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

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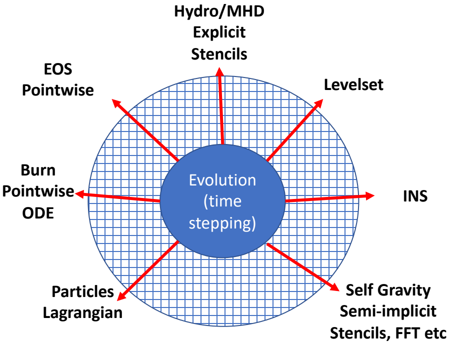
Pronouns: he/him/his/himself

Outline

Background: Multi-physics simulations with Flash-X[1]



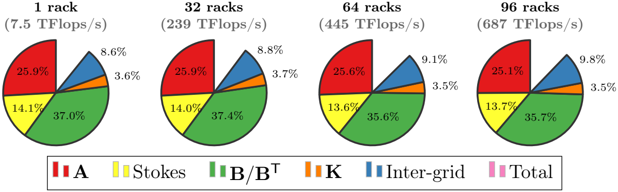
(Credit: A. Dubey)

- 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[2]



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

$\mathbf{A}$, Stokes, $\mathbf{B}/\mathbf{B}^\top$, $\mathbf{K}$ represent PDE operators.

Observe

- Highly optimized matrix-free apply routines dominate with $\sim$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

[2] 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

[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[3]
- 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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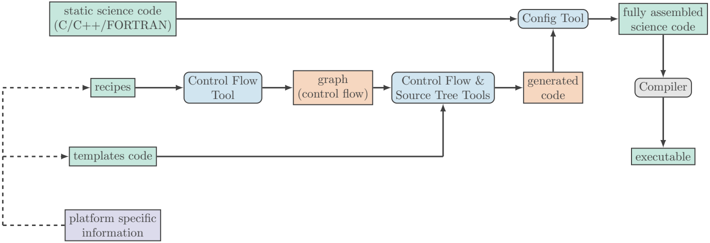
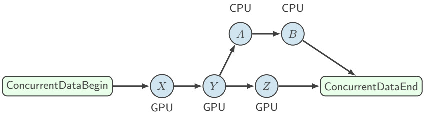
Generating code from recipes and code templates



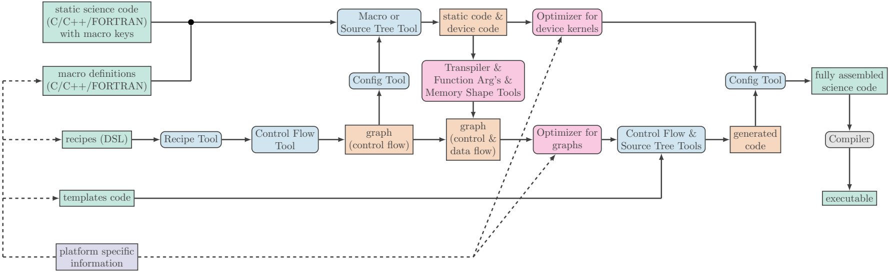
Chain of code generation tools (example above).

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




```
# 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

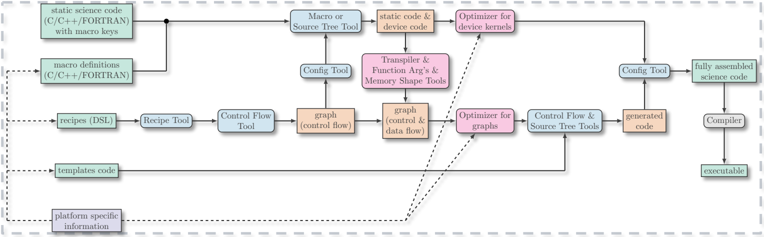


Fig: Example toolchain with full spectrum of tools

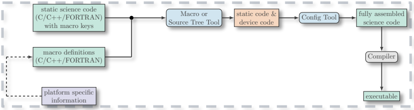


Fig: Example toolchain without recipe tools

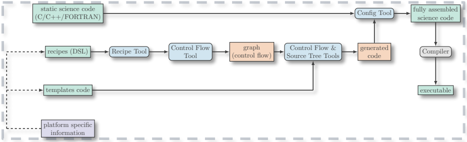


Fig: Example toolchain with recipe tools

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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

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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).

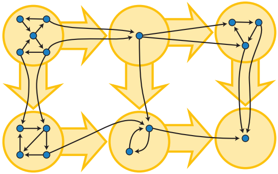

Illustration of a quotient graph
(Credit: wikipedia.org)

Subgraph: Nodes of G in the same block (orange circle) form a subgraph.

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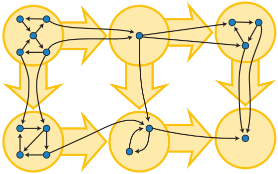

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5. Traversal of the coarse quotient graph yields the call sequence, thus the apply routine / driver code

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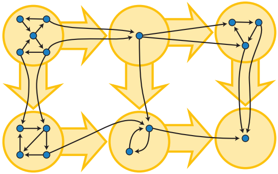

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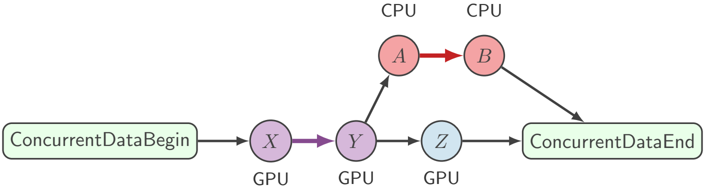
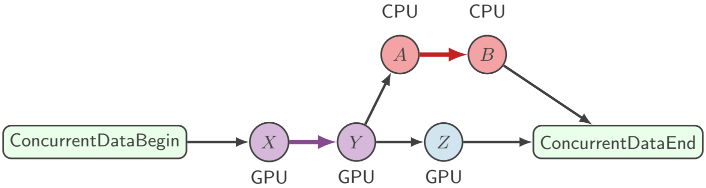
Previous example of a recipe and control flow graph

- 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 $Y \to A$

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
    // 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 data
  return 0;
}
```

Outline

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

Rudi, Johann, A. Cristiano I. Malossi, Tobin Isaac, Georg Stadler, Michael Gurnis, Peter W. J. Staar, Yves Ineichen, Costas Bekas, Alessandro Curioni, and Omar Ghattas (2015). "An Extreme-Scale Implicit Solver for Complex PDEs: Highly Heterogeneous Flow in Earth's Mantle." In: *SC15: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, 5:1–5:12.

Rudi, Johann, Jared O'Neal, Mohamed Wahib, Anshu Dubey, and Klaus Weide (2021). *CodeFlow: Code Generation System for FLASH-X Orchestration Runtime*. Tech. rep. ANL-21/17. Argonne National Laboratory, Lemont, IL.