drops-udf

OCTA UDF support for `drops`
version 0.2.0
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Table of Contents

1 Introduction

`drops-udf` is an OCTA UDF support interface for `drops`. You can use the OCTA UDF files for input / output for `drops` by using `drops-udf`. For further information about `drops`, see the documents of `drops`.

2 Install drops-udf

You can build and install drops-udf if the binary package of your system is not available, or if you want to customize the drops-udf. The sourca package of drops-udf is using GNU Automake and GNU Autoconf, therefore you can build and install drops-udf just like usual free software. Note that drops-udf requires drops and you have to install it before build drops.

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

```
$ zcat drops-udf-0.2.0.tar.gz | tar tvf -
```

or if you are using GNU tar, do

```
$ tar zxvf drops-udf-0.2.0.tar.gz
```

Then the source directory will extracted. Move to the directory drops-0.2.0.

```
$ cd drops-udf-0.2.0
```

To build drops-udf, do configure-make-make install just like other free software.

```
$ ./configure
$ make
$ su -
# make install
```

Now drops-udf will be installed under /usr/local of your system. 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 drops-udf,

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

will help you.

3 Invoking drops-udf

The format for running the drops-udf program is:

```
$ dropsudf option ...
```

dropsudf supports the following options:

--input=*input*
-i *input* Read the parameters for simulation from the input file *input*. If no input file is specified, drops will read the input file named dropsin.udf.

--psi=*psi*
-d *psi* Read the initial value of the psi-field from the file psi. The psi-field input file psi must be the gzipped plain text. You can create one easily by using gzip. By default, drops set the psi-field to be homogeneous. This options is passed to drops.

--external=*external*
-e *external*
Read the external force field from the file external. The external force input file density must be the gzipped plain text. You can create one easily by using gzip. By default, drops does not apply any external force to the system. This options is passed to drops.

-I *directory*
Add *directory* to the search paths. This option is passed to xudfpp.

-D *name*[=*definition*]
Define macro *name* (= *definition*). This option is passed to xudfpp.

--help
-h Show summary of options.

--version
-v Show version of program.

4 Tutorial

In this section, we show a simple example for using `dropsudf`. The input file for `dropsudf` is the OCTA UDF file. Here we use the following input OCTA UDF file (the parameters or conditions are the same as the tutorial data for the `drops`).

```
\begin{header}
    \begin{def}
        EngineType : string;
        EngineVersion : string;
        IOType : string;
        ProjectName : string;
        Comment : string;
    \end{def}
    \begin{data}
        EngineType : "drops (drops-udf)"
        EngineVersion : "0.1.0"
        IOType : "in"
        ProjectName : "drops-udf"
        Comment : "an input file for the AB diblock copolymer melt"
    \end{data}
\end{header}

\begin{def}
    class polymer :
    {
        N : double
        f[] : double
        a[][] : int
        monomer[] : string
        lambda : double
    }

    condition :
    {
        optimize_lattice : select {"true", "false"}

        use_multigrid_solver : select {"true", "false"}

        dynamics_simulation : select {"true", "false"}

        save_psi_sequential : select {"true", "false"}
        save_density_sequential : select {"true", "false"}
        save_chemical_potential_sequential : select {"true", "false"}
        save_free_energy_sequential : select {"true", "false"}
        save_geometry_sequential : select {"true", "false"}

        error_tolerance : double
```

```
    seed : int
    noise : double
    initial_noise : double

    phi_min : double

    iteration_max : int
    interval : int
    omega : double
}

file :
{
    wisdom : string
    output : string
}

multigrid :
{
    n_cycle : int
    n_pre : int
    n_post : int
    error_tolerance : double
}

geometry :
{
    dimension : int

    nx : int
    ny : int
    nz : int

    lx : int
    ly : int
    lz : int
}

blend :
{
    polymer[] : string
    volume_fraction[] : double
}

monomer :
{
    name[] : string
```

```
        b[] : double
        chi[][] : double
    }

    AB_diblock : polymer
\end{def}

\begin{data}
    condition :
    {
        "false",

        "false",

        "false",

        "false",
        "false",
        "false",
        "false",
        "false",

        1.0e-12,
        19876,
        0.0e-2,
        1.0e-3,

        -1.0,

        5000,
        500,
        0.1
    }

    file :
    {
        "fftw.wisdom",
        "dropsout.udf"
    }

    multigrid :
    {
        10,
        5,
        5,
        1.0e-4
    }
```

```
geometry :
{
    1,

    256,
    1,
    1,

    32,
    1,
    1
}

blend :
{
    [
        "AB_diblock"
    ],
    [
        1
    ]
}

monomer :
{
    [
        "A",
        "B"
    ],
    [
        1,
        1
    ],
    [
        [ 0, 3.0 ],
        [ 0, 0 ]
    ]
}

AB_diblock :
{
    40,
    [
        0.5,
        0.5
    ],
```

```
        [
            [ 0, 1 ],
            [ 0, 0 ]
        ],
        [
            "A",
            "B"
        ],
        20
    }
\end{data}
```

The input file is a bit verbose, but its parameters and conditions are equivalent to the Lua input file for `drops`. The datail format will be found in the section 'Input File Format'.

