ExaHyPE, an Exascale Hyperbolic PDE Engine

Jean-Matthieu Gallard
Technical University of Munich (TUM)
Department of Informatics
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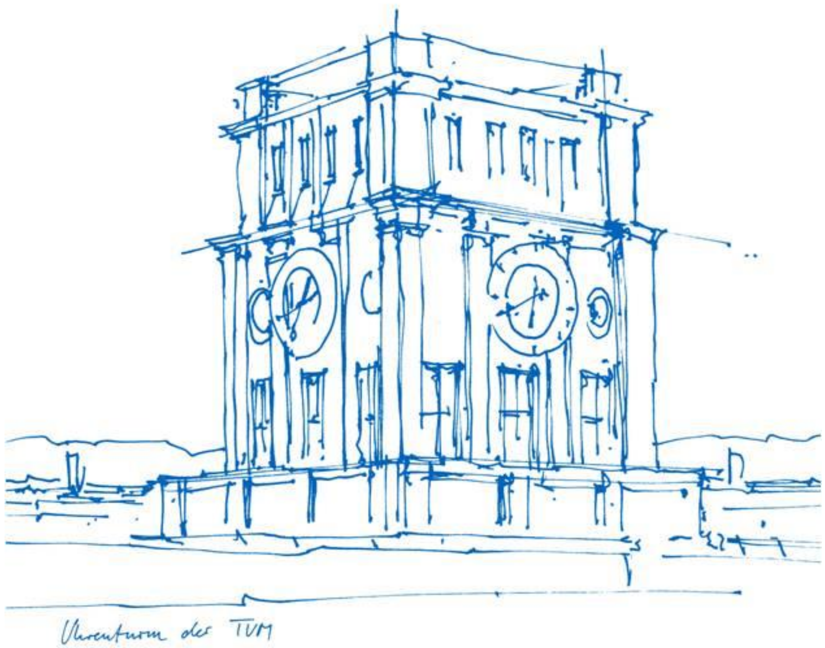


The ExaHyPE Project

Horizon 2020 project in the FETHPC call

“Towards Exascale High Performance Computing”

(New mathematical and algorithmic approaches)

ExaHyPE participants:

- **TUM:** Michael Bader, Jean-Matthieu Gallard, Leonhard Rannabauer
- **Durham Univ.:** Tobias Weinzierl, Dominic Charrier, Benjamin Hazelwood
- **Univ. Trento:** Michael Dumbser, Francesco Fambri, Maurizio Tavelli
- **LMU Munich:** Alice Gabriel, Kenneth Duru
- **Frankfurt IAS:** Luciano Rezzolla, Sven Köppel, Alejandro Cruz Osorio
- **RSC:** Alexander Moskowsky & Co.
- **BayFOR:** Robert Iberl, Teresa Kindermann (project management)
- associated: Leibniz Supercomputing Centre and JSCC RAS

