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

Document Information

Contract Number	288777
Project Website	www.montblanc-project.eu
Contractual Deadline	M24
Dissemination Level	RE
Nature	Report
Coordinator	Nico Sanna (CINECA)
Contributors	All Mont-Blanc Partners
Reviewer	N. Puzovic (BSC), T. Palfer-Sollier (BULL)
Keywords	Kernels, OmpSs, ARM

Notices:
The research leading to these results has received funding from the European Community's Seventh Framework Programme [FP7/2007-2013] under grant agreement n° 288777.

Change Log

Version	Description of Change
v0.1	Initial Draft released to the European Commission
v0.2	First proposed template to the partners of the Consortium
v0.3	First proposed draft after contributions from the partners of the Consortium
v0.4	Version reviewed by the internal reviewers
V1.0	Final version for the European Commission

Table of Contents

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

http://wiki.montblanc-project.eu/index.php5/WP3_Optimized_application_kernels

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:

T3.2. Porting of the kernels (m6:m24)
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.

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:

FILE	Description
`Euterpe_kernels.doc`	The supporting information material for EUTERPE kernels
`Euterpe_krsaa.tar`	The first part of the code/test archives in tar/gzip format
`Euterpe_krsab.tar`	The second part of the code/test archives in tar/gzip format

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:

FILE	Description
`README_QE-GPU.docx`	The supporting information material for GPU version of QuantumESPRESSO
`QE-GPU.tgz`	The QuantumESPRESSO archive in tar/gzip format

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:

FILE	Description
`README_BigDFT.doc`	The supporting information for BigDFT
`Bigdft-1.7-dev.28.tgz`	The BigDFT archive in tar/gzip format

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 sequentally 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:

FILE	Description
README_HimenoBench.docx	The supporting information material for HIMENO
HimenoBench.tgz	The HIMENO archive in tar/gzip format
README_COSMO_Opcode.docx	The supporting information material for COSMO OpCode
COSMO_Opcode.tgz	The COSMO OpCode archive in tar/gzip format

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:

FILE	Description
`MP2C_README.doc`	The supporting information material for MP2C thermostat kernel
`MP2C_del_3_4.tar.gz`	The MP2C thermostat code archive in tar/gzip format

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:

FILE	Description
`HYDRO_README.doc`	The supporting information material for HYDRO kernel
`HYDRO.tar.gz`	The HYDRO code archive in tar/gzip format

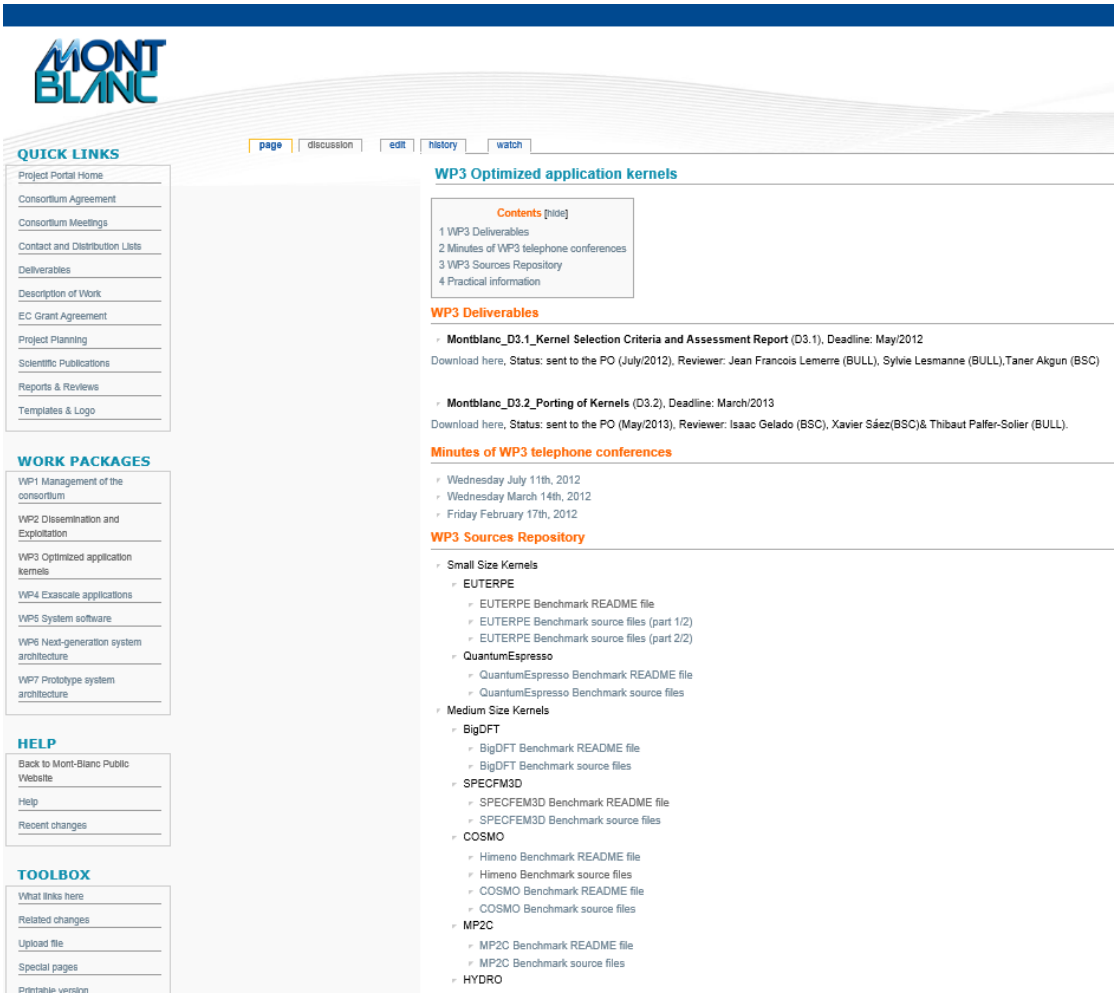
All the details on how to compile, run and test the various version included into the archives are fully detailed in the accompanying README files.

