

ExaHyPE Guidebook

http://www.exahype.eu

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Preamble

ExaHyPE is a collection of open source tools. It is mainly written in C++, Java and Matlab.

Dependencies and prerequisites

ExaHyPE's core routines can be used if you have a recently new C++ compiler (C++11 has to be supported) and Java distribution installed.

- ExaHyPE source code depends only on MPI and Intel's TBB or OpenMP if you want to run it with distributed or shared memory support. There are no further dependencies or libraries required. All examples from this guidebook run and have been tested with GCC 4.2 and Intel 12 or later. Earlier compiler versions might work.
- ExaHyPE's setup environment relies on Java, as parts of it come along as jar files
- ExaHyPE's default build environment uses make and tr, i.e. only standard Unix commands.

The guidebook assumes that you use a Linux system. It all should work on Windows and Mac as well, but we haven't tested it in detail.

Who should read this document

This guidebook is written similar to a tutorial in a hands-on style. It addresses users of ExaHyPE. It is not meant to help developers or replace code documentation. Using the guidebook requires a decent knowledge of the application domain modelled via a hyperbolic equation system. It does not require deep programming knowledge.

Everything in this guidebook runs out-of-the-box by following the written text only. There are however few additional steps that advanced users might want to try out. Those do not come along with very detailed step-by-step descriptions. They are marked with an (optional) postfix in the title. Standard or new users should just skip these sections.

 $\begin{array}{c} {\rm June}~9,~2016\\ {\rm The}~{\tt ExaHyPE}~{\rm team} \end{array}$

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1. Download (and install)

ExaHyPE does not require any real installation. It is basically just a download. Please visit www.exahype.eu to get particular ExaHyPE source code variants. All remarks here refer to the latest ExaHyPE release.

Each release consists of three major source code packages:

- 1. The actual ExaHyPE sources is a tar.gz archive. It contains the actual engine with all mesh organisation, computational kernels, load balancing components, and so forth.
- 2. ExaHyPE is based upon the PDE solver framework Peano (peano-framework.org) which provides the underlying adaptive mesh refinement (AMR) data structures as well as mesh traversal algorithms.
- 3. The engine is used through a Java toolbox that provides the opportunity to configure the engine to a particular setup. The sources for the latter typically are not required, but they are available from the ExaHyPE home page.

A complete download/setup reads as follows:

You might choose to maintain a different directory structure or rely on a previous Peano or ExaHyPE installation. In this case, you have to adopt pathes in your ExaHyPE scripts.

Dry run

To check whether you are ready to use ExaHyPE, type in

> java -jar exahype.jar

This should give you the following welcome message:

The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671698 (ExaHyPE). It is based upon the PDE framework Peano (www.peano-framework.org).

ERROR: Please provide input file as argument

Using a newer/other Peano version (optional)

ExaHyPE is based upon the PDE solver framework Peano (www.peano-framework.org). With the present scripts, you use the newest stable Peano release. As Peano is still improved, it might make sense to download a new archive from time to time.

ExaHyPE uses a couple of Peano toolboxes. These toolboxes are part of Peano's framework, but they are not by default included in the release. While normal Peano users have to download them manually, we provide a snapshot with ExaHyPE. These snapshots are help in ExaHyPE's Peano directory. If you want to try newer versions, download the corresponding toolboxes from Peano's webpage and extract them manually into ExaHyPE's Peano subdirectory.

If you use Peano in several projects, it might make sense to skip the download of the archive into ExaHyPE's Peano directory and instead add two symbolic links with ln -s in the Peano directory to Peano's peano and tarch directory.

2. Setup a first experiment

ExaHyPE is written for high performance computing experiments. Our philosophy is write one code specification per experiment/machine/setup configuration and sacrifice flexibility in exchange for performance. Because of this, ExaHyPE specification files act on the one hand as configuration files that are passed into the executable for a run. On the other hand, a specification file tailors the executable, i.e. is used to generate some source code. The compiler can, at hands of the specification, optimise aggressively in several places. ExaHyPE prefers to run the compiler more often rather than working with one or few generic executables.

An ExaHyPE specification is a text file where you specify exactly what you want to solve in which way. This file¹ is handed over to our ExaHyPE toolkit, a small Java application generating all required code. This code (also linking to all other required resources such as parameter sets or input files) then is handed over to a compiler. You end up with an executable that may run without the Java toolkit or any additional sources from ExaHyPE. It however rereads the specification file again for input files or some parameters, e.g. We could have worked with two different files, a specification file used to generate code and a config file, but decided to have everything in one place.

