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FACULTY OF ENGINEERING

Generating Highly Parallel Geometric Multigrid Solvers with the ExaStencils Approach

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Motivation

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void Smoother() {
for (int fragmentIdx = 0; fragmentIdx < 1; ++fragmentIdx) {if (isValidForSubdomain) {if ((neighbor_isValid[1]&&neighbor_isRemote[1])) {
#pragma omp parallel for schedule(static) num_threads(27)
for (int w = 0; (w<1); w += 1) {for (int z = 1; (z<98); z += 1) {for (int y = 1; (y<98); y += 1) {for (int x = 100; (x<101); x += 1) {buffer_Send_0[1][((((((w*9409)+x)+y)+(z*97))-198)] = slottedFieldData_Solution[slot][5][((((((w*1019304)+x)+(y*104))+(z*10296))];}}}}}}}
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#pragma omp critical
{ MPI_Isend(buffer_Send_0[1], 9409, MPI_DOUBLE, neighbor_remoteRank[1], (((unsigned int)commId << 20)+((unsigned int)(neighbor_fragCommId[1]) << 10)), mpiCommunicator, &mpiRequest_Send_0[1]); }
reqOutstanding_Send_0[1] = true;}}};
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int x = iterationOffsetBegin[0];
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for (; (x<_upper); x += 1) {
slottedFieldData_Solution[((curSlot_Solution[1]+1)%2)][1][(((x+(y*12))+(z*108))+124)] = ((slottedFieldData_Solution[(curSlot_Solution[1]%2)][1][(((x+(y*12))+(z*108))+124)]*2.000000e-01)+(((((((fieldData_RHS[1][((x+(y*8))+(z*56))]+slottedFieldData_Solution[(curSlot_Solution[1]%2)][1][(((
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curSlot_Solution[1] = ((curSlot_Solution[1]+1)%2);
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```

MPI

OpenMP

SIMD extensions

Motivation

Why not concentrate on the algorithmic description?

```
1  Function Smoother () : Unit {
2    communicate Solution
3    loop over Solution {
4      Solution = Solution + 0.8 * (1.0 / diag(Laplace)) *
        (RHS - Laplace * Solution)
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- Productivity
  - Algorithm description at high-level
  - Hide low-level details from programmer
- Portability
  - Support different target platforms from the same description
  - Support different target languages from the same description
- Performance
  - Portable: high performance on different target platforms
  - Competitive: comparable performance to hand-written code

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ExaSlang

ExaSlang Layer 4

Properties

- Procedural
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Specification of

- Operations depending on the multigrid level
- Loops over computational domain
- Communication and data exchange
- Interface to 3rd-party code

Data Types

Simple and aggregate data types

- `Real`, `Integer`, `String`, `Boolean`
- `Complex<Real>`, `Complex<Integer>`

Algorithmic data types

`Field`

- Correspond to discretized (mathematical) variables
- Communication scheme via `Layout`
- Specify `Slot` number for multiple copies

`Stencil`

- Correspond to discretized (mathematical) operators
- (Nearly) arbitrary expressions possible

Computations

Loop over computational domain split into `loop over fragments`

- Fragments stem from distribution across different cluster nodes
- Corresponds to global operation
- Optionally: reduction operators

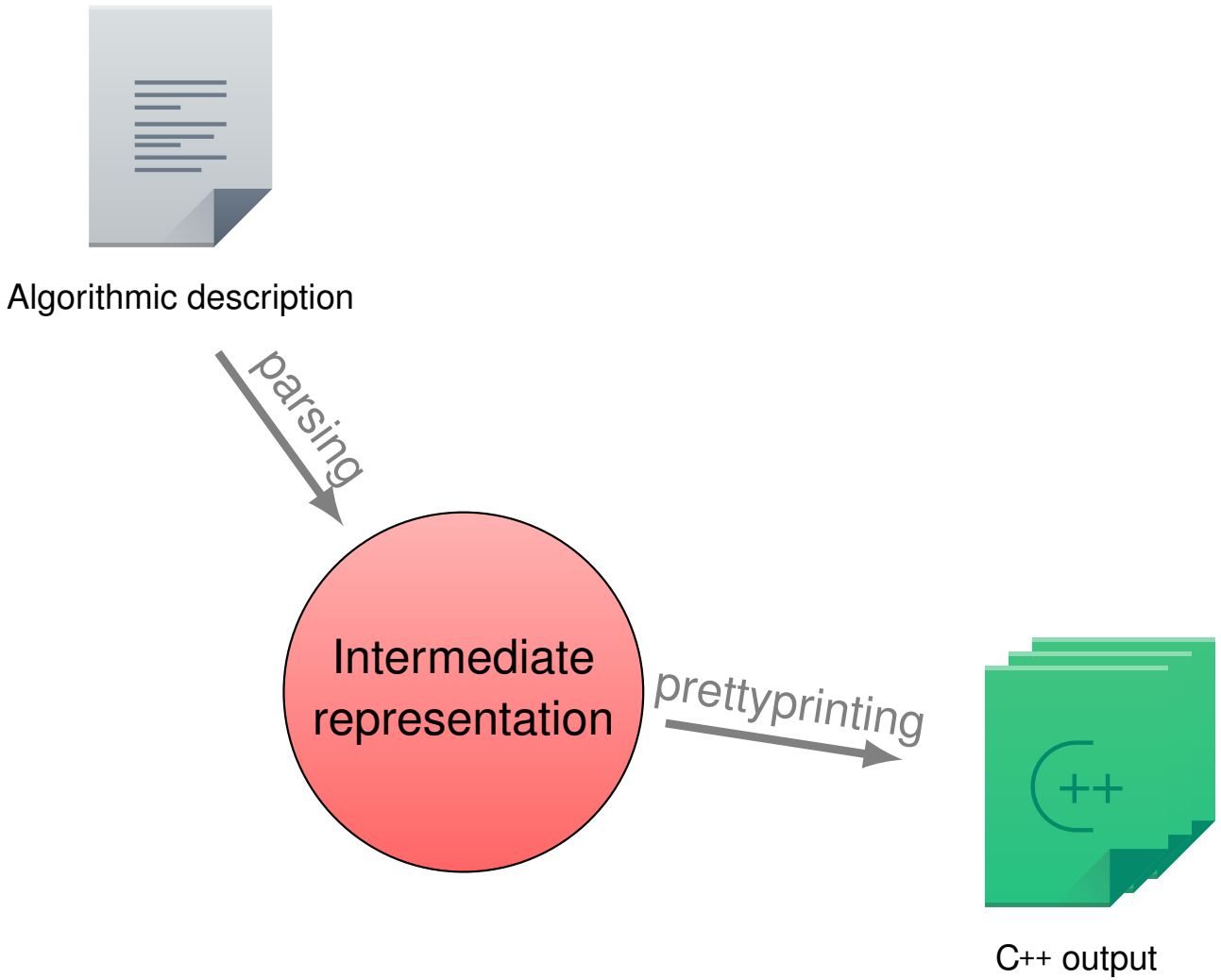
and `loop over <field>`

- Iteration over parts of fields possible
- Corresponds to local operation
- Optionally: Reduction operators

