# Machine Programming

Lecture 16 – LLM for Software Testing: Static Analysis

## Logistics – Week 9

- Assignment 3: Coding LLM Agents
  - <a href="https://github.com/machine-programming/assignment-3">https://github.com/machine-programming/assignment-3</a>
  - Fully functional web-app agent. Due: Oct 23 (Thu)
- Forming groups for your final projects!
  - Form a group of 2-3 before This Thursday (Oct 19 Oct 23)

#### Module 3: Overview

# - What should the program do? 1. Syntax/Semantics/Functional correctness 2. Comprehensive test coverage 3. Has no security flaw 4. Optimized for runtime speed 5. ... Structural Specification

#### **Synthesis Strategy**

- How do we find such a program?

**Enumeration**: Bottom-up and Top-Dowr

#### **Programming with Large Language Models**

- Next token predicti Fixed ompting, controlled decoding
- Iterative refinement, agentic frameworks and tool use
- Pre-training, fine-tuning, reinforcement learning

- What is the space of the programs?

**General Purpose Programming Language**Python / Java / C / Rust / ...

**Domain Specific Languages**SQL / LEAN / ROCQ / DATALOG / PDDL / ...

# Software Analysis

Testing and Dynamic Analysis

## Forms of Software Analysis

#### Static Analysis

Examine code without concrete execution

- Taint analysis
- Reachability analysis
- Abstract interpretation
- Symbolic execution
- ..

#### **Dynamic Analysis**

Observes program behavior while executing

- Unit testing
- Fuzzing
- Property-based testing
- Penetration testing
- ...

**Unit Testing** 

Human-written tests in the form of concrete input-output

assert f(2) == 4

**Unit Testing** 

Human-written tests in the form of concrete

ie form of concr input-output Fuzzing

Randomly generating test inputs

**Unit Testing** 

Human-written tests in the form of concrete input-output

assert f(2) == 4

Fuzzing

Randomly generating test inputs

for i in 0..10<sup>4</sup>: x = gen\_input() f(x)

**Property-based testing** 

Randomly generating test inputs, but with properties checking outputs

```
for i in 0..10<sup>4</sup>:
  x = gen_input()
  y = f(x)
  assert property(x,y)
```

**Unit Testing** 

Human-written tests in the form of concrete input-output

assert f(2) == 4

Fuzzing

Randomly generating test inputs

for i in 0..10^4:
 x = gen\_input()
 f(x)

Property-based testing

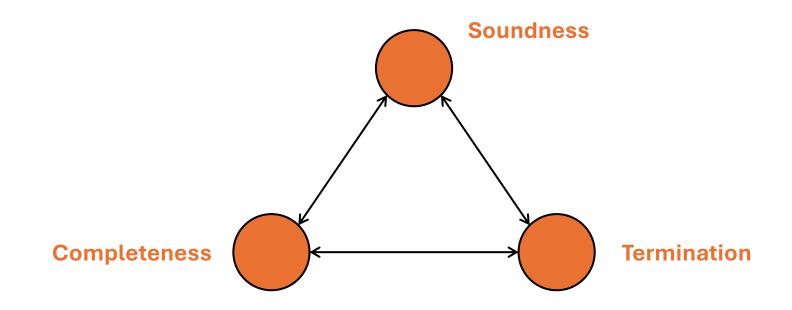
Randomly generating test inputs, but with properties checking outputs

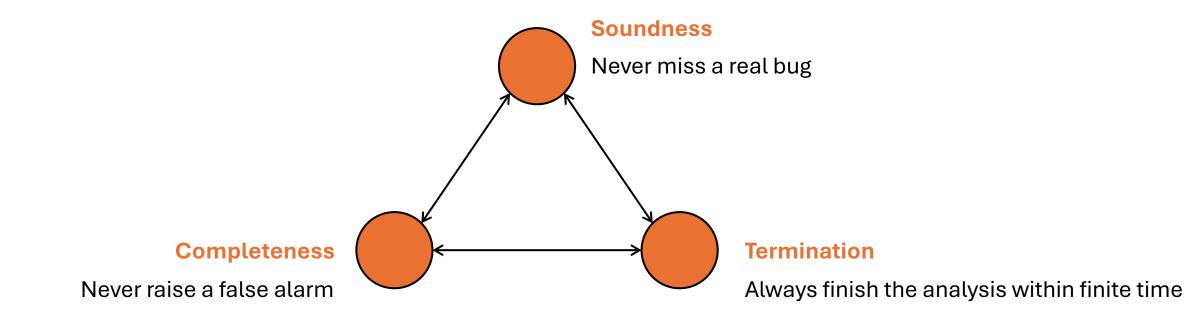
```
for i in 0..10^4:
    x = gen_input()
    y = f(x)
    assert property(x,y)
```

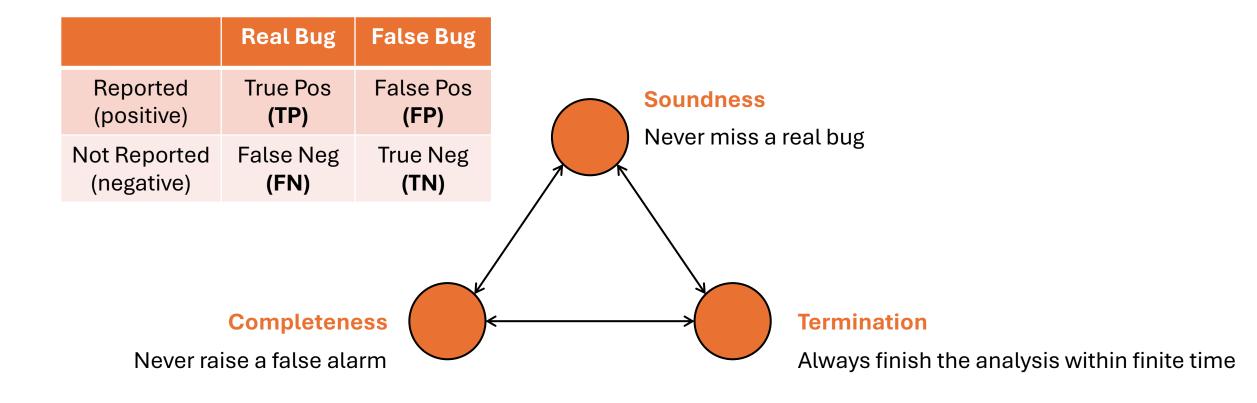
Penetration testing

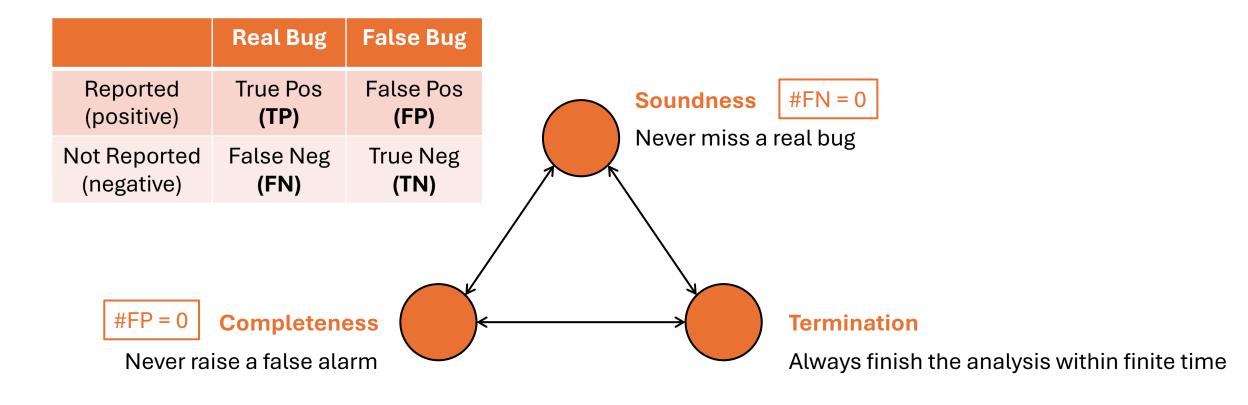
Crafting adversarial inputs to trigger vulnerabilities rather than getting outputs

```
try:
   f(very_bad_input)
   assert false
except:
   assert no_bad_behavior
```









#### Dynamic Analysis:

#### **Unit Testing**

- (assuming tests are correct)

#### **Fuzzing**

- (assuming harness is real)

Completeness

Never raise a false alarm



**Termination** 

Always finish the analysis within finite time

#### Program – Line coverage: 5/5 (100%)

```
def calculate_interest(balance: float, months: int) -> float:
    rate = 0.02 # 2% per month
    if months > 12:
        rate = 0.03 # higher rate for long-term deposits
    return balance * rate / months
```

