

GPUSPH Installation Guide

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1 Introduction

GPUSPH is an implementation of Smoothed Particle Hydrodynamics (SPH) on NVIDIA CUDA-enabled graphics cards. The first version of GPUSPH was developed by Alexis Héroult, guided by SPHysics, and presented at the Third SPHERIC Workshop in Lausanne, Switzerland in 2008. The graphics processing unit (GPU) implementation came from GPU-LAVA, a lava flow program, developed by Héroult and Bilotta at INGV in Catania, Italy. The present version of GPUSPH is open source, licensed under the GNU General Public License (www.gnu.org/licenses/gpl.txt). Smoothed Particle Hydrodynamics (SPH) is a Lagrangian meshless numerical method that was developed in astrophysics by Lucy (1977) and Gingold and Monaghan (1977). Its first application to free surface flows (e.g. dam breaks and waves) was by Monaghan et al. (1994). Since in SPH the interactions between particles involve many neighbors (several hundreds in three dimensions), it suffers from high computational costs. This motivated the development of massively parallel SPH codes, in particular codes running on graphics cards due to their performance and relatively low cost.

The development of sophisticated graphics cards is driven by the demands of advanced computer gaming, in particular to handle three-dimensional graphics for the computer display. Each of these graphics cards has numerous streaming processors to do the mathematics of image rotation, resizing etc. With the advent of the *CUDA* programming language from NVIDIA in 2007, simple C++ language can be used to access the mathematical power of these massively parallel cards. For computer simulations that are not data-intensive, GPU programming provides supercomputer capabilities at commodity prices.

Some timing information can be found in Héroult et al. (2010), showing that using the GPU is far faster (orders of magnitude) than using a CPU to compute SPH models. Speedups of 100 can be achieved for parts of the code when compared to serial versions of the code.

The first version of GPUSPH was running on NVIDIA's Compute Capability (CC) 1.x cards, GeForce 8xxx cards. From this first version we tested GPUSPH on all NVIDIA architectures (from Fermi CC 2.x to the latest Pascal CC 6.x). NVIDIA dropped support for CC 1.x and will soon do it for CC 2.x. So at the moment GPUSPH will run on any card with CC 2.x or higher (from Fermi up) but we expect to drop soon the support for CC 2.x. When done GPUSPH will run on any card with CC 3.x or higher (from Kepler up).

This guide is divided into several sections. First, the installation and set-up of the GPUSPH code is explained and some example problems to illustrate its use are

provided. The second chapter goes through all the steps necessary to build a new simulation and post-process the results. The third chapter deals with an overview of SPH, with which the reader should have some familiarity. Finally we discuss the nature of the GPUSPH program in some detail.

2 Installation of GPUSPH

The first step to run GPUSPH is to install the NVIDIA company's CUDA compilers and libraries (directions given below). CUDA is an extension of the C++ language to allow C++ to talk to the graphics card.

The second step is to install the open source software, CHRONO, which simulates rigid body dynamics. This library is used for any rigid objects that move, such as floating objects or objects moved by fluid flow.

The third step is to obtain, compile and run GPUSPH.

Remark: to run multi-node simulations, you also need to install OpenMP ($\geq 1.8.4$).

2.1 Installing CUDA

Ensure that your computer has an NVIDIA graphics card that is CUDA enabled. The NVIDIA website has a list of all the CUDA-enabled graphics cards: www.nvidia.com/object/cuda_gpus.html. You can check whether CUDA is already installed on your machine by launching the command:

```
nvidia-smi
```

from the terminal. If CUDA is installed it will give you information on the current state of the NVIDIA graphics card(s) on the machine.

Note: GPUSPH runs on cards with Compute Capability at least 2.0

Remark: regarding the choice of the GPU, the more CUDA cores and the more memory on the card, the better. Anyway a mid range mobile GPU's like GT750m/GT840 with 1 or 2GB of memory is sufficient to run significant simulations. A laptop with such a GPU will be a perfect mobile developing and testing platform.

The GPU programming language CUDA can be obtained from the NVIDIA website, CUDA Zone. The CUDA Toolkit and CUDA Software Development Kit (SDK) need to be installed for your operating system along with the video driver. These packages include the CUDA compiler `nvcc`, which is needed to develop executable code, and the graphics card driver that allows your program to access the GPU card.

