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Flavours of GPU kernels in ExaHyPE

SYCL's impact on algorithms, data structures and implementations

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Outline

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ExaHyPE

High-performance computing strategy

Finite Volumes

Migrating from OpenMP to SYCL

Conclusion

Two application challenges

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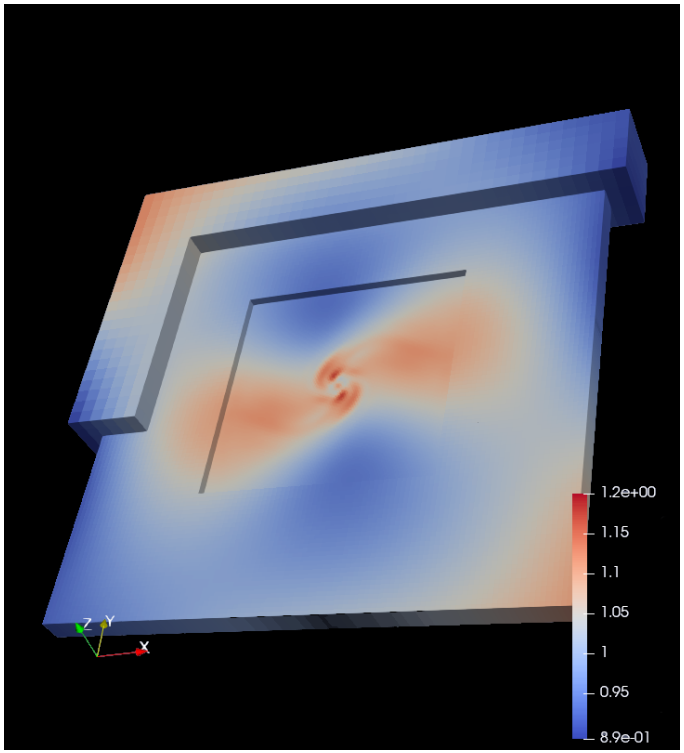

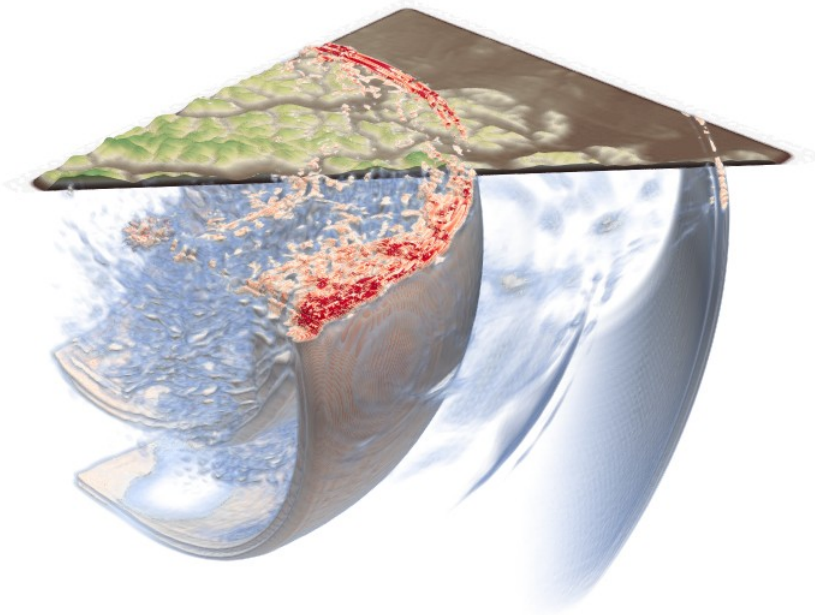

Work by groups of B. Li et al (Institute for Computational Cosmology) and M. Bader et al (TUM)

Chris Johnson: “Before every great invention was the discovery of a new tool”[+].

[+] From an interview in the video “The Golden Age of Computing”.

