## ChemLAB COMS W4115 - Programming Languages & Translators Professor Stephen Edwards

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## Introduction

ChemLab is a language that will allow users to conveniently manipulate chemical elements. It can be used to solve chemistry and organic chemistry problems including, but not limited to, stoichiometeric calculations, oxidation-reduction reactions, acid-base reactions, gas stoichiometry, chemical equilibrium, thermodynamics, stereochemistry, and electrochemistry. It may also be used for intensive study of a molecule's properties such as chirality or aromaticity. These questions are mostly procedural and there is a general approach to solving each specific type of problem. For example, to determine the molecular formula of a compound: 1) use the mass percents and molar mass to determine the mass of each element present in 1 mole of compound 2) determine the number of moles of each element present in 1 mole of compound. Albeit these problems can generally be distilled down to a series of plug-and-chug math calculations, these calculations can become extremely tedious to work out by hand as molecules and compounds become more complex (imagine having to balance a chemical equation with Botox:  $C_{6760}H_{10447}N_{1743}O_{2010}S_{32}$ ). Our language can be used to easily create programs to solve such problems through the use of our specially designed data types and utilities.

## Language Tutorial

## 1.1 Program Execution

To compile a .chem program, simply use the compilation shell script with your .chem file as the only argument. ./compile.sh yourProgram.chem

After compilation, if there are no errors, there will be a Java program that gets created. One can the compile the Java program into an executable using javac.

### 1.2 Variables

Variables in ChemLAB must be declared as a specific type. To use a variable, declare the type of the variable, and assign it to the value that you want like this:

```
int myNum = 5;
String hello = "World";
```

### 1.3 Control Flow

```
ChemLAB supports "if/else" statements:
if(10>6){
print("inside the if");
else{
print("inside the else");
```

```
}
ChemLAB supports "while loops":
while(i > 0){
print(i);
i = i-1;
}
```

### 1.4 Functions

Functions are the basis of ChemLAB. Functions can be passed any amount of parameters and are declared using the function keyword. The parameters within a function declaration must have type specifications.

This is a function that takes in two parameters:

```
function add (int a, int b){
  return a+b;
}
This is a function that takes in no parameters:
function noParam(){
  print("Hello World");
  return 1;
}
```

## 1.5 Printing to stdout

```
To print to stdout, simply use the built-in function "print" print(6); print("Hello World");
```

# Language Reference Manual

## Project Plan

Like any project, careful planning and organization is paramount to the success of the project. More importantly however, is the methodical execution of the plan. Although we originally developed a roadmap for success as well as implemented a number of project management systems, we did not follow the plan as intended. This section outlines our proposed plans for making ChemLAB happen and the actual process that we went through.

### 3.1 Proposed Plan

We had originally planned to use the waterfall model in our software development process in which we would first develop a design for our language, followed by implementation, and finally testing. The idea was for all team members to dedicate complete focus to each stage in the project. Especially since we only had three members on our team, our roles were not as distinct and everyone had the chance to work, at least in some capacity, in all the roles. We intended to meet consistently each week on for at least two hours. During our meetings, each member was suppose to give an update about what he or she had been working on the past week as well as plans for the upcoming week and any challenges he or she faced that required the attention of the rest of the group. To help facilitate communication and the planning of meetings, we used Doodle to vote on what times were best for meetings. Also, in order to improve team dynamics, we planned to meet at least once every two weeks outside the context of school in order to hang out and have fun. Development would occur mostly on Mac OS and Windows 7, using the latest versions of OCaml, Ocamllex, and OCamlyacc for the compiler. We used Github for version control and makefiles to ease the work of compiling and testing code. The project timeline that we had laid out at the beginning was as follows:

• Sept 24th: Proposal Due Date

• Oct 2nd: ChemLAB syntax roughly decided upon

• Oct 23th: Scanner/Parser/AST unambiguous and working

• Oct 27th: LRM Due Date

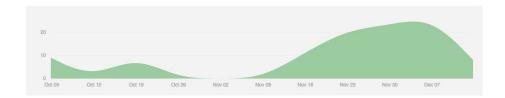
• Nov 9th: Architectural design finalized

• Dec 5th: Compile works, all tests passed

• Dec 12th: Project report and slides completed

• Dec 17th: Final Project Due Date

### 3.2 What Actually Happened



This graph was pulled from Github reflecting the number of commits being made over the span of this semester. Due to schedule conflicts and a false sense of security, we did not start intensely working on the project until after Thanksgiving break. Since we did not coordinate the development of the Scanner, AST, and parser with the writing of the LRM, our language did not have as concrete a structure as we had hoped. Furthermore, we did not have enough time to implement some of the features in our language such as object-orientation or more built-in functions. As we were developing the software, we did make sure to allow testing at all steps in the design process. In the test script, we had identifiers for how far in the compilation process we wanted the program to run. Thus, we were able to maintain testing capabilities even before all of our code was ready. We discuss the testing procedure in more detail in a subsequent section.

## 3.3 Team Responsibilities

This subsection describes the contributions made by each team member:

• Project Proposal - Gabriel L/Alice C/Martin O

- Scanner Gabriel L
- AST Alice C/Gabriel L/Martin O
- Parser Alice C/Martin O
- $\bullet\,$  LRM Gabriel L
- Code Generation Alice C
- Semantic Analyzer -Gabriel L/Martin O
- Testing Martin O
- $\bullet\,$  Final Report Gabriel L/Martin O

## 3.4 Project Log

We add later

# Architectural Design

Test Plan

# Lessons Learned

## Appendix A

## Code Listing

### ../ast.ml

```
type operator = Add | Sub | Mul | Div | Equal | Neq | Lt | Leq | Gt | Geq
    type re = And | Or
    type bool = True | False
    type data_type = IntType | BooleanType | StringType | DoubleType |
        ElementType | MoleculeType | EquationType
    type variable =
7
    Var of string
9
    type expr =
10
         Binop of expr * operator * expr
11
         \mathbf{Brela} \ \mathbf{of} \ \mathbf{expr} \ * \ \mathbf{re} \ * \ \mathbf{expr}
12
         Int of int
13
         String of string
14
         Boolean of bool
15
         Double of float
16
         Asn of string * expr
17
         Equation of string * variable list * variable list
18
         Concat of expr * expr
19
         \mathbf{Seq} \ \mathbf{of} \ \mathbf{expr} \ * \ \mathbf{expr}
20
         Print of expr
21
         List of expr list
22
         Call of string * expr list
23
         Access of expr * string
24
         Draw of string * int * int
25
         Null
26
        Noexpr
27
28
    type stmt =
29
         Block of stmt list
      Expr of expr
```

```
Return of expr
32
        If of expr * stmt * stmt
33
        For \mathbf{of} expr * expr * expr * stmt
34
        While of expr * stmt
35
      | Print of expr
36
37
    type variable_decl = {
38
     vname : string;
39
      vtype : data_type;
40
41
42
    type element_decl = {
43
     name : string;
44
      mass : int;
45
      electrons : int;
46
      charge : int;
47
48
    type molecule_decl = {
49
50
     mname : string;
51
      elements: variable list;
52
53
54
   type rule =
55
        Balance of string
56
        | Mass of string
57
58
    type par_decl = {
59
     paramname : string; (* Name of the variable *)
60
      paramtype : data_type; (* Name of variable type *)
61
62
    type func_decl = {
63
64
      fname : string;
65
      formals : par_decl list;
      locals: variable_decl list;
66
67
      elements : element_decl list;
68
      molecules : molecule_decl list;
69
      rules : rule list;
70
      body: stmt list;
71
72
73
    (* type program = {
74
      gdecls : var_decl list;
75
      fdecls : func_decl list
76
77
    *)
   type program = func_decl list
```