#### Test 1

```
def test_short_term_interest():
    assert calculate_interest(1000, 6) == pytest.approx(3.33)
```

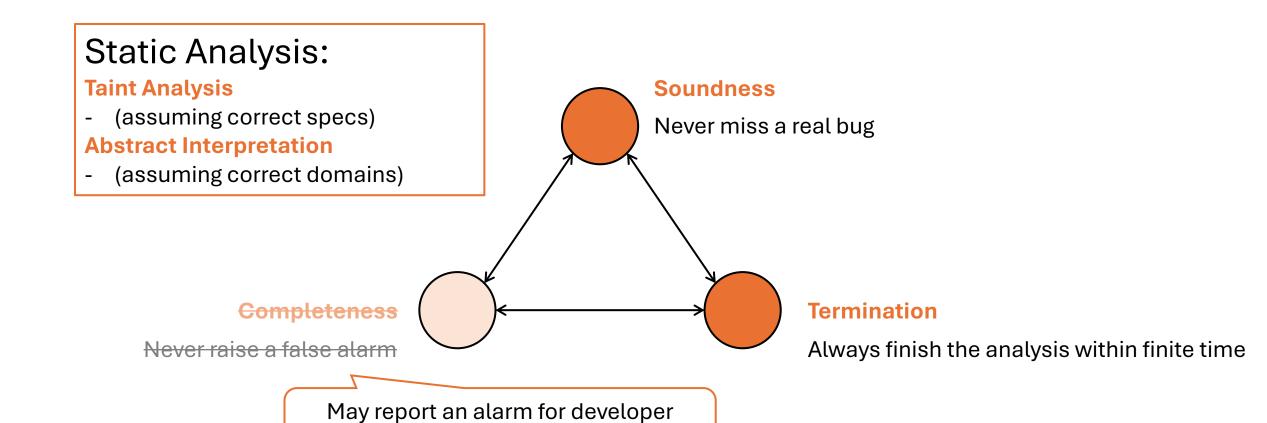
#### Test 2

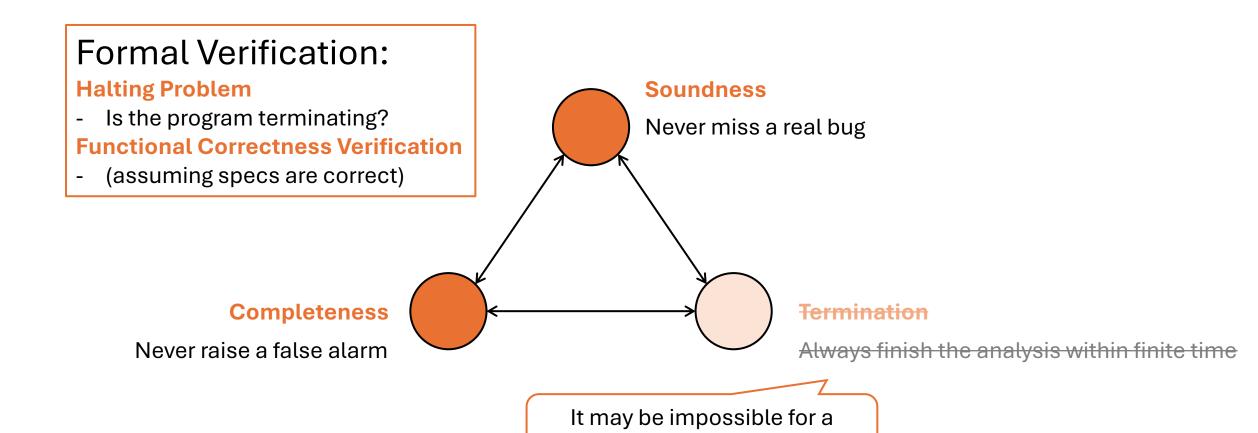
```
def test_long_term_interest():
   assert calculate_interest(1000, 24) == pytest.approx(1000 * 0.03 / 24)
```

#### Test 3 (Assume that this test case is not there)

```
def test_zero_months_divide_by_zero(): # covers implicit error path
  assert calculate_interest(1000, 0) == 0
```

confirmation, and that is rejected



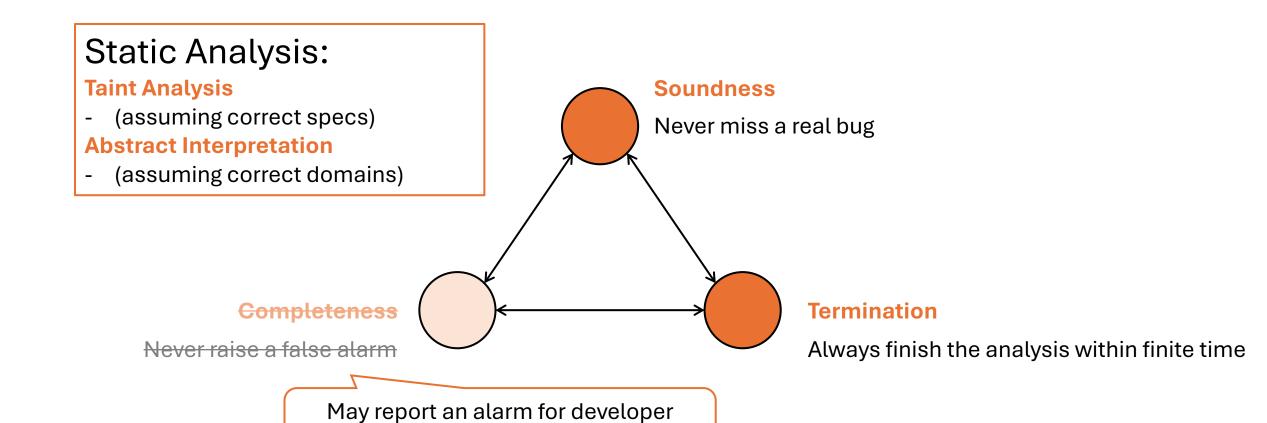


verifier to terminate

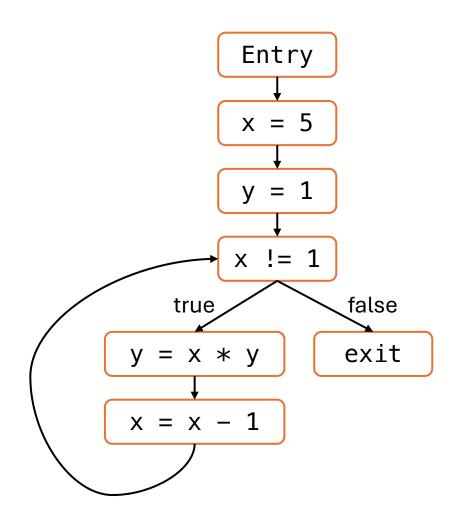
# Software Analysis

Static Analysis

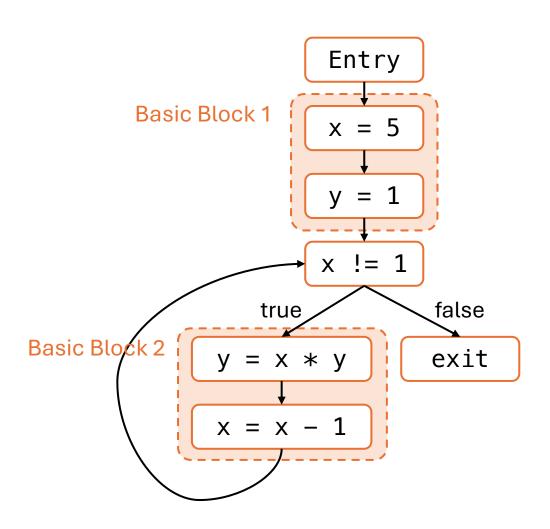
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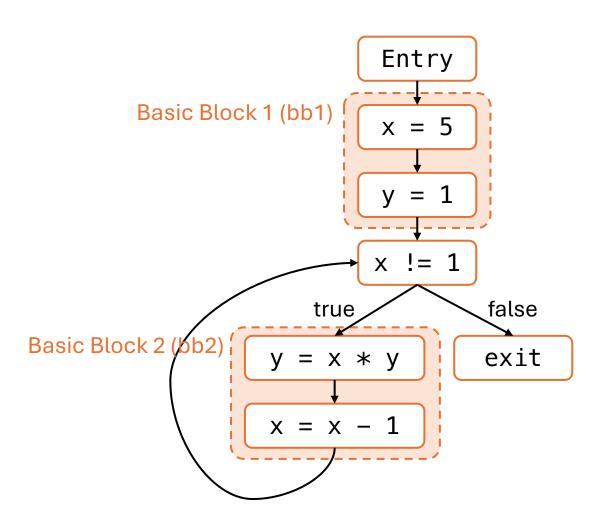
- Premise:
  - An abstract representation of imperative programs
  - Illustrating how "control" (execution) flows through the code
- A graph representation
  - Summarizes the flow of control in all possible runs of the program
- Goal:
  - Help all sorts of static analysis by providing the birds eye view



```
int x = 5;
int y = 1;
while (x != 1) {
   y = x * y;
   x = x - 1;
}
```

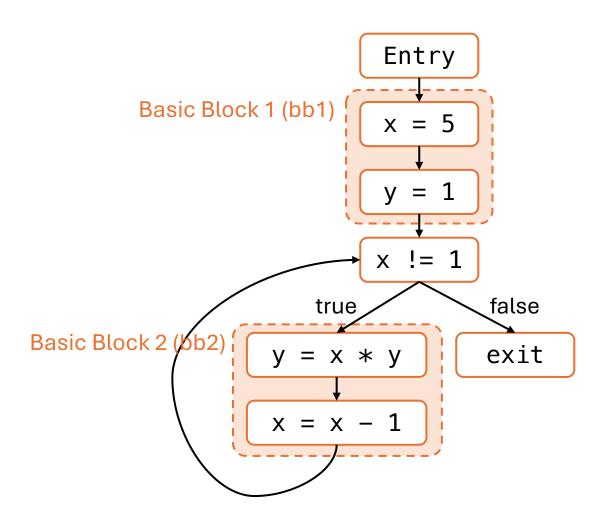


```
int x = 5;
int y = 1;
while (x != 1) {
   y = x * y;
   x = x - 1;
}
```



```
bb1 {
  int x = 5;
  int y = 1;
  while (x != 1) {
    y = x * y;
    x = x - 1;
}
```

#### Control-Flow Graphs: Traces



```
bb1 {
  int x = 5;
  int y = 1;
  while (x != 1) {
    y = x * y;
    x = x - 1;
  }
```

#### **Execution Trace**

```
Entry \rightarrow bb1 \rightarrow cond

\rightarrow bb2 \rightarrow cond // (x == 5)

\rightarrow bb2 \rightarrow cond // (x == 4)

\rightarrow bb2 \rightarrow cond // (x == 3)

\rightarrow bb2 \rightarrow cond // (x == 2)

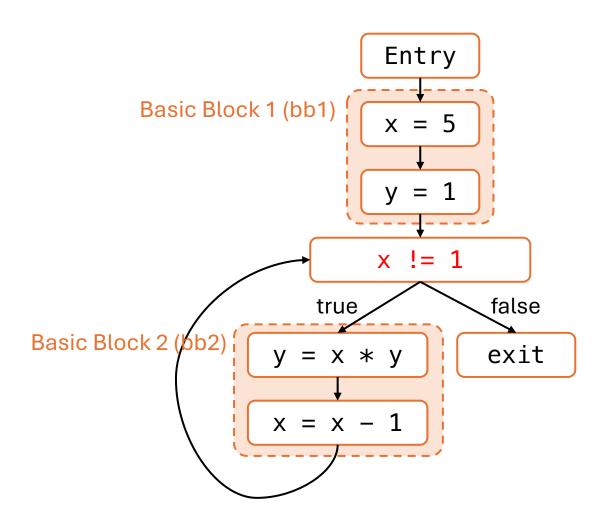
\rightarrow bb2 \rightarrow cond // (x == 1)

\rightarrow exit
```

## **Dataflow Analysis**

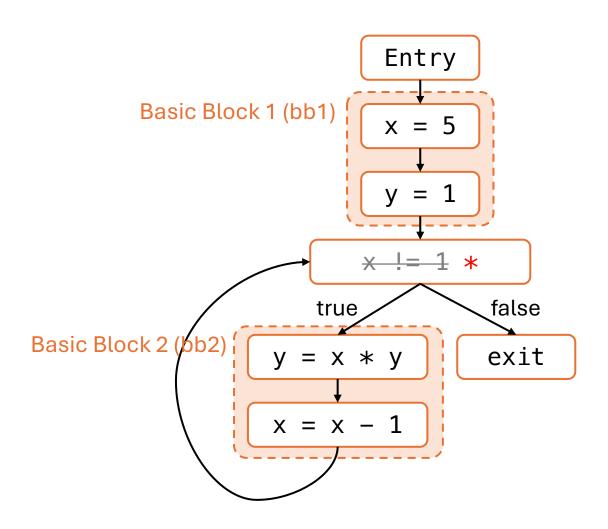
- Building on control-flow analysis
  - Abstracts away control-flow conditions
- Considers all paths possible in actual runs (sound)
- Including paths that are never realizable (incomplete)

