

# ML-Guided IBP Reduction

Neural Network Guided Integration-by-Parts Reduction of  
Feynman Integrals

Two-Loop Triangle-Box Topology

## The Problem

- ▶ **IBP reduction:** Express complex Feynman integrals as linear combinations of simpler “master” integrals
- ▶ **Challenge:** Exponential search space of IBP identities
- ▶ **Traditional approaches:** Laporta algorithm, Kira, FIRE

# Triangle-Box Topology

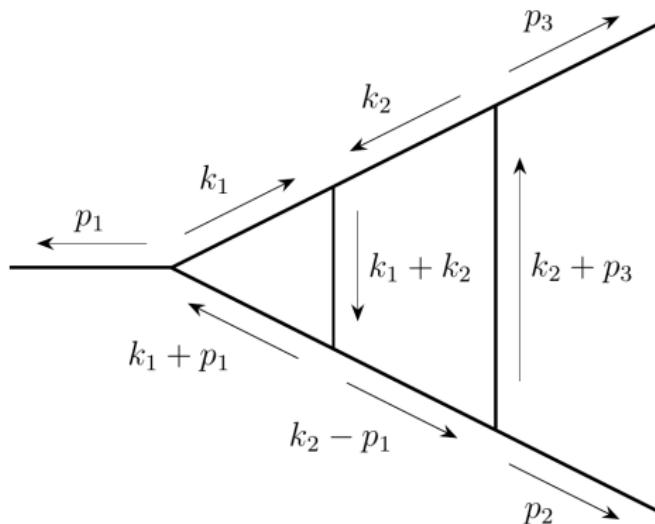


Figure 1: Triangle-Box Feynman Diagram

*Two-loop integral with 6 propagators + 1 ISP. From arXiv:2502.05121.*

# Propagators and ISP

6 Propagators (denominators)

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$$\begin{array}{lll} D_1 = k_1^2 & D_2 = k_2^2 & D_3 = (k_1 + k_2)^2 \\ \hline D_4 = (k_1 + p_1)^2 & D_5 = (k_2 + p_3)^2 & D_6 = (k_2 - p_1)^2 \end{array}$$

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1 ISP (irreducible scalar product)

$D_7 = (k_1 + p_3)^2$  — needed to complete basis, appears in numerator

# Integral Notation

$$I[a_1, a_2, a_3, a_4, a_5, a_6, a_7]$$

$$I(a_1, \dots, a_7) = \int \frac{d^D k_1 d^D k_2}{\prod_{i=1}^7 D_i^{a_i}}$$

## Index Meaning

- ▶  $a_i > 0$ : **propagator** in denominator (power  $a_i$ )
- ▶  $a_i < 0$ : **numerator** insertion (ISP to power  $|a_i|$ )
- ▶  $a_i = 0$ :  $D_i$  absent

## Example

$$I[1, 1, 1, 1, 1, 1, -3] = \text{top sector integral with } D_7^3 \text{ in numerator}$$

# Kinematics and Masses

## External Masses

- ▶  $p_1^2 = m_1^2, p_2^2 = m_2^2, p_3^2 = m_3^2$
- ▶ Physics depends on ratios  $m_2/m_1, m_3/m_1$

## Our Numerical Setup

- ▶ Work over **finite field**  $\mathbb{F}_p$  with  $p = 1009$
- ▶ Fixed random values:  $d = 41, m_1 = 1, m_2 = 31, m_3 = 47$
- ▶ Exact integer arithmetic (no floating point errors)

# IBP Identities

## Source

Integration by parts under the integral sign:

$$0 = \int d^D k_1 d^D k_2 \frac{\partial}{\partial k_l^\mu} \frac{q^\mu}{\prod_i D_i^{a_i}}$$

## For Triangle-Box

- ▶ **8 IBP operators:** 2 loop momenta  $\times$  4 vectors  
 $\{k_1, k_2, p_1, p_2\}$
- ▶ **1 LI identity:** from Lorentz invariance
- ▶ Each identity relates integrals with shifted indices  $a_i$