#### ../scanner.mll

```
{ open Parser }
2
3
    rule token = parse
        [', ', '\t', '\r', '\n']
4
                                          { token lexbuf }
                                 { comment lexbuf }
5
6
         ,(,
                                   { LPAREN }
 7
                                   RPAREN }
8
                                   LBRACKET }
9
                                   RBRACKET }
10
                                   LCURLY }
11
                                   RCURLY }
12
                                 { STRINGDECL }
13
                                           { SEMI }
         ': '
14
                                            COLON }
15
                                            COMMA }
16
                                            ACCESS }
17
                                            PLUS }
18
                                            MINUS }
19
         ,_{*},
                                            TIMES }
20
                                            DIVIDE }
        ,%,
21
                                            MOD }
22
         '=
                                            ASSIGN }
23
                                 { ARROW
         , ~ ,
24
                                            CONCAT }
25
        "___"
                                            EQ }
        "!="
26
                                            NEQ }
27
        ,<,
                                            LT }
28
        "<="
                                            LEQ }
        ,>,
29
                                            GT }
        ">="
30
                                            GEQ }
31
        "&&"
                                            AND }
32
        " | ]"
                                          { OR }
        , į ,
33
                                          { NOT }
        " i f"
34
                                   { IF }
        "else"
35
                                   { ELSE }
        "while"
36
                                   { WHILE }
                                 { FOR }
37
        "for"
38
        " int"
                                   { INT }
39
        "double"
                                      { DOUBLE }
40
        "string"
                                   { STRING }
        "boolean"
41
                                      { BOOLEAN }
42
        "element"
                                      { ELEMENT }
43
        "molecule"
                                      { MOLECULE}
44
        "equation"
                                      { EQUATION }
45
        "Balance"
                                   { BALANCE }
        "mass"
46
                                      { ATTRIBUTE(attr) }
                    as attr
        "charge"
47
                                        { ATTRIBUTE(attr)
                     as attr
        "electrons" as attr
48
                                        { ATTRIBUTE(attr) }
        "function"
49
                                      { FUNCTION }
```

```
"object"
50
                                 { OBJECT }
51
       "return"
                                 { RETURN }
52
       "true"
                               { BOOLEAN_LIT(true) }
53
       "false"
                               { BOOLEAN_LIT(false) }
       "print"
54
                               { PRINT }
       "Call"
55
                             { CALL }
       "Draw"
56
                             { DRAW }
57
       ['0' - '9'] + as lxm
                                     { INT_LIT(int_of_string lxm) }
       ('0') | ['1'-'9']+['0'-'9']*)(['.']['0'-'9']+)? as lxm { DOUBLE_LIT(
         float_of_string lxm) }
       59
       ;,,, [,,,,]* ,,, as lxm
60
                                      { STRING_LIT(lxm) }
       ['A'-'Z']['a'-'z']* as lxm
                                      { ELEMENT_LIT(lxm)}
61
62
       (['A'-'Z']['a'-'z']*['0'-'9']*)+ as lxm
                                                  { MOLECULE_LIT(lxm)}
63
       eof
                                     { EOF }
                               { raise (Failure("illegal character " ^
64
     as char
65
                           Char.escaped char)) }
66
67
   and comment = parse
68
       " */"
                     { token lexbuf }
69
                   { comment lexbuf }
```

