Dislocation Depinning Simulator

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Contents

1 Introduction

This is the user guide to the Dislocation Depinning Simulator (DDS). This simulator models the dislocation depinning on pinning sites in 2D.

2 Model

Our depinning model consists of a lattice of size $L_x \times L_y$ (with PBC in direction x) Sites have a binary values corresponding to plastic slip. The boundaries between different-valued sites represent dislocation segments. These segments are of either edge or screw character. The resolved shear stress τ acting on a segment at position $\boldsymbol{r}$ is the sum of three contributions:

$$\tau(\boldsymbol{r}) = \tau_{\text{ext}}(\boldsymbol{r}) + \tau_{\text{self}}(\boldsymbol{r}) + \tau_{\text{pin}}(\boldsymbol{r}), \tag{1}$$

where these are the external stress, the stress from the self-intercation of the dislocation and the pinning field, respectively. The self-stress at the ith segment is the sum of the contributions of all the other segments (and their images in direction x which ensure the PBC):

$$\tau_{\text{self}}(\boldsymbol{r}_i) = \sum_j^{\{s\}} \tau_s(\boldsymbol{r}_i - \boldsymbol{r}_j) + \sum_j^{\{e\}} \tau_e(\boldsymbol{r}_i - \boldsymbol{r}_j), \tag{2}$$

where the interactions are summed over the set of the other screw segments $\{s\}$ and edge segments $\{e\}$. At each time step a dislocation segment is chosen randomly (with uniform probability) and it is moved with one cell in the direction of net force acting on the segment.

3 Building DDS

3.1 Compilation

After navigating to folder `src` call

```
mkdir ../build
cd ../build
cmake ../src
make
```

which results a binary file in folder `build`.

3.2 Prepocessor directives

Header file `general.h` defines the following relevant constant.

identifier	hard-coded value	description
`N_EWALD`	2	Number of image/ghost segments on each side

The header also may define macros that control output file generation.

identifier	description
`SAVE_LATTICE`	Saves configuration in *lattice* format after each n_{lat} step.
`SAVE_SEGMENTS`	Saves configuration in *segments* format after n_{seg} each step.
`SAVE_PINNING_FIELD`	Saves pinning field $\tau_{\mathrm{pin}}(\boldsymbol{r})$.

4 Executing DDS

The simulator can be executed in the following way.

```
<path to build>/depinning <path to control file> <path to pinning field file>
   <path to output directory>
```

One example is the following.

```
./build/depinning "test.ctrl" "pin.fld" "results/"
```

Note: output directory will be created upon execution.

5 Setting up initial configurations

5.1 Initial dislocation configuration

The type of the initial configuration is hard-coded at this version. The configuration is a single straight horizontal dislocation line which is `initial_height` sites above of the bottom boundary of the lattice. The Burgers vector of the dislocation can be controlled with parameter `vertaical_burgers`.

Implementing a different initial dislocation configuration can be done manually in the code by modifying the entries of variable `lattice`. If an entry is `true`, the corresponding site has already been invaded by the dislocation. If it is `false`, it is yet to be invaded.

5.2 Pinning stress field

The pinning stress field is read from file with the path to it given when executing. The file should contain `Lx`×`Ly` pinning stress values (floating point numbers) separated with white space. Note: dimensions `Lx` and `Ly` should be added as input parameter and should be consistent with the pinning field file.

6 Output files

6.1 Configuration files

6.1.1 Lattice files

Lattice files contain the information about configurations. The location and name format is

```
<outout directory>/lattice/<configuration id>.lat
```

where the configuration id start from 0 and increases by one with each time step. Consequently, if not every configuration is saved, configuration ids may not be subsequent integers.

The files contain an array of size (Ly×Lx). Each value correspond to lattice site. If the site has already been invaded by the dislocation line, its value is 1, otherwise it is 0. where the configuration id start from 0 and increases by one with each time step. Consequently, if only stable configurations are saved, configuration ids may not be subsequent integers.