Download the relevant driver for your machine from: <http://www.nvidia.com/Download/index.aspx?lang=en-us> and the CUDA toolkit from: <https://developer.nvidia.com/cuda-downloads> Follow the instructions provided by NVIDIA for the installation.

To ensure that all is installed correctly and working, you should compile and run the SDK examples, which include many programs that illustrate the capabilities of CUDA and the GPU; for example, NVIDIA's sorting program `radixSort` is used by GPUSPH to organize the neighbor list. Some interesting SDK programs are `fluidsGL` and `particles`. To compile the SDK programs, after the SDK is installed, go to `/Developer/GPUComputing/C` and (on a unix/linux or mac machine), type `make` on a terminal window command line. This should create a directory of executable examples located within the `C` directory called `bin/darwin/release` for the mac and `bin/linux/release` for a linux machine. In this directory, type `./fluidsGL` to run the `fluidsGL` example. You should see a green window open on your desktop. Use the mouse to stir up the fluid. The example program `Particles` is worth playing with as well, as it provided a basis for developing GPUSPH.

2.2 Installing GPUSPH

The GPUSPH source code is hosted on GitHub. The project's GitHub page is <http://github.com/GPUSPH/gpusph>.

To obtain the GPUSPH code, you can either use the `git` revision control system, or download a `.zipped` archive of a specific version. This manual refers to version 5.0 of GPUSPH.

If you have `git` installed, you can use

```
git clone https://github.com/GPUSPH/gpusph.git
cd gpusph
git checkout v5.0
```

to get version 5.0 specifically. Otherwise, download the `.zipped` archive from <http://github.com/GPUSPH/gpusph/archive/v5.0.zip>, and then

```
unzip v5.0.zip
cd gpusph-5.0
```

(you may remove `v5.0.zip` afterwards).

Within the top directory, you can find the `Makefile`, a `src` directory (holding the main GPUSPH source), a `scripts` directory (holding various auxiliary scripts), a copy of the license, settings to produce internal documentation with Doxygen, and a sample Digital Elevation Model (DEM) data file.

The most interesting source files in `src` are the `Problems`. A few sample problems are shipped with GPUSPH, showing how to employ specific features. You can get a list of the available problems by running

```
make list-problems
```

To build and test GPUSPH, you can run

```
make test
```

which should automatically detect your configuration, such as the compute capability of your GPU as well as the availability of optional libraries such as MPI (for multi-node support) or HDF5 (to read HDF5SPH data files).

When the building completes, you will have some new directories (`build` and `dist`) and a GPUSPH soft link to the compiled binary. `make test` will also automatically run `./GPUSPH` for you.

After building, simply running `./GPUSPH` will run the program again.

2.3 Installing the CHRONO library

The CHRONO website provides information for how to install CHRONO: http://api.chrono.projectchrono.org/tutorial_install_chrono.html

Remark: There is no need for the Irrlicht library with GPUSPH.

In this section we summarize the steps for the CHRONO library installation. To install CHRONO, besides the GPUSPH requirements you need to have `cmake` installed and a `cmake` interface like `ccmake` on Linux.

First, create a directory where to install CHRONO:

```
mkdir install_chrono
```

In that directory, clone the CHRONO repository from Github in a source directory:

```
cd install_chrono
git clone https://github.com/projectchrono/chrono.git source
```

This command will download the CHRONO repository in a folder named `source`.

Create a folder where to build CHRONO:

```
mkdir build
```

From the build repository, run `cmake`:

```
cmake ../source
```

Configure the compilation options with `ccmake`:

```
ccmake .
```

set the following options to off:

```
ENABLE_MODULE_CASCADE           OFF
ENABLE_MODULE_COSIMULATION       OFF
ENABLE_MODULE_FEA                 OFF
ENABLE_MODULE_FSI                 OFF
ENABLE_MODULE_IRRLICHT           OFF
ENABLE_MODULE_MATLAB              OFF
ENABLE_MODULE_MKL                 OFF
ENABLE_MODULE_OPENGL              OFF
ENABLE_MODULE_PARALLEL            OFF
ENABLE_MODULE_POSTPROCESS         OFF
ENABLE_MODULE_PYTHON              OFF
ENABLE_MODULE_VEHICLE             OFF
ENABLE_OPENMP                     OFF
```

Once this is done, you can compile the CHRONO project (still from the `build` folder):

```
make
```

and install the library (also from the `build` folder):

```
sudo make install
```

3 Choosing the GPUSPH Problem and other compilation options

You can test a different problem by using:

```
make OtherProblem test
```

where `OtherProblem` is the name of a different problem. You can get a list of available problems with `make list-problems`.