## Result

All integrals reduce to **16 master integrals**

# The Memory Wall

Traditional IBP codes hit **memory limits** as integrals grow more complex:

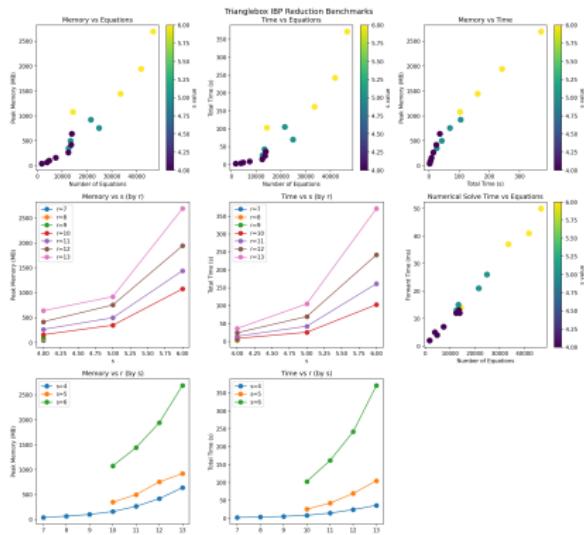


Figure 2: Kira Memory Scaling

*Kira benchmarks: Memory grows exponentially with integral weight ( $r$ ), reaching 2.5+ GB for  $r=13$ .*

## Our Solution

- ▶ **ML-guided beam search:** Train a neural network to score IBP actions
- ▶ **Hierarchical reduction:** Process sectors from highest to lowest
- ▶ **Parallel execution:** Distribute across Condor cluster for ~10x speedup
- ▶ **Constant memory:** Each one-step reduction is independent - no system accumulation

# The Action Space: Key Innovation

## Why Traditional IBP is Hard

- ▶ Infinite possible IBP identities (any seed, any operator)
- ▶ No clear way to choose which identity to apply
- ▶ Laporta: build giant linear system, solve globally

## Our Approach: Finite Action Space

- ▶ Restrict to actions that **solve for a specific target integral**
- ▶ Each action = (IBP operator, seed shift)
- ▶ Enumerate only **valid actions** that eliminate the target
- ▶ Enables ML: classification over finite action set

## Action Representation

Action = (ibp\_op, delta)

- ▶ **ibp\_op**: Which IBP/LI operator (0-15)
- ▶ **delta**: Shift from target to seed integral

## Example

Target:  $I[2,0,1,0,1,1,0]$ , Action: (3, (-1,0,0,0,0,0,0))

IBP eq (op=3, seed=[1,0,1,0,1,1,0]):

$$c_1 \cdot I[2,0,1,0,1,1,0] + c_2 \cdot I[1,0,1, \dots] + \dots = 0$$

↑ target

Solve for target → express in terms of simpler integrals

# Direct vs Indirect Actions

## Direct Actions

- ▶ Target appears directly in the raw IBP equation
- ▶ Straightforward: apply IBP, solve for target

## Indirect Actions (Key Innovation)

- ▶ Target does **not** appear in raw IBP equation
- ▶ But appears **after applying substitutions** from previous steps

Raw IBP:  $c_1 \cdot I[A] + c_2 \cdot I[B] = 0$  (no target)

After subs:  $c_1 \cdot I[A] + c_2 \cdot (\dots + c_3 \cdot I[\text{target}] + \dots) = 0$   
↑ target appears!

Indirect actions leverage reduction history for deeper reductions

# Subsector Filtering

## The Problem

Arbitrary IBP actions can introduce integrals in **higher sectors** → explosion

## Solution: Subsector Constraint

Only allow actions where all resulting integrals are in **subsectors** of target

## Sector Hierarchy

Sector 63 [1,1,1,1,1,1] (6 propagators)

↓ subsectors

Sector 62 [0,1,1,1,1,1] (5 propagators)

Sector 61 [1,0,1,1,1,1] (5 propagators)

↓

...lower sectors...