## **Abstracting Control-Flow Graphs**



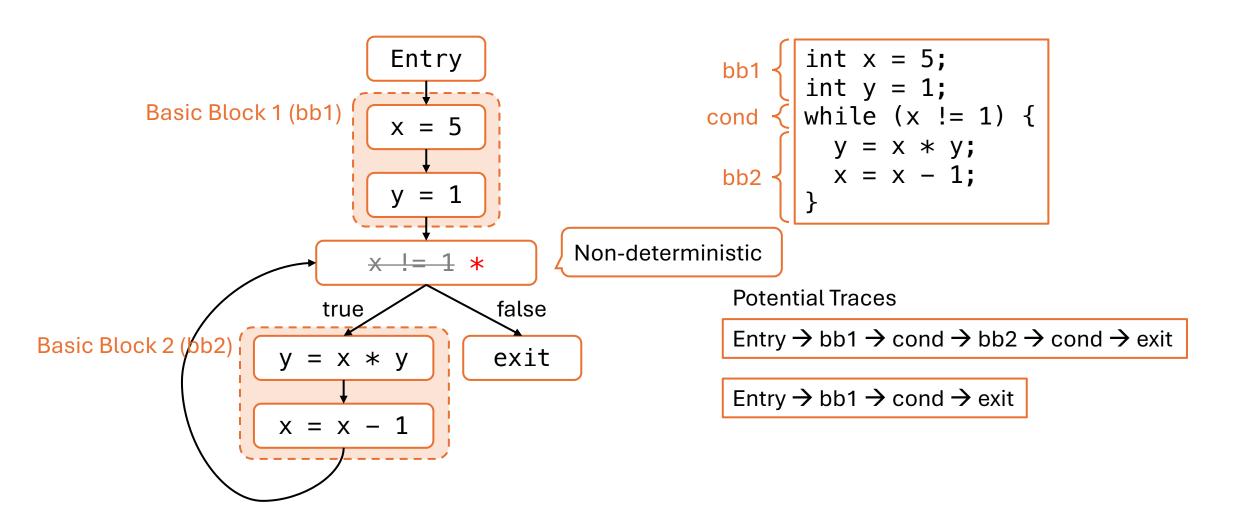
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## **Abstracting Control-Flow Graphs**



```
bb1 {
  int x = 5;
  int y = 1;
  while (x != 1) {
    y = x * y;
    x = x - 1;
  }
```

## **Abstracting Control-Flow Graphs**



#### Modern Dataflow Analyses

#### Interval Analysis

- Check memory safety (integer overflows, buffer overruns, ...)

#### **Taint Analysis**

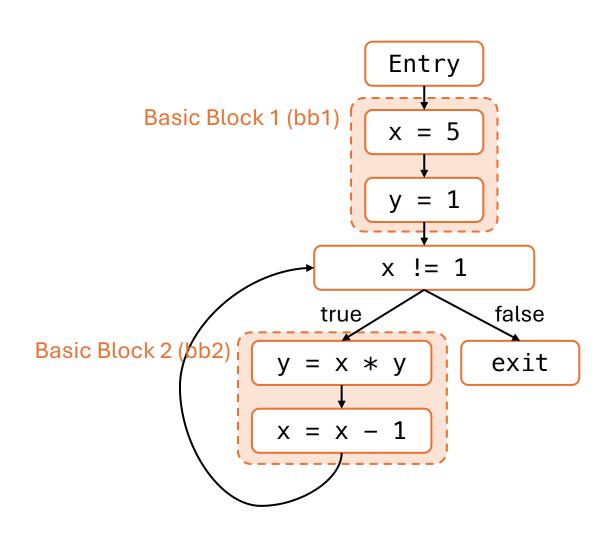
- Check information flow (Sensitive data leak, code injection, ...)

#### Type-State Analysis

- Temporal safety properties (APIs of protocols, libraries, ...)

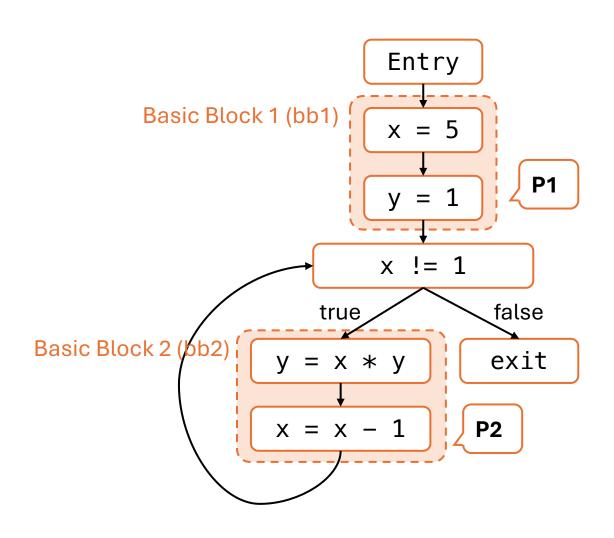
#### Concurrency Analysis

- Concurrency safety properties (dataraces, deadlocks, ...)



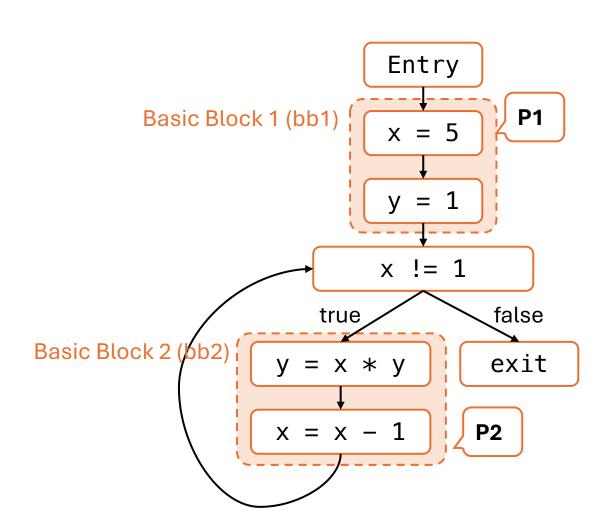
#### • Goal:

- Determine whether a program point containing a piece of data (definition of a variable) can flow to another program point
- Reduced to...
  - Path finding problem in a graph



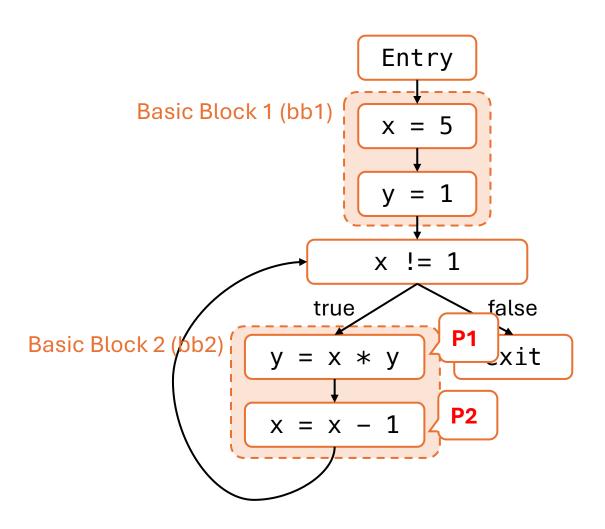
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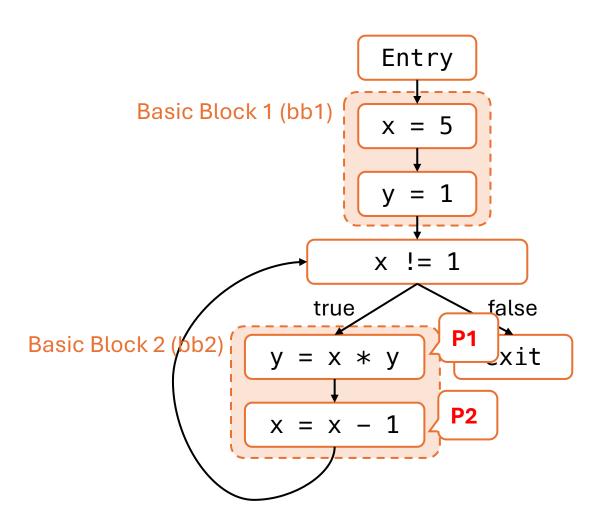


#### • Goal:

- Determine whether a program point containing a piece of data (definition of a variable) can flow to another program point
- Reduced to...
  - Path finding problem in a graph
- Example:
  - Does information defined in P1 flow to P2?

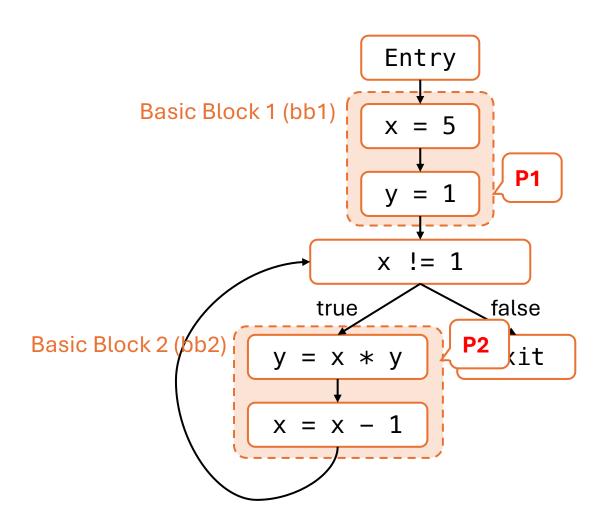


 Does information defined in P1 flow to P2?

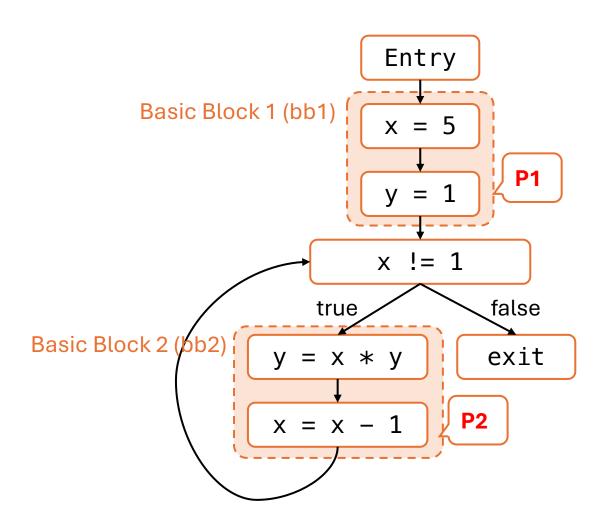


 Does information defined in P1 flow to P2?