6.1.2 Segment files

Segment files contain the information about configurations. The location and name format is

```
<outout directory>/segment/<configuration id>.seg
```

where the configuration id start from 0 and increases by one with each time step. Consequently, if not every configuration is saved, configuration ids may not be subsequent integers. Each row corresponds to a dislocation segment.

column	description
1	The x coordinate of the center of the segment.
2	The y coordinate of the center of the segment.

Coordinates of the centers of sites are integers starting from 0. Consequently, the segment coordinates are half-integers.

6.1.3 Memory need and recommendations

Lattice and segment files both contain all the information about the configurations and they can be converted into each other. The lattice files, however, typically need significantly more memory. Thus, usually the use of segment files is recommended. The space need of the two file types is summarized in the following table. L is the total dislocation length (that is, the number of segments).

file type	data type	file size	memory need [B]
lattice	int	LxLy	4LxLy
segment	double	L	$8L$

The size of segments files can only exceed the size of lattice files in very extreme cases and it cannot be more than 16LxLy. In a typical simulation with Lx=Ly$= 256$ and $L \approx 2$Lx the size of a lattice and segment file are 256MB and 4MB, respectively.

6.2 Stress file

Stress file `stress` contains the external stress value at each simulation step. The external stress may have a non-zero initial value, but the simulation step counter and the slipped area is zero initially. The stress file is located here:

```
<outout directory>/stress
```

column	description
1	Simulation steps elapsed
2	Slipped area measured in cell area
3	The value of external stress

6.3 Time file

Time file `time` contains the total simulation time measured in seconds. The file is located here:

```
<outout directory>/time
```

Note: the simulation time is also printed to the standard output upon the termination of the simulation.

6.4 Pinning file

Pinning file

```
<outout directory>/pinning.fld
```

contain the information about the pinning field. The files contain an array of size (`Ly`$\times$`Lx`). Each value correspond to the pinning stress at a lattice site.

6.5 Metadata file

Metadata file

```
<outout directory>/meta
```

contains relevant metadata such as the random seed, elastic and lattice parameters, etc. which are organized in groups in the file.

column	description
1	Description of the parameter.
2	Identifier of the variable used in the code.
3	Value of the parameter in simulation units.

7 Control file parameters

Elastic parameters

parameter	data type	default value	description
mu	double	1.0	Shear modulus. Self interaction is directly proportional to this value, therefore, it simply scales the (external and pinning) stress values.
Poisson	double	0.35	Poisson ratio.
Burgers	double	1.0	Length of the Burgers vector. Should not be modified: a Burgers vector different from the cell size my cause problems with the line tension.
cellsize	double	1.0	Linear size of the simulation cell. Should not be modified in this version.
spring_constant	double	0.01	The extent of stress drop due to plastic strain increment. If the number of slipped cells is changed with $\Delta A = \pm 1$, the external stress changes with $-A$`spring_constant`

Configuration parameters

parameter	data type	default value	description
Lx	int	100	Width of the lattice in cells.
Ly	int	100	Width of the lattice in cells.
initial_height	int	50	Initial vertical position of the dislocation line. `initial_height` rows of cells are below the initially straight dislocation line.
vertical_burgers	int	0	Determines the character of the horizontal dislocation segments. Zero and non-zero values mean those are of screw and edge character, respectively.

Loading parameters

parameter	data type	default value	description
stress_init	double	0.0	The initial value of the external stress.
stress_rate	double	0.0	The external stress rate. Note: the external stress does not execatly change with this rate as it it also affected by the plastic strain and parameter `spring_constant`.

Other parameters

parameter	data type	default value	description
seed	int	0	The seed that controls the pseudo-random segment choice for the dynamics.

8 Termination of DDS

In normal circumstances the simulation terminates when any of these conditions are met:

a) Any of the segments reaches a limit set near to the top end of the simulation box. In a typical setup when a dislocation line is moving from bottom to top, this is the expected termination message.

b) Any of the segments reaches a limit set near to the bottom end of the simulation box. In a typical setup this may be unexpected and possible this is due to initially locating the dislocation too close to the bottom end.

c) All the dislocation segments annihilate. In a typical setup this may be unexpected but my happen if loop(s) are created instead of a straight dislocation line.

In any other case the simulation should not terminate during normal functioning.