D3.4 Package containing the optimized codes of the public kernels ported
Version 1.0

Document Information

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<thead>
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<th>288777</th>
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</thead>
<tbody>
<tr>
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<td><a href="http://www.montblanc-project.eu">www.montblanc-project.eu</a></td>
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## Change Log

<table>
<thead>
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<th>Description of Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>v0.1</td>
<td>Initial Draft released to the European Commission</td>
</tr>
<tr>
<td>v0.2</td>
<td>First proposed template to the partners of the Consortium</td>
</tr>
<tr>
<td>v0.3</td>
<td>First proposed draft after contributions from the partners of the Consortium</td>
</tr>
<tr>
<td>v0.4</td>
<td>Version reviewed by the internal reviewers</td>
</tr>
<tr>
<td>V1.0</td>
<td>Final version for the European Commission</td>
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Executive Summary

This report refers to the activities planned in WP3 under Task 3.2.

After completion of WP3 activities in P2 of the Mont-Blanc workplan, we setup a repository containing the source and supporting files for all the kernels object of this workpackage. The repository can be accessed at the URL


In this document we report the details about the structure of the repository with some brief description of the content therein.
1 Introduction

This report refers to the activities planned in WP3 under Task 3.2 highlighted below:

<table>
<thead>
<tr>
<th>T3.2. Porting of the kernels (m6:m24)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The aim of this task is to provide a ported version of the source code for each kernel selected in Task 3.1 and run them on the target platform. Critical aspects of the porting will be pointed out for each kernel and overcome by means of specific actions. Recovery strategies will be identified and applied if necessary. This activity will also provide assistance to Task 4.1 in enabling the full applications containing one or more of the selected kernels to the platform.</td>
</tr>
</tbody>
</table>

In the following we report the structure of archive files containing the sources and tests of all the kernels of WP3. All the archives are provided with a “README” file where the details on the compilation and executions of the kernels are reported in full detail. Wherever necessary, we also report in the following sections additional comments and information regarding a specific kernel or its archive.
2 Small Size Kernels

In the following we report the structure of archive files containing the sources and tests of the various small-size kernels of WP3. All the archives are provided with a “README” file where the details on the compilation and executions of the kernels are reported in full detail. Wherever necessary, we also report in this section additional comments and information regarding a specific kernel or its archive.

2.1 EUTERPE
The files for the kernels versions of EUTERPE used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euterpe_kernels.doc</td>
<td>The supporting information material for EUTERPE kernels</td>
</tr>
<tr>
<td>Euterpe_krsaa.tar</td>
<td>The first part of the code/test archives in tar/gzip format</td>
</tr>
<tr>
<td>Euterpe_krsab.tar</td>
<td>The second part of the code/test archives in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run and test the various version included into the archives are fully detailed in the accompanying README files.

2.2 QuantumESPRESSO
The archives and supporting files for the versions of QuantumESPRESSO used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>README_QE-GPU.docx</td>
<td>The supporting information material for GPU version of QuantumESPRESSO</td>
</tr>
<tr>
<td>QE-GPU.tgz</td>
<td>The QuantumESPRESSO archive in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run and test the various versions included into the archives are fully detailed in the accompanying README file.
3 Medium Size Kernels

In the following we report the structure of archive files containing the sources and tests of the various medium-size kernels of WP3. All the archives are provided with a “README” file where the details on the compilation and executions of the kernels are reported in full detail. Wherever necessary, we also report in this section additional comments and information regarding a specific kernel or its archive.

3.1 The preconditioning kernel of BigDFT

The archives and supporting files for the version of BigDFT used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>README_BigDFT.doc</td>
<td>The supporting information for BigDFT</td>
</tr>
<tr>
<td>Bigdft-1.7-dev.28.tgz</td>
<td>The BigDFT archive in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run, test and benchmark the provided BigDFT source tree are detailed in the accompanying README file.

3.2 The reduced, non-production version of SPECFEM3D

The file SPECFEM3D.kernel.tar.gz contains the source code for the SPECFEM3D kernel. In order to execute this kernel, it is necessary to:

1. Create the derivative matrices
2. Create the mesh for the number of MPI processes to use
3. Compile and execute the kernel

3.2.1 Create the derivative matrices

It is mandatory to create the small derivative matrices as a first step. It generates a small ASCII file DATABASES_FOR_SOLVER/matrices.dat (once generated, it is not necessary to do this again):

```
cd define_matrices
  csh make_all.csh
  ./xcreate_matrices
  cd..
```

3.2.2 Create the mesh for the number of processes to use

The mesh is defined statically to avoid its dynamic allocation and a balanced load. The number of processes to use is defined by the product of NPROC_XI times NPROC_eta values (which
are found in file `DATA/Par_file` of the mesher directory). NOTE: MPI can be deactivated if needed to run in serial mode on a "single mesh slice".

```
cd mesher_for_MPI_GPU_CPU/
edit DATA/Par_file to fit your needs
edit Makefile and comment out line "MPIFLAGS = -DUSE_MPI" if needed
make all

and then type either

./xmeshfem3D or
mpirun -np num_processes_to_use_here./xmeshfem3D
cd ..
```

The mesh will be generated in the directory `DATABASES_FOR_SOLVER`.

### 3.2.3 Compile and execute the kernel
The kernel can be compiled after generating the mesh.

```
cd src
make all
```

A binary called `xspecfem3D` should be generated and can be executed sequentially or in parallel using:

```
./xspecfem3D
or
mpirun -np num_processes_to_use_here./xspecfem3D
```

### 3.3 The reduced, non-production version of COSMO
The archives and supporting files for the versions of COSMO and HIMENO used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>README_HimenoBench.docx</td>
<td>The supporting information material for HIMENO</td>
</tr>
<tr>
<td>HimenoBench.tgz</td>
<td>The HIMENO archive in tar/gzip format</td>
</tr>
<tr>
<td>README_COSMO_Opcode.docx</td>
<td>The supporting information material for COSMO OpCode</td>
</tr>
<tr>
<td>COSMO_Opcode.tgz</td>
<td>The COSMO OpCode archive in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run and test the various version included into the archives are fully detailed in the accompanying README files.
### 3.4 The thermostat routine of MP2C

The files for the Thermostat routine of the MP2C version used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP2C_README.doc</td>
<td>The supporting information material for MP2C thermostat kernel</td>
</tr>
<tr>
<td>MP2C_del_3_4.tar.gz</td>
<td>The MP2C thermostat code archive in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run and test the various version included into the archives are fully detailed in the accompanying README files.

### 3.5 The “Hydro” kernel

The files for the Thermostat routine of the MP2C version used in WP3 are as follows:

<table>
<thead>
<tr>
<th>FILE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRO_README.doc</td>
<td>The supporting information material for HYDRO kernel</td>
</tr>
<tr>
<td>HYDRO.tar.gz</td>
<td>The HYDRO code archive in tar/gzip format</td>
</tr>
</tbody>
</table>

All the details on how to compile, run and test the various version included into the archives are fully detailed in the accompanying README files.
4 The WP3 software repository

The repository of the archives and the supporting files were uploaded into the wiki page of the Mont-Blanc project portal and accessible under the terms of the CA at the URL:


In the figure below we report a snapshot of the repository page at the date of delivery of D3.3:

5 Conclusions and next steps

The repository of WP3 sources and related test files of the kernels in WP4 will be continuously updated during P3 of the Mont-Blanc project workplan.
References