**YES** 



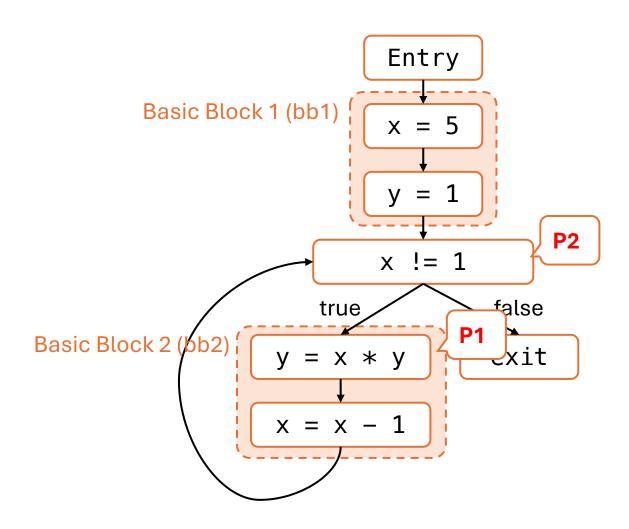
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 Does information defined in P1 flow to P2?

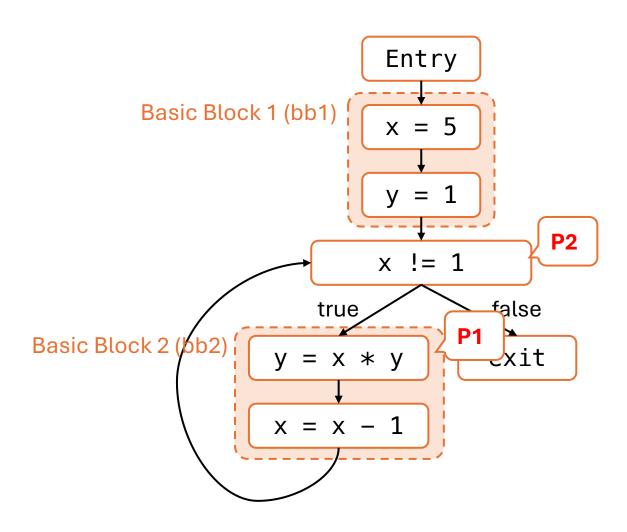
NO

### Reaching Definitions Analysis: Quiz



 Does information defined in P1 flow to P2?

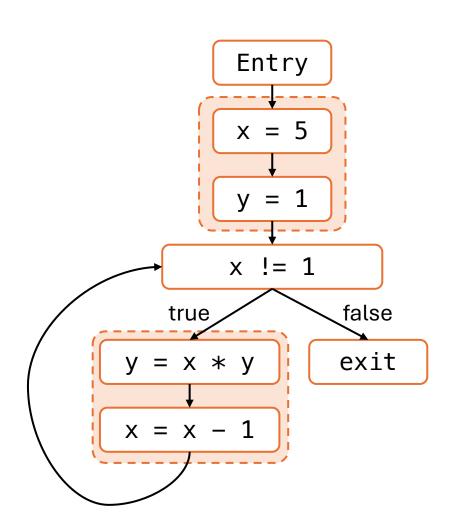
## Reaching Definitions Analysis: Quiz



 Does information defined in P1 flow to P2?

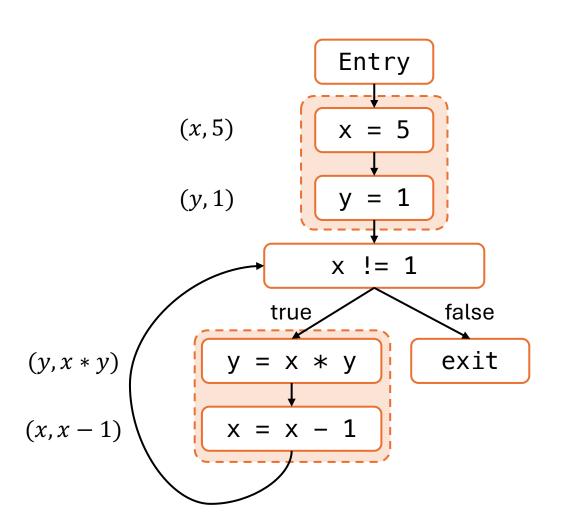
**YES** 

## How to Compute Reaching Definitions?



- For each node n, we denote
  - IN(n) = nodes which can reach n
  - OUT(n) = nodes which can go beyond n
- Dataflow analysis computes IN(n) and OUT(n) for each node
- Chaotic Iteration:
  - Starting from them being empty
  - Repeat operations to populate them
  - Until the two sets stop changing

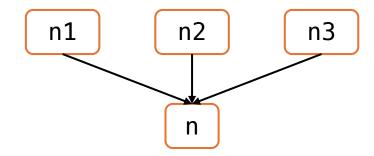
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# How to Compute? Flow-in

$$IN(n) = \bigcup_{m \in predecessors(n)} OUT(m)$$



 $IN(n) = OUT(n_1) \cup OUT(n_2) \cup OUT(n_3)$ 

## How to Compute? Flow-out

$$OUT(n) = (IN(n) - KILL(n)) \cup GEN(n)$$

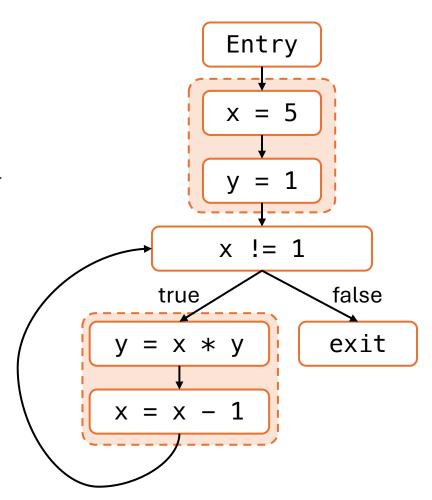
$$IN(n)$$
 $n$ 
 $OUT(n)$ 

n: 
$$y = x * y$$
  $GEN(n) = \{(y, n)\}$   $KILL(n) = \{(y, 5)\}$ 

n: 
$$X != 1$$
  $GEN(n) = {}$   $KILL(n) = {}$ 

### Chaotic Iteration for Dataflow Analysis

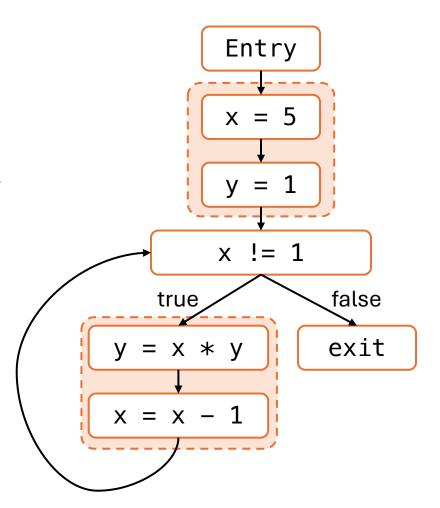
- for (each node n in control-flow graph):
  - $IN(n) = \{\}$
  - $OUT(n) = \{\}$
  - $GEN(n) = \{(v,n)\}$  if n is an assignment else  $\{\}$
- repeat:
  - for (each node n):
    - IN(n) = flow-in(n)
    - OUT(n) = flow-out(n)
- until all the IN(n) and OUT(n) stops changing



### Chaotic Iteration for Dataflow Analysis

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**Question:** Does it always terminate?

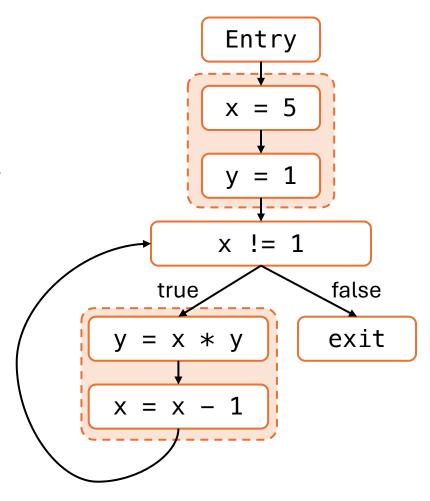


## Chaotic Iteration for Dataflow Analysis

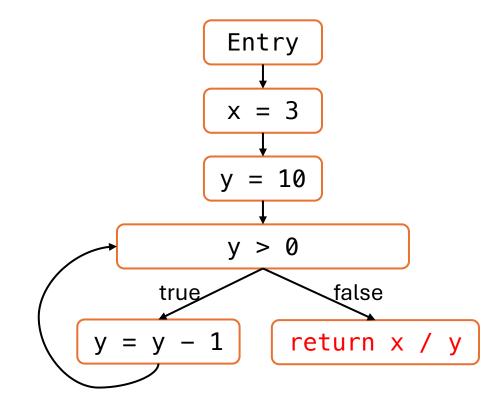
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- until all the IN(n) and OUT(n) stops changing

**Question:** Does it always terminate?

**Answer:** Yes!



- Question:
  - With Dataflow analysis, can we tell whether there could be a divide-byzero vulnerability?

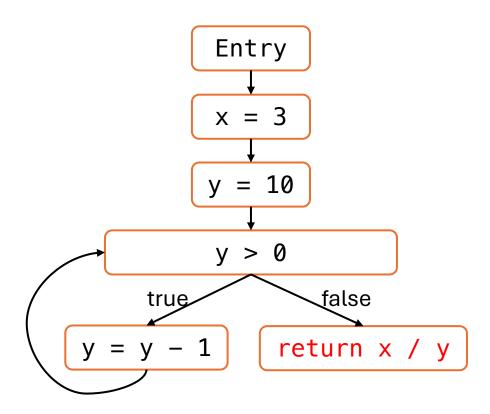


### Question:

 With Dataflow analysis, can we tell whether there could be a divide-byzero vulnerability?

