

Generating optimal HPC code with ML

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PASC23



Outline

Intro

What is code generation? Not ChatGPT!

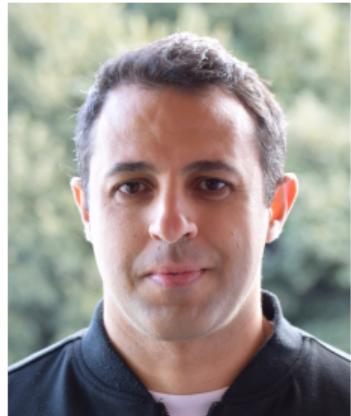
Representation? + HPC = Polyhedral

Democratise Polyhedral: a polyhedral mini-tutorial

Current status: Tadashi

RIKEN Center for Computational Science

High Performance Artificial Intelligence Systems Research Team



Mohamed Wahib
HPC+compilers

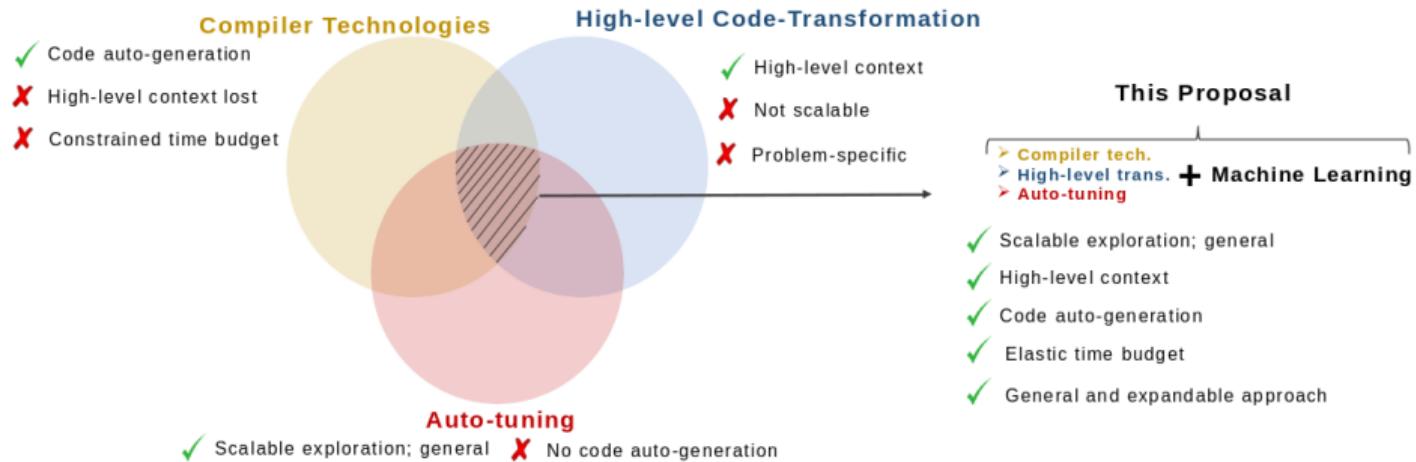


Aleksandr Drozd
HPC+AI



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HPC+math

Motivation/Overview



What **is** code generations?

The ultimate goal: “Hey AI, optimise this code!”

- ▶ Source to source transformations
- ▶ Targeting high-level optimisations.
 - ▶ Here High-level optimisations are code transformations which exploit deeper insight, an overview of the overall structure/context of the application
 - ▶ This is in contrast to low-level, local transformations performed by compilers.
- ▶ Something with practical use/impact.

Fundamental requirement: **the transformations need correct/legal**.

What is **not** code generation? (at least in this context)

Code generations (by ML) is very popular:

- ▶ ChatGPT, Co-pilot, generative models
- ▶ Deepmind's "new" sort algorithm¹ and "new" matrix multiplication²
- ▶ NLP: code from human languages/commit messages

Code generation in general:

- ▶ Compilers: compiler pass

¹ Mankowitz et al, Faster sorting algorithms discovered using deep reinforcement learning

² Fawzi et al, Discovering faster matrix multiplication algorithms with reinforcement learning

The (potential) problem with LLMs/generative models

Deepmind¹ found algorithms using unittests, however **tests don't guarantee correctness/legality.**

- ▶ Primary purpose of testing is to check *human* code.
- ▶ Writing tests is hard, especially ones that ensure full coverage.
- ▶ Not universal: each program needs new unittests.
 - ▶ Writing an AI to write unittests is just moving the goalpost (how do we know tests written by AI ensure correctness/legality).