#### ../parser.mly

```
1
   %{ open Ast
2
      let parse_error s = (* Called by parser on error *)
3
       print_endline s;
4
       flush stdout
   %}
5
6
   %token SEMI LPAREN RPAREN LBRACKET RBRACKET LCURLY RCURLY COMMA STRINGDECL
       COLON ACCESS CONCAT NOT OBJECT ARROW
   %token PLUS MINUS TIMES DIVIDE MOD PRINT ASSIGN
   %token EQ NEQ LT LEQ GT GEQ EQUAL
9
10
   %token RETURN IF ELSE FOR WHILE INT DOUBLE STRING BOOLEAN ELEMENT MOLECULE
11
       EQUATION FUNCTION
12
   %token INT DOUBLE STRING BOOLEAN ELEMENT MOLECULE EQUATION FUNCTION
13
   %token CALL ACCESS DRAW
14
   %token BALANCE MASS CHARGE ELECTRONS
15
   %token AND OR
   %token INT BOOLEAN STRING DOUBLE
16
   %token <string> DATATYPE ATTRIBUTE
17
   |%token <bool> BOOLEAN_LIT
18
19
   |%token <string> ELEMENT_LIT
   |%token <string> MOLECULE_LIT
   |%token <string> STRING_LIT
21
   %token <string> ID
   %token <int> INT_LIT
  |%token <float > DOUBLE_LIT
```

```
%token EOF
26
27
   %nonassoc NOELSE
28
   %nonassoc ELSE
29
   %right ASSIGN
30
   %left ACCESS
   %left OR
   %left AND
33
   %left EQ NEQ
34
   %left LT GT LEQ GEQ
   %left PLUS MINUS
36
   %left TIMES DIVIDE
37
   %start program
   %type <Ast.program> program
40
41
   %%
42
   program:
43
     { [] }
                                                         { ($2 :: $1) }
44
      | program fdecl
45
46
   id:
                                                   { $1 }
47
     ID
                                                       { $1 }
48
      | STRING_LIT
49
       ELEMENT_LIT
                                                         { $1 }
                                                         { $1 }
50
      | MOLECULE_LIT
51
52
   var:
     id {Var($1)}
53
54
55
56
   vdecl:
57
      datatype ID SEMI
58
      \{ \{ \text{vname} = \$2 ; \}
59
       vtype = $1;
60
      } }
61
62
    vdecl_list:
63
      | vdecl_list vdecl {($2::$1)}
64
65
66
   stmt:
                                       { Expr($1) }
67
       expr SEMI
68
                                           { Return($2)}
       RETURN expr SEMI
                                             69
       LCURLY stmt_list RCURLY
70
       IF LPAREN expr RPAREN stmt %prec NOELSE
71
       IF LPAREN expr RPAREN stmt ELSE stmt
                                                     { If($3, $5, $7)}
       FOR LPAREN expr SEMI expr SEMI expr RPAREN stmt \{ For(\$3, \$5, \$7, \$9) \}
72
73
       WHILE LPAREN expr RPAREN stmt
                                                     { While ($3, $5) }
74
       PRINT expr SEMI
                                           { Print($2)}
```

```
75
 76
    stmt_list:
 77
       /* nothing */ { [] }
 78
       | stmt_list stmt { ($2 :: $1) }
 79
 80
    datatype:
                 \{ IntType \}
 81
         INT
 82
        BOOLEAN
                    { BooleanType }
 83
        STRING { StringType }
 84
       | DOUBLE { DoubleType }
 85
 86
    expr:
                                              { Int($1) }
 87
      INT_LIT
 88
       | id
                                           { String($1) }
        PRINT expr SEMI { Print($2)}
 89
 90
        EQUATION id LCURLY element_list ARROW element_list RCURLY
                                                                         { Equation ($2
           , \$4, \$6) \}
 91
         expr PLUS expr
                                                  \{ Binop(\$1, Add, \$3) \}
                                                    { Binop($1, Sub, $3) }
 92
         expr MINUS expr
                                                     Binop($1, Mul, $3) }
 93
         expr TIMES expr
 94
         expr DIVIDE expr
                                                    \{ Binop(\$1, Div, \$3) \}
 95
         expr LT expr
                                                  \{ Binop(\$1, Lt, \$3) \}
                                                  \{ Binop(\$1, Gt, \$3) \}
96
         expr GT expr
         expr LEQ expr
97
                                                  \{ Binop(\$1, Leq, \$3) \}
98
         expr AND expr
                                                          { Brela($1, And, $3) }
99
         expr OR expr
                                                          { Brela($1, Or, $3) }
100
         id ASSIGN expr
                                                  \{ Asn(\$1, \$3) \}
                                                    { Concat($1, $3) }
101
         expr CONCAT expr
        CALL id LPAREN actuals_opt RPAREN
102
                                                            \{ Call(\$2, \$4) \}
103
                                                      { Access($1, $3) }
         expr ACCESS ATTRIBUTE
        DRAW LPAREN STRING_LIT COMMA INT_LIT COMMA INT_LIT COMMA INT_LIT COMMA
104
          INT_LIT COMMA INT_LIT COMMA INT_LIT COMMA INT_LIT RPAREN
           { Draw($3, $5, $7, $9, $11, $13, $15, $17, $19) }
105
106
107
108
    edecl:
      ELEMENT id LPAREN INT_LIT COMMA INT_LIT COMMA INT_LIT RPAREN SEMI
109
110
111
         name = $2;
112
         mass = \$4;
113
         electrons = \$6;
114
         charge = \$8
115
116
      }}
117
118
     edecl_list:
119
                                 { [] }
120
        | edecl_list edecl
                                   { List.rev ($2 :: $1)}
121
```

```
122
123
    mdecl:
124
      MOLECULE id LCURLY element_list RCURLY SEMI
125
126
        mname = \$2;
127
        elements = \$4;
128
129
130
    m decl_list:
131
      { [] }
      | mdecl_list mdecl { ($2 :: $1) }
132
133
134
    element_list:
135
      var
                         { [$1] }
136
      | element_list COMMA var { ($3 :: $1)}
137
138
     rule:
139
      BALANCE LPAREN id RPAREN SEMI {Balance($3)}
140
141
142
     rule_list:
143
      {[]}
      144
145
146
    formals_opt:
147
      /* nothing */
                             { [] }
                             { List.rev $1 }
148
      | formal_list
149
150
    formal_list:
                           { [$1] }
151
      param_decl
      | formal_list COMMA param_decl { $3 :: $1 }
152
153
154
    actuals_opt:
155
       /* nothing */
                               { List.rev $1 }
156
      | actuals_list
157
158
    actuals_list:
159
                                     { [$1] }
        expr
      | actuals_list COMMA expr
160
                                    { $3 :: $1 }
161
162
    param_decl:
163
      datatype id
        \{ \{ paramname = \$2; \}
164
165
          paramtype = $1 } }
166
167
168
      FUNCTION id LPAREN formals_opt RPAREN LCURLY vdecl_list edecl_list
          mdecl_list rule_list stmt_list RCURLY
169
170
        fname = \$2;
```

```
171 | formals = $4;

172 | locals = List.rev $7;

173 | elements = List.rev $8;

174 | molecules = List.rev $9;

175 | rules = List.rev $10;

176 | body = List.rev $11

177 | }
```