```
1  Function NormResidual @(coarsest and finest) () : Real {
2    Variable res : Real = 0
3    loop over fragments with reduction(+ : res) {
4      loop over Residual @current with reduction(+ : res) {
5        res += Residual @current * Residual @current
6    }}
7    return ( sqrt(res) )
8  }
```

ExaStencils Framework

Abstract workflow:



ExaStencils Framework

Using a simple 1-step concept, we can do some refinements, e. g.,

```
1  loop over Solution {
2    // ....
3  }
```

is being processed to

```
1  for (int z = start_z; z < stop_z; z += 1) {
2    for (int y = start_y; y < stop_y; y += 1) {
3      for (int x = start_x; x < stop_x; x += 1) {
4        // ....
5      }
6    }
7  }
```

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4        // ....
5      }
6    }
7  }
```

But what about the calculations? What about more complex things? Optional code modifications? Parallelization? Vectorization? Blocking? Color splitting?

➔ Very cumbersome with 1-step approach. Need something more flexible!

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ExaStencils Framework

ExaStencils Framework

Current workflow

1. DSL input (Layer 4) is parsed
2. Parsed input is checked for errors and transformed into the IR
3. Many smaller, specialized transformations are applied
4. C++ output is prettyprinted

ExaStencils Framework

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Concepts

- Major program modifications take place only in IR
- IR can be printed to C++ code
- Small transformations can be enabled and arranged according to needs
- Central instance keeps track of generated program: StateManager
- Variant generation by duplicating program at different transformation stages

ExaStencils Framework

Transformations

- Transform program state into another one
- Are applied to program state in depth-first order
- May be applied to only a part of the program state
- Are grouped together in Strategies

ExaStencils Framework

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Strategies

- Are applied in transactions
- Standard strategy that linearly executes all transformations is provided
- Custom strategies possible

ExaStencils Framework

Transactions

- Before execution, a snapshot of the program state is made
- May be committed or aborted

Checkpoints

- A copy of program state during compilation
- Restoration of program states
- Acceleration of variant generation for design space exploration