Hyperbolic equation systems

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ExaHyPE's vision: The engine ExaHyPE allows groups with decent computational background to write an exascale solver for

$$\frac{\partial}{\partial t} Q + \nabla \cdot \mathbf{F}(Q) + \sum_i \mathcal{B}_i \frac{\partial Q}{\partial x_i} = \mathbf{S}(Q).$$

User:

- Pick numerical scheme (FV, RKFD, RKDG, ADER-DG)
- Supplement BCs, initial conditions
- Implement PDE terms
- Indicate where to refine
- ...
- Do **not** care about all the code environment, meshing, numerics

Engine:

- Constrain to a small, fixed set of ingredients
- Generate actual simulation code (glue code, numerical kernels, ...)
- Determine *where*, *when*, *in which order* and *how* to call compute kernels

Disclaimer: Concepts inherited from underlying AMR framework Peano, prototyped in ExaHyPE, all rewritten from scratch in ExaHyPE 2 (cmp. ACM TOMS).

ExaHyPE 2's Python scripts

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```
import peano4
import exahype2

my_solver    = exahype2.solvers.rkdg.rusanov.GlobalAdaptiveTimeStepWithEnclaveTasking(
 name               = "CCZ4DG8RK4",
 rk_order           = 4,
 polynomials        = exahype2.solvers.GaussLegendreBasis(8),
 unknowns           = 59,
 [...]

my_solver.set_implementation(
 boundary_conditions  = exahype2.solvers.rkdg.PDETerms.Empty_Implementation,
 flux                 = exahype2.solvers.rkdg.PDETerms.None,
 ncp                  = """
  // my_code_snippets
 """
 [...]

project = exahype2.Project( ... )
project.add_solver( my_solver )
project.set_global_simulation_parameters(
 dimensions = 3,
 offset = [0.0,0.0,0.0],
 size   = [1.0,1.0,1.0],
 [...]

project.set_load_balancing( ... )
project.set_Peano4_installation("../../..", peano4.output.CompileMode.Release)
peano4_project = project.generate_Peano4_project()
peano4_project.output.makefile.parse_configure_script_outcome( "../../.." )
peano4_project.generate()
```

Callbacks in ExaHyPE 2

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```
double examples::exahype2::euler::Euler::maxEigenvalue( ... ) {
  constexpr double gamma = 1.4;
  const double irho = 1./Q[0];
  #if Dimensions==3
  const double p = (gamma-1) * (Q[4] - 0.5*irho*(Q[1]*Q[1]+Q[2]*Q[2]+Q[3]*Q[3]));
  #else
  const double p = (gamma-1) * (Q[4] - 0.5*irho*(Q[1]*Q[1]+Q[2]*Q[2]));
  #endif
  const double u_n = Q[normal + 1] * irho;
  const double c   = std::sqrt(gamma * p * irho);
  return std::max( std::abs(u_n-c), std::abs(u_n+c) );
}
```

(Example above: Euler equations, i.e. nothing fancy but textbook by R. LeVeque)

- Python API yields plain Makefile/CMake
- Glue code all generated
  (meshing, load balancing, algorithm phases, plotting, ...)
- Empty stubs for physics/application domain-specific ingredients
  (Python may inject C code snippets directly or use SymPy

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Classic domain decomposition: MPI+X

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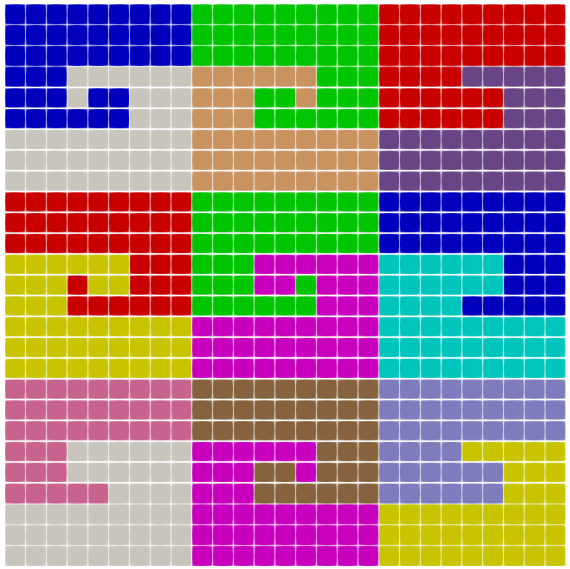

SFC-based domain partitioning of regular grid for 18 ranks/cores.

