

MIKE Powered by DHI

GPU - Guidelines



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1 Background

Since the release of MIKE 2016, all of the Flexible Mesh models, with MIKE 21 Spectral Waves FM being the only exception, are capable of utilising graphics processing units (GPUs) for parallelisation. Reaching optimal performance of the GPU is not always straightforward. There are a number of pitfalls that should be avoided and a number of things worth keeping in mind.

These guidelines are divided into four sections and will address some of the issues related to: Hardware, GPU Configuration and Model Setup. Finally, the fourth section consists of a number of Frequently Asked Questions (FAQs).

2 Hardware

Some of the things worth considering are related to the GPU hardware and the installation of it:

- Only NVIDIA GPUs of compute capability 2.0 or higher are supported. A list of GPUs and their compute capability is found at: <https://developer.nvidia.com/cuda-gpus>.
- A GPU is not just a GPU. Some GPUs are suitable for gaming, some for visualisation and others for scientific computations.
To obtain good performance in a scientific computing context the GPU should have a high number of Streaming Multiprocessors and cores (shading units). Other important specifications are the amount of memory and the bandwidth. An essential value is the theoretical double precision floating-point performance (FLOPS rate). Some GPUs have excellent single precision floating-point performance, but less impressive double precision floating-point performance.
- When installing the GPU in the computer, make sure to install the GPU to the fastest PCI Express slot available. Otherwise, an unnecessary data transfer bottleneck may have been created. When utilising multiple GPUs the PCI Express slots should have identical speed in order to obtain optimal performance.
- Among the fastest PCI Express slots available, choose the slot with the most physical space around the GPU, such that down-clocking due to reaching the heat limit (GPU driver specified) and the risk of computer shut down due to overheating are reduced. Potentially, an extra cooling system is needed to ensure a sufficient heat transportation.
- Make sure that the computer has a power supply, which is large enough to cover the total power consumption of all the installed GPUs.
- When utilising multiple GPUs the best performance is obtained using identical GPUs. Otherwise, the GPU with the lowest performance dictates the overall performance.
- Some graphics cards consist of two GPUs, e.g. GeForce GTX Titan Z and Tesla K80. The MIKE software recognises these dual graphics cards as two individual GPUs. Hence, to fully utilise these graphics cards a license permitting multiple GPU usage is required.

3 GPU Configuration

After having installed the GPU there are a few things to consider with respect to configuration:

- Use the latest NVIDIA driver supporting the considered GPU. Drivers can be found at <http://www.nvidia.com/Download/index.aspx>.
- For older graphics card drivers it is not possible to utilise the GPU when accessing the machine remotely using Microsoft Remote Desktop Connection. The only exception is when the GPU supports TCC (Tesla Compute Cluster) mode, which is the case for the NVIDIA Tesla family of graphics cards. For GPUs not supporting TCC mode it is necessary to install a third-party VNC client in order to use remote login.
For newer graphics card drivers it is possible to utilise the GPU when using remote login through Microsoft Remote Desktop Connection. However, it still might be necessary to use a third-party VNC client in order to gain access to the NVIDIA Control Panel when using remote login.
- A few NVIDIA GeForce GPUs have a CUDA Double Precision switch, which can be enabled from the NVIDIA Control Panel. The default setting for the MIKE FM models capable of utilising GPUs is to perform the floating-point calculations taking place on the GPU in double precision. Hence, enabling the CUDA Double Precision switch will improve performance of the models significantly. Note that not all GPUs have this feature. Please see the FAQ in Section 5.2 for information on how to determine whether or not the GPU has this switch and how to enable it.
- The NVIDIA Tesla GPUs support ECC (Error Correcting Code) memory protection, which helps reducing data errors. However, by disabling this feature it is possible to increase performance. In the benchmarking reports mentioned in Section 5.4 ECC was disabled.