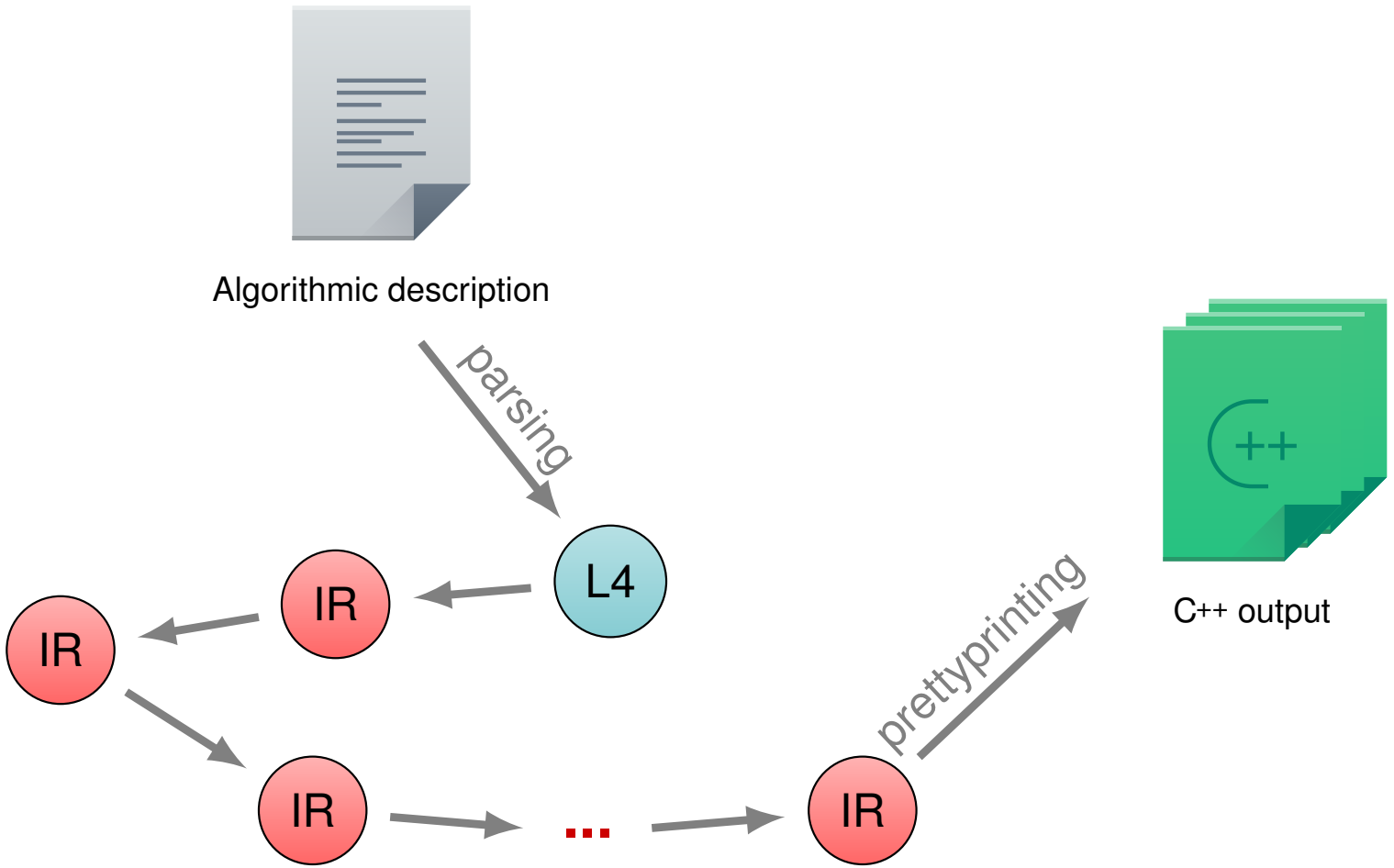
ExaStencils Framework

Example transformations:

```
1  var s = DefaultStrategy("example strategy")
2
3  // rename a certain function
4  s += Transformation("rename stencil", {
5    case x : Stencil if(x.identifier == "foo")
6      =>
7      {
8        if(x.entries.length != 7) error("invalid stencil size")
9        x.identifier = "bar"; x
10     }
11 })
12
13 // evaluate additions
14 s += Transformation("eval adds", {
15   case AdditionExpression(l : IntegerConstant, r : IntegerConstant)
16     => IntegerConstant(l + r)
17 })
18
19 s.apply // execute transformations sequentially
```

ExaStencils Framework

Implemented workflow:



ExaStencils Framework

```
1  Function Smoother () : Unit {
2    communicate Solution
3    loop over Solution {
4      Solution = Solution + 0.8 * (1.0 / diag(Laplace)) *
         (RHS - Laplace * Solution)
5    }
6  }
```

- Program control flow and calculations can be transformed to C++
- What about parallelism?

