

The ExaHyPE story & Profiling for ExaHyPE

Part I

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www.exahype.eu

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Introduction

What this presentation is not about:

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

Introduction

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- ▶ **Demo session** ;-(

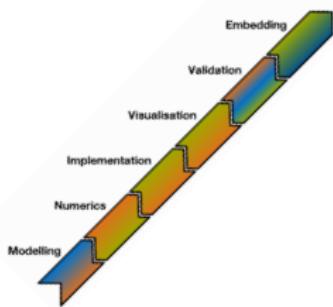
What this presentation is about:

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

Context & Motivation

Important aspects in the context of Scientific Computing:

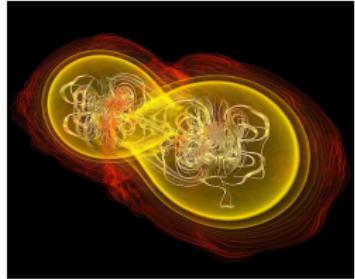
Simulation Pipeline



Exascale Computing



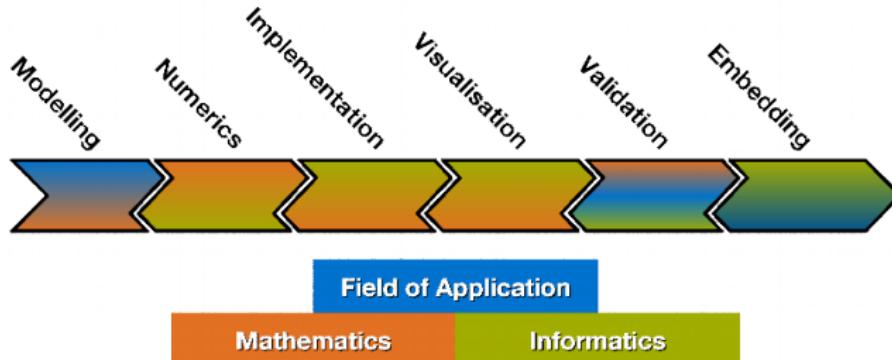
Hyperbolic Conservation Laws



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), 2015)

Exascale Computing

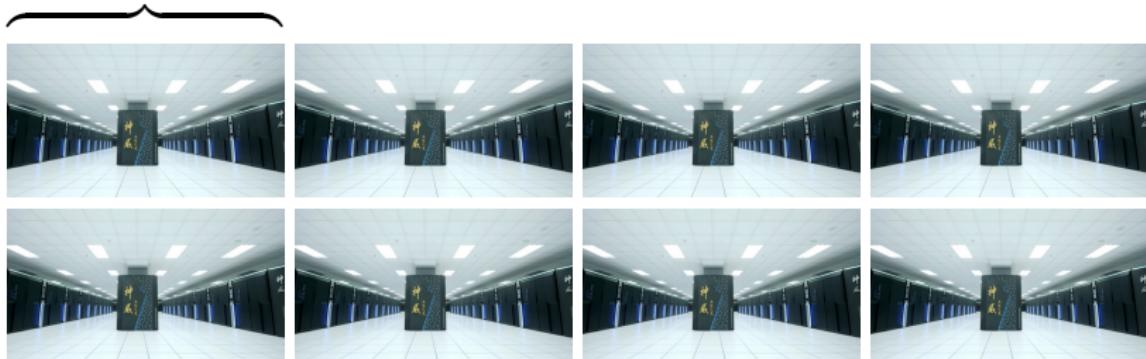
Major challenges*:

- ▶ **Energy** consumption
- ▶ Multi-level **parallelism** on hybrid architectures
- ▶ Fault tolerance and **resilience**
- ▶ Memory and network **bandwidth bottlenecks**
- ▶ ...