- Adaptive Cartesian mesh based upon spacetrees
- SFC-based non-overlapping domain decomposition
- Boundary data exchange hidden
- Rebalancing triggered by callbacks

Realisation:

- No difference between MPI and shared memory parallelisation
- Both MPI+shared memory: SPMD+BSP

$\Rightarrow$ Inappropriate for many cores (boundary exchange overhead)

$\Rightarrow$ Struggles with imbalances (due to AMR or non-linear compute kernels, e.g.)

Enclave tasking

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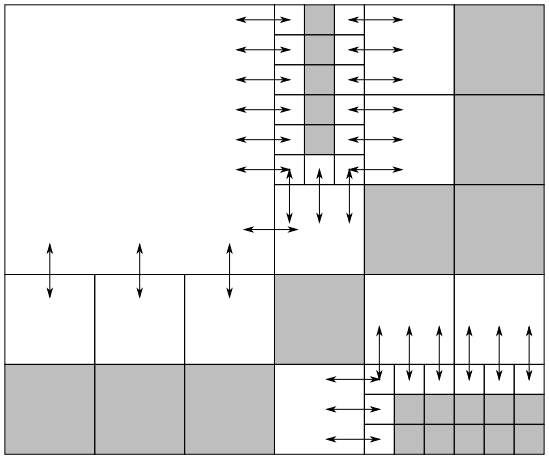

- Mark all cells along MPI boundary and resolution transitions
  (those are involved in MPI and might refine/coarsen)
  - reordering of these cells challenging
  - these cells are along critical path in task graph (latency sensitive)

  $\Rightarrow$ skeleton grid
- Remaining cells define real tasks
  - overlap with MPI and AMR
  - compensate for BSP imbalances

  $\Rightarrow$ enclave cells

Task classification and GPU offloading

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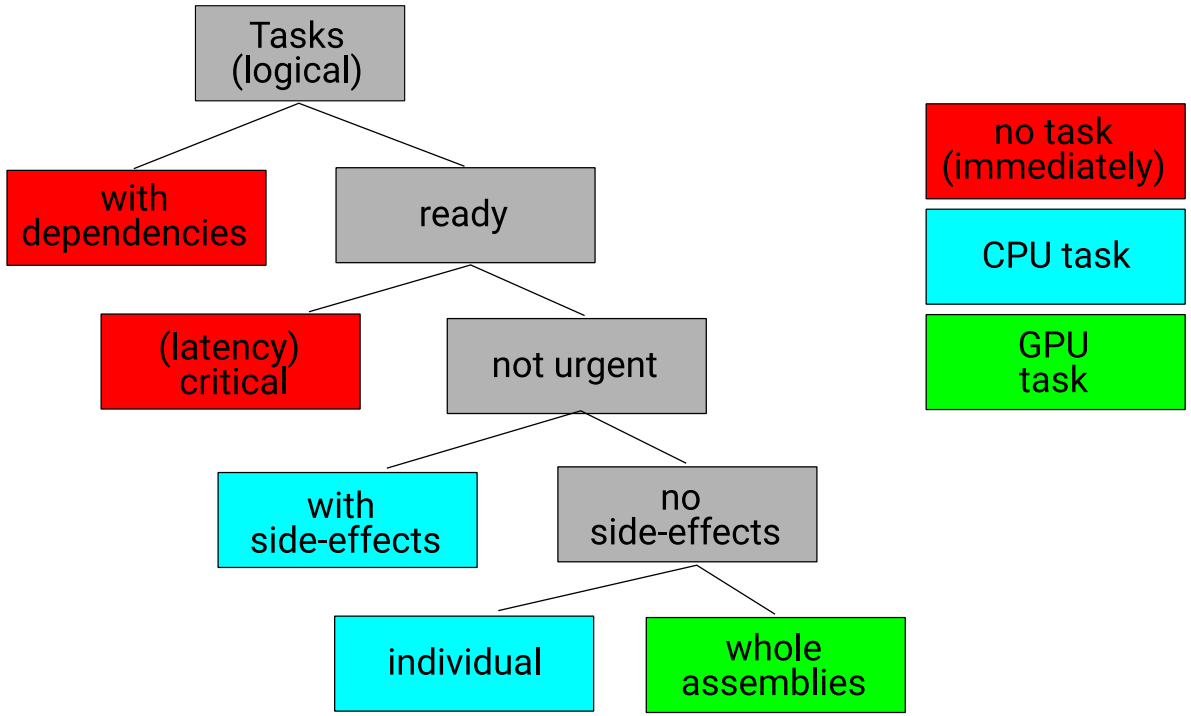