There are a number of other options available. A complete list of the options and their description can be obtained by running `make help-options`. All options (with the exception of `plain` and `echo`) are persistent across compilations, so they can be set once with `make option=value`, and subsequent executions of `make` will remember the `value` set.

The `make` options are listed below:

- `target_arch` - if set to 32, force compilation for 32 bit architecture
- `problem` - Name of the problem. Since version 5, you can just use the problem name as a target to build that particular test case.
- `dbg` - 0 no debugging, 1 enable debugging
- `compute` - 11, 12, 13, 20, 21, 30, 35, etc: compute capability to compile for (default: autodetect)
- `fastmath` - Enable or disable fastmath. Default: 0 (disabled)
- `mpi` - 0 do not use MPI (no multi-node support), 1 use MPI (enable multi-node support). Default: autodetect
- `hdf5` - 0 do not use HDF5, 1 use HDF5, 2 use HDF5 and HDF5 requires MPI. Default: autodetect
- `verbose` - 0 quiet compiler, 1 ptx assembler, 2 all warnings
- `plain` - 0 fancy line-recycling stage announce, 1 plain multi-line stage announce
- `echo` - 0 silent, 1 show commands
- `chrono` - 0 do not use the CHRONO library, 1 use the CHRONO library

To view your current make options type `make show` instead of `make`.

4 Example Problems

Simulations in GPUSPH are defined in terms of **Problems**. Some example problems are provided with GPUSPH itself, to illustrate the basics of problem design, and how to use the fundamental building blocks provided by GPUSPH. Such building blocks include a variety of geometrical shapes to describe the (fixed) solid boundaries of the domain, as well as a number of objects that move following prescribed laws, such as gates, pistons and paddles.

These objects are designed to offer great flexibility in their use, far beyond what is shown in the sample problems. This flexibility should allow you to create very complex simulations by combining the objects appropriately.

The number of particles used in the test problems is deliberately taken as a small number, simply to allow for fast execution times even on older hardware. One of the

first tests to try is to increase the resolution by reducing the size of the particles. For example, by reducing the particle size from the default of 0.025m to the smaller 0.02m, `DamBreak3D` would run with 21,252 particles instead of the default 10,664.

This can be done in two ways. A permanent change comes about by editing the problem file (e.g. `DamBreak3D.cc`) and changing the value passed as argument of `set_deltap()` (e.g., replace `set_deltap(0.025f);` with `set_deltap(0.02f);`). The second way is to specify the particle size at runtime using the appropriate command line option (described below): e.g. `./GPUSPH --deltap 0.02`.

4.1 DamBreak3D

`DamBreak3D` is a case originally used by Gomez-Gesteira and Dalrymple (2004) for testing a prototype version of SPHysics. It is based on some experiments done by Arnason (2005) at the University of Washington. We assume an instantaneous breaking dam and the resulting flow impinging onto a rectangular object. The whole problem is contained within a bounding box, which extends 1.6m in length (x axis), 0.67m in width (y axis), and 0.4m in height. This is the experimental box. The fluid behind the dam is a rectangular box of water at one end of the tank at time equal to zero. The dam is assumed to break instantaneously so that the column of water, confined on three sides, collapses into the tank. In the tank there is a vertical rectangular object – the collapsing water column impacts on the tank and then flows up the front face of the object and around the sides. Finally the water hits the back wall of the tank. A screenshot of the simulation at time 0.6s is provided in the Figure 1.