#### ../semantic.ml

```
open Ast
    open Str
3
   \mathbf{type} \ \mathrm{env} \, = \, \{
4
5
     mutable functions : func_decl list;
6
 7
8
    let function_equal_name name = function
9
      func-> func.fname = name
10
11
    let function_fparam_name name = function
12
      par -> par.paramname = name
13
14
    let function_var_name name = function
15
      variable -> variable.vname = name
16
17
    (* Checks whether a function has been defined duplicately *)
    let function_exist func env =
18
19
      let name = func.fname in
20
         \mathbf{try}
21
           let _ = List.find (function_equal_name name) env.functions in
22
             let e = "Duplicate function: "^ name ^" has been defined more than
                 once" in
23
                raise (Failure e)
24
        with Not-found -> false
25
26
27
    (*Checks if function has been declared*)
28
    let exist_function_name name env = List.exists (function_equal_name name) env
        . functions
29
30
31
    let get_function_by_name name env =
32
33
           let result = List.find (function_equal_name name) env.functions in
34
35
      with Not_found -> raise (Failure ("Function" ^ name ^ " has not been declared
36
37
```

```
let get_formal_by_name name func =
39
40
        let result = List.find(function_fparam_name name) func.formals in
41
42
      with Not-found -> raise (Failure ("Formal Param" ^ name ^ " has not been
         declared!"))
43
44
    let get_variable_by_name name func =
45
      \mathbf{try}
46
        let result = List.find(function_var_name name) func.locals in
47
      with Not_found -> raise (Failure ("Local Variable" ^ name ^ "has not been
48
         declared!"))
49
50
51
    let count_function_params func = function
52
      a \rightarrow let f count b =
      if b = a
53
54
        then count+1
55
        else count
56
    in
57
      let count = List.fold_left f 0 func.formals in
58
        if count > 0
59
          then raise (Failure ("Duplicate parameter in function" ^ func.fname))
60
          else count
61
62
    let count_function_variables func = function
63
64
      a \rightarrow let f count b =
65
      if b = a
66
        then count+1
67
        else count
68
    in
69
      let count = List.fold_left f 0 func.locals in
70
        if count > 0
71
          then raise (Failure ("Duplicate variable in function" ^ func.fname))
72
          else count
73
74
    (*Determines if a formal paramter with the given name
                                                               fpname
       the given function*)
76
    let exists_formal_param func fpname =
77
78
    List.exists (function_fparam_name fpname) func.formals
    with Not-found -> raise (Failure ("Formal Parameter" ^ fpname ^ " should
79
       exist but was not found in function " ^ func.fname))
80
81
82
    (*Determines if a variable declaration with the given name
                                                                   v n a m e
                                                                               exists
        in the given functioin*)
```

```
83
    let exists_variable_decl func vname =
84
85
86
     List.exists (function_var_name vname) func.locals
    with Not-found -> raise (Failure ("Variable " ^ vname ^ " should exist but
87
        was not found in function " ^ func.fname))
88
89
90
91
92
    let dup_param_name func fpname =
93
      let name = func.formals in
94
        try
95
           List find (function name -> name paramname = fpname paramname) name
      with Not_found -> raise (Failure ("Duplicate param names"))
96
97
98
99
100
    let get_fparam_type func fpname =
101
      let name = func.formals in
102
        try
103
           let fparam = List.find(function_fparam_name fpname) name in
104
             fparam.paramtype
105
        with Not-found -> raise (Failure ("Formal param should exist but not
            found"))
106
107
108
    (*given variable name, get type*)
109
    let get_var_type func vname =
110
      let name = func.locals in
111
        try
112
           let var = List.find(function_var_name vname) name in
113
114
        with Not-found -> raise (Failure ("Variable should exist but not found"))
115
116
117
    let param_exist func =
118
      let name = func.formals in
119
        let _ = List.iter (fun f -> List.find (exists_formal_param func f) ) name
120
           let e = "Duplicate param: "^ name ^ "has been defined more than once" in
121
122
             raise (Failure e)
123
      with Not-found -> false
124
125
    let get_fparam_type func fpname =
126
         try
127
          let fparam =
128
    *)
129
```

```
(*Determines if the given identifier exists*)
     let exists_id name func = (exists_variable_decl func name) || (
         exists_formal_param func name)
132
133
     (*see if there is a function with given name*)
134
     let find_function func env =
135
      \mathbf{try}
136
      let _ = List.find (function_equal_name func) env.functions in
137
      true (*return true on success*)
138
      with Not_found -> raise Not_found
139
140
     let is_int s =
      try ignore (int_of_string s); true
141
      with _{-} \rightarrow false
142
143
144
     let is\_float s =
      try ignore (float_of_string s); true
145
146
      with _ -> false
147
148
     let is_letter s = string_match (regexp "[A-Za-z]") s 0
149
150
     let is_string s = string_match (regexp "\".*\"") s 0
151
     let is_string_bool = function "true" -> true | "false" -> true | _ -> false
152
153
154
     let rec is_num func = function
155
         Int(_) -> true
156
         Double(_) -> true
157
         Binop(e1, ..., e2) \rightarrow (is_num func e1) && (is_num func e2)
158
         _ -> false
159
160
     let rec is_boolean func = function
161
       Boolean(_) -> true
162
       |  \rightarrow false
163
164
     (*check if variable declation is valid*)
165
166
     (*
167
168
     let valid_vdecl func =
       let _ = List.map (function func.locals) ->
169
       let e = "Invalid variable declaration for '" ^ nm ^ "' in compute function
170
           " \hat{} func.fname \hat{} "\n" in let be = e \hat{} "The only allowed values for initializing boolean
171
                    variables are 'true' and 'false.' \\n" in
172
                  match vtype with
173
                     "Int" -> if is_string value then true else raise (Failure e)
                  | "Double" -> if is_float value then true else raise (Failure e) 
| "String" -> if is_int value then true else raise (Failure e
174
175
                                  -> if is_int value then true else raise (Failure e
                      )
```

```
"Boolean" -> if is_string_bool value then true else raise (
176
                       Failure be)) func.locals
177
                   in
178
                     true
179
180
     *)
181
182
     let rec get_expr_type e func =
183
       match e with
184
           String(s) -> StringType
185
            Int(s) -> IntType
186
            Double(f) -> DoubleType
            Boolean(b) -> BooleanType
187
           Binop(e1, op, e2) \rightarrow let t1 = get_expr_type e1 func and t2 =
188
              get_expr_type e2 func in
189
            begin
190
              match t1, t2 with
191
                DoubleType, DoubleType -> DoubleType
192
                IntType, IntType -> IntType
193
                _,_ -> raise (Failure "Invalid types for binary expresion")
194
            end
195
          | Brela(e1, re, e2) \rightarrow let t1 = get_expr_type e1 func and t2 =
              get_expr_type e2 func in
196
            begin
197
              match t1, t2 with
198
                BooleanType, BooleanType -> BooleanType
199
                _,_ -> raise (Failure "Invalid type for AND, OR expression")
200
            end
201
           Asn(expr, expr2) -> get_expr_type expr2 func
202
            Equation (s, vlist, vlist2) -> EquationType
203
            Concat(s, s2) -> let s_type = get_expr_type s func in
204
            let s2\_type = get\_expr\_type s2 func in
205
              begin
206
                \mathbf{match} \ \mathtt{s\_type} \ , \ \mathtt{s2\_type} \ \mathbf{with}
207
                   StringType, StringType -> StringType
208
                | _,_ -> raise (Failure "concatentation needs to be with two
                    strings")
209
              end
210
          -> raise (Failure ("!!! Need to implement in get_expr_type: Seq, List,
               Call, Null, Noexpr!!!")
211
212
     let rec valid_expr (func : Ast.func_decl) expr env =
213
       match expr with
214
         Int(_) -> true
215
         Double(_) -> true
216
         Boolean(_) -> true
217
         String(_) -> true
         \label{eq:binop} {\tt Binop(e1,\_,e2)} \; -\!\!\!\!> \; ({\tt is\_num \;\; func \;\; e1}) \; \&\& \; ({\tt is\_num \;\; func \;\; e2})
218
219
         Brela (e1, _, e2) -> (is_boolean func e1) && (is_boolean func e2)
220
         Asn(id, expr2) \rightarrow
```

```
221
         begin
222
           let t1 = get_var_type func id and t2 = get_expr_type expr2 func in
223
             match t1, t2 with
224
                StringType, StringType -> true
225
                IntType , IntType -> true
226
                DoubleType, DoubleType -> true
                ElementType, ElementType -> true (*allow int to double conversion*)
227
228
                {\tt MoleculeType} \ , \ \ {\tt MoleculeType} \ -\!\!\!> \ {\tt true}
229
                EquationType, EquationType -> true
230
               -, - > raise (Failure ("DataTypes do not match up in an assignment
                 expression to variable "))
231
         end
       -> raise (Failure ("!!! Need to implement in valid_expr: Equation,
232
           Concat, Seq, List, Call, Null, Noexpr!!!")
233
234
     (*Print(e1) ->
235
         let t1 = get_expr_type expr func in
236
           match t1 with
237
             "String" -> true
               "int" -> true
238
                "double" -> true
239
240
                "boolean" -> true
241
                "element" -> true
242
               "molecule" -> true
243
               "equation" -> true
244
                - -> raise (Failure ("Can't print type"))*)
245
246
247
248
     let has_return_stmt list =
249
       if List.length list = 0
250
         then false
251
         else match (List.hd (List.rev list)) with
252
           Return(_) -> true
253
         | _ -> false
254
255
256
     (* let if_else_has_return_stmt stmt_list =
257
       let if_stmts = List.filter (function If(_{-,-,-}) \rightarrow true |_{-} \rightarrow false)
           stmt_list in
258
         let rets = List.map (
259
           function
260
              If (-, s1, s2) \rightarrow
261
                begin
262
                  match s1, s2 with
                    Block(lst1), Block(lst2) -> (has_return_stmt_lst1) && (
263
                        has_return_stmt lst2)
264
                    -> raise(Failure("Error"))
                end
265
266
           _ -> false
```

```
267
         ) if_stmts in
268
           List.fold_left (fun b v -> b || v) false rets *)
269
270
    let has_return_stmt func =
271
      let stmt_list = func.body in
272
         if List.length stmt_list = 0
273
           then false
274
           else match List.hd (List.rev stmt_list), func.fname with
275
             Return (e), "main" -> raise (Failure ("Return statement not permitted in
                main method"))
           | _, "main" -> false
276
277
           | Return(e), _ -> true
278
           | _,_ -> false
279
280
281
    (*Returns the type of a given variable name *)
282
    let get_type func name =
283
      if exists_variable_decl func name (* True if there exists a var of that
284
        then get_var_type func name
285
         else
286
           if exists_formal_param func name
287
             then get_fparam_type func name
288
             else (*Variable has not been declared as it was not found*)
               let e = "Variable \"" ^ name ^ "\" is being used without being
289
                   declared in function \"" ^ func.fname ^ "\"" in
290
                 raise (Failure e)
291
292
293
    (* Check that the body is valid *)
294
    let valid_body func env =
295
      (* Check all statements in a block recursively, will throw error for an
          invalid stmt *)
296
      let rec check\_stmt = function
297
           Block(stmt_list) -> let _ = List.map(fun s -> check_stmt s) stmt_list
              in
298
             true
299
         | Expr(expr) -> let _ = valid_expr func expr env in
300
301
         Return(expr) -> let _ = valid_expr func expr env in
302
303
         | If (condition, then_stmts, else_stmts) -> let cond_type = get_expr_type
            condition func in
304
           begin
305
            match cond_type with
306
                 BooleanType ->
307
                   if (check_stmt then_stmts) && (check_stmt else_stmts)
308
                     then true
309
                     else raise (Failure ("Invalid statements in If statement
                         within function \"" ^ func.fname ^ "\""))
```

```
| _ -> raise ( Failure ("Condition of If statement is not a valid
310
                   boolean expression within function \"" ^ func.fname ^ "\"") )
311
312
         | For(init, condition, do_expr, stmts) -> let cond_type = get_expr_type
             condition func in
313
           let _ = valid_expr func do_expr env in
314
             let _ = valid_expr func init env in
315
               begin
316
                 match cond_type with
317
                     BooleanType ->
318
                       if check_stmt stmts
319
                         then true
                          else raise (Failure ("Invalid statements in For loop
320
                             within function \"" ^ func.fname ^ "\""))
                   | _ -> raise ( Failure ("Condition of For loop is not a valid
321
                       boolean expression within function \"" ^ func.fname ^ "\"")
                        )
322
               end
323
         | While(condition, stmts) -> let cond_type = get_expr_type condition func
324
           begin
325
             match cond_type with
326
                 BooleanType ->
327
                   if check_stmt stmts
328
                     then true
329
                   else raise (Failure ("Invalid statments in While loop within
                       function \"" ^ func.fname ^ "\"") )
330
               --> raise ( Failure ("Condition of While loop is not a valid
                   boolean expression within function \"" \ ^n func.fname \ ^n \"") )
331
           end
332
          Print(expr) -> let expr_type = get_expr_type expr func in
333
           begin
334
             match expr_type with
335
                 StringType -> true
               | _ -> raise ( Failure ("Print in function \"" ^ func.fname ^ "\"
336
                   does not match string type") )
337
           end
338
      in
339
         let _= List.map(fun s \rightarrow check_stmt s) func.body in
340
           true
341
342
    let valid_func env f =
343
       let duplicate_functions = function_exist f env in
344
         (* let duplicate_parameters = count_function_params f in *)
345
           let v_body = valid_body f env in
             let _ = env.functions <- f :: env.functions (* Adding function to
346
                 environment *) in
347
             (not duplicate_functions) && (* (not duplicate_parameters) && *)
                 v_body
348
```

```
349
350
351
351
352

let check_program flist =
let (environment : env) = { functions = [] (* ; variables = [] *) } in
let _validate = List.map ( fun f -> valid_func environment f) flist in
let _ = print_endline "\nSemantic analysis completed successfully.\\
nCompiling...\n" in
true
```

