FORTRAN TO PYTHON INTERFACE GENERATOR WITH AN APPLICATION TO AEROSPACE ENGINEERING

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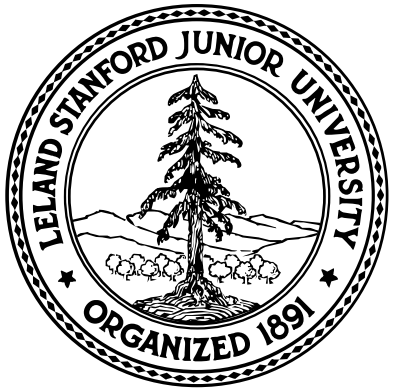

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Outline

- Motivation for using Python to wrap Fortran
- What is f2py and how does it work?
- Simple example
- f2py features
- Future work
- Engineering application
- Conclusions

Motivation

- Fortran is still here:
  - Large number of numerical libraries and legacy code
  - Programming language of choice in most engineering applications
  - Very efficient for numerical applications
- Often necessary to "glue" different applications
  - Need for scripting, file parsing or object-oriented features
  - Not necessarily in the same language
- Python is a good choice that fulfills these needs.
- f2py automates the wrapping process.

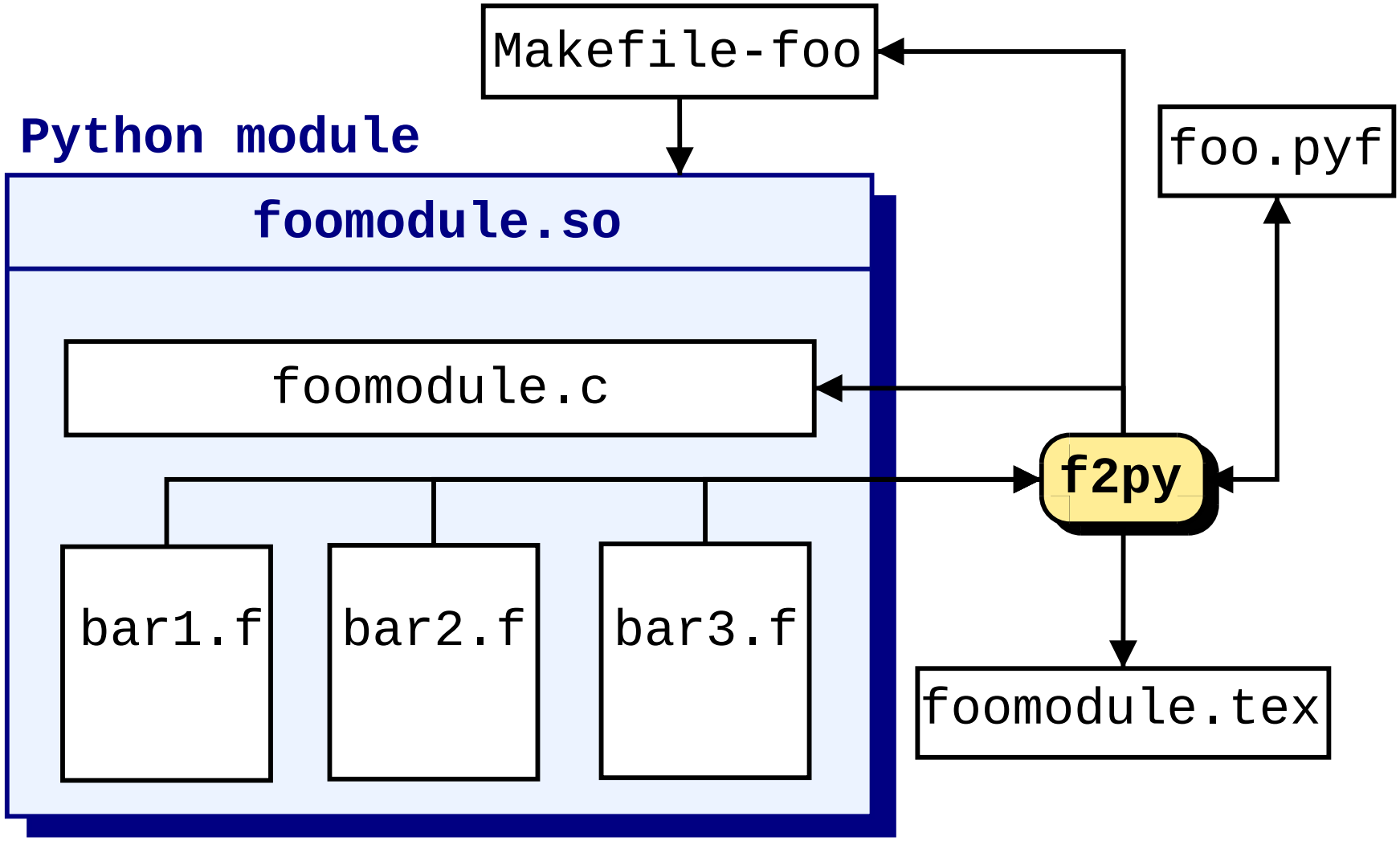
What is f2py?

