The ExaHyPE story & Profiling for ExaHyPE
Part I

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www.exahype.eu

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The project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 671698 (ExaHyPE).

Introduction

Topics not covered by this presentation

- Numerics deep dive (ADER-DG, Limiting, etc.)
- Performance analysis case studies and scaling graphs (next time)
- Demo session ;-(

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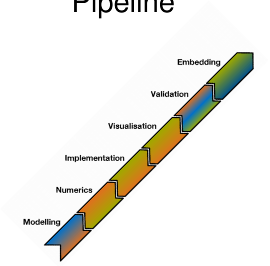
Topics covered by this presentation

- **Context** and **motivation** behind the project
- Overview on **key objectives** of ExaHyPE
- Summary on **techniques** employed by the framework
- Current state and next steps on the agenda
- Profiling infrastructure for ExaHyPE

Context & Motivation

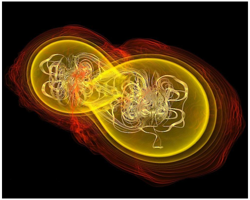
Important aspects in the context of Scientific Computing

Simulation Pipeline



Exascale computing

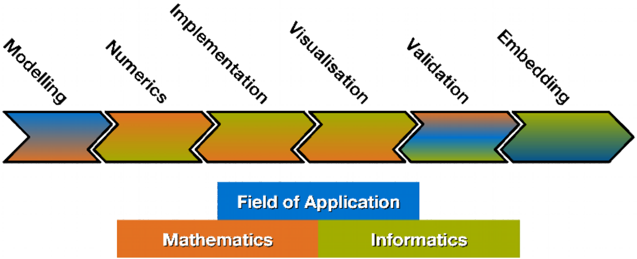
Hyperbolic PDEs



Simulation Pipeline

Observations from practice

- All steps are repeated over and over again!
- Nobody can be an expert in everything!
- Why not focus on what you are best in and consider the other problems solved?



The Simulation Pipeline
via Hans-Joachim Bungartz: Modeling and Simulation (IN2010)

Exascale Computing

Major challenges*

- Energy consumption
- Multi-level parallelism on hybrid architectures
- Fault tolerance and resilience
- Memory and bandwidth as bottleneck
- ...

*E.g. according to the U.S. DOE (source: science.energy.gov/ascr/research/scidac/exascale-challenges/).

Exascale Computing

Sunway TaihuLight, Wuxi, China, 2016
125 PFlop/s, 15.3 MW, 237M USD

An exascale system, Europe, 2020?

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148 SuperMUCs don't fit on a slide…

Hyperbolic PDEs

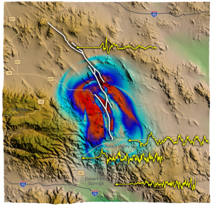
General form

$$\frac{\partial}{\partial t}[\boldsymbol{u}]_v + \frac{\partial}{\partial x_d}[\boldsymbol{F}(\boldsymbol{u})]_{vd} = [\boldsymbol{s}(\boldsymbol{u})]_v\,,$$

where $v \in \{1, 2, \ldots, V\}$ and $\boldsymbol{F} = [\boldsymbol{f}_1, \boldsymbol{f}_2, \ldots, \boldsymbol{f}_D]$ and $\frac{\partial [\boldsymbol{f}_d]_i}{\partial x_j}$ has real eigenvalues for all $d \in \{1, 2, \ldots, D\}$.

