OAK RIDGE National Laboratory

Automated Fortran–C++ Bindings for Large-Scale Scientific Applications

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github.com/swig-fortran

Overview

- Introduction
- Tools
- SWIG+Fortran
- Strategies
- Example libraries

Introduction

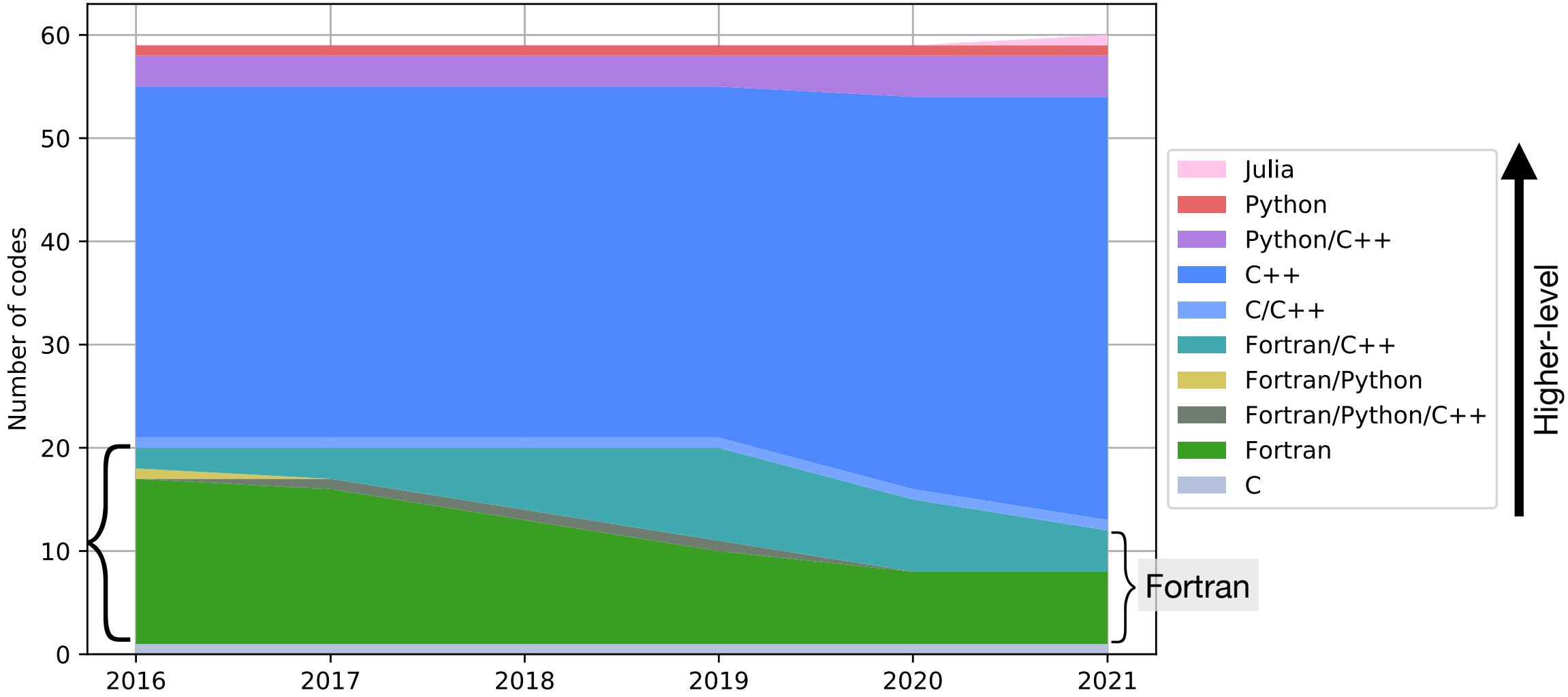
How did I get involved?

