Optimaiden implementation development

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Desiderata

- Code works across language and library version changes (~~Python~~)
- Hight abstraction level, memory safe (~~C~~, C++ (?))
- Describes compiler-checked library interfaces (~~Perl~~, ~~PhP~~)

(Amiard et al. 2022)

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(Amiard et al. 2022)

Code example

Space group symbol decoder

```
   C 2y (x-y, x+y, z),   C 2y (1/2*a - 1/2*b, 1/2*a + 1/2*b, c)
```

```
Get_Hall_Symbol_Inversions (Symbol, Pos, N_Inversions);
Get_Hall_Symbol_Centerings (Symbol, Pos, Centering, N_Centering);

for Axis_Number in 1..4 loop
   Get_Hall_Symbol_Rotation (Symbol, Pos, Symmetry_Operators,
                             N_Symmetry_Operators,
                             Preceeding_Axis_Direction,
                             Preceeding_Axis_Order, Axis_Number);
end loop;

Get_Change_Of_Basis (Symbol, Pos, Change_Of_Basis);

Apply_Change_Of_Basis
  (
   Symmetry_Operators, N_Symmetry_Operators,
   Centering, N_Centering,
   Inversions, N_Inversions,
   Change_Of_Basis
  );

Build_Group (Symmetry_Operators, N_Symmetry_Operators);
```

(Hall 1981a)
(Hall 1981b)

Code example

The interface

```
with Symmetry_Operations; use Symmetry_Operations;

package Hall_Symbol_Parser is

   Debug_Print_Matrices : Boolean := False;

   function Decode_Hall_Symbol (Symbol : in String)
                                return Symmetry_Operator_Array;

end Hall_Symbol_Parser;
```

```
saulius@starta optimaiden/ $ make -W src/optimaiden.adb
alr build
...
 Build finished successfully in 1.10 seconds.
```

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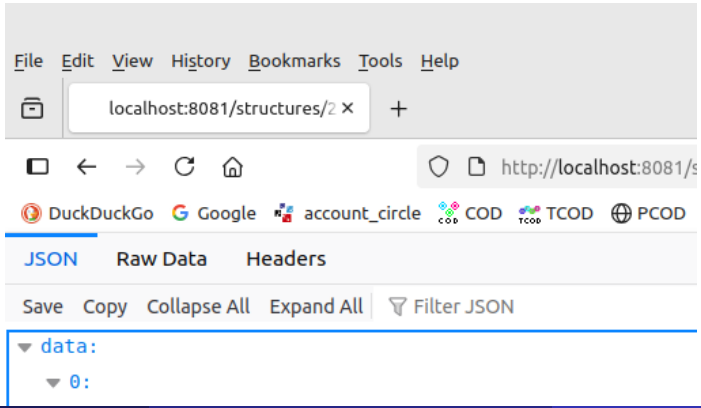

Filter language

Tools at hand:

- AYacc :)
- AFelx :)
- Grammatiker (OPTIMADE EBNF $\rightarrow$ AYacc)
- GNAT (of course :)

Filter grammar

```
ebnf2ayacc Filter.ebnf > Filter.y
```

```
(* BEGIN EBNF GRAMMAR Filter *)
(* The top-level 'filter' rule: *)

Filter = [Spaces], Expression ;

(* Values *)

OrderedConstant = String | Number ;
UnorderedConstant = ( TRUE | FALSE ) ;

Value = ( UnorderedConstant | OrderedValue ) ;
```

```
%token ONLY_TOKEN
%token ANY_TOKEN

%token TRUE_TOKEN
%token FALSE_TOKEN

%token IDENTIFIER_TOKEN
%token NUMBER_TOKEN

%%

Filter : optional__Spaces Expression
;
OrderedConstant : String | Number
;
UnorderedConstant : grouped__TRUEs
;
Value : grouped__UnorderedConstants
;
```

Ada compilation

```
for I in 1 .. Argument_Count loop
    YYInput_Definition.Start_Parsing (Argument (I));
    Put_Line ("Parsing string: """ & Buffer & """");
    YYParse;
end loop;
```

```
saulius@starta optimaiden/ $ ./bin/parse_filter 'nelements > 3 AND _cod_formula ST
Parsing string: "nelements > 3 AND _cod_formula STARTS WITH "C6""
>>> Token: IDENTIFIER_TOKEN, "nelements"
>>> Token: NUMBER_TOKEN, "3" ( 3.00000E+00)
>>> Getting number:  3.00000E+00
>>> Token: IDENTIFIER_TOKEN, "_cod_formula"
```

Future plans

- Connect to SQL (Ada libraries exist – report by Yaroslav Rozdobudko)
- Generate serving code from the formal OPTIMADE spec. (Swagger? Y.R.);
- Use formal property definitions to generate responses (A.M.)
- Split the task into Ada packages :);