* e.g. according to the U.S. Department of Energy: science.energy.gov/ascr/research/scidac/exascale-challenges/

Exascale Computing

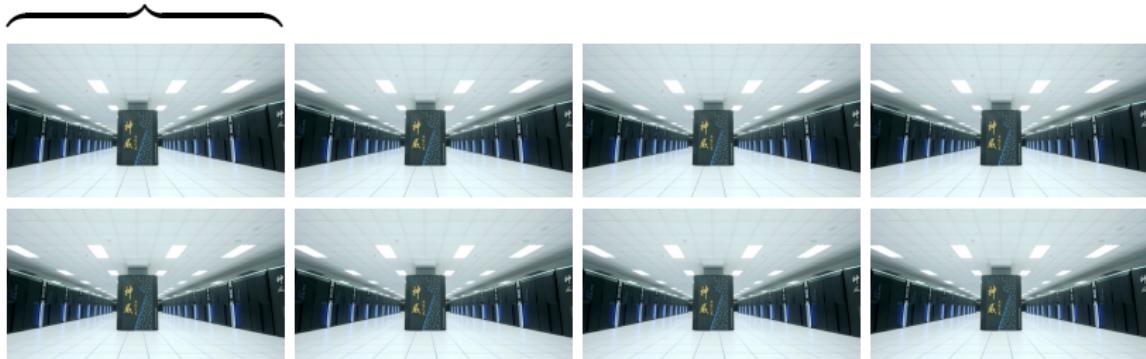
Sunway TaihuLight, Wuxi, China, 2016
125 PFlop/s, 15.3 MW, 237M USD



An exascale system, Europe, 2020?

Exascale Computing

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An exascale system, Europe, 2020?

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

Hyperbolic Conservation Laws

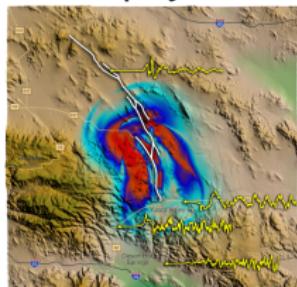
General form:

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

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

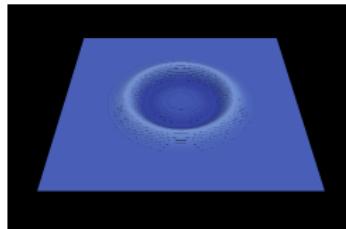
Areas of application:

Geophysics



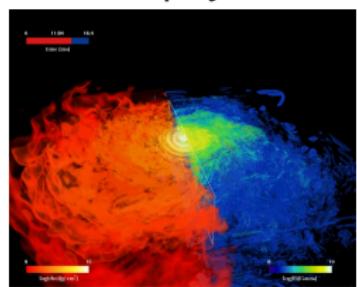
Simulation of ground shaking of the 1992 Landers Earthquake
(via Alexander Heinecke, 2014)

Gas dynamics



Simulated pressure wave in a compressible gas
(via Dominic E. Charrier, 2016)

Astrophysics



Simulation of the merger of two magnetized neutron stars
(via Luciano Rezzolla, 2008)

Hyperbolic Conservation Laws

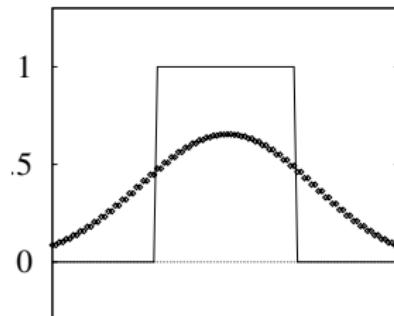
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Challenges:

- ▶ 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, 2009)

Hyperbolic Conservation Laws

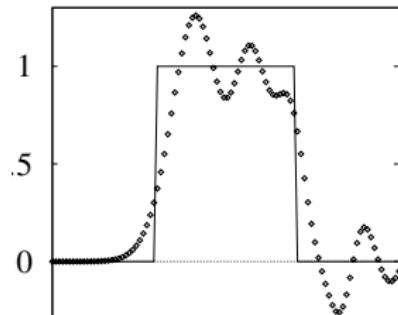
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ExaHyPE: The Project

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
 - ▶ In correspondence with Europe's **2020 exascale strategy**
- ▶ Goal: Become **the engine** for large HCL simulations!

