

The ExaHyPE story & Profiling for ExaHyPE

Part I

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<http://exahype.eu>

August 2016

Introduction

Topics not covered by this presentation

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

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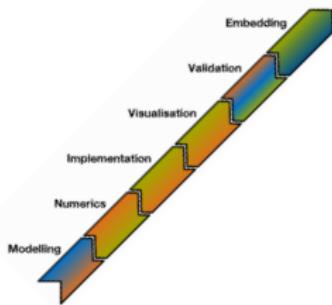
Topics covered by this presentation

- ▶ 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

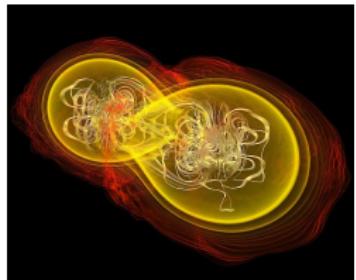
Simulation Pipeline



Exascale computing



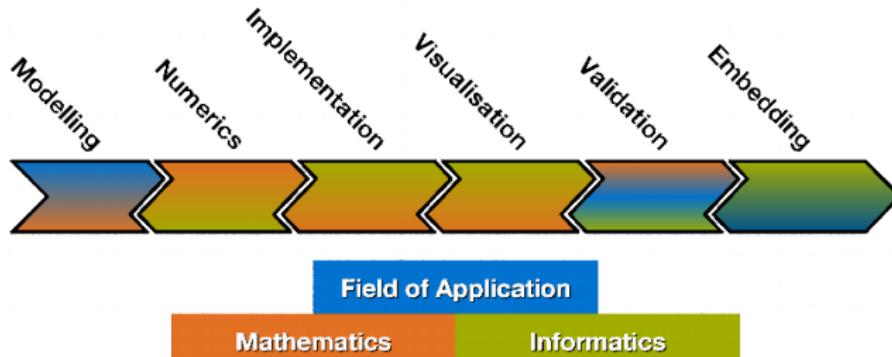
Hyperbolic PDEs



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

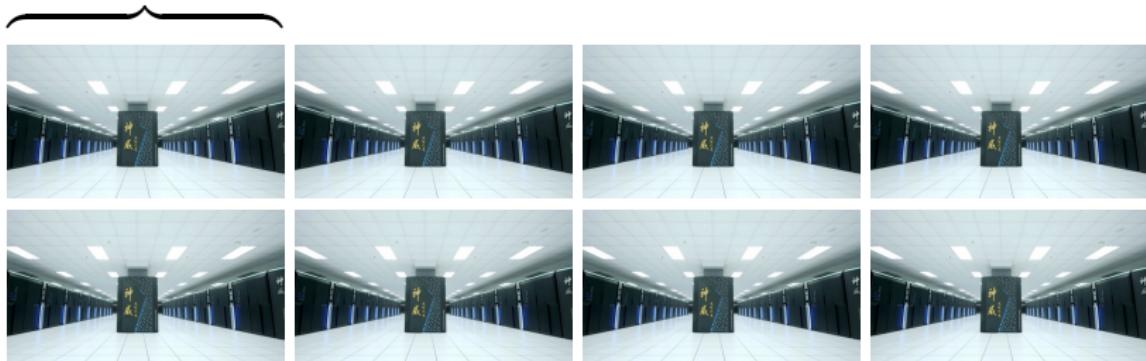
Sunway TaihuLight, Wuxi, China, 2016
125 PFlop/s, 15.3 MW, 237M USD



An exascale system, Europe, 2020?

Exascale Computing

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148 SuperMUCs don't fit on a slide...

Hyperbolic PDEs

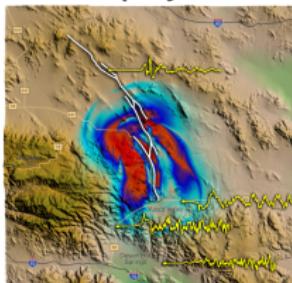
General form

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

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

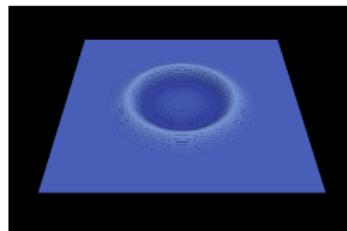
Areas of application

Geophysics



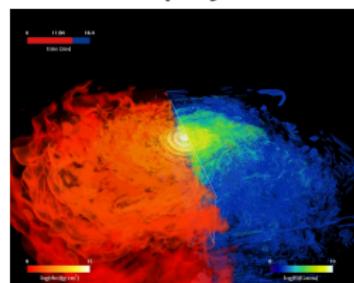
Simulation of ground shaking of the 1992 Landers Earthquake