- SCALE (1969–present): Fortran/C++
- VERA: multiphysics, C++/Fortran
- MPACT: hand-wrapped calls to C++ Trilinos

Project background

- Exascale Computing Project: at inception, many scientific app codes were primarily Fortran
- Numerical/scientific libraries are primarily C/C++
- Expose Trilinos solver library to Fortran app developers: ForTrilinos product

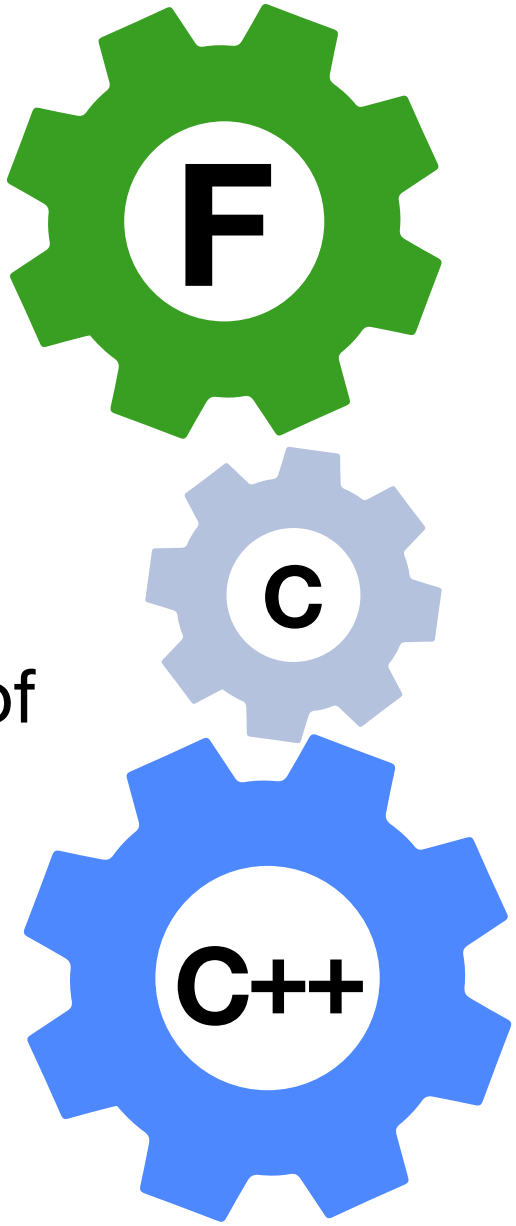
ECP: more exascale, less Fortran



ECP application codes over time *(credit: Tom Evans)*

Motivation

- C++ library developers: expand user base, more opportunities for development and follow-on funding
- Fortran scientific app developers: use newly exposed algorithms and tools for your code
- Multiphysics project integration: in-memory coupling of C++ physics code to Fortran physics code
- Transitioning application teams: bite-size migration from Fortran to C++



Tools

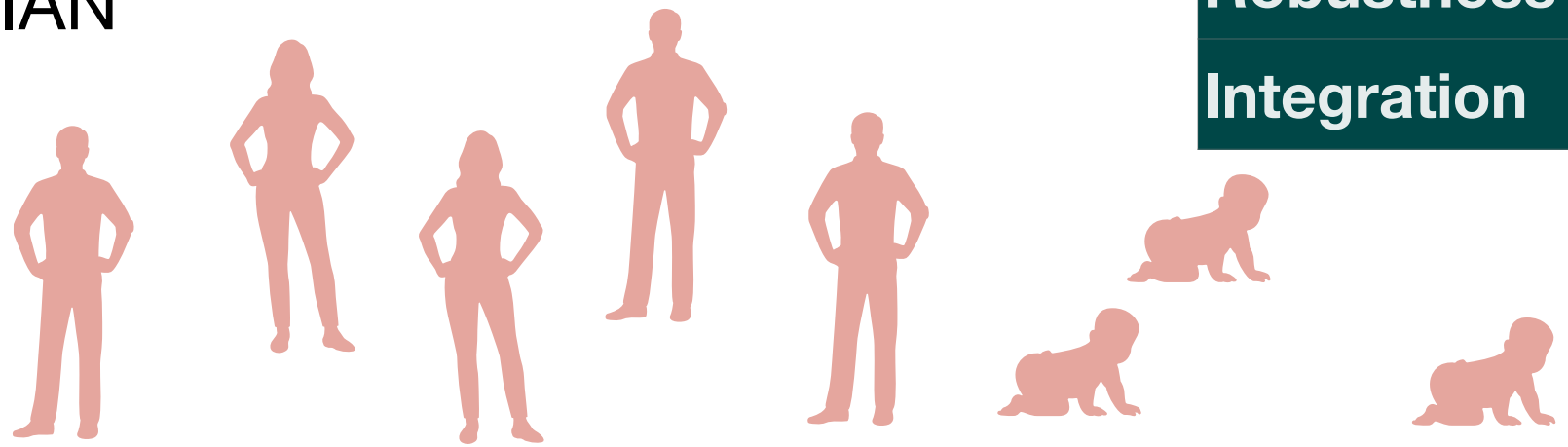
Wrapper “report card”