5 Reporting Bugs

If you find a bug in `dropsudf`, please send electronic mail to uneyama@ton.scphys.kyoto-u.ac.jp. Include the version number, which you can find by running '`dropsudf --version`'. Also include in your message the output that the program produced and the output you expected.

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

6 Input File Format

The input file is the OCTA UDF file. It is converted into Lua script for `drops` by `dropsudf`. Thus, most of the parameters is the same as the `drops` input file. In this section, the OCTA UDF variable definition for the input file and the difference between the `dropsudf` input and `drops` is shown.

6.1 Simulation Condition

```
condition :
{
    optimize_lattice : select {"true", "false"}

    use_multigrid_solver : select {"true", "false"}

    dynamics_simulation : select {"true", "false"}

    save_psi_sequential : select {"true", "false"}
    save_density_sequential : select {"true", "false"}
    save_chemical_potential_sequential : select {"true", "false"}
    save_free_energy_sequential : select {"true", "false"}
    save_geometry_sequential : select {"true", "false"}

    error_tolerance : double
    seed : int
    noise : double
    initial_noise : double

    phi_min : double

    iteration_max : int
    interval : int
    omega : double
}
```

`condition` is the same as the Lua input file, except for the type of some variables. For the `bool` type cannot be used directly in the OCTA UDF, the `bool` type are replaced by the `select` type which can be set to `"true"` or `"false"`.

6.2 Input / Output Files

```
file :
{
    wisdom : string
    output : string
}
```

`file` is majory different from the Lua input file. This is because `dropsudf` uses the OCTA UDF file as the output. Many output file names and its templates is not appear in the `dropsudf` input. The new variable is:

`file.output`
: (*string*)

  `dropsudf` output OCTA UDF file name (for the density field, the chemical potential field, the psi-field, the free energy and the geometry). The single data as well as the sequential data will be stored in this OCTA UDF file. Also note that no OpenDX file is created by `dropsudf`.

6.3 Multigrid Solver

```
multigrid :
{
    n_cycle : int
    n_pre : int
    n_post : int
    error_tolerance : double
}
```

`multigird` is completely the same as the Lua input file.

6.4 Geometry of Simulation Box

```
geometry :
{
    dimension : int

    nx : int
    ny : int
    nz : int

    lx : int
    ly : int
    lz : int
}
```

`geometry` is completely the same as the Lua input file.

6.5 Polymer Blend

```
blend :
{
    polymer[] : string
    volume_fraction[] : double
}
```

`blend` is completely the same as the Lua input file.

6.6 Monomer Species

The information about monomers is set as the `monomer` table.

```
monomer :
```

```
{
    name[] : string
    b[] : double
    chi[][] : double
}
```

`monomer` is completely the same as the Lua input file.

6.7 Polymer Species

```
class polymer :
{
    N : double
    f[] : double
    a[][] : int
    monomer[] : string
}

polymer : polymer
```

The definition for polymer species is like the Lua input file but there are some differences. First, the type of *polymer* is changed from the table (the structure, in the word of OCTA UDF) to the `polymer` class. `polymer` class have the same structure as the table for `polymer` in the Lua input file, but the type of `a` is changed from `bool` to `int` (for the OCTA UDF cannot handle `bool` type).

7 Output File Format

In this section, the variable definition for the output OCTA UDF file by `dropsudf` is shown.

```
position[][] : double

psi[][] : double
phi[][] : double
mu[][] : double

free_energy :
{
    total : double
    long_range : double
    local : double
    short_range : double
}

geometry :
{
    dimension : int

    nx : int
    ny : int
    nz : int

    lx : double
    ly : double
    lz : double
}
```

`position` (*array of array of double*)
: Array of position vectors.

`psi` (*array of array of double*)
: The output value of the psi-field. The first index corresponds to the position and the second index corresponds to the component type.

`phi` (*array of array of double*)
: The output value of the density field. The first index corresponds to the position and the second index corresponds to the component type.

`mu` (*array of array of double*)
: The output value of the chemical potential field. The first index corresponds to the position and the second index corresponds to the component type.

`free_energy.total`
(*double*)
: The total free energy per unit volume.

`free_energy.long_range`
(*double*)

The long range part of the free energy.

`free_energy.local`
(*double*)

The local part of the free energy.

`free_energy.total`
(*double*)

The short range part of the free energy.

`geometry.dimension`
The dimensions of the system.

`geometry.nx`
Number of divison in the x-axis direction.

`geometry.ny`
Number of divison in the y-axis direction.

`geometry.nz`
Number of divison in the z-axis direction.

`geometry.lx`
Length of the edge of the simulation box in the x-axis direction.

`geometry.ly`
Length of the edge of the simulation box in the y-axis direction.

`geometry.lz`
Length of the edge of the simulation box in the z-axis direction.

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```
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```

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