Tool for creating Fortran to Python interfaces.

Wrappers created with f2py enable the following operations:

- Call Fortran routines from Python
  - Fortran 77/90/95 routines
  - Fortran 90/95 module routines
- Access Fortran data from Python
  - Fortran 77 common block variables
  - Fortran 90/95 module variables
- Call Python functions from Fortran

How Does it Work?



Example: Wrapping Simple Fortran 77 Routines

1. Generate interface
   ```
   > f2py foo.f bar.f -m
   foobar -h foobar.pyf
   ```

2. Edit signature file, `foobar.pyf` (optional).

3. Build module
   ```
   > make -f Makefile-foobar
   ```

4. Python session
   ```
   >>> import foobar
   ...
   ```

```
! Fortran file foo.f:
      subroutine foo(a)
      integer a
      a = a + 5
      end
```

```
! Fortran file bar.f:
      function bar(a,b)
      integer a,b,bar
      bar = a + b
      end
```

Step 1: Generate Interface

```
> f2py foo.f bar.f -m foobar -h foobar.pyf

Reading fortran codes...
        Reading file 'foo.f'
        Reading file 'bar.f'
Post-processing...
        Block: foobar
                        Block: foo
                        Block: bar
Saving signatures to file "foobar.pyf"
Creating 'Makefile-foobar'...
        Linker: ld ('Linker for MIPSpro 7 Compilers' 7.30.)
        Fortran compiler: f77 ('MIPSpro 7 Compilers' 7.30)
        C compiler: cc ('MIPSpro 7 Compilers' 7.30)
Stopping. Edit the signature file and then run f2py on the signature
        file: f2py foobar.pyf
        Or run GNU make to build shared module: gmake -f Makefile-<modulename>
```

Step 2 (Optional): Edit Signature File, `foobar.pyf`

```
!%f90 -*- f90 -*-
module foobar ! in
    interface  ! in :foobar
        subroutine foo(a) ! in :foobar:foo.f
            integer :: a
        end subroutine foo
        function bar(a,b) ! in :foobar:bar.f
            integer :: a
            integer :: b
            integer :: bar
        end function bar
    end interface
end module foobar

! This file was auto-generated with f2py (version:1.218).
! See http://cens.ioc.ee/projects/f2py2e/
```

Step 3: Build Module

```
> gmake -f Makefile-foobar

/usr/bin/f2py foobar.pyf
Reading fortran codes...
        Reading file 'foobar.pyf'
Post-processing...
        Block: foobar
                        Block: foo
                        Block: bar
Keeping existing 'Makefile-foobar'. Use --overwrite-makefile to overwrite.
Building modules...
        Building module "foobar"
                Constructing wrapper function "foo"
                  foo(a)
                Constructing wrapper function "bar"
                  bar = bar(a,b)
        Wrote C/API module "foobar" to file "foobarmodule.c"
        Documentation is saved to file "foobarmodule.tex"
Run GNU make to build shared modules: gmake -f Makefile-<modulename> [test]
cc -mips4 -n32  -I/usr/local/include/python1.5/Numeric -I/usr/local/include/python1.5
-c -o foobarmodule.o foobarmodule.c
f77 -mips4 -n32     -c -o foo.o foo.f
f77 -mips4 -n32     -c -o bar.o bar.f
ld -shared -s  -o foobarmodule.so foobarmodule.o  foo.o bar.o -L/usr/lib32 -lftn -lc -lfortran
```

