Role-Oriented Code Generation in ExaHyPE

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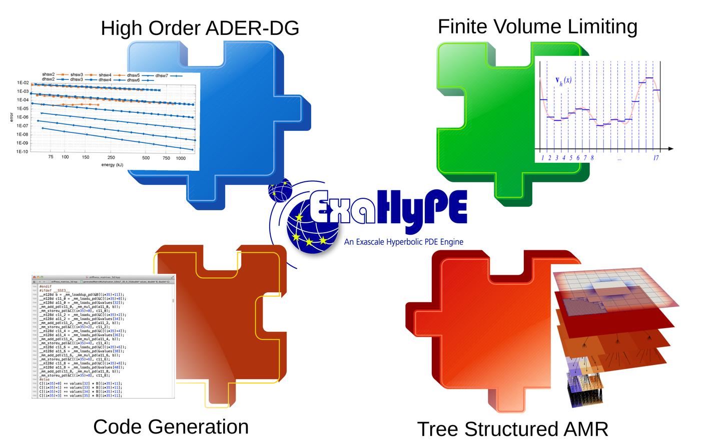
Towards an Exascale *PDE Engine*

ExaHyPE [1] is designed to enable medium-sized interdisciplinary research teams to quickly realise extreme-scale simulations of grand challenges.

The ExaHyPE Engine solves systems of first-order hyperbolic PDEs of the form:

$$\mathbf{P}\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{Q}, \nabla \mathbf{Q}) + \sum_{i=1}^{d} \mathbf{B}_i(\mathbf{Q}) \frac{\partial \mathbf{Q}}{\partial x_i} = \mathbf{S}(\mathbf{Q}) + \sum \delta$$

ExaHyPE employs higher-order ADER-DG on tree-structured adaptive Cartesian grids using a-posteriori subcell Finite-Volume limiting [4]:



"What's an Engine?"

Similar to a "game engine", we aim for efficient core functionality but also application flexibility:

- **fixed parallel AMR framework**: Peano [3] (tree-structured adaptive Cartesian grids; MPI+Tasking parallelism, load balancing) → www.peano-framework.org
- **fixed numerics**: high-order discontinuous Galerkin with ADER time-stepping (ADER-DG) with a-posteriori Finite-Volume subcell limiting
- **flexible w.r.t. applications**: hyperbolic PDEs stemming from conservation laws

Code generation is our means to manage software complexity.

Role-Oriented Code Generation:

We have observed the following roles for software development on the engine and on its applications:

- **application expert(s)**: implements the PDE system, problem-specific initial/boundary conditions, etc., for a given application; desires straightforward user API that hides complexity of solver and optimisation
- **algorithms expert(s)**: implements efficient numerical schemes; shall design architecture-oblivious algorithms via custom macros that isolate low-level optimisation
- **optimisation expert(s)**: performs hardware-aware optimisation on performance-critical components of the solver – relies on abstractions by algorithmic templates.

Any role might be adopted by multiple users.
Any user may adopt multiple roles.

ExaHyPE's *Toolkit* and *Code Generator* [2] thus provide separate views for each role.
Toolkit and Code Generator are stand-alone applications based on the Jinja2 templating engine.

References

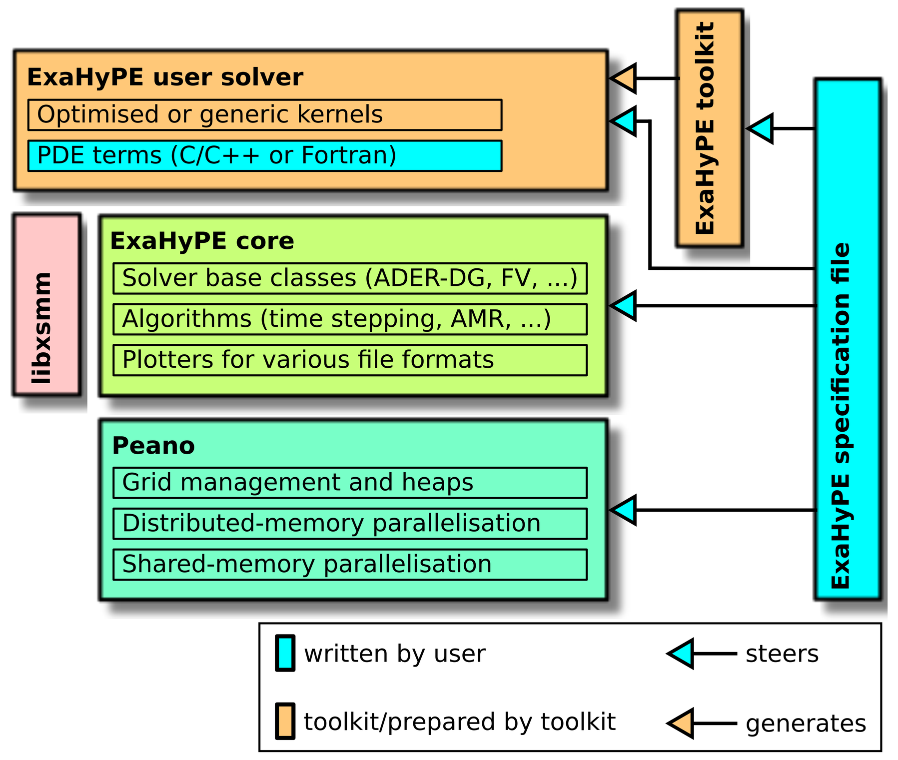
[1] A. Reinarz et al.: *ExaHyPE: An engine for parallel dynamically adaptive simulations of wave problems.* Comp. Phys. Comm. 254, 2020. http://dx.doi.org/10.1016/j.cpc.2020.107251

