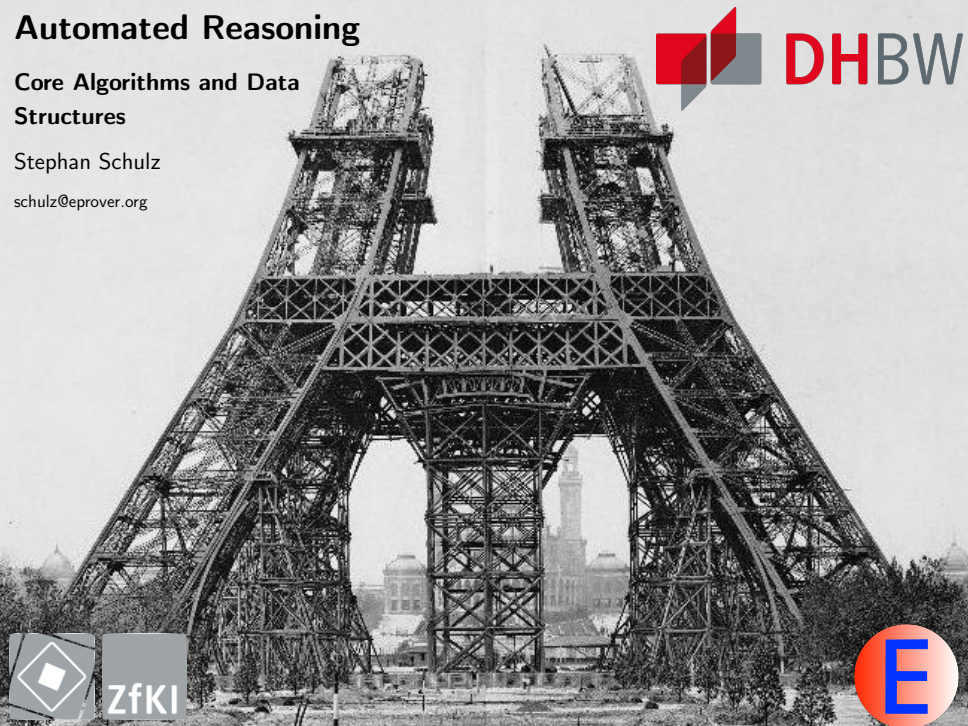


# Automated Reasoning

Core Algorithms and Data  
Structures

Stephan Schulz

[schulz@eprover.org](mailto:schulz@eprover.org)



## Abstract

We will look at some core concepts shared by nearly all modern automated theorem provers and related systems – terms, substitutions, unification, matching, as well as their applications, including paramodulation/superposition, rewriting, and subsumption. I will present actual code examples from PyRes and E, and discuss some implementation details.

We will then also attempt to develop a new, unification-based clause selection heuristic for E, and evaluate if it is a useful contribution to the portfolio of strategies.

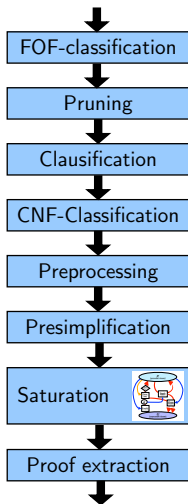
Participants are encouraged to bring a laptop with a UNIX/Linux style C development system, and/or a recent Python-3 installation for the practical work.

# Contents

- 1 Introduction
- 2 Basics
- 3 Implementing unification (Python)
- 4 Unification in C
- 5 Use case: Clause evaluation heuristics
- 6 References and Image credits