Step 4: Python Session

```
>>> import foobar
>>> print foobar.__doc__
This module 'foobar' is auto-generated with f2py (version:1.218).
The following functions are available:
  foo(a)
  bar = bar(a,b)
.
>>> print foobar.foo.__doc__
Function signature:
  foo(a)
Required arguments:
  a : input int

>>> print foobar.bar(2,3)
5
>>> from Numeric import *
>>> a = array(3)
>>> print a,foobar.foo(a),a
3 None 8
```

Main Features

1. Support for all Fortran intrinsic types.

2. Support for different types of dimension specifications, e.g.:
```
real a(5), b(3:8), c(*)
integer n
parameter (n=3)
real d(n,5)
```

3. Call Fortran 77/90/95 routines and Fortran 90/95 module routines.

4. Access Fortran 77 common blocks.

5. Access Fortran 90/95 module data, including allocatable data.

Main Features

6. Supported compilers:
   - GNU project C Compiler (gcc)
   - Compaq Fortran
   - VAST/f90 Fortran
   - Absoft f77/f90
   - MIPSpro 7 Compilers
7. Supported platforms:
   - Intel/Alpha Linux
   - HP-UX
   - IRIX64
8. Documentation:
   - f2py User's Guide
   - Mailing list: `f2py-users@cens.ioc.ee`
   - Homepage: `http://cens.ioc.ee/projects/f2py2e`
   - Development under CVS, GNU LGPL.

Supported Argument Attributes

- `intent(<intent>)`: `in`, `out`, `inout`, `hide` or a combination.
- `dimension(<dimspec>)`
- `depend([<names>])`: dependency on arguments in `<names>`.
- `check([<C booleanexpr>])`: verify the size of input arguments.
- `note(<LaTeX text>)`: used for adding notes to the module documentation.
- `optional, required`
- `external`: used for call-back arguments.
- `allocatable`: used for Fortran 90/95 allocatable arrays.

Accessing Fortran 77 Common Block Data

Python:

```
>>> import foo
>>> print foo.__doc__
Functions:
  bar()
COMMON blocks:
  /fun/ i,r(4)
.
>>> foo.fun.r=range(5)
>>> foo.fun.i=13
>>> foo.bar()
 i= 13
 r=  0.  1.  2.  3.
>>> print foo.fun.__doc__
i - 'i'-scalar
r - 'f'-array(4)
```

Fortran:

```
!Fortran file foo.f:
      subroutine bar()
      integer i
      real r(4)
      common /fun/ i,r
      write(*,*) "i=",i
      write(*,*) "r=",r
      end
```

Accessing Fortran 90 Module Data

Python:

```
>>> import foo
>>> print foo.__doc__
Functions:
  bar()
Fortran 90/95 modules:
  fun --- r,i.
>>> foo.fun.r = range(4)
>>> foo.bar()
 i= 0
 r= 0.E+0,  1.,  2.,  3.
>>> foo.fun.i = 17
>>> foo.fun.r = range(7)
>>> foo.bar()
 i= 17
 r= 0.E+0,  1.,  2.,  3.,  4.,  5.,  6.
```

Fortran:

```
!Fortran file fun.f90
module fun
  integer i
  real, allocatable :: r(:)
end module fun
subroutine bar()
  use fun
  write(*,*) "i=",i
  write(*,*) "r=",r
end subroutine bar
# re-allocation
```

Calling Python Functions from Fortran

Python:

```
>>> def bar(i,a):
...       print 'i=',i
...       a[:] = [1,3,2,5,7]
>>> foo.fun(bar)
i= 4
a= 1.0 3.0 2.0 5.0 7.0
>>> print foo.fun.__doc__
fun - Function signature:
  fun(bar,[bar_extra_args])
Required arguments:
  bar : call-back function
Optional arguments:
  bar_extra_args := () input tuple
Call-back functions:
  def bar(e_4_e,a): return
  Required arguments:
    e_4_e : input int
    a : input rank-1 array('f') with bounds (5)
```

Fortran:

```
subroutine fun(bar)
external bar
real a(5)
call bar(4,a)
write(*,*) "a=",a
end
```

