The ExaHyPE story & Profiling for ExaHyPE
Part I

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August 2016

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

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** ;-(

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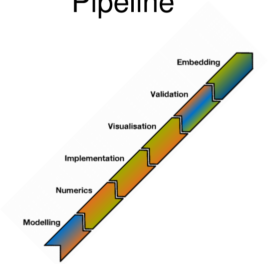
What this presentation is about:

- **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

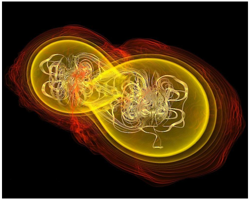
Important aspects in the context of Scientific Computing:

Simulation Pipeline



Exascale Computing

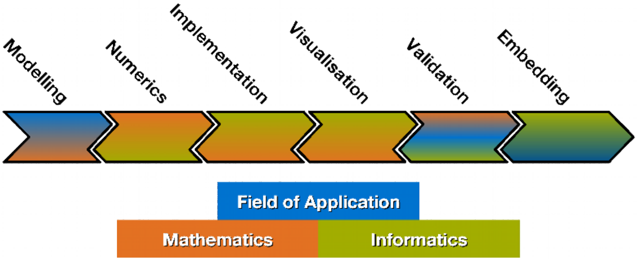
Hyperbolic Conservation Laws



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?

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

Hyperbolic Conservation Laws

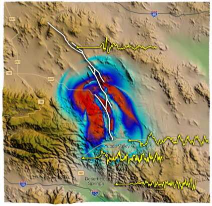
General form:

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

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

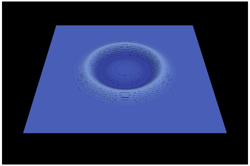
Areas of application:

Geophysics



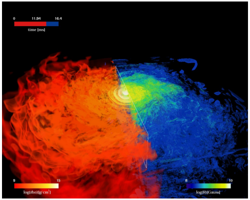
Simulation of ground shaking of the 1992 Landers Earthquake (via Alexander Heinecke, 2014)

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)

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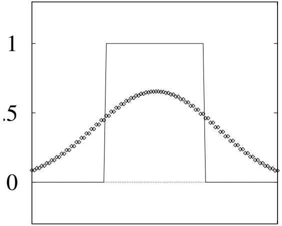
Challenges:

- 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)

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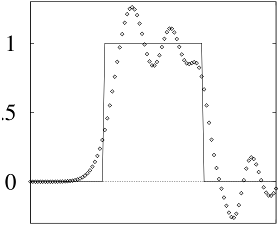

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ExaHyPE: The Project

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**

ExaHyPE: The Project

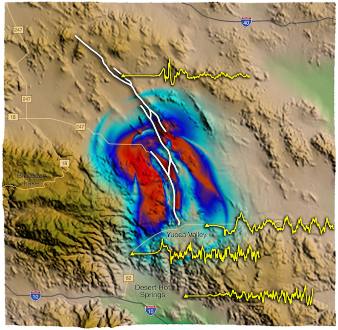
Objectives:

- **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,)

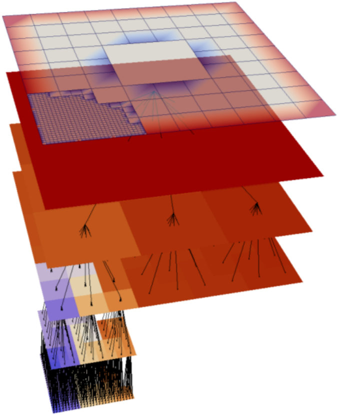


Simulation of the 1992 Landers Earthquake
(via Alexander Heinecke, 2014)

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)

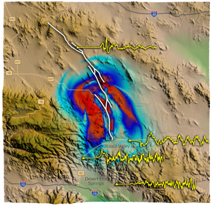
ExaHyPE: Applications

Hyperbolic Conservation Laws:

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

Initial focus:

Geophysics



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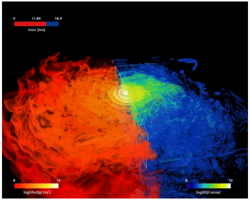

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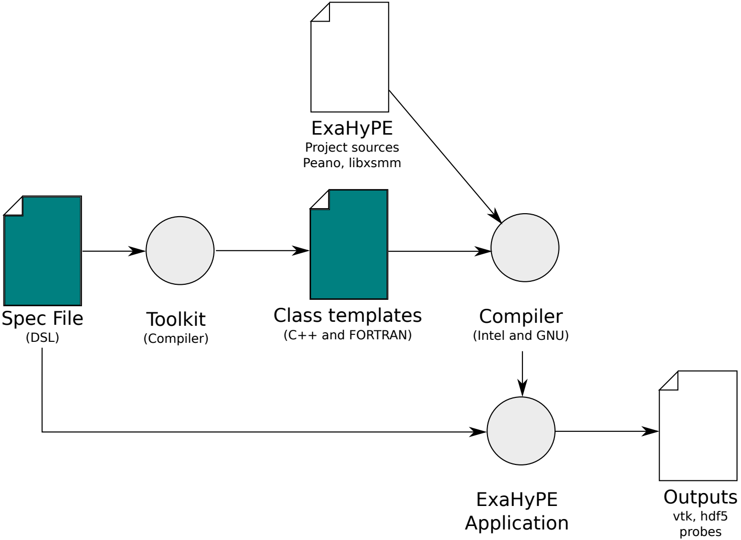
ExaHyPE: From a User's Perspective