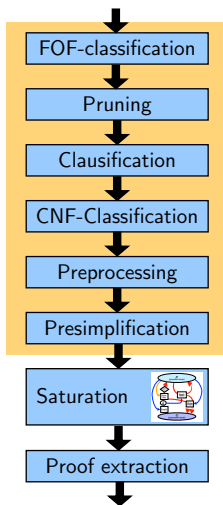
## **Introduction**

# Refutational Theorem Proving in First-Order Logic



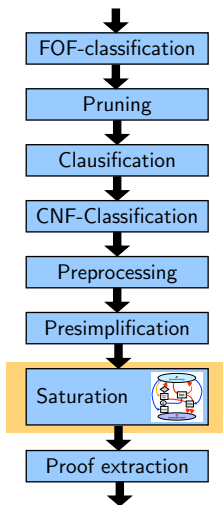
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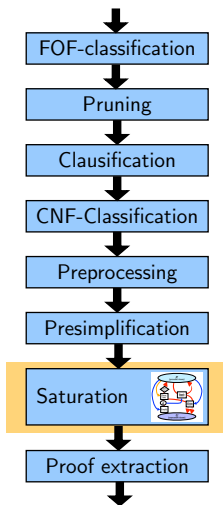
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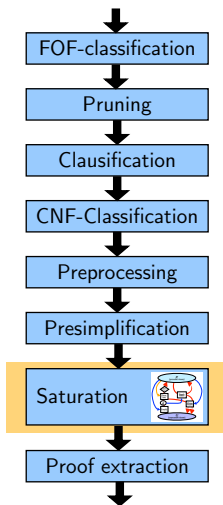
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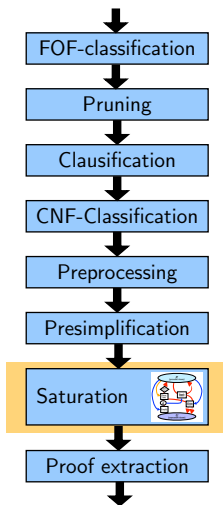


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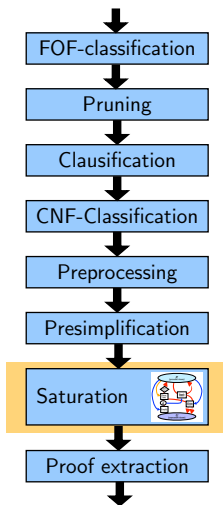
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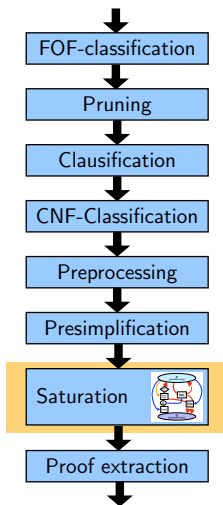
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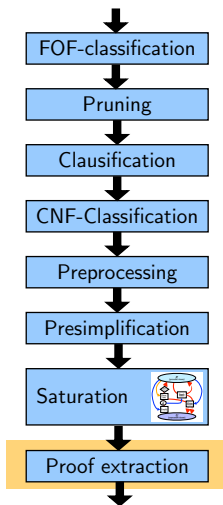
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    - 5 Desired result: Empty clause
- ▶ Do a lot of post-processing
  - ▶ Result: Proof object

# Saturation

- ▶ Assume a set of clauses  $C$
- ▶ While the set is not saturated do...
  - ▶ Pick matching premises and an inference rule
  - ▶ Apply the inference rule to the premises and add the result to  $C$
  - ▶ Perform **simplification** to remove **redundant** clauses from  $C$

(Equality Resolution)

$$\frac{u \not\preceq v \vee R}{\sigma(R)} \quad \text{if } \sigma = \text{mgu}(u, v), \dots$$

(Deletion of resolved literals)

$$\frac{s \not\preceq s \vee R}{R}$$

(Superposition into negative literals)

$$\frac{s \simeq t \vee S \quad u \not\preceq v \vee R}{\sigma(u[p \leftarrow t] \not\preceq v \vee S \vee R)} \quad \text{if } \sigma = \text{mgu}(u|_p, s), \dots$$

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## Generating inference rules

- Necessary for completeness
- Increase size of proof state

(Superposition into negative literals)

$$\frac{s \simeq t \vee S \quad u \not\preceq v \vee R}{\sigma(u[p \leftarrow t] \not\preceq v \vee S \vee R)} \quad \begin{array}{l} \text{if } \sigma = \text{mgu}(u|_p, s), \\ \sigma(s) \not\preceq \sigma(t), \dots \end{array}$$

## Simplification rules

- Critical for performance
- Reduce size of proof state

(Rewriting of negative literals)

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## Local (single premise)

- Easy to keep track of
- Cheap to implement

## Non-local (multiple premises)

- Harder to keep track of (pairs of clauses!)
- Expensive to implement (find partners)

(Superposition into negative literals)

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>99% of generated clauses

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>90% of cpu time

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## Basics

# First-Order Terms

## Definition (First-order terms)

We assume a set  $F$  of function symbols with associated arities (e.g.  $\{f/2, g/1, a/0, b/9\}$ ) and a set of first-order variables

$V = \{X, Y, Z, \dots\}$ . The set  $T(F, V)$  of **terms** is defined as follows:

- ▶  $V \subseteq T(F, V)$  (any variable is a term)
- ▶ If  $t_1, \dots, t_n$  are in  $T(F, V)$  and  $f/n \in F$ , then  $f(t_1, \dots, t_n) \in T(F, V)$  (an  $n$ -ary function symbol with  $n$  argument terms is a term)
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- 
- ▶ Examples (over the  $F, V$  given above):
    - ▶  $f(X, g(Y))$
    - ▶  $a()$  (usually written as  $a$  without parentheses -  $a$  is a **constant**)
    - ▶  $g(g(g(f(Y, b))))$

## Definition (Substitution)

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Let  $\sigma, \tau$  be two substitutions

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We can compute  $\tau \circ \sigma$  explicitly:

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Special case:  $\tau$  is of the form  $\{X \mapsto t\}$  and  $X$  is not bound by  $\sigma$ :

$$\tau \circ \sigma = \{X \mapsto \tau(\sigma(X)) \mid X \text{ is bound by } \sigma\} \cup \tau$$

## Definition (Unifier, most general unifier)

Let  $s, t$  be two terms.

A **unifier** for  $s, t$ ...

- ▶ is a substitution  $\sigma$
- ▶ such that  $\sigma(s) = \sigma(t)$ .

A unifier  $\sigma$  for  $s, t$  is called a **most general unifier** ...

- ▶ if every other unifier  $\sigma'$  of  $s, t$  can be written as  $\tau \circ \sigma$  for some substitution  $\tau$



## Definition (Unifier, most general unifier)

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- ▶ Fact: MGUs can be found systematically

# Why is unification interesting?

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# Why is unification interesting?

- ▶ *The calculus says I need unifiers!*
- ▶ But why?
  - ▶ Terms represent **sets of objects**
  - ▶ Atomic formulas are statements about sets of objects
  - ▶ ...and so are clauses
- ▶ To usefully combine different knowledge fragments, they need to talk about a common set of objects
  - ▶ Unification determines if such a set exists...
  - ▶ ...and in the success case gives us a description of this common set

Unification finds **common instances** of terms/atoms/clauses, i.e. the intersection of the domains they make useful statements about!

# Observations on unification

- 1  $abs(X), dir(X)$  can never be unified
  - ▶ The first symbol is always different
- 2  $X, sqrt(X)$  can never be unified
  - ▶ No matter what is used for  $X$ , a  $sqrt$  always remains
  - ▶ “Occurs-Check”
- 3  $X, sqrt(a)$  unifies with  $\sigma = \{X \mapsto sqrt(a)\}$ 
  - ▶ A variable paired with most terms is fine
- 4  $add(X, a), add(b, Y)$  unifies with  $\sigma = \{X \mapsto b, Y \mapsto a\}$ 
  - ▶ The unifier can be composed from those necessary to unify particular subterms



# Unification as parallel equation solving

Fact: The unification problem becomes **simpler** when you consider it for sets of pairs of terms!

- ▶ Given:  $C = \{s_1 = t_1, s_2 = t_2, \dots, s_n = t_n\}$ 
  - ▶ Search **common mgu**  $\sigma$  with
    - ▶  $\sigma(s_1) = \sigma(t_1)$
    - ▶  $\sigma(s_2) = \sigma(t_2)$
    - ▶  $\dots$
    - ▶  $\sigma(s_n) = \sigma(t_n)$
- ▶ Use a transformation system ([LMM88])
  - ▶ State:  $C, \sigma$ 
    - ▶  $C$ : Set of equations to be solved
    - ▶  $\sigma$ : Candidate unifier
  - ▶ Initial state for finding  $\text{mgu}(s, t)$ :  $\{s = t\}, \{\}$
  - ▶ Termination:  $\{\}, \sigma$

# Unification: Transformation system

$$\text{Deletion: } \frac{\{t = t\} \cup C, \sigma}{C, \sigma}$$

$$\text{Bind: } \frac{\{X = t\} \cup C, \sigma}{\{X \mapsto t\}(C), \{X \mapsto t\} \circ \sigma} \text{ if } X \notin \text{Vars}(t)$$

$$\text{Orient: } \frac{\{t = X\} \cup C, \sigma}{\{X = t\} \cup C, \sigma} \text{ if } t \text{ is not a variable}$$

$$\text{Decompose: } \frac{\{f(s_1, \dots, s_n) = f(t_1, \dots, t_n)\} \cup C, \sigma}{\{s_1 = t_1, \dots, s_n = t_n\} \cup C, \sigma}$$

$$\text{Occurs: } \frac{\{X = t\} \cup C, \sigma}{\text{FAIL}} \text{ if } X \in \text{Vars}(t), t \neq X$$

$$\text{Conflict: } \frac{\{f(s_1, \dots, s_n) = g(t_1, \dots, t_m)\} \cup C, \sigma}{\text{FAIL}} \text{ if } f \neq g$$