Plans for the Future

1. Use `distutils`, replacing current Makefile approach. Need Fortran compiler support from `distutils`.

2. Support for MS Windows? Very little familiarity with Fortran compilers under Windows.

3. Find a better solution for C-Fortran array transpose problem.

4. GUI for manipulating signature files (a good excuse to learn wxPython).

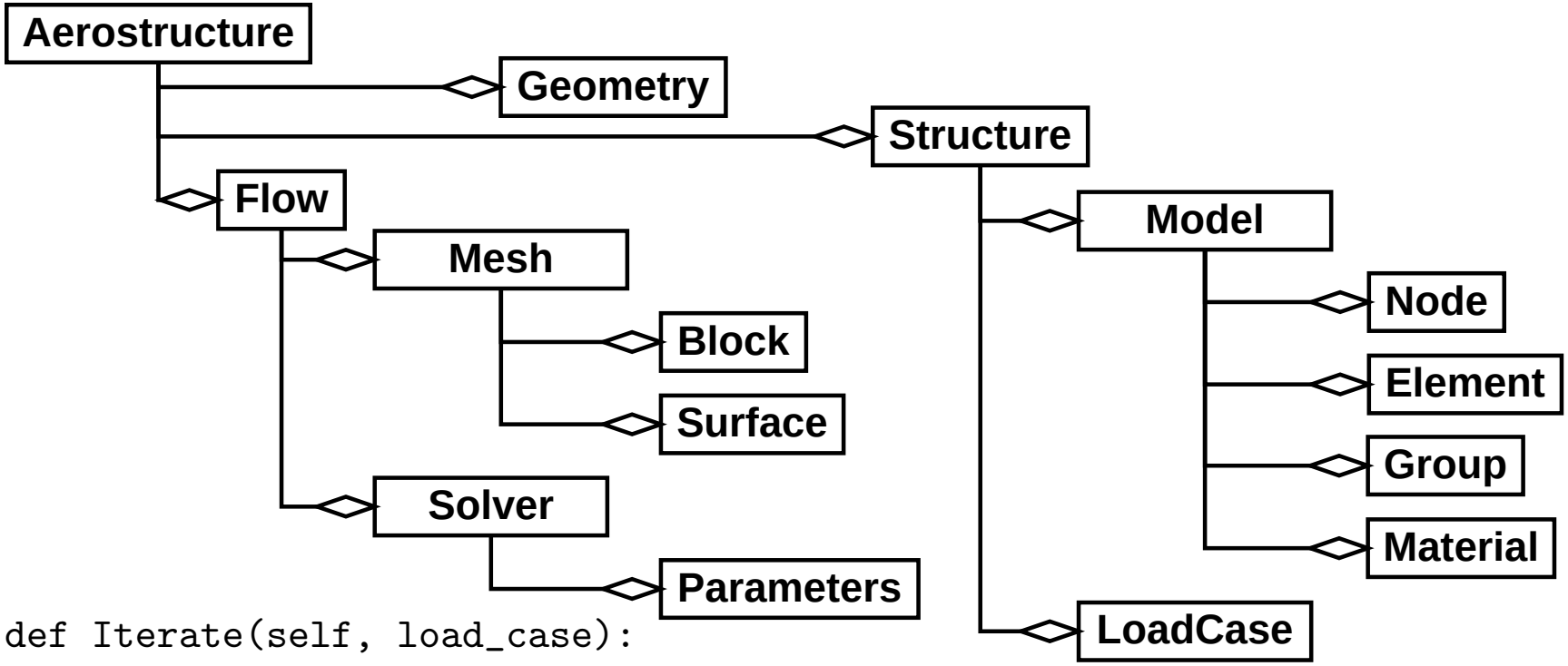
5. Maintain a repository for signature files.

6. f2py – 3rd Edition.

