Domain-specific Optimisation for the High-level Synthesis of CellML-based Simulation Accelerators

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Te Whare Wānanga o Tāmaki Makaurau

CellML

- Standard to model biomedical problems
- Differential equations describe interaction between components

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$$alpha\_m = \frac{-(V+47)}{e^{-\frac{V+47}{10}} - 1}$$

$$beta\_m = 40 \times e^{-0.056 \times (V+72)}$$

$$\frac{dm}{dt} = alpha\_m \times (1-m) - (beta\_m \times m)$$

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$$\frac{dm}{dt} = alpha\_m \times (1-m) - (beta\_m \times m)$$

C Code Generation Service

```
ALGEBRAIC[1] = -1.0 * (STATES[0] + 47.0)
               / (exp(-0.1 * (STATES[0] + 47.0)) - 1.0);
ALGEBRAIC[8] = 40.0 * exp(-0.056 * (STATES[0] + 72.0));
RATES[1]     = ALGEBRAIC[1] * (1.0 - STATES[1])
               - ALGEBRAIC[8] * STATES[1];
```

Hardware-accelerated cell simulation

- Numerical integration
- Cells can be treated independently for some time
- ODoST (Yu et al., 2015): fully-spatial, fully-pipelined FPGA accelerators from a model's equation system
- Instantiate as many pipelines as fit on the FPGA

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Fewer resources per pipeline → **More throughput**

Approach

- Fully-spatial computation
  = every SW instruction becomes HW operator

- SW compiler's architecture independent optimisations

  - eliminate redundant operations, or

  - replace "expensive" ops by "cheaper" ones

- Try unsafe floating-point transformations

Cost model

- Estimation of resource demand → guide opts
- Based on relative, per operator ALM and DSP usage on Stratix IV

$$c(op) = \left\| \begin{pmatrix} \frac{n_{\mathrm{ALM}}(op)}{212480} \\ \frac{n_{\mathrm{DSP}}(op)}{1024} \end{pmatrix} \right\|$$

- Allows transformation with a Pareto improvement
- Resulting order of operation costs
  Add < Exp < Mul < Div < Log < Pow

Adding LLVM to the mix

- Sequential computation in C generated from CellML equations → idiomatic DSL-like structure
- Use clang/LLVM as frontend
- Optimise on LLVM-IR (existing and custom opts)
- Reconstruct C code for ODoST input

Identifying redundancies

- Array accesses, function calls hinder optimisation

```
… = -0.1*(STATES[0]+50.0) / (exp(-(STATES[0]+50.0)/10.0) - 1.0);
```

same value?