#### Answer:

 We can tag the nodes with additional information such as abstract domains

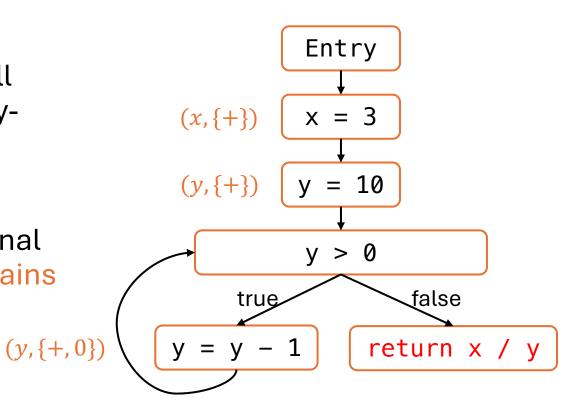


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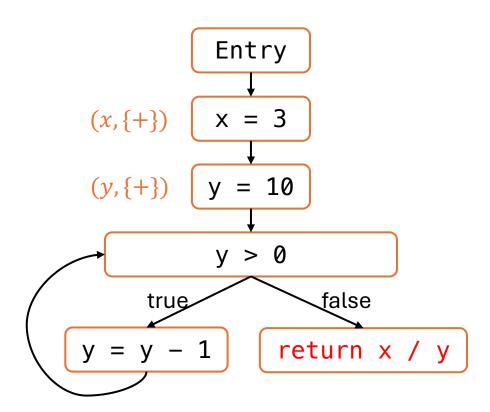


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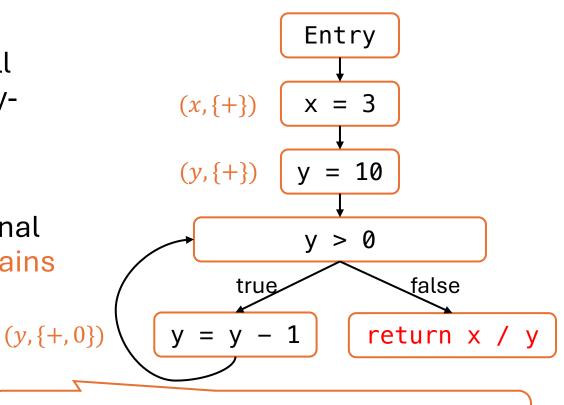
### Question:

 With Dataflow analysis, can we tell whether there could be a divide-byzero vulnerability?

### Answer:

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Abstract Domain:  $\{+, 0, -\}$ 



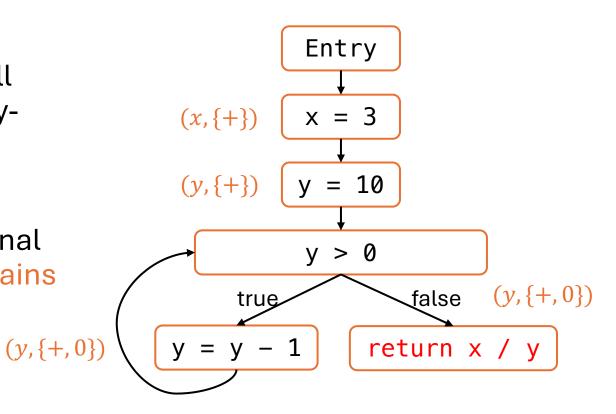
**Question:** At the end of analysis, for this node, can y be tagged with abstract domain  $\{+, 0, -\}$ ?

### Question:

 With Dataflow analysis, can we tell whether there could be a divide-byzero vulnerability?

### Answer:

 We can tag the nodes with additional information such as abstract domains



### **Arithmetic of Abstract Domains**

```
\{+\} + \{+\} \rightarrow \{+\}
\{+\} - \{+\} \rightarrow \{+, 0, -\} Specialization: \{+\} - 1 \rightarrow \{+, 0\}
\{+\} * \{+\} \rightarrow \{+\}
\{+\} + \{0\} \rightarrow \{+\}
\{+\} - \{0\} \rightarrow \{+\}
\{+\} * \{0\} \rightarrow \{0\}
\{+\} + \{-\} \rightarrow \{+, 0, -\} Specialization: \{+\} + (-1) \rightarrow \{+, 0\}
\{+\} - \{-\} \rightarrow \{+\}
\{+\} * \{-\} \rightarrow \{-\}
```

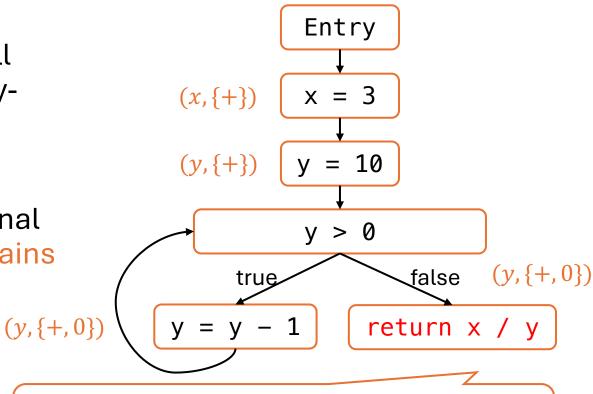
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Abstract Domain:  $\{+, 0, -\}$ 



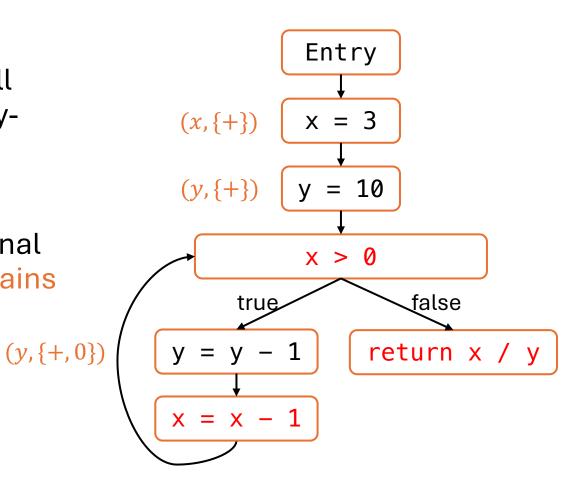
Since y is tagged with abstract domain 0, there IS a potential divide-by-zero vulnerability!

### Question:

 With Dataflow analysis, can we tell whether there could be a divide-byzero vulnerability?

### Answer:

 We can tag the nodes with additional information such as abstract domains

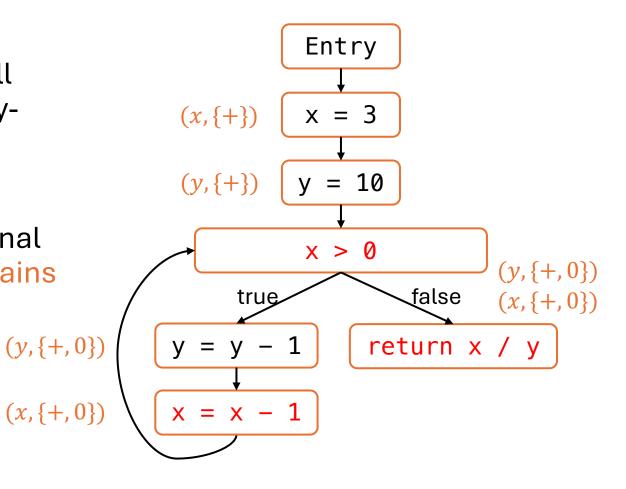


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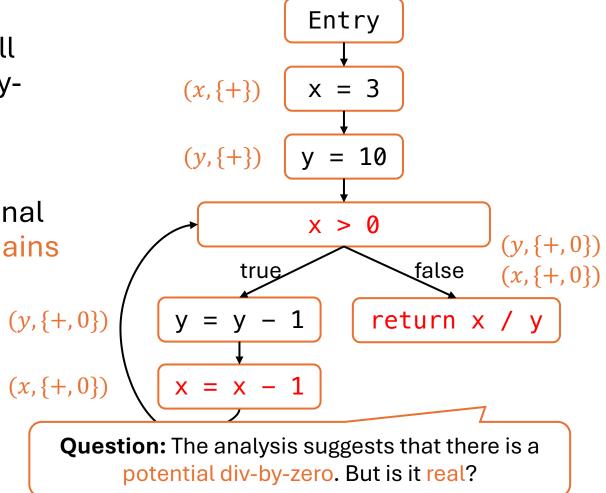


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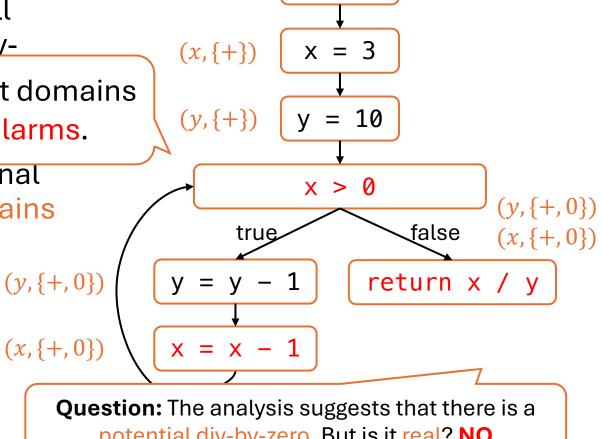


- Question:
  - With Dataflow analysis, can we tell whether there could be a divide-by-