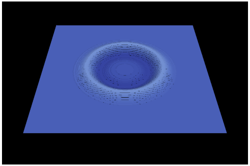
Areas of application

Geophysics



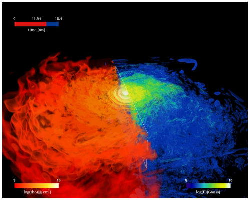
Simulation of ground shaking of the 1992 Landers Earthquake

Gas dynamics



Simulated pressure wave in a compressible gas

Astrophysics



Simulation of the merger of two magnetized neutron stars

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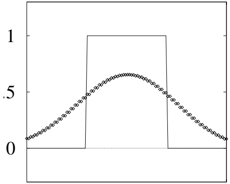
Challenges

- Long-term accuracy
- Stability at shocks
- Time step restrictions (e.g. for stiff source terms)
- Arithmetic density and data locality



Example Linear Advection (via Eleuterio F. Toro: Riemann solvers and numerical methods for fluid dynamics)

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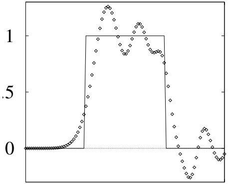

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The ExaHyPE project

Vision

- Three pillars of scientific progress:
  Theory, Experiment and Simulation
- Programming (exascale) supercomputers is a key challenge
- The ExaHyPE project seeks to address the software aspect of supercomputer development
  - Development of new mathematical and algorithmic approaches
  - Initial focus on applications in geo- and astrophysics
  - Correspondence with Europe's 2020 exascale strategy

The ExaHyPE project

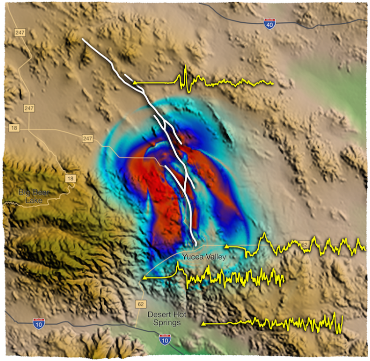
Objectives

- Energy efficiency on tomorrow's supercomputing hardware
- Scalable algorithms through well-balanced dynamic adaptivity
- Compute-bound simulations in spite of slow memory and networks
- Extreme parallelism on unreliable hardware

The ExaHyPE project

Benefit

- Simulation of risk scenarios
- Fundamental scientific findings
- Open-source



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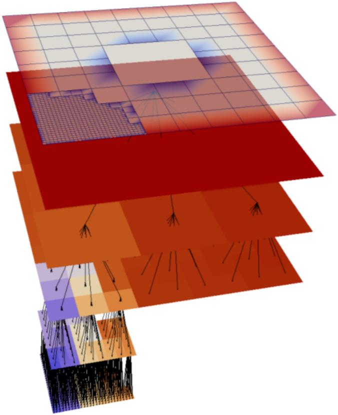
The ExaHyPE project

Approach

- High-order space-time Discontinuous Galerkin method (ADER-DG) with a-posteriori FVM based subcell limiting
- Dynamically adaptive Cartesian grids (AMR), space filling curves and dynamic load balancing (Peano)
- Hardware specific optimization of dominant compute kernels (libxsmm)



Adaptive Grid (via Weinzierl)

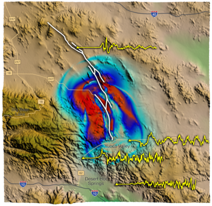
Exahype: Applications

Hyperbolic PDEs

$$\frac{\partial}{\partial t}[\boldsymbol{u}]_v + \frac{\partial}{\partial x_d}[\boldsymbol{F}(\boldsymbol{u})]_{vd} = [\boldsymbol{s}(\boldsymbol{u})]_v$$