**Result:** Reductions flow downward through sector hierarchy

# Why This Works

## Finite + Learnable

- ▶ Typically 10-100 valid actions per state
- ▶ Model learns which actions lead to successful reductions

## Hierarchical Structure

- ▶ Subsector filtering ensures monotonic progress
- ▶ Never introduces integrals harder than current target

## Substitution Chains

- ▶ Indirect actions enable multi-step reasoning
- ▶ Model implicitly learns useful substitution patterns

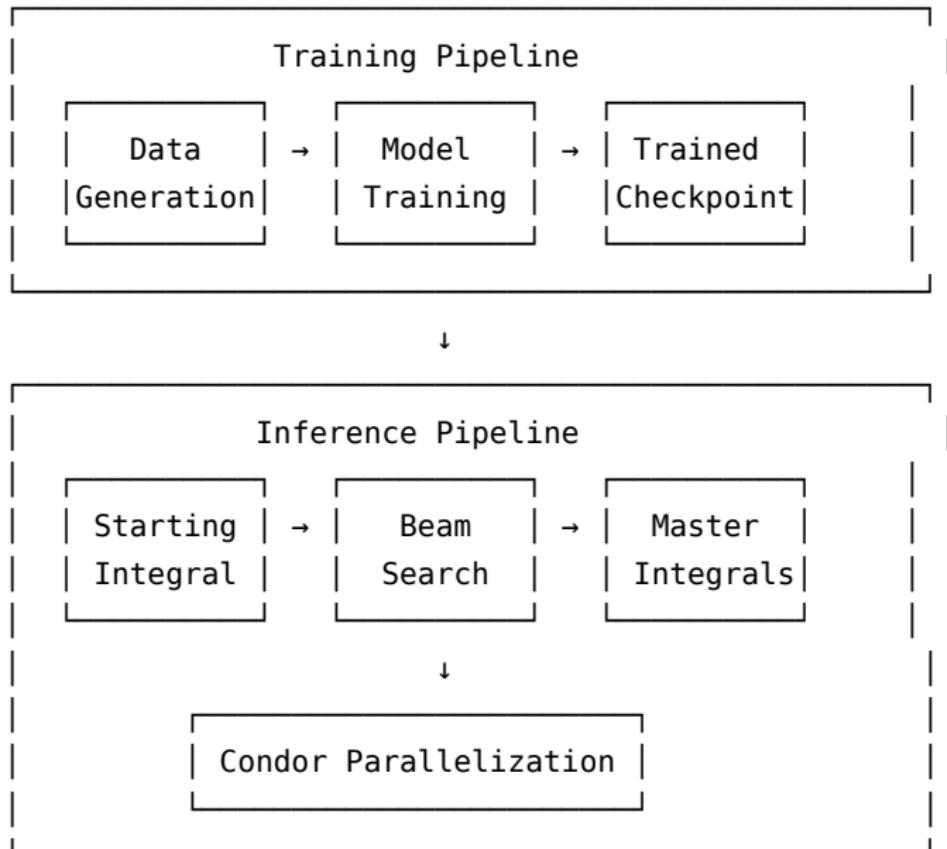
## Key Results

### Triangle-Box Topology (arXiv:2502.05121)

Integral	Weight	Seq.	Par.	Speedup	Masters
$I[2,0,2,0,1,1,0]$	(6,0)	5 min	-	-	4
$I[1,1,1,1,1,1,-3]$	(6,3)	73 min	12 min	6x	16
$I[3,2,1,3,2,2,-6]$	(13,6)	<b>~20 hr</b>	<b>115 min</b>	<b>~10x</b>	16

- ▶ Results match Kira exactly
- ▶ Reduces to exact 16 paper masters from arXiv:2502.05121

