CoGL

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Description

CoGL is a stand-alone meso-scale simulation code used to analyze pattern formation in ferroelastic materials using the Ginzburg–Landau approach. It models transitions from a face-centered cubic parent phase to a body-centered tetragonal product phase due to either a rapid decrease in temperature or an external deformation. By solving the force balance equations that use a nonlinear elastic free-energy functional and also incorporate inertial and viscous forces, the strains are computed at each point on a regular three-dimensional grid. The code allows the study of nucleation and growth of phase changes on loading-unloading and heating-cooling protocols as a function of strain rates.

The simulation code itself is relatively short (a few hundred lines of code), consisting mainly of gradient and Laplacian computations over the grid. Two versions of the code are included here: the original serial Fortran code written by the domain scientists, and a data-parallel implementation using the PISTON framework. PISTON is a portable, data-parallel framework developed at Los Alamos using NVIDIA's Thrust library. It allows an application developer to compile and run his/her code on different parallel accelerator and multi-core architectures, making efficient use of the available parallelism on each. This is accomplished by constraining the developer to writing algorithms using a limited set of data-parallel primitives, each of which is efficiently implemented for each target architecture.

In the PISTON version of CoGL, the simulation is computed primarily using data-parallel transform primitives, in which, for example, each thread computes the gradient at one grid cell. In an extended version of this proxy app, not included here, more complex isosurface, threshold, and cut surface visualization algorithms already implemented in PISTON can be applied to the strain field computed by the simulation and rendered in-situ as the simulation is running.

Preliminary testing on a single node has shown that the PISTON implementation compiled to an OpenMP backend and run on multiple cores scales well with the number of cores and outperforms the equivalent serial C++ code and especially the original Fortran code. The PISTON implementation compiled to a CUDA backend and run on a GPU improves parallel performance even further. Furthermore, when the simulation is run on the GPU, rendering can be implemented with limited additional performance cost because all the data can be kept on the card using CUDA's interop feature.

This simulation was described in the following paper (http://www.sciencedirect.com/science/article/pii/S1359645406000668):

Rajeev Ahluwalia, Turab Lookman, and Avadh Saxena. "Dynamic strain loading of cubic to tetragonal martensites", *Acta Materialia*, Volume 54, Issue 8, May 2006, Pages 2109-2120.

Instructions

The dependencies are CUDA (https://developer.nvidia.com/cuda-downloads), which includes the Thrust library; CMake (http://www.cmake.org/cmake/resources/software.html), for configuring the build; OpenGL, GLEW, and GLUT (available with most package installers such as apt-get or yum); and PISTON (https://github.com/losalamos/PISTON). Like Thrust, PISTON is only used through the inclusion of header files, so there is no need to build anything in PISTON itself. CoGL has been tested on Linux and Mac operating systems. PISTON-based programs have also been run on Windows machines, but CoGL itself has not been tested on Windows, so it should be possible to get it to run on Windows, but may take a little effort. We have in the past had some trouble installing GLEW on Macs, so the necessary GLEW header and library for Mac are included in the mac subdirectory. See the end of this readme for licensing notes about this redistribution. An NVIDIA GPU that supports CUDA with double-precision is necessary to run the CUDA-based CoGL executable.

There are three executables that can be built. The original FORTRAN program written by the domain scientists is in fortran subdirectory, and can be built using the Makefile in that directory, resulting in the coglFOR executable. The other two executables, coglGPU (which uses the Thrust CUDA backend) and coglOMP (which uses the Thrust OpenMP backend), can be built using the standard CMake build process (http://www.cmake.org/cmake/help/runningcmake.html). The DATA_DIR CMake configuration path should be set to the InitData directory within the CoGL directory, where files containing initial conditions are included. The PISTON_DIR CMake configuration path should be set to the location where PISTON is installed. Whether interop is used or not with coglGPU can be controlled using the ENABLE_INTEROP CMake variable.

Running coglGPU or coglOMP without any command-line parameters will result in a GLUT window launching, which will show a rendering of the cubical grid, colored according to the e2 deviatoric strain value, along with numbers written to the console that can be used to validate correctness. The view may be rotated using the left mouse button and zoomed using the right mouse button. It takes a few thousand time steps before “interesting” things begin to happen. Running coglFOR will only output these numbers, without any graphical output. Running coglGPU or coglOMP with a single command-line argument that is an integer greater than zero will result in that many time steps being run and timed, without any rendering. In order to run coglGPU in this render-free mode, interop must be disabled in the CMake configuration.