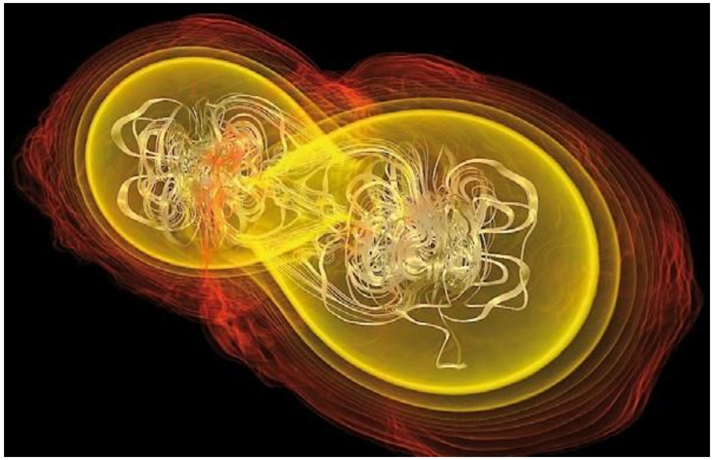
Outline

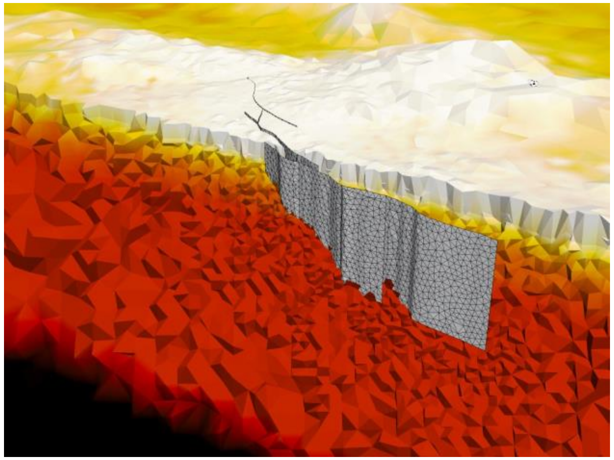
1. What is ExaHyPE
2. ExaHyPE’s component
3. Code Generation
4. Some benchmarks
5. Outlook

Towards an Exascale Hyperbolic PDE Engine

ExaHyPE Goal: a PDE “engine” (as in “game engine”)

- Enable medium-sized interdisciplinary research teams to realize extreme-scale simulations of grand challenges within one year
- Focus on hyperbolic conservation laws and specific numerics
- Concentrate on two specific grand challenges in the project:





Towards an Exascale Hyperbolic PDE Engine

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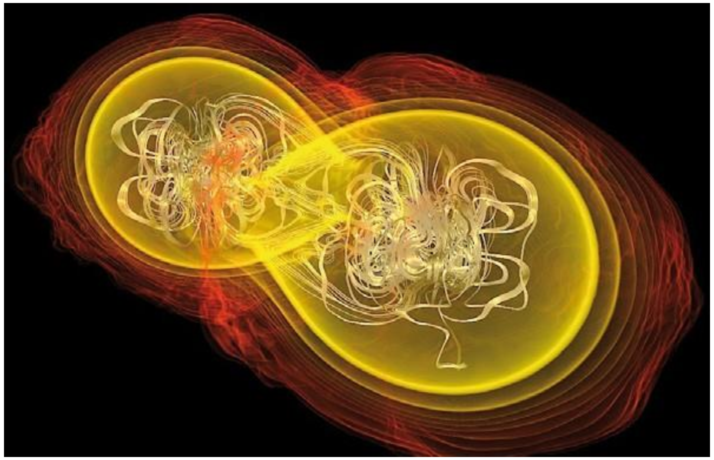

Astrophysics: merger of binary system of neutron stars (FIAS)

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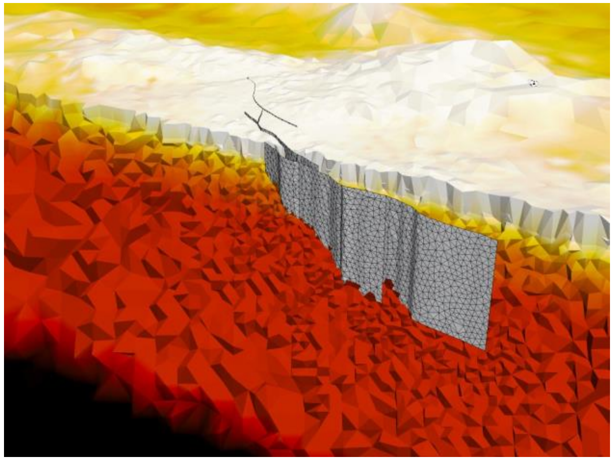
Seismology: regional earthquake simulation (LMU)