# System Architecture



## Part 1: Data Generation

# Data Generation: Two-Phase Approach

## Phase 1: Scrambling

1. Choose a **random sector** from 63 non-trivial sectors
2. Start from random linear combination of **that sector's masters**
3. Apply random IBP identities to increase complexity
4. **Record** each IBP used:  $[(op_1, seed_1), (op_2, seed_2), \dots]$
5. Only use IBPs that stay within target sector (no higher sectors)

## Phase 2: Unscrambling (Oracle)

Replay the scramble in reverse to generate training samples

# Unscrambling: Step by Step

At each step:

1. Find **target** = highest-weight non-master in expression
2. Look up which recorded IBP can eliminate target (**oracle**)
3. Enumerate **all valid actions** that could eliminate target
4. Record training sample: (expr, target, valid\_actions, oracle\_choice)
5. Apply action: add target → solution to substitutions
6. Repeat until only masters remain

Key: Oracle provides perfect labels

- ▶ No expensive search needed — answer comes from scramble record
- ▶ Model learns to predict oracle's choice among valid alternatives

# Data Generation: Coverage

## Sector Coverage

- ▶ All 63 non-trivial sectors covered
- ▶ Uses 16 paper masters for their respective sectors
- ▶ Uses corner integrals for remaining sectors

## Dataset Statistics

Split	Samples	Size
Train	946,168	3.8 GB
Validation	118,271	480 MB
Test	~118,000	480 MB

# Data Format

Each training sample contains:

```
{  
    'sector_mask': [1,0,1,0,1,1],  # 6-bit sector encoding  
    'expr': [                      # Current expression  
        ([1,0,2,0,1,1,0], 107),     # (integral, coefficient)  
        ([1,0,1,0,1,1,0], 303),  
        ...  
    ],  
    'subs': [                      # Substitution history  
        (key_integral, [(repl_int1, coeff1), ...]),  
        ...  
    ],  
    'target_integral': [1,0,2,0,1,1,0], # Integral to eliminate  
    'valid_actions': [(ibp_op, delta), ...],  
    'label': 3  # Index of correct action  
}
```

## Part 2: Model Architecture

# Model: IBPActionClassifierV5

## Overview

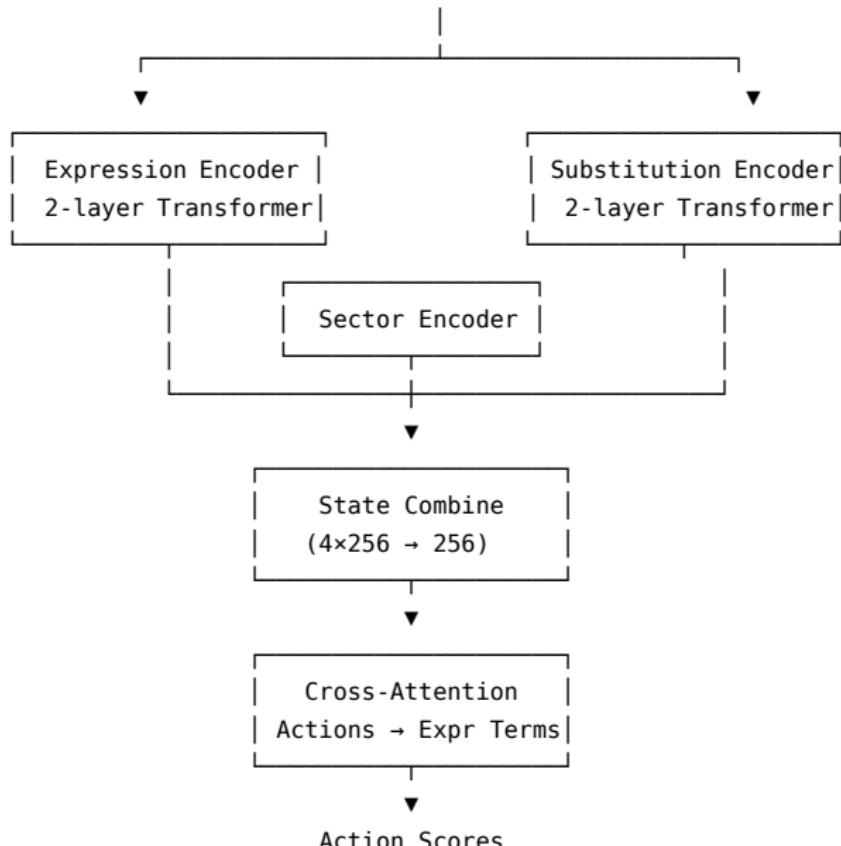
- ▶ **Task:** Score candidate IBP actions given current reduction state
- ▶ **Architecture:** Transformer-based with specialized encoders
- ▶ **Parameters:** 7.7M
- ▶ **Best validation accuracy:** 90.77%