Conclusions

- Some aspects of OPTIMADE implemenation (e.g. filter grammar) can be generated automatically from the *formal* OPTIMADE spec. in any language;
- Ada gives just enought tools to implement OPTIMADE within reasonable time and with reasonable effort.
- Ada allows us to produce a protable and maintainable implementation of OPTIMADE;

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Useful links

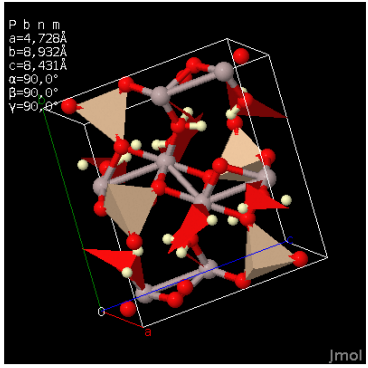
Ada code and Ada books

Code: https://github.com/sauliusg/

Ada books: https://bookauthority.org/books/best-ada-books

Open-access Ada books from AdaCore: https://learn.adacore.com/

Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

References I

Amiard, Raphaël et al. (Apr. 2022). *Learning Ada*. Ed. by Richard Kenner. URL: https://learn.adacore.com/pdf_books/learning-ada.pdf WEB: https://learn.adacore.com/. AdaCore. URL: https://learn.adacore.com/pdf_books/learning-ada.pdf.

Gražulis, Saulius et al. (2009). "Crystallography Open Database – an open-access collection of crystal structures". In: *Journal of Applied Crystallography* 42, pp. 726–729. DOI: 10.1107/S0021889809016690. URL: http://dx.doi.org/10.1107/S0021889809016690.

Hall, S. R. (July 1981a). "Space-group notation with an explicit origin". In: *Acta Crystallographica Section A* 37.4, pp. 517–525. DOI: 10.1107/s0567739481001228.

— (Nov. 1981b). "Space-group notation with an explicit origin; erratum". In: *Acta Crystallographica Section A* 37.6, pp. 921–921. DOI: 10.1107/s0567739481001976.

Spare slides

Just in case someone asks...

Ada CIF parser

Multi language programming

`cod-tools` CIF parser: svn://www.crystallography.net/cod-tools

```
procedure Parse_Cif_From_File_With_Error_Code (Filename : char_array;
                                               CO : Cif_Option_T)
      with Import => True,
      Convention => C,
      External_Name => "parse_cif_from_file_with_error_code";


task Cif_Parser_Task is
   entry Begin_Parsing (Cif_Filename : Unbounded_String;
                        Cif_Options : Cif_Option_T);
end Cif_Parser_Task;
```

Ada popularity

Growing ?!

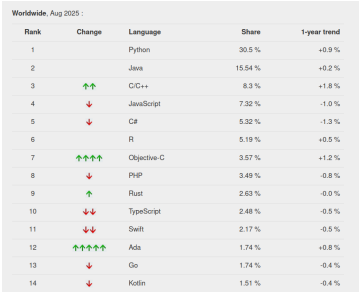
(All URLs accessed 2025-08-21)

“Why is 40-year-old programming language Ada hot again?”
https://www.developer-tech.com/news/why-is-40-year-old-programming-language-ada-hot-again/

“2025: ‘Golden Oldie’ Ada Hits Popularity Milestone”
https://www.techrepublic.com/article/news-tiobe-analysis-july-2025/

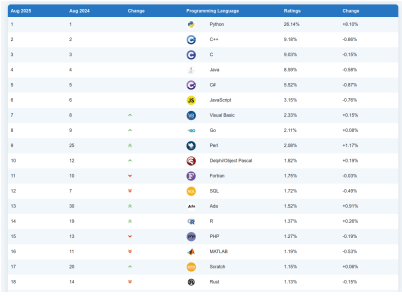
https://pypl.github.io/PYPL.html

https://www.tiobe.com/tiobe-index/



Worldwide, Aug 2025 :

Rank	Change	Language	Share	1-year trend
1		Python	30.5 %	+0.9 %
2		Java	15.54 %	+0.2 %
3	↑↑	C/C++	8.3 %	+1.8 %
4	↓	JavaScript	7.32 %	-1.0 %
5	↓	C#	5.32 %	-1.3 %
6		R	5.19 %	+0.5 %
7	↑↑↑↑	Objective-C	3.57 %	+1.2 %
8	↓	PHP	3.49 %	-0.8 %
9	↑	Rust	2.63 %	-0.0 %
10	↓↓	TypeScript	2.48 %	-0.5 %
11	↓↓	Swift	2.17 %	-0.5 %
12	↑↑↑↑↑	Ada	1.74 %	+0.8 %
13	↓	Go	1.74 %	-0.4 %
14	↓	Kotlin	1.51 %	-0.4 %