A trivial project

A trivial project in ExaHyPE is described by the following specification file:

```
exahype-project TrivialProject
peano-path = ./Peano/peano
tarch-path = ./Peano/tarch
multiscalelinkedcell-path = ./Peano/multiscalelinkedcell
exahype-path = ./ExaHyPE

output-directory = ./Applications/trivialproject

architecture = noarch

computational-domain
dimension = 2
width = 1.0
offset = 0.0, 0.0
end-time = 10.0
end computational-domain
```

¹Some examples can be found in the Toolkit directory or on the ExaHyPE webpage. They have the extension exahype.

end exahype-project

Most parameters should be rather self-explanatory. You might have to adopt some of the paths. Note ExaHyPE supports both two- and three-dimensional setups. We hand the file over to the toolkit

```
java -jar ExaHyPE.jar examples/trivial-project-2d.exahype
```

and observe that the toolkit has created a new directory Applications/trivialproject. We change into this directory and type in

```
make
```

which gives us an executable. The toolkit plots additional information how to switch into debug versions of the code or how to switch to another compiler through environment variables. For most systems, the defaults should do. We finally run this first ExaHyPE application with

```
./ExaHyPE <yourpath>/trivial-project-2d.exahype
```

Within the section computational-domain, all entries except the dimension can be changed before application startup: If you change their value, there is no need to recompile or to rerun the toolkit again.

A simple 2d Euler flow

So far, the simulation run neither computes anything nor does it give you any output. We close this section with a brief demonstration how to realise a 2d Euler flow within ExaHyPE. ExaHyPE's fundamental idea is that the user specifies all PDEs she wants to solve within the specification file. We start with a solve of the compressible Euler equations via the ADER-DG method. For this type of solver, the engine needs to know how many unknowns the solved PDE has and which polynomial order shall be used. We do not have any material involved, so we set the field parameters to 0.

For the actual computations, there are three types of kernels (PDE solver realisations) that can be used within ExaHyPE. You can either write the whole solver yourself, you can make ExaHyPE realise the solver while you specify the flux update operations, or you can use a pre-defined ExaHyPE kernel which gives you the best performance. Available options are described and detailed in Chapter D. For the time being, we use kernel = generic::fluxes::nonlinear, the generic kernels for non-linear PDEs, where PDE-specific functions, e.g. the flux function, yet have to be specified by us.

In the present example, we rely on the latter variant. We also stick to a regular grid simulation for the time being. The specification file then is

```
exahype-project MyEuler

peano-path = ./Peano/peano
tarch-path = ./Peano/tarch
```

```
{\it multiscale linked cell-path} = ./{\it Peano/multiscale linked cell}
 shared memory oracles-path = ./Peano/shared memory oracles
 exahype-path = ./ExaHyPE
 output-directory = ./Applications/guidebook-chapter-2
 architecture = noarch
computational-domain
   dimension = 2
   width = 1.0
   offset = 0.0, 0.0
   end-time = 0.4
 end computational-domain
 solver ADER-DG MyEulerSolver
   unknowns = 5
   parameters = 0
   order = 3
   kernel = generic::fluxes::nonlinear
   language = C
   plot vtk::ascii
     time = 0.0
     repeat = 0.05
     filename = ./solution
   end plot
 end solver
 shared-memory
   identifier = dummy
   cores = 2
   properties-file = shared memory. properties
 end shared-memory
 optimisation
   fuse-algorithmic-steps = on
 end optimisation
end exahype-project
```

We run the toolkit and end up with a new directory Applications/guidebook-chapter-2. Within this directory, there is a file MySolver.cpp that we have to complete as follows:

```
#include "MySolver.h"

MyEuler::MySolver( int kernelNumber):
    exahype::solvers::Solver("MySolver",exahype::solvers::Solver::ADER_DG,kernelNumber,5,3+1) {
    int MyEuler::MySolver::getMinimumTreeDepth() const {
        return 3;
    }
}
```

```
// ...
void MyEuler::MySolver::adjustedSolutionValues(...) {
  if (tarch::la::equals(t, 0.0)) {
    const double GAMMA = 1.4;
    Q[0] = 1.;
    Q[1] = 0.;
    Q[2] = 0.;
    Q[3] = 0.;
    Q[4] =
        1. / (GAMMA - 1) +
        std::exp(-((x[0]-0.5)*(x[0]-0.5)+(x[1]-0.5)*(x[1]-0.5)) /
                  (0.05 *0.05)) *
            1.0e-3:
bool Euler2d::MyEulerSolver::hasToAdjustSolution(...) {
  if (tarch::la::equals(t, 0.0)) {
    return true;
  return false;
```

Actually, only proper initial conditions have to be provided. The remainder is pregenerated.

To set the initial conditions, we need to implement two of the pregenerated functions: We specify that we want to adjust the solution values at time t=0 in function hasToAdjustSolutionValues and then set initial conditions via the function adjustedSolutionValues. We clarify the semantics of the arguments of hasToAdjustSolutionValues and adjustedSolutionValues in Chapter 4. For the time being, we compile and run the code.