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:

http://wiki.montblanc-project.eu/index.php5/WP3_Optimized_application_kernels

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

[1] **OmpSs**. A. Duran, E. Ayguadé, R. Badia, J. Labarta, L. Martinell, X. Martorell, and J. Planas. OmpSs: A proposal for programming heterogeneous multi-core architecture. Parallel Processing Letters, 21:173-193, 2011.

[2] **EUTERPE**. X. Sàez, A. Soba, E. Sànchez, R. Kleiber, F. Castejòn, and J. M. Cela. Improvements of the particle-in-cell code EUTERPE for petascaling machines. Computer Physics Communications, 182:2047-2051, September 2011.

[3] **QuantumESPRESSO**. Paolo Giannozzi, Stefano Baroni, Nicola Bonini, Matteo Calandra, Roberto Car, Carlo Cavazzoni, Davide Ceresoli, Guido L Chiarotti, Matteo Cococcioni, Ismaila Dabo, Andrea Dal Corso, Stefano de Gironcoli, Stefano Fabris, Guido Fratesi, Ralph Gebauer, Uwe Gerstmann, Christos Gougoussis, Anton Kokalj, Michele Lazzeri, Layla Martin-Samos, Nicola Marzari, Francesco Mauri, Riccardo Mazzarello, Stefano Paolini, Alfredo Pasquarello, Lorenzo Paulatto, Carlo Sbraccia, Sandro Scandolo, Gabriele Sclauzero, Ari P Seitsonen, Alexander Smogunov, Paolo Umari, and Renata MWentzcovitch. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics: Condensed Matter, 21(39):395502 (19pp), 2009.

[4] **BigDFT**. L. Genovese, B. Videau, M. Ospici, T. Deutsch, S. Goedecker, and J.-F. Mhaut. Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus Mécanique, 339:149-164, 2011. http://inac.cea.fr/L_Sim/BigDFT/.

[5] **SPECFEM3D**. http://www.geodynamics.org/cig/software/specfem3d-globe.

[6] **HIMENO**. http://www.cs.berkeley.edu/~mhoemmen/pubs/thesis.pdf

[7] **COSMO**. A. Montani, D. Cesari, C. Marsigli, and T. Paccagnella. Seven years of activity in the field of mesoscale ensemble forecasting by the COSMO-LEPS system: main achievements and open challenges. Technical report, Deutscher Wetterdienst, 2010.

[8] **COSMO-OPCODE**. http://www.hp2c.ch/projects/opcode/

[9] **MP2C**. G. Sutmann and W. Frings. Extending scalability of MP^{2}C to more than 250k compute cores. Technical report, Forschungszentrum J□lich, 2010.

[10] **RAMSES-HYDRO**. R. Osmont, D. Pomar□ede, V. Gautard, R. Teyssier, and B. Thooris. Monitoring and control of the RAMSES simulation program. In Proceedings of the CCP2007 Conference on Computational Physics, Brussels, Belgium, 2007.