Identifying redundancies

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```
… = -0.1*(STATES[0]+50.0) / (exp(-(STATES[0]+50.0)/10.0) - 1.0);
```

same value?

- But we know:
  - Input arrays do not alias or overlap
  - Function calls are mathematical operators, side effect-free

Identifying redundancies

- Augment the IR with this domain knowledge to help alias analysis
    - Mark input pointers as `noalias`
    - Map function calls to LLVM intrinsics
- LLVM's global value numbering can now identify expressions across the whole equation system
- Equation system ≅ Dataflow graph

Existing optimisation patterns in LLVM

- -instcombine pass
  - Constant folding & algebraic identities
  - Add < Mul < Div in software compiler as well

Existing optimisation patterns in LLVM

- -instcombine pass
  - Constant folding & algebraic identities
  - Add < Mul < Div in software compiler as well
  - Some transformations only if unsafe FP transformations are allowed
    e.g. $x/c = x \cdot 1/c$ only safe if reciprocal is exact

Domain-specific optimisations

Higher-order powers

- Equations contain x^p with an integer constant
- $8 \cdot c(\text{Mul}) < 1 \cdot c(\text{Pow})$
- Use Knuth’s binary exponentiation method

Op	*ALM*	*DSP*	*c(•)*
Mul	132	4	0.39
Pow	2058	31	3.18

  - lower generic power operator to short sequence of multiplications
  - Example: $x^6 = (\underbrace{(x \cdot x)}_{:= y} \cdot y) \cdot y$

A closer look at the exponential function

$$e^{x + \underline{c}} \cdot \underline{d}$$

Common pattern!

constants underlined

Add < Exp < Mul < …

A closer look at the exponential function

$$e^{x + \underline{c}} \cdot \underline{d}$$

<u>constants</u>
underlined

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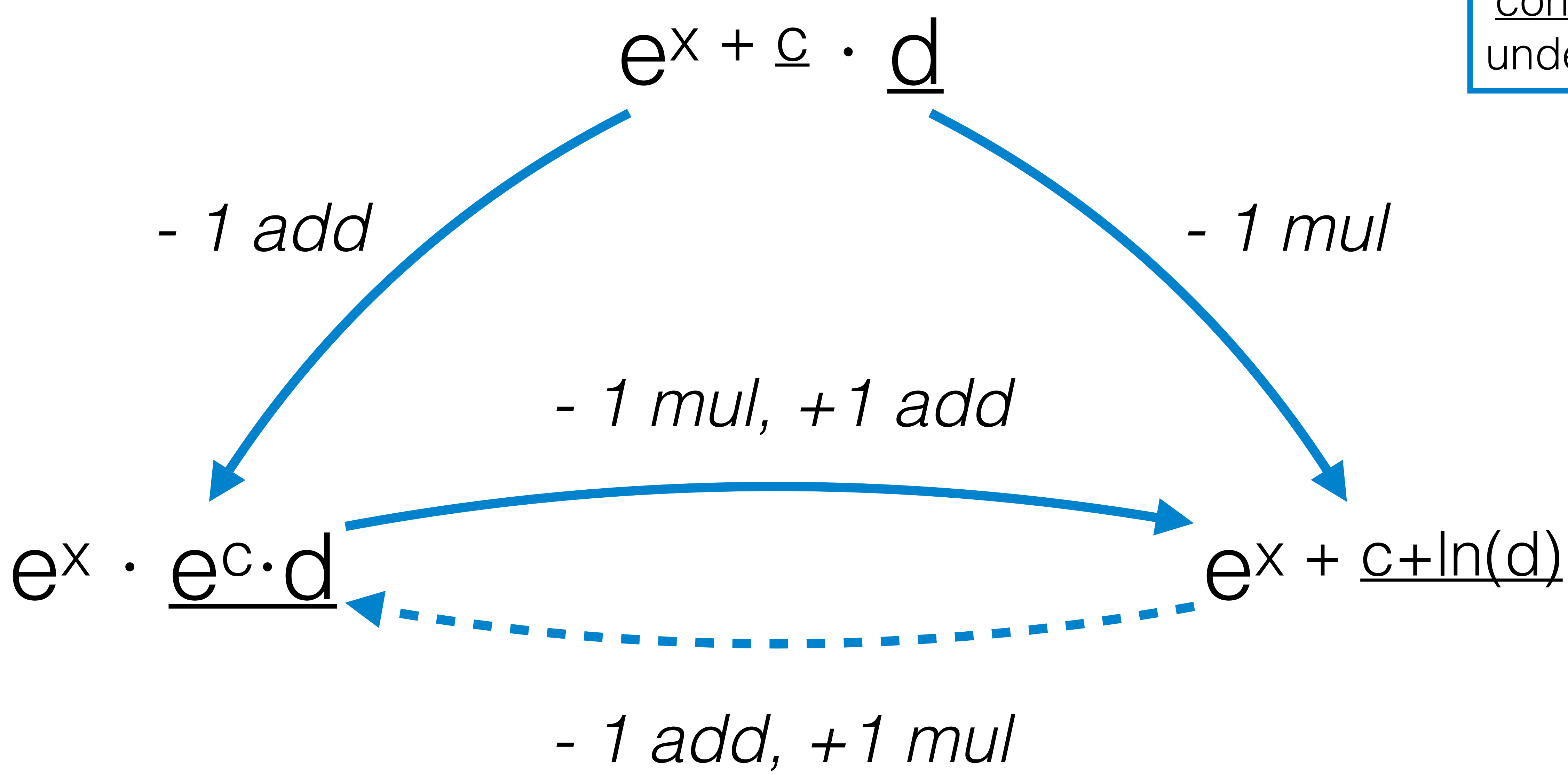