A remark on material parameters

In ExaHyPE, we do not really distinguish unknowns that are subject to a PDE from parameters on the user side. If you have 4 unknowns and 3 (material) parameters, all functions just seem to handle 4+3=7 variables. We only distinguish the values in the script file as we obviously do not want to run any PDE kernel (unknown update) on top of the material parameters. For them, we restrict to a subset of all the variables—namely the first 4 in the example above. To the user, we do not distinguish material parameters from unknowns. When you set up the initial condition, e.g., you will be passed 7 unknowns.

Plots

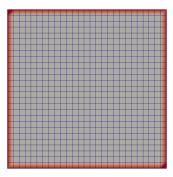
Still, the simulation does not give any output besides status messages on the terminal. We have to add appropriate plotters. ExaHyPE offers a couple of predefined export mechanisms. Within each solver section, we may use an arbitrary number of plotters to pipe the result at certain time steps into files. We start with

```
solver ADER-DG MySolver
unknowns = 5
parameters = 0
order = 3
kernel = kernel::euler2d

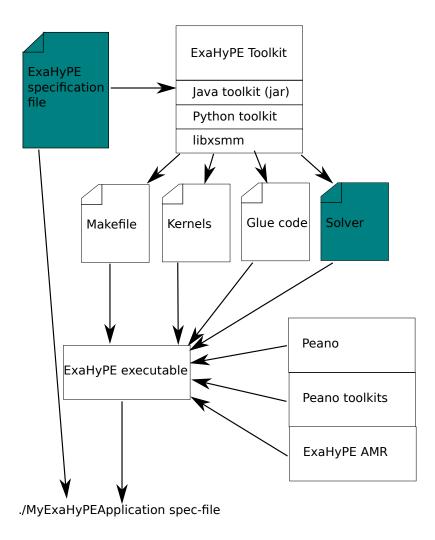
plot vtk::binary
time = 0.0
repeat = 0.02
filename = ./solution
end plot
end solver
...
```

and postpone a detailed explanation to later chapters. For the time being, it is sufficient to note that this operation writes VTK binary files (they can be read in by Paraview or VisIt, e.g.) into files named solution... .vtk. The first file is written at time 0, i.e. at startup time. From hereon, we obtain a new snapshot every 0.02 simulation intervals.

Once you have inserted the plotter into your specification file, invoke the toolkit again, compile the code and run the simulation. You obtain a sequence of files yielding images similar to



3. ExaHyPE architecture



- 1. The user writes a specification file (text format) that holds all required data ranging from paths, which parallelisation to use, computational domain up to a specification which kind of solvers will exist and which numerical schemes they realise.
- 2. This specification file is handed over to the ExaHyPE toolkit which is a Java tool. It internally relies on Python scripts and invokes the libxsmm generator driver as well. A local build of the libxsmm's code generation driver is therefore a prerequisite for using optimised kernels.
- 3. The toolkit yields a couple of files (Makefile, glue code, helper files, ...). Among them is also one C++ implementation class per solver that was spec-

ified in the specification file. The output directory in the specification file defines where all these generated files go to.

- 4. a) Within each C++ implementation file, the user can code solver behaviour such as initial conditions, mesh refinement control, and so forth.
 - b) The whole build environment is generated. A simple make thus at any time should create the ExaHyPE executable.
- 5. If you run your ExaHyPE executable, you have to hand over the specification file again. Obviously, many entries in there (simulation time or number of threads to be used) are not evaluated at compile time but at startup. You don't have to recompile your whole application if you change the number of threads to be used.

To summarise, the blueish text files are the only files you typically have to change yourself. All the remainder is generated and assembled according to the specification file.

3.1. Switching between Generic and Optimised Kernels

Driven by the choice in the specification file, ExaHyPE chooses either generic kernels or optimised kernels. If you switch between the generic and the optimised kernels, you have to use the toolkit to regenerate the glue code.

4. ADER-DG solvers with user-defined kernels

In this chapter, we introduce ExaHyPE's kernels that allow the user to specify flux and eigenvalue functions for the kernels (for linear problems), but leaves everything else to ExaHyPE. The resulting code can run in parallel and scale, but its single node performance might remain poor, as we do not rely on ExaHyPE's high performance kernel. Therefore, the present coding strategy is well-suited for rapid prototyping of new solvers. To outline the steps a user has to perform to define his own fluxes and state-depending initial values, we again consider the compressible Euler equations with d=2. This is the example we also used in Chapter 2.