**Dataflow Analysis** with  $\{+, 0, -\}$  abstract domains reported a false positive div-by-zero alarms.

 We can tag the nodes with additional information such as abstract domains

Abstract Domain:  $\{+, 0, -\}$ 

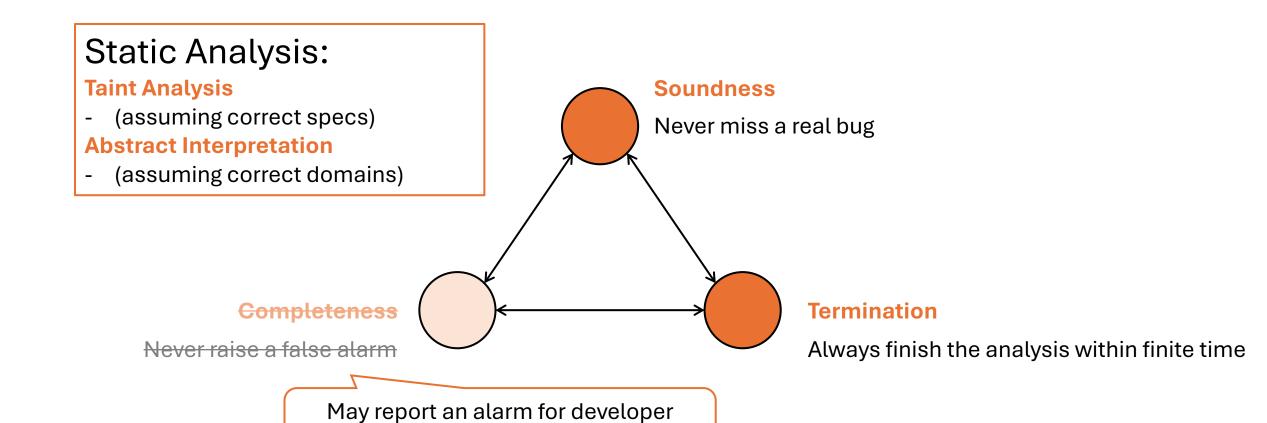


Entry

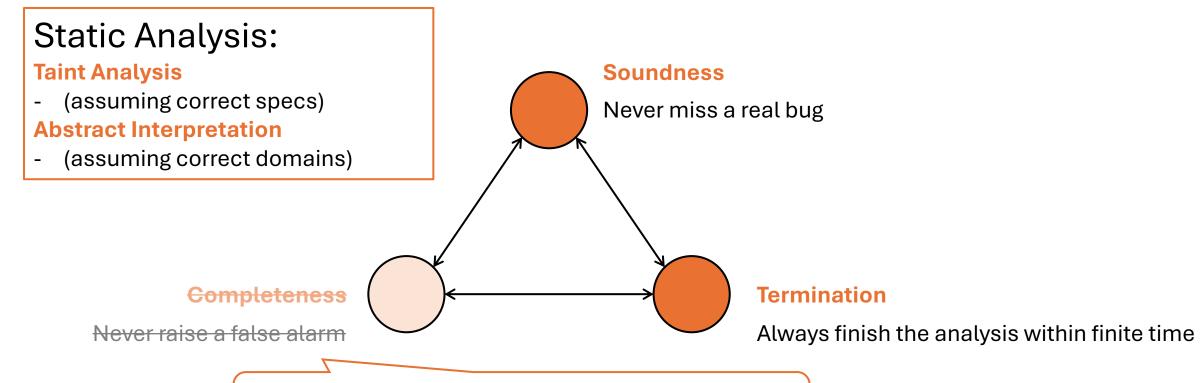
**Question:** The analysis suggests that there is a potential div-by-zero. But is it real? NO

# Software Testing: Impossible Triangle

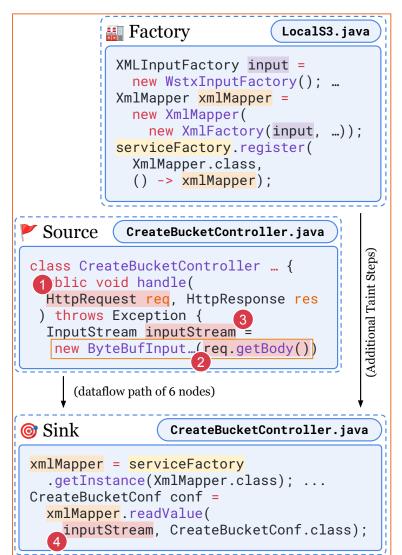
confirmation, and that is rejected



## Software Testing: Impossible Triangle



Dataflow Analysis & Abstract Domain generalizes to entire space of input, but loses precision



GitHub Advisory Database / GitHub Reviewed / CVE-2025-27136

#### LocalS3 CreateBucketConfiguration Endpoint XML External Entity (XXE) Injection

(Moderate severity) (GitHub Reviewed) Published on Mar 8 in Robothy/local-s3 · Updated on Mar 14

#### **Steps to Reproduce**

1. Create an XML document that includes an external entity declaration pointing to the internal target:

2. Send a PUT request to create a new bucket with this configuration:

```
curl -X PUT http://app/test-bucket-2 -H 'Content-Type: application/xml' -d @payload.xml
```

3. Retrieve the bucket location to see the resolved entity content:

```
curl http://app/test-bucket-2/?location
```

When these steps are executed, the server processes the XML, resolves the external entity by making a request to the internal URL, and includes the response in the bucket's location constraint. The attacker can then retrieve this information through the bucket location endpoint.

- Goal:
  - See how a program point with "tainted information" may flow through the code
  - How is it "Manifested" into a real vulnerability

```
Factory
                                 LocalS3.java
            XMLInputFactory input =
              new WstxInputFactory(); ...
            XmlMapper xmlMapper =
              new XmlMapper(
                new XmlFactory(input, ...));
            serviceFactory.register(
              XmlMapper.class,
              () -> xmlMapper);
Source
             CreateBucketController.java
                                           Steps)
 class CreateBucketController ... {
 ablic void handle(
   HttpRequest reg, HttpResponse res
  ) throws Exception {
   InputStream inputStream =
    new ByteBufInput...(req.getBody())
      (dataflow path of 6 nodes)
Sink
                   CreateBucketController.java
 xmlMapper = serviceFactory
   .getInstance(XmlMapper.class); ...
 CreateBucketConf conf =
   xmlMapper.readValue(
     inputStream, CreateBucketConf.class);
```