- Hold GPU-fitting tasks back
- Deploy en bloc to device
  (classic offloading model)

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Disclaimer

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- Finite Volumes
  (same principles hold for all numerical schemes)
- Rusanov
  (everything else too complicated with CCZ4)
- Generic, application-agnostic kernels
  (see outlook)
- OpenMP
  (production back-end)
- Study only these enclave tasks
  (omit meshing/AMR, MPI, . . .)

Rusanov

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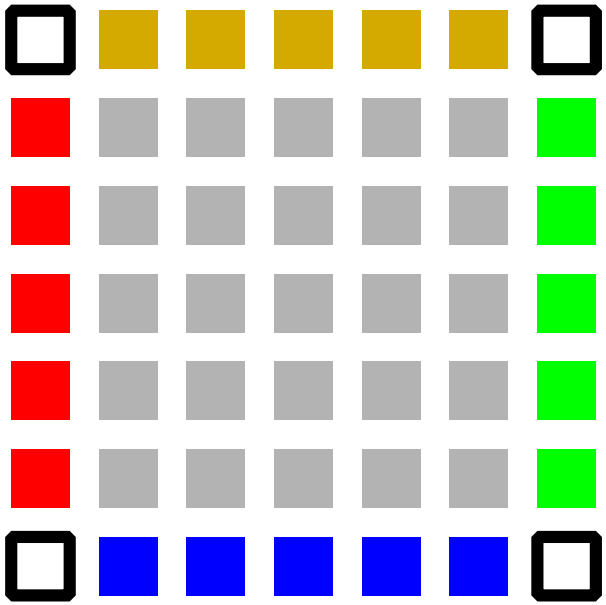
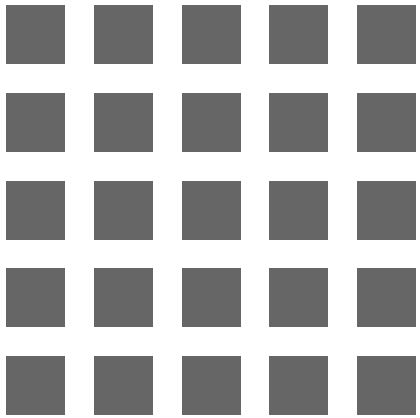