## Unification algorithm (sketch)

```
def mgu(s, t):  
    C = {s=t}  
    sigma = {}  
    while C != {}:  
        remove arbitrary s=t from C  
        apply the matching rule to s=t, C, sigma  
        (modifying sigma and C as appropriate)  
        if result==FAIL:  
            return FAIL  
    return sigma
```



# Example

$C$	$\sigma$	Rule
$\{f(f(X, g(g(Y))), X) = f(f(Z, Z), U)\}$	$\{\}$	Decompose
$\{f(X, g(g(Y))) = f(Z, Z), X = U\}$	$\{\}$	Bind ( $X$ )
$\{f(U, g(g(Y))) = f(Z, Z)\}$	$\{X \mapsto U\}$	Decompose
$\{U = Z, g(g(Y)) = Z\}$	$\{X \mapsto U\}$	Bind ( $U$ )
$\{g(g(Y)) = Z\}$	$\{X \mapsto Z,$ $U \mapsto Z\}$	Orient
$\{Z = g(g(Y))\}$	$\{X \mapsto Z,$ $U \mapsto Z\}$	Bind ( $Z$ )
$\{\}$	$\{X \mapsto g(g(Y)),$ $U \mapsto g(g(Y)),$ $Z \mapsto g(g(Y))\}$	

## Pretty Code

# Python: Terms

- ▶ Terms are implemented as Python lists (equivalent to LISP s-expressions)
  - ▶ Variables are plain strings: "X", "Y", ...
  - ▶ Function symbols are plain strings: "f", "g", "sqrt", ...
  - ▶ Composite terms:  $[f, t_1, \dots, t_n]$ 
    - ▶  $f$  is the function symbol
    - ▶ The  $t_i$  represent the subterms
- ▶ Example:  $f(f(X, a), g(a))$ 
  - ▶ Python representation: `["f", ["f", "X", ["a"]], ["g", ["a"]]]`
- ▶ Functions include:
  - ▶ `termIsVar(t)` - return true if  $t$  is a variable
  - ▶ `termIsCompound(t)` - return true if  $t$  is not a variable
  - ▶ `termFunc(t)` - return the function symbol of compound term  $t$
  - ▶ `termArgs(t)` - return the argument list of compound term  $t$

# Python substitutions (basics)

```
class Substitution(object):
    def __init__(self, init = []):
        self.subst = {}
        for i in init:
            self.subst[i[0]] = i[1]

    def value(self, var):
        if var in self.subst:
            return self.subst[var]
        else:
            return var

    def apply(self, term):
        if termIsVar(term):
            return self.value(term)
        else:
            res = [termFunc(t)]
            args = [self.apply(x) for x in termArgs(term)]
            res.extend(args)
            return res
```

## Python substitutions (extension)

```
def isBound(self, var):  
    return var in self.subst  
  
def modifyBinding(self, binding):  
    var, term = binding  
    if self.isBound(var):  
        res = self.value(var)  
    else:  
        res = None  
    if term == None:  
        if self.isBound(var):  
            del self.subst[var]  
    else:  
        self.subst[var] = term  
    return res
```

## Python substitutions (limited composition)

```
def composeBinding(self, binding):
    tmpsubst = Substitution([binding])
    var, term = binding
    vars = self.subst.keys()
    for x in vars:
        bound = self.subst[x]
        self.subst[x] = tmpsubst.apply(bound)
    if not var in self.subst:
        self.subst[var] = term
```

## Python: Occurs check

```
def occursCheck(x, t):  
    """  
    --- Perform an occurs-check, i.e. determine if the variable  
    --- x occurs in the term t. If that is the case (and  
    --- t != x), the two can never be unified.  
    --- """  
    if termIsCompound(t):  
        for i in termArgs(t):  
            if occursCheck(x, i):  
                return True  
        return False  
    else:  
        return x == t
```