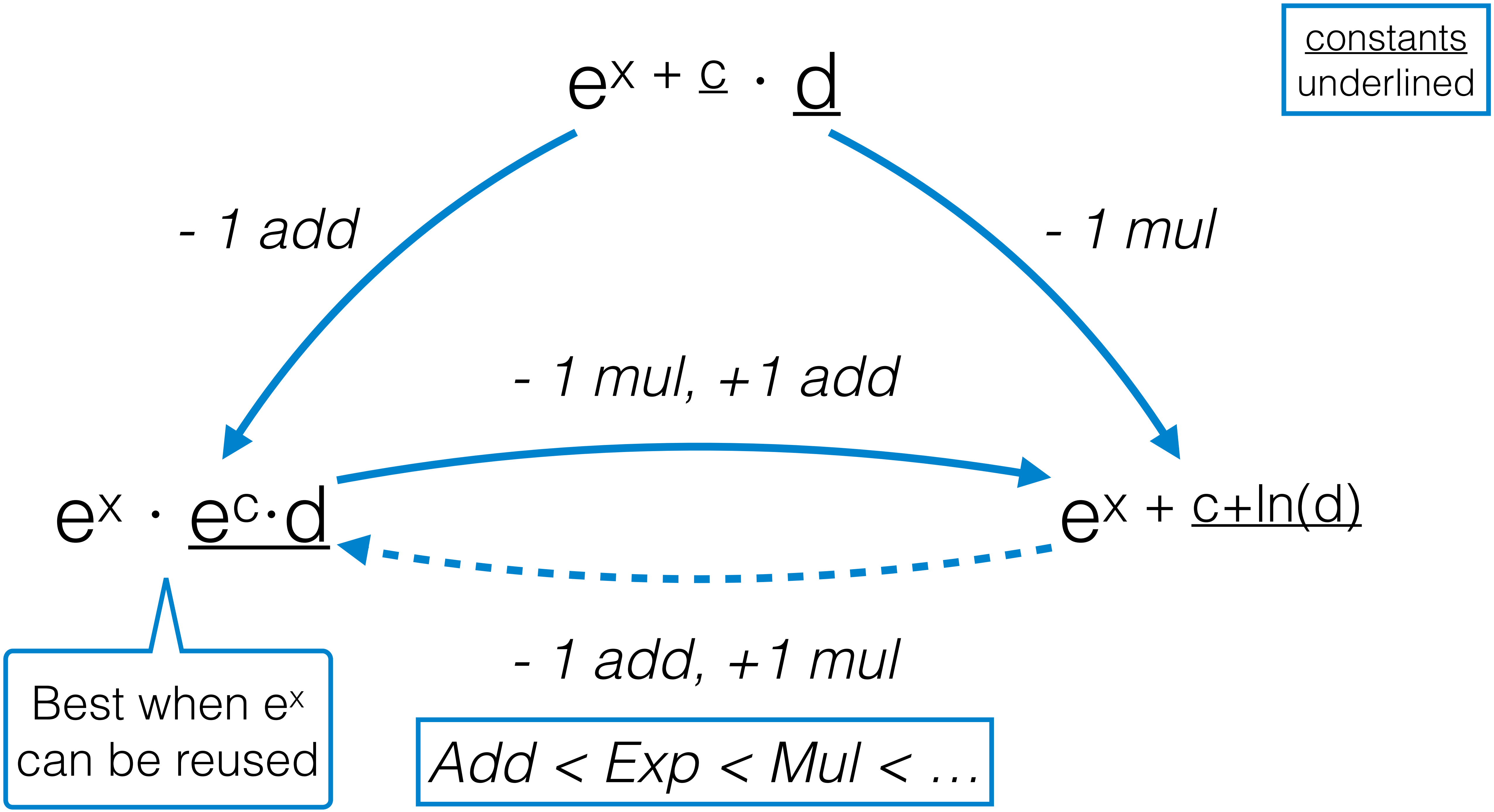
A closer look at the exponential function

constants underlined



Add < Exp < Mul < …

A closer look at the exponential function



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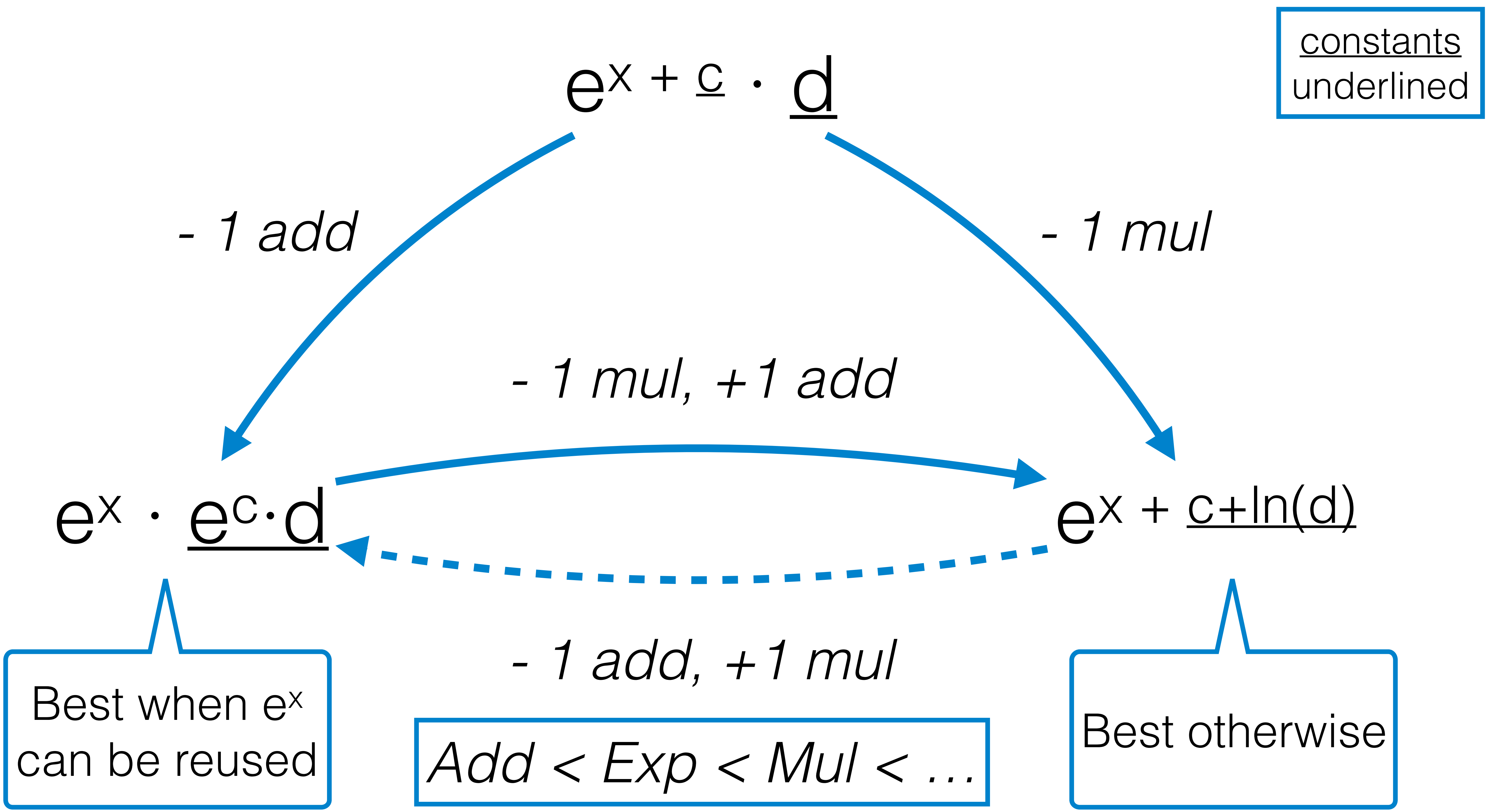


Multiple Constant Multiplication

- x is multiplied with a set of constants c_i
- Can trade 1 multiplication for 1 addition if:
  - $c_2 = 2 \cdot c_1 \quad \rightarrow \quad x \cdot c_2 = (x \cdot c_1) + (x \cdot c_1)$
  - $c_4 = c_3 + 1 \quad \rightarrow \quad x \cdot c_4 = (x \cdot c_3) + x$
- Handle factors in ascending order of absolute values
  - Works also for chains of constants, e.g. 2, 3, 4, 6

Results

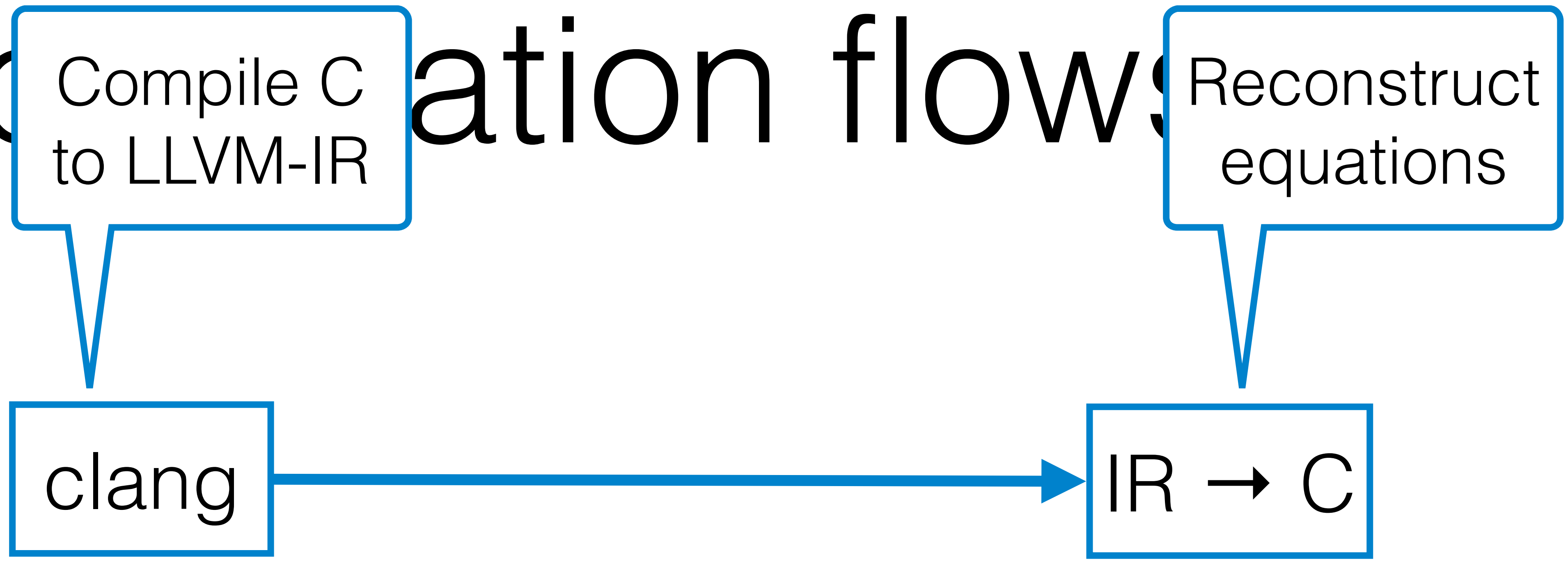
Compilation flows

Compilation flows

NoOpt:

Co ation flows

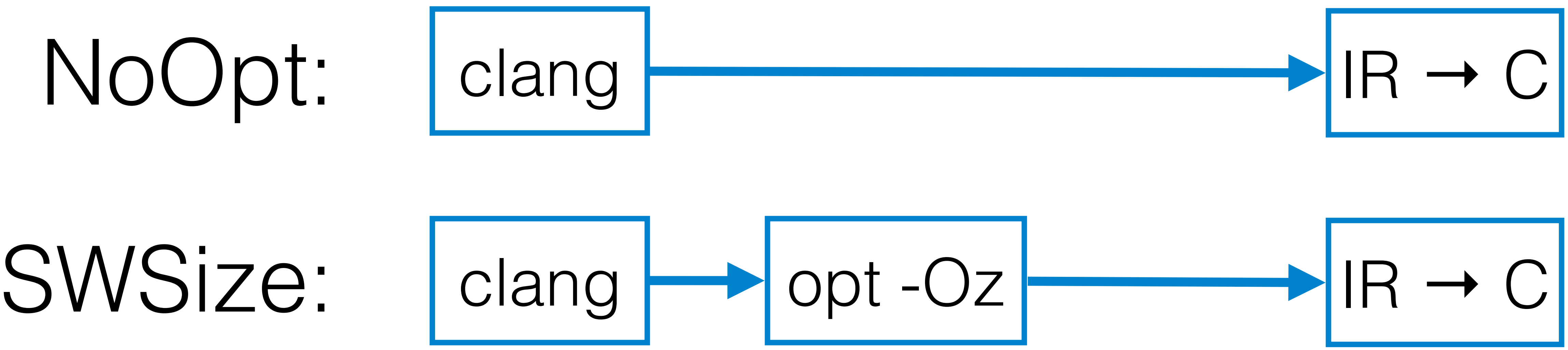
NoOpt:



Compilation flows

NoOpt:

Compilation flows