4 Model Setup

When setting up the model there are a few things to keep in mind regarding performance:

- In order to obtain good performance for the MIKE FM models using GPU parallelisation the number of wet elements in the domain should be sufficiently large. Here, the emphasis is on the wording “wet elements”, since it is not sufficient to have a huge number of elements representing the domain if there is almost no water in the domain.
For the test cases presented in the benchmarking reports (see section 5.4) the maximum performance of the GeForce GTX Titan GPU is reached only after using around 400.000 or more wet elements in the domain for each GPU. If the model domain for each GPU is described using only a small number of elements, then the MIKE FM models could in fact be slower when utilising the GPU than when not utilising it.
- Only output what is necessary, and only when it is necessary. Writing output from the GPU is time consuming due to transferring data from GPU memory to CPU memory.
- Depending on the accuracy needed in the model results, it might be preferable to perform the floating-point calculations taking place on the GPU in single precision instead of double precision, which is the default setting for the MIKE FM models. The reason is that some GPUs have a significantly higher processing power when performing single precision floating-point calculations rather than double precision floating-point calculations. Hence, for these GPUs a significant performance increase is expected when switching from double precision GPU calculations to single precision GPU calculations.
However, be aware that single precision calculations are by definition less accurate than double precision calculations, which to some degree will affect the modelling results. Please, see section 5.3 on how to instruct the MIKE FM models to use single precision GPU calculations.

5 Frequently Asked Questions

This section lists a few FAQs related to the usage of GPU. For the full list of FAQs for the MIKE software, please visit <http://faq.dhigroup.com/>.

5.1 Why does the MIKE software not find my GPU?

If the GPU is not recognised by the MIKE software it may be due to an outdated GPU driver. Please try updating the driver. Drivers are found at this webpage: <http://www.nvidia.com/Download/index.aspx>.

Alternatively, the GPU might not be supported by the MIKE software. Only NVIDIA GPUs of compute capability 2.0 or higher are supported. A list of GPUs and their compute capability is found at: <https://developer.nvidia.com/cuda-gpus>.

If the GPU has been successfully recognised by the MIKE software, then the “Parallelization” tab in the “Launch Settings” dialog in the respective MIKE FM editor will look similar to the left picture in Figure 5.1. Otherwise it will look similar to the right picture in Figure 5.1.

