdx.x*blockDim.x + threadIdx.x;
25     float sum = 0.f;
26     for (int j = 0; j < n; ++j) sum += a[row*n+j]*b[j*n+col];
27     c[row*n+col] = sum;
28 }

```

Listing 1: Different versions of matrix matrix multiplication

Code snippets for serial, OpenMP parallel and CUDA parallel for archetypal matrix matrix multiplication are given in Listings 1. There are several advantages of OpenMP as a programming paradigm for GPGPUs

- ✓ OpenMP is efficient at expressing loop-level parallelism in applications, which is an ideal target for utilizing GPU's highly parallel computing units to accelerate data-parallel computations
- ✓ The concept of a master thread and a pool of worker threads in OpenMP's fork-join model represents well the relationship between the master thread running in a host CPU and a pool of threads in a GPU device
- ✓ Incremental parallelization of applications, which is one of OpenMP's features, can add the same benefit to GPGPU programming

Algorithm 2: GMRES

```

/*  $A$  is of size  $n \times n$ ,  $b$  is of size  $n \times 1$  */
1  $q \leftarrow 0$ ;
2  $x_0 \leftarrow x^*$ ; // Initial guess
3 while Not converged do
4      $r_q = b - Ax_q$ ;
5      $v_1 \leftarrow \frac{r_q}{\|r_q\|}$ ;
6     if  $q=0$  then
7          $\beta \leftarrow \|r_q\|$ ;
8     for  $j = 1, 2, \dots, m$  do
9          $W_j = Av_j$ ; // Columns of  $W$ 
10         $\hat{v}_{j+1} \leftarrow W_j$ ;
11        for  $i = 1, 2, \dots, j$  do
12             $H_{i,j} \leftarrow v_i^T W_j$ ; // Elements of  $H$ 
13             $\hat{v}_{j+1} \leftarrow \hat{v}_{j+1} - v_i H_{i,j}$ ;
14         $H_{j+1,j} \leftarrow \|\hat{v}_{j+1}\|$ ;
15         $v_{j+1} \leftarrow \frac{\hat{v}_{j+1}}{H_{j+1,j}}$ ;
16    Find  $y$  s.t.  $\|\beta e_1 - Hy\|$  is minimized; //  $e_1$  is the first column of  $(m+1) \times (m+1)$  identity
    matrix,  $H$  is of size  $(m+1) \times m$ ,  $y$  is of size  $m \times 1$ 
17     $x_{q+1} = x_q + Wy$ ; // Refined guess,  $W$  is of size  $n \times m$ 
18     $q \leftarrow q + 1$ ;

```

3.4 Krylov subspace solver and OpenMP implementation

The governing PDEs (Eqs. (1) and (9)) are discretized using finite element method and finite volume method respectively, and the resulting system of algebraic equations is solved using Krylov space methods [39–42], which generate a sequence of iterates x_n that are approximate solutions. In these algorithms, x_n belongs to an affine space that grows with n :

$$x_n - x_0 \in \text{span}(r_0, Ar_0, \dots, A^{n-1}r_0)$$

where $r_0 := b - Ax_0$ is the initial residual. The algebraic system of equations resulting from the flow equations (Eqs. (9)) are solved using GMRES [42] as shown in Algorithm 2. In a nutshell, the residuals at each iteration are QR-factorized, and guesses are refined using the solution of a least-squares problem.

```

1 // Triggering the OpenMP functionality
2 #ifdef _OPENMP
3 #pragma omp parallel
4 #pragma omp master
5 n_threads = omp_get_num_threads();
6 #else
7 n_threads = 1;
8 #endif
9 // Code piece of the Block GMRES solver implementation offloaded onto
  OpenMP threads
10 #pragma omp parallel for
11 for (int conn = 0; conn < nConns; conn++){
12     memcpy (mOffd_cpy_row_wised+ConnToRowIndex[2*conn]*nComps2, mOffd_A+
        conn*nComps2, BlockSize);

```



```

13  memcpy (mOffd_cpy_row_wised+ConnToRowIndex[2*conn+1]*nComps2, mOffD_B
    +conn*nComps2, BlockSize);
14 }
15 #pragma omp parallel for private (ib)
16 for (iw=0; iw<nW; iw++){
17     int n_wr = 0;
18     for (ib=0; ib<nWPerfs[iw]; ib++) n_wr += nImpVars[mWLoc[iw][ib]];
19     memcpy(mRWJ_cpy1[iw], mRWJ[iw], n_wr*sizeof(double));
20     memcpy(mWRJ_cpy1[iw], mWRJ[iw], n_wr*sizeof(double));
21     mWWJ_cpy1[iw][0] = mWWJ[iw][0];
22     memcpy(mRWJ_cpy2[iw], mRWJ[iw], n_wr*sizeof(double));
23     memcpy(mWRJ_cpy2[iw], mWRJ[iw], n_wr*sizeof(double));
24     mWWJ_cpy2[iw][0] = mWWJ[iw][0];
25 }

```

Listing 2: Triggering the OpenMP functionality

The code snippets in the flow simulator that have evidence of OpenMP usage are provided in Listings 2.

4 Conclusions and Outlook

Due to the similarity between OpenMP and CUDA programming models, we should be able to convert OpenMP parallelism, especially loop-level parallelism, into the forms that best express parallelism in CUDA. However, the baseline translation of existing OpenMP programs does not always yield good performance. Performance gaps are due to architectural differences between traditional shared-memory multi-processors (SMPs), served by OpenMP, and stream architectures, adopted by most GPUs. Even though the OpenMP programming model is platform-independent, most existing OpenMP programs were tuned to traditional shared-memory multiprocessors. We refer to stream architectures as those that operate on a large data space (or stream) in parallel, typically in an SIMD manner and tuned for fast access to regular, consecutive elements of the data stream. In GPU architectures, optimization techniques designed for CPU-based algorithms may not perform well [7]. Also, GPUs face bigger challenges in handling irregular applications than SMPs, because of the stream architectures' preference for regular access patterns. Handling all these issues is part of future work.

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