[2] J.-M. Gallard et al.: *Role-oriented code generation in an engine for solving hyperbolic PDE systems.* 2019 Int. Workshop on Softw. Eng. for HPC-Enabled Research (SE-HER), SC19.

[3] T. Weinzierl: *The Peano software—parallel, automaton-based, dynamically adaptive grid traversals.* ACM Trans. Math. Softw. 45(2): 14, 2019.

[4] O. Zanotti, F. Fambri, M. Dumbser, A. Hidalgo: *Space-time adaptive ADER discontinuous Galerkin finite element schemes with a posteriori sub-cell finite volume limiting.* Computers & Fluids 118, 2015, p. 204–224.

How to Create Code that is Easy to Use & Extend, Flexible, Efficient, . . . ?



Using the ExaHyPE Toolkit:

1. create a specification file that defines the domain, PDE system, required architecture, parallelisation, etc.
2. ExaHyPE toolkit creates glue code, application-specific template classes and core routines (tailored to application and architecture)
3. implement the application classes with PDE- and scenario-specific methods:
   - `flux(...)`, `ncp(...)`, ... for PDE terms (conservative fluxes, non-conservative products, etc.)
   - `eigenvalues(...)` to compute eigenvalues (for Riemann solvers)
   - `boundaryValues(...)`, etc.

Jinjia2 Templates and Model-View-Controller Design

ExaHyPE Toolkit and Code Generator follow a Model-View-Controller Design – e.g., for the Toolkit:

- **Controller**: builds multiple contexts from the specification file, such as type of PDE, choice of numerical solver, architecture, etc.
- **Model**: responsible for generating a specific View – e.g., generate the glue code for either a finite volume solver or an ADER-DG solver
- **View**: Jinja2 template engine is invoked to render templates that are tailored to Model-provided contexts.

Jinjia2 templates allow "logic" in the code representation, while keeping it close to the generated code and easily readable and expandable. For example

```
{% if initA %}
{{allocateArray('A', nDof)}}
for(int i=0; i<{{nDof}}; ++i) {
  A[i] = B[i+{{nDof*nVar}}] * {{C}}[i];
}
{% endif %}
```

may generate the following code:

```
double A[5] __attribute__((aligned(32)));
for(int i=0; i<5; ++i) {
  A[i] = B[i+20] * foo[i]
}
```

Creating an ExaHyPE Application: View for the Application Expert

Specification file:

```
exahype-project Elastic
  peano-kernel-path const  = ./Peano
  exahype-path const       = ./ExaHyPE
  output-directory const   = ./Elastic

  computational-domain
    dimension const      = 3
    width                = 1.0, 1.0, 1.0
    offset               = 0.0, 0.0, 0.0
    end-time             = 1.0
  end computational-domain

  solver ADER-DG ElasticWaveSolver
    variables const   = v:3,sigma:6
    parameters const  = rho:1,cp:1,cs:1
    order const       = 7
    maximum-mesh-size    = 2e-2
    maximum-mesh-depth   = 2
    time-stepping        = global
    terms const = flux,ncp,
     material_parameters,point_sources
    optimisation const   = optimised
    language const       = C
    basis                = Lobatto
  end solver
end exahype-project
```