For the Euler equations

$$\frac{\partial}{\partial t} \mathbf{Q} + \mathbf{\nabla} \cdot \mathbf{F}(\mathbf{Q}) = 0 \quad \text{with} \quad \mathbf{Q} = \begin{pmatrix} \rho \\ \mathbf{v} \\ E \end{pmatrix} \quad \text{and} \quad \mathbf{F} = \begin{pmatrix} \mathbf{v} \\ \frac{1}{\rho} \mathbf{v} \otimes \mathbf{v} + pI \\ \frac{1}{\rho} \mathbf{v} (E + p) \end{pmatrix}$$

supplemented by initial values $\mathbf{Q}(0) = \mathbf{Q}_0$ and appropriate boundary conditions, we rewrite the conserved quantities \mathbf{Q} and fluxes \mathbf{F} into an equation over five state unknowns

$$\mathbf{Q} = \begin{pmatrix} Q_0 \\ Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{pmatrix} = \begin{pmatrix} \rho \\ v_x \\ v_y \\ v_z \\ E \end{pmatrix}$$

which are discretised over Ω .

Here, ρ denotes the mass density, $\mathbf{v} \in \mathbb{R}^d$ denotes the velocity vector, E denotes the energy, and p denotes the fluid pressure. For our 2d setup, the velocity in z-direction v_z is set to zero.

Introducing the adiabatic index γ , the fluid pressure is here defined as

$$p = (\gamma - 1) \left(E - \frac{1}{2} \mathbf{v}^2 / \rho \right).$$

A corresponding specification file euler-2d.exahype for this setup is

```
/**
    *Example code of Chapter 3 in ExaHyPE codebook
    */
exahype-project Euler2d
```

```
peano-path = ./Peano/peano
 tarch-path = ./Peano/tarch
 multiscalelinkedcell-path = ./Peano/multiscalelinkedcell
 exahype-path = ./ExaHyPE
 output-directory = ./Applications/eulerflow2d
 architecture = noarch
 computational-domain
   dimension = 2
   width = 1.0
   offset = 0.0, 0.0
   end-time = 0.4
 end computational-domain
 solver ADER-DG MyEulerSolver
   unknowns = 5
   parameters = 0
   order = 3
   kernel = generic::fluxes::nonlinear
   plot vtk::binary
     time = 0.0
     repeat = 0.05
     filename = ./solution
   end plot
 end solver
end exahype-project
```

The script sets some paths in the preamble before it specifies the computational domain and the simulation time frame in the environment computational-domain.

In the next lines, a solver of type ADER-DG is specified and assigned the name MyEulerSolver. The kernel type of the solver is set to generic::fluxes::nonlinear. This tells the ExaHyPE engine that we do not provide it with problem specific and highly optimized ADER-DG kernels. Instead we tell it to use some generic partially optimized ADER-DG kernels that can be applied to virtually any hyperbolic problem. In this case, the user is only required to provide the ExaHyPE engine with problem specific flux (and eigenvalue) definitions.

Within the solver environment, there is also a plotter specified. The specified plotter is configured to write binary VTK output by setting its identifier to vtk::binary. The plotter is further configured to write out a snapshot of the solution of the associated solver every 0.05 time intervals. The first snapshot is set to be written at time t=0.

Once we are satisfied with the parameters in our ExaHyPE specification file, we hand it over to the ExaHyPE toolkit:

```
java -jar <mypath>/ExaHyPE.jar Euler2d.exahype
```

4.1. Study the generated code

We obtain a new directory (equalling output-directory from the specification file) and change into this file. It contains a makefile, some helper files, and a new class MyEulerSolver. This new class was generated according to the solver entry ADER-DG MyEulerSolver that we have specified in our script.

Class MyEulerSolver is divided into three source code files: First, there is a header that we might want to extend later on. For the time being, it suits our needs. There is further an implementation file with an addendum _generated. This is a file we should never edit since it is overwritten every time we use the toolkit to generate code for our problem. Finally, there is another implementation file that we will use to realise the actual solver behaviour. Here, we will specify the aforementioned user defined flux and eigenvalue definitions that are necessary if we want to use the generic ADER-DG kernels.

Before we start to do so, it might be reasonable to compile the overall code once and to doublecheck whether we can visualise the resulting outputs. This should all be straightforward. Please verify that any output you visualise holds only zero values since the initial values are set to zero at the moment.

If you translate in debug mode or with assertions, ExaHyPE might even stop with an assertion.