ExaHyPE: The Project

Objectives:

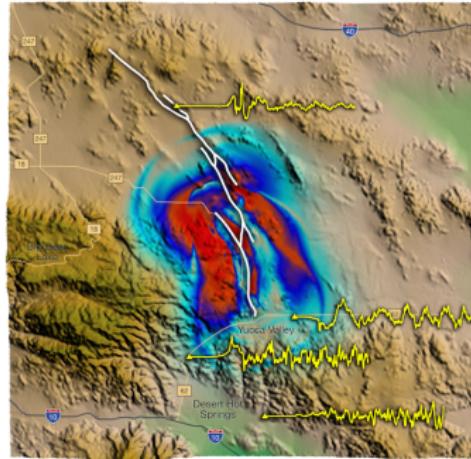
- ▶ **Energy efficiency** on tomorrow's supercomputing hardware
- ▶ Scalable algorithms through well-balanced **dynamic adaptivity**
- ▶ **Compute-bound** simulations in spite of slow memory and networks
- ▶ Extreme parallelism on **unreliable hardware**



ExaHyPE: The Project

Benefit:

- ▶ Simulation of **risk scenarios**
 - ▶ Assess the effects of earthquake and aftershocks
 - ▶ Quantify seismic hazards
- ▶ Enable fundamental **scientific findings**
 - ▶ Study some of the longest-standing mysteries in astrophysics...
 - ▶ ... and other disciplines
- ▶ **Open-source** (BSD3, 



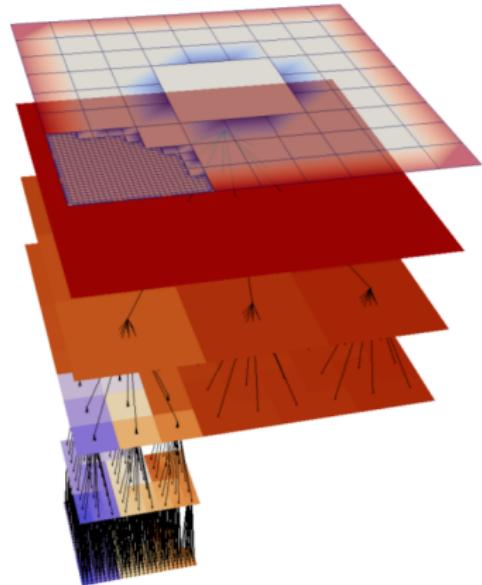
Simulation of the 1992 Landers Earthquake

(via Alexander Heinecke, 2014)

ExaHyPE: The 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 grids in Peano
(via Tobias Weinzierl, 2014)

ExaHyPE: Applications

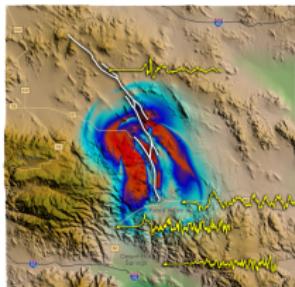
Hyperbolic Conservation Laws:

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Initial focus:

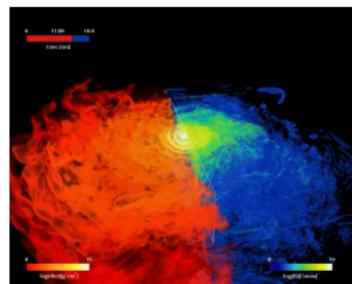


Geophysics



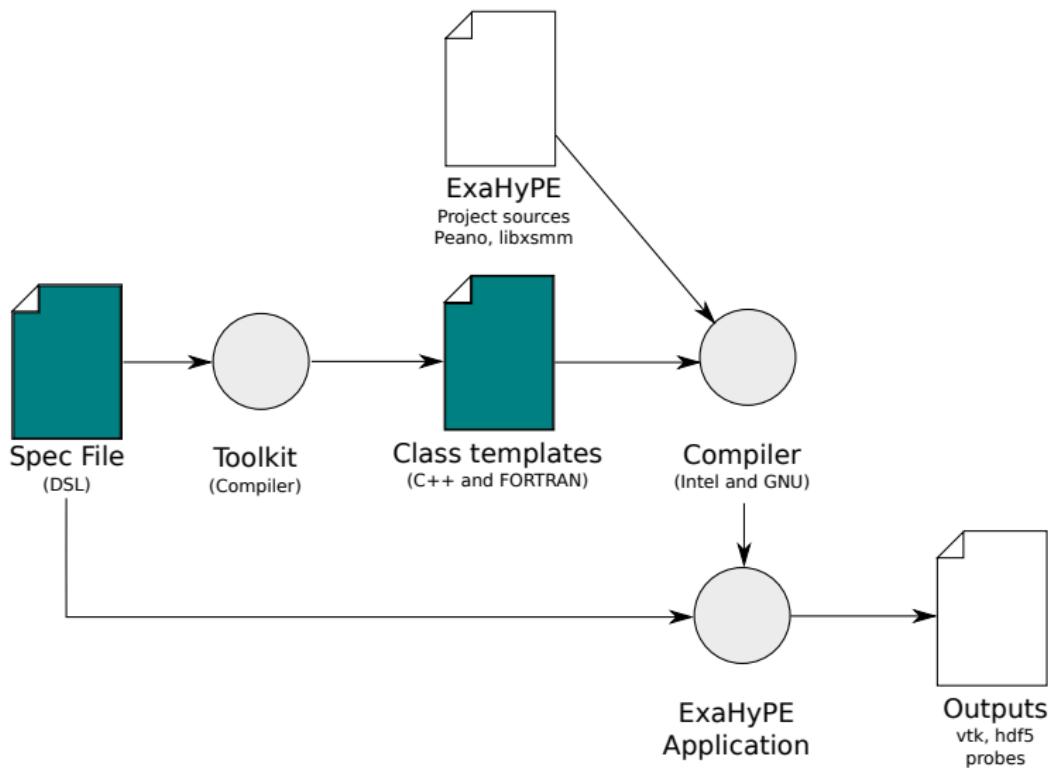
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ExaHyPE: From a User's Perspective