## Key Innovation (V5)

Full substitution encoding - encode not just the key integral but the complete replacement expression

# Model Architecture Diagram

Inputs: Expression, Target, Substitutions, Sector, Actions



## Component Details

Component	Purpose
<b>Expression Encoder</b>	Encode expression + target
<b>Substitution Encoder</b>	Encode reduction history
<b>Sector Encoder</b>	Condition on sector
<b>Cross-Attention Scorer</b>	Score actions vs expression

All use 2-layer architectures (Transformer or cross-attention)

## Model Hyperparameters

- ▶ Embedding dimension: 256, Attention heads: 4
- ▶ Total parameters: 7,696,709

## Part 3: Training

# Training Configuration

```
epochs = 30
batch_size = 256
learning_rate = 0.0004
weight_decay = 1e-5
optimizer = AdamW
```

## Training Results

- ▶ **Best checkpoint:** Epoch 22
- ▶ **Validation accuracy:** 90.77% (top-1)
- ▶ **Top-5 accuracy:** ~98%
- ▶ **Training time:** ~800s per epoch on GPU

# Training Curves

## Key Observations

- ▶ Model converges by epoch 20-25
- ▶ Validation accuracy plateaus at ~91%
- ▶ No significant overfitting observed
- ▶ Top-5 accuracy very high (~98%) - beam search can recover from top-1 mistakes

## Part 4: Beam Search Inference

# Beam Search Algorithm

Each Step (beam width = 20)

1. Start with **20 states** in the beam
2. For each state, identify **target** = max weight non-master
3. Model ranks valid actions; expand **top 20 actions per state**
4. This produces ~**400 candidate states**
5. Sort by (max\_weight, n\_non\_masters, -model\_score)
6. Keep **top 20** → new beam

Termination

- ▶ Stop when best state contains **only master integrals**
- ▶ Model guides *which actions to try*; weight reduction decides *what to keep*

# Beam Search Optimizations

## P1: Equation Caching ( $\sim 3\text{-}10x$ speedup)

- ▶ IBP equation generation is expensive (sympy operations)
- ▶ Cache `get_raw_equation` results
- ▶ Reuse across beam states with shared history

## P2: Batched Inference ( $\sim 50x$ speedup)

- ▶ Prepare all action candidates as numpy arrays
- ▶ Single batched forward pass through model
- ▶ Eliminates per-action inference overhead

## Combined Effect

- ▶ Per-step time: 10-90s  $\rightarrow$  0.1-5s
- ▶ Makes deep reductions feasible

# Hierarchical Reduction Strategy

## Algorithm

1. Find highest-level sector with non-master integrals
2. Run beam search to eliminate all non-masters in that sector
3. Move to next highest sector
4. Repeat until only masters remain

Example: I[2,0,2,0,1,1,0]

Sector	Level	Steps
53	4	53
52	3	17
49	3	4
37	3	42
21	3	46
...	...	...
<b>Total</b>	-	<b>176</b>

# Beam Restart Strategy (V11+)

## Problem

After weight improvement, beam often contains suboptimal states that will never succeed

## Solution: Beam Restart

1. Run beam search until weight improves
2. **Stop and restart** with only the best state
3. Prunes dead ends, enables deeper exploration

