

Comp. Science on Today’s Hardware

Computational science software must run at an appreciable fraction of peak performance on many different machines:

- Nvidia GPUs
- Intel/AMD wide-vector CPUs (AVX-256, AVX-512)
- Intel/AMD GPUs
- ...

Programming Challenges

- Array/vector architectures
- High memory latency
- Limited on-chip memory

Simplification: Use CL/CUDA abstract machine model for all of them

Still: Machine-specific trade-offs/capacities

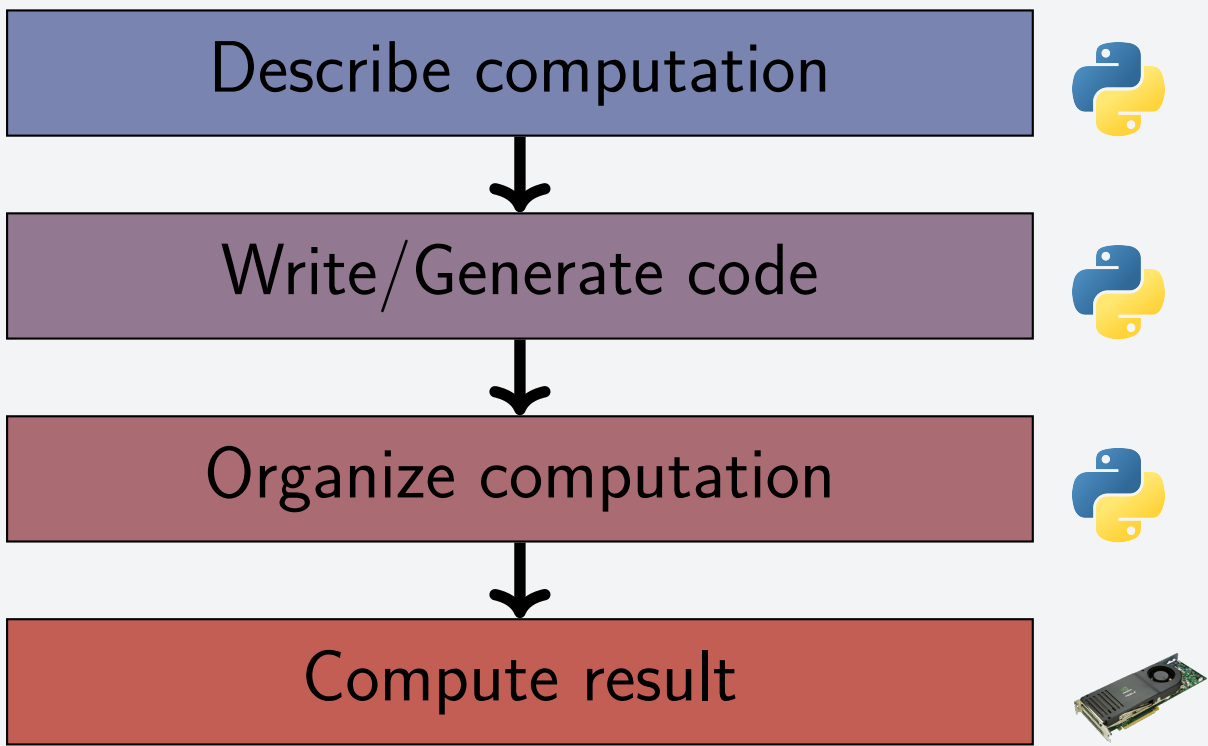
Therefore: Machine-specific code needed

And: Many dialects (OpenCL, CUDA, ISPC, OpenMP+Pragma SIMD, ...)

Competing Approaches

- C++ Metaprogramming
- Libraries

PyOpenCL/PyCUDA: HPC in Python



Loopy

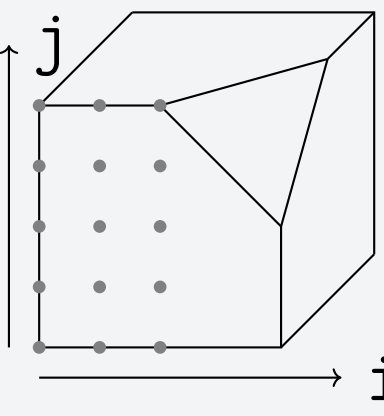
Loopy is a code generator for computation with arrays.