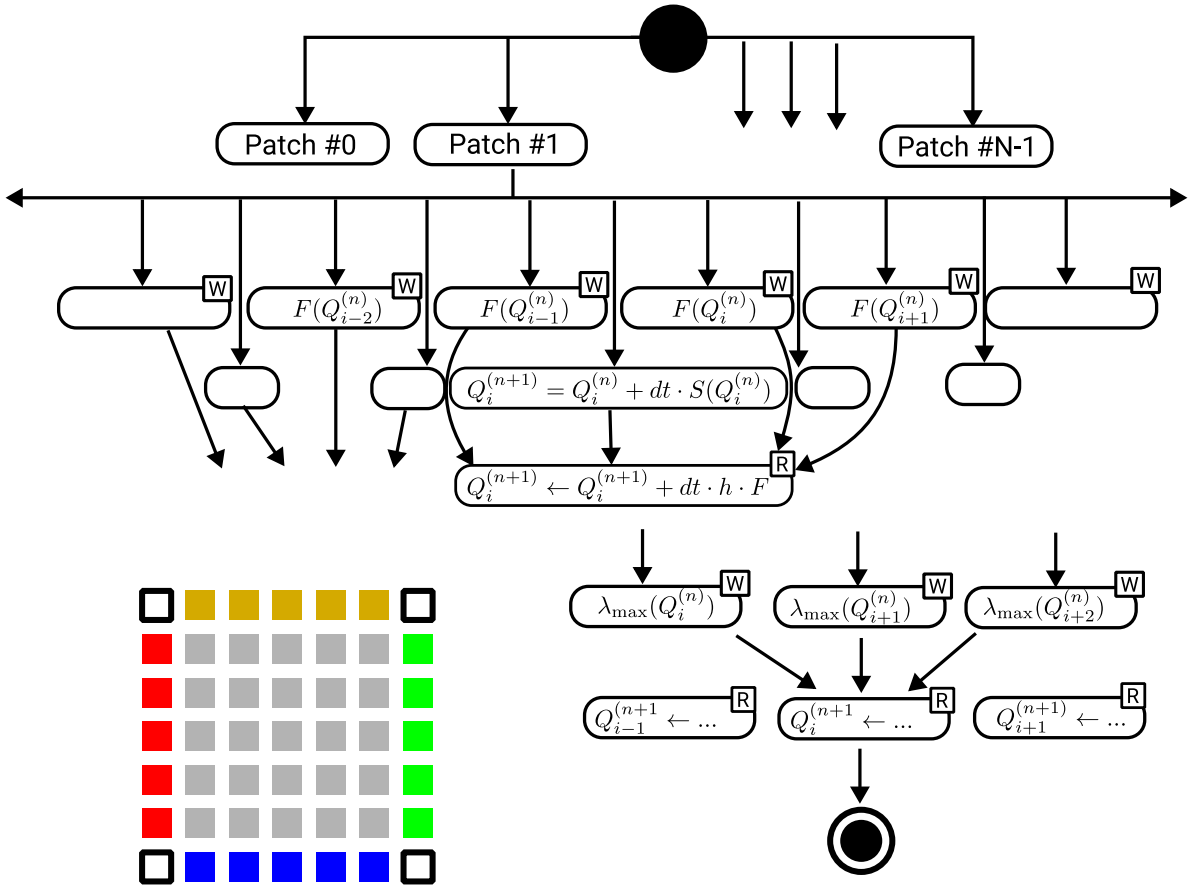


- Halo layer valid
- Array of structures (AoS)
- Numerics blueprint

$$Q_i^{(n+1)} = Q_i^{(n)} + dt \cdot S(Q_i^{(n)}) + dt \cdot h \cdot F_{i-\frac{1}{2}}(Q^{(n)}) + dt \cdot h \cdot F_{i+\frac{1}{2}}(Q^{(n)})$$

$$F_{i+\frac{1}{2}}(Q^{(n)}) = \frac{1}{2}F(Q_i^{(n)}) + \frac{1}{2}F(Q_{i+1}^{(n)}) - \frac{\max\left(\lambda_{\max}(Q_{i+1}^{(n)}), \lambda_{\max}(Q_i^{(n)})\right)}{2}\left(Q_{i+1}^{(n)} - Q_i^{(n)}\right)$$

Rusanov graph



- Outer loop over patches $n \in \{0, \ldots, N-1\}$
- Per PDE term: Compute data (write to temp array; concurrent)—update $Q^{(n+1)}$ (read; concurrent fan in/gather)
- Computations per PDE term concurrent (cmp. $\lambda_{\max}(Q^{(n)})$ vs. $F(Q^{(n)})$)
- Flexibility to order temporary data

Patch-wise Finite Volume Rusanov kernels

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```
// commit to certain order
exahype2::enumerator::AoS0ALexicographicEnumerator fluxHostEnumerator(...);

// allocate temp buffers -> do on GPU
double* tempFluxX = new double[fluxHostEnumerator.size()];