Gas dynamics



Simulated pressure wave in a compressible gas

Astrophysics



Simulation of the merger of two magnetized neutron stars

Hyperbolic PDEs

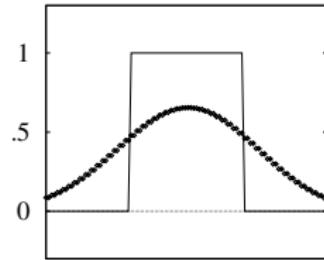
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Challenges

- ▶ 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)

Hyperbolic PDEs

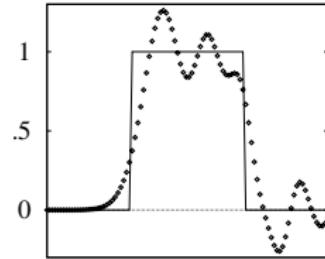
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The ExaHyPE project

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

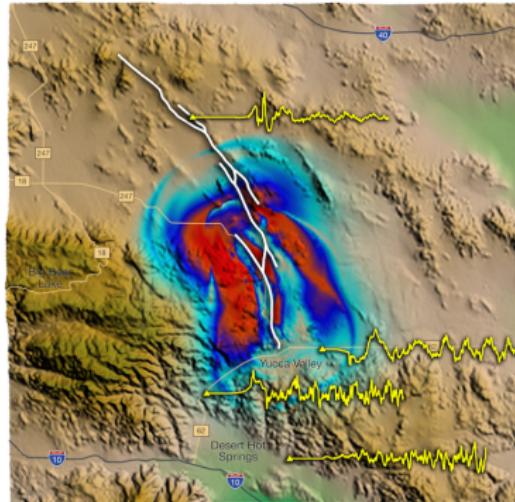
- ▶ Energy efficiency on tomorrow's supercomputing hardware
- ▶ Scalable algorithms through well-balanced dynamic adaptivity
- ▶ Compute-bound simulations in spite of slow memory and networks
- ▶ Extreme parallelism on unreliable hardware



The ExaHyPE project

Benefit

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

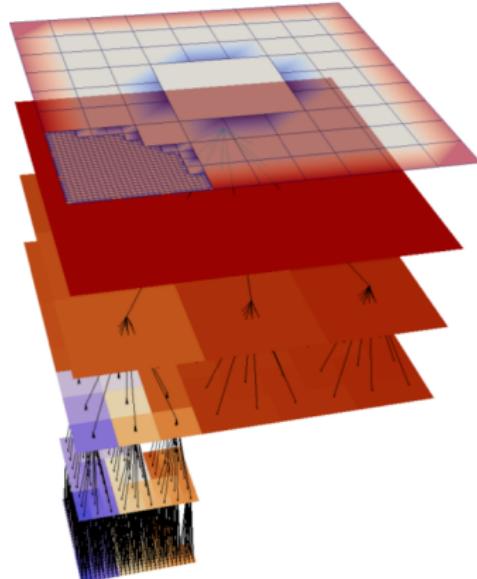


Simulation of ground shaking of the 1992 Landers Earthquake

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 (libxsimm)



Adaptive Grid (via Weinzierl)