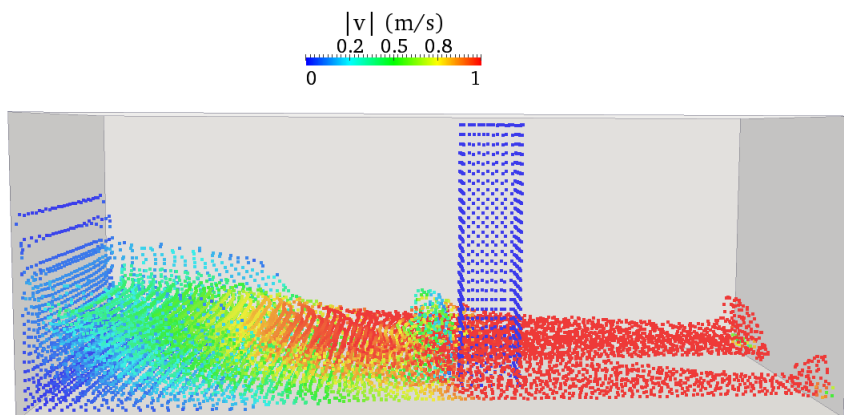


Figure 1: Screenshot of the `DamBreak3D` simulation at time 0.6s.

4.2 DamBreakGate

In most laboratory experiments of dam breaks, the dam takes a certain amount of time to move out of the way. The example problem `DamBreakGate` illustrates the use of moving boundaries with prescribed motions. The problem is set up the same way as the `DamBreak3D` case, but there is a moving gate that is raised vertically with a linearly varying velocity. In this case, the gate will move with a velocity that is zero when the problem starts and that linearly increases with time until the gate is outside the domain. The effect on the dam break is that the escaping water is affected by the gate motion. (See Crespo et al. (2008)'s SPH modeling of János et al. (2004)'s experiment, where a moving gate was important.)

The moving gate is created by defining its geometry with a geometry type `GT_MOVING_BODY`, and overriding the Problem `moving_bodies_callback` function to determine the linear and angular velocity of the body.

A screenshot of the simulation at time 0.8s is provided in the Figure 2.

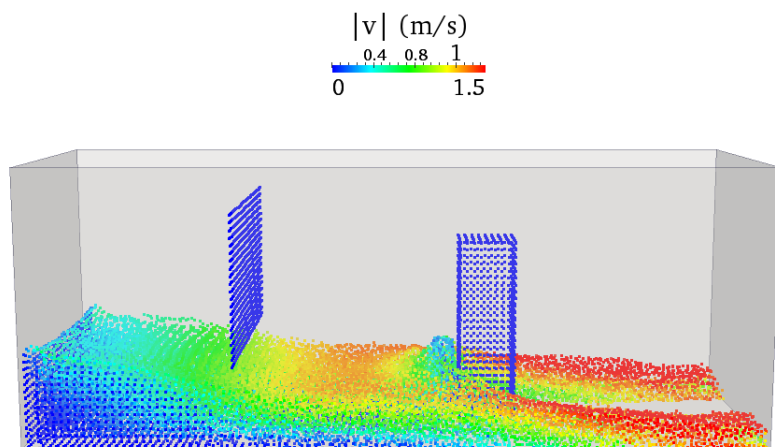


Figure 2: Screenshot of the `DamBreakGate` simulation at time 0.8s.

4.3 OpenChannel

This problem represents an instantaneous start up of a highly viscous and dense fluid flow in an open channel on a 9 deg slope. The channel is rectangular in cross-section (1m wide and 0.7m deep) and the computed length of the infinitely long channel is 2m. The side walls are fixed (Leonard-Jones boundary force) while the computational

ends of the domain are periodic, so that a particle leaving the downstream end of the model domain enters the upstream end at the same place, 2m upstream.

The periodic boundary here is used in the x direction, although boundaries in other problems can be periodic in the other directions as well. The key parameter in the problem statement is the simulation framework `periodicity`, which can be set to any combination of `PERIODIC_X`, `PERIODIC_Y`, `PERIODIC_Z` to indicate periodicity along each of the axes. Figure 3 shows the shape of the velocity field in the channel after time convergence.

