frisca

Fast rheology simulation cores by single chain slip-spring models
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1 Introduction

Polymer solutions or melts with large molecular weights exhibit characteristic rheological properties due to the 'entanglements' [The Theory of Polymer Dynamics]. The macroscopic flows of 'entangled' polymeric materials become much different from flows of Newtonian fluids. To perform flow simulations of entangled polymeric materials efficiently, fast rheology simulation models are clealry demanding.

The slip-spring model [Likhtman-2005], which mimics the entanglements by spring like objects which slides (slips) on polymer chains, is one of rheology models of entangled polymers. The slip-spring model is simple and enables us to perform efficient simulations. Recently, the slip-spring model is slightly modified to achieve further efficient simulations and fast simulations on a GPU [Uneyama-2011]. The macroscopic flow simulations of polymeric materials are expected to be accelerated by using the slip-spring based rheology simulation models.

`frisca` is the package of fast rheology simulator cores based on the single chain slip-spring type models. It contains simulator cores work both on a CPU and on a GPU. `frisca` contains four simulator cores. Two different slip-spring based models are employed; the standard single chain slip-spring model `frisca`, and the corase-grained single chain slip-spring model `frisca-cg`. Their implementaions on a GPU are also provided. The GPU versions are name `frisca-gpu` and `frisca-cg-gpu`.

Simulator cores of `frisca` can simulate stress tensors of entanged polymers under given deformations. `frisca` is designed to be embedded to other simulators such as particle based hydrodhynamics simulation models [Murashima-Taniguchi-2011]. Because of its high numerical efficiency, `frisca` enables macroscopic flow simulations with reasonable computational costs.

2 Compilation of frisca

2.1 To Download the Latest Version of frisca

The latest version of frisca is available at the following URL. Access the web page and download the latest version via HTTP (FTP is not supported).

http://www.scl.kyoto-u.ac.jp/~uneyama/frisca.html

2.2 Build from the Source

You need to build frisca from the source package to use it. (Binary packages are not provided due to some poratability and tuning problems.) The source package of frisca is using GNU Autoconf, therefore you can build it like other free software packages. However, because frisca is designed to be embedded to other simulator programs, it is not directly installed to your system. To use frisca as a rheology simulator of other simulator programs, it is better to copy simulator core directories (subdirectories under src/) directly into other source trees and modify Makefile or other setting files.

Note that frisca requires HDF5 (http://www.hdfgroup.org/HDF5/). If you want to build the GPU version simulator cores, frisca also requires CUDA toolkit and CUDA SDK (http://developer.nvidia.com/cuda-downloads). You have to install them before building frisca. CUDA Toolkit version 2.1 or later are supported. Devices of compute capability 1.1 or later are supported (devices of compute capability 1.3 or later are recommended).

The source package is distributed as a gzipped tar archive file, thus first you need to extract it. To extract the archive, do

```
$ zcat frisca-0.1.0.tar.gz | tar xvf -
```

or if you are using GNU tar, do

```
$ tar zxvf frisca-0.1.0.tar.gz
```

Then the source directory will extracted. Move to the directory frisca-0.1.0.

```
$ cd frisca-0.1.0
```

To build frisca, do configure-make just like other free software packages.

```
$ ./configure
$ make
```

Now library files for simulator cores and simple simulator programs using frisca will be built and stored under src/ and examples/ subdirectories. If you have an error messages and the compilation is aborted, some commands or libraries may be missing. Install the required packages and retry.

If you want to customize or tune frisca,

```
$ ./configure --help
```

will help you.

2.3 Build with CUDA

If you use GPU version (CUDA version) simulator cores of `frisca`, the simulation speeds can be accelerated largely. To build GPU version simulator cores, you need to specify `--enable-cuda` option for the `configure` script.

```
$ ./configure --enable-cuda
```

If the CUDA toolkit and CUDA SDK are installed to default paths, `configure` will automatically detect them. If the toolkit is not detected, you should set the path properly. If the SDK is not detected, then you should manually specify the path for it.

```
$ ./configure --enable-cuda --with-cuda-sdkdir=/path/to/nvidia/cuda/sdk
```

where `/path/to/nvidia/cuda/sdk` is the path for the SDK.