Exahype: Applications

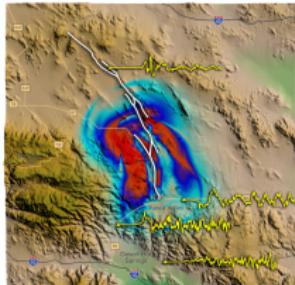
Hyperbolic PDEs

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

Initial Focus

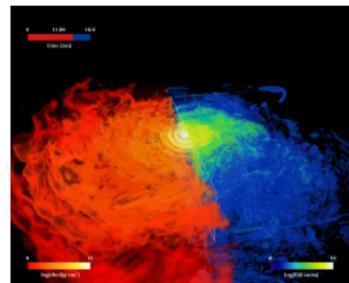


Geophysics



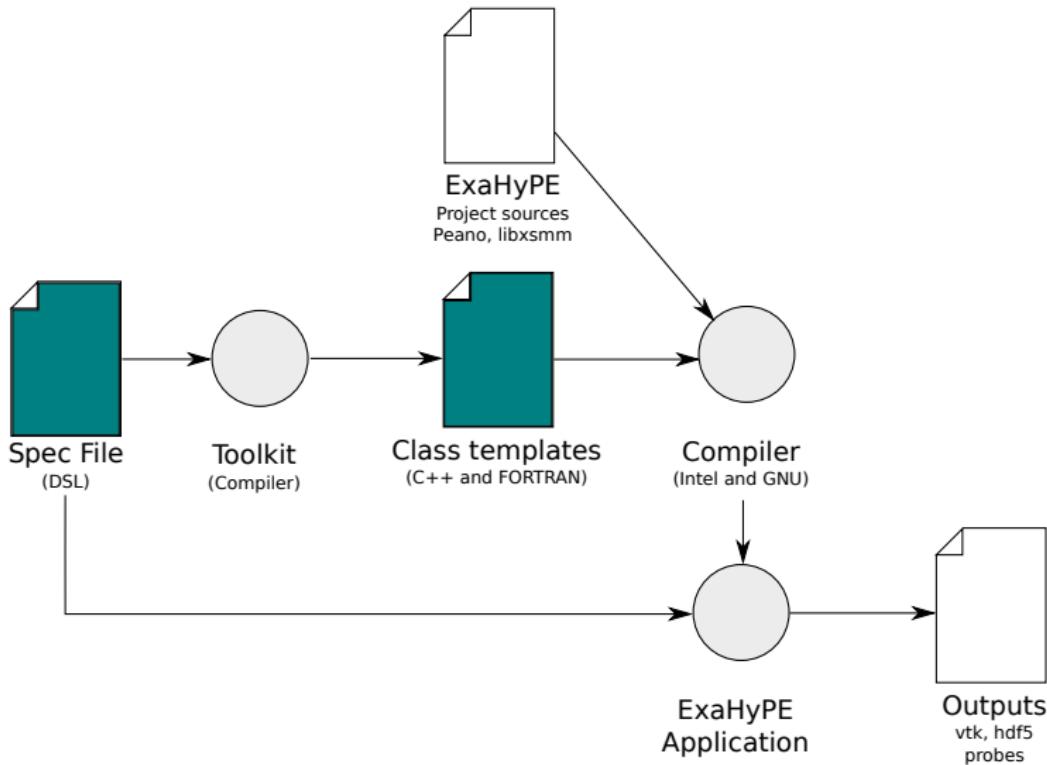
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Gas dynamics