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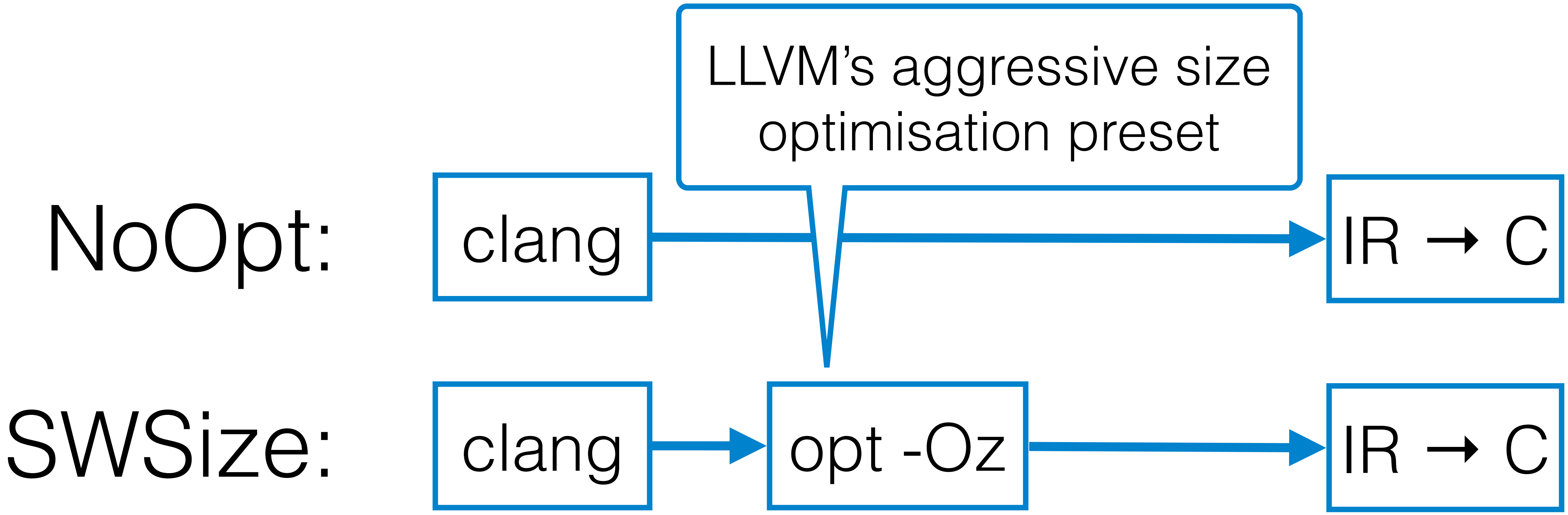

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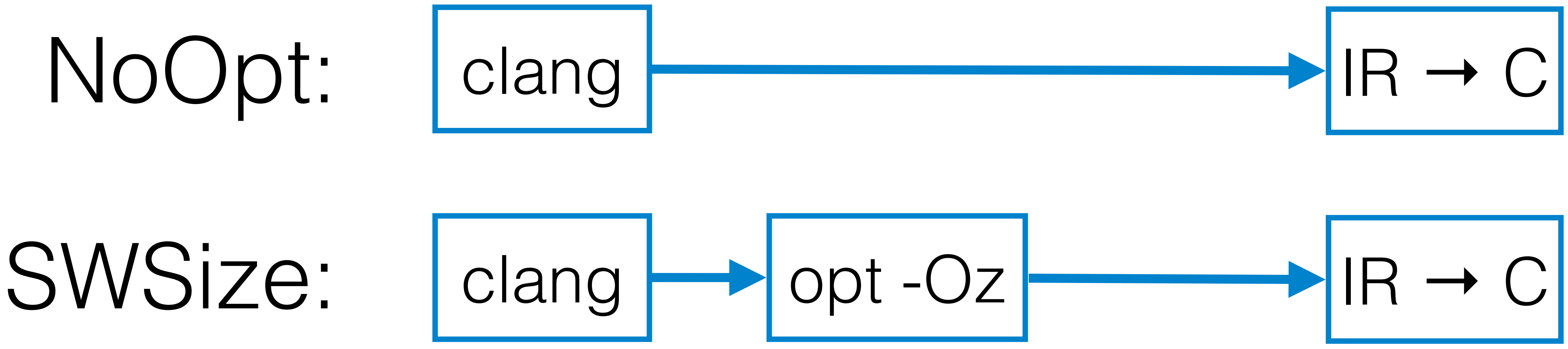

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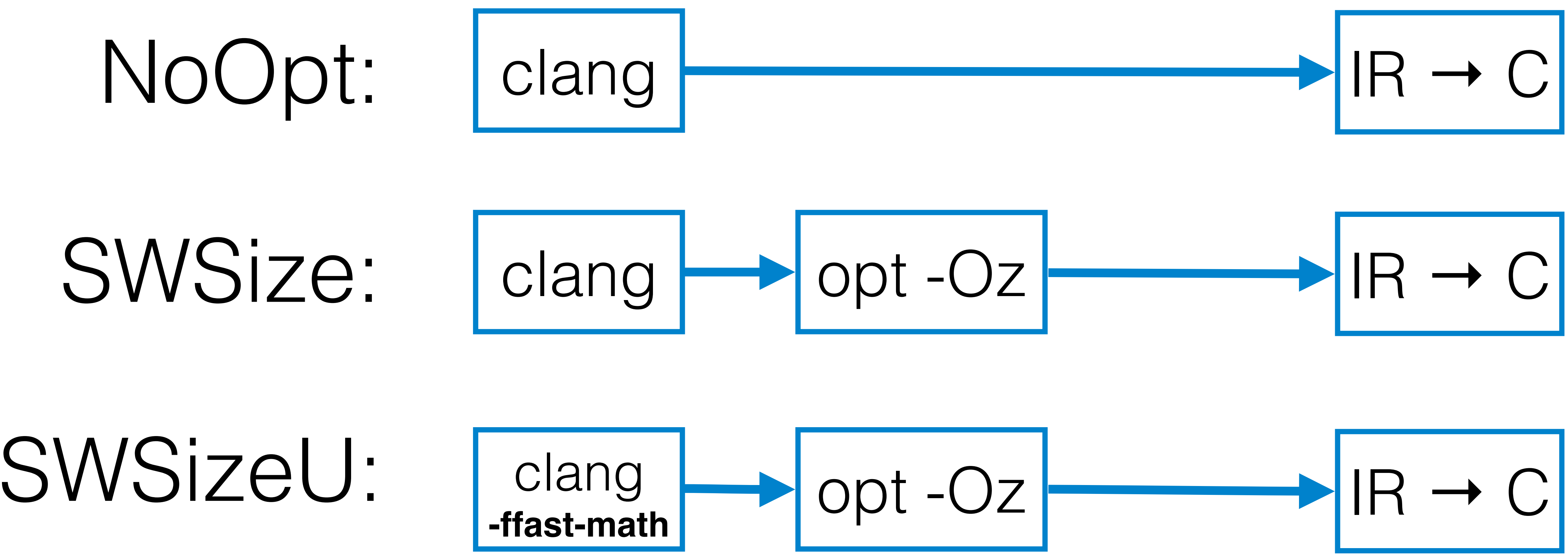

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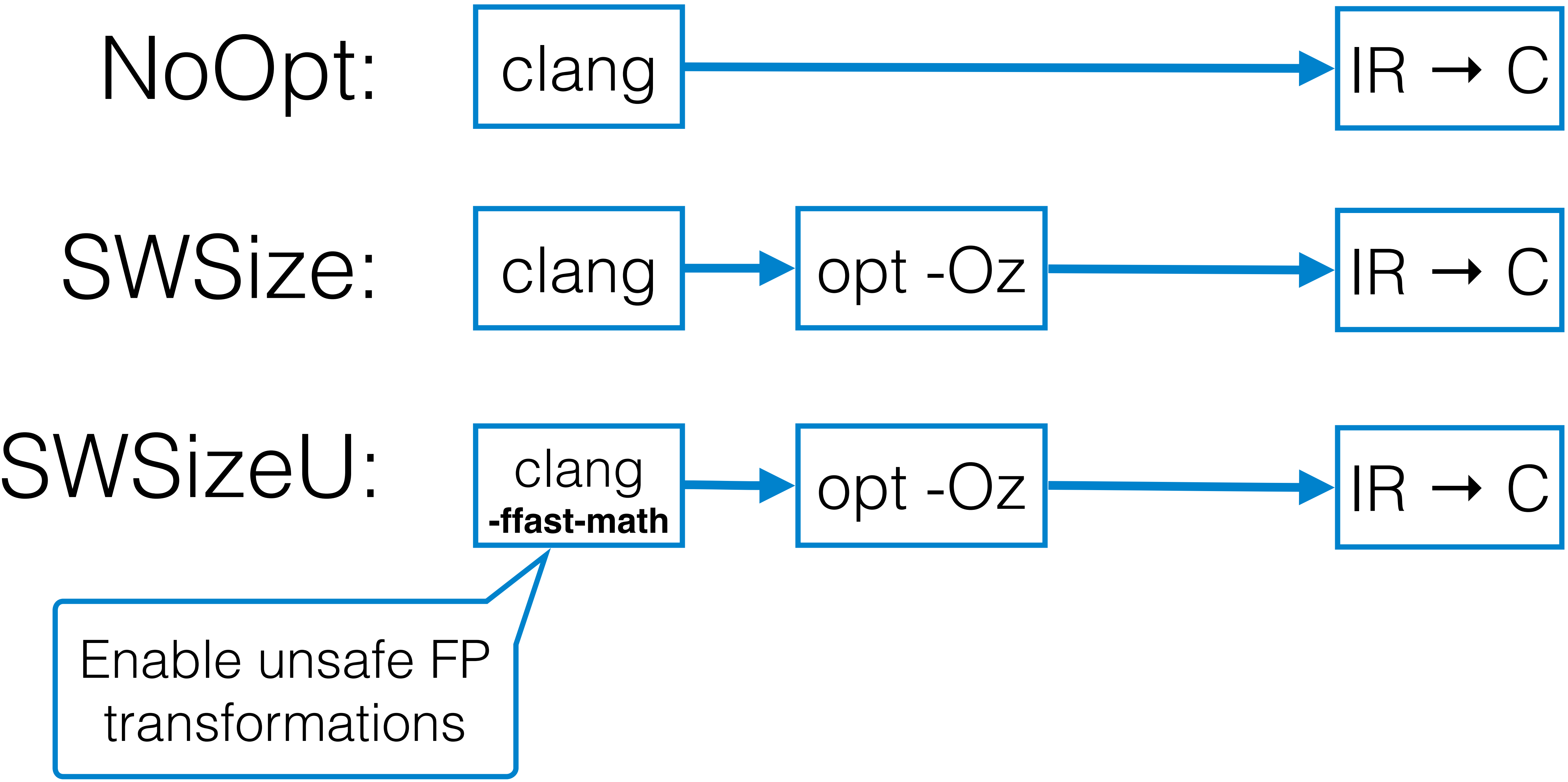

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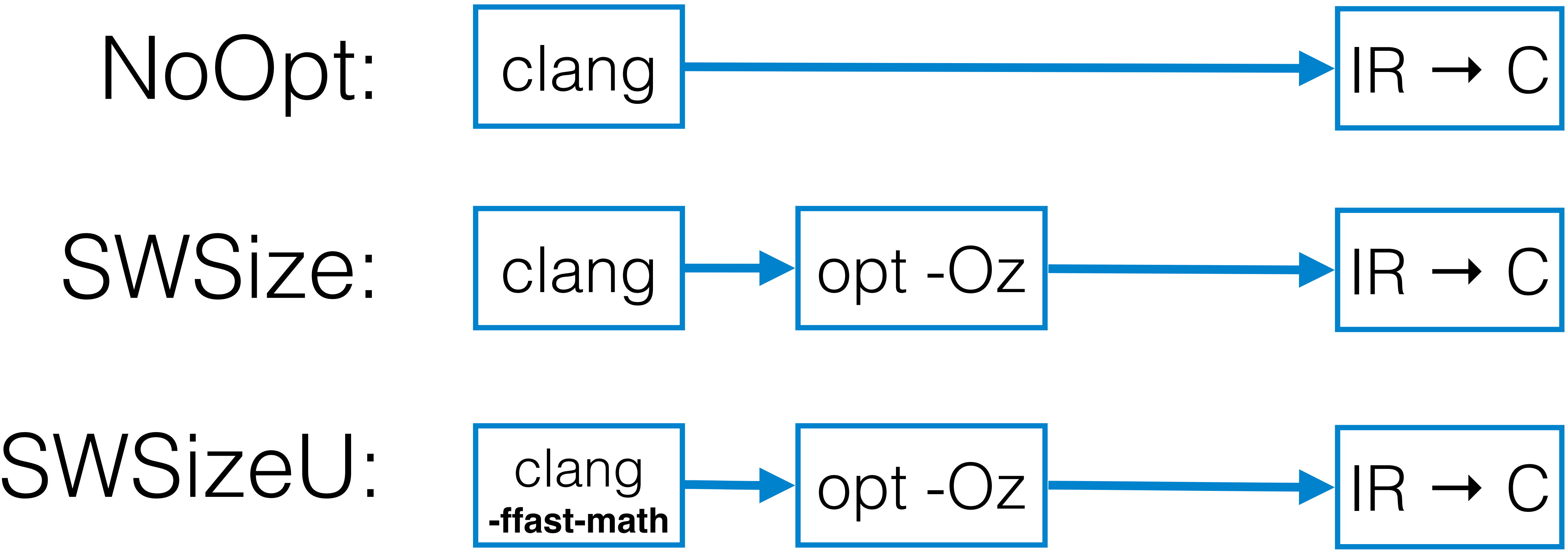

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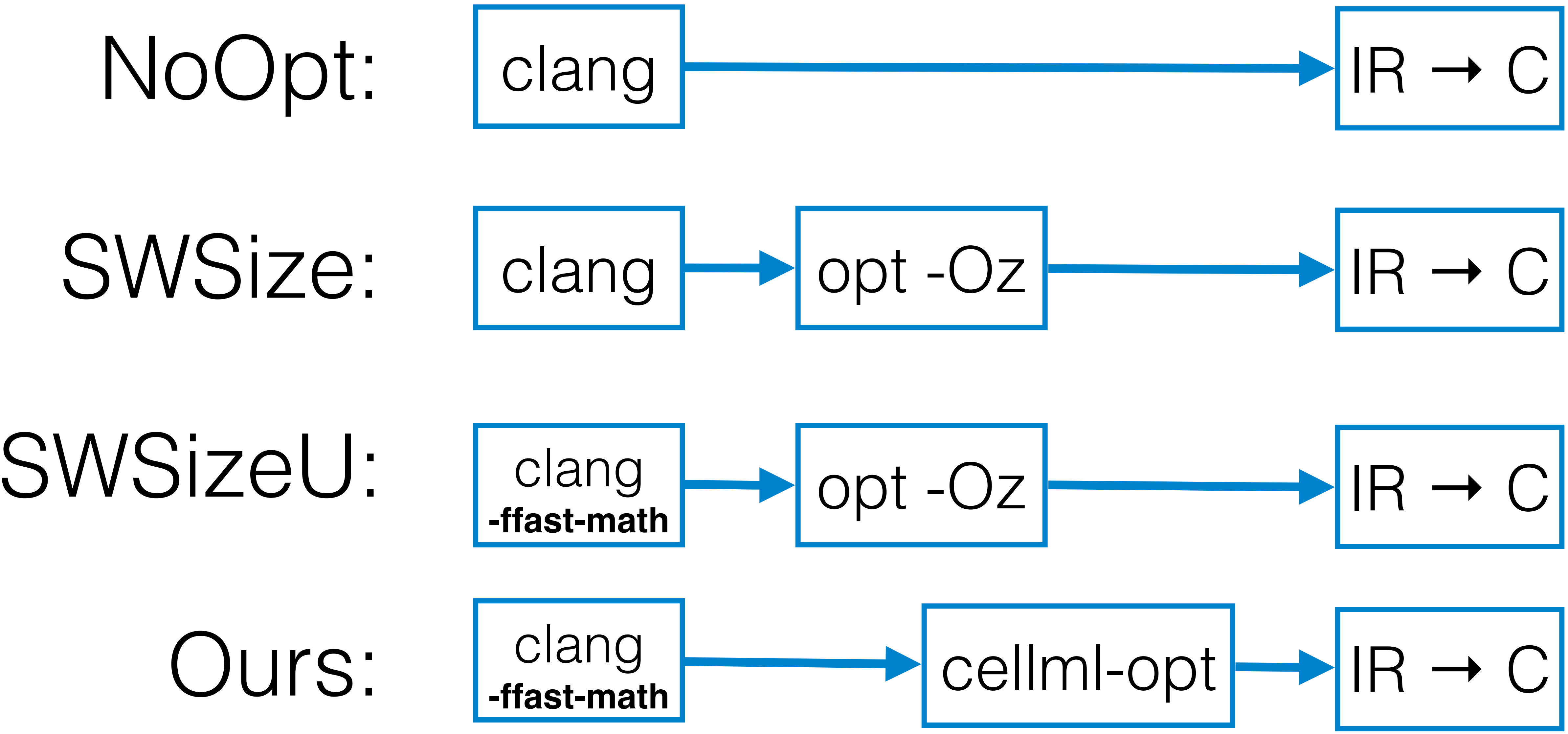

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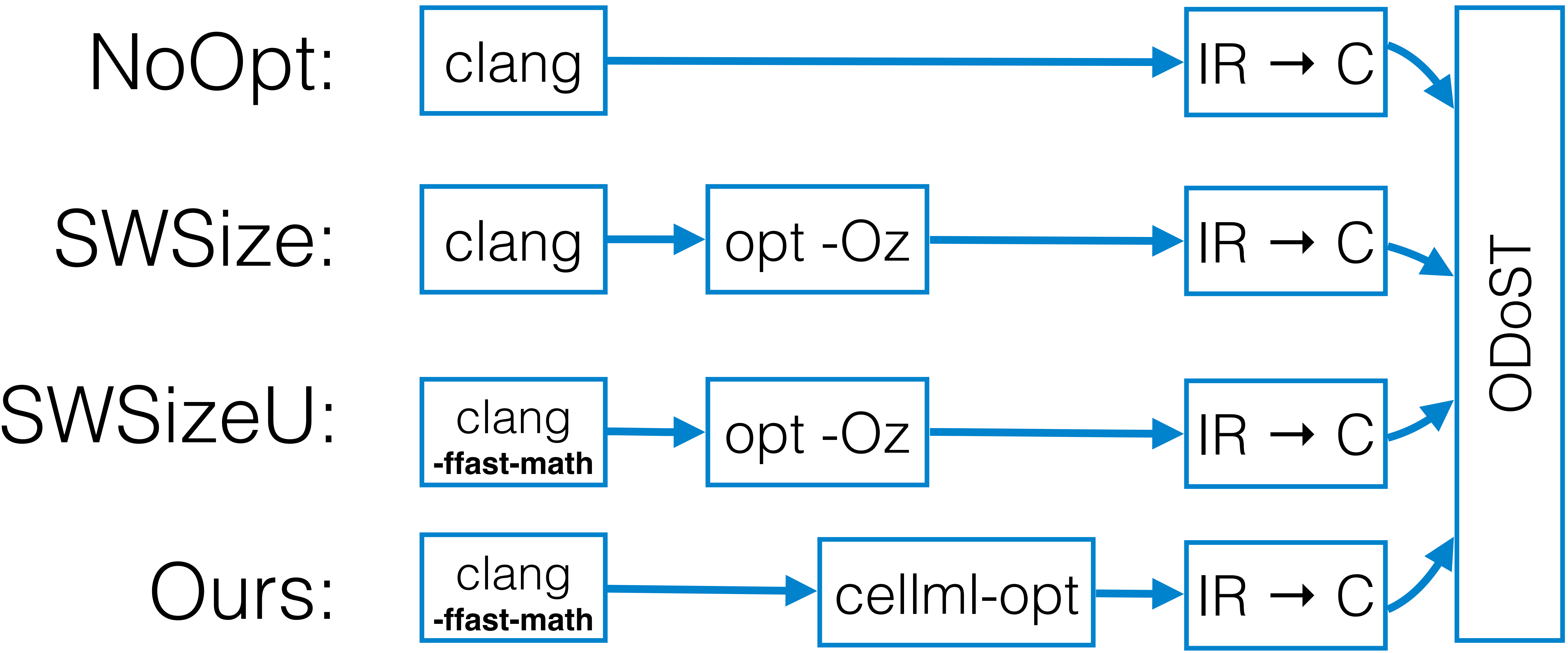
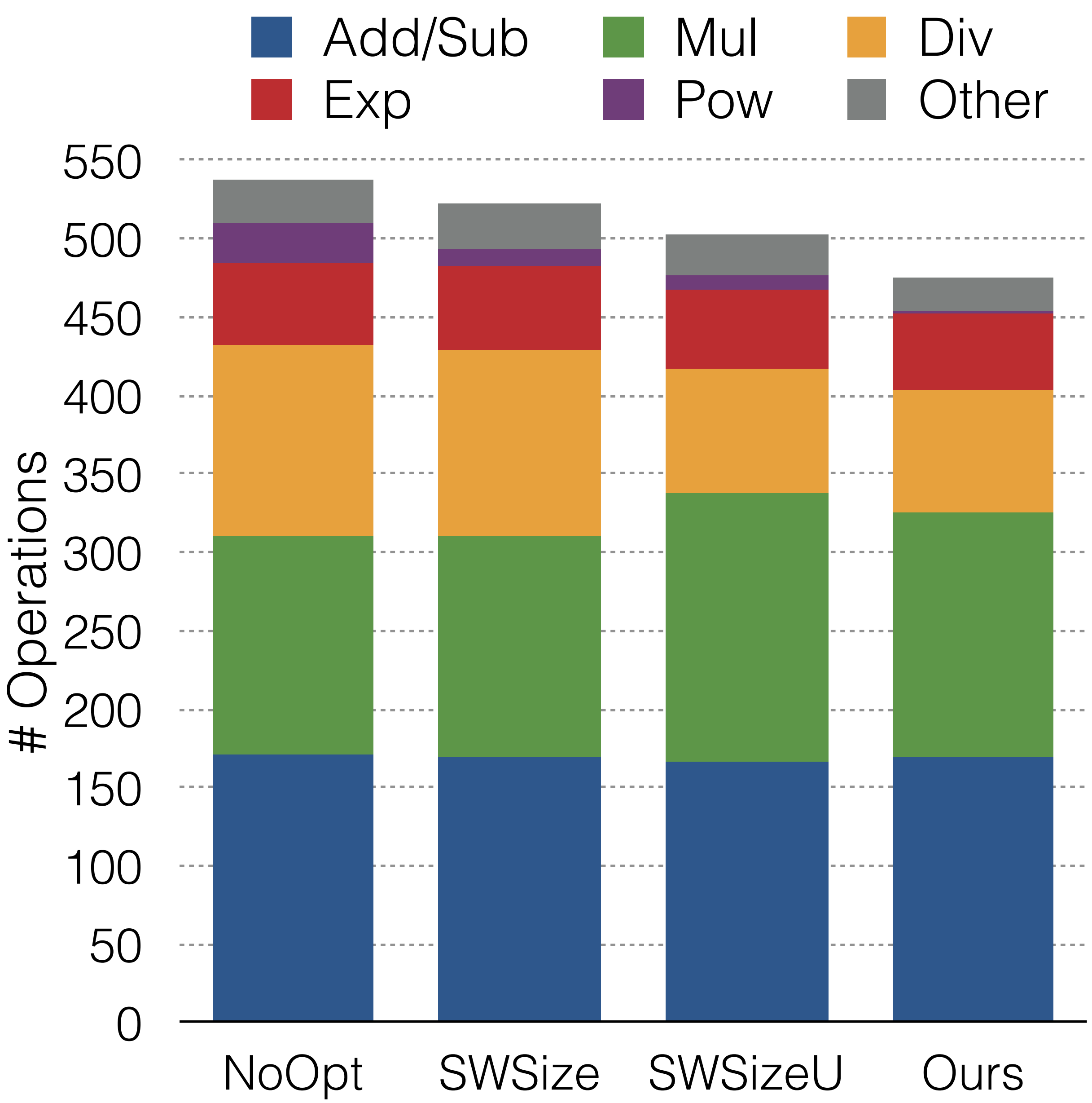


Error measurement

- Generic driver, 1000 integration steps of 1 μs each, starting at t = 1.0 s
- Compare computed values **before / after optimisation**, calculate relative error