- Simple recursive descent

# Python Unification

```
def mguTermList(l1, l2, subst):
    while(len(l1)!=0):
        t1 = l1.pop(0)
        t2 = l2.pop(0)
        if termsIsVar(t1):
            if t1==t2:
                continue
            if occursCheck(t1, t2):
                return None
            new_binding = Substitution([(t1, t2)])
            l1 = [new_binding(t) for t in l1]
            l2 = [new_binding(t) for t in l2]
            subst.composeBinding((t1, t2))
        elif termsIsVar(t2):
            [symmetric case elided]
        else:
            if termFunc(t1) != termFunc(t2):
                return None
            l1.extend(termArgs(t1))
            l2.extend(termArgs(t2))
    return subst
```



## Hacking Time

# Beyond unification

- ▶ For heuristic evaluation, we want to go beyond unification success/failure
- ▶ We want a measure of "how close" two terms are to being unifiable
- ▶ Idea: Compute a **unification distance**
  - ▶ For unifiable term pairs the distance is 0
  - ▶ Otherwise, collect all unsolved equations
    - ▶ Compute numerical score from these unsolved equations
    - ▶ ...e.g. summing up the size of all terms involved
- ▶ Example: Trying to unify  $f(g(a), f(X, a))$  and  $f(g(b), f(g(X), Y))$ 
  - ▶ Repeated decomposition yields  $a = b$ ,  $X = g(X)$ ,  $a = Y$
  - ▶ The green equation is solvable, the red ones yield a unification distance of  $(1+1)+(1+2)=5$

## Exercise: Implement unification distance

- ▶ Implement unification distance in PyRes
- ▶ Suggestions:
  - ▶ Use the file `unification.py`
  - ▶ Steal what you can (we have limited time)
  - ▶ Integrate test code into the unit tests at the end of the file
  - ▶ To run the unit tests, just run the file (`./unification.py`)
  - ▶ What is the unification distance of  $p(a, b, c, X, Y)$  and  $p(b, c, d, f(a), f(Y))$ ?
- ▶ Reminder: `git clone`  
`https://github.com/eprover/PyRes.git`
- ▶ To run an example:
  - ▶ `cd PyRes`
  - ▶ `./pyres-fof.py -tifbp -HPickGiven5 -nlargest EXAMPLES/PUZ001+1.p`

# A note on matching

- ▶ *Matching* is the task of finding a substitution  $\sigma$  with  $\sigma(s) = t$ 
  - ▶ Substitution is only applied to one term (the *matching* term)
- ▶ Differences:
  - ▶ No occurs-check necessary
  - ▶ A binding once made is *invariant*
  - ▶ In particular: No composition of bindings
  - ▶  $X = X$  cannot be discarded, but must be bound
- ▶ Result: Matching is in  $\Theta(n)$ 
  - ▶ One linear pass is enough
  - ▶ Check `matching.py` for details in PyRes

## **Performance Code**

# PyRes vs. Performance

- ▶ PyRes is written with the aim of clarity
  - ▶ Performance is a secondary consideration
  - ▶ Python is not a high-performance language
- ▶ Can we do better?
  - ▶ Algorithmically?
  - ▶ Data-structure-wise?
  - ▶ Choosing a different language?

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**Yes, yes, and yes!**

- ▶ In practice, nearly all unification attempts fail!
  - ▶ No paramodulation into/resolution on first-order variables
  - ▶ 10 different function symbols  $\Rightarrow \approx 90\%$  conflict on the first symbol
- ▶ Efficient unification: Detect failures early
  - ▶ Prefer equations matching **Decompose** and **Conflict**
  - ▶ Delay equations matching **Orient**, **Bind**, **Occurs**
  - ▶ **Deletion** is only needed for equations of the form  $X = X$  (Why?)



# Data types in C

From E/cte\_termtypes.h:

```
typedef struct termcell
{
    FunCode          f_code;      /* Top symbol of term */
    TermProperties    properties; /* Boolean flags */
    int               arity;
    struct termcell* binding;      /* For variable bindings,
                                   potentially for temporary
                                   rewrites */

    [...a lot of members elided...]
    struct termcell* args[];      /* Flexible array member contain
                                   the arguments */
} TermCell, *Term_p, **TermRef;
```

- ▶ Function symbol/variable encoded as FunCode (i.e. long)
- ▶ Arguments as flexible array member