Initial Focus

Geophysics



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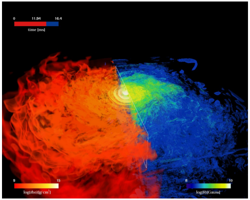
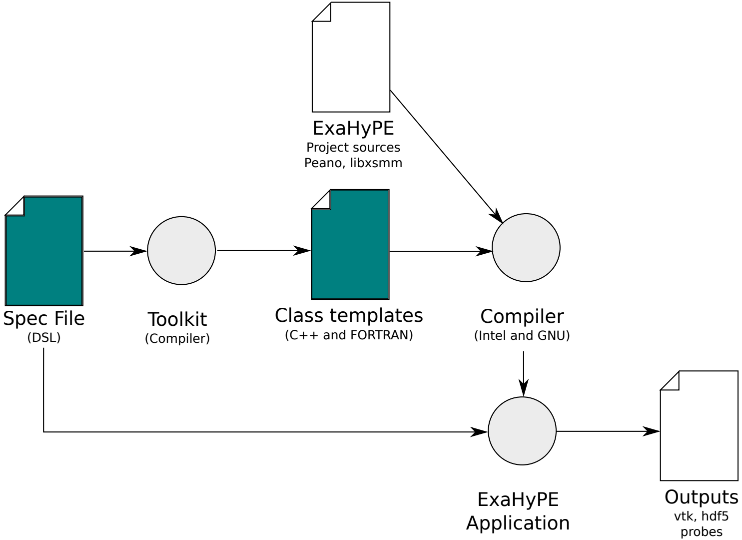


Simulation of the merger of two magnetized neutron stars

Exahype: As a user



Exahype: As a user

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

libxsmm-path                 = ../mypath
output-directory             = ./Applications/eulerflow2d
architecture                 = noarch

computational-domain
  dimension                  = 2
  width                      = 1.0
  offset                     = 0.0, 0.0
  end-time                   = 0.1
end computational-domain


solver ADER-DG MyEulerSolver
  unknowns   = 5
  parameters = 0
  order      = 3
  kernel     = generic::fluxes::nonlinear
  language   = C
  /* language  = Fortran */

  plot vtk::binary
    time     = 0.0
    repeat   = 0.05
    filename = ./solution
  end plot
end solver

shared-memory
  identifier                 = dummy
  cores                      = 2
  properties-file            = sharedmemory.properties
end shared-memory