4.2. Setting up the experiment

To set up the experiment, we open the implementation file Euler2d.cpp of the class Euler2d. There are two routines (getMinimumTreeDepth and adjustedSolutionValues that allow us to setup the initial grid. We leave the default setting for the tree depth—we can use it later to set up adaptive initial grids as well—and focus on the initial values. The implementation of the initial values might look as follows¹:

¹The exact names of the parameters might change with newer ExaHyPE versions and additional parameters might drop in, but the principle always remains the same.

```
) *1.0e-3;
}
}
```

The above routine enables us to specify time dependent solution values. It further enables us to add source term contributions to the solution values. While the routine itself is more or less self-explaining, we nevertheless highlight a few details:

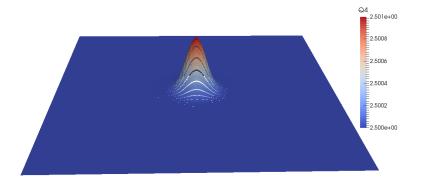
- We only want to impose initial conditions so we check if the time t is zero with respect to some tolerance in the first line of the routine.
- While the unknown pointer Q itself does not give any hint about the actual size of the array it points at, we know by construction that we have five unknowns per grid point and thus choose the iteration space accordingly. Note that as usual for C type languages indexing of the array starts with zero.
- The spatial position **x** is given as a pointer to a double array of size **dimension** which you have previously specified in the script **euler-2d.exahype**. Note that the indexing of the arrays starts here of course also with zero.

The routine adjustedSolutionValues must always be paired with the routine hasToAdjustSolution that specifies when and in which grid cell we want to adjust solution values:

```
bool Euler2d::MyEulerSolver::hasToAdjustSolution(
    const tarch::la::Vector<DIMENSIONS,double>& center,
    const tarch::la::Vector<DIMENSIONS,double>& dx,
    double t
) {
    if (tarch::la::equals( t, 0.0 ,1e-15 )) { // @todo precision
        return true;
    }
    return false;
}
```

The routine's arguments center and dx refer to the center point of the cell and to its extent in each coordinate direction. The simulation time is here again denoted by t.

We conclude our experimental setup with a compile run and a first test run. This time we get a meaningful image and definitely not a program stop for an assertion, as we have set all initial values properly. However, nothing happens so far; which is not surprising given that we haven't specified any fluxes yet.



4.3. Realising the fluxes

To realise the fluxes, we have to fill the functions flux and eigenvalues in file MyEulerSolver.cpp with code. As we rely on the kernel mode generic::fluxes::nonlinear, ExaHyPE autonomously realises all steps of ADER-DG and only calls back to the solver for the flux and eigenvalue evaluations.

```
void Euler2d::MyEulerSolver::flux(
 const double* const Q,
 double* f,
 double* g
 const double GAMMA = 1.4;
 const double irho = 1.0/Q[0];
 const double p = (GAMMA-1)^*(Q[4] - 0.5^*(Q[1]*Q[1] + Q[2]*Q[2]) *irho);
 f[0] = Q[1];
 f[1] = irho*Q[1]*Q[1] + p;
 f[2] = irho*Q[1]*Q[2];
 f[3] = irho*Q[1]*Q[3];
 f[4] = irho*Q[1]*(Q[4]+p);
 g[0] = Q[2];
 g[1] = irho*Q[2]*Q[1];
 g[2] = irho*Q[2]*Q[2] + p;
 g[3] = irho*Q[2]*Q[3];
 g[4] = irho*Q[2]*(Q[4]+p);
```

```
void Euler2d::MyEulerSolver::eigenvalues(
   const double* const Q,
   const int normalNonZeroIndex,
   double* lambda
) {
   const double GAMMA = 1.4;

   double irho = 1.0/Q[0];
   double p = (GAMMA-1)*( Q[4] -0.5* (Q[1]*Q[1] + Q[2]*Q[2]) *irho );
```

```
double u_n = Q[normalNonZeroIndex+1] *irho;

double c = std::sqrt(GAMMA *p *irho);

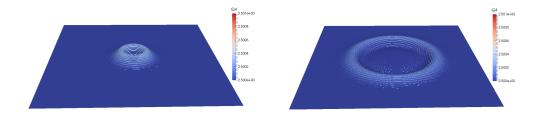
lambda[0] = u_n-c;

lambda[1] = u_n;
 lambda[2] = u_n;
 lambda[3] = u_n;

lambda[4] = u_n+c;
}
```

The implementation of function flux is again very straightforward. The code basically mimics the definition of the flux tensor $\mathbf{F}(\mathbf{Q}) = (\mathbf{f}(\mathbf{Q}), \mathbf{g}(\mathbf{Q}))^{\mathrm{T}}$. As the creators of the Euler2d project, we naturally know the size of the parameters \mathbf{Q} , \mathbf{f} , and \mathbf{g} which is identical to the number of state unknowns. The same holds for the size of the array of eigenvalues the pointer lambda appearing in the signature and body of function eigenvalues refers to which is also identical to the number of state unknowns.