#pragma omp target teams distribute device(targetDevice) \
 ...
for (int patchIndex=0; patchIndex<numberOfCells; patchIndex++) {
 if (Dimensions==2 and evaluateSource) {
  #pragma omp parallel for simd collapse(2)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = 0; x < numberOfVolumesPerAxisInPatch; x++) {
   internal::copySolutionAndAddSourceTerm_LoopBody<Solver>(
    ...

 if (Dimensions==2 and evaluateFlux) {
  #pragma omp parallel for simd collapse(2)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = -1; x < numberOfVolumesPerAxisInPatch+1; x++) {
   internal::evaluateFlux<Solver>(
    ...

  #pragma omp parallel for simd collapse(2)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = 0; x < numberOfVolumesPerAxisInPatch; x++) {
   internal::updateWithFlux<Solver>(
    ...
}
```

- Hide temp enumeration
- Distribute loop over patches among SMs/warps
- Collapse internal d-dimensional/$d+1$-dimensional `parallel for` loops

Batched Finite Volume Rusanov kernels

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```
if (Dimensions==2 and evaluateSource) {
  #pragma omp target teams distribute device(targetDevice) \
              parallel for simd collapse(3)
  for (int patchIndex=0; patchIndex<numberOfCells; patchIndex++)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = 0; x < numberOfVolumesPerAxisInPatch; x++) {
   internal::copySolutionAndAddSourceTerm_LoopBody<Solver>(
    ...

f (Dimensions==2 and evaluateFlux) {
  #pragma omp target teams distribute device(targetDevice) \
              parallel for simd collapse(3)
  for (int patchIndex=0; patchIndex<numberOfCells; patchIndex++)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = -1; x < numberOfVolumesPerAxisInPatch+1; x++) {
   internal::evaluateFlux<Solver>(
    ...

  #pragma omp parallel for simd collapse(2)
  for (int patchIndex=0; patchIndex<numberOfCells; patchIndex++)
  for (int y = 0; y < numberOfVolumesPerAxisInPatch; y++)
  for (int x = 0; x < numberOfVolumesPerAxisInPatch; x++) {
   internal::updateWithFlux<Solver>(
    ...
}
```

- Hide temp enumeration
- Distribute loop over patches among SMs/warps
- Collapse internal d-dimensional/$d+1$-dimensional loops
- Use `parallel for` for collapsed loops

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Batched kernels in SYCL

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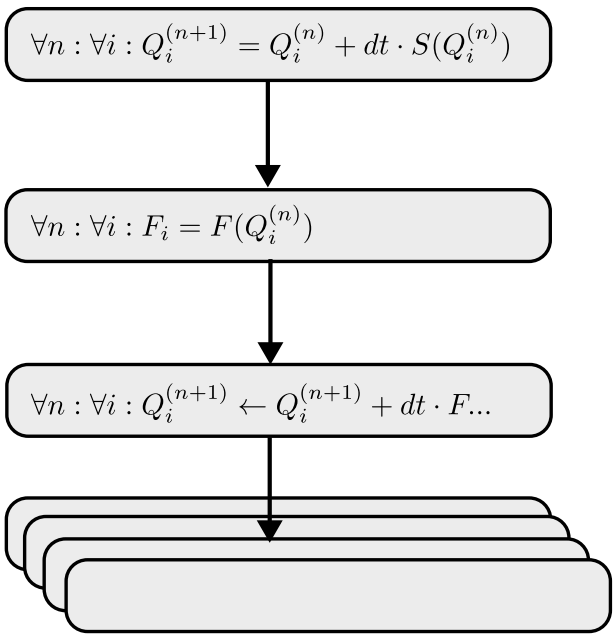

- Sequence of steps
  - OpenMP: Sequence of nested loops
  - SYCL: Sequence of kernels

  (ignore concurrency between steps)
- Parallel, collapsed loop
  - OpenMP: Collapse and `parallel for`
  - SYCL: `range`
- Tuning
  - OpenMP: annotations
  - SYCL: `nd_range` and partial serialisation
    (required anyway due to lack of 4d/5d ranges)
- Degenerated DAG

