Transformation from DSL to Source Code for Multi-Physics Simulations with Flash-X

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Pronouns: he/him/his/himself
Outline

Background, Motivation, and Overview

Code Generation Toolkit

Control Flow Graphs

Conclusion
Background: Multi-physics simulations with Flash-X\(^1\)

- Flash-X’s source code (FORTRAN & C++) is configured before compilation such that only desired physics units are included in the binary.
- Physics units can be further decomposed into implementations for specific hardware platforms.

\(^1\)Flash-X is a new application code derived from FLASH.
Performance of simulation relies on apply routines

Relative time spend in apply routines of a PDE solver

1 rack (7.5 TFlops/s)
32 racks (239 TFlops/s)
64 racks (445 TFlops/s)
96 racks (687 TFlops/s)

25.9% 8.6% 25.9% 8.8%
14.1% 37.0% 14.0% 37.4%
8.6% 3.6% 8.8% 3.7%

A, Stokes, B/Bᵀ, K represent PDE operators.

Measured on IBM BlueGene/Q architecture (1 rack = 16,384 cores)

Observe

- Highly optimized matrix-free apply routines dominate with ~80% of time
- Optimization of apply routines and its kernels is (highly) platform dependent
- Transition to new heterogeneous architectures, such as, single- or multi-GPU nodes from different vendors (Nvidia, AMD, Intel), involves substantial transformations and optimizations of code at many levels of abstraction

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=Rudi et al. (2015), In: Proceedings of SC’15
Motivation and overview

Time stepping in Flash-X (and linear & nonlinear solvers in most other applications)

- Every iteration requires applying an operator of the underlying multi-physics PDE
- The operators are matrix-free apply routines
- Optimized kernels carry out computations on each grid cell

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3 presented by Tom Klosterman (SIAM PP22 MS79)
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**Challenges arising due to heterogeneous platforms**

- **Kernels** must be optimized for each platform → for now, leave this to skilled developers taking advantage of the Macro processor

- **Apply routines** (loops over kernels) must be written for each platform → opportunity for developer-guided automation

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Propose: Automate generation of apply routines / driver code

▶ Recipes: Create a concise domain specific language (DSL)
▶ Orthogonalize: Separate domain knowledge and platform knowledge
▶ Code generation tool kit: Transform recipes to human-readable source code
▶ Hints: Users provide platform-dependent code optimizations hints, thus, tools remain simple and avoid exploring an intractable search space

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Generating code from recipes and code templates

Chain of code generation tools (example above).

Example recipe (right) and resulting control flow graph (bottom).

```python
# create new, empty graph
g = ControlFlowGraph()

# add nodes to graph
dIn = g.linkNode(ConcurrentDataBegin())(g.root)

wX = g.linkNode(Work(name='X'))(dIn)
wY = g.linkNode(Work(name='Y'))(wX)
wZ = g.linkNode(Work(name='Z'))(wY)
wA = g.linkNode(Work(name='A'))(wX)
wB = g.linkNode(Work(name='B'))(wA)

dOut = g.linkNode(ConcurrentDataEnd())([wB, wZ])

# set node attributes
g.setNodeAttribute([wA, wB], 'device', 'CPU')
g.setNodeAttribute([wX, wY, wZ], 'device', 'GPU')
```
Overview of all components of code generation toolkit

- Input and output files shown as green boxes
- Intermediate outputs shown as orange boxes (can be inspected by humans)
- Code generation tools are blue boxes (currently in development)
- Optimization tools are pink boxes (future development)
Developers can select and combine tools

Fig: Example toolchain with full spectrum of tools

Fig: Example toolchain without recipe tools

Fig: Example toolchain with recipe tools
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Process control flow graphs into hierarchical graphs

Approach

1. Create a (flat) control flow graph where nodes (blue) represent computational work (i.e., kernels) and edges represent dependencies between kernels and data flow
Process control flow graphs into hierarchical graphs

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2. Assign attributes to nodes representing which device it will execute on (e.g., CPU, GPU).

3. Extract a hierarchical graph consisting of a quotient graph and subgraphs (orange) (which group kernels that will run on same device).

**Definitions**

**Quotient graph:** The nodes of a quotient graph $Q$ of $G$ form blocks of a partition of the nodes of $G$ ($Q$ contains orange circles, $G$ contains blue circles).

**Subgraph:** Nodes of $G$ in the same block (orange circle) form a subgraph.
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4. Generate **device specific subroutines** for aggregated device specific kernels (subgraphs).

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5. Traversal of the coarse quotient graph yields the call sequence, thus the apply routine / driver code.

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**Previous example of a recipe and control flow graph**

- Mark edges with a **device change attribute** (CPU-to-GPU or GPU-to-CPU) between any of the connected nodes.
- Condensation of nodes that are connected by edges **without** device change.

Subgraph for **CPU** includes work/kernels $A$ and $B$.

Subgraph for **GPU** includes work/kernels $X$ and $Y$.

$Z$ cannot be combined with $X$, $Y$ because of concurrent edge $Y \rightarrow A$.
Previous example: code generated from hierarchical control flow graph

```
// define task-function for GPU
void gpu_taskfn_00() {
    X_GPU();
    Y_GPU();
}

// define task-function for CPU
void cpu_taskfn_01() {
    A_CPU();
    B_CPU();
}

int main(int argc, char* argv[]) {
    // begin concurrent data
    { // begin concurrent work
        // execute task-function on GPU
        gpu_taskfn_00();
        { // begin concurrent work
            // execute work on GPU
            Y_GPU();
            // execute task-function on CPU
            cpu_taskfn_01();
        } // end concurrent work
    } // end concurrent work
    return 0;
}
```
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Broader impact: Tools for performance portability

Tools are broadly applicable

- Do not assume a programming language (e.g., FORTRAN, C, ...) or parallelization framework (e.g., CUDA, HIP, OpenMP, OpenACC, ...)
- Do not try to infer optimizations, avoiding intractable search space and corner cases
- Ease burdens and increase productivity of developers working with scientific codes, in terms of code maintenance and platform migration
- Allow software communities to work together and separate concerns/tasks

Tools are flexible

- Each tool is simple and independent
- Multiple tools can be composed into toolchains or pipelines
- Developers can select tools they need and build their own portability framework (avoid one-solution-fits-all)
References I