It should be possible to build the OpenMP-based executable (coglOMP) on a system without CUDA. In this case, it will be necessary to separately download the Thrust library (http://code.google.com/p/thrust/downloads/list), and set THRUST_DIR in the CMake configuration to point to its location (and set USE_CUDA to OFF). While this has been tested for some PISTON-based programs, it has not been explicitly tested with CoGL, so please contact the authors directly if this does not work.

Several parameters may be modified at the top of the CoGLSim.h file. On systems that are slow or have a relatively small amount of memory on the CPU or GPU, it may be desirable to decrease the grid

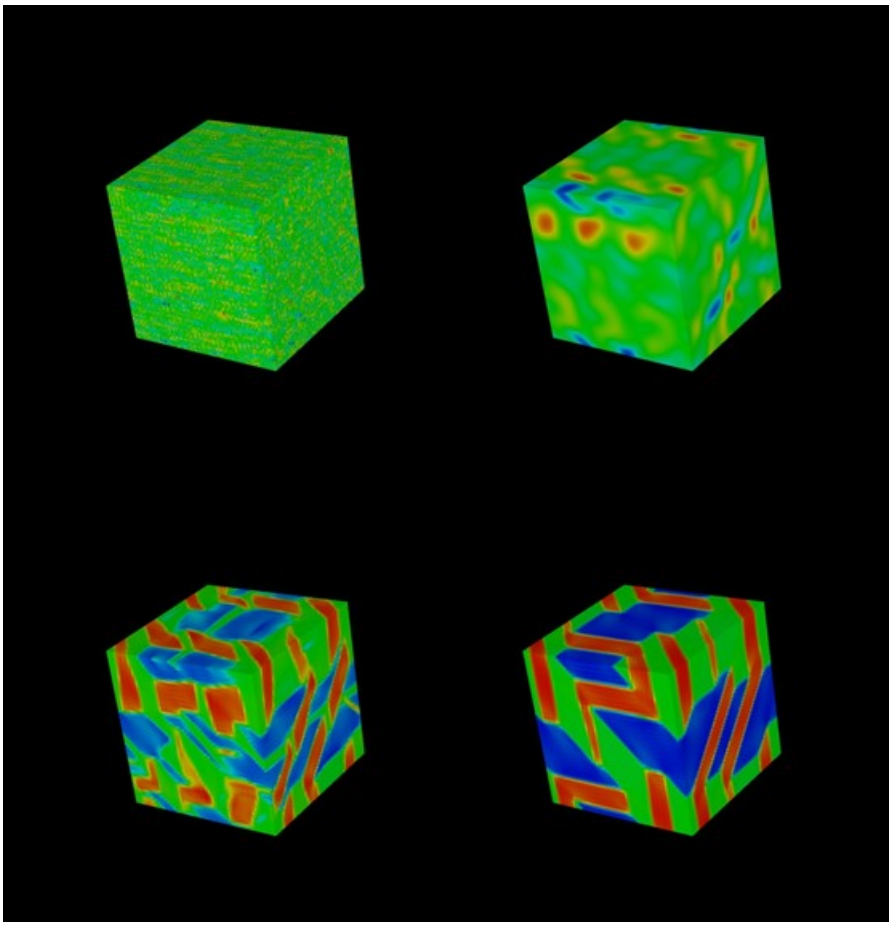
dimension (DIM). One might experiment with uncommenting the #defines for PRECOMPUTE_INDICES, OPTIMIZE_KERNEL_DIVISIONS, and/or OPTIMIZE_KERNEL_BRANCHES in order to compare performance with these variations.

This release of CoGL is a somewhat simplified version which does not include additional visualization operators, such as isosurface, threshold, and cut surface. It only renders each cell as a cube. Since only the surface of the grid is visible, this can result in a lot of "wasted" rendering of interior cubes. If you are interested in this version with the additional visualization operators, please contact the authors.

GLEW Redistribution Notes

From http://glew.sourceforge.net/glew.txt :

Sample frames



Four selected time steps (3000, 15,000, 25,000, and 200,000) from the CoGL simulation, plotting the grid points colored according to the deviatoric strain value, showing how the strain field evolves when a parent cubic lattice changes to a daughter tetragonal structure.