Performance: human ‘in the loop’ for the foreseeable future.

- Capture math at a high level; target number crunching
- Progressively ‘lower’ through manual transformations
- Observe and control optimization steps
- ‘Help me write the CUDA C/ISPC/... I would write’

Loopy: Program Representation

Polyhedron



Statement(s)

b[i] = sum(j, A[i,j] * x[j])

Summary

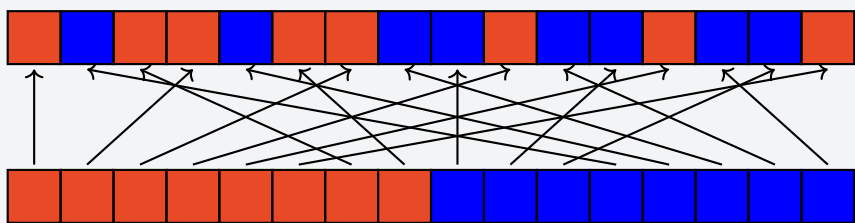
Tree of Polyhedra
+ Statements
+ Dependencies
= Semantics

{[i,j]:
0<=i<n and
0<=j<n and
...}

Vector Shuffles via Array Access

Vector shuffles complement shared memory as an efficient means of communication.

- less synchronization
- less energy expense
- harder to program

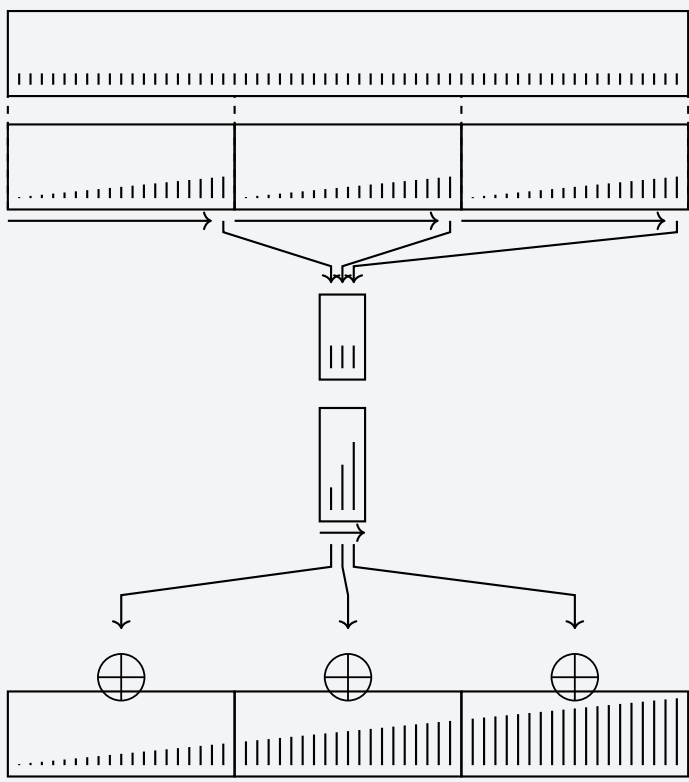


Idea: Represent them in Loopy’s intermediate representation, make them reachable by transforms (e.g. for SoA/AoS transpose)

Transformation, Efficiency for Scan

Scan/prefix sums are a core parallel primitive [Blelloch ‘93], with uses in, e.g.:

- threads with variable-size output
- sorting
- filtering



Idea: Allow Loopy to represent and transform scans

Transform Addressing

Core difficulty in program transformation: Transform addressing, i.e. specifying where a transform should apply.

