

make ENV=ICC/ICC_MKL_OMP (classic version)
make ENV=ICC/ICC_MKL_OMP HDF5=ON (new version)

Dear All

As you might have realized after using KAPSEL, the output options were not very flexible. If you chose to output field data, you had no choice but to output all of it (velocity, phi field, pressure, 5 components of the stress tensor), which would quickly increase the file size to unmanageable proportions. Furthermore, there were only two direct options to visualize the data, either gourmet or AVS/Express. The former was only useful for small systems, the latter was a commercial product. The latest version of KAPSEL, which you can download from the git repository, contains new output options that will hopefully help you in the visualization and analysis of your simulation data.

In this updated version, we have added support for the [hdf5 format](#) (which looks to become the standard input/output library for scientific simulation codes) to handle all data OUTPUT (fluid & particles). For the moment, all INPUT is still handled using UDF (you can still enable output.udf for particle data if you wish). There is even an hdf viewer/editor, similar to gourmet, which you can download from [here](#).

However, this viewer is not capable of visualizing the data, for this, we use the [xdmf format](#), as a simple xml wrapper, to tell applications such as [Paraview](#) and [Visit](#) how to load the data (both are free, both support xdmf natively).

Howto:

Compile:

Compilation is the same as before. Make sure the hdf5 library (version 1.8) is installed (modify the Makefile accordingly). You do not need to install the xdmf library

Input:

Old define/input files will continue to work. To use the new functionality choose 'EXTENDED' as FilteType (before you could only choose ASCII/BINARY). The EXTENDED options are as follows

-Driver

Format = HDF5 (no other options available at this time)

-Print_particle

First = n (only data for particles n, n+1, n+2, ..., N_total - 1 will be printed)

-Print_field

Crop = YES/NO (crop field data to hyperslab along x, y, or z direction)

Yes:

Slab = YZ/XZ/XY (print slab parallel to yz/xz/xy planes, perpendicular to x/y/z axis)

Start = n (start position : 0, 1, 2, ..., N_grid-1)

Width= n (number of planes to include in slab)

Vel : YES/NO (print fluid velocity)

Phi : YES/NO (print particle phi field)

Charge : YES/NO (print charge density fields for Electrolyte simulations)

Pressure: YES/NO (print pressure field)

Tau : YES/NO (print stress tensor field)

Visualize:

To generate the xdmf files simply run the h5kapsel2xdmf.py python script which has been added to the Tools/ directory

>\$./h5kapsel2xdmf.py data.conf

where data.conf is the configuration file written by kapsel to the output directory. This will generate two files: data_fluid.xdmf and data_particle.xdmf which you can directly load into paraview/visit.

For data analysis, you can use the [h5py](#) python package to access the trajectory data. Together with [Mayavi](#), this should also give you an additional visualization alternative (you can continue to use gourmet thanks to this python interface as well).

Example:

Attached is an example of the new input.udf/define.udf files for a system of 48 particles sedimenting in the -x direction (LX=128, LY=64, LZ=32).

The first 12 particles are skipped.

Only the fluid velocity data is saved, and only for a YZ slab of thickness 8 starting at (x) position 60. I have also included a brief howto guide to visualize this using Paraview.

Implementation Notes:

If you have modified a previous version of KAPSEL, and would like to incorporate the new changes, it should be possible to do this with very little work. The main modifications are in sp_3d_ns.cxx, where all references to AVS output routines have been replaced with calls to corresponding output functions which prepare all data and then call the specific writer (avs/hdf5/etc). The AVS code has not been modified. The new output writers are implemented using a virtual base class. It is therefore very easy to add new output writers. For a detailed view of the changes please see commit 3b8a7f3 in the git repository (feature/output_data branch).

ps. Feel free to forward this information to anyone I have forgotten. Also, please let us know if you find any bugs.

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