CVE-2025-27136

- Goal:
  - See how a program point with "tainted information" may flow through the code
  - How is it "Manifested" into a real vulnerability
- Taint Specification:
  - Source: the HttpRequest parameter to a handle function of a Java Servlet
  - Sink: the readValue function of XmlMapper

```
Factory
                                 LocalS3.java
            XMLInputFactory input =
              new WstxInputFactory(); ...
            XmlMapper xmlMapper =
              new XmlMapper(
                new XmlFactory(input, ...));
            serviceFactory.register(
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Source
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```

IRIS: LLM-ASSISTED STATIC ANALYSIS FOR DETECTING SECURITY VULNERABILITIES

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University of Pennsylvania
mhnaik@cis.upenn.edu

#### IRIS: LLM-ASSISTED STATIC ANALYSIS FOR cronutils/validation/CronValidator.java cronutils/parser/CronParser.java @override /\*\* Parse string with cron ex(3)ssion. ... \*/ public / lean is Valid( public Cron parse(final String expression) { String value, ConstraintValidatorContext context) { try { /\* ... \*/ } catch { throw new IllegalArgumentException( cronParser.parse(value).valida(5); // ... 4 ing.format("Failed to parse '%s'. %s", catch (IllegalArgumentException e) { expression, e.getMessage()), e); context .buildConstraintViolationWithTemplate(e.getMessage()) .addConstraintViolation(); // ...

Figure 2: An example of Code Injection (CWE-94) vulnerability found in cron-utils (CVE-2021-41269) that CodeQL fails to detect. We number the program points of the vulnerable path.

### IRIS: LLM-Assisted Static Analysis for

DETECT cronutils/validation/CronValidator.java cronutils/parser/CronParser.java @override /\*\* Parse string with cron ex[3]ssion. ... \*/ public / lean isValid( public Cron parse(final String expression) -String value, ConstraintValidatorContext context) { try { /\* ... \*/ } catch { **Ziyang Li** throw new IllegalArgumentException( University of cronParser.parse(value).valida 5(); // ... (4)ing.format("Failed to parse '%s'. %s", catch (IllegalArgumentException e) { expression, e.getMessage()), e); liby99@ci context .buildConstraintViolationWithTemplate(e.getMessage()) .addConstraintViolation(); // ...

Figure 2: An example of Code Injection (CWE-94) vulnerability found in cron-utils (CVE-2021-41269) that CodeQL fails to detect. We number the program points of the vulnerable path.

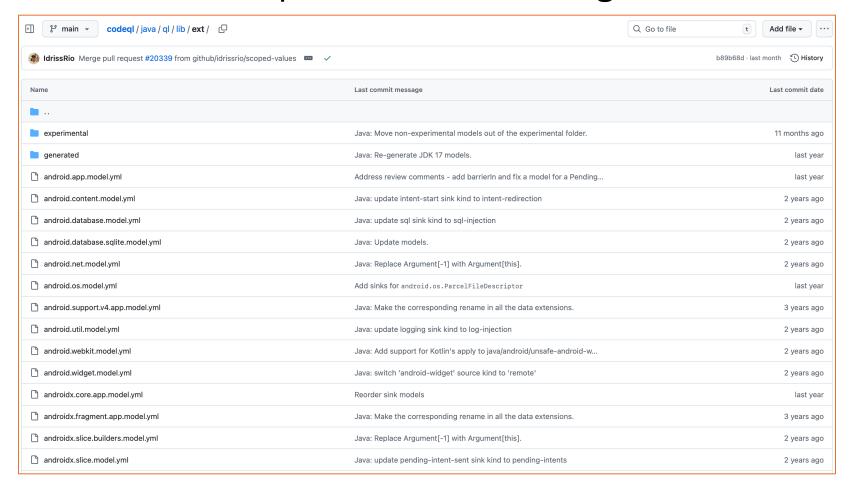
#### Taint Specification:

**Source**: the value parameter to the isValue function of a CronValidator

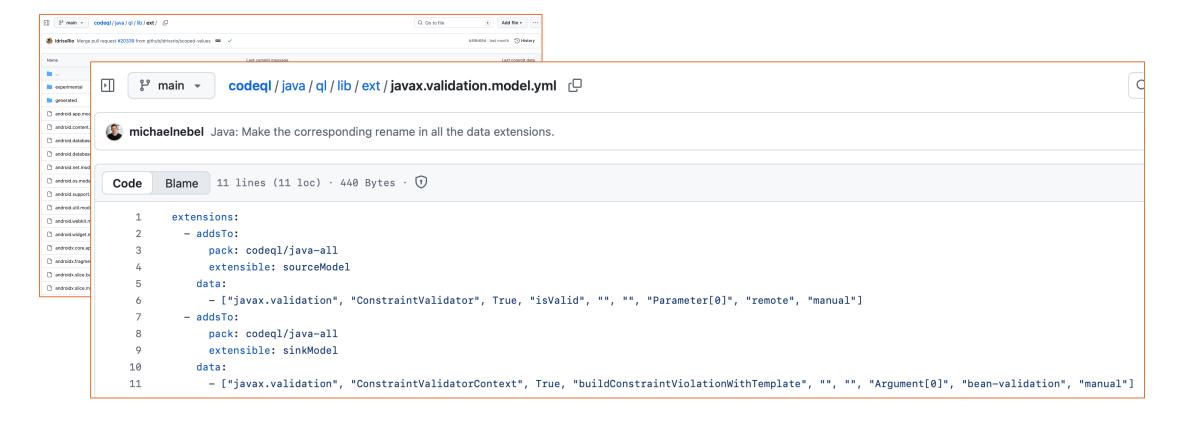
**Sink**: the buildConstraintViolationWithTemplate function of ConstraintValidatorContext

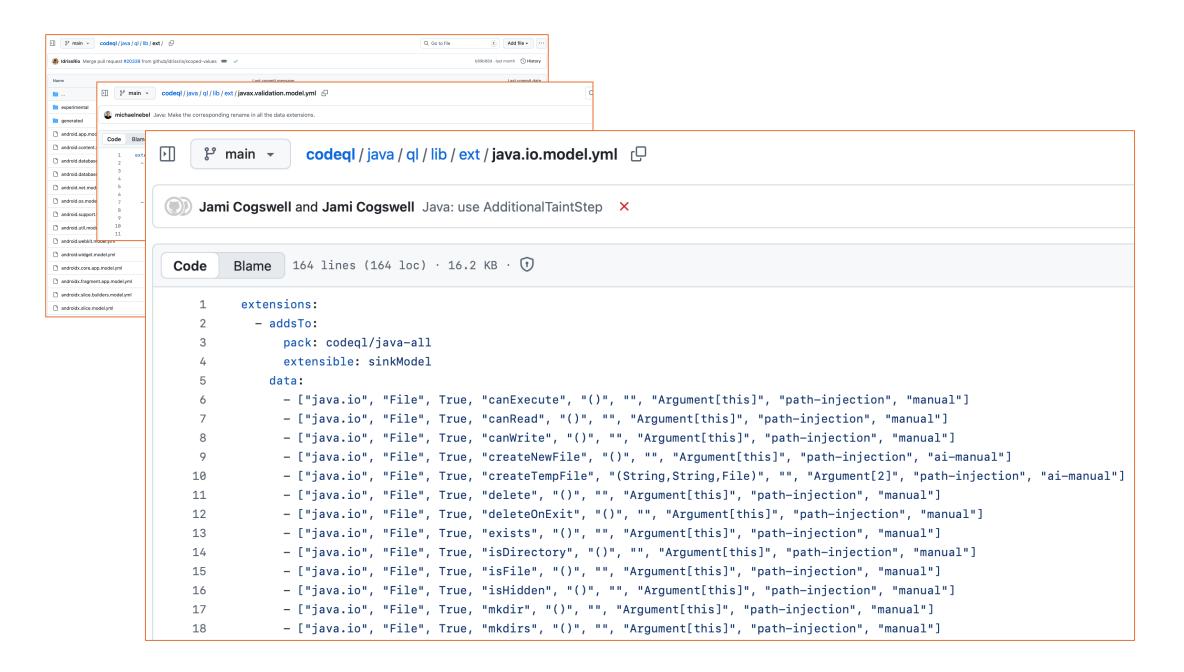
Where are those taint specifications coming from?

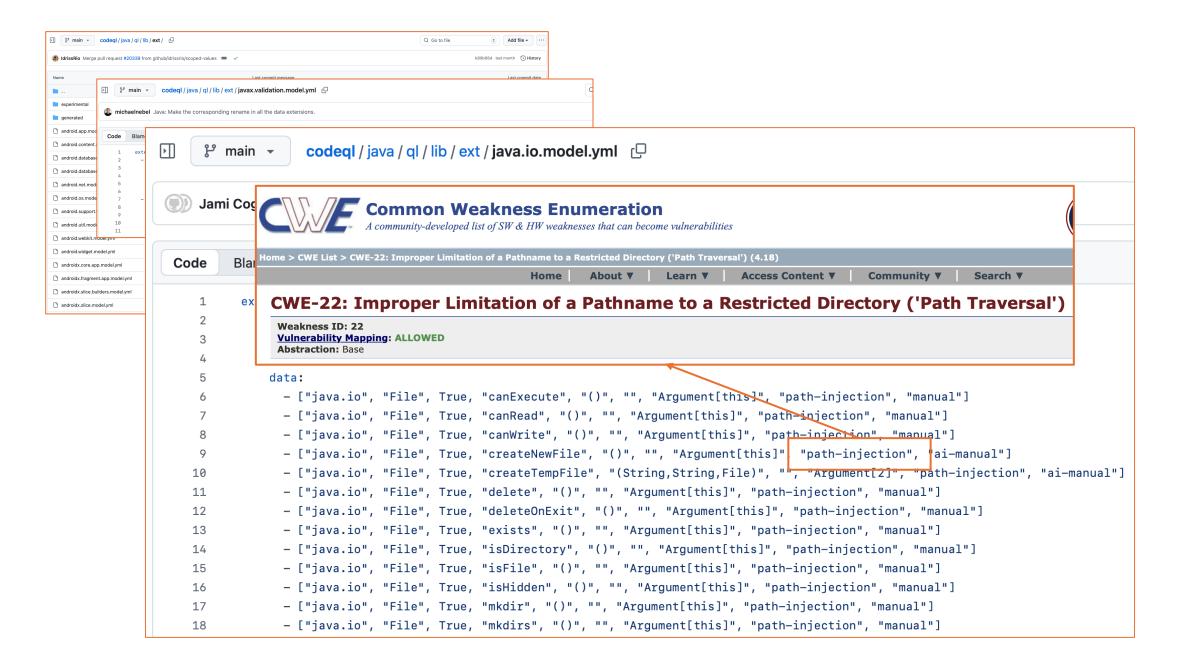
Where are those taint specifications coming from?



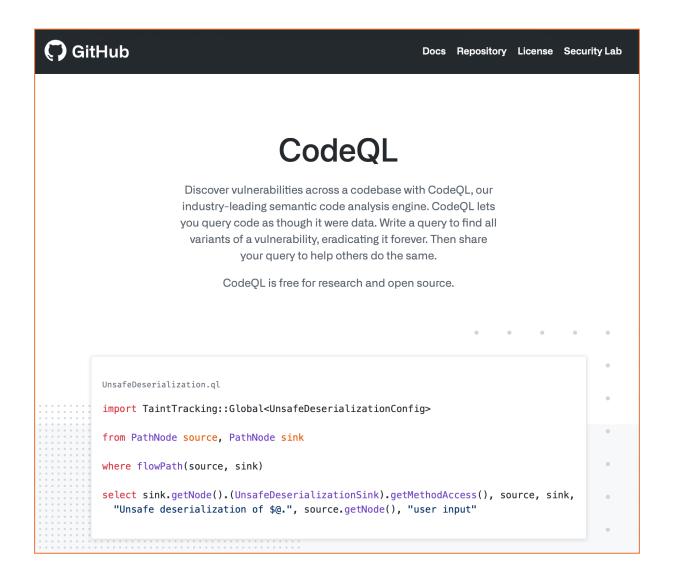
Where are those taint specifications coming from?







# Dataflow Analysis in Real Life: CodeQL



#### 1 /\*\* \* @name Uncontrolled data used in path expression \* Odescription Accessing paths influenced by users can allow an attacker to access un \* @kind path-problem \* Oproblem.severity error GitHub \* @security-severity 7.5 \* Oprecision high \* @id java/path-injection 9 \* @tags security 10 external/cwe/cwe-022 external/cwe/cwe-023 11 12 external/cwe/cwe-036 13 external/cwe/cwe-073 \*/ 14 15 16 import java Unsafe 17 import semmle.code.java.security.TaintedPathQuery 18 import TaintedPathFlow::PathGraph from 19 where 20 from TaintedPathFlow::PathNode source, TaintedPathFlow::PathNode sink seled 21 where TaintedPathFlow::flowPath(source, sink) select sink.getNode(), source, sink, "This path depends on a \$0.", source.getNode(), 22 23 "user-provided value"

### Dataflow Analysis in Real Life: CodeQL

- Question:
  - When we have a programming language for static analysis...
  - Can we Synthesize Program in this language?

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# IRIS: LLM-Assisted Static Analysis for Detecting Security Vulnerabilities

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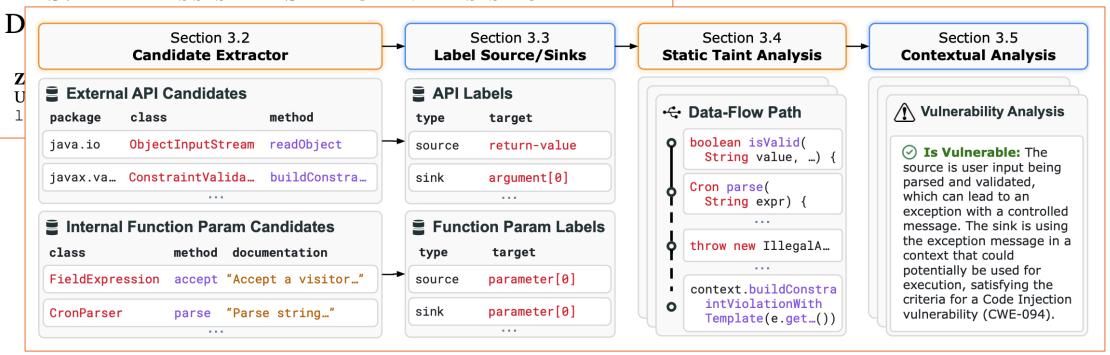
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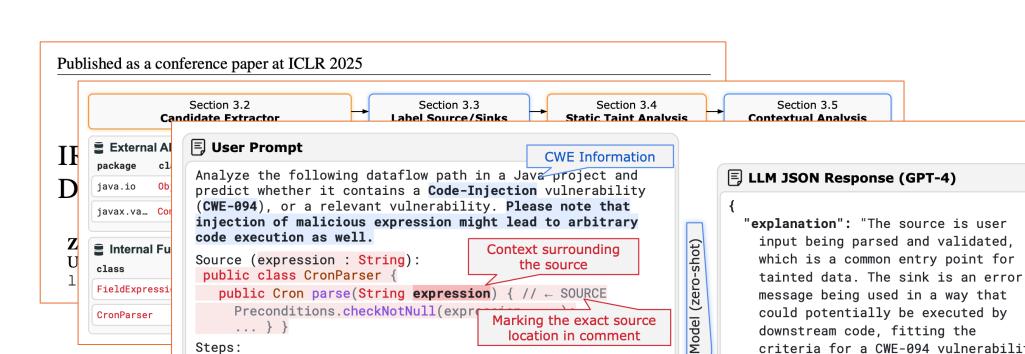
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#### IRIS: LLM-Assisted Static Analysis for





- Step 1 [CronParser.java]: String rep = expr.replace(...);

public class CronValidator implements ConstraintValidator {

ctx.build...(e.getMessage()).addCo...(); // 

SINK

Context surrounding

the sink

public boolean isValid(String value, ...) {

ctx.disableDefaultCor \_\_aintViolation();

Steps:

Sink (getMessage(...)):

} catch (IllegalArgu

return false;

} ... } }

location in comment

Marking the exact sink

location in comment

Intermediate Steps

Language

downstream code, fitting the

criteria for a CWE-094 vulnerability

if the error message is mishandled. However, without evidence of the

error message being executed, it's

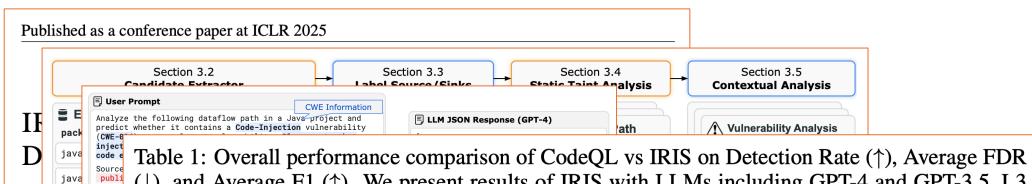
solely based on this dataflow.",

"source\_is\_false\_positive": false,

"sink\_is\_false\_positive": false,

"is\_vulnerable": true

speculative to confirm vulnerability



Steps: - Step

Sink

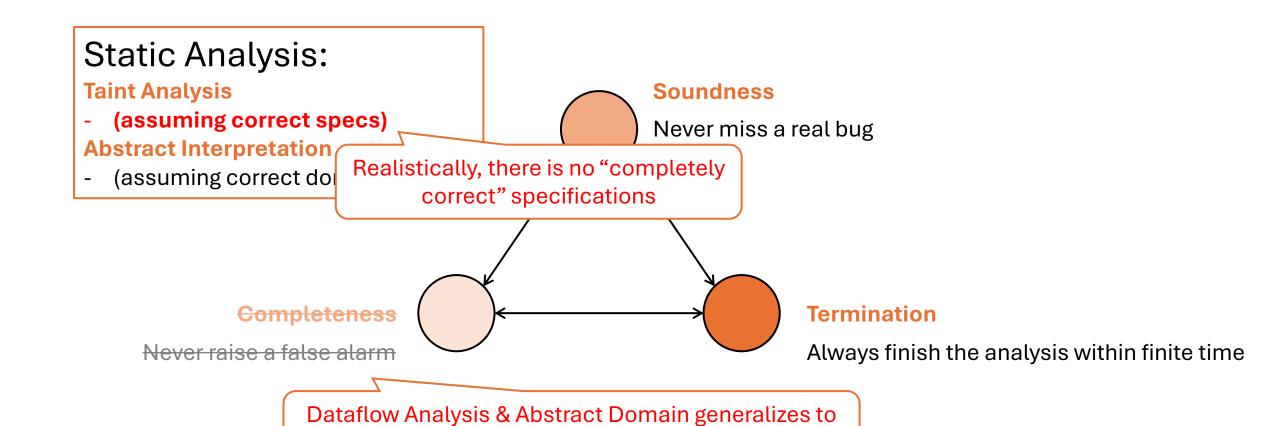
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Table 1: Overall performance comparison of CodeQL vs IRIS on Detection Rate (↑), Average FDR (↓), and Average F1 (↑). We present results of IRIS with LLMs including GPT-4 and GPT-3.5, L3 8B and 70B, Q2.5C 32B, G2 27B, and DSC 7B.

	Method	<b>#Detected</b> (/120)	<b>Detection Rate</b> $(\%)$	Avg FDR (%)	Avg F1 Score
	CodeQL	27	22.50	90.03	0.076
IRIS +	GPT-4 GPT-3.5 L3 8B L3 70B Q2.5C 32B	<b>55</b> († 28) 47 († 20) 41 († 14) 54 († 27) 47 († 20)	<b>45.83</b> († 23.33) 39.17 († 16.67) 34.17 († 11.67) 45.00 († 22.50) 39.17 († 16.67)	84.82 (\$\dagger\$ 5.21) 90.42 (\$\dagger\$ 0.39) 95.55 (\$\dagger\$ 5.52) 90.96 (\$\dagger\$ 0.93) 92.38 (\$\dagger\$ 2.35)	$0.177 (\uparrow 0.101)$ $0.096 (\uparrow 0.020)$ $0.058 (\downarrow 0.018)$ $0.113 (\uparrow 0.037)$ $0.097 (\uparrow 0.021)$
	G2 27B DSC 7B	45 († 18) 52 († 25)	$37.50 (\uparrow 15.00)$ $43.33 (\uparrow 20.83)$	91.23 († 1.20) 95.40 († 5.37)	0.100 († 0.024) 0.062 (\psi 0.014)

## Software Testing: Impossible Triangle



entire space of input, but loses precision