➔ Affects nearly all parts of the generated program

➔ Requires major changes and concepts for

  - distributing the data and the work
  - keeping the data synchronized

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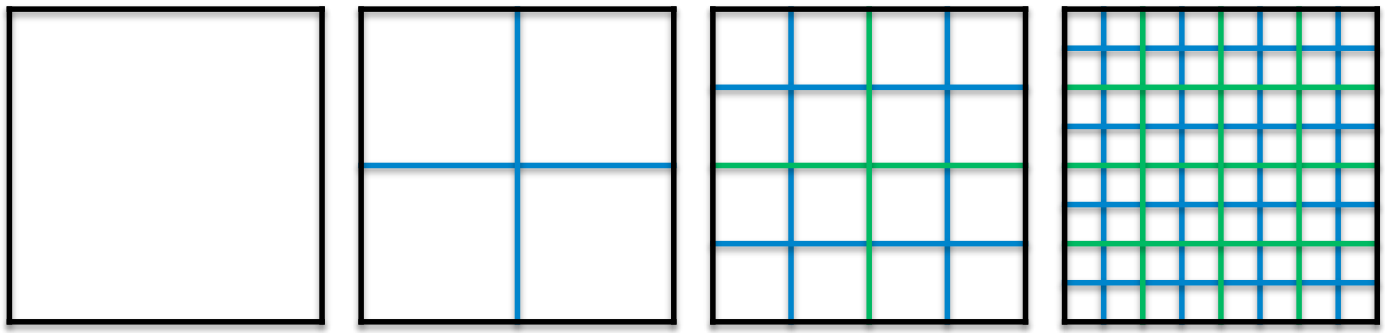
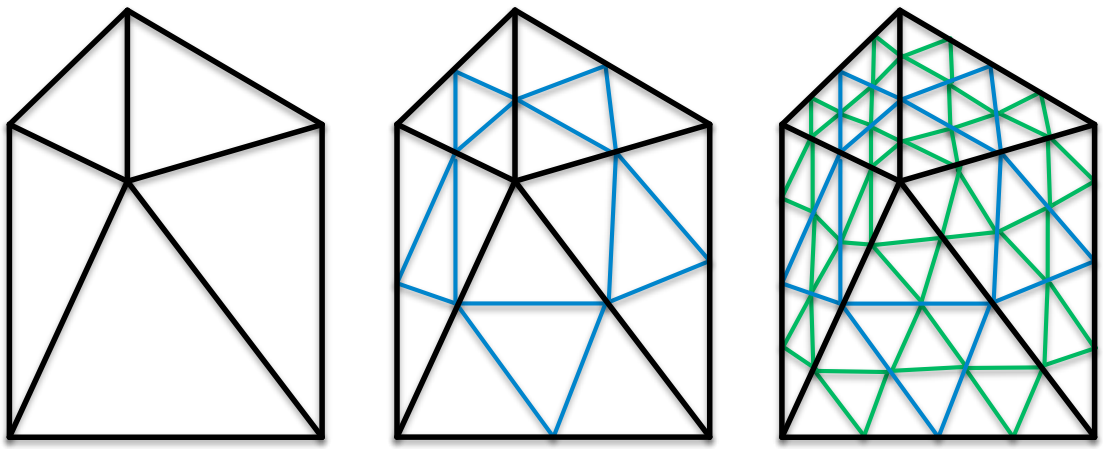
Partitioning the Computational Domain(s)

Domain Partitioning – Our Scope

- Uniform grids



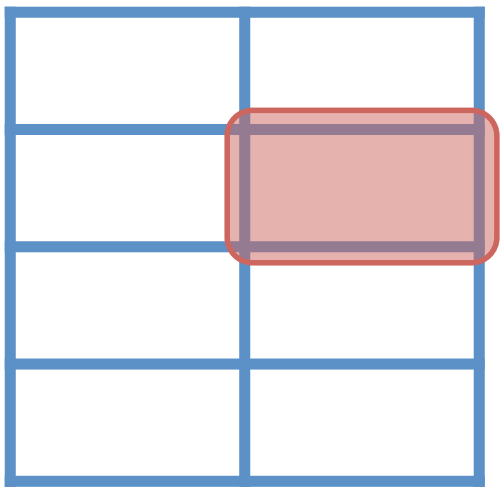
- Block-Structured grids



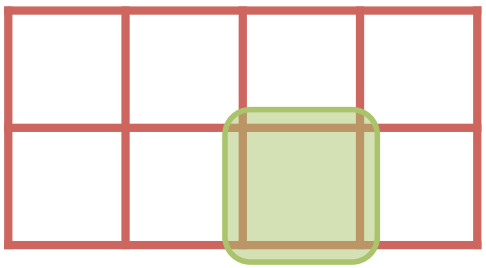
Domain Partitioning – Concept

- Easy for regular domains

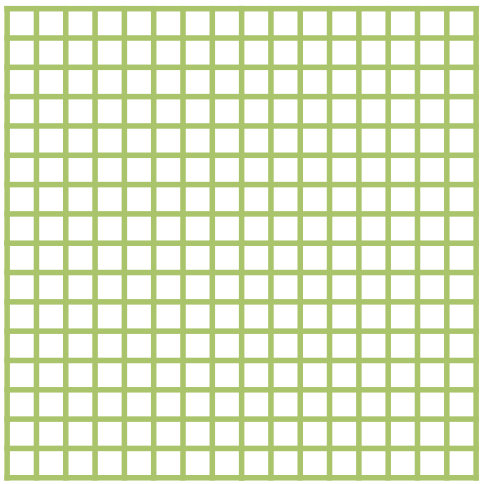
Each **domain** consists of one or more **blocks**



Each **block** consists of one or more **fragments**



Each **fragment** consists of several **data points** / **cells**



- More complicated for HHG

Domain Partitioning – Mapping to Parallelism

- Domain partition maps directly to parallelization strategy, e. g. using MPI and OMP
  - Each **block** corresponds to one *MPI* rank
  - Each **fragment** corresponds to one *OMP* rank
  - Pure *MPI* corresponds to one **fragment** per **block**
  - Pure *OMP* corresponds to one **block**
  - Hybrid *MPI*/*OMP* corresponds to multiple **blocks** and multiple **fragments** per **block**
  - Optional transformation: aggregate all **fragments** within one block and *OMP* parallelize field operations directly
- Easy to map to different interfaces, e. g. MPI and CUDA

Domain Partitioning – User Interface

- Two different ways:
  - Load domain information from file (work in progress)
  - If supported by domain shape and partition: generate req. information on the fly
- All domains are specified in Layer 4

```
1 Domain global< [ -1, -1, -1 ] to [ 1, 1, 1 ] >
2 Domain sthSmaller< [ -0.75, -0.75, -1 ] to [ 0.75, 0.75, 1 ] >
```