Notation must be:

- compact
- specific
- human-readable

Idea: A query language acting on the program representation

A Transform-Capable Array Package

numpy code is widespread, e.g.:

- neural nets
- computational science
- image processing

numpy code could use GPUs well, but not robustly high performance without help.

```
result[1:-1] = v[2:] - v[:-2]
result[0] = v[1] - v[0]
result[-1] = v[-1] - v[-2]
```

- Many realizations of “lazy numpy”
- For automatic differentiation, performance

Ideas:

- a reusable lazy array package
- connect it to Loopy codegen
- allow user intervention for performance
- replace PyOpenCL/PyCUDA array objects

Graphical Transform User Interface

Instructions

out[i, j] = sum(k, in[i, k])

OpenCL

Domain

{ [i, j, k]: 0<=i,j<n and 0<=k<4 }

Kernel

ARGUMENTS:

	Space	Dtype	Shape
in	Global	float32	(n,4)
out	Global	float32	(n,4)
n	ValueArg	int32	

DOMAINS:

[n]-> {[i,j,k]: 0<=i<n and 0<=j<n and 0<=k<4 }

INDEX IMPLEMENTATION TAGS:

i: lid(0), Add tag...
j: none, Add tag...
k: unroll, Add tag...

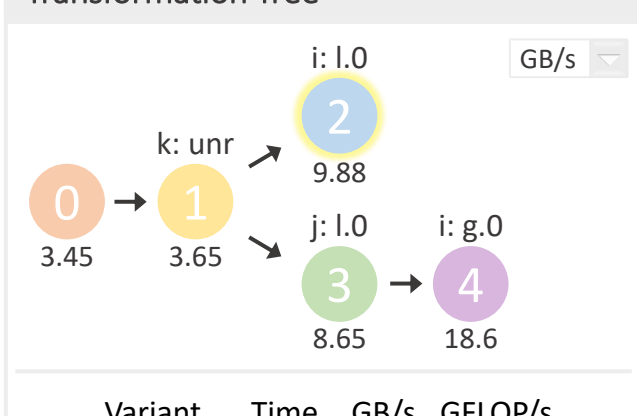
INSTRUCTIONS:

0[i,j] out[i,j] <- reduce(sum, [k], in[i,k]) #insn

Output

```
kernel void loopy_kernel(  
int const n, _global float const *in,  
_global float *out)  
{  
float acc_k;  
for (int j = 0; j <= -1 + n; ++j)  
{  
acc_k = 0.0f;  
acc_k = acc_k + in[4 * lid(0)];  
acc_k = acc_k + in[4 * lid(0) + 1];  
acc_k = acc_k + in[4 * lid(0) + 2];  
acc_k = acc_k + in[4 * lid(0) + 3];  
out[n * lid(0) + j] = acc_k;  
}  
}
```

Transformation Tree



Variant	Time	GB/s	GFLOP/s
2	0.0023	9.88	1.976

- Improves Transform Discoverability
- Eases Experimentation
- Supports Performance Modeling

(Ask for a demo!)

Loopy Usage Example

```
import loopy as lp  
k = lp.make_kernel(  
    "{ [i]: 0<=i<n }",  
    "out[i]=2*a[i]"  
)  
  
k = lp.split_iname(k, "i", 128)  
k = lp.tag_inames(k, "i_outer: g.0")  
k = lp.tag_inames(k, "i_inner: l.0")
```

Loopy: Summary

Github:

<https://github.com/inducer/loopy>

- One intermediate representation from math to low-level machine code
 - Shared medium between human and machine
- Transformations to cover the difference
- Make near-peak performance accessible by manual transformation
- Allow autotuning/automated search to be implemented “on top”

A user quote about Loopy’s IR:

We believe that loopy’s level of abstraction hits this sweet spot needed for a high performance code generation workflow. [Kempf et al. ‘18]

Known Science Users

- Firedrake finite element framework: <https://arxiv.org/abs/1903.08243>
- Dune PDElab finite element framework: <http://arxiv.org/abs/1812.08075>
- Pystella stencil-based cosmology solver: <https://arxiv.org/abs/1909.12843>, <https://arxiv.org/abs/1909.12842>
- Computational neuroscience: <https://doi.org/10.3389/fninf.2018.00068>
- SIMD/SIMT for chemical kinetics: <https://doi.org/10.1016/j.combustflame.2018.09.008>