- Certain, model specific deviation is acceptable
  - e.g. precision of “wet biology experiments” ~ 0.01 %

Ten Tusscher, K. H. W. J., Noble, D., Noble, P. J., & Panfilov, A. V. (2004). A model for human ventricular tissue.

Example model



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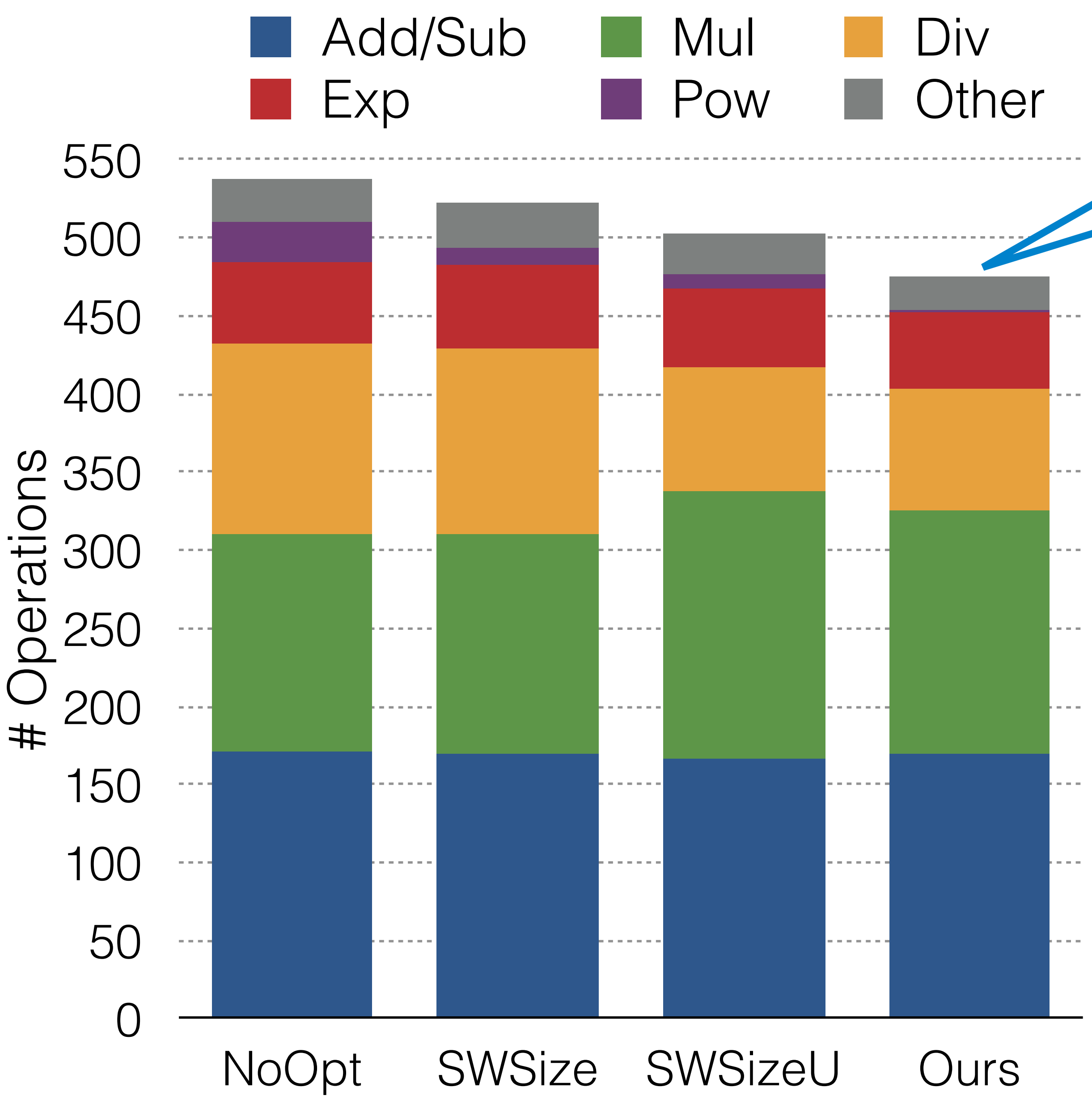

Least total number of operations

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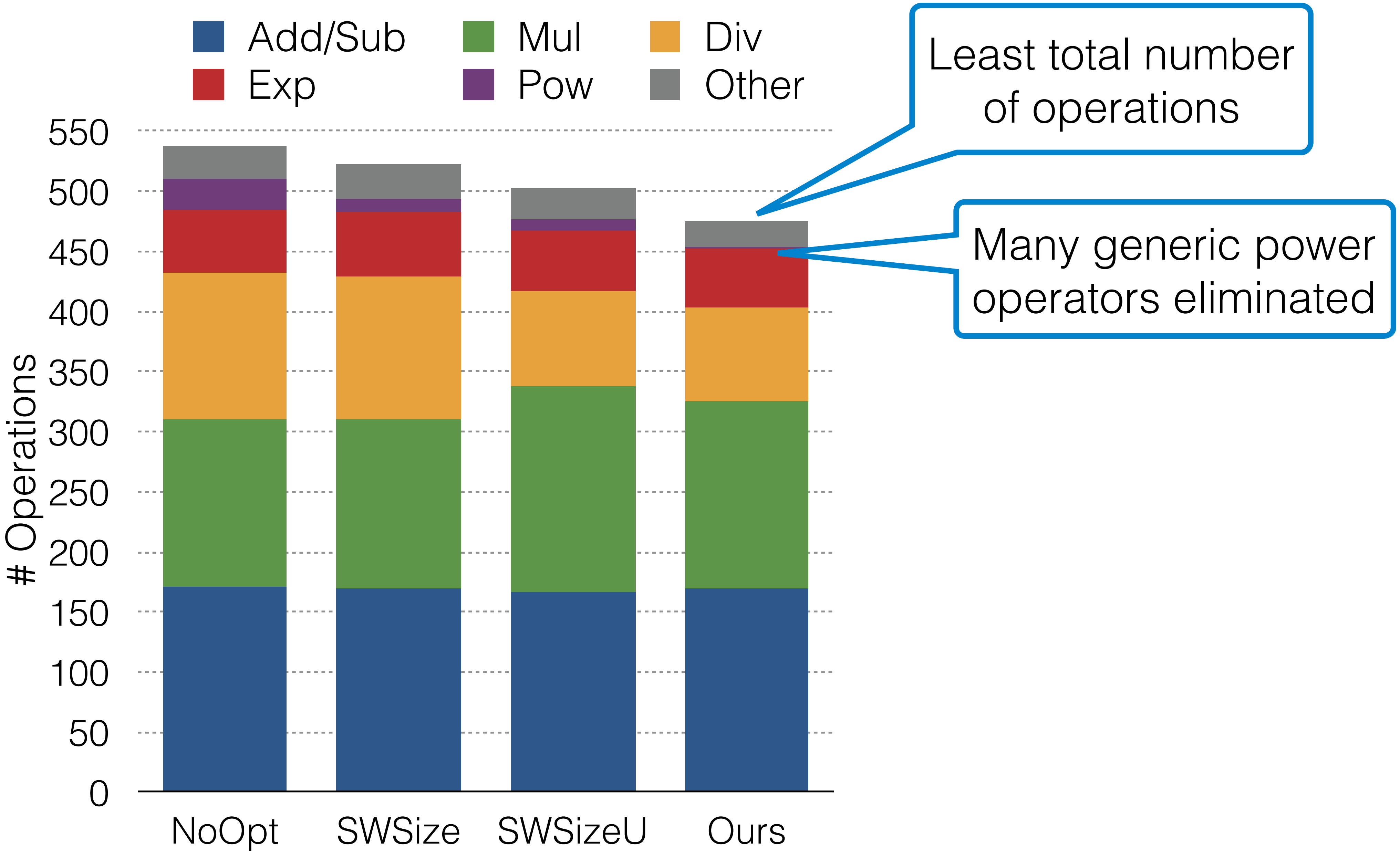

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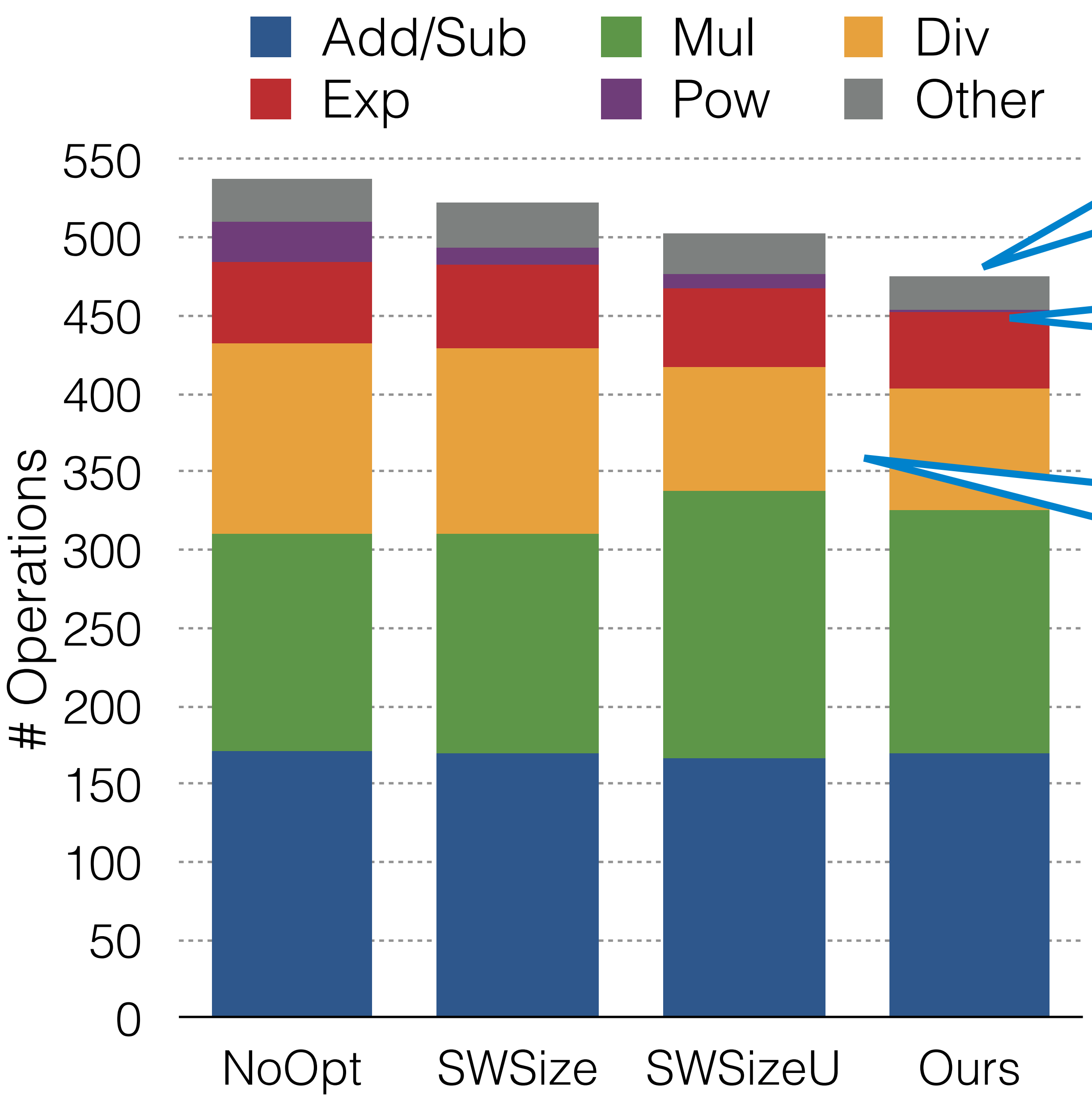

Least total number of operations

Many generic power operators eliminated

Transform many div to mul when unsafe FP is allowed

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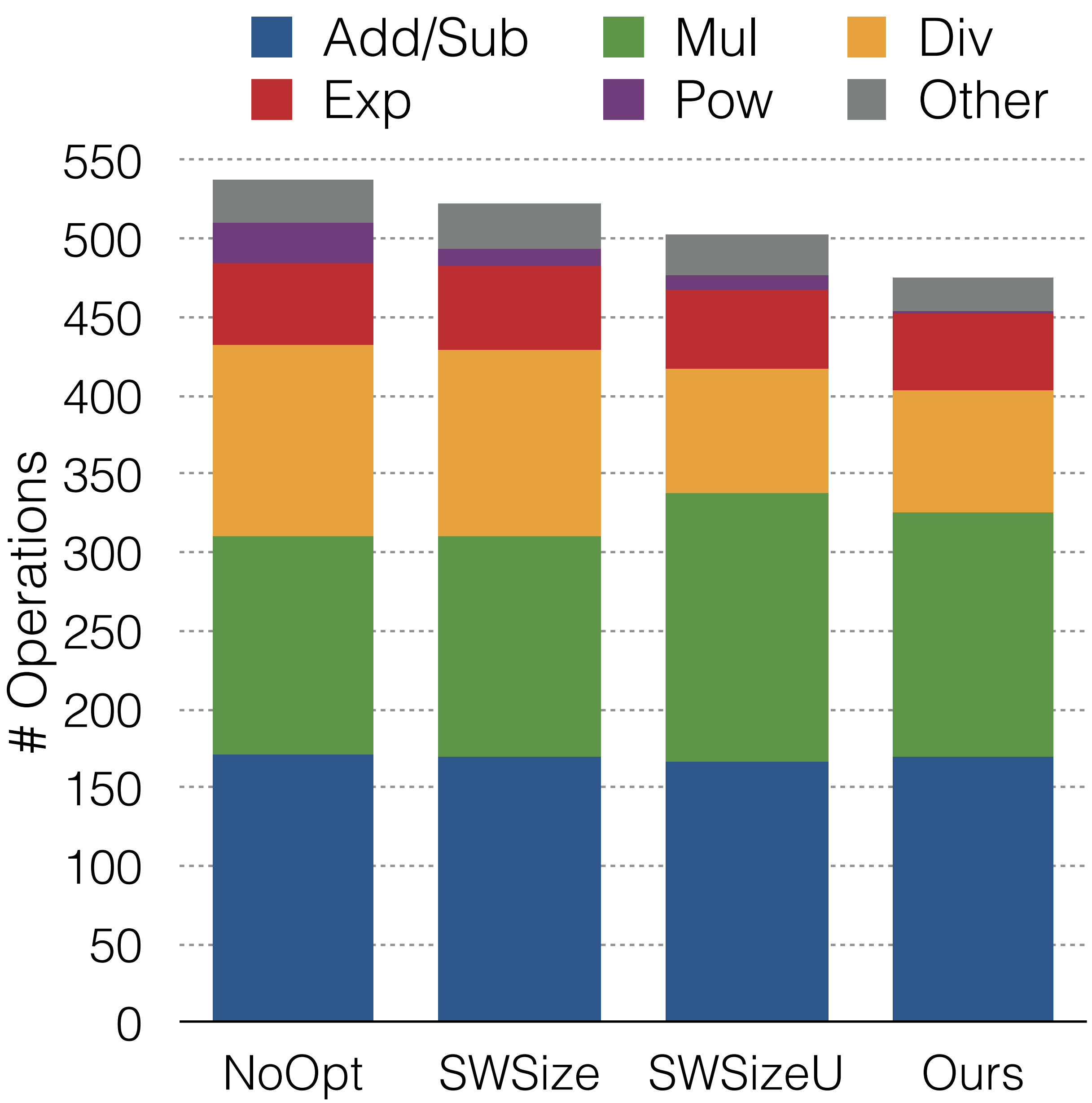

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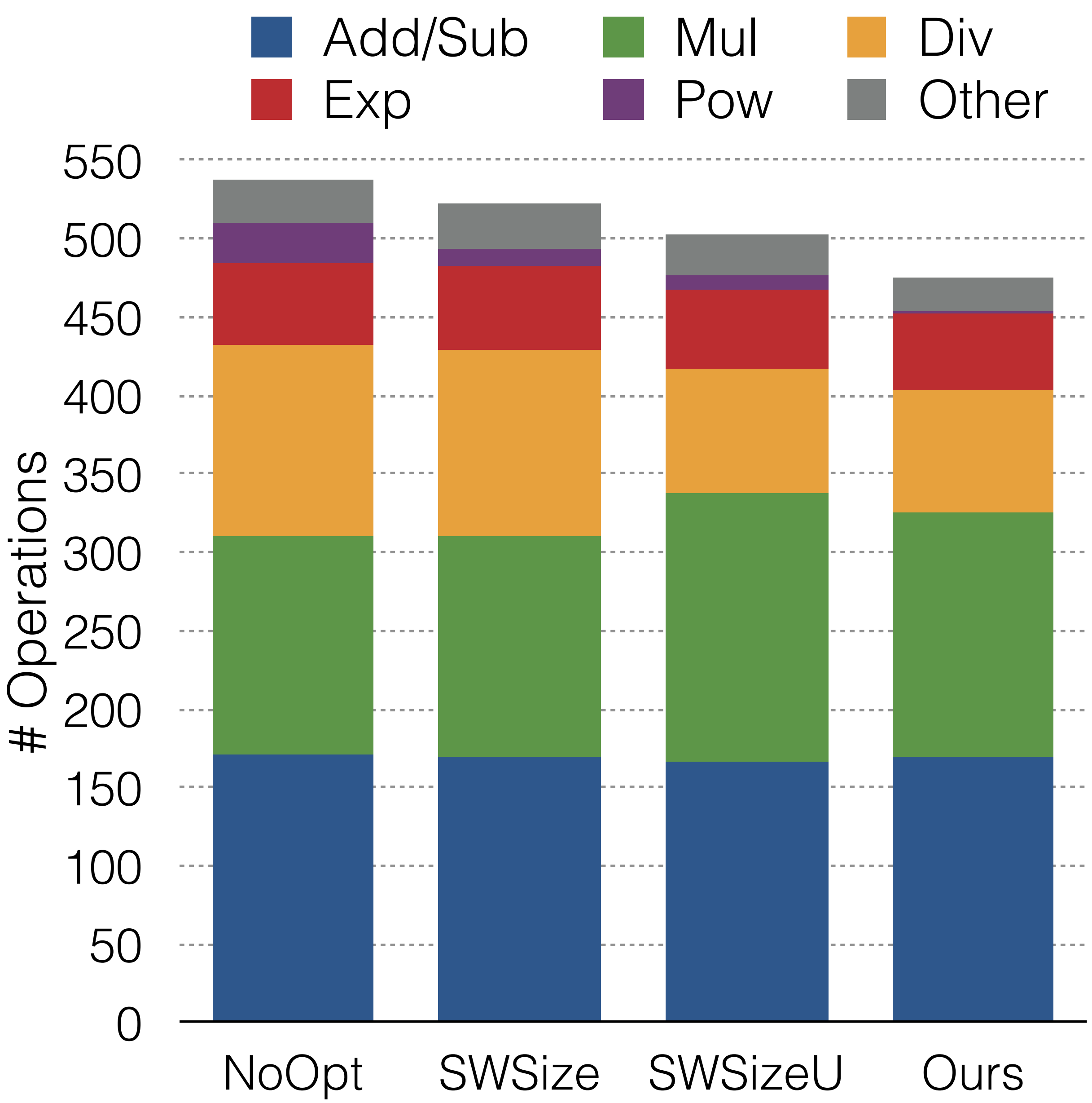