- **Portability**: Does it use standardized interoperability?
- **Reusability**: How much manual duplication needed for new interfaces?
- **Capability**: Does the Fortran interface have parity with the C++?
- **Maintainability**: Do changes to the C++ code automatically update the Fortran interface?
- **Robustness**: Is it possible for silent failures to creep in?
- **Integration**: How much overhead is needed to get the glue code working in development/deployment?

Hand-rolled binding code

- Often based on hand-rolled C interface layer
- Often targets F77/90 using configure-time bindings
- Examples: SuperLU, STRUMPACK, TASMANIAN

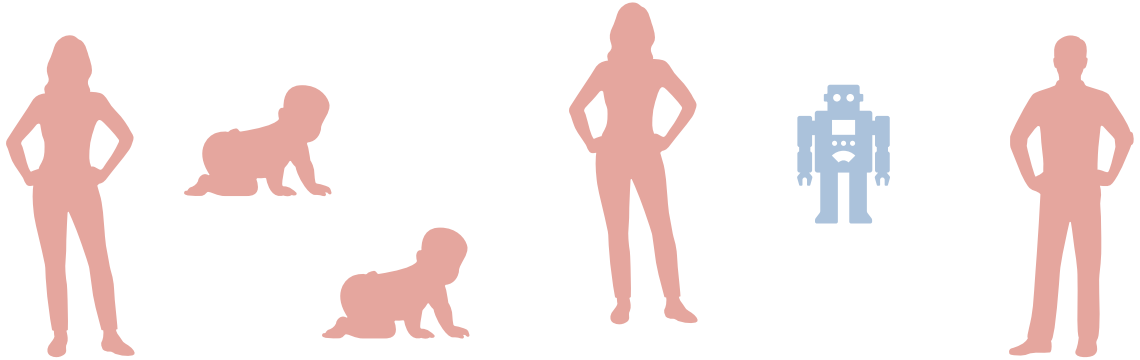
Portability	😕
Reusablity	😵
Capability	😐
Maintainability	😵
Robustness	😰
Integration	😒/🙂



Project-specific scripts

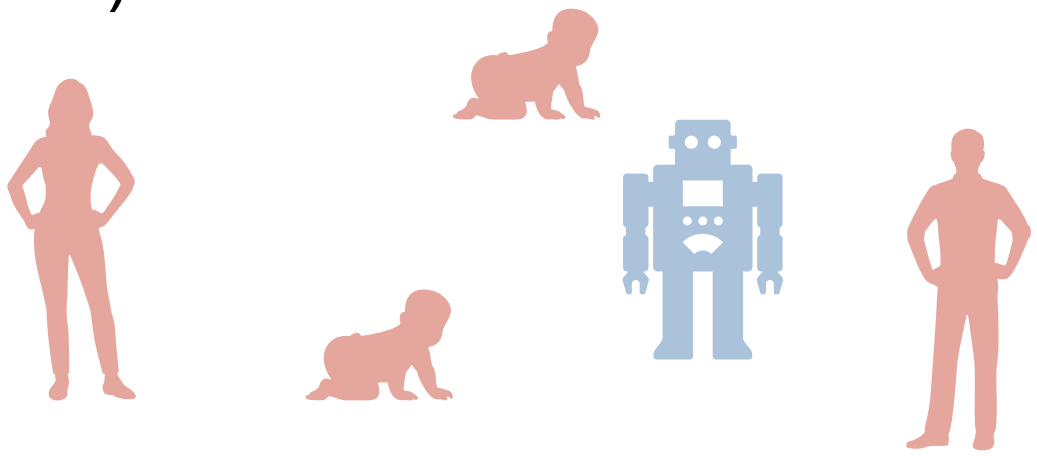
- Text processing engines hardcoded to a particular project's data types, header formatting
- Simple translations of function signatures and types to "glue code"
- Examples: MPICH, HDF5, Silo, PETSc