- Actual partition is specified through the number of blocks and fragments in each dimension
- Using this information domain setup code is generated

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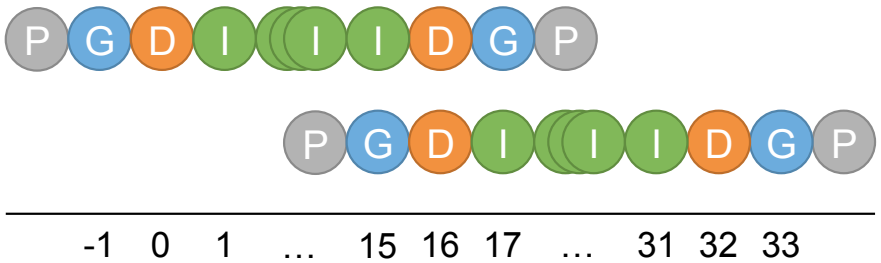
Communication

Communication – Requirements

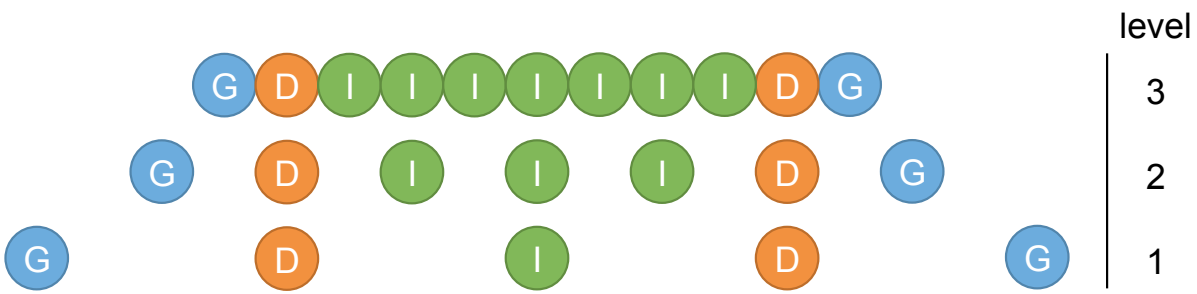
- Data needs to be exchanged between different processes . . .
  - . . . locally and/or remotely (i. e. between fragments within and/or across blocks)
  - . . . with different patterns (e. g. 6P/26P in 3D)
  - . . . for specific regions in the grids (e. g. when using temporal blocking)
  - . . . for multiple data layouts
  - . . . using MPI data types if reasonable
  - . . . asynchronously
- However, it is not feasible to. . .
  - . . . implement every possible case
  - . . . extensively use templates and defines
  - . . . trade variability for performance (e. g. using PGAS)

Communication – Requirements

- Fields (data mapped to fragments) are (logically) split into different regions: padding (P), ghost (G), duplicate (D) and inner (I) points