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

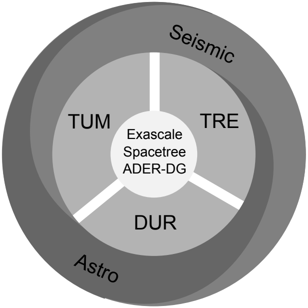
Current state:

- ADER-DG (unlimited) and FVM solver
- 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



Associated Partner

Profiling for ExaHyPE: Motivation

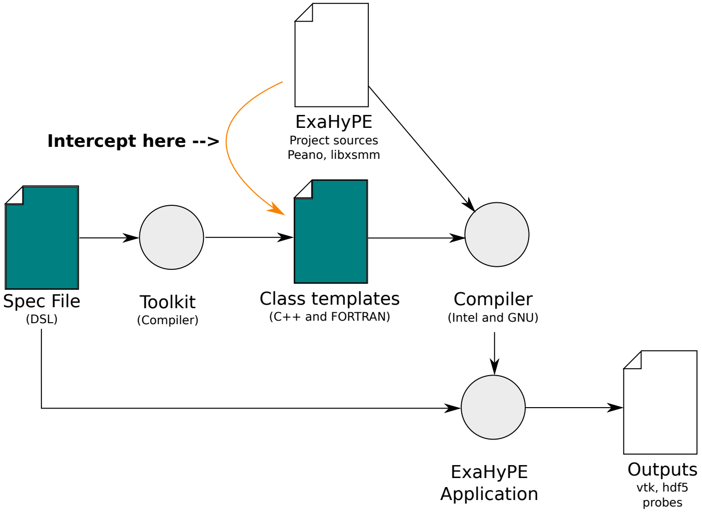
You can't optimize for what you don't measure!

Profiling provides metrics to

- obtain a **baseline**,
- **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



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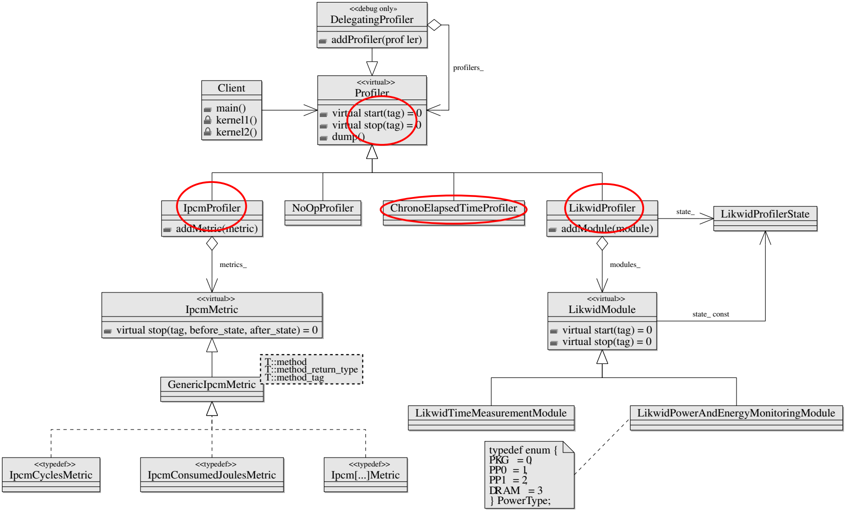

Profiling for ExaHyPE: Metrics

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 (I, 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!**

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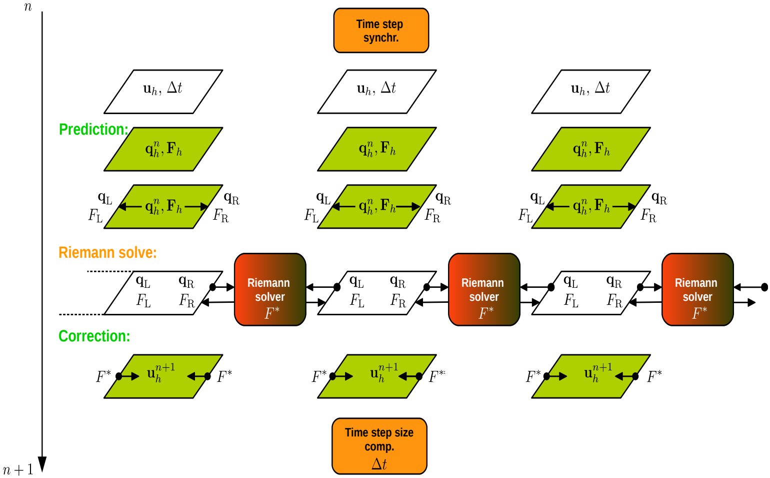
ADER-DG



via Dominic E. Charrier, 2016