Portability	🙃
Reusablity	😐
Capability	😐
Maintainability	😒
Robustness	🙂
Integration	😟/🙂



Automated code generators (manual C++ declaration)

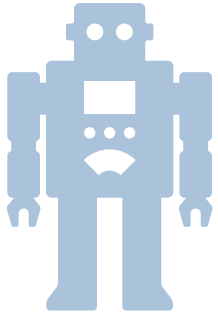
- CIX: in-house ORNL tool (template substitution)
- Shroud: recent LLNL development (custom YAML)

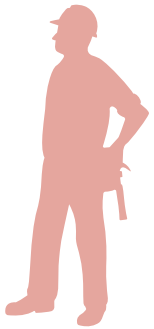


Portability	😊
Reusablity	😊
Capability	😊
Maintainability	😣
Robustness	🙂
Integration	😒/🙂

Automated code generators (integrated C++ parsing)

- SWIG+Fortran: fork of Simplified Wrapper Interface Generator





Portability	😊
Reusablity	😊
Capability	🥳
Maintainability	🤓
Robustness	🥳
Integration	😇

SWIG+Fortran

SWIG: *Simplified Wrapper and Interface Generator*

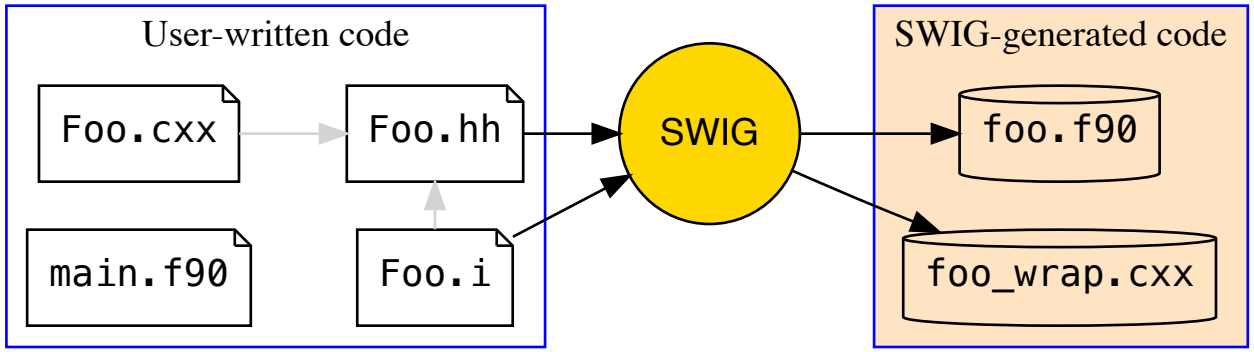
- Generate *interfaces* to existing C and C++ code and data types so that a *target language* can invoke functions and use the data
- "Glue" code: flat C-linkage wrappers to C++ functions, corresponding interfaces in target language
- Does *not* couple target languages to other target languages
- Does *not* parse target languages or create C++ proxy wrappers

Supported Languages

- Allegro CL
- C#
- CFFI
- CLISP
- Chicken
- D
- Go
- Guile
- Java
- Javascript
- Lua
- Modula-3
- Mzscheme
- OCAML
- Octave
- Perl
- PHP
- Python
- R
- Ruby
- Scilab
- Tcl
- UFFI