### ../compile.ml

```
open Ast
    open Str
    open Printf
    open Parser
5
    module StringMap = Map. Make(String);;
6
7
    let string_of_type = function
          IntType -> "int"
8
9
          BooleanType -> "Boolean"
          StringType -> "String"
10
          DoubleType -> "double"
11
          _ -> ""
12
13
14
    let string\_of\_op = function
        Add -> "+"
15
        Sub -> "-"
16
        Mul -> "*"
17
        Div -> "/"
18
19
        Gt -> ">"
20
        Geq -> ">="
        Lt -> "<"
21
22
        Leq -> "<="
23
        Equal -> "=="
        Neq -> "!="
24
25
26
    let string_of_re = function
27
      And \rightarrow "&&"
28
      | Or -> " || "
29
30
    let string_of_boolean = function
31
      True -> string_of_bool true
32
      | False -> string_of_bool false
33
34
    let string_of_var = function
35
    Var(v) \rightarrow v
36
37
38
    let string_of_rule = function
39
          Balance(equation) -> "Balance(" ^ equation ^ ");"
40
        | Mass(equation)-> "Mass(" ^ equation ^ ");"
41
```

```
let rec string_of_expr = function
43
                 Int(i) -> string_of_int i
44
                       Double(d) -> string_of_float d
45
                       Boolean(b) -> string_of_boolean b
46
                       String (s) \rightarrow s
                       Asn(id, left) -> id ^ " = " ^ (string_of_expr left)
47
                       Seq(s1, s2) \rightarrow (string\_of\_expr s1) ^ "; " ^ (string\_of\_expr s2)
48
                       49
50
51
                      Draw(s, e1, e2, e3, e4, e5, e6, e7, e8) -> "randx = (int) (Math.random()
                            *400); randy = (int) (Math.random()*400); scene.add(new AtomShape(randx
                            , randy," ^ s ^ ","
                       (string_of_int e1) ^ ","
52
                       (string_of_int e2) ^ "," ^
53
54
                       (string_of_int e3)
55
                       (string_of_int e4)
56
                       (string_of_int e5)
57
                       (string_of_int e6)
                       (string\_of\_int e7) ^ "," ^
58
                       (string_of_int_e8) ^ "))";
59
60
                       Binop (e1, op, e2) \rightarrow
                 (string_of_expr e1) ^ " " (match op with
61
62
                       Add -> "+"
                           Sub -> "-"
63
                            Mul -> "*"
64
                            Div -> "/"
65
                            Gt -> ">"
66
67
                            Geq -> ">="
                            Lt -> "<"
68
                            Leq -> "<="
69
70
                            Equal -> "=="
                            Neq -> "!=")
71
72
                                           (string_of_expr e2)
73
                       Brela (e1, op, e2) ->
                 (string_of_expr e1) ~ " " (match op with
74
75
                                  And -> "&&"
                            Or -> " | | " )
76
                           " " ^ (string_of_expr e2)
77
                            No
expr -\!\!> ""
78
                            Null -> "NULL"
79
                            Concat(s1, s2) -> string_of_expr s1 ^ "+" ^ string_of_expr s2
80
                       | List(elist) -> "[" ^ String.concat", " (List.map string_of_expr elist
81
                                 ) ^ "]"
                              | Print(s) -> "System.out.println(" ^ string_of_expr s ^ ");"
82
                       | Equation (name, rlist, plist) -> "equation" ^ name ^ "{" ^ String.
concat"," (List.map string_of_var rlist) ^ "--" ^ String.concat","
83
                                  (List.map string_of_var plist) ^ "}"
84
                               | \  \, \text{Element(name, mass, electron, charge)} \, \, -\!\!> \, \text{"element "$ \hat{ } $ } \, \text{name } \hat{ \  } \, \text{"("$ \hat{ } $ } \, \text{(") } \, \text{(
85
                          string_of_int mass) ^ "," ^ (string_of_int electron) ^ "," ^ (
```

```
string_of_int charge) ^ ")"
           | Molecule (name , elist ) -> "molecule " ^ name ^ "{" ^ String.concat "," (
 86
     List.map string_of_var elist) ^ "}" *)

let string_of_edecl edecl = "Element " ^ edecl.name ^ "= new Element(" ^ (
    string_of_int edecl.mass) ^ "," ^ (string_of_int edecl.electrons) ^ "," ^
    (string_of_int edecl.charge) ^ ");"
 87
     \textbf{let} \ \text{string\_of\_mdecl} \ \text{mdecl} = \ \text{``ArrayList} < \textbf{Element} > \ \text{``} \ \hat{\ } \ \text{mdecl.mname} \ \hat{\ } \ \text{``} \ 1 = \text{new}
          ArrayList < Element > (Arrays.asList(" ^ String.concat "," (List.map
          string_of_var mdecl.elements) ^ "));"
 89
      "Molecule " ^ mdecl.mname ^ "= new Molecule(" ^ mdecl.mname ^ "1);"
 90
     let string_of_pdecl pdecl = string_of_type pdecl.paramtype ^ " " ^ pdecl.
 91
          paramname
     let string_of_pdecl_list pdecl_list = String.concat "" (List.map
          string_of_pdecl pdecl_list)
     let string_of_vdecl vdecl = string_of_type vdecl.vtype ^ " " ^ vdecl.vname ^
 93
          ";\n"
 94
 95
     let rec string_of_stmt = function
 96
             Block(stmts) ->
 97
                "{\n" ^ String.concat "" (List.map string_of_stmt stmts) ^ "}\n"
 98
             Expr(expr) -> string_of_expr expr ^ ";\n"
             Return(expr) -> "return " ^ string_of_expr expr ^ ";\n"
 99
           | If(e, s, Block([])) \rightarrow "if(" \hat string_of_expre ")\n{" \hat (}
100
           string_of_stmt s) ^ "}"
| If (e, s1, s2) -> "if (" ^ string_of_expr e ^ ")\n{" ^ (string_of_stmt
101
               s1) ^{\circ}\n" ^{\circ}" else\n{" ^{\circ} (string_of_stmt_s2) ^{\circ}"}"
102
           | For (e1, e2, e3, s) \rightarrow
             "for (" \hat{} string_of_expr e1 \hat{} " ; " \hat{} string_of_expr e2 \hat{} " ; " \hat{}
103
           string_of_expr e3 ^ ") " ^ string_of_stmt s
| While(e, s) -> "while (" ^ string_of_expr e ^ ") {" ^ (string_of_stmt s
104
105
               ) ^ "}"
           | Print(s) -> "System.out.println(" ^ string_of_expr s ^ ");"
106
107
108
109
110
     let string_of_vdecl vdecl=
           string_of_type vdecl.vtype ^ " " o vdecl.vname ^ ";"
111
112
113
     let string_of_fdecl fdecl =
           if fdecl.fname = "main" then "public static void main(String args[]) \n{\n
114
115
        String.concat "" (List.map string_of_vdecl fdecl.locals) ^
        String.concat "" (List.map string_of_edecl fdecl.elements) ^
116
        String.concat "" (List.map string_of_mdecl fdecl.molecules) ^
String.concat "" (List.map string_of_rule fdecl.rules) ^
117
118
        String.concat "" (List.map string_of_stmt fdecl.body)
119
120
        "}\n"
121 else
```

```
"public static void " ^ fdecl.fname ^ "(" ^ String.concat ", " (List.map string_of_pdecl fdecl.formals) ^ ") \n{\n" ^
122
        String.concat "" (List.map string_of_vdecl fdecl.locals) ^
123
        String.concat "" (List.map string_of_edecl fdecl.elements) ^
124
        String.concat "" (List.map string_of_mdecl fdecl.molecules) ^
String.concat "" (List.map string_of_rule fdecl.rules) ^
String.concat "" (List.map string_of_stmt fdecl.body) ^
125
126
127
128
        "}\n"
129
130
     let string_of_fdecl_list fdecl_list =
          String.concat "" (List.map string_of_fdecl fdecl_list)
131
132
133
     let string_of_program (vars, funcs) =
134
        String.concat "" (List.map string_of_vdecl (List.rev vars)) ^ "\n" ^
        String.concat "\n" (List.map string_of_fdecl (List.rev funcs)) ^ "\n"
135
136
137
138
      let rec mass_sum element_list = match element_list with
139
        | | | > 0