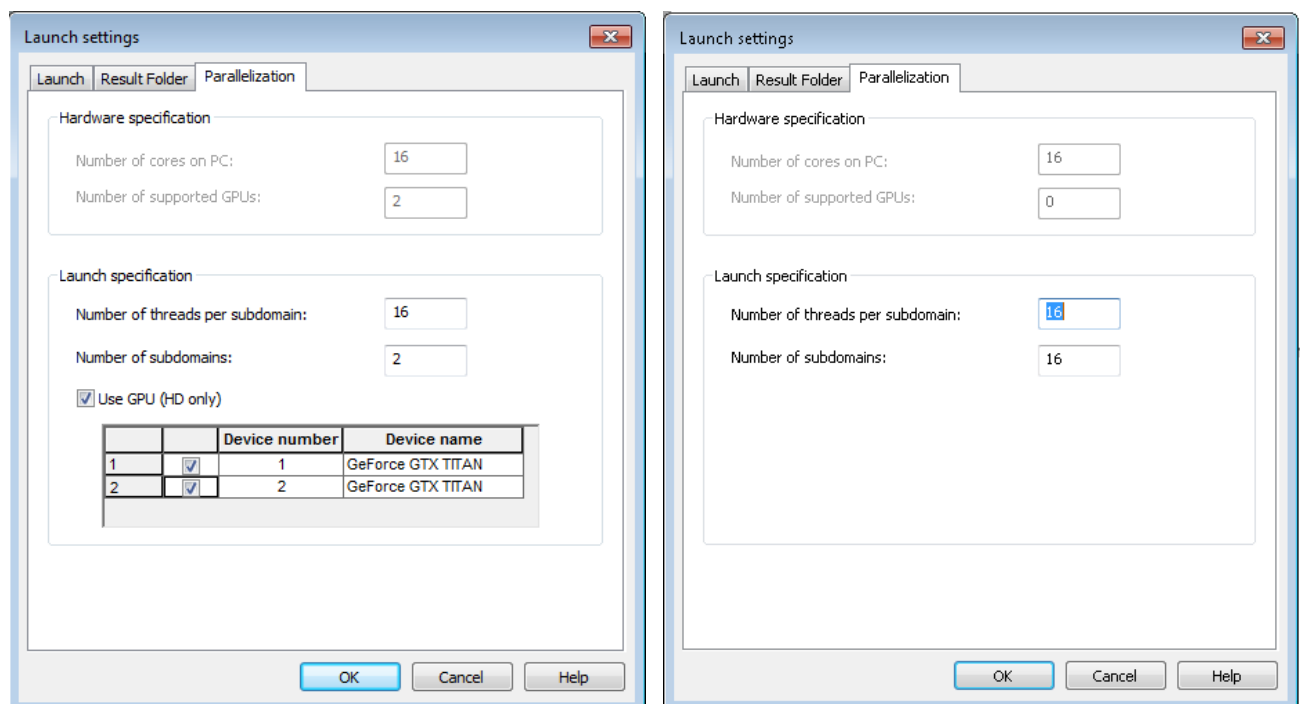


Figure 5.1 *Left:* Dialog where the GPUs have been recognised. *Right:* Dialog where the GPUs have not been recognised

5.2 Does my GPU have a CUDA Double Precision switch?

A few NVIDIA GeForce GPUs have a CUDA Double Precision switch, which can be enabled from the NVIDIA Control Panel. By enabling this switch more of the GPU's processing power is dedicated to performing double precision floating-point calculations.

This feature is only available for some GeForce GPUs, e.g. GeForce GTX 580, GeForce GTX Titan, GeForce GTX Titan Black, GeForce GTX Titan-Z and possibly others.

Since the default setting for the MIKE software is to use double precision floating-point calculations on the GPU, enabling this switch will improve performance of the GPU simulations significantly.

Please note, that the NVIDIA Tesla GPUs does not have this switch, since these GPUs are designed explicitly for doing numerical calculations.

If the GPU has a CUDA Double Precision switch, then it can be enabled as illustrated in Figure 5.2. If the switch is not there, then the GPU does not support this feature.