Implementation of flux function:

```
void Elastic::ElasticWaveSolver
  ::flux(const double* const Q,
         double** const F) {
  VariableShortcuts s;
  double sigma_xx=Q[s.sigma + 0];
  double sigma_yy=Q[s.sigma + 1];
  double sigma_zz=Q[s.sigma + 2];
  double sigma_xy=Q[s.sigma + 3];
  double sigma_xz=Q[s.sigma + 4];
  double sigma_yz=Q[s.sigma + 5];
  F[0][ s.v + 0] = -sigma_xx;
  F[0][ s.v + 1] = -sigma_xy;
  F[0][ s.v + 2] = -sigma_xz;
  F[1][ s.v + 0] = -sigma_xy;
  F[1][ s.v + 1] = -sigma_yy;
  F[1][ s.v + 2] = -sigma_yz;
  F[2][ s.v + 0] = -sigma_xz;
  F[2][ s.v + 1] = -sigma_yz;
  F[2][ s.v + 2] = -sigma_zz;
}
```

Download the ExaHyPE engine from: www.ExaHyPE.org

ExaHyPE was developed as a joint project of:

in particular by:

Dominic Charrier, Benjamin Hazelwood, Tobias Weinzierl (University of Durham), Michael Dumbser, Francesco Fambri, Maurizio Tavelli, Olindo Zannotti (University of Trento), Alice Gabriel, Kenneth Duru (Ludwig-Maximilians-University Munich), Luke Bovard, Sven Köppel, Luciano Rezzolla (Frankfurt Institute for Advanced Studies), Jean-Mathieu Gallard, Leonhard Rannabauer, Anne Reinarz, Philipp Samfaß, Angelika Schwarz and Vasco Varduhn (Technical University of Munich).
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Architecture-Oblivious Templates and Architecture-Aware Optimisation Macros

Using Jinja2's macros and variables, we can design architecture-oblivious *algorithmic templates* that are rendered by Jinja2 with custom made architecture-aware *optimisation macros*.
This keeps the development of new numerical schemes and low-level architecture-aware optimisation separated and the roles of algorithm and optimisation expert independent from one another.

Example: tensor contraction to compute the x-component of the gradient of state tensor Q (variable `lQi`):

Algorithm expert provides *"loop over GEMM"* implementation using macros (provided by the optimisation expert) for matrix multiplication (`matmul`) and index calculation (`idx`) to extract matrix slices:

```
for (int yz=0; yz<{{nDof*nDof3D}}; yz++) {
  {{matmul('gradQ_x', 'lQi', 'dudxT', 'gradQ',
           idx(0,yz,0,0), '0', idx(0,yz,0,0))}}
}
```

$$\forall z,y,k,n\colon\ \nabla Q_{z,y,x,n} = \sum_{k} \Delta_{x,k} \cdot Q_{z,y,k,n}$$

Depending on the context – number of degrees of freedom (`nDof`), used architecture, etc. – the Code Generator resolves the template variables, using hardware-specific padding in the index for the tensor offsets and matrix dimensions (here AVX2). The architecture-aware `matmul` macro selects a hardware-efficient backend for matrix multiplication, for example using the Eigen library [8].

```
for (int yz=0; yz<36; yz++) {
  Map< Matrix<double,12,6>, Aligned, OuterStride<12> > lQi_m(lQi+yz*72);
  Map< Matrix<double,6,6>,  Aligned, OuterStride<8> >  dudxT_m(dudxT);
  Map< Matrix<double,12,6>, Aligned, OuterStride<12> > gradQ_m(gradQ+yz*72);

  gradQ_m.noalias() = lQi_m * dudxT_m ;
}
```

For an AVX-512 architecture (Intel Skylake), the template would be rendered with padding to a different SIMD width (16 instead of 12) and calling the highly optimised GEMM function generated by LIBXSMM [9]:

```
for (int yz = 0; yz < 36; yz++) {
  gemm_16_6_6_gradQ_x(lQi+yz*96, dudxT, gradQ+yz*96);
}
```