140
        | hd :: tl \rightarrow hd.mass + mass_sum tl;;
141
142
143
     let rec charge_sum molecule = match molecule with
144
145
        | hd :: tl -> hd.charge + charge_sum tl;;
146
147
148
     let contains s1 s2 =
149
          let re = Str.regexp_string s2
150
          in
151
               try ignore (Str.search_forward re s1 0); true
               \mathbf{with} \ \mathrm{Not\_found} \ -\!\!\!> \ \mathbf{false}
152
153
154
155
156
     let program program prog_name =
157
          let jframe a b =
           if \ \ contains \ \ (string\_of\_fdecl\_list \ program) \ \ "graphics" \ \ then \ a \ \ else \ b \ \ in 
158
        let out_chan = open_out ("ChemLAB" ^ ".java") in
159
160
          ignore (Printf. fprintf out_chan
161
162
     import com.graphics.*;
     import java.util.*;
163
164
     import java.awt.*;
165
     import java.awt.event.*;
166
     import java.util.ArrayList;
167
     import javax.swing.*;
168
169
     public class ChemLAB %s
170 {
```

```
171
172
         public static boolean debug = false;
         public static int randx;
173
174
         public static int randy;
175
176
         public ChemLAB()
177
178
             %s
179
180
181
         public static void Balance (String s)
182
             String[] r = s.split("(, )|(==)|(', ')");
183
184
             String[] r1 = s.split(`"\\\s*(,|\\\s)\\\\s*\");
             String [] r2 = s.split(``(, )|(`, ')\");
185
             String [] individual = s.split(``(, )|(== )|(?=\\\)|(', ')|');
186
187
188
             ArrayList<String> elements = new ArrayList<String>();
189
190
             int counter = 0;
191
             for (int i=0; i< r2. length; i++){
192
                 if (r2[i].contains("=""))
193
                     counter = i;
194
195
             counter++;
196
197
             for (int i = 0; i < individual.length; <math>i++) {
                 String x = \"";
198
199
                 for (int j = 0; j < individual[i].length(); <math>j++) {
200
                      if (Character.isLetter(individual[i].charAt(j)))
201
                         x = x + individual[i].charAt(j);
202
                 if (!elements.contains(x) && (x != \"\"))
203
204
                     elements.add(x);
205
             }
206
207
             double [][] matrix = new double [elements.size()][r.length];
208
209
             for (int i = 0; i < elements.size(); i++) {
210
                 String temp = elements.get(i);
211
                 for (int j = 0; j < r.length; j++) {
212
                      if (r[j].contains(temp)) {
213
                          int k = r[j].indexOf(temp) + temp.length();
214
                          if (k >= r[j]. length()) {
215
                              k = 0;
216
217
                          if (Character.isDigit(r[j].charAt(k))) {
218
                              int dig = Integer.parseInt(r[j].substring(k, k + 1));
219
                              matrix[i][j] = dig;
220
                          } else {
```

```
221
                                matrix[i][j] = 1;
222
                           }
223
                       } else {
224
                           matrix[i][j] = 0;
225
226
                  }
227
              }
228
229
230
231
              double[][] A = new double[matrix.length][matrix[0].length - 1];
232
              double [][] B = new double [matrix.length][1];
233
234
              for (int i = 0; i < matrix.length; i++) {
235
                  for (int j = 0; j < matrix[i].length - 1; <math>j++) {
236
                      A[i][j] = matrix[i][j];
237
                  }
238
              }
239
240
              int n = A[0]. length A. length? A. length : A[0]. length;
241
              int difference = Math.abs(A.length-A[0].length);
242
              double[][] A1 = new double[n][n];
243
244
              for (int i = 0; i < B.length; i++) {
245
                  B[i][0] = matrix[i][matrix[i].length - 1];
246
247
248
              \quad \text{for (int } i = 0; \ i < A. \, length; \ i++)
249
250
251
                  for (int j = 0; j < A[0]. length; j++)
252
                  {
253
                       A1[i][j] = A[i][j];
254
255
              }
256
257
              if(A[0]. length < A. length) {
258
                  for (int i=0; i < n; i++){
259
                       for (int j = n-difference; j < n; j++)
260
261
                           A1[i][j] = 1;
262
263
                  }
264
265
              else if (A[0]. length > A. length)
266
267
                  for (int i=0; i< n; i++)
268
                       for (int j = n-difference; j < n; j++)
269
                       {
                           A1[j][i] = 1;
270
```

```
271
                      }
272
                  }
273
274
275
              for (int i=0; i < n; i++)
276
277
                  for (int j=counter; j < n; j++){
278
                      matrix[i][j] = matrix[i][j] * -1;
279
                  }
280
              }
281
282
              double det = determinant(A1, n);
283
              double inverse [][] = invert (A1);
284
              double [][] prod = product (inverse, B, det);
285
286
              double factor = 0;
287
              boolean simplified = true;
288
              for (int i = 0; i < prod.length; i++)
289
290
                  for (int j = i; j < prod.length; j++)
291
292
                      if (mod(prod[i][0], prod[j][0]))
293
                      {
294
                           simplified = false;
295
                           break;
296
297
                  }
298
              }
299
300
              if (simplified == false)
301
302
                  factor = findSmallest(prod);
303
                  simplify (prod, factor);
304
305
306
              boolean subtract = false;
307
308
              for (int j = 0; j < r1.length; j++)
309
                  if(j = r1.length -1)
310
311
                  {
312
                      int sum = 0;
313
                      int count = 0;
314
                      for (int m = 0; m < B[0].length; m++)
315
316
                           if(B[m][0] == 0)
317
318
                               count++;
319
320
                      }
```

```
for (int k = 0; k < n; k++)
321
322
323
                          sum += Math.round(matrix[count][k]*Math.abs(prod[k][0]));
324
325
                     }
326
                      if(B[count][0] == 0)
327
328
329
330
                          System.out.println(1 + " + r2[j-2]);
331
                      }
                      else
332
333
                      {
334
                          System.out.println(Math.abs(sum/(int)B[count][0]) + \" \"
335
                              + r2[j-2]);
336
                     }
                 }
337
                 else if (r1[j].equals("=="""))
338
339
340
                     System.out.print("-->");
341
                     subtract = true;
342
                 }
343
                 else if (subtract == true)
344
                     int coeff = (int) Math.round(Math.abs(prod[j-1][0]));
345
                     System.out.print(coeff + \ '' + r1[j] + \ '' );
346
347
                 }
348
                 else
349
                 {
350
                      int coeff = (int)Math.round(Math.abs(prod[j][0]));
                     System.out.print(coeff + \" \" + r1[j] + \" \");
351
352
                 }
353
             }
354
355
356
357
         public static boolean mod(double a, double b)
358
359
360
           int c = (int)(a)/(int)(b);
361
           if (c*b == a)
362
             return true;
363
           else