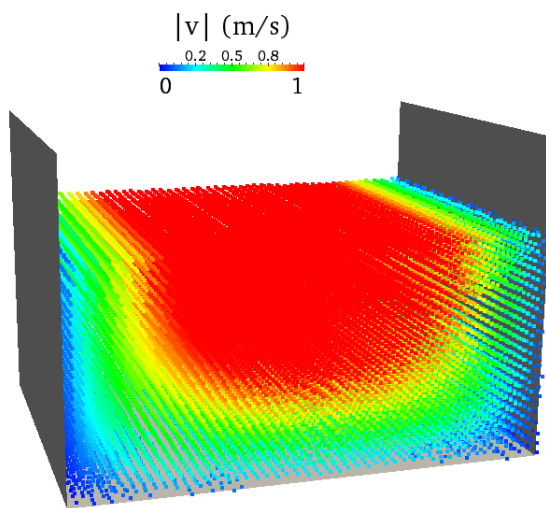


Figure 3: Screenshot of the OpenChannel simulation after time convergence.

4.4 WaveTank

WaveTank uses a moving boundary to create a paddle wavemaker at one end of a wave tank with a sloping bottom (bottom slope is 4.2364 deg). The wavemaker motion is controlled by the `moving_bodies_callback` function. In this case, the length of the paddle is 1.0m and the paddle pivots about an origin `m_origin`; here, the pivot is located 0.1344m below the bottom and 0.13m from the front wall of the tank. To specify the paddle motion, the angular frequency of the motion ($2\pi/T$, where $T = 1$ s is the wave period), and the wave paddle stroke at the water surface ($S = 0.1$ m) are given in the variables `mb_omega` and `mb_amplitude`. To change the

stroke and the frequency of the wave paddle, you must change these variables in the problem file, `WaveTank.cc`. Figure 4 shows a screenshot of the simulation at time 9s.

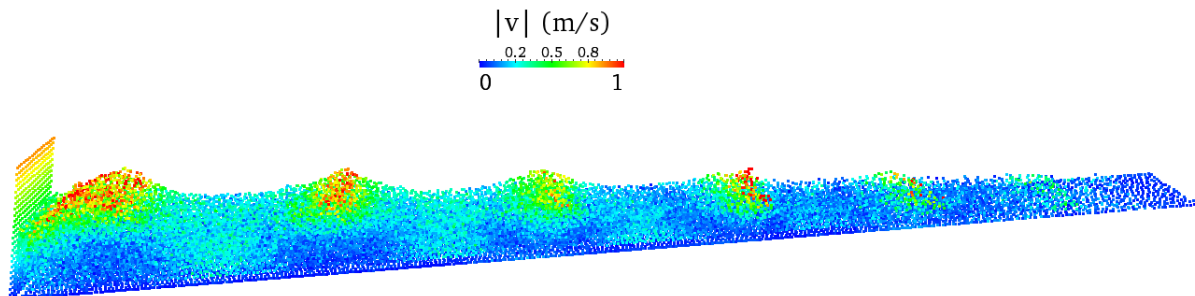


Figure 4: Screenshot of the WaveTank simulation at time 9s.

4.5 SolitaryWave

SolitaryWave is similar in set up to the WaveTank example, except that a piston moving boundary is used. The motion of a vertical plate is determined by the method of Goring (1979), available in PDF format from: <http://caltechkhr.library.caltech.edu/50/>. The full excursion (stroke) of the paddle is the variable `S`.

4.6 Seiche

The Seiche problem is to examine the influence of shaking on a rectangular container of size: $\ell = 0.707\text{m}$, $w = \ell/2$, and depth, $H = 0.5\text{m}$. The purpose of the example is to illustrate the ability to vary gravity in a problem. As the problem starts, there is water in the container. After 0.3s, gravity is modified by adding a component in the x direction, such that the total gravity vector is `set_gravity(3.*sin(9.8*(t-m_gtstart)), 0.0, -9` which means that the container is shaken with a sinusoidal motion with angular frequency of 9.8s^{-1} (period = 0.64s), with a magnitude of 3m/s^2 until time `m_gtend=3.0` is reached, when the gravity vector once again returns to the vertical acceleration of gravity. After this time, the seiching motion starts to decrease in amplitude.

The variation of gravity with time (and any stop (`m_gtend`) and start times) is prescribed in a user-supplied (in the problem) `g_callback` function.