- Duplicate points allow for intuitive mapping between levels



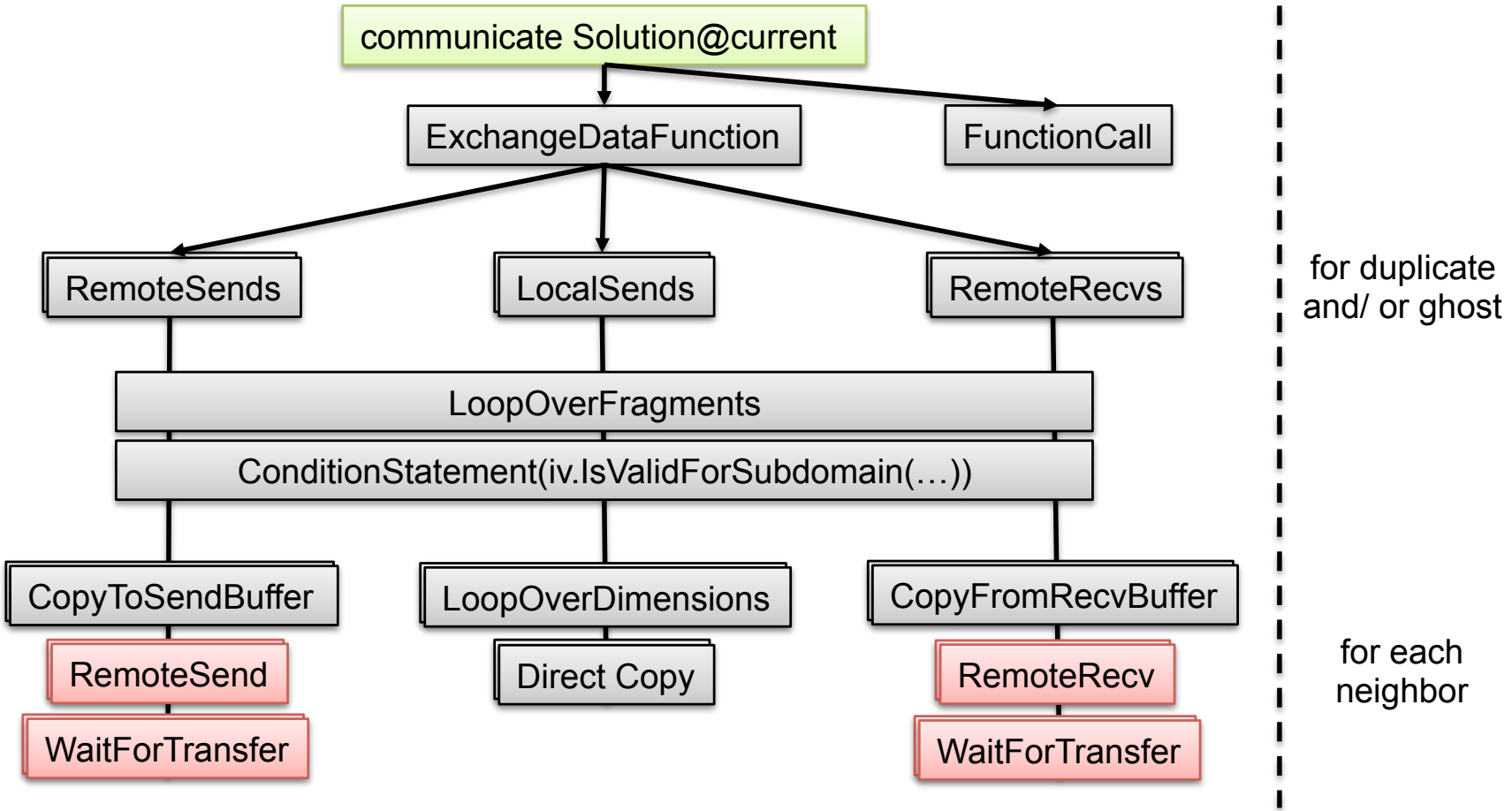
Communication – User Interface

- Communication statements are added automatically (wip) or specified by the user

```
1  /* communicates all applicable layers */
2  communicate Solution@current
3  /* communicates only ghost layers */
4  communicate ghost of Solution[curSlot]@current
5  /* communicates duplicate and first two ghost layers */
6  communicate dup ghost [ 0, 1 ] of Solution[curSlot]@current
7  /* starts asynchronous communicate */
8  begin communicate Residual@current
```

- Basic (Layer 4) communicate statements are synchronous with respect to the computations
- Actual realization, i. e. usage of synchronous and/ or asynchronous MPI operations is up to the generator