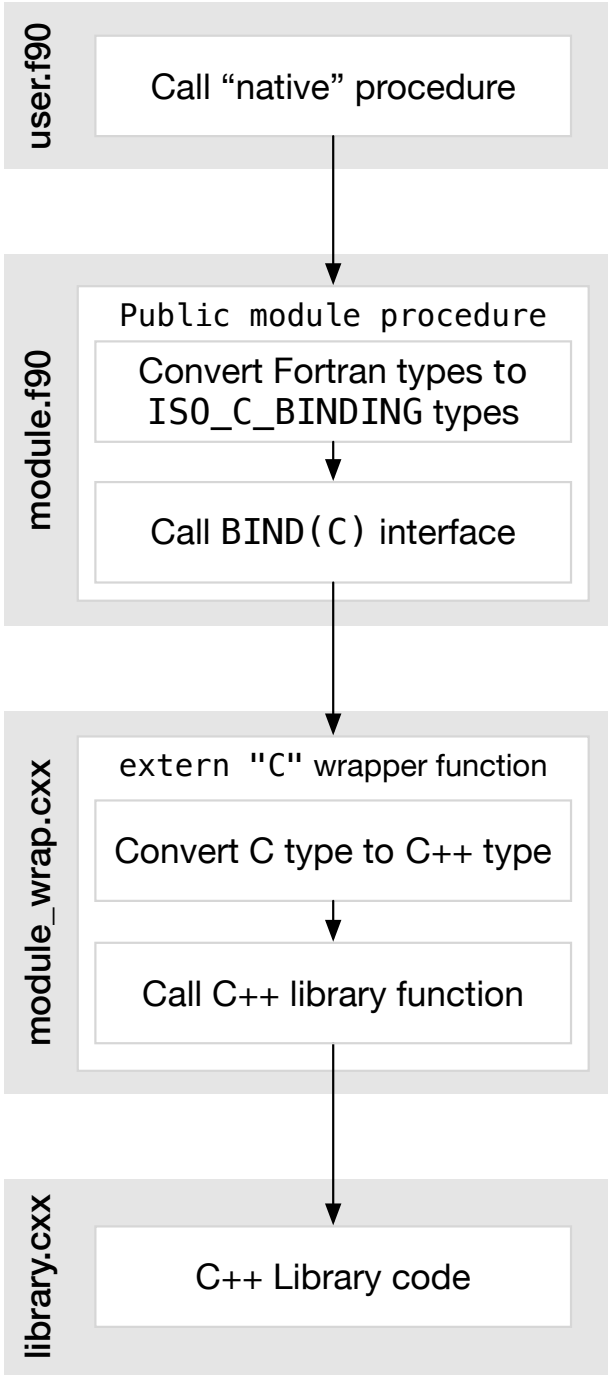
SWIG execution sequence

- SWIG reads `.i` interface file which may `%include` other C/C++ headers to parse them
  - Interface file can be as little as a couple of lines for simple interfaces
  - More difficult C++/Fortran conversions require more interface code
- SWIG *generates source code files*: `.cxx` and `.f90`
  - This wrapper code can be distributed like regular source files
  - Library users *don't need to know SWIG*



Control flow and data conversion

- Fortran 2003 standard defines C-compatible datatypes
- Use only Fortran-compatible ISO C datatypes
- Minimize data movement of numerical arrays



Features

- **Primitive types**
- Enumerations
- **Classes** (with inheritance)
- C strings and std::string
- Function pointers
- **Arrays** and `std::vector`

- **Function overloading**
- **Template instantiation**
- Compile-time constants
- **Exception handling**
- **OpenACC and Thrust**

Addition with “native” int: input and generated C code

```c
#ifndef simplest_h
#define simplest_h
int add(int a, int b);
#endif
```

simplest.h

```
%module simplest

%typemap(ftype, in="integer, intent(in)")
  int "integer"
%typemap(fin) int "$1 = int($input, C_INT)"
%typemap(fout) int "$result = int($1)"
%include "simplest.h"
```

simplest.i

```c
SWIGEXPORT int _wrap_add(
    int const *farg1,
    int const *farg2) {
  int fresult ;
  int arg1 ;
  int arg2 ;
  int result;
  arg1 = (int)(*farg1);
  arg2 = (int)(*farg2);
  result = (int)add(arg1,arg2);
  fresult = (int)(result);
  return fresult;
}
```