To optimize the simulator cores for your GPU, you may want to specify `NVCFLAGS` and `GPUARCH`. For example, the following setting will give the optimized binaries for Fermi architecture GPUs.

```
$ ./configure --enable-cuda NVCFLAGS=-O3 GPUARCH=sm_20
```

(It should be noted here that `--fast-math` option is automatically set and thus you do not need to set it by yourself.) Also, to optimize and tune the number of threads launched on a GPU, change the numbers of blocks and threads. These numbers are defined in `threads_gpu.h` header files in `src/frisca-gpu` and `src/frisca-cg-gpu`.

If you embed `frisca` to other source trees, you will need to manually set these variables. In each simulator core subdirectories, there is `Makefile` which works solely by itself. It will be the easiest way to directly edit the target `Makefile` for your environment.

3 Example

To use `frisca` as an embedded rheology simulator, the main simulator program is required. As a simple example, the simple simulator for start-up shear flow is presented in the following section.

3.1 Simple Start-Up Shear Flow Simulator

The main routine of the start-up shear flow simulator with `frisca` simulator core is shown and explained below. The full source code is stored in `examples/frisca`.

First, the simulator is allocated on the memory and then initialized.

```
z_max = calculate_estimate_for_z_max(n,n0);
state = allocate_simulator_state(m,n,z_max);

initialize_simulator_state(state,seed,n_s,n0,zeta_s);
```

The functions `allocate_simulator_state()` and `initialize_simulator_state()` allocate and initialize the state of a simulator, respectively. `calculate_estimate_for_z_max()` gives the estimate value of `z_max`, which is requried for the memory allocation.

Second, the dynamics simulation is performed and the stress tensor is calculated.

```
for(i = 0;i < p;i++)
{
    get_stress_tensor(state,sigma);
    printf("%f %f %f %f %f %f\n",
           sigma[0],sigma[1],sigma[2],sigma[3],sigma[4],sigma[5]);

    perform_simulation(state,iterations,dt,kappa);
}
```

Here, the function `perform_simulation()` performs the dynamics simulation by integrating the time evolution equations. The function `get_stress_tensor()` gives the average stress tensor for a chain. Thus calculated stress tensor can be used for other simulators such as the macroscopic fluid simulator. (In this example code, the stress tensor is just printed out.)

Third, after the simulation is completed, the simulator state is stored to an output file and then the memory for the simulator state is freed.

```
store_simulator_state_to_file("frisca_state.h5",state);

free_simulator_state(state);
```

The function `store_simulator_state_to_file()` stores the current simulator state to the output HDF5 file. (The stored state can be loaded by the function `load_simulator_state_from_file()`.) `store_simulator_state_to_file()` can be omitted if the state is not needed to be stored. Finally, the function `free_simulator_state` frees the memory allocated for the simulator state.

4 Reporting Bugs

Currently, the error handling routines in `frisca` is not complete and therefore `frisca` may suddenly stops if some input error or calculation error is caused. Especially, parameters are not strictly checked and care should be paid.

If you find a bug in `frisca`, please send electronic mail to uneyama@scl.kyoto-u.ac.jp with the version number and simulator core name. Please describe the problem in detail, for example, how and/or when the program works wrong.

If you have other questions, comments or suggestions about `frisca`, contact the author via electronic mail to uneyama@scl.kyoto-u.ac.jp. The author will try to help you out, although he may not have time to fix your problems.

5 References

[Likhtman-2005] A. E. Likhtman, *Macromolecules* **38**, 6128 (2005).

[Uneyama-2011] T. Uneyama, *Nihon Reoroji Gakkaishi (J. Soc. Rheol. Jpn.)* **39**, 135 (2011).

[Murashima-Taniguchi-2011] T. Murashima and T. Taniguchi, *Europhys. Lett.* **96**, 18002 (2011).

[The Theory of Polymer Dynamics] M. Doi an S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford University Press (1986).

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