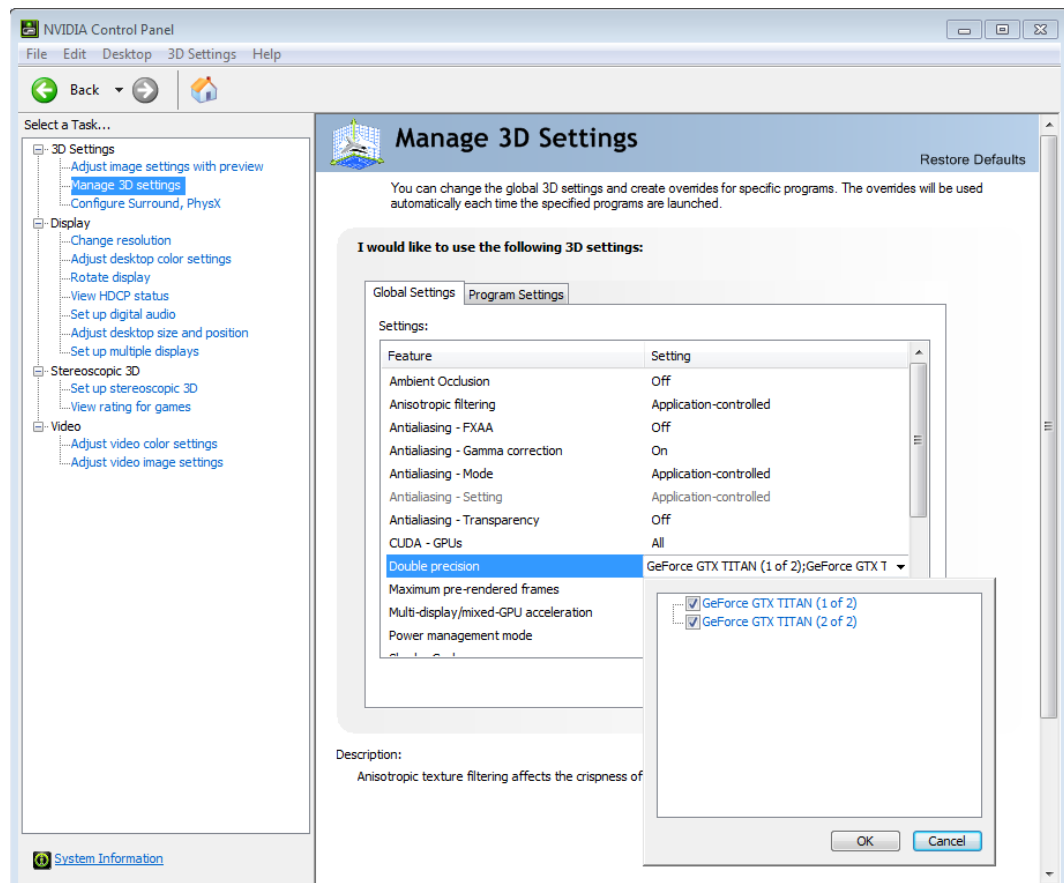


Figure 5.2 Screenshot of the NVIDIA Control panel showing how to enable the CUDA Double precision switch

5.3 How do I force MIKE to use single precision GPU calculations?

The default setting for the MIKE FM models is to perform the floating-point calculations taking place on the GPU in double precision, since double precision calculations are more accurate than single precision calculations.

It is, however, possible to force the calculations taking place on the GPU to be performed in single precision. The reason for this is that some GPUs have a significantly higher processing power when performing single precision floating-point calculations rather than double precision floating-point calculations. Hence, switching to single precision calculations for these GPUs might lead to a significant performance increase.

Be aware, that switching to single precision calculations will affect the accuracy of the model results to some degree. Whether this is a problem or not depends on the specific model.

Single precision GPU calculations are enabled from within MIKE Zero → File → Options → User Settings → Simulation Settings → “Use single precision GPU calculations” checkbox, please see Figure 5.3.