The normal vectors that are involved in ExaHyPE's ADER-DG kernels always coincide with the (positively signed) Cartesian unit vectors. Thus, the eigenvalues function is only supplied with the index of the single component that is non-zero within these normal vectors. In function eigenvalues, the aforementioned index corresponds to the parameter normalNonZeroIndex. A rebuild and rerun should yield results similar to



5. Shared memory parallelisation

ExaHyPE currently supports shared memory parallelisation through Intel's Threading Building Blocks (TBB) and OpenMP. We recommend using the TBB variant that is typically one step ahead of the OpenMP support. To make an ExaHyPE project use multi- and manycore architectures, please add a shared-memory configuration block to your specification file:

```
shared-memory
strategy = dummy
cores = 4
properties-file = sharedmemory.properties
end shared-memory
```

Rerun the ExaHyPE toolkit afterwards, and recompile your code. For the compilation, we assume that the environment variables TBB_INC and TBB_SHLIB are set¹. If you use OpenMP, your compiler has to support OpenMP. The toolkit checks whether the environment variables are properly set and gives advise if this is not the case.

Whenever you configure your project with shared memory support, the **default** build variant is a shared memory build (with TBB or OpenMP, respectively). However, you always are able to rebuild without shared memory support or a different shared memory model just by manually redefining environment variables and by rerunning the makefile. There is no need to rerun the toolkit again. Also not that all arguments within the **shared-memory** environment are read at startup time. If you change the core count, there's no need to recompile. The same statements holds for the other parameters.

For users familiar with OpenMP, we emphasise that we do set the thread count manually within the code. OpenMP requires, per default, all users to control the thread count via environment variables. In ExaHyPE, the value of the environment variable and the value in the config file thus should match. You'll obtain a warning otherwise.

For most users, the dummy strategy should be sufficient. While the field **cores** is self-explaining, the properties file is neglected for the dummy strategy. If you use a more sophisticated strategy, it however makes a difference. More sophisticated strategies are subject of discussion next.

¹ TBB_INC=-I/mypath/include and TBB_SHLIB="-L/mypath/lib64/intel64/gcc4.4 -ltbb" are typical environment values.

Table 5.1.: Parameter choices for the multicore configuration. All values are read at program startup. There is no need to rerun the toolkit if you change any of them.

Parameter	Options	Description
strategy	dummy autotuning sampling	The shared memory efficiency is very sensitive to a multitude of parameters that threshold the size of minimal problems deployed to one task, decide which code fragments shall run in parallel, and so forth. Three shared memory strategies for these parameters are provided at the moment. dummy uses some default values that have proven to be reasonably robust and yield acceptable speed. sampling tests different choices and plots information on well-suited variants to the terminal. autotuning tries to find the best choice on-the-fly.
cores	> 0	Number of cores that shall be used.
properties-file	filename	The sampling and the autotuning strategy can write their results into files and reuse these results in follow-up runs. If no (valid) file is provided, they both start from scratch and without any history. If the file name is empty or invalid, no output data is dumped. The entry is ignored if you use the dummy strategy.

Autotuning and tailoring

Shared memory performance can be very sensitive to machine-specific tuning parameters. We thus encourage high performance applications to use ExaHyPE's autotuning strategy. This strategy loads a set of tuning parameters from the properties file—if a file does exist—incrementally tries to improve these architecture-specific properties, and then dumps the values again into the property file.

This means that first runs might be really slow, but the runtime improves throughout the development. For production runs, you then have a well-suited parameter file at hands for the autotuning. The autotuning switches off automatically as soon as it has to believe that best-case parameters are found. However, it could be that these parameters are local runtime minima.

If you prefer to get the whole picture, you might want to run the sampling. However, the parameter space is huge, i.e. getting a valid picture might require several days. The output of the sampling is written into the specified properties file and then allows you to identify global best case parameters.

Once the autotuning strategy has found a (local) best-case configuration, it marks these configurations as valid and does not continue to search. As a result, also timing overheads are reduced. As all strategies write text configuration files, it is possible to configure the autotuning manually with proper parameter choices and to switch off the actual autotuning at the same time. You might for example search for optimal choices with the sampling and then feed these values into the autotuning.

It is obvious that proper property files depend on the machine you are using. They reflect your computer's properties. Please note that very good property files also depend on the

- choice of cores to be used,
- MPI usage and balancing,
- application type, and even
- input data/simulation scenario.

It thus might make sense to work with various property files for your experiments.

Hybrid parallelisation

This section discusses the interplay of the shared memory parallelisation with MPI. It is written for HPC experts. For most users, no changes have to be made to the shared memory parallelisation when they turn on MPI as well.

This subsection yet has to be written.

6. Optimisation

6.1. High-level tuning

ExaHyPE realises few high level optimisations that you can switch on and off at code startup through the specification file. To gain access to these optimisations, add a paragraph

```
optimisation
fuse-algorithmic-steps = off
end optimisation
```

at the end of your specification file.

Step fusion. Each time step of an ExaHyPE solver consists of four phases: local ADER-DG predictor, projection of the prediction onto the cell phases, solve of the Riemann problem, and update of the predicted solution. We may speed up the code if we fuse these four steps into one grid traversal. To do so, we set fuse-algorithmic-steps.