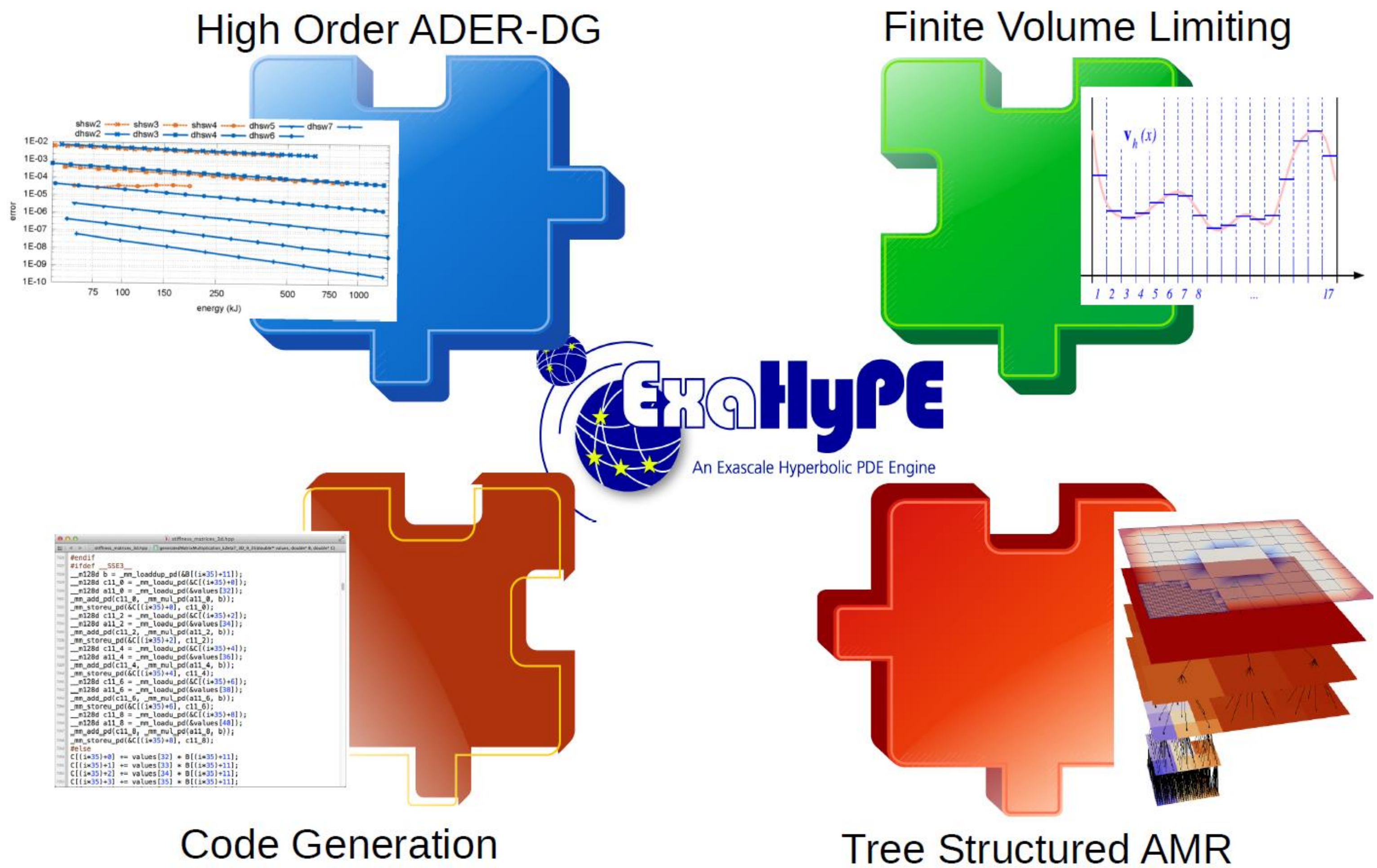
Towards an Exascale Hyperbolic PDE Engine

Requirements for Exascale Algorithms:

- Avoid data-transfer/communication and synchronisation
- Maximize arithmetic intensity and maximize “science per flop”/“science per Watt”
- Dynamic load balancing with lightweight adaptive response

➔ Focus on **High Order Discretisation** and **Adaptivity** in Space and Time

Components of the ExaHyPE Engine



Engine Architecture and Application Interface

Application Layer – user provides:

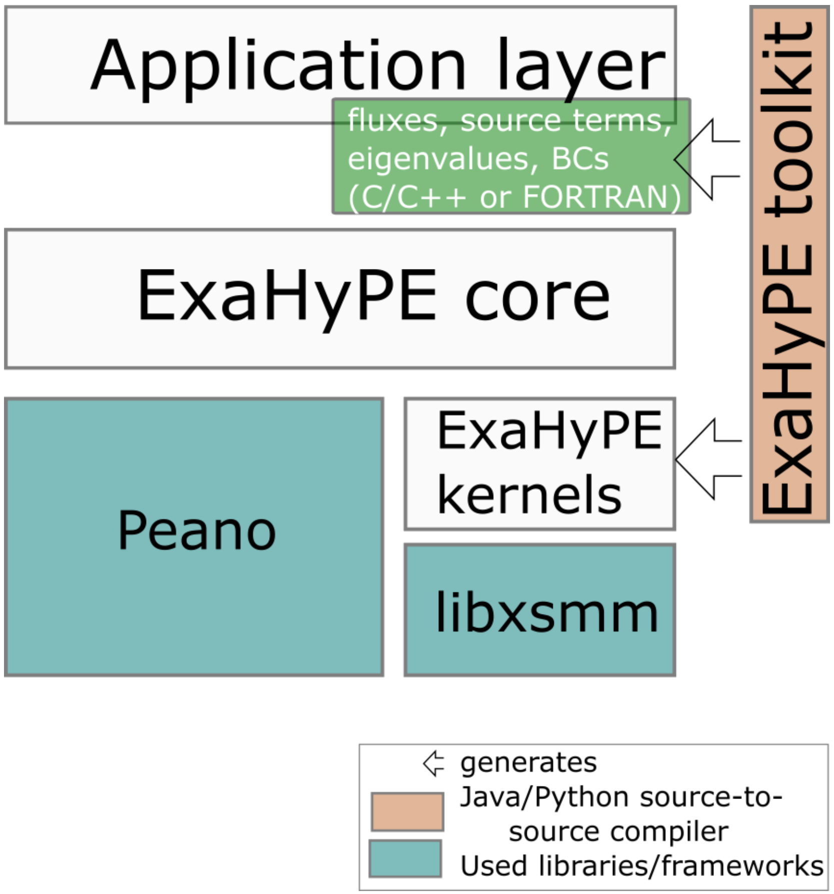
- C/Fortran code for PDEs

ExaHyPE toolkit generates:

- core routines, templates for application-specific functions
- kernels tailored to discretization order, number of quantities, etc.

Peano framework:

- hybrid MPI+Intel TBB parallelism
- data structures for parallel AMR



Code Generation: Optimizations and Constraints

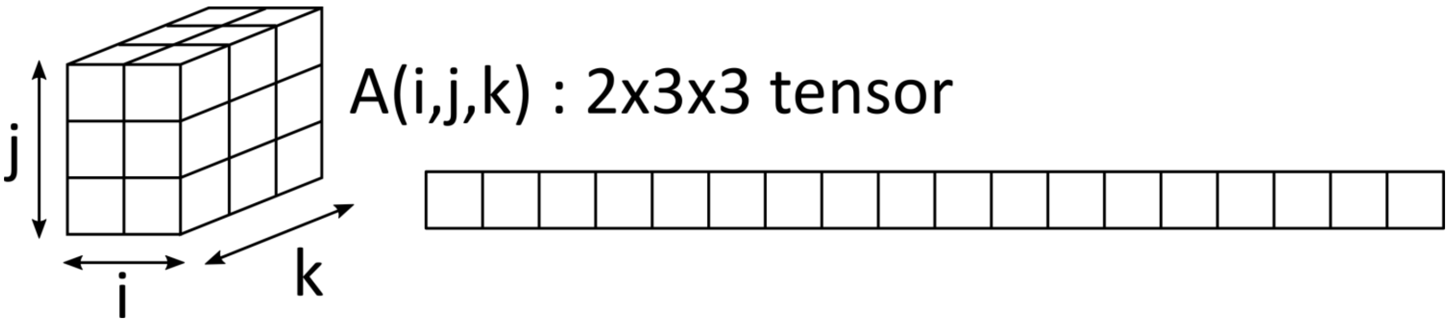
Desired Optimizations:

- Loop vectorization
- Efficient data access
- Matrix-tensor multiplications: Intel's Libxsmm