4.7 DEMExample

This is an example showing how to use GPUSPH's support for Digital Elevation Models (DEMs). It loads the topography of the bottom of the domain from a file called `half_wave0.1m.txt`, shipped with GPUSPH. A different DEM can be used, by either changing the name in the source `DEMExample.cu` file, or by providing the new name as argument to the `--dem` command-line option to GPUSPH.

5 GPUSPH Command Line Options

When running from the command line, there are several options available to you to alter some aspects of the GPUSPH run.

- device *integer*** Choose which GPU(s) to use for the run. On the command line: `./GPUSPH --device N`, where N is the (integer) number of the device you wish to use. To find the number associated with each of your CUDA-enabled devices (graphics cards), you can use the CUDA SDK program `DeviceQueryDrv`. If you only have one CUDA-enabled GPU, the only possible choice for N is 0, which is the default. If you want to run the simulation on several GPUs, the command is: `./GPUSPH --device i,j,k`
- deltap *float*** Change the resolution (inter-particle spacing) at which the problem should be run.
- tend *float*** The model time in seconds when you wish the model to stop.
- dt *float*** Force the use of the fixed, specified time-step, even if the problem would use dynamic time-stepping otherwise.
- dem *string*** For the Problem DEMExample: the name of the DEM file to use.
- resume *fname*** Resume from the given file (HotStart file saved by HotWriter).
- checkpoint-every *float*** HotStart checkpoints will be created every VAL seconds of simulated time (float VAL, 0 disables).
- checkpoints *integer*** Number of HotStart checkpoints to keep.
- maxiter *integer*** Break after this many iterations.
- dir *string*** Use given directory for dumps instead of date-based one.

- nosave** Disable all file dumps but the last.
- gpudirect** Enable GPUDirect for RDMA (requires a CUDA-aware MPI library).
- striping** Enable computation/transfer overlap in multi-GPU (usually convenient for 3+ devices).
- asynccmpi** Enable asynchronous network transfers (requires GPUDirect and 1 process per device).
- num-hosts *integer*** Uses multiple processes per node by specifying the number of nodes.
- byslot-scheduling** MPI scheduler is filling hosts first, as opposite to round robin scheduling.
- debug *flags*** Enable specified debug flags.
- help** Show the help and exit.

5.1 Debugging GPUSPH execution

To assist developers when introducing new GPUSPH features, it is possible to trace the execution of the simulator, providing insight on the evolution of some of the internal structures using the provided debug flags. Multiple debug flags can be enabled in a single run, by passing a comma-separated list as an argument to **--debug**. For example:

```
./GPUSPH --debug print_step,inspect_buffer_access
```

The `validate_init_position` debug option is also useful for users that want to further validate their initial setup.

The debug flags currently supported are:

print_step print each step and command as it is being executed;

neibs debug the neighbors list on host, saving it to file;

forces debug forces on host, saving them to file;

numerical_density debug relative density variation on host, saving it to file;

inspect_preforce inspect pre-force particle status; this saves the particle system status before each force computation;

inspect_pregamma inspect pre-gamma integration particle status; this saves the particle system status before the gamma integration kernel execution;

inspect_buffer_access inspect buffer access; show how each buffer is being accessed (reading or writing, and from which state) during execution of each command; note that this needs compile-time support, by enabling `#define DEBUG_BUFFER_ACCESS 1` in `src/buffer.h`;

inspect_buffer_lists inspect the state of the particle system and its buffer lists (states and free buffer pool) after each command;

check_buffer_update check buffer update; this is used to check that all and only modified buffers are exchanged in an `UPDATE_EXTERNAL` call;

check_buffer_consistency check buffer consistency; when this is enabled, after every command GPUSPH will verify that the shared parts of the subdomains in multi-GPU simulations are consistent across devices; note this needs compile-time support, by adding `-DINSPECT_DEVICE_MEMORY` to `CPPFLAGS` in `Makefile.local`;

clobber_invalid_buffers clobber invalid buffers; when this is true, every time a buffer is marked invalid, its content will be clobbered (reset to the initial value, typically NAN or equivalent); useful to check that stale data is not being used inadvertently; note that this needs compile-time support, by enabling `#define DEBUG_BUFFER_ACCESS 1` in `src/buffer.h`;

validate_init_positions throw an exception (instead of just warning) if a particle is out of bounds during initialization of the problem;

benchmark_command_runtimes measure (and show) command runtimes.