6.2. Optimised Kernels

ExaHyPEoffers optimised compute kernels. Given a specification file, the toolkit triggers the code generator to output optimised compute kernels for this specific setup.

Prerequisites The code generator exhibits two dependencies. First, the code generator requires Python 3. Second, it relies on Intel's libxsmm generator driver. You therefore have to clone the libxsmm repository https://github.com/hfp/libxsmm and build your local generator driver

```
make generator
```

to obtain the executable in path/to/libxsmm/bin/libxsmm_gemm_generator.

Microarchitecture The optimised kernels explicitly use the instruction set available on the target processor. You therefore have to define its microarchitecture in the specification file. The specification file terms the processor architecture just architecture. Here are the supported options for this flag.

Architecture	Meaning
noarch	unspecified
wsm	Westmere
snb	Sandy Bridge
hsw	Haswell
knc	Knights Corner (Xeon Phi)
knl	Knights Landing (Xeon Phi)

You can identify the microarchitecture of your processor through amplxe-gui, an analysis tool part of Intel VTune Amplifier. Alternatively, you can obtain the 'model name' via

cat /proc/cpuinfo

and search for it on http://ark.intel.com.

Set the architecture flag to 'noarch' if the microarchitecture of your processor is not supported. You will nevertheless obtain semi-optimised kernels. The default makefile utilises the flags march=native (gcc) respectively xHost (icc). The compiler queries what hardware features are available and optimises the kernels to some degree.

7. Postprocessing, plotting & logs

7.1. Dumps and visualisation of the whole setup

The table below gives a brief overview over available plotter types. They are distinguished by their identifier in the specification file. While the number of plotters and their type have to be fixed at compile time—if you want to introduce a new plotter, you have to rerun the ExaHyPE toolkit and rebuild your code—all other parameters are read at runtime.

Identifier	Description
vtk-binary	Write a VTK binary file.
vtk-text	Write a VTK text file.

7.2. Logging

ExaHyPE creates a large number of log files; notably if you build in debug or assert mode. Which data actually is written to the terminal can be controlled via a file exahype.log-filter. This file has to be held in your executable's directory. It specifies exactly which class of ExaHyPE is allowed to plot or not. The specification works hierarchically, i.e. we start from the most specific class identifier and then work backwards to find an appropriate policy.

<pre># Level # (info or debug)</pre>	Trace	Rank (-1 means all ranks)	Black or white list entry
debug debug	tarch peano	-1 -1	black black
info	tarch	-1	black
info		-1	black
info	peano::u	tils::UserInterface -1	white
info	exahype	-1	white

If no file exahype.log-filter is found in the working directory, a default configuration is chosen by the code. Please note that a sound performance analysis requires several log statements to be switched on. For a detailed description, please study Peano's handbook or the produced report pages as well as the report scripts.

A. The ExaHyPE toolbox

The ExaHyPE toolbox is a small Java toolkit. It acts as sole interface for users, i.e. non-developers. We decided to realise it in Java for several reasons:

- 1. We can realise lots of syntax checks without blowing up the C++ code.
- 2. We have to generate code fragments in ExaHyPE. The order of the methods chosen for example has an impact on kernel calls and mapping variants. This is easy in Java.
- 3. We prefer not to have several interfaces. With a Java front-end, we can directly generate the configuration rather than parsing configurations again.

A.1. Rebuild the toolbox

To build the toolbox, we rely on ant.

ant target

where target is from

- createParser. Recreates the Java parser. ExaHyPE's Java parser relies on SableCC. The parser has to be regenerated if and only if you change the grammar or you have to rebuild the tool without a previous build.
- compile. Translate the toolkit.
- dist. Pack the translated files into one jar file.
- clean. Clean up the compiled and temporary files.

B. Frequently asked developer questions & problems

• MPI plus TBB deadlocks or is very slow

On several systems, we have encountered problems when we tried to use multithreaded MPI. As a result, we disable multithreaded MPI usage by default in the makefile (switch -DnoMultipleThreadsMayTriggerMPICalls). You might want to try to enable multithreaded MPI again with

- -DMultipleThreadsMayTriggerMPICalls, but we cannot guarantee that it works properly. It is trial & error depending on your compiler/MPI/cluster choice.
- To be continued ...

C. Frequently asked user & problems

• How do I modify the computational domain?

Open the specification file and alter the width. The entry specifies the dimensions of the computational domain. Please note that ExaHyPE only supports square/cube domains as it works on cube/square cells only. You might have to extend your problem's domain accordingly. width is read at startup time, i.e. there's no need to rerun any script or recompile once you have changed the entry. Just relaunch your simulation.

• How do I alter the time step size?

ExaHyPE implements three time stepping schemes (global time stepping, local time stepping, anarchic time stepping). You can configure them within your generated solver class in your application directory. Once you have chosen the time stepping scheme, the code autonomously determines the biggest stable time step size that is permitted. Nothing has to be done.