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

```

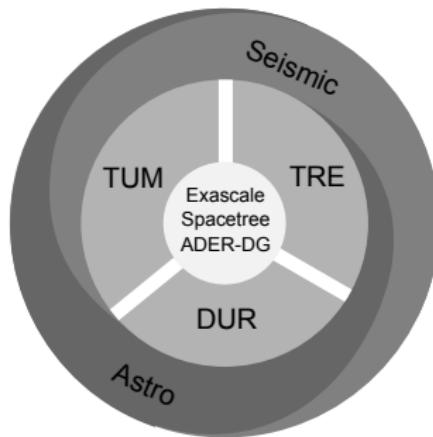
Implement:

- ▶ Flux
- ▶ Eigenvalues
- ▶ Source
- ▶ Initial conditions





Exahype: Consortium



UNIVERSITÀ DEGLI STUDI
DI TRENTO



Durham
University



FIAS Frankfurt Institute
for Advanced Studies



Bavarian
Research Alliance

Associated Partner



Exahype: Profiling motivation

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

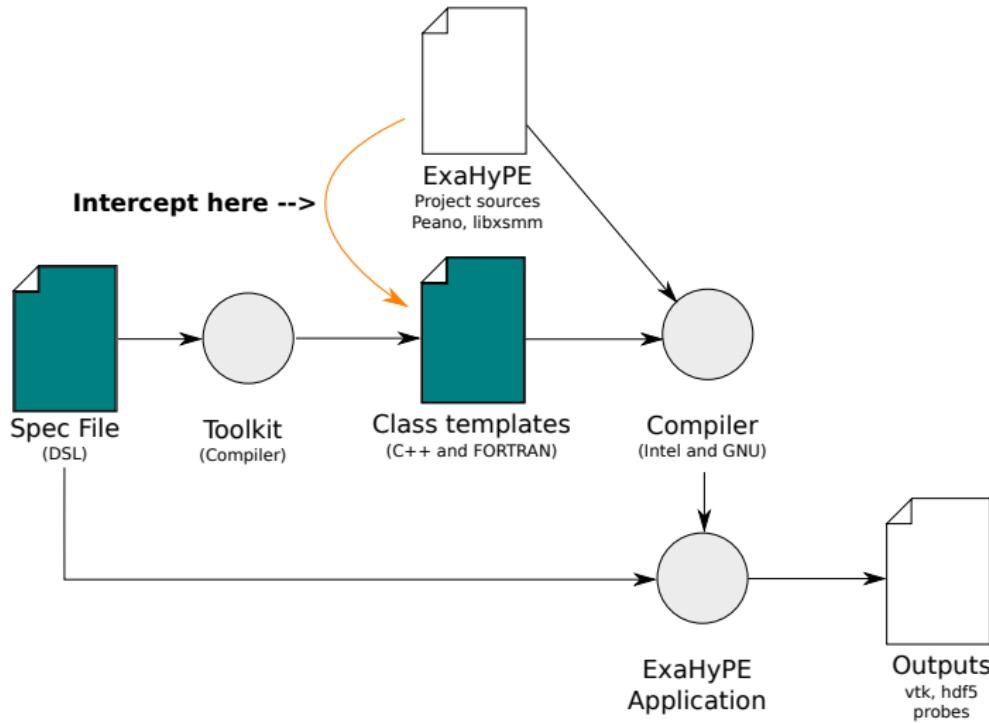
Profiling provides metrics to

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

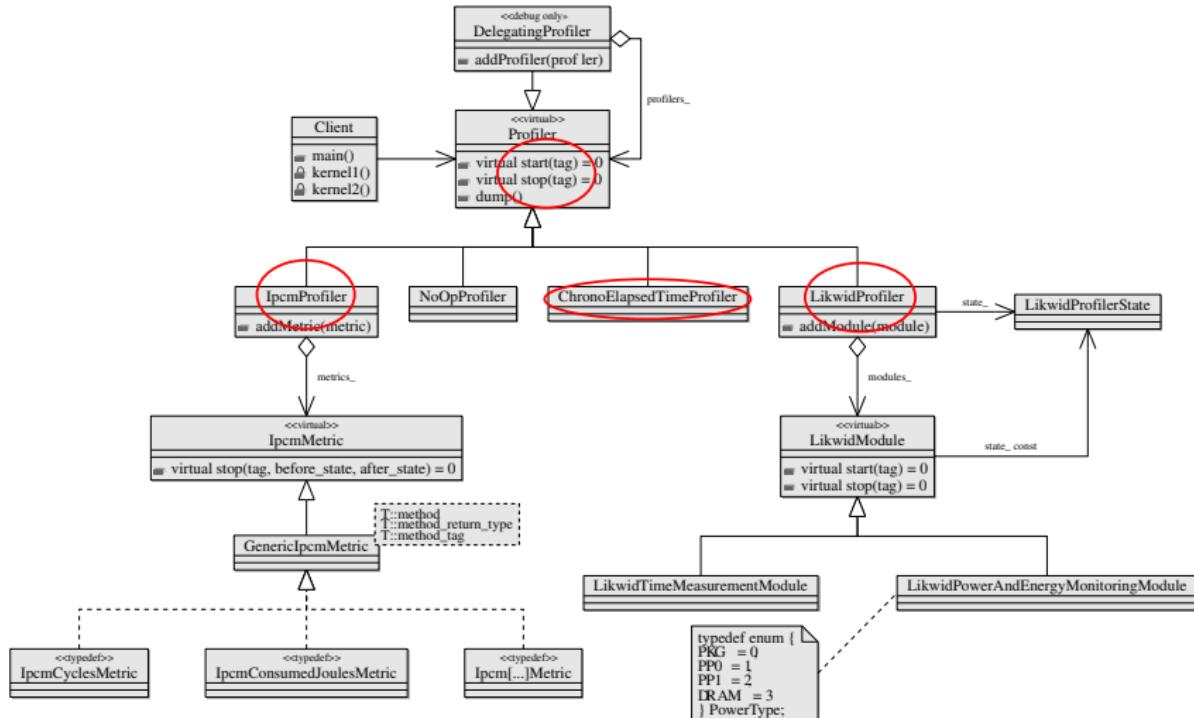


We don't need a third one
of these on campus!

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 (L1, L2, L3)
- ▶ Cycles lost due to cache misses (L2, L3)
- ▶ Instructions retired, branch prediction ratio
- ▶ ...



Exahype: Profiling next steps

Q & A

Funding...

ADER-DG