6 Running multi-node simulations

GPUSPH can distribute the computation of a simulation on multiple GPU devices attached to different nodes of a cluster in different ways.

Say we want to launch a simulation on N nodes, each with D devices (with CUDA device numbers ranging from 0 to $D-1$); the total number of devices in the simulation will be $N \times D$. We can run either:

- one process per node, D GPUs per process

- 2 processes per node, $D/2$ GPUs per process
- 4 processes per node, $D/4$ GPUs per process
- etc.

Additionally, some MPI implementations have built-in support for CUDA, which allows for faster communication between devices on different nodes. Experimental support for this feature can be enabled in GPUSPH with the `--gpudirect` command-line option.

The best decision on how to distribute the computation across nodes and devices depends on the queue policy of the cluster, on the network topology, on simple a posteriori performance tests, on the capabilities of the MPI implementation, etc.

If we wanted to run the simulation on all the devices of one node, we would run in an interactive shell:

```
./GPUSPH --device 0,1,...D-1
```

Running the same simulation on multiple nodes only requires to run the same command within the reference MPI launcher (usually a script called `mpirun`); GPUSPH will retrieve the necessary information about the launch environment directly from the MPI runtime and will organize the node-to-node communication accordingly.

```
mpirun -np N ./GPUSPH --device 0,1,...D-1
```

This command leaves to MPI the choice of which nodes to use in the network, if more than N are available. It is always safe to provide MPI a list of hostnames corresponding to the nodes chosen to run the simulation. If the file containing the list of hostnames is called `myhostsfile`, a typical syntax will be:

```
mpirun -np N -hostfile ./myhostsfile \  
./GPUSPH --device 0,1,...D-1
```

Please note the syntax may vary from one MPI library to another. For example, MVAPICH uses `-hostfile` while OpenMPI `--hostfile`.

Let us now see the command line options needed to run the same simulation with more processes (and thus on more nodes) and a smaller number of devices per process. In this case we need to inform both the MPI runtime and GPUSPH. For the former, we simply decrease the number of processes to start (with the `-np` option); for the latter, we need to shorten appropriately the list of devices passed with the `--device` option. If our aim is to run $N * 2$ processes each using $D/2$ devices, we then run:

```
mpirun -np N*2 -hostfile ./myhostsfile \  
./GPUSPH --device 0,1,...D/2-1
```


Here we need to take care of a few important details. If the list of available hosts contains at least $N * 2$ hostnames, the MPI runtime will start every process on a different physical node. But what happens if the list is shorter (e.g. N hosts only), or if we want anyway to use a smaller number of nodes (for example because part of the cluster is already used by other processes)? The MPI runtime will start multiple processes per node and the GPU device numbers will be likely to conflict (i.e. two different processes might try to use the same GPU device for different parts of the simulation domain, causing a performance slowdown or a failure if the CUDA devices are set in “exclusive mode”). In this case, we must inform GPUSPH that the number of physical hosts (i.e. nodes) is smaller than the number of processes, so that it will shift the GPU device numbers of the appropriate processes and no GPU device will be accessed by two processes. The corresponding option is `--num-hosts`:

```
mpirun -np N*2 -hostfile ./myhostsfile \
--num-hosts N ./GPUSPH --device 0,1,...D/2-1
```

But there is another important detail. There are different ways the MPI runtime can distribute the processes across the nodes. Two very common policies are “by slot” (fill-first) and “by node” (round robin). The scheduling policy affects the association between the process ranks and the CUDA device numbers, so GPUSPH must be informed about it to use the appropriate offsets. GPUSPH assumes a round robin schedule is being used; if this is not true, the `--byslot-scheduling` option must be passed:

```
mpirun -np N*2 -hostfile ./myhostsfile \
--num-hosts N --byslot-scheduling \
./GPUSPH --device 0,1,...D/2-1
```

There is no optimal policy in general as its performance depends on the node load and the node-to-node connection speed. It is worth trying both to check whether one is more performant than the other. The default policy is usually “by slot”(fill-first, usually preferred by non GPU-based softwares) but it is always safer to explicitly set it for every run. In OpenMPI the corresponding options are `--byslot` and `--bynode`. One final possibility is to run one process per device. This is the most consuming option from the point of view of the host memory, since every process will allocate on host the whole simulation scenario, but it might be useful if the GPUDirect feature is being used but the MPI runtime does not support multiple devices per process, or if the amount of data to be saved on file is large or the saving frequency is very high, so that saving would benefit from a parallel dump (every process saves its part of the simulation independently from the other processes).