## Impact

- ▶ Essential for high-weight integrals
- ▶  $I[1,1,1,1,1,1,-3]$ : 1,416 steps across 45 sectors
- ▶  $I[3,2,1,3,2,2,-6]$ : 46,345 steps across 62 sectors

## Part 5: Parallelization

# Parallelization Motivation

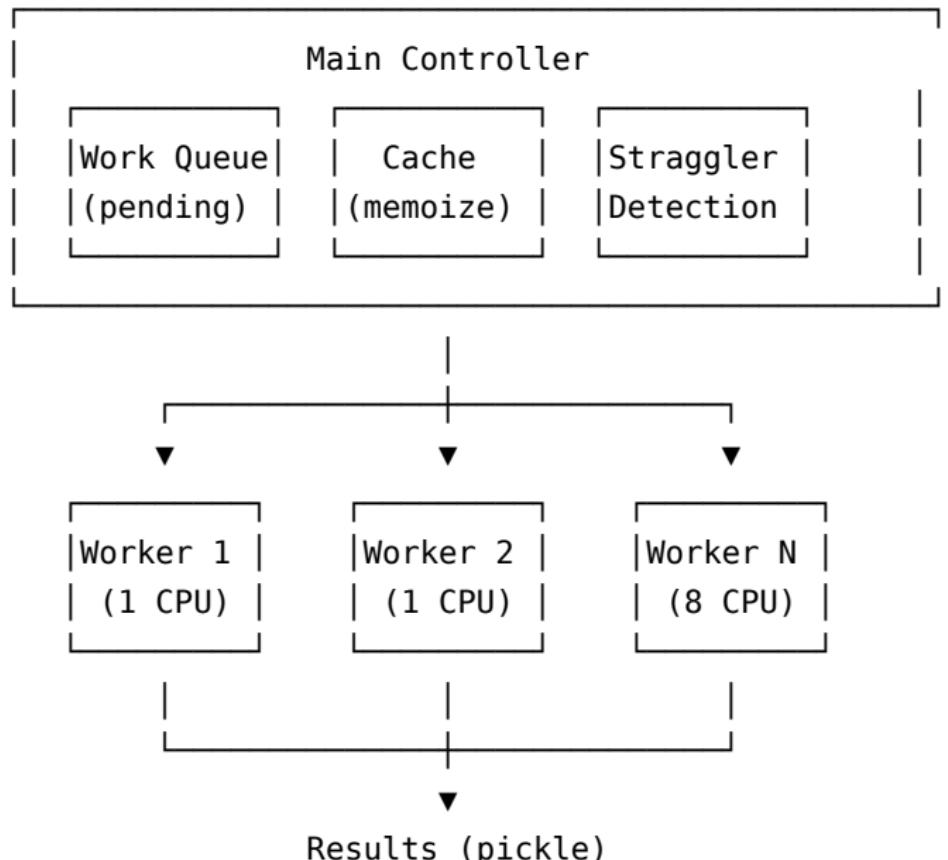
## The Bottleneck

- ▶ Sequential reduction of  $I[3,2,1,3,2,2,-6]$  takes ~20 hours
- ▶ Single-threaded beam search on CPU
- ▶ Many independent integrals could be processed in parallel

## Key Insight

Each one-step reduction is independent - distribute across workers!

# Async Parallel Architecture



# Key Parallelization Features

## 1. Async Work Distribution

- ▶ Submit all pending non-masters immediately
- ▶ Don't wait for level synchronization
- ▶ Process results as they arrive

## 2. Memoization Cache

- ▶ Store: integral → reduced expression
- ▶ Avoid redundant work (~55,000 cache hits!)
- ▶ Critical when stragglers produce already-cached results

## 3. Straggler Detection

- ▶ Jobs >30 min are killed and resubmitted
- ▶ Resubmit with 8 CPUs (parallel beam search)
- ▶ Prevents slow integrals from blocking progress