simplest_wrap.c

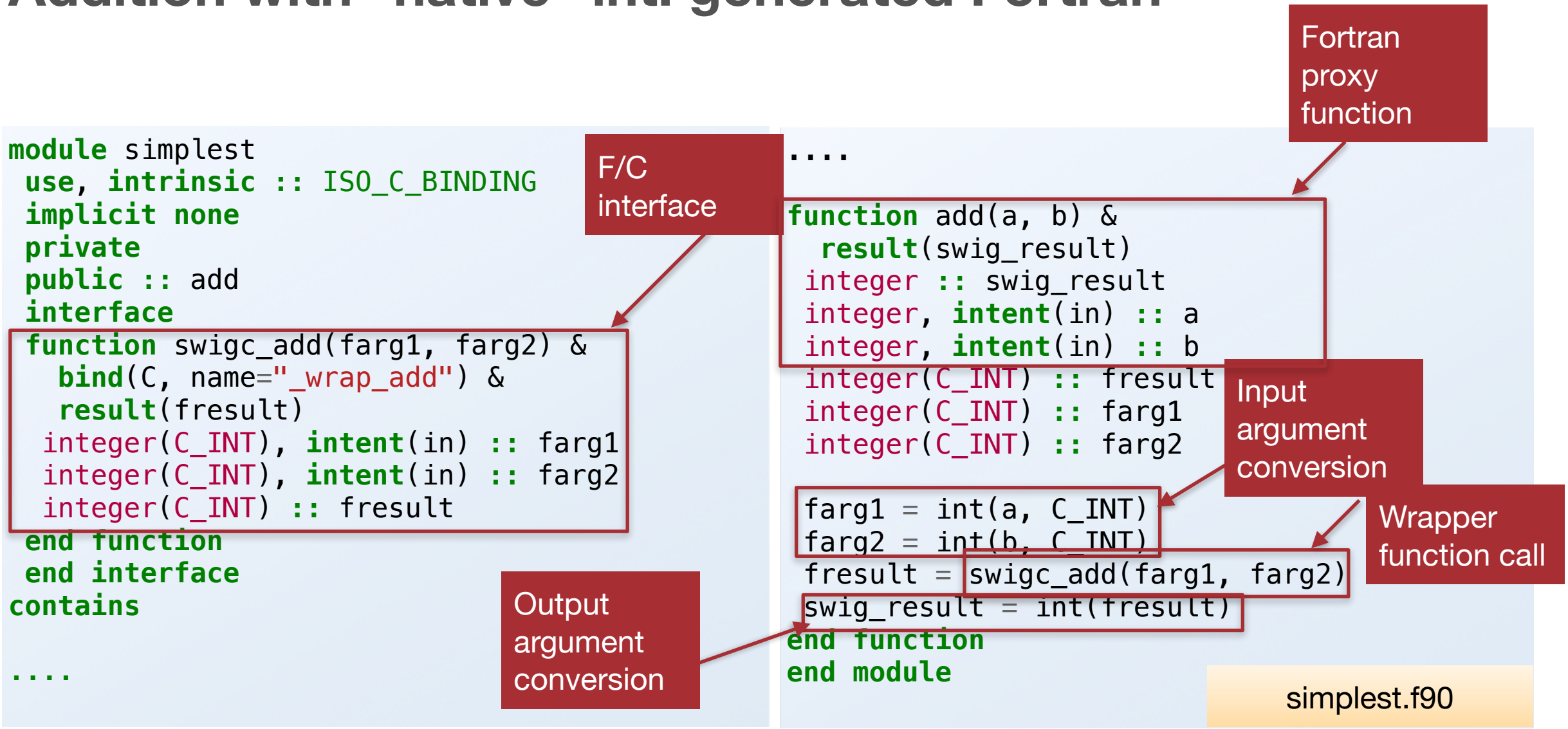
F/C interface

Input argument conversion

Wrapped function call

Output argument conversion

Addition with “native” int: generated Fortran



Simple addition function: the part app devs care about

```c
SWIGEXPORT int swigc_add(int const *farg1,
int const *farg2);
```

simplest_wrap.c

```
module simplest
 use, intrinsic :: ISO_C_BINDING
 …
contains
function add(a, b) &
  result(swig_result)
 integer :: swig_result
 integer, intent(in) :: a
 integer, intent(in) :: b
 …
end function
end module
```

simplest.f90

```
program main
  use simplest, only : add
  write (0,*) add(10, 20)
end program
```

main.f90

```
$ ./main.exe
          30
```

Automatic `BIND(C)` wrapping

```
%module bindc

%fortranbindc;
%fortran_struct(Point)

%inline {
typedef struct { float x, y, z; } Point;
void print_point(const Point* p);
void make_point(Point* pt,
                const float xyz[3]);
}
```