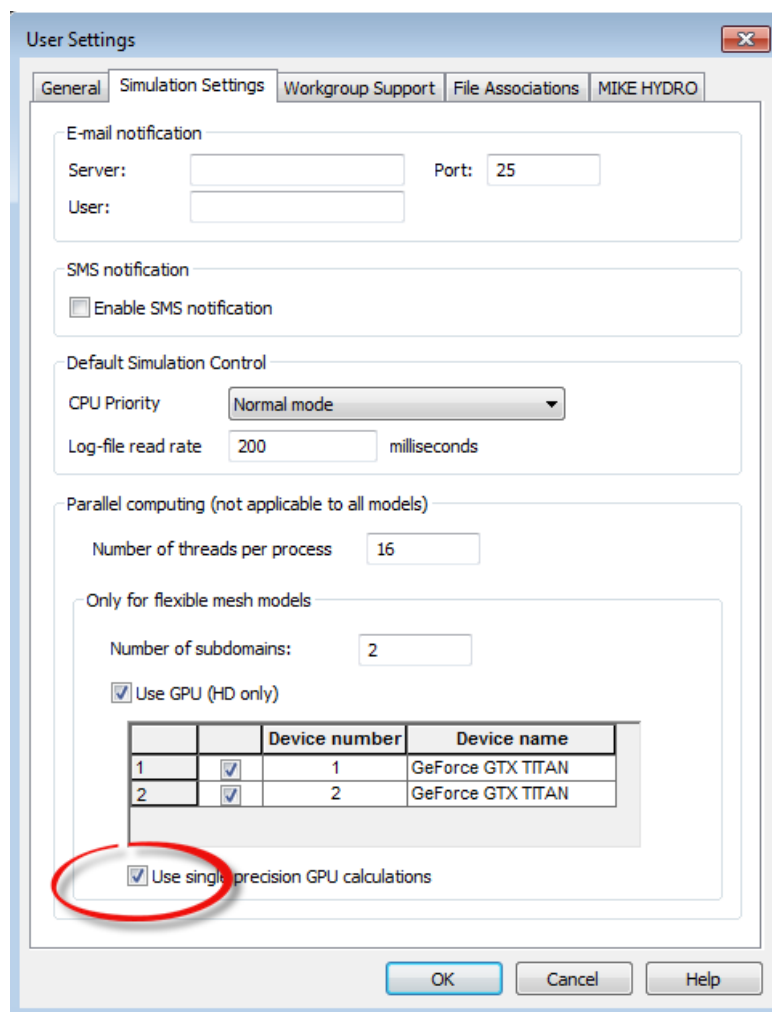


Figure 5.3 How to enable single precision GPU calculations from within MIKE Zero

5.4 Which GPUs have been tested by DHI?

Extensive benchmarking have been done for both MIKE 21 Flow Model FM utilising GPU and MIKE 3 Flow Model FM utilising GPU. The tests have been conducted using a number of different GPUs. The benchmarking results for MIKE 21 Flow Model FM and MIKE 3 Flow Model FM, respectively, are presented in the following two reports:

[MIKE 21 Graphical Processing Units \(GPU\) benchmarking report](#)

and

[MIKE 3 Graphical Processing Units \(GPU\) benchmarking report](#)

5.5 How many subdomains and threads should I use?

Launching a simulation from within the MIKE FM editors makes the “Launch settings” dialog appear. On the “Parallelization” tab in this dialog the user can specify which parallelisation technique to use for the simulation, please see Figure 5.4.

The number of subdomains specifies the number of domains to decompose the model domain into. Generally, this number should not exceed the number of CPU cores available on the machine. When utilising GPUs, this number should reflect the number of GPUs to use for the simulation. In rare occasions it might be beneficial, from a performance perspective, to use more subdomains than GPUs, but never less subdomains than GPUs.

The number of threads per subdomain specifies the number of OpenMP threads to use for each subdomain during the simulation. As a rule of thumb, this number times the number of subdomains should be less than or (preferably) equal to the total number of CPU cores available on the machine.

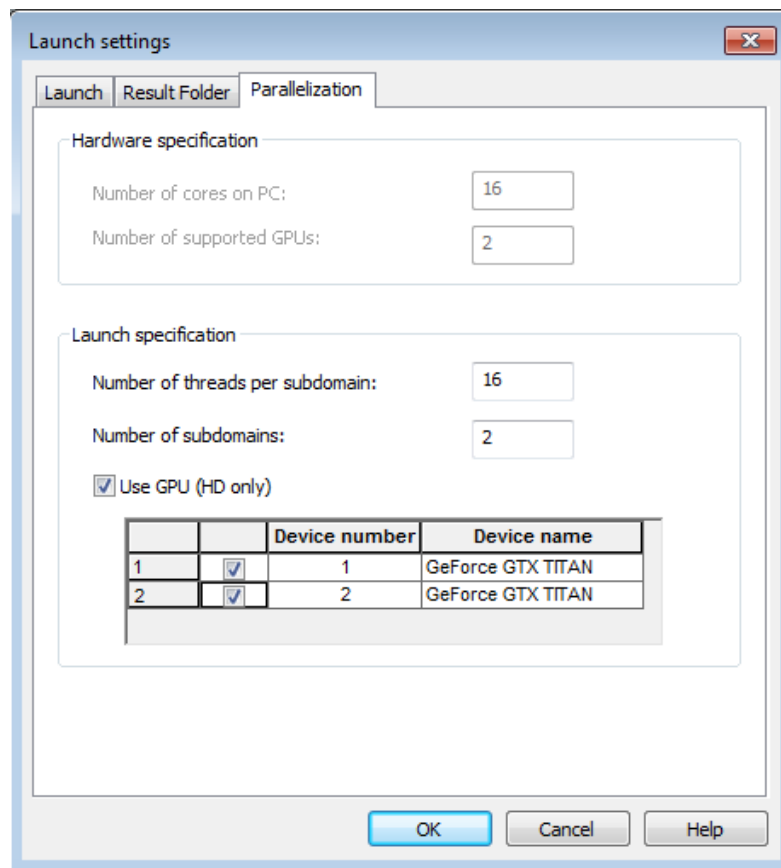


Figure 5.4 The “Launch Settings” dialog where parallelisation technique is specified

5.6 How do I run GPU simulations in batch?

There are a couple of possibilities on how to run GPU simulations in batch.