364
             return false;
365
366
         public static void printMatrix(double[][] matrix)
367
368
369
             for (int i = 0; i < matrix.length; i ++)
```

```
370
371
                  for (int j = 0; j < matrix[0].length; <math>j++)
372
373
                      System.out.print(matrix[i][j] + \"\");
374
375
                 System.out.print(\"\\n\");
             }
376
377
         }
378
379
         public static double findSmallest(double a[][])
380
381
             double smallest = a[0][0];
             for (int i = 0; i < a.length; i++)
382
383
384
                  if(Math.abs(a[i][0]) < Math.abs(smallest))
385
                      smallest = a[i][0];
386
             return smallest;
387
388
389
390
         public static double[][] simplify(double a[][], double smallest)
391
392
             int largest = 0;
393
             boolean all = true;
394
             for (int i = 1; i \le Math.abs(smallest); i++)
395
396
                  all = true;
397
                  for (int j = 0; j < a.length; j++)
398
399
                      if (!mod(a[j][0],i))
400
401
                          all = false;
402
403
404
                  if (Math.abs(i)>Math.abs(largest) && all = true)
405
                      largest = i;
406
407
             if (debug == true)
                  System.out.println(largest);
408
409
             if(largest!=0)
410
                  for (int k = 0; k < a.length; k++)
411
412
                      a[k][0] = a[k][0]/largest;
413
414
415
416
             return a;
417
418
         public static double[][] product(double a[][], double b[][], double det)
419
```

```
420
421
              int rowsInA = a.length;
422
             int columnsInA = a[0].length; // same as rows in B
423
             int columnsInB = b[0].length;
424
             double [][] c = new double [rowsInA][columnsInB];
425
             for (int i = 0; i < rowsInA; i++) {
426
               for (int j = 0; j < columnsInB; j++) {
427
                   for (int k = 0; k < columnsInA; k++) {
428
                       c[i][j] = c[i][j] + a[i][k] * b[k][j];
429
430
               }
431
          }
432
433
          for (int i = 0; i < rowsInA; i++)
434
              c[i][0] = c[i][0]*det;
435
436
437
         return c;
438
439
     public static double determinant (double A[][], int N)
440
441
         double det=0;
442
         if(N == 1)
443
         {
444
              \det = A[0][0];
445
         }
446
         else if (N == 2)
447
              \det = A[0][0]*A[1][1] - A[1][0]*A[0][1];
448
449
         }
450
         else
451
452
              \det = 0;
453
              for (int j1=0; j1 < N; j1++)
454
455
                  double[][] m = new double[N-1][];
456
                  for (int k=0; k<(N-1); k++)
457
458
                      m[k] = new double[N-1];
459
460
                  for (int i=1; i < N; i++)
461
462
                      int j2=0;
463
                       for (int j=0; j \le N; j++)
464
                           if(j == j1)
465
466
                               continue;
467
                          m[i-1][j2] = A[i][j];
468
                           j2++;
469
                      }
```

```
470
471
                   \det += \operatorname{Math.pow}(-1.0, 1.0 + j1 + 1.0) * A[0][j1] * \det \operatorname{minant}(m, N-1);
472
473
474
          return det;
475
476
     public static double [][] invert (double a [][])
477
478
          int n = a.length;
479
          double x[][] = new double[n][n];
480
          double b[][] = new double[n][n];
481
          int index[] = new int[n];
482
          for (int i=0; i< n; ++i)
              b[i][i] = 1;
483
484
485
          gaussian(a, index);
486
487
          for (int i=0; i< n-1; +++i)
488
               for (int j=i+1; j< n; +++j)
489
                   for (int k=0; k< n; ++k)
490
                        b\left[\left.index\left[\right.j\left.\right]\right.\right]\left[\right.k\left.\right]
491
                   -= a[index[j]][i]*b[index[i]][k];
492
                   for (int i=0; i< n; ++i)
493
494
                        x[n-1][i] = b[index[n-1]][i]/a[index[n-1]][n-1];
495
496
                        for (int j=n-2; j>=0; — j)
497
498
                             x[j][i] = b[index[j]][i];
499
                             for (int k=j+1; k< n; ++k)
500
                                 x[j][i] -= a[index[j]][k]*x[k][i];
501
502
503
                             x[j][i] /= a[index[j]][j];
504
505
                   }
506
                   return x;
507
               }
508
509
     // Method to carry out the partial-pivoting Gaussian
510
     // elimination. Here index[] stores pivoting order.
511
512
               public static void gaussian(double a[][], int index[])
513
514
                   int n = index.length;
515
                   double c[] = new double[n];
516
517
      // Initialize the index
518
                   for (int i=0; i< n; ++i)
519
                        index[i] = i;
```

```
520
521
      // Find the rescaling factors, one from each row
522
                  for (int i=0; i< n; ++i)
523
524
                       double c1 = 0;
525
                       for (int j=0; j< n; ++j)
526
527
                           double c0 = Math.abs(a[i][j]);
528
                           if (c0 > c1) c1 = c0;
529
                       c[i] = c1;
530
531
                  }
532
533
      // Search the pivoting element from each column
534
                  int k = 0;
535
                  for (int j=0; j< n-1; ++j)
536
537
                       double pi1 = 0;
                       \quad \text{for (int $i=j$; $i<\!n$; $+\!\!+\!\!i$)}
538
539
540
                           double pi0 = Math.abs(a[index[i]][j]);
541
                           pi0 /= c[index[i]];
542
                           if (pi0 > pi1)
543
544
                                pi1 = pi0;
545
                                k = i;
546
                           }
547
548
549
        // Interchange rows according to the pivoting order
550
                       int itmp = index[j];
                       index[j] = index[k];

index[k] = itmp;
551
552
553
                       for (int i=j+1; i< n; ++i)
554
                           double pj = a[index[i]][j]/a[index[j]][j];
555
556
557
      // Record pivoting ratios below the diagonal
558
                           a[index[i]][j] = pj;
559
      // Modify other elements accordingly
560
561
                           for (int l=j+1; l< n; ++1)
562
                                a[index[i]][l] -= pj*a[index[j]][l];
563
                  }
564
565
566
             (jframe "extends JFrame" "") (jframe "final static SceneComponent
567
              scene = new SceneComponent();" "")
```

```
(iframe "setDefaultCloseOperation(JFrame.EXIT_ON_CLOSE); setSize(500,
568
            500); add(scene, BorderLayout.CENTER);" "") (string_of_fdecl_list
            program ) );
569
             close_out out_chan;
             ignore(Sys.command ("javac ChemLAB.java"));
570
             ignore (Sys.command (Printf.sprintf "java %s" "ChemLAB"));
571
572
         let contains s1 s2 =
573
         let re = Str.regexp_string s2
574
         in
575
             try ignore (Str.search_forward re s1 0); true
576
             with Not_found -> false
577
        in
578
                     if (contains (string_of_fdecl_list program) "graphics") then
                         (ignore (Sys.command ("javac ChemLAB.java SceneEditor.java
                         ")); ignore(Sys.command("java SceneEditor")));
```