Application to Aerospace Engineering

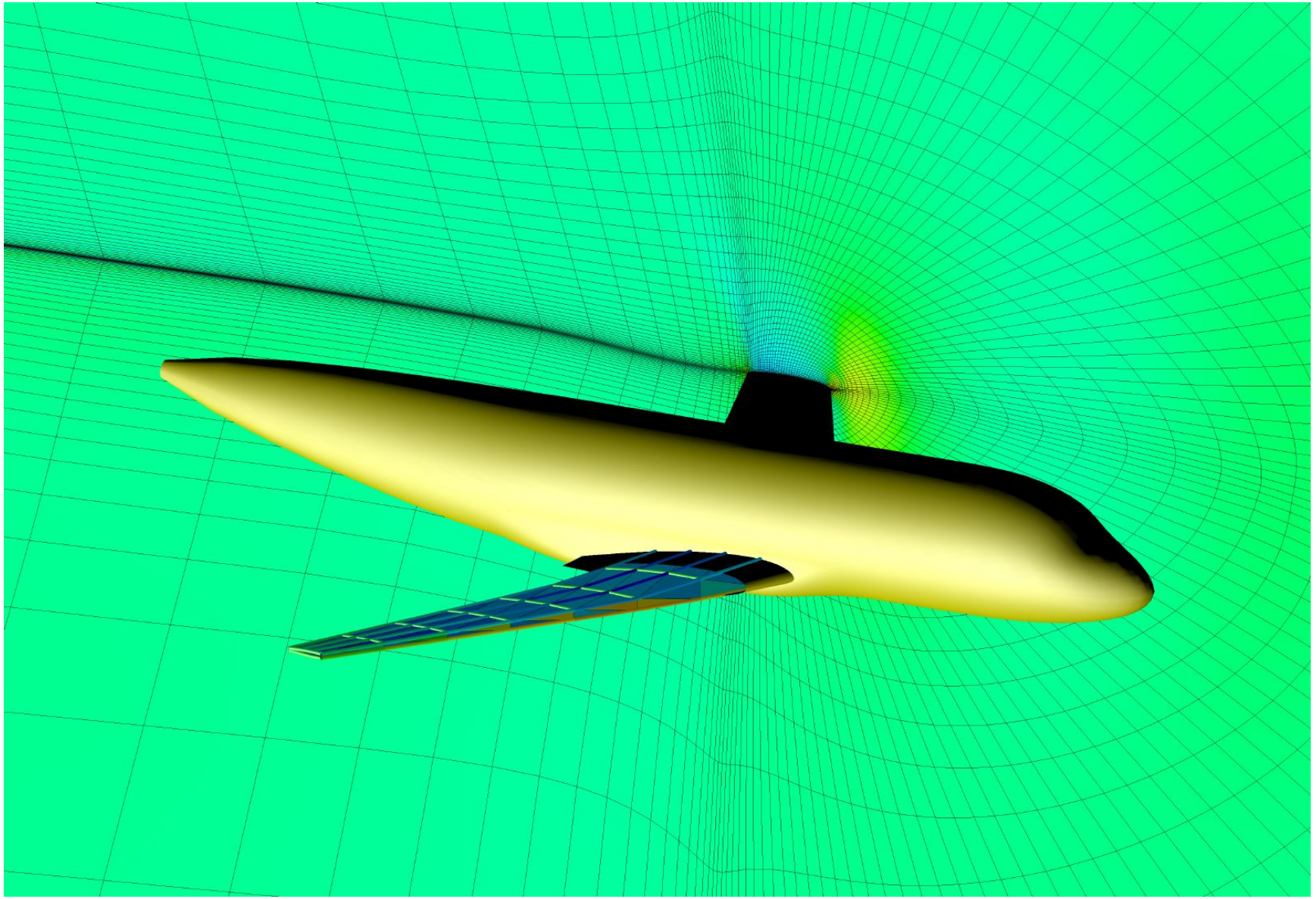
- Aero-structural design optimization framework:
  - 3D Computational fluid dynamics
  - Structural finite-element model
  - Geometry engine and database
- Motivation:
  - User friendly interface for using large Fortran solvers.
  - A better way for scripting or gluing Fortran programs.
  - Object-oriented framework to facilitate extensibility for more complex design problems.
- Requirements:
  - Access to Fortran 77 common blocks and Fortran 90 modules.
  - Wrapping process as automated as possible.

Python Module Design




```
def Iterate(self, load_case):
  """Iterates the aero-structural solution."""
  self.flow.Iterate()
  self._UpdateStructuralLoads()
  self.structure.CalcDisplacements(load_case)
  self.structure.CalcStresses(load_case)
  self._UpdateFlowMesh()
  return
```

Aero-Structural Model and Solution



Conclusions

- Presented a tool for creating Python wrappers for Fortran programs automatically.
- The tool was used in a complex aerospace engineering application.
- In practice, f2py was shown to provide:
  - An extremely versatile interface
  - A high level of automation
  - Robustness
- f2py has the potential to become the standard tool for wrapping Fortran with Python.