Optimised Kernels: Vectorisation and Minimisation of Memory Footprint

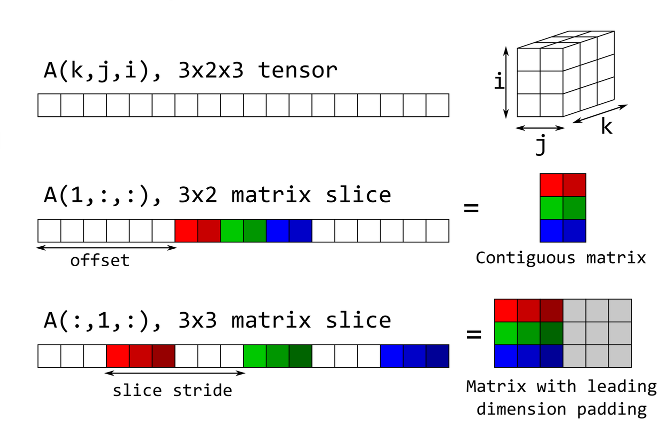
ExaSeis faces conflicting demands for data layout:

- DG tensor operations are turned into sequences of matrix multiplications ("loop over GEMM") → suggests quantities as leading dimension (AoS)
- evaluation of fluxes loops over integration points calling user-functions (`flux()`, e.g.) → suggests integration points as leading dimension (SoA)
- choose AoSoA as data layout: → single out one dimension
- In addition: provide dimensional `flux()` function to reduce the memory footprint ⇝ changes API ("View" for application expert)

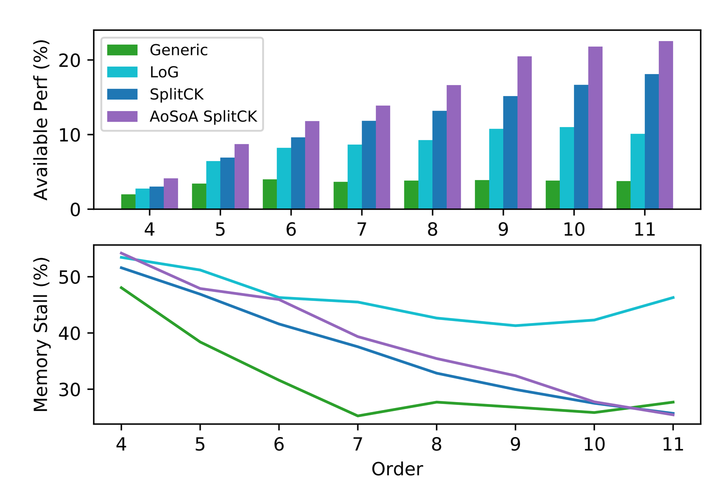
```
//scalar formulation of flux_x
void flux_x(double* Q, double* F) {
  F[0] = -(Q[0]+Q[3]+Q[4]);
  F[1] = -(Q[1]+Q[3]+Q[5]);
  F[2] = -(Q[2]+Q[4]+Q[5]);
}

//vectorized formulation of flux_x
void flux_x_vect(double* Q, double* F) {
  #pragma omp simd aligned(Q,F:ALIGNMENT)
  for(int i=0; i<VLENGTH; i++) {
    F[0*VSTRIDE+i] = -(Q[0*VSTRIDE+i]
        +Q[3*VSTRIDE+i]+Q[4*VSTRIDE+i]);
    F[1*VSTRIDE+i] = -(Q[1*VSTRIDE+i]
        +Q[3*VSTRIDE+i]+Q[5*VSTRIDE+i]);
    F[2*VSTRIDE+i] = -(Q[2*VSTRIDE+i]
        +Q[4*VSTRIDE+i]+Q[5*VSTRIDE+i]);
  }
}
```

Extracting matrix slices from a tensor A:



Example performance of seismic wave propagation (LOH.1 benchmark) on curvilinear meshes [7]:



- significantly reduces the L2-cache footprint
- 5.7× speedup for order 10 compared to generic implementation.

References

[5] K. Duru et al.: *A new discontinuous Galerkin method for elastic waves with physically motivated numerical fluxes.* J. Comp. Phys. 386, 2019, submitted

[6] K. Duru et al.: *A stable discontinuous Galerkin method for the perfectly matched layer for elastodynamics in first order form.* Numerische Mathematik 146, p. 729–782, 2020.