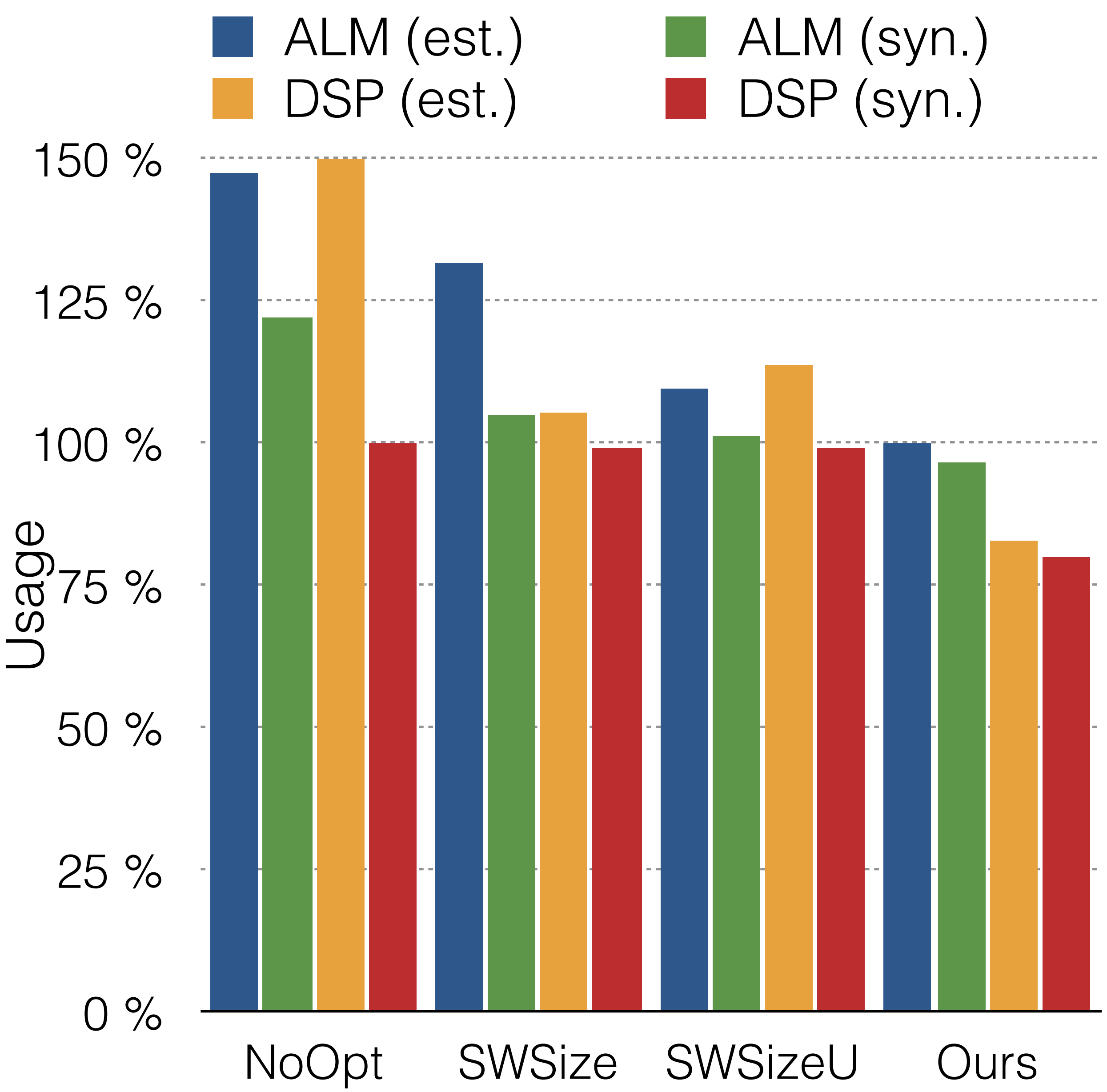

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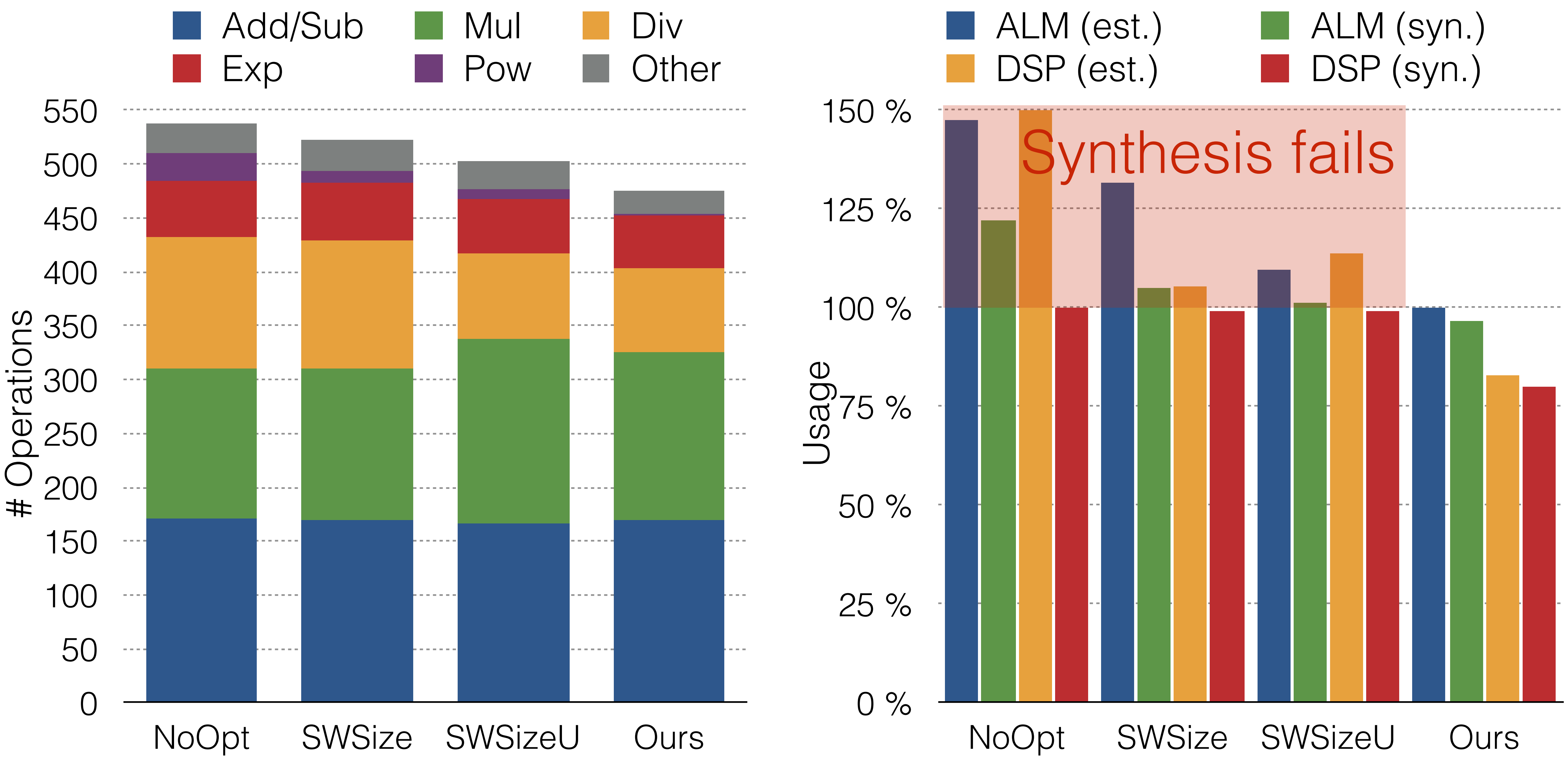

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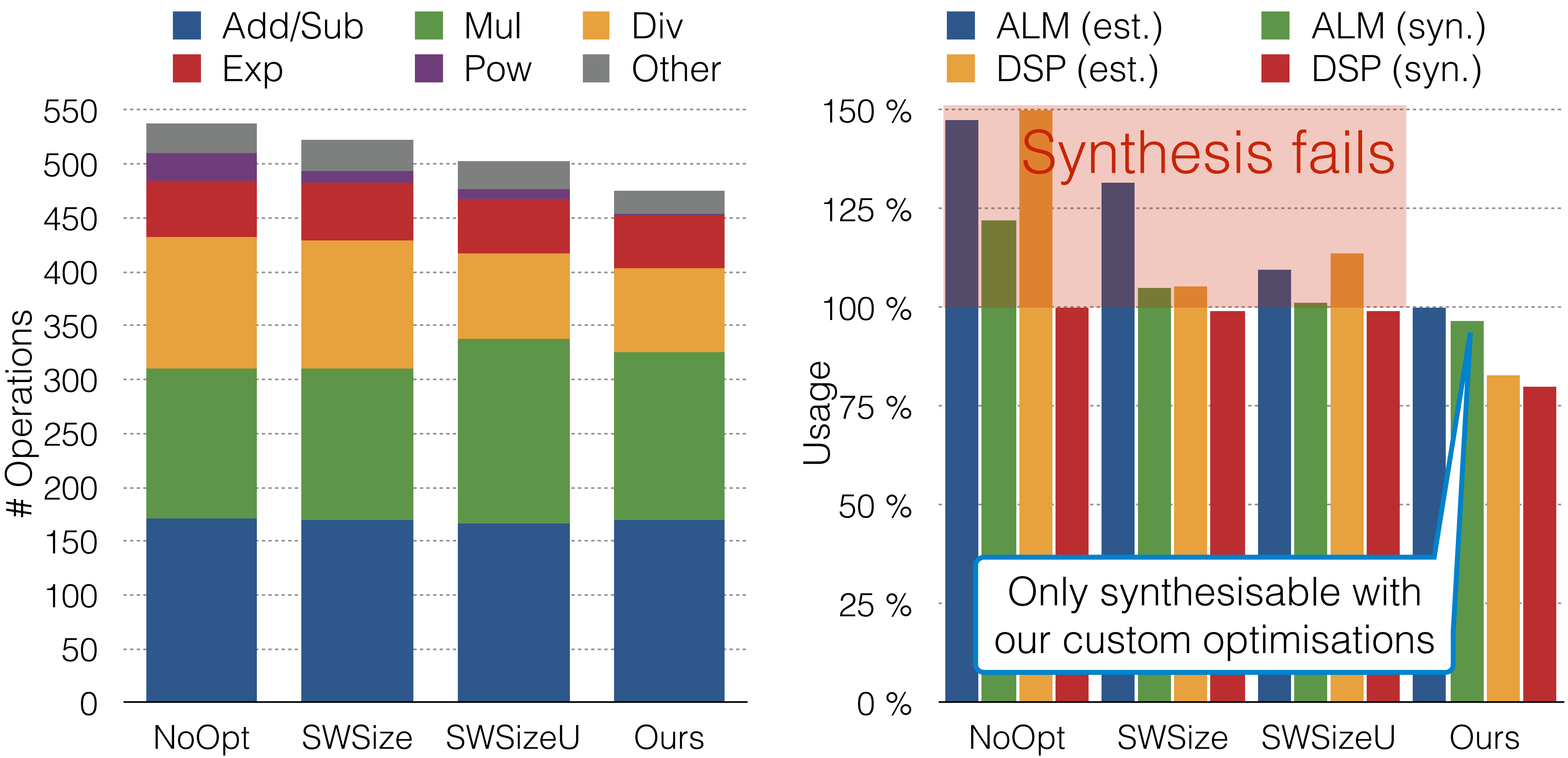

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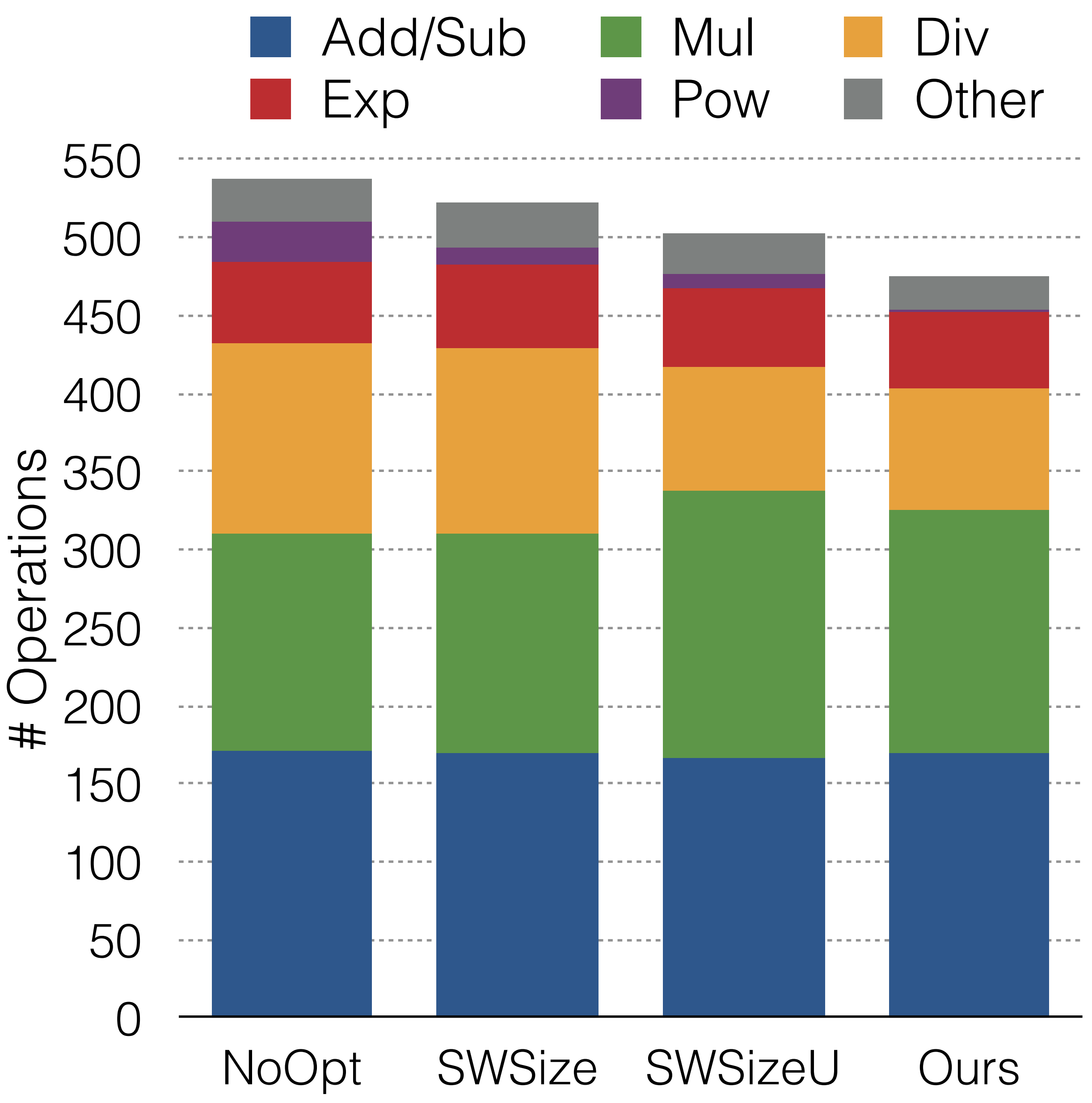

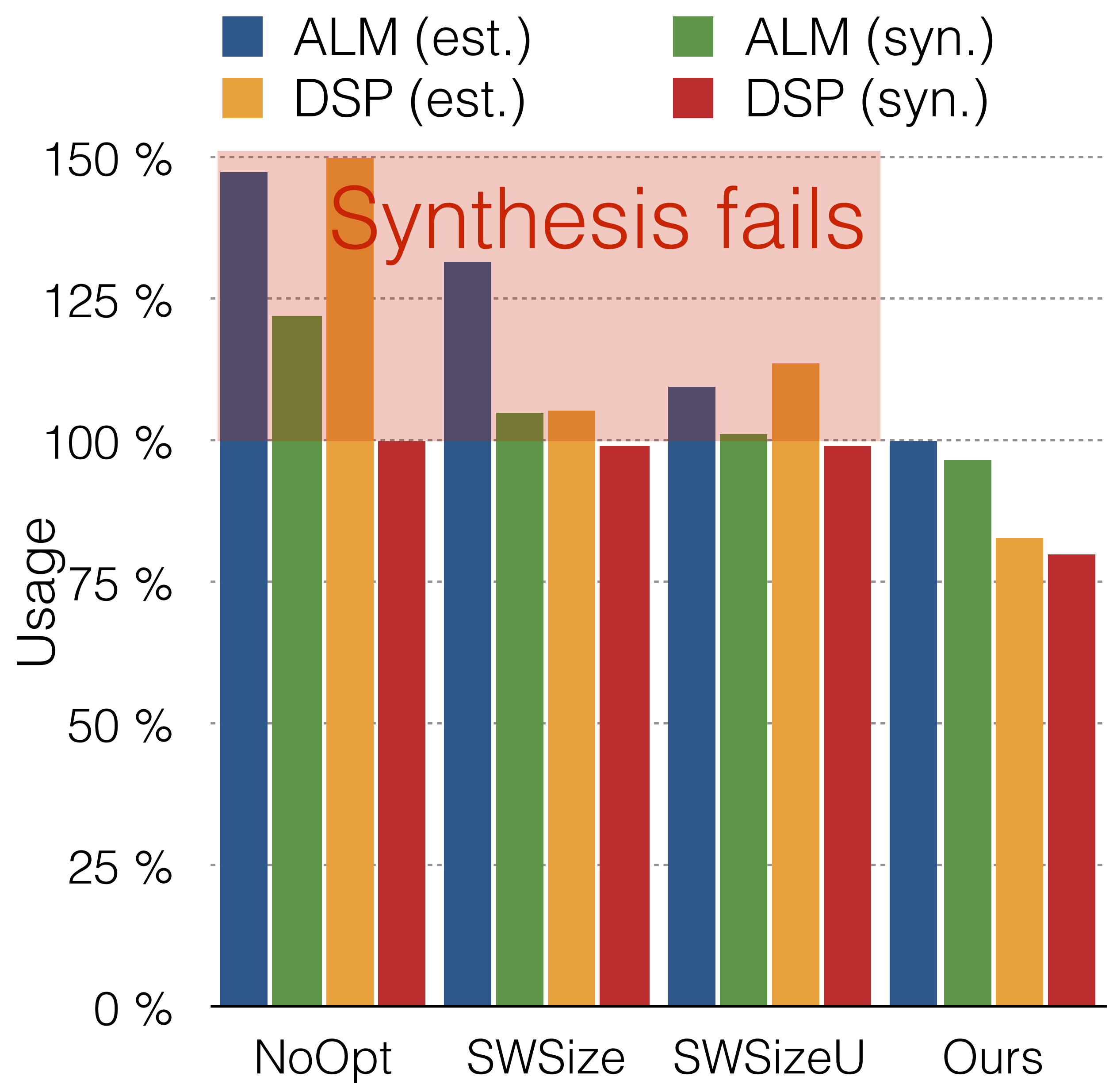

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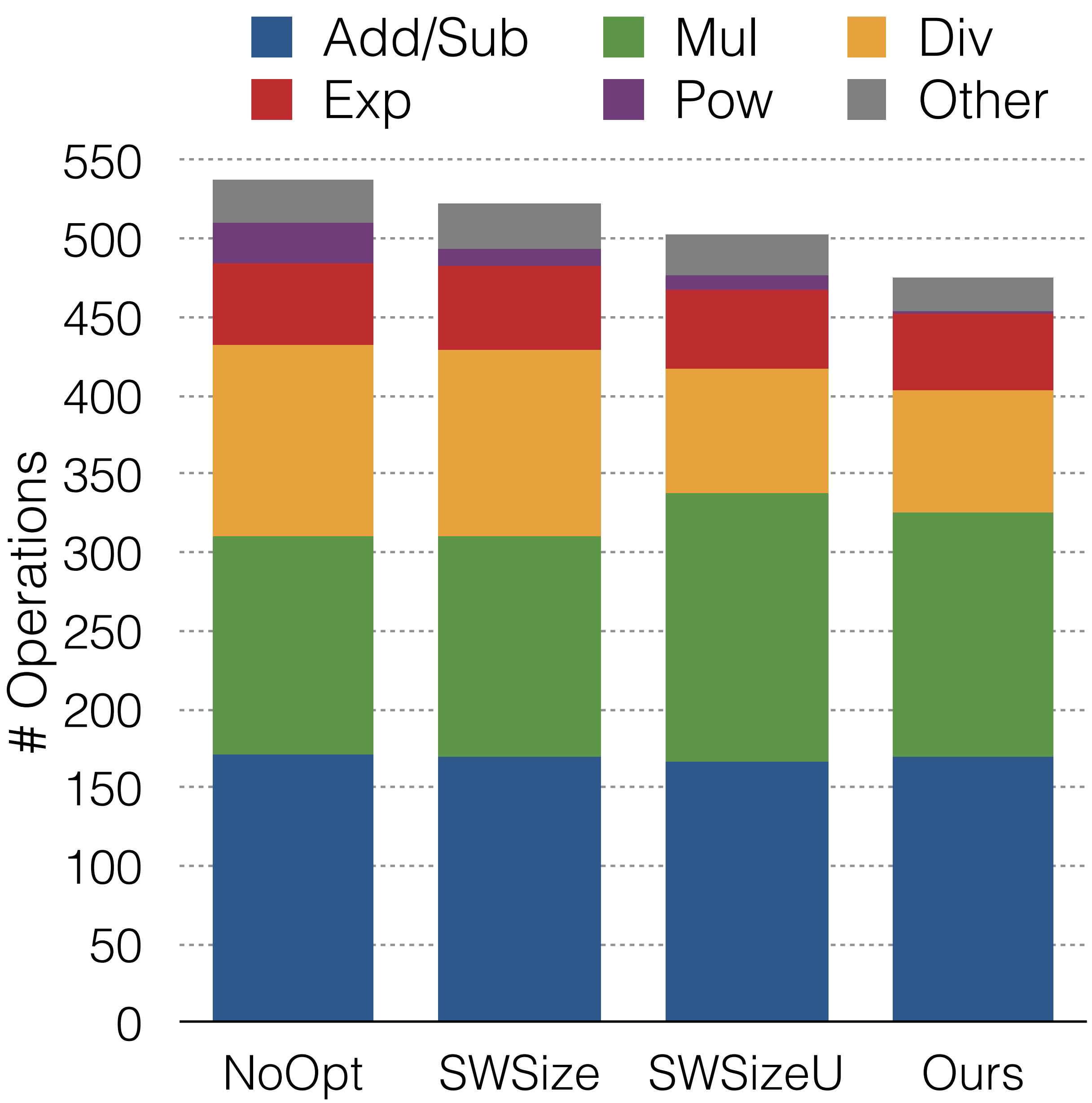

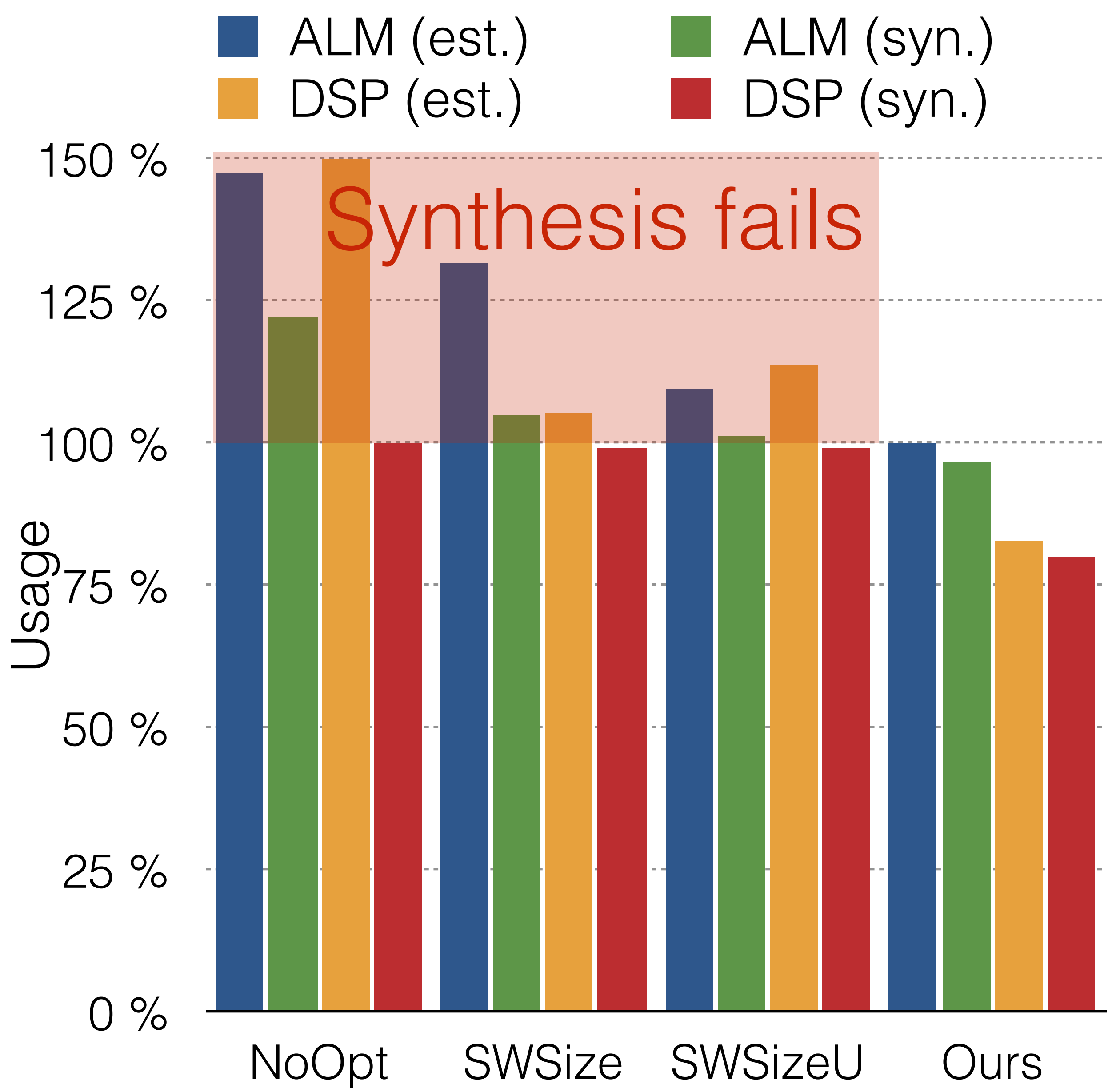

	SWSizeU	Ours
Rel. Err [%]	0.00054	0.0012
F_{max} [MHz]	-	111

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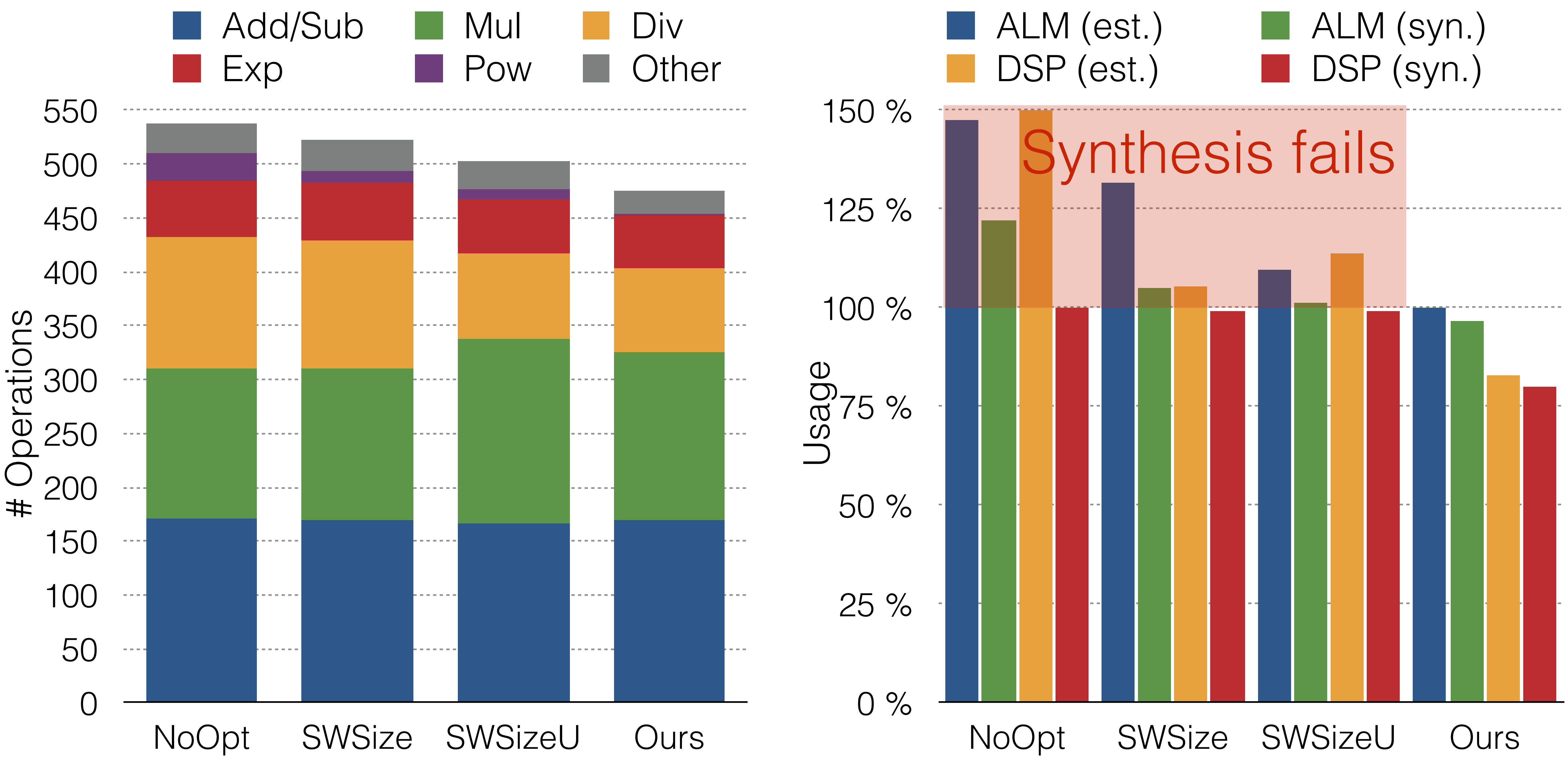

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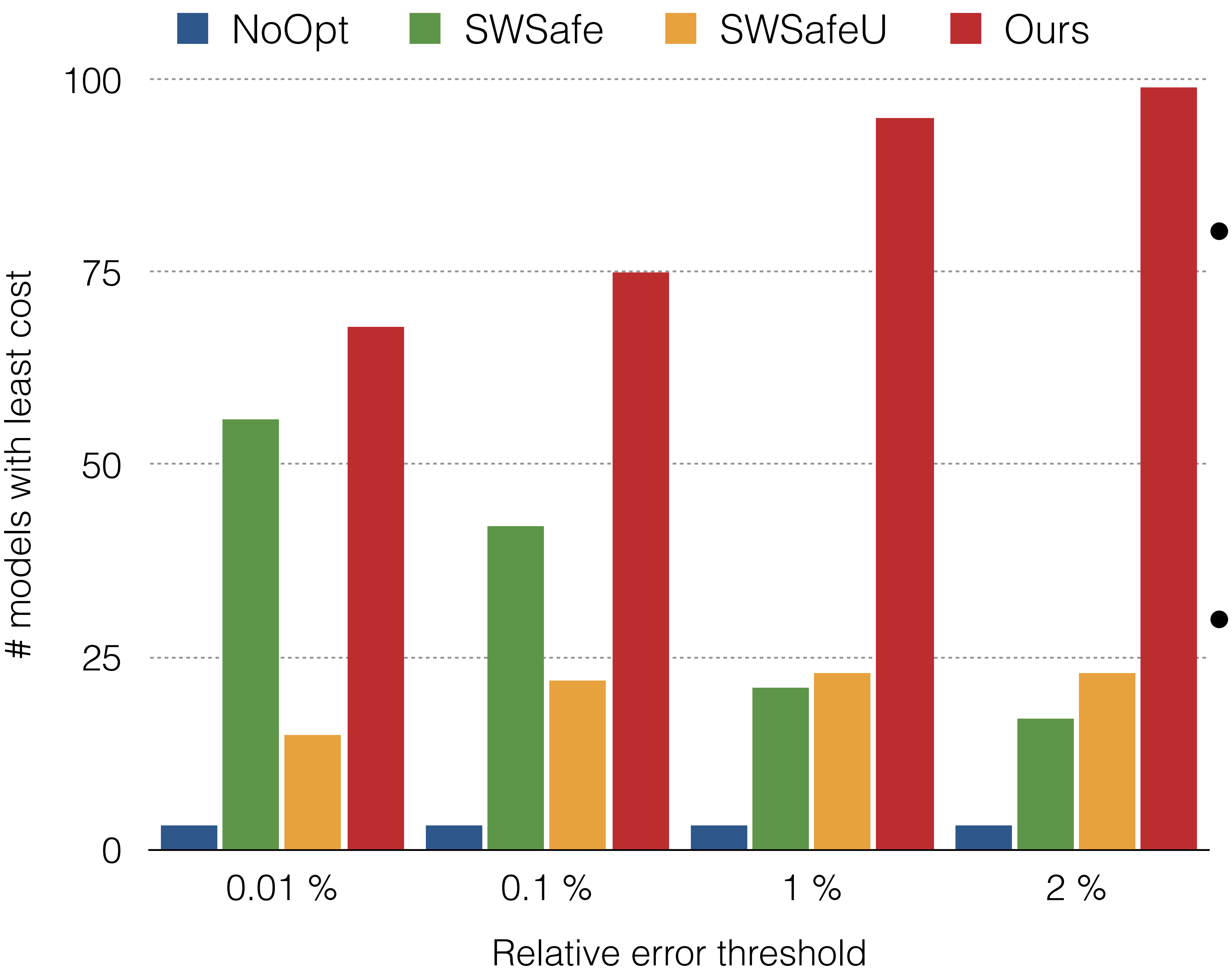
Slightly larger error

General applicability

- 146 models from the CellML repository
  (> 20 equations, operators available as intrinsics, converge in input interval, 2+ curation stars)