optimisation
  fuse-algorithmic-steps     = off
end optimisation

end exahype-project
```

+

Implement:

- Flux
- Eigenvalues
- Source
- Initial conditions

Exahype: Agenda

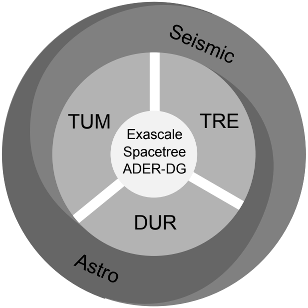
Current state

- ADER-DG (unlimited) and FVM solver available
- Shared- and distributed-memory parallelization
- Static AMR
- Shu vertex analytic benchmark
- Advanced output tooling

Next steps

- ADER-DG with a-posteriori subcell limiting
- Dynamic AMR
- Improved load balancing
- Petascale prototype
- Additional analytic benchmarks
- Parallel IO

Exahype: Consortium



UNIVERSITÀ DEGLI STUDI DI TRENTO

Durham University

FIAS Frankfurt Institute for Advanced Studies

Technische Universität München

LMU Ludwig-Maximilians-Universität München

RSC

Bavarian Research Alliance

Associated Partner lrz

Exahype: Profiling motivation

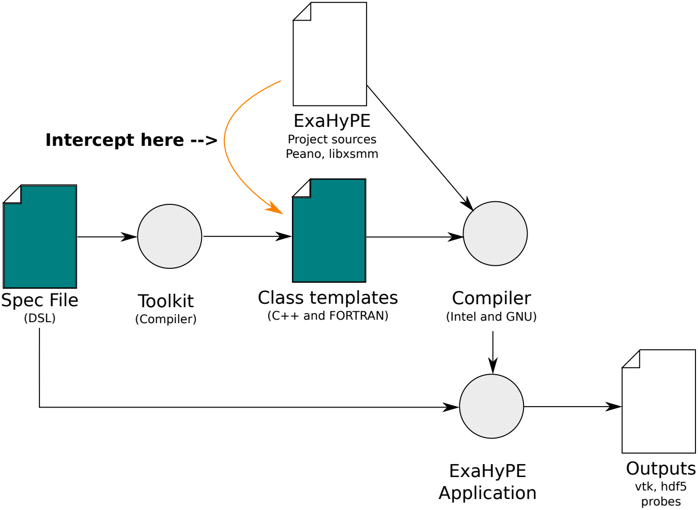
You can't optimize for what you don't measure!

Profiling provides metrics to

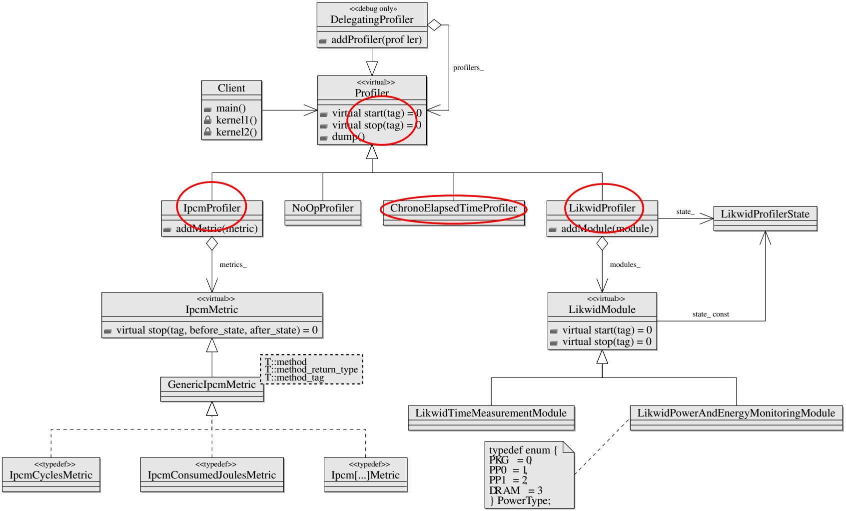
- obtain a **baseline**
- **track progress** of optimization efforts
- **compare** solution to other state of the art solutions

We don't need a third one of these on campus!

Exahype: Profiling arch



Exahype: Profiling arch



Exahype: Profiling

What we can measure

- Kernel call count
- Wall clock time, cycles
- Read/write RAM
- Flop/s (estimate)
- Energy consumption (Core, RAM, package; estimate)
- Cache hits/misses/ratio (I, L2, L3)
- Cycles lost due to cache misses (L2, L3)
- Instructions retired, branch prediction ratio
- ...

Exahype: Profiling next steps

Profiling: Next steps

- Comparison generic vs. optimized kernels vs. Fortran baseline (cell update time)
- **Case study**: Quick optimization of generic kernels, usage of profiling in practice
- Polynomial degree $\rightarrow$ energy
- Analytic benchmark + AMR, fixed error: Polynomial degree $\rightarrow$ energy (real world sweet spot)
- ...

Profiling for ExaHyPE - Part II

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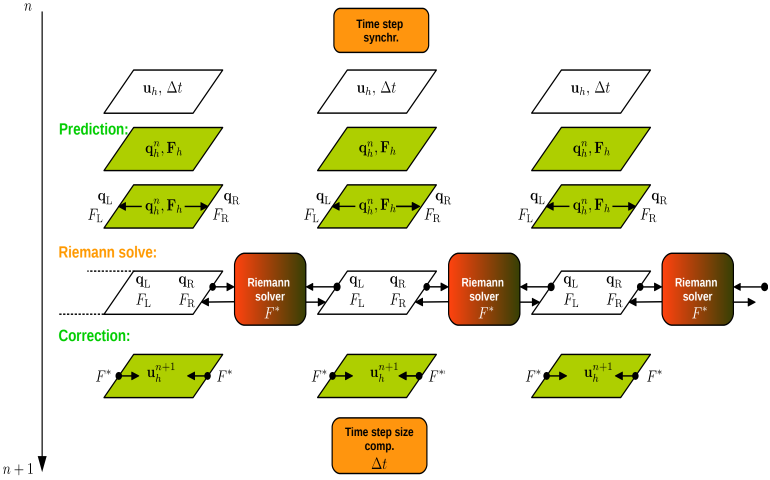
ADER-DG



via Dominic