The first possibility is to use the MzLaunch.exe application, which is installed with the MIKE Zero installation, please see Figure 5.5.

In Figure 5.5, the first call to MzLaunch.exe is followed by the optional parameter -gpu 1, which instructs MzLaunch.exe to utilise the GPU using 1 subdomain. The second call instructs MzLaunch.exe to utilise the GPU using 2 subdomains. When using more than one subdomain, the application will automatically distribute the work over the same number of GPUs, if available.

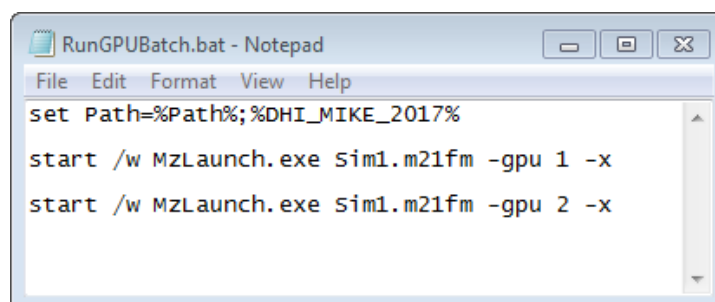


Figure 5.5 Calling the MzLaunch.exe application with optional parameters for utilising the GPU

The second possibility for running GPU simulations in batch is to call the computational engine directly, without using the MzLaunch.exe application. The tricky part here is to figure out which executable to use for which setup-file. A job normally maintained by the MzLaunch.exe application.

The following table illustrates which executable being associated to which type of setup-file:

Table 5.1 Associating computational engines with file extensions.

Model	Executable	Single precision calculations	File extension
MIKE 21 Flow model FM	FemEngineHDGPU.exe	No	.m21fm
MIKE 21 Flow model FM	FemEngineHDGPUSP.exe	Yes	.m21fm
MIKE 3 Flow model FM	FemEngineHDGPU.exe	No	.m3fm
MIKE 3 Flow model FM	FemEngineHDGPUSP.exe	Yes	.m3fm
MIKE 21/3 Coupled Model FM	FemEngineGPU.exe	No	.mfm
MIKE 21/3 Coupled Model FM	FemEngineGPUSP.exe	Yes	.mfm
MIKE FLOOD	FemEngineMFGPU.exe	No	.couple
MIKE FLOOD	FemEngineMFGPUSP.exe	Yes	.couple

The commands given in Figure 5.6 illustrate three different ways of utilising the GPU by calling the computational engine directly. The command “set OMP_NUM_THREADS” specifies the number of threads used by each subdomain in the simulation.

The first call does not use the “mpiexec” command, meaning that only a single subdomain is used in the simulation. In this case the application automatically determines which GPU to use, if more are available.

The second command is used when more subdomains are used in the simulation. Again, the application automatically determines which GPU to use, if more are available.

The third command is used when more subdomains are used in the simulation and the user would like to specify which GPUs to use for the simulation. In this case the user has specified to use two GPUs (one for each subdomain), and the user would like to utilise GPU number 1 and GPU number 2. The syntax for specifying the optional parameters is:

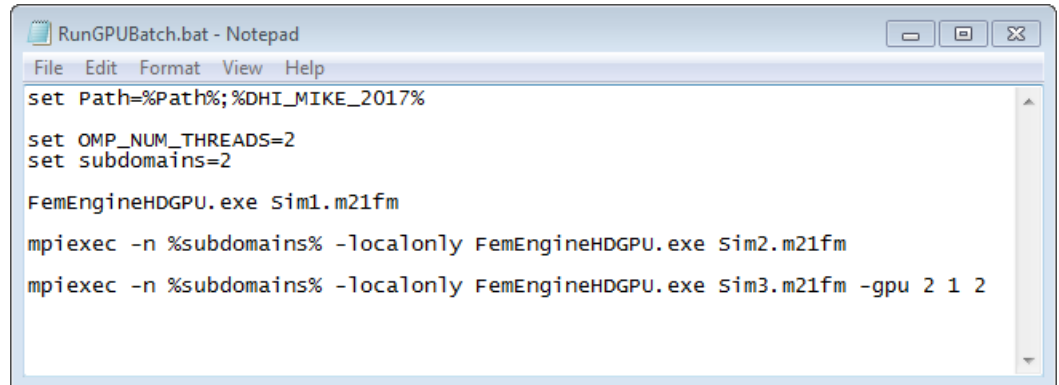
-gpu NumberOfGPUs GPU1 GPU2

This means that if the user has 4 GPUs available on the machine, but only wants to use 3 of these, namely GPU1, GPU2 and GPU4, in the simulation, then the optional parameters would be:

-gpu 3 1 2 4

Of course, here the number of subdomains needs to be at least 3, since the user wants to use 3 GPUs.

The numbering of the GPUs refer to the numbers assigned to each GPU by the computational engine. This numbering is listed in the top of the simulation log file, please see Figure 5.7.



```

set Path=%Path%;%DHI_MIKE_2017%

set OMP_NUM_THREADS=2
set subdomains=2

FemEngineHDGPU.exe sim1.m21fm

mpiexec -n %subdomains% -localonly FemEngineHDGPU.exe sim2.m21fm

mpiexec -n %subdomains% -localonly FemEngineHDGPU.exe sim3.m21fm -gpu 2 1 2
    
```

Figure 5.6 Calling the computational GPU engine directly for a MIKE 21 Flow Model FM simulation

```

===== CUDA GPU Device Information =====
Number of GPU devices      : 1
GPU device number         : 1
GPU device name           : NVS 5400M
CUDA Compute Capability   : 2.1

Selected device number    : 1

number_of_threadsPerBlock : 128 (default)
=====
    
```

Figure 5.7 Section of the simulation log file showing GPU device information and the numbering assigned by the computational engine

Even though the above example only considers the FemEngineHDGPU.exe application and the .m21fm file format, the procedure is exactly the same for the other executables and file formats listed in Table 5.1.

5.7 Why did my GPU simulation crash?

There can be a number of reasons why the simulation does not complete successfully ranging from wrong model input to hardware failure.

Most commonly, the reason for the simulation to stop is when a numerical blow-up happens in the model. This type of crash is reported in the log file and it is most often caused by wrong or self-contradictory input to the model, which causes the model to be unstable.

Typically, this kind of crash is not related specifically to the utilisation of GPUs. This can be tested by running the simulation with GPU utilisation and then once more without utilising the GPU. If the blow-up happens in both simulations, then it is not related to utilisation of the GPU.

In other occasions, the progress bar in the model editor goes directly to 100% without the model creating a log file. Often, this crash happens because the user has insufficient

write-privileges to the folder where the model setup is located. In such case, the crash would also happen when not utilising the GPU.

Alternatively, the reason might be an error in the GPU hardware. This type of error can be tricky to find, but one approach is to replace the GPU suspected of creating the error with a different GPU and check if the error still occurs.

In very rare occasions, the crash happens in the middle of an otherwise perfectly running simulation without leaving any message in the log file and the system is shut down and rebooted. Again, the reason can be faulty GPU hardware or perhaps a power supply which is not large enough to cover the total power consumption of the different hardware in the computer. However, it is also a possibility that the system was close to overheating and shut down as a safety measure. Indications of this might be found in the Windows Event Viewer. Since the GPU generates a lot of heat, it is important to have a good airflow inside the computer cabinet and a cooling system which ensures sufficient heat transportation.