Example of bad unittests

Original

```
double gold(double input[N]) {
    double result = 0;
    for (int i = 0; i < N; i++)
        result += input[i];
    return result;
}
```

Unittest

```
void unittest(int kpass) {
    srand((unsigned int)time(NULL));
    double input[N];
    for (int k = 0; k < kpass; k++) {
        for (int i = 0; i < N; i++)
            input[i] = (double)rand();
        compare(input);
    }
}
```

```
Equal? yes; delta: 0.0000000000000000; gold: 2243918836.000000; cgpt: 2243918836.000000;
Equal? yes; delta: 0.0000000000000000; gold: 4117298770.000000; cgpt: 4117298770.000000;
...
Equal? yes; delta: 0.0000000000000000; gold: 3835775724.000000; cgpt: 3835775724.000000;
And now for some tricky input:
Equal? no ; delta: 0.0000005960464477539; gold: 400000000.000000; cgpt: 400000000.000000;
```

Transformed

```
double cgpt(double input[N]) {
    double result = 0;
    for (int i = N - 1; i >= 0; i--)
        result += input[i];
    return result;
}
```

Main

```
int main(int argc, char *argv[]) {
    unittest(10);
    double tricky_input[] = {400000000, 9e-8, 9e-8};
    printf("And now for some tricky input:\n");
    compare(tricky_input);
    return 0;
}
```

Representation

One of the first questions we have was: When training the ML model, which representation(s) do we use?

Representations at different compiler passes:

1. Source code
2. Abstract Syntax Tree (AST)
3. Intermediate Representation(s) (IR), e.g. LLVM IR
4. Assembly code
5. Binary code

Other representations:

1. Graphical representations³ (call flow data flow graph)
2. Polyhedral model

³Cummins et al, ProGraML: Graph-based Deep Learning for Program Optimization and Analysis

HPC codes, just the right ratio of difficult

The next question: How to constrain the problemspace, to make it more feasible while still keeping it relevant/impactful?

We target HPC/scientific codes (e.g. stencils, simulations) because:

- ▶ The plethora of research papers describing optimisations of HPC codes is evidence that this is **not a solved problem**.
- ▶ HPC codes usually contain deep and **complex nested loops**, but **each loop separately is regular** (regular memory accesses and boundaries).
- ▶ We have **experience** with optimising such codes.

Polyhedral model

Why polyhedral? “Best bang for the buck.”

- ▶ Reasonable restrictions.
- ▶ Mathematically provable correctness/legality.
- ▶ Compact way to express optimisation opportunities (e.g. parallelism)
- ▶ Compact way to express big transformations (e.g. schedule of the tile)

Reasonable restrictions

SCoP/SANA⁴: Most is true for HPC codes

- ▶ **Static control**: control does not depend on input data
- ▶ **Affine**: all relevant expressions are (quasi-)affine
- ▶ **No Aliasing**: essentially no pointer manipulations

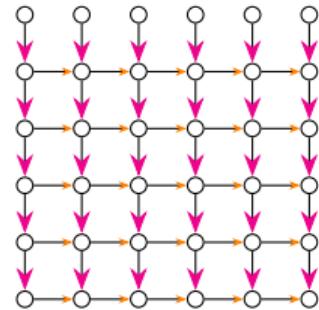
These restrictions can be relaxed if care is taken.

⁴Verdoolaege, Polyhedral compilation without polyhedra

Working example

Dependency in the outer loop, inner loop can be parallel:

```
for(int i = 1; i < N; i++)  
    for(int j = 0; j < M; j++)  
S1: a[i][j] += a[i-1][j];
```



Components of polyhedral compilation

- ▶ SCoP extraction
- ▶ Dependency analysis
- ▶ Find a schedule θ
- ▶ Legality check
- ▶ Generate the new source code

Polyhedral basics

Everything can be represented as a matrix

- ▶ Statements: S_1 (S_1 is a label). $S_1: a[i][j] += a[i-1][j];$
- ▶ Statement instances $S_1(i, j)$ (i, j are symbols for integer variables)
- ▶ Domain of S_1 : $\{S_1(i, j) : 1 \leq i \leq N - 1, 0 \leq j \leq M - 1\}$ (N is a symbolic constant, unknown but not changing)
- ▶ Dependency graph: $e_1 : S_1(i_s, j_s) \rightarrow S_1(i_t, j_t)$ (between statement instances)
 - ▶ Notation: s = source (before), t = target (after)
 - ▶ Dependency polyhedron: $P_e = \{S_1(i_s, j_s, i_t, j_t) : i_s = i_t - 1, j_s = j_t\}$

Dependency check

Original: $\theta_0 : S_1(i, j) \rightarrow (i, j)$

- ▶ **Dependencies** are maps between event instances: $S_1(i - 1, j) \rightarrow S_1(i, j)$
- ▶ **Schedules** are maps from statement instances to (multidimensional) time

Apply the schedule to the range and domain

- ▶ Dependency: $S_1(i - 1, j) \rightarrow S_1(i, j)$
- ▶ Map to time: $(i - 1, j) \prec (i, j)$ (\prec is the lexicographic order) or
- ▶ $(i, j) - (i - 1, j) = (1, 0) \succ 0$ OK!
- ▶ $\theta(\vec{s}) \prec \theta(\vec{t})$ for the dependency $\vec{s} \rightarrow \vec{t}$
- ▶ $\delta(i, j) \succ 0$ where $\delta(i, j) = \theta(i, j) - \theta(i - 1, j)$

Expressing Transformations

Swap loops $\theta_1 : S_1(i, j) \rightarrow (j, i)$

- ▶ Check: $(j, i) - (j, i - 1) = (0, 1) \succ 0$ OK!
- ▶ You can start get θ_1 from scratch, but you can also modify θ_0 : in this case $\theta_1 = T \circ \theta_0$ where $T = (i, j) \mapsto (j, i)$. $\theta_1 : S_1(i, j) \xrightarrow{\theta_0} (i, j) \xrightarrow{T} (j, i)$
- ▶ The zero in $\delta = (0, 1)$ we can parallelise the j loop

Reverse j $\theta_2 : S_1(i, j) \rightarrow (i, -j)$

- ▶ Check: $(i, -j) - (i - 1, -j) = (1, 0) \succ 0$ OK!