Patch-wise realisation in SYCL

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```
::sycl::queue& queue = tarch::accelerator::getSYCLQueue(targetDevice);
[...]
double* tempFluxX ::sycl::malloc_device<double>(fluxEnumerator.size(), queue);
[...]
queue.submit(
 [&](::sycl::handler &handle) {
  handle.parallel_for(   // or parallel_for_work_groups
   ::sycl::range<1>{numberOfPatches},
   [=] (::sycl::item<1> i) {
    int patchIndex = i[0];

    if (Dimensions==2 and evaluateSource) {
     handle.parallel_for(   // or parallel_for_work_items
      ::sycl::range<2>{numberOfVolumesPerAxisInPatch,numberOfVolumesPerAxisInPatch},
      [&] (::sycl::item<2> i) {
       int x          = i[0];
       int y          = i[1];
       internal::copySolutionAndAddSourceTerm_LoopBody<Solver>(
       [...]
    if (Dimensions==2) {
     handle.parallel_for(
      ::sycl::range<2>{numberOfVolumesPerAxisInPatch,numberOfVolumesPerAxisInPatch+2*solversHaloSize},
      [=] (::sycl::item<2> i) {
       int y          = i[0];
       int x          = i[1]-solversHaloSize;
       internal::computeMaxEigenvalue_LoopBody<Solver>(
       [...]
```

- Multiple nested `parallel_for` regions within kernel
- Different iteration ranges

$\Rightarrow$ 1:1 translation not possible

A proper compute-DAG in SYCL

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```
std::vector< ::sycl::event > copySolutionEvent(numberOfPatches);
if (Dimensions==2 and evaluateSource) {
 for (int patchIndex = 0; patchIndex<numberOfPatches; patchIndex++) {
  copySolutionEvent[patchIndex] = queue.submit(
   [&](::sycl::handler &handle) {
   handle.parallel_for(
    ::sycl::range<2>{numberOfVolumesPerAxisInPatch,numberOfVolumesPerAxisInPatch},
    [=] (::sycl::item<2> i) {
     int x          = i[0];
     int y          = i[1];
     internal::copySolutionAndAddSourceTerm_LoopBody<Solver>(
     [...]


  updateWithEigenvalueEvent[patchIndex] = queue.submit(
   [&](::sycl::handler &handle) {
    handle.depends_on(copySolutionEvent[patchIndex]);
    [...]
```

- Smallish compute kernels
- Individual dependencies

  (no address magic required)

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Before we continue

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- Paper on batching vs. patch-wise on CPUs:
  B. Li, H. Schulz, T. Weinzierl, H. Zhang: Dynamic task fusion for a block-structured finite volume solver over a dynamically adaptive mesh with local time stepping, ISC High Performance 2022, LNCS 13289, 2022, pp. 153–173
- Paper on GPU offloading:
  M. Wille, T. Weinzierl, G. Brito Gadeschi, M. Bader: Efficient GPU Offloading with OpenMP for a Hyperbolic Finite Volume Solver on Dynamically Adaptive Meshes, ISC High Performance 2023, LNCS (accepted)
- Benchmark suite: www.peano-framework.org
  - ExaHyPE 2 shipped extension of AMR framework Peano
  - Guidebook (pdf) part of repository
  - Benchmarks read-to-use
- Waiting for Intel GPUs
  (Codeplay release of NVIDIA bindings appreciated)

Conclusion and future work

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- Features in SYCL missing (?)
  - Multiple parallel fors per kernel with different ranges
    (compute max range and add masking)
  - Ranges for $d \geq 4$
    (any implicit linearisation is **not** performance-portable)
- All realisations possible with all GPUisation approaches

$\Rightarrow$ Realisation language favors algorithm flavour

- Batched and patch-wise kernels only two out of many realisations

$\Rightarrow$ Graph focus (in theory) very powerful

- Performance
  - Graph-based approach outperform loop parallelism
  - Performance portable (spread over multiple cores, e.g.)

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