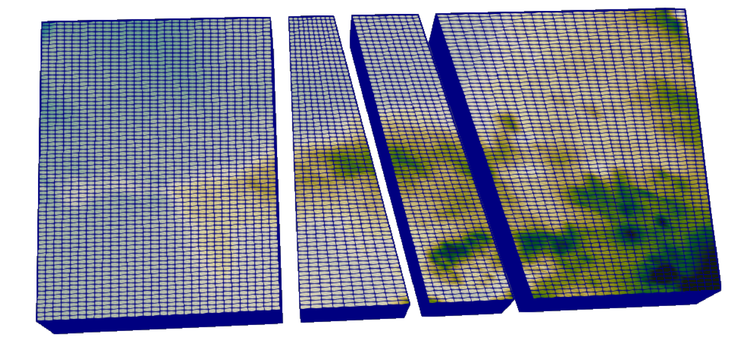
[7] J.-M. Gallard, L. Rannabauer, A. Reinarz, M. Bader: *Vectorization and minimization of memory footprint for linear high-order discontinuous Galerkin schemes.* In: 21st IEEE Int. Workshop on Parallel & Distributed Scientific and Engineering Computing (PDSEC-2020), 2020.

[8] G. Guennebaud et al.: *Eigen v3* `http://eigen.tuxfamily.org`

[9] A. Heinecke et al.: *LIBXSMM: accelerating small matrix multiplications by runtime code generation.* In: SC16: Int. Conf. for HPC, Netw., Storage and Analysis, 2016, pp. 981–991.

ChEESE Pilot Demonstrator: Towards UQ for Seismic Hazard Analysis

We link *ExaSeis* – the collection of seismic wave propagation models in ExaHyPE – to the MUQ C++ toolbox for uncertainty quantification (muq.mit.edu) and plan to experiment with novel UQ-based approaches to seismic hazard analysis.



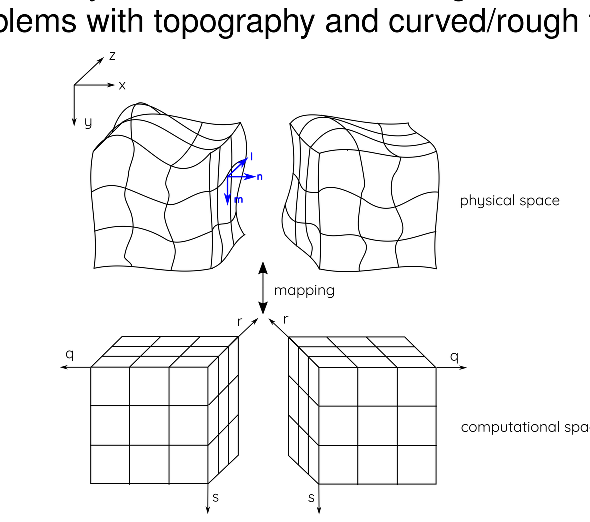
Curvilinear mesh aligned to topography and three planar fault planes of the bookshelf-type South Iceland Seismic Zone.

ADER-DG on Curvilinear Meshes

To fit ExaHyPE's Cartesian meshes to domains with topography and multiple faults (incl. slightly curved and/or rough faults), we developed a curvilinear method that maps Cartesian to curvilinear elements:

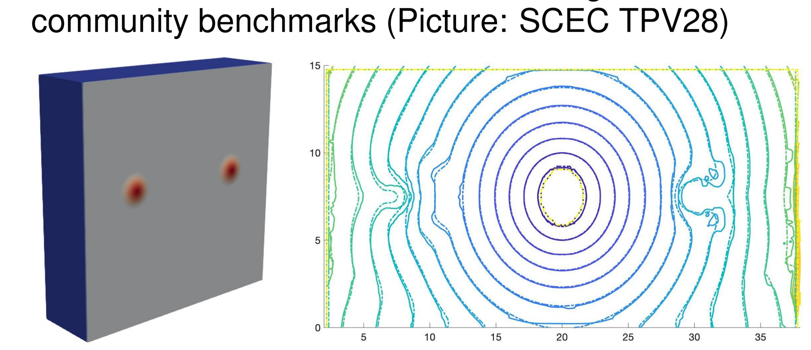
- retains the tensor structure of the DG basis
- flux and source terms of the system are transformed with the element Jacobian
- but: eigenvalues (and thus the time-step size) highly depend on the perturbation introduced by the topography

Allows fully automated initial mesh generation for problems with topography and curved/rough faults!



Multi-Physics Dynamic Rupture

We simulate multi-physics spontaneous dynamic rupture, across complex fault geometries.
The automated mesh generator allows to model fault structures, including branches, by defining a k-d-tree.
The rupture is incorporated as boundary condition, which we solve with a new developed physics based Riemann solver. Our code is verified against community benchmarks (Picture: SCEC TPV28)



TPV28 benchmark (vertical strike-slip fault with two hills): setup (left) and rupture contours computed by ExaSeis (right).

Acknowledgements

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