Reverse i $\theta_3 : S_1(i, j) \rightarrow (-i, j)$

- ▶ Check: $(-i, j) - (-(i - 1), j) = (-1, 0) \not\succ 0$ ILLEGAL!

More transformations

Diagonal from $(0, 0)$ $\theta_4 : S_1(i, j) \rightarrow (i + j, j)$:

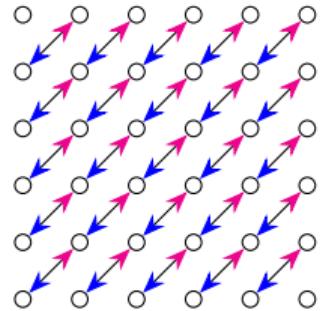
- ▶ Check: $(i + j, j) - (i - 1 + j, j) = (1, 0)$: OK!

Alternative diagonal from $(0, 0)$ $\theta_5 : S_1(i, j) \rightarrow (i + j, i)$

- ▶ Check: $(i + j, i) - (i - 1 + j, i - 1) = (1, 1)$: OK!

Tiling: $\theta(i, j) = (\lfloor i/T \rfloor, \lfloor j/T \rfloor, i \bmod T, j \bmod T)$

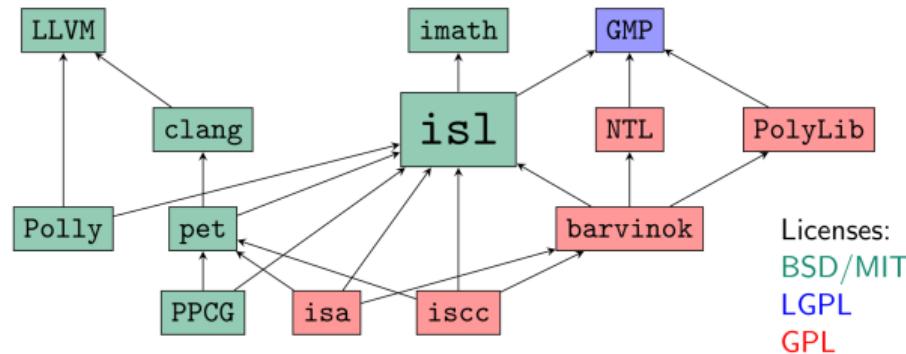
- ▶ $(\lfloor i/T \rfloor, \lfloor j/T \rfloor, i \bmod T, j \bmod T) - (\lfloor (i-1)/T \rfloor, \lfloor j/T \rfloor, (i-1) \bmod T, j \bmod T)$
- ▶ The delta: $(q_i, 0, r_i, 0)$ where $q_i = \lfloor i/T \rfloor - \lfloor (i-1)/T \rfloor$,
 - ▶ here $q_i = 1$ if $i | T$ and $q_i = 0$ when $i \nmid T$
 - ▶ $r_i = 1 - q_i T$ which is $1 - T < 0$ if $i | T$
 - ▶ when $i | T$: $(1, 0, 1 - T, 0) \succ 0$; when $i \nmid T$: $(0, 0, 1, 0) \succ 0$: OK!



Tools

A slide from Verdoollaeghe, “Polyhedral compilation without polyhedra”.

isl and Related Libraries and Tools



isl: manipulates parametric affine sets and relations

barvinok: counts elements in parametric affine sets and relations

pet: extracts polyhedral model from clang AST

PPCG: Polyhedral Parallel Code Generator

iscc: interactive calculator

isa: prototype tool set including derivation of process networks and equivalence checker

Tadashi

Ultimate goal: legality check

- ▶ Ask <random LLM/generative model> to optimise your code, and have a tool to check the legality of the output the model produced!
- ▶ Very difficult: which original statement corresponds to which transformed statement?

正:Tadashi

- ▶ Uses polyhedral.
- ▶ Checks the legal of any schedule.
 - ▶ Quite easy to do with the ISL library.
- ▶ Generates⁵ the transformed code (if the transformation is legal).

⁵work in progress.

Restrictions and relaxations

The restrictions

1. Polyhedral is oblivious to the statements
2. Polyhedral is oblivious to the hardware
3. Bending the SANA/SCoP rules

And how to bend them

1. More involved **data flow analysis**
2. The δ encodes info about parallelism and data locality
 - ▶ Transformations **in** and **after** polyhedral
3. Approximations and/or pw-qpolynomial

A framework to automate the process