Communication – Node Progression

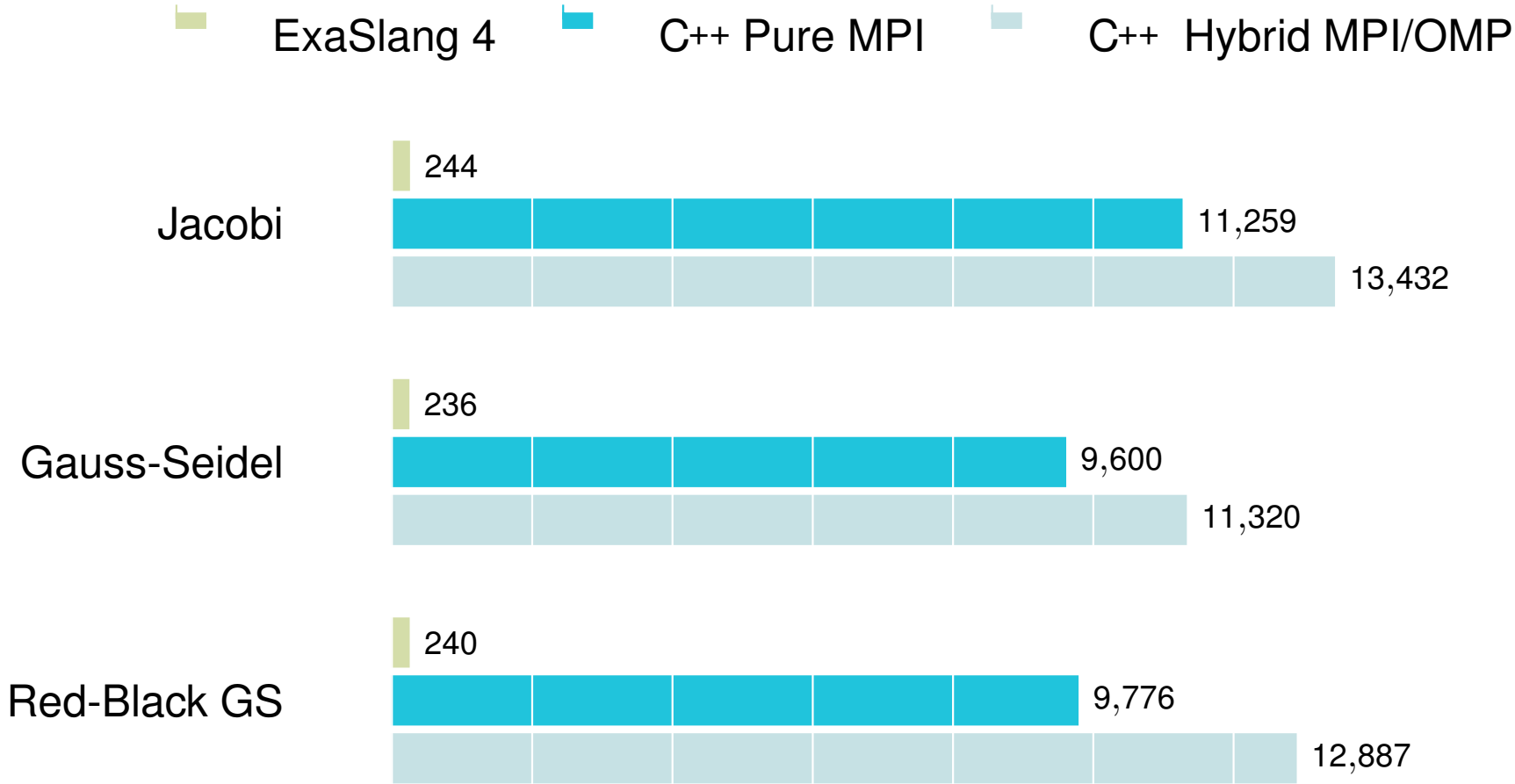


Results

Benchmark Problem and System

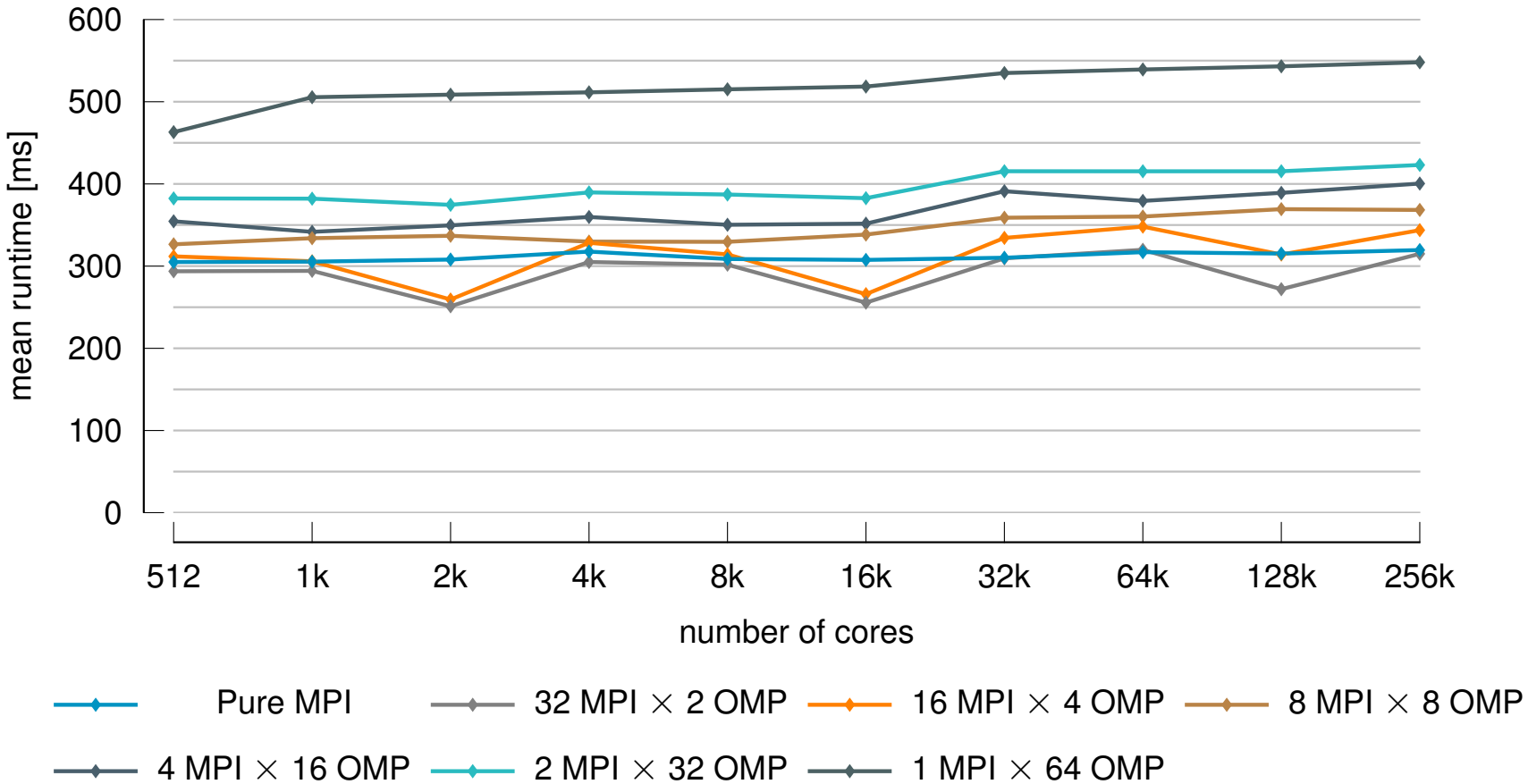
- Target system
  - JUQUEEN supercomputer located in Jülich, Germany
  - 458,752 cores / 28,672 nodes (1.6 GHz, 16 cores each, four-way multithreading)
- Regarded problem
  - 3D finite differences discretization of Poisson's equation ($\Delta\phi = f$) with Dirichlet boundary conditions
  - V(3,3) cycle, parallel CG as coarse grid solver
  - Jacobi, Gauss-Seidel or red-black Gauss-Seidel smoother
  - Pure MPI or hybrid MPI/OMP parallelization
  - 64 threads per node, roughly 10^6 unknowns per core
  - Code optimized through polyhedral loop transformations, 2-way unrolling and address precalculation on finer levels as well as custom MPI data types
  - Vectorization and blocking are work in progress