Aug 2025	Aug 2024	Change	Programming Language	Ratings	Change
1	1		Python	26.14%	+8.13%
2	2		C++	9.18%	-0.88%
3	3		C	9.03%	-0.15%
4	4		Java	8.89%	-0.68%
5	5		C#	5.52%	-0.87%
6	6		JavaScript	3.15%	-0.76%
7	8	↑	Visual Basic	2.33%	+0.15%
8	9	↑	Go	2.11%	+0.08%
9	25	⇑	Perl	2.08%	+1.17%
10	12	↑	Delphi/Object Pascal	1.82%	+0.19%
11	10	↓	Fortran	1.79%	-0.03%
12	7	⇓	SQL	1.72%	-0.49%
13	38	⇑	Ada	1.52%	+0.91%
14	19	⇑	R	1.37%	+0.28%
15	13	↓	PHP	1.27%	-0.19%
16	11	⇓	MATLAB	1.19%	-0.53%
17	28	↑	Scratch	1.15%	+0.06%
18	14	⇓	Rust	1.13%	-0.15%

Example: dihedral angle calculation

The assignment

```
Write a Perl*) program that calculates torsion angles for DNA and RNA
macromolecules. Compute the following angles: alpha, beta.

*) Note: Ada programs are acceptable; in that case all native Perl
   features mentioned in this specification SHOULD be replaced by the
   corresponding Ada features.

NB: for this particular assignment, you MAY NOT use external libraries
to read PDB files or calculate dihedral angles; these functions MUST
be implemented in the program.
```

NOTE: Students could chose a set of atoms for their individual assignment

Full assignment text: https://tinyurl.com/yp24aad4

Example: dihedral angle calculation

The vector algebra code

```
type Vector_3D is array (1 .. 3) of Long_Float;

function "-" (V, W : Vector_3D) return Vector_3D is
begin
   return (V(1) - W(1),  V(2) - W(2), V(3) - W(3));
end;
```

Example given to the students

```
type Vector_3D is record
   X, Y, Z : Float;
end record;

function "-" (V1, V2 : Vector_3D) return Vector_3D is
begin
    return (V1.X - V2.X, V1.Y - V2.Y, V1.Z - V2.Z);
end;
```

Version designed by the students (Martynas Mažuolis)

Example: dihedral angle calculation

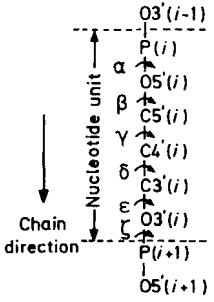
Angle definition and calculation

```
Function Dihedral_angle (Atoms: Chemical_Atom_Set) return float is
        Vector1 : Vector_3D := to_vector(Atoms.Atom_Array(1)) - to_vec..
        Vector2 : Vector_3D := to_vector(Atoms.Atom_Array(2)) - to_vec..
        Vector3 : Vector_3D := to_vector(Atoms.Atom_Array(3)) - to_vec..
        Angle1 : Bond_Angle := Angle(Vector1, Vector2);
        Angle2 : Bond_Angle := Angle(Vector2, Vector3);
        Normal1 : Vector_3D := Cross(Vector1, Vector2);
        Normal2 : Vector_3D := Cross(Vector2, Vector3);
        NX: Vector_3D := Cross(Normal1, Normal2);
        Sign : float := (if Vector2*NX >= 0.0 then 1.0 else -1.0);
        Dihedral : Float := Angle(Normal1, Normal2)*Sign;

        begin
        pragma Assert(Atoms.N>=4);
    return Dihedral;

        end;
```

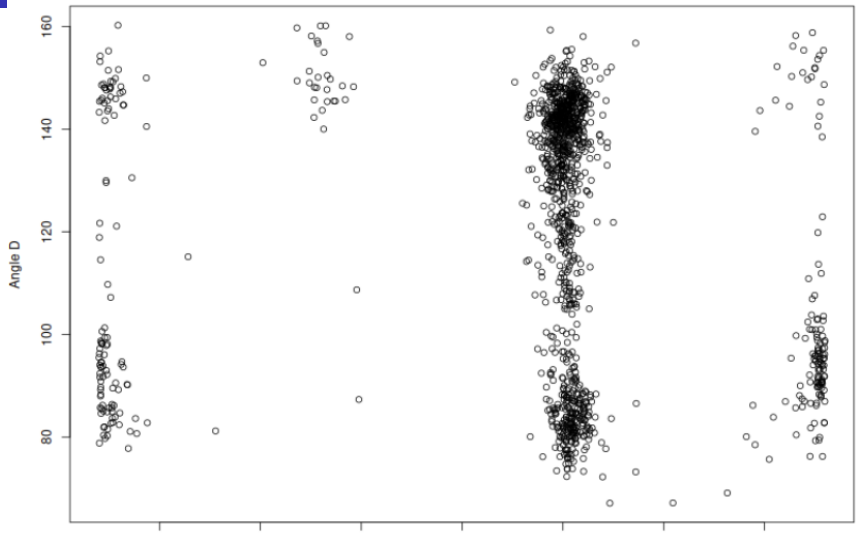
Version designed by the students (Viktorija Jugai)

Example: dihedral angle calculation

Results on the whole PDB



(IUPAC-IUB, **IIJCBN1983**)



Result computed by Aušrinė Zeleckytė