ExaHyPE: From a User's Perspective

```

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

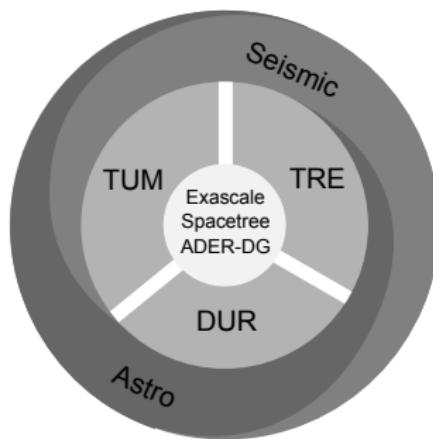
Current state:

- ▶ ADER-DG (unlimited) and FVM **solvers**
- ▶ Shared- and distributed-memory **parallelization**
- ▶ Static mesh refinement
- ▶ "Shu vortex" **analytic benchmark**
- ▶ Advanced **export** capabilities

Next steps:

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

ExaHyPE: Summary



UNIVERSITÀ DEGLI STUDI
DI TRENTO



Durham
University



FIAS Frankfurt Institute
for Advanced Studies



Bavarian
Research Alliance

Associated Partner



Profiling for ExaHyPE: Motivation

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

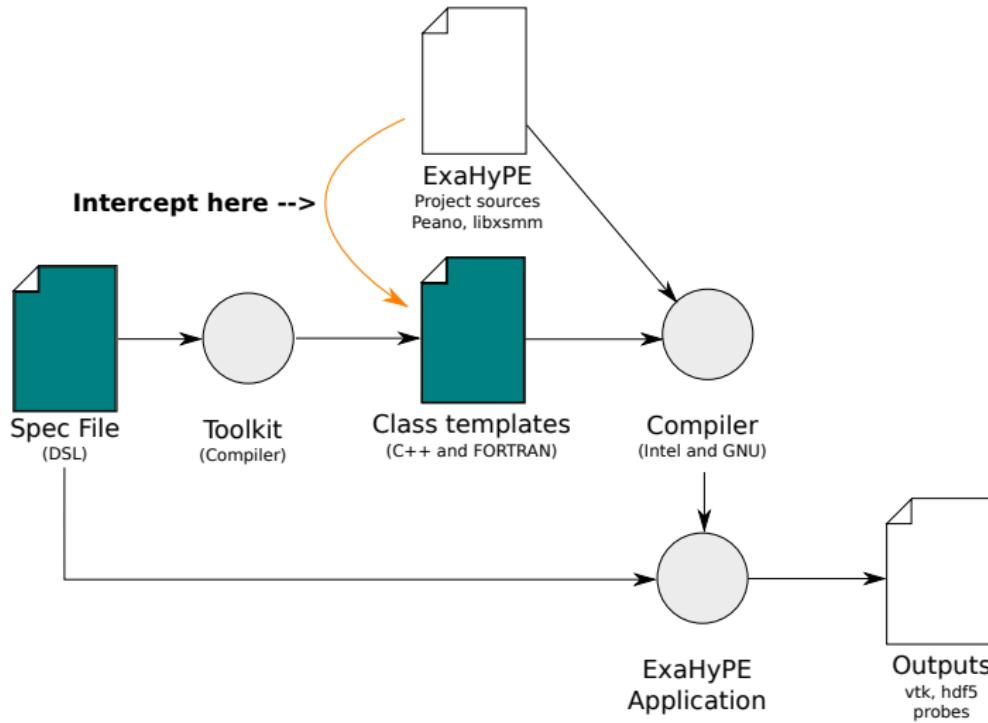
Profiling provides metrics to

- ▶ obtain a **baseline**,
- ▶ **guide** and **track progress** of optimization efforts,
- ▶ **compare** current status to other state of the art solutions.

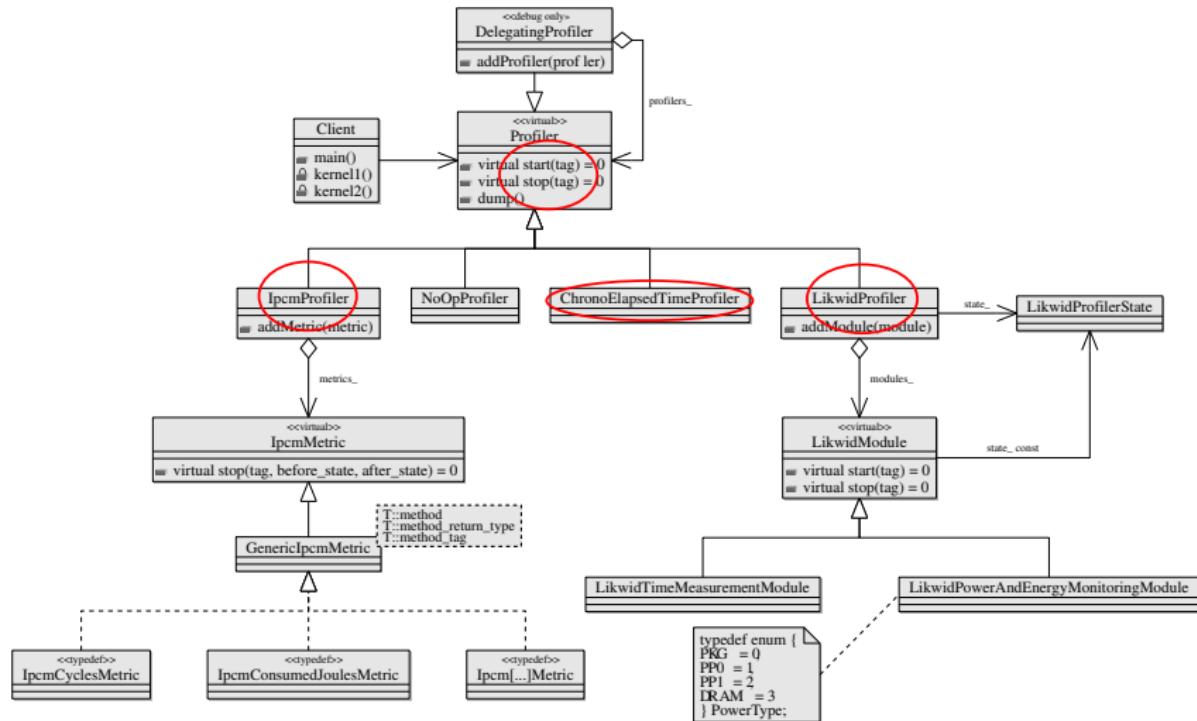


We don't need a third one
of these on campus!

Profiling for ExaHyPE: Architecture



Profiling for ExaHyPE: Architecture



Profiling for ExaHyPE: Metrics

What we can measure at the moment:

- ▶ Kernel call counts
- ▶ Cycles and wall clock time
- ▶ RAM reads/writes
- ▶ **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
- ▶ ...

Profiling for ExaHyPE: Outlook

Profiling: Next steps

- ▶ Comparison **cell update time**:
Generic C++ vs. optimized C++ vs. Fortran baseline
- ▶ **Case study**: Fast, **metric-driven optimization** of generic kernels
- ▶ Relation polynomial degree, energy consumption/runtime
+ **explanation** based on **profiling insights**
- ▶ Analytic benchmark, AMR, fixed error:
Relation polynomial degree, energy consumption
Goal: Find real world **break-even point**
- ▶ ...

Profiling for ExaHyPE - Part II

Conclusion

Key aspects:

1. Exascale Computing is about both hardware and **software**
2. ExaHyPE as an **answer to future challenges** in Scientific Computing
3. **Frameworks** are necessary to manage the increasing complexity in HPC
4. Profiling is important: **Measure, then optimize!**

The ExaHyPE story & Profiling for ExaHyPE

Part I

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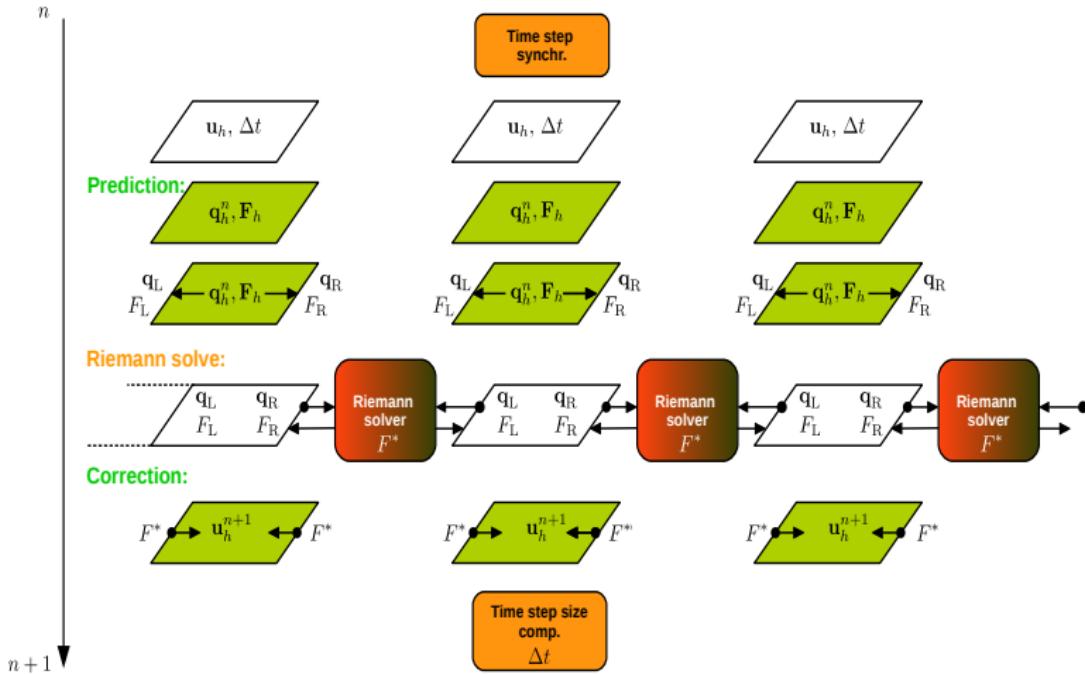
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ADER-DG



via Dominic E. Charrier, 2016