Finally, let’s see some practical examples. Suppose our cluster has 12 nodes, each

equipped with 4 GPU devices. We need to run a simulation on 12 devices. To run 3 processes on 3 hosts, each using 4 devices, we will run:

```
mpirun -np 3 -hostfile ./myhostsfile ./GPUSPH --device 0,1,2,3
```

To run 6 processes on 6 hosts, each using 2 devices, we will run:

```
mpirun -np 6 -hostfile ./myhostsfile ./GPUSPH --device 0,1
```

Note that another simulation can be run simultaneously on the remaining 2 devices of the same nodes, with:

```
mpirun -np 6 -hostfile ./myhostsfile ./GPUSPH --device 2,3
```

To run 6 processes on 3 hosts, each using 2 devices, we will run:

```
mpirun -np 6 -hostfile ./myhostsfile_with3hosts \  
--num-hosts 3 ./GPUSPH --device 0,1
```

(-byslot-scheduling might also be necessary)

To run 12 processes on 12 hosts, each using 1 device, we will run:

```
mpirun -np 12 -hostfile ./myhostsfile ./GPUSPH --device 0
```

Note that another simulation can be run simultaneously on one of the free devices of each node (e.g. device number 3), with:

```
mpirun -np 12 -hostfile ./myhostsfile ./GPUSPH --device 3
```

Please note the options for the MPI library always precede the GPUSPH executable name. If the MPI library supports it, we also suggest enabling the option to tag each line of the output with the process rank that has generated it; in OpenMPI, the option is called `--tag-output` while in MVAPICH `-prepend-rank`. This will come very helpful when the logs need to be analyzed (tip: use `grep` to separate the logs if they are multiplexed).

If you need to use any queue-management system, remember to inform it about the desired topology, coherently with the options passed to GPUSPH. For example, with PBS you would set the `nodes` and `ppn` parameters for the number of hosts and processes per host, respectively.

7 Installing pre/post processing tools

7.1 Installing SALOME

You can download SALOME from: <http://www.salome-platform.org/downloads/current-version>

For this you need to register on the SALOME website. Then, follow the installation instructions from the SALOME website and the installer.

Remark: SALOME is used for SA boundary pre-processing, to generate an STL mesh of the boundaries. You can of course use another mesher of your choice for this step.

7.2 Installing CRIXUS

Crixus is a preprocessing tool for GPUSPH.

Prerequisites:

- `cmake` \geq 2.8
- `cuda`
- `hdf5` \geq 1.8.7

Getting CRIXUS:

```
git clone https://github.com/Azrael3000/Crixus.git
cd Crixus.git
```

Compiling Crixus: Crixus uses CMake for compilation. Let us assume that you have CRIXUS in a `Crixus.git` directory. and you want the building to happen in `Crixus.git/build` then follow the commands below:

```
mkdir build
cd build
cmake ..
make
```

Note that you should not run `cmake` in the main Crixus folder.

The binary is then located at `Crixus.git/build/bin/Release/Crixus`. Note that `make install` is not supported yet. To easily change the parameters of `cmake` you can use `ccmake` instead.

If `hdf5` cannot be found due to lacking environmental variable you can edit the main `CMakeLists.txt` which has a commented line that reads:

```
#set(ENV{HDF5_ROOT} "/your/path/to/hdf5")
```

Uncomment it and set the respective `hdf5` path in order to use your custom installation.

To finish the installation it is recommended to add the path to the CRIXUS binary to your `PATH` environment variable. Add this line in `~/.bashrc`:

```
export PATH=/your_path/Crixus.git/build/bin/Release/Crixus:$PATH
```

where /your_path is your path to the CRIXUS directory.

7.3 Installing PARAVIEW

PARAVIEW is directly available from the Linux packages.

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