```
X Vuln Patch
                        LocalS3.java:124-125
                                                      Sanitizer Query
                                                                                                               xml_xxe_cve_2025_27136.ql
 + input.setProperty(SUPPORT_DTD, false);
                                                       class XmlXxeSanitizer extends DataFlow::Node { XmlXxeSanitizer() {
                                                         exists(MethodCall setPropCall |
                                                           setPropCall.getMethod().hasQName("...", "...", "setProperty") and
                                                           exists(Field f | setPropCall.getArgument(0) = f.getAnAccess() and
          Factory
                                LocalS3.java
                                                             f.hasName("SUPPORT_DTD") and ... ) and
                                                           exists(Field f | setPropCall.getArgument(1) = f.getAnAccess() and
           XMLInputFactory input =
                                                             f.hasName("false") and ... ) and ... ) } } // 12 lines omitted...
             new WstxInputFactory(); ...
           XmlMapper xmlMapper =
             new XmlMapper(
                                                     Taint Steps
                                                                                                               xml_xxe_cve_2025_27136.ql
               new XmlFactory(input, ...));
           serviceFactory.register(
                                                       predicate serviceRegisterFlowStep(DataFlow::Node n1, DataFlow::Node n2) {
             XmlMapper.class,
                                                         exists(MethodCall register, VarAccess xmlMapperVar |
             () -> xmlMapper);
                                                           register.getMethod().hasName("register") and
                                                           register.getMethod().getDeclType().hasQName("...", "ServiceFactory") and
                                                           exists(LambdaExpr lambda | lambda.getExprBody() = xmlMapperVar and ...)
            CreateBucketController.java
Source
                                                         or ... } // 40 lines omitted for other additional taint steps...
                                          (Additional Taint Steps)
class CreateBucketController ... {
 public void handle(
                                                      Source Query
                                                                                                               xml_xxe_cve_2025_27136.ql
  HttpRequest req, HttpResponse res
  ) throws Exception {
                                                       class HttpRequestSource extends DataFlow::Node { HttpRequestSource() {
   InputStream inputStream =
                                                         exists(MethodCall getBodyCall | this.asExpr() = getBodyCall
   new ByteBufInput...(req.getBody())
                                                           getBodyCall.getMethod().hasName("getBody") and
                                                           getBodyCall.getQualifier().getType().hasQName("...", "HttpRequest") and
                                                          or ... } } // 9 lines omitted for other types of sources
      (dataflow path of 6 nodes)
Sink
                  CreateBucketController.java
                                                     Sink Ouerv
                                                                                                              xml_xxe_cve_2025_27136.ql
xmlMapper = serviceFactory
                                                       class XmlParsingXxeSink extends DataFlow::Node { XmlParsingXxeSink() {
   .getInstance(XmlMapper.class); ...
                                                         exists(MethodCall call | this.asExpr() = call.getArgument(0) and
 CreateBucketConf conf =
                                                           call.getMethod().hasName("readValue") and
   xmlMapper.readValue(
                                                           call.getMethod().getDeclType().hasQName("...", "XmlMapper")
     inputStream, CreateBucketConf.class);
                                                       }} // 6 lines omitted...
```

# Automated Static Vulnerability Detection via a Holistic Neuro-symbolic Approach

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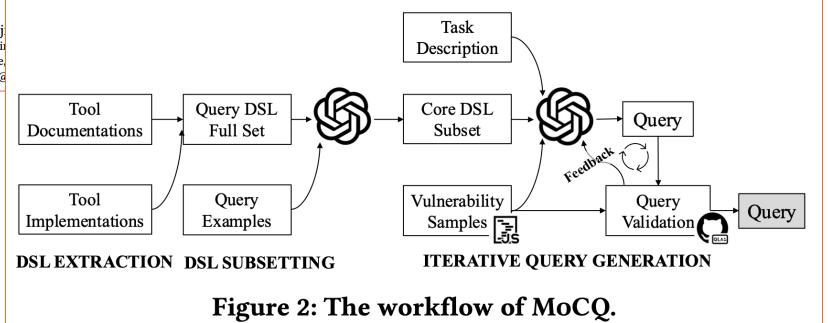
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#### Automated Static Vulnerability Detection via a Holistic Neuro-symbolic Approach

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#### Automated Static Vulnerability Detection via a Holistic

F Colu New pl268 Task Description

#### Tool Documentations

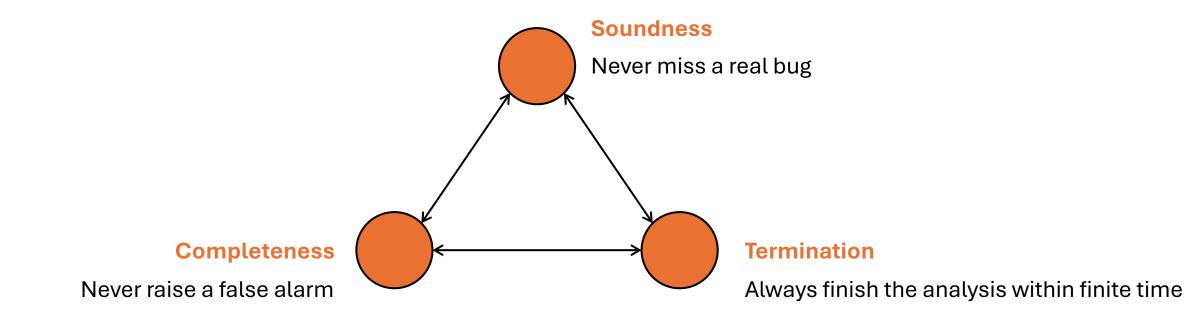
#### Table 1: New vulnerabilities discovered by MoCQ.

Tool Implementations

DSL EXTRACT

Project	Vul. Type	Experts'	MoCQ	Status
forkcms [42]	PHP SQLi	<b>✓</b>	<b>✓</b>	Reported
SyliusCmsPlugin [39]	PHP XSS	×	$\checkmark$	Reported
parse-static-imports [43]	JS Cmd.	×	$\checkmark$	Acknowledged
es2015-proxy [41]	JS Proto.	×	$\checkmark$	Acknowledged
web-worker [45]	JS Proto.	$\checkmark$	$\checkmark$	Reported
koa-send [46]	JS Proto.	$\checkmark$	$\checkmark$	Acknowledged
content-type [40]	JS Proto.	×	$\checkmark$	Reported

## Software Testing: Impossible Triangle



### Logistics – Week 9

- Assignment 3: Coding LLM Agents
  - <a href="https://github.com/machine-programming/assignment-3">https://github.com/machine-programming/assignment-3</a>
  - Fully functional web-app agent. Due: Oct 23 (Thu)
- Forming groups for your final projects!
  - Form a group of 2-3 before This Thursday (Oct 19 Oct 23)