- 4 thresholds for maximum relative error per model
- Use the cost model to estimate impact of transformations

Least cost per flow



- Count models with least cost after optimisation with a given flow
- If error > threshold, fall-back to SWSafe

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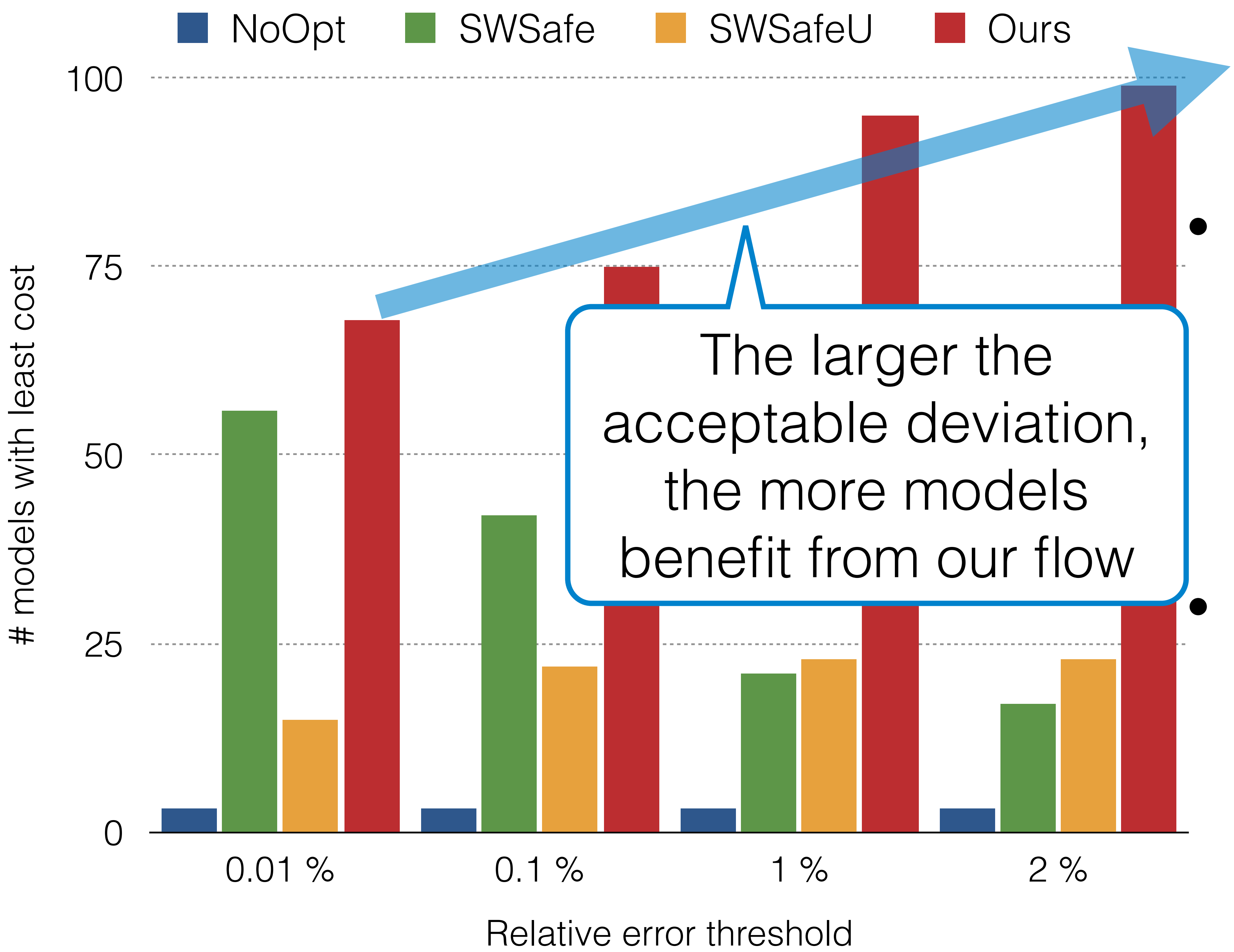

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Summary

- Size reduction after synthesis in 4 example models
  - Our recipe: up to 25 % less ALM, 20 % less DSP
  - Never worse than unoptimised (c.f. other flows)
- Broad applicability for domain-specific optimisations across 146 models

Future work

- Cost model served us well as quantitive instrument
  - Estimation of DSP usage ok
  - More accurate estimation of ALM demand needed
- A priori error analysis instead of empirical study

Thank you!