Only generate interface code

Don't create proxy class

bindc.i

```
module bindc
…
 type, bind(C), public :: Point
  real(C_FLOAT), public :: x
  real(C_FLOAT), public :: y
  real(C_FLOAT), public :: z
 end type Point
…
interface
 subroutine print_point(p) &
   bind(C, name="print_point")
  use, intrinsic :: ISO_C_BINDING
  import :: point
  type(Point), intent(in) :: p
 end subroutine
 subroutine make_point(pt, xyz) &
   bind(C, name="make_point")
  use, intrinsic :: ISO_C_BINDING
  import :: point
  type(Point) :: pt
  real(C_FLOAT), dimension(3), intent(in) :: xyz
 end subroutine
end interface
end module
```

bindc.f90

Templated class

```
template<typename T>
class Thing {
    T val_;
  public:
    Thing(T val);
    T get() const;
};

template<typename T>
void print_thing(const Thing<T>& t);
```

Insert raw C++ code into generated wrapper file

Instantiate templates at SWIG time

Tell SWIG to parse the header file

```
%module "templated"

%{
#include "templated.hpp"
%}
%include "templated.hpp"

// Instantiate templated classes
%template(Thing_Int)  Thing<int>;
%template(Thing_Dbl)  Thing<double>;

// Instantiate and overload a function
%template(print_thing)  print_thing<int>;
%template(print_thing)  print_thing<double>;
```

templated.i

Templated class: generated Fortran wrapper code

```
module templated
…
integer, parameter, public :: swig_cmem_own_bit = 0
integer, parameter, public :: swig_cmem_rvalue_bit = 1

type, bind(C) :: SwigClassWrapper
 type(C_PTR), public :: cptr = C_NULL_PTR
 integer(C_INT), public :: cmemflags = 0
end type
! class Thing< int >
type, public :: Thing_Int
 type(SwigClassWrapper), public :: swigdata
contains
 procedure :: get => swigf_Thing_Int_get
 procedure :: release => swigf_release_Thing_Int
 procedure, private :: swigf_Thing_Int_op_assign__
 generic :: assignment(=) => swigf_Thing_Int_op_assign__
end type Thing_Int
interface Thing_Int
 module procedure swigf_create_Thing_Int
end interface
! class Thing< double >
type, public :: Thing_Dbl
 …
end type Thing_Dbl
…
```

Memory ownership

Opaque class wrapper

Fortran proxy class

Second template instantiation

```
interface print_thing
  module procedure swigf_print_thing__SWIG_1,
swigf_print_thing__SWIG_2
 end interface
 public :: print_thing
interface
  subroutine swigc_delete_Thing_Int(farg1)
    bind(C, name="_wrap_delete_Thing_Int")
…
contains
subroutine swigf_release_Thing_Int(self)
  use, intrinsic :: ISO_C_BINDING
  class(Thing_Int), intent(inout) :: self
  type(SwigClassWrapper) :: farg1
  farg1 = self%swigdata
  if (btest(farg1%cmemflags, swig_cmem_own_bit)) then
    call swigc_delete_Thing_Int(farg1)
  endif
  farg1%cptr = C_NULL_PTR
  farg1%cmemflags = 0
  self%swigdata = farg1
end subroutine
…
end module
```

Overloaded function

Call delete if we “own” the memory

templated.f90 (2/2)

Exception handling

```
%module except
%include <std_except.i>
%exception {
  SWIG_check_unhandled_exception();
  try {
    $action
  }
  catch (const std::exception& e) {
    SWIG_exception(SWIG_RuntimeError, e.what());
  }
}
%{
#include <stdexcept>
#include <iostream>
%}
%inline {
void do_it(int i) {
  if (i < 0)
    throw std::logic_error("N00000");
  std::cout << "Yes! I got " << i
    << std::endl;
}
void do_it_again(int i) { do_it(i); }
}
```

Replaced with wrapper call

```
program main
  use except, only : do_it, do_it_again, ierr, get_serr
  call do_it(-3)
  if (ierr /= 0) then