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```

- ▶ Function symbol/variable encoded as FunCode (i.e. long)
- ▶ Arguments as flexible array member
- ▶ Variable binding directly in the term cell

# Shared terms and shared variable bindings

- ▶ E aggressively **shares** terms [Sch25]
  - ▶ Every long-lived term is represented only once
  - ▶ Variables are even more aggressively shared - every variable corresponds to exactly one term cell (even in unshared terms)
  - ▶ Originally inspired by DeDam [NRV97], although the relationship is hard to recognise now. . .
- ▶ What does that mean?
  - ▶ If we bind a variable anywhere, we bind a variable everywhere
  - ▶ Some application of substitutions to complex structures can be done locally (if we have the variables in hand)

## Substitutions in E

```
typedef PStack_p    Subst_p ;
```

# Substitutions in E

```
typedef PStack_p    Subst_p ;
```

- ▶ A substitution is just a stack (of term cell pointers)
  - ▶ When a variable is bound, the binding is recorded in the term cell
  - ▶ The fact that this binding is part of a substitution is recorded by pushing the variable onto the substitution
  - ▶ In other words, a single binding is the pair  $(v, v \rightarrow \text{binding})$
  - ▶ Each bound variable (representing the binding) is on the stack
- ▶ Allows for fast backtracking
- ▶ Since variables are shared, adding a binding is the same as composing a new binding with the substitution!
- ▶ Big performance gain
  - ▶ Intermediate results are represented implicitly
  - ▶ Deleting them is nearly free

# Backtracking substitutions

```
PStackPointer SubstAddBinding(Subst_p subst, Term_p var,
                               Term_p bind)
{
    PStackPointer ret = PStackGetSP(subst);
    var->binding = bind;
    PStackPushP(subst, var);
    return ret;
}

bool SubstBacktrackSingle(Subst_p subst)
{
    Term_p handle;
    if (PStackEmpty(subst))
    {
        return false;
    }
    handle = PStackPopP(subst);
    handle->binding = NULL;
    return true;
}
```

# Substitution code

```
int SubstBacktrackToPos(Subst_p subst , PStackPointer pos)
{
    int ret = 0;
    while(PStackGetSP(subst) > pos)
    {
        SubstBacktrackSingle(subst);
        ret++;
    }
    return ret;
}
```

```
int SubstBacktrack(Subst_p subst)
{
    int ret = 0;
    while(SubstBacktrackSingle(subst))
    {
        ret++;
    }
    return ret;
}
```

## Unification code in E - Prologue

```
bool SubstComputeMgu(Term_p t1, Term_p t2, Subst_p subst)
{
    if ((TermCellQueryProp(t1, TPPredPos) && TermIsFreeVar(t2)) ||
        (TermCellQueryProp(t2, TPPredPos) && TermIsFreeVar(t1)))
    {
        return false;
    }
    PStackPointer backtrack = PStackGetSP(subst); /* For backtra

    bool res = true;
    PQueue_p jobs = PQueueAlloc();

    PQueueStoreP(jobs, t1);
    PQueueStoreP(jobs, t2);
}
```



## Unification code in E - Orient, Bind

```
while (!PQueueEmpty(jobs))
{
    t2 = TermDerefAlways(PQueueGetLastP(jobs));
    t1 = TermDerefAlways(PQueueGetLastP(jobs));
    if (TermIsFreeVar(t2))
    {
        SWAP(t1, t2);
    }
    if (TermIsFreeVar(t1))
    {
        if (t1 != t2)
        {
            if ((t1->type != t2->type) || OccurCheck(t2, t1))
            {
                res = false;
                break;
            }
            else
            {
                SubstAddBinding(subst, t1, t2);
            }
        }
    }
}
```

## Unification code in E - Conflict

```
else
{
    if(t1->f_code != t2->f_code)
    {
        res = false;
        break;
    }
    else
    {
```

## Unification code in E - Decompose

```
for(int i=t1->arity-1; i>=0; i--)
{
    /* Delay variable bindings */
    if(TermlsFreeVar(t1->args[i]) ||
        TermlsFreeVar(t2->args[i]))
    {
        PQueueBuryP(jobs, t2->args[i]);
        PQueueBuryP(jobs, t1->args[i]);
    }
    else
    {
        PQueueStoreP(jobs, t1->args[i]);
        PQueueStoreP(jobs, t2->args[i]);
    }
}
}
```