Generated Lines of Code



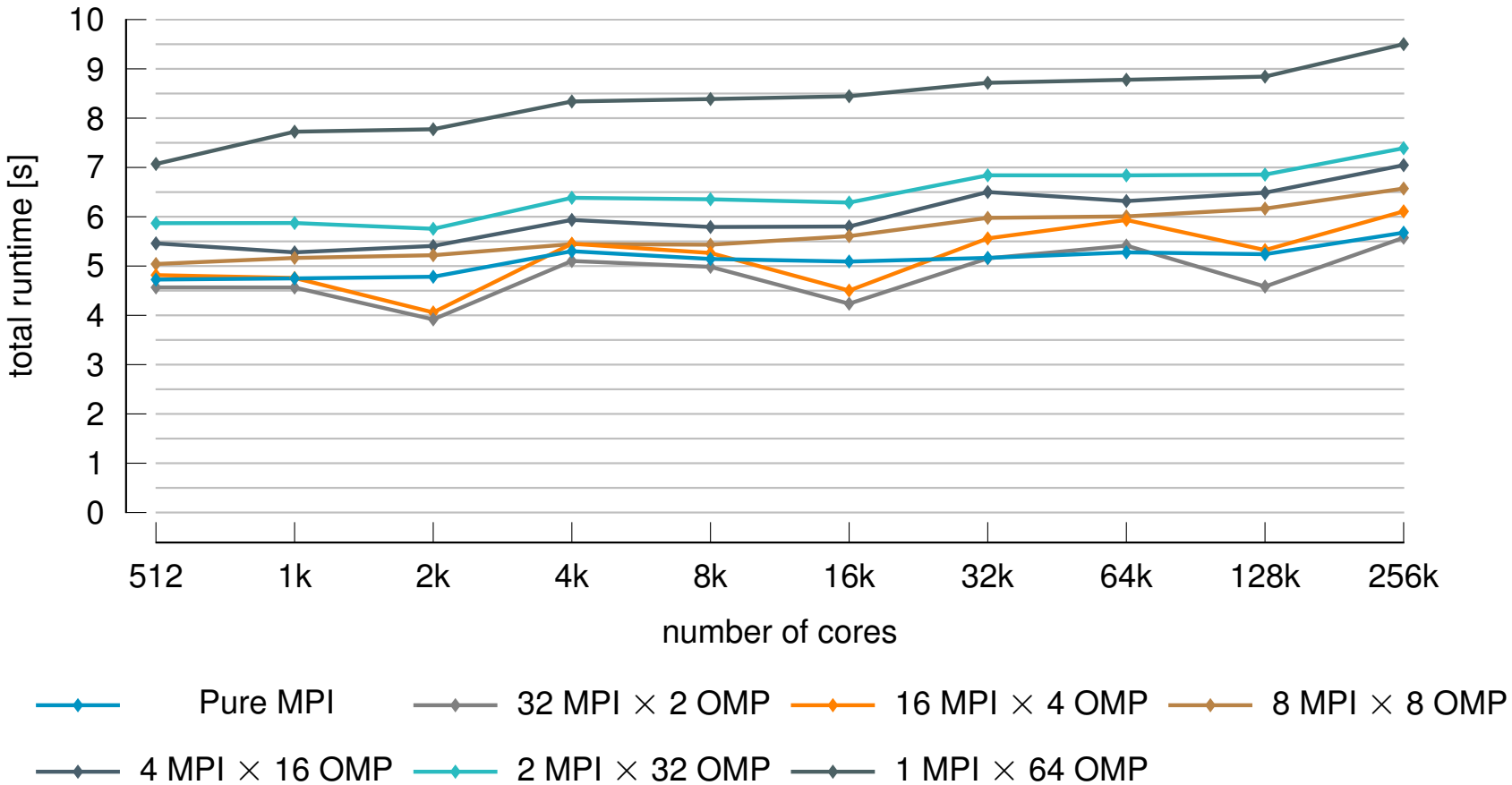
Weak Scalability

- Mean time per V-cycle
- V(3,3) with Jacobi and CG



Weak Scalability

- Time to solution
- V(3,3) with Jacobi and CG



Conclusion

Conclusion

- Transformation framework for generating massively parallel geometric multigrid solvers from an abstract representation
- Specialized DSLs allow for concise algorithmic descriptions (Productivity)
- Generated code is automatically tuned towards target platforms using, e. g., OpenMP, MPI and intrinsics (Portability)
- Performance and scalability are not yet optimal but already quite good (Performance)

Next Steps

- Applications
- Abstract DSL layers (ExaSlang 1 to 3)
- Target platform description language
- End-user tool support (e. g. editors)
- Variant generation and exploration (in combination with. . .)
- Convergence analysis
- Extended performance optimizations (e. g. color-partitioned memory) and examination of their impacts on, e. g., communication functions
- More in-depth analysis of performance potentials in overlapping communication and computation
- ((Multi-)GPU support)
- (HHG data structures)

Thanks for listening. Questions?

ExaStencils – Advanced Stencil Code Engineering

http://www.exastencils.org

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