Only global rently. You c configure yet.

• How do I alter the time step size (advanced)?

You may however choose the time step size yourself if you do not rely on the generated kernels but write a whole solver yourself (see solver variant user::defined in Section 4) from scratch.

- How do I change the spatial resolution statically? The spatial resolution (mesh width) is tied to a particular solver/problem. ExaHyPE thus wants to tell the kernel/grid per solver which resolution you require. For this, have a look into getMinimumTreeDepth(). Here, you tell the code how fine the start grid has to be.
- How do I change the resolution dynamically? The dynamic AMR is realised along the same lines as the static refinement. You have to implement refinementCriterion in your solver which tells ExaHyPE where you want to refine. How this is realised—notably how all the ranks and cores synchronise—is hidden away from the user code and decided in the kernel.
- To be continued ...

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D. Solver Kernels

The kernel variants below are offered for the ADER-DG solver type. The last column indicates whether we offer FORTRAN support for these.

Kernel	Description	F
user::defined	Only function signatures are generated. All responsibility which and how kernels are realised is up to the user. We basically only hand over large double arrays. This is the lowest level of abstraction.	yes
generic::fluxes::nonlinear	Default ADER-DG routines are used, but they make no assumptions on the fluxes. The toolkit will ask you to provide fluxes, eigenvalues, and so forth which are then used within nested for loops generically. This is the second level of abstraction and well-suited for fast prototyping.	yes
generic::fluxes::linear	Similar to generic::fluxes::nonlinear. Given the explicit notion of a linear flux, the underlying generic source code however is simpler. This variant is faster.	yes
optimised::fluxes::nonlinear	Equals generic::fluxes::nonlinear from a user's point of view. However, the underlying ADER-DG routines/loops all are optimised through libxsmm.	no
optimised::fluxes::linear	Optimised version of optimised::fluxes::nonlinear that removes any non-linear iteration.	no
kernel::euler2d	These are optimised kernels that solves the Euler equations in two or three dimensions. They mirror the example from Chapter 4. As we fix the PDE, no fluxes, eigenvalues, have to be written by the user and the resulting kernel is very aggressively optimised.	t.b.a.

The following kernel variants are offered for the Finite-Volume solver type:

Kernel	Effect
user::defined	Only function signatures are generated. All responsibility which and how kernels are realised is up to the user. We basically only hand over large double arrays. This is the lowest level of abstraction.
t.b.d.	

E. Datastructures in the Optimised Kernels

Matrix	Memory Layout	Size
Kxi	[[Kxi];0]	$(nDOF+Pad) \times nDOF$
iK1	analogous to Kxi	
dudx	analogous to Kxi	
FRCoeff	[FRCoeff]	$1 \times nDOF$
FLCoeff	analogous to FRCoeff	
F0	[F0;0]	$1 \times (\text{nDOF+Pad})$
equidistantGridProjector1d fineGridProjector1d	analogous to generic version analogous to generic version	

Table E.1.: Structure of the system matrices in the optimised kernels.

Name	Memory Layout	Meaning		
	2D			
weights2 weights3		quadrature weights + Padding outer product of quadrature weights + Padding		
3D				
weights2 weights3	$[w_i w_j, 0] \\ [w_i w_j w_k, 0]$	outer product of quadrature weights + Padding all combinations of quadrature weights + Padding		

Table E.2.: Variables holding combinations of quadrature weights employed in the optimised kernels.

Variable	Ordering	Size	
rhs, rhs0	(nVar,nDOFx,nDOFy,nDOFz,nDOFt)	$nVar \cdot nDOF^4$	
lFbnd	(nDOFx, nDOFy, nVar)	$((nDOFx \cdot nDOFy)+Pad) \cdot nVar$	
lQbnd	(nDOFx, nDOFy, nVar)	$((nDOFx \cdot nDOFy)+Pad) \cdot nVar$	
lqh (nonlinear)	(nVar, nDOFt, nDOFx, nDOFy, nDOFz)	$(nVar+Pad)\cdot nDOF^4$	
lqh (linear)	(nVar, nDOFx, nDOFy, nDOFz,nDOFt,)	$(nVar+Pad)\cdot nDOF^4$	
lFh	(nVar,nDOFx,nDOFy,nDOFz,nDOFt,d)	$(nVar+Pad)\cdot nDOF^4\cdot d$	
temporary variables			
QavL, QavR	(nVar)	(nVar+Pad)	
lambdaL, lambdaR	(nVar)	(nVar+Pad)	
$\mathrm{tmp_bnd}$	(nDOFx, nDOFy, nVar)	$((nDOFx \cdot nDOFy)+Pad) \cdot nVar$	

Table E.3.: Data layout (Fortran notation) used in the optimised kernels.