# Parallel Performance

## I[3,2,1,3,2,2,-6] Results

Metric	Value
Time (sequential)	~20 hours
Time (parallel)	<b>115 minutes</b>
<b>Speedup</b>	~10x
Jobs submitted	21,096
Stragglers resubmitted	24
Cache hits	55,075
Final masters	16

## Part 6: Results

## Validation Against Kira

$I[2,0,2,0,1,1,0]$  Coefficient Comparison (mod 1009)

Master Integral	Kira	Our Result	Match
$I[1, -1, 1, 0, 1, 1, 0]$	107	107	Exact
$I[1, 0, 1, 0, 1, 1, 0]$	303	303	Exact
$I[1, 0, 1, 0, 1, 0, 0]$	752	752	Exact
$I[0, 1, 1, 1, 0, 0, 0]$	915	—	Symmetry
$I[1, 0, 1, 0, 0, 1, 0]$	—	915	Symmetry

**4th master:**  $I[0, 1, 1, 1, 0, 0, 0]$  and  $I[1, 0, 1, 0, 0, 1, 0]$  related by  
k1  $\leftrightarrow$  k2 loop exchange symmetry

**Result:** Perfect agreement with Kira!

## Scaling Results

Integral	Weight	Time	Steps	Masters
I[2,0,2,0,1,1,0]	(6,0)	5 min*	526	4
I[1,1,1,1,1,1,-3]	(6,3)	12 min*	1,416	16
I[3,2,1,3,2,2,-6]	(13,6)	<b>115 min*</b>	131,769	16

\*With parallel execution (async hierarchical)

## Final Reduction Example

$I[3,2,1,3,2,2,-6] \rightarrow 16$  Paper Masters

Final expression (mod 1009):

171 \*  $I[1,0,1,1,1,1,0]$

854 \*  $I[1,1,0,1,1,1,0]$

377 \*  $I[1,1,1,1,1,0,0]$

160 \*  $I[-1,1,1,1,1,0,0]$

100 \*  $I[0,1,1,1,1,0,0]$

647 \*  $I[1,-1,1,0,1,1,0]$

9 \*  $I[1,-1,1,1,1,0,0]$

... (16 masters total)

Matches arXiv:2502.05121 basis exactly!

## Part 7: Conclusions

## Key Contributions

1. **ML-guided IBP reduction** that matches professional software (Kira)
2. **Constant memory usage** - avoids the memory wall of traditional approaches
3. **Hierarchical beam search** with restart strategy for deep reductions
4. **Async parallel execution** with ~10x speedup
5. **Straggler handling** for robust distributed computing
6. **Paper-masters-only mode** for clean minimal basis

# Technical Innovations

## Model

- ▶ Full substitution encoding (V5)
- ▶ Cross-attention action scoring
- ▶ Target-aware expression encoding

## Inference

- ▶ Equation caching (3-10x speedup)
- ▶ Batched model inference (50x speedup)
- ▶ Beam restart strategy

## Parallelization

- ▶ Async one-step distribution
- ▶ Memoization cache (~55k hits)
- ▶ Automatic straggler resubmission

## Future Work

1. **GPU workers** for faster beam search
2. **Adaptive timeouts** based on sector statistics
3. **More integrals** - test on other two-loop families
4. **Training on successful paths** - use reduction results to improve model
5. **Path optimization** - shorten saved reduction paths

# Code Availability

**Repository:** [github.com/davidshih17/RL\\_IBPrediction\\_claude](https://github.com/davidshih17/RL_IBPrediction_claude)

## Key Files

- ▶ `models/classifier_v5.py` - Model architecture
- ▶ `scripts/eval/hierarchical_reduction_async.py` - Parallel reduction
- ▶ `scripts/eval/reduce_integral_onestep_worker.py` - Condor worker
- ▶ `docs/parallelization.md` - Detailed documentation

# Thank You

Questions?

Contact

- ▶ Repository:  
[github.com/davidshih17/RL\\_IBPrediction\\_claude](https://github.com/davidshih17/RL_IBPrediction_claude)
- ▶ arXiv: 2502.05121 (paper masters reference)