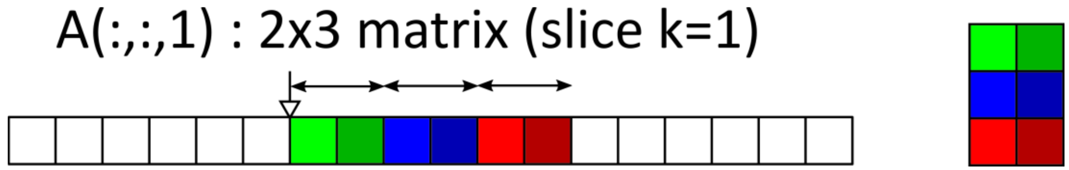
Constraints posed by:

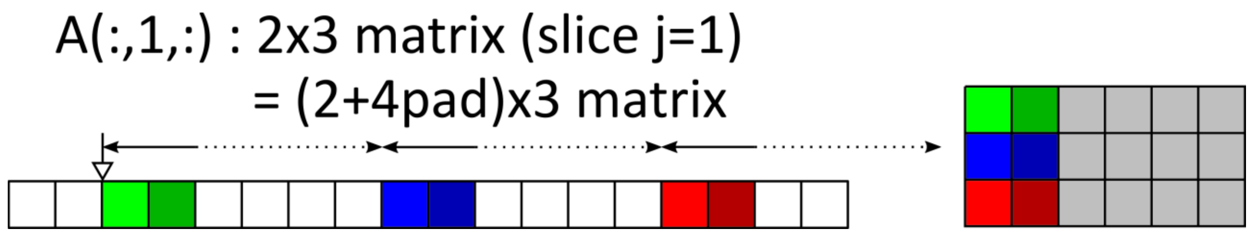
- Memory access: seamless integration with other user code fragments required
- Matrix multiplication: Libxsmm doesn't implement entire BLAS

Libxsmm: Accessing Matrices in Tensor



Fortran notations vs stride access for matrix multiplication:





Benchmark cases

Cases:

- EulerFlow 3D
  - No sources, no NCP
  - 5 quantities

- GRMHD
  - No sources, but NCP
  - 19 quantities

- Z4 Kerr-Schild
  - Sources + NCP
  - 54 quantities

Hardware:

- Intel Xeon E5-2697v3 (HSW)
- Single core measurements

Compiler:

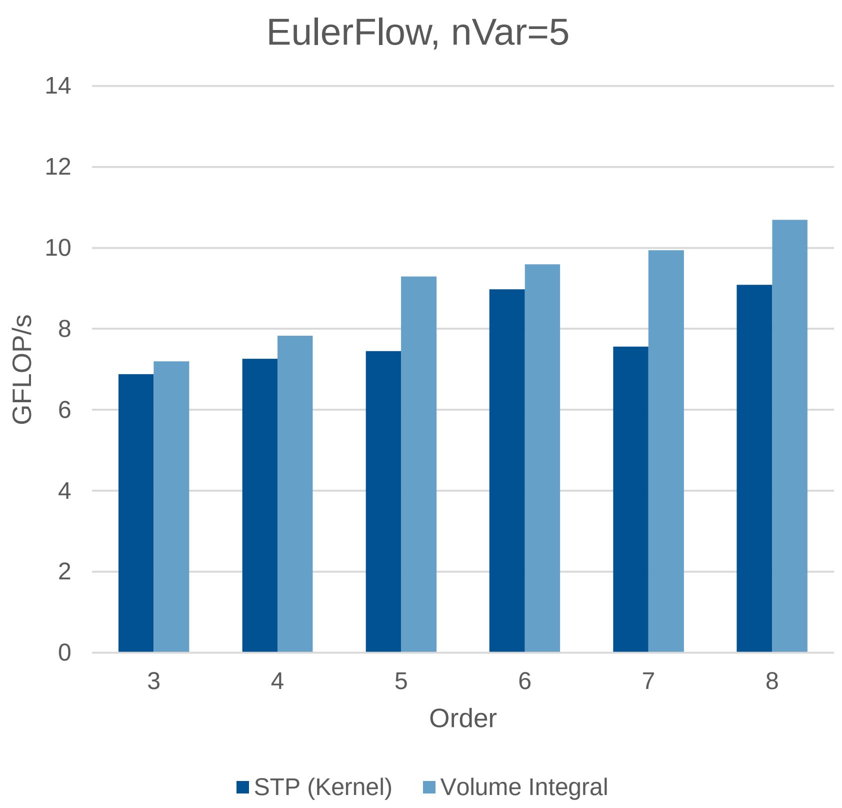
- Intel compiler 16.0.4 for C++ (icpc)
- gfortran v4.9
- Aggressive optimization options