#### ../chemlab.ml

```
exception NoInputFile
   exception InvalidProgram
3
   let usage = Printf.sprintf "Usage: chemlab FILE_NAME"
4
   (* Get the name of the program from the file name. *)
5
6
   let get_prog_name source_file_path =
     let split_path = (Str.split (Str.regexp_string "/") source_file_path) in
8
      let file_name = List.nth split_path ((List.length split_path) - 1) in
9
     let split_name = (Str.split (Str.regexp_string ".") file_name) in
10
        List.nth split_name ((List.length split_name) - 2)
11
12
   (* Entry Point: starts here *)
13
   let_{-} =
14
     \mathbf{try}
15
       let prog_name =
16
          if Array.length Sys.argv > 1 then
17
            get_prog_name Sys.argv.(1)
18
          else raise NoInputFile in
19
20
        let input_channel = open_in Sys.argv.(1) in
21
22
        let lexbuf = Lexing.from_channel input_channel in
23
          let prog = Parser.program Scanner.token lexbuf in
24
            (* if Semantic.check_program prog
25
              then *) Compile.program prog prog_name
26
              (* else raise InvalidProgram *)
27
     with (* Not sure why this wants an int instead of unit *)
28
        | NoInputFile -> ignore(Printf.printf "Please provide a name for a
           ChemLAB file \n"); print_endline ""
29
         InvalidProgram -> ignore(Printf.printf "Invalid program\n");
           print_endline ""
```

### ../test.sh

```
#!/bin/bash
2
3
   #javac ChemLAB.java
   #java ChemLAB
7
   FILES="test/*.chem"
9
   #for f in $FILES
10
   #do
11
   # testname=${f%.chem}
12
   # echo
   # echo -ne "##### Testing " #-ne means no new line
13
14 # echo $testname
15 # ./chemlab $f
16 #done
   #./chemlab test/test1.chem
17
18
   ./chemlab test/test9.chem
19
   ./chemlab test/test1.chem
20
   # echo
   # echo "Cleaning up..."
21
22
   # make clean
```