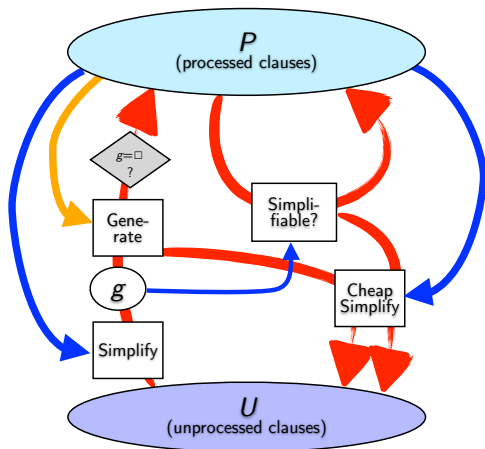
## Unification code in E - Epilogue

```
PQueueFree(jobs);  
  
if (!res)  
{  
    SubstBacktrackToPos(subst, backtrack);  
}  
return res;  
}
```

(see E/TERMS/cte\_match\_mgu\_1-1.[ch])

## Using Unification Distance

## Given Clause Loop



- ▶ While there are unprocessed clauses ...
  - ▶ ... **heuristically pick** given clause from  $U$
  - ▶ ... and process it
- ▶ Goal: Generate **empty clause**
- ▶ Choice point: Pick the next given clause
  - ▶ Based on heuristic weight (small is beautiful)

# Unification distance in clause evaluation

- ▶ We are in an equational context:
  - ▶ Literals are equations or disequations
  - ▶ Goal: Empty clause (get rid of all literals)
- ▶ Consider  $a \not\simeq X \vee f(X, a) \simeq a$ 
  - ▶ Implicational form:  $a \simeq X \rightarrow f(X, a) \simeq a$
  - ▶ So: If we can solve the first literal, the second becomes available for rewriting
  - ▶ So: Negative literals that can be resolved (by unification) are desirable
  - ▶ Maybe: Negative literals that can be **nearly** resolved are too?
- ▶ Idea: Base literal evaluation on unification distance
  - ▶ Sum them up (cleverly) for clauses
  - ▶ Cleverly: What do we do for positive literals?

# Hacking session 2

- ▶ Reminder: E lives at <https://www.eprover.org>
- ▶ ...or at <https://github.com/eprover/eprover>
  - ▶ ...which also displays the installation information
- ▶ Option 1:
  - ▶ Improve the PyRes unification algorithm
  - ▶ Steal ideas from the C version
- ▶ Option 2:
  - ▶ Implement unification distance in E
  - ▶ Use it to implement a new clause evaluation heuristic



# Clause evaluation in E

- ▶ All relevant code is in E/HEURISTICS/
- ▶ Each clause evaluation function needs 3 C functions:
  - ▶ `WFCB_p MyEvalParse((Scanner_p in, OCB_p ocb, ProofState_p state)`
  - ▶ `WFCB_p MyEvalInit(ClausePrioFun prio_fun, ...)` (which will only be called from `MyEvalParse()`)
  - ▶ `double MyEvalCompute(void* data, Clause_p clause)` (which will be called for each clause)
- ▶ You need to register your new function in `che_wfcbadm.in.c`
  - ▶ External name goes into `WeightFunParseFunNames[]`
  - ▶ Parse function goes into `WeightFunParseFun[]` (at the corresponding index)
- ▶ Check e.g. `TPTPTypeWeight*` in `HEURISTICS/che_varweights.h` for a simple example

# Conclusion

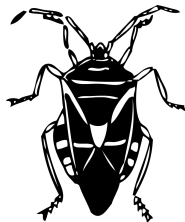
- ▶ First steps into some data structures
  - ▶ Terms
  - ▶ Substitutions
- ▶ Unification as equation solving ...
  - ▶ ...not as a theoretical approach, but as a practical implementation
- ▶ Some hacking experience with real ATPs gained(?!?)

# Conclusion

- ▶ First steps into some data structures
  - ▶ Terms
  - ▶ Substitutions
- ▶ Unification as equation solving ...
  - ▶ ...not as a theoretical approach, but as a practical implementation
- ▶ Some hacking experience with real ATPs gained(!?)

**I hope you had fun!**

- Bug reports for E should include:
  - The exact command line leading to the bug
  - All input files needed to reproduce the bug
  - A description of what seems to be wrong
  - **The output of `eprover --version`**



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  - ▶ *Tour Eiffel* under construction  
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- ▶ Others: Painstakingly drawn by the author