  -fast -fstrict-aliasing -std=c++0x

  -restrict -no-ipo -ip -xCORE-AVX2 -fma

Gflops measurements, single core HSW

- Small number of quantities: scaling with order
- Big number of quantities: plateau instead of further scaling



Probable cause of the plateau in libxsmm

Libxsmm called on sliding slices of the tensor to perform Matrix-Matrix multiplications

*gemm(&A[i*X],&B[0],&C[i*Y]);*

Problem:

A and C slices not reused

↳ A and C not in L1 cache

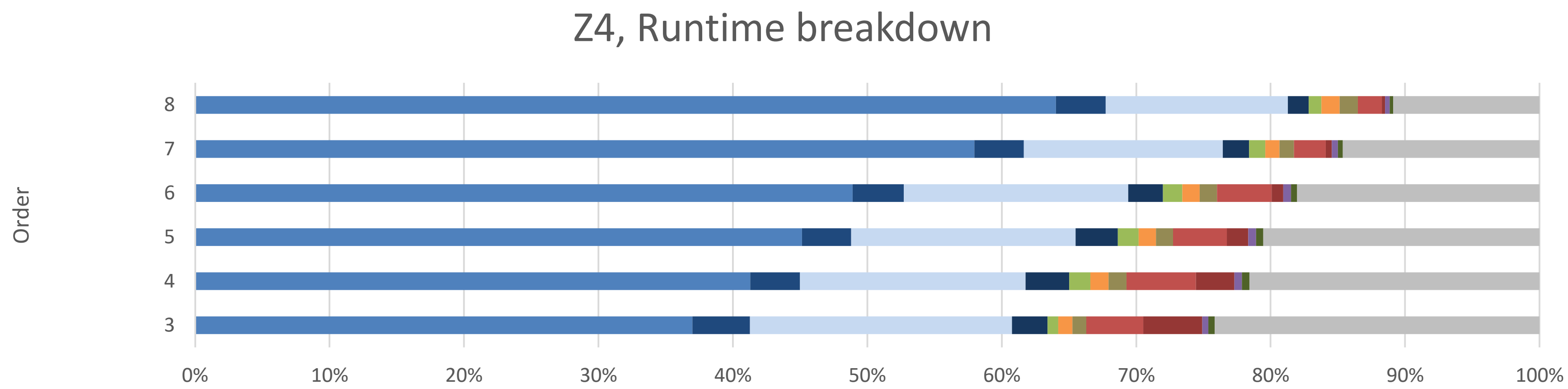
↳ need to be fetched from L2/L3/RAM

↳ bottleneck in performances

Solution:

Customize generated gemms to use L1 prefetching

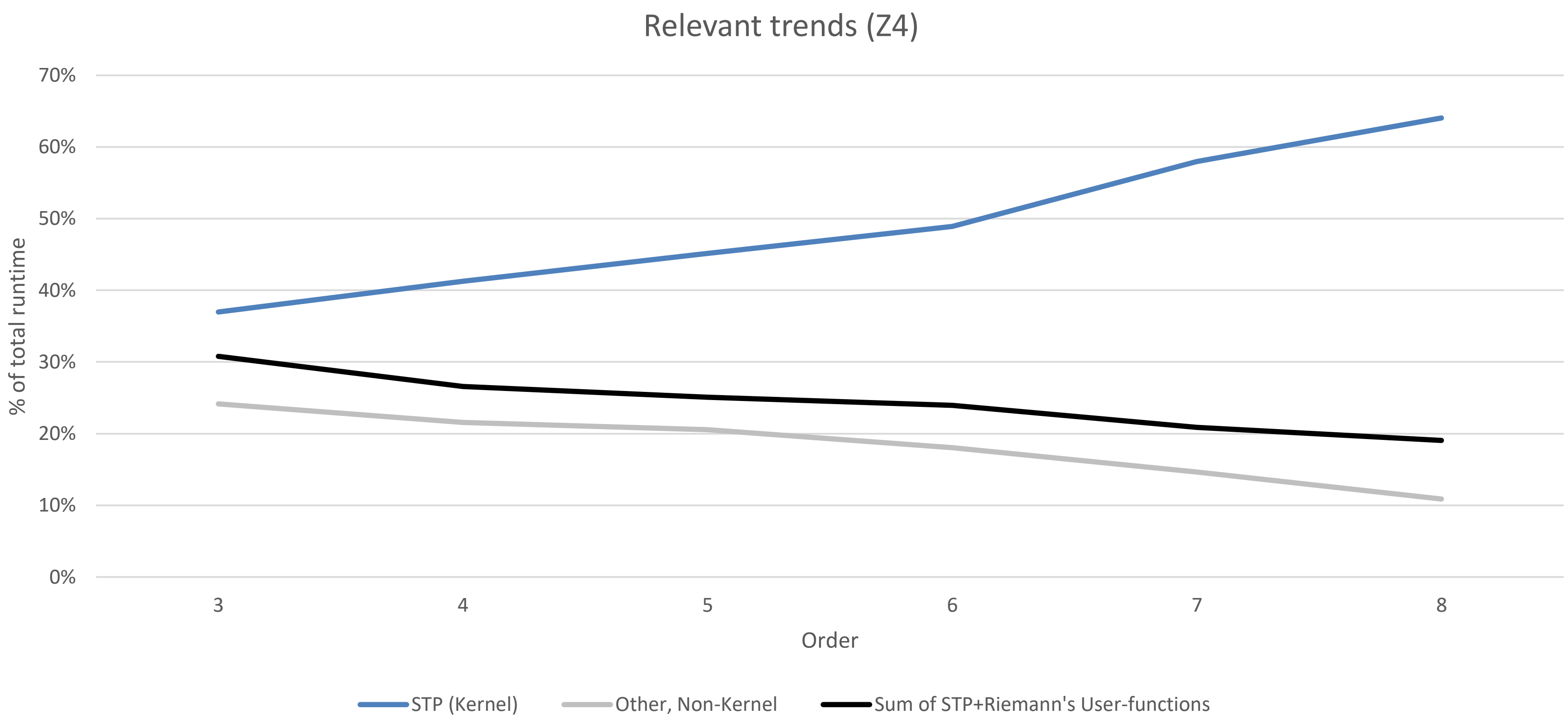
Runtime Breakdown



	3	4	5	6	7	8
STP (Kernel)	36.99%	41.28%	45.14%	48.90%	57.97%	64.03%
STP (NCP)	4.29%	3.71%	3.67%	3.81%	3.66%	3.71%
STP (Flux)	19.47%	16.77%	16.68%	16.70%	14.81%	13.54%
STP (Source)	2.64%	3.25%	3.14%	2.58%	1.97%	1.55%
Boundary Cond.	0.81%	1.57%	1.56%	1.44%	1.20%	0.95%
Volume Integral	1.05%	1.35%	1.28%	1.30%	1.07%	1.35%
Surface Integral	1.05%	1.35%	1.28%	1.30%	1.07%	1.35%
Riemann (Kernel)	4.23%	5.15%	3.99%	4.07%	2.37%	1.78%
Riemann (NCP)	4.40%	2.86%	1.60%	0.85%	0.44%	0.24%
Solution Up.	0.43%	0.58%	0.59%	0.58%	0.45%	0.34%
StableTimeStep	0.49%	0.56%	0.54%	0.46%	0.38%	0.26%
Other, Non-Kernel	24.15%	21.57%	20.54%	18.03%	14.63%	10.89%

Runtime Breakdown trends

- Overhead and user function cost goes down (relatively)
- SpaceTimePredictor becomes more and more dominant



Outlook

- Optimized kernels make ExaHyPE faster than the Fortran prototype from Trento.
- User functions not negligible anymore.
- Bottleneck with libxsmm identified, potential solution proof of concept tested successfully.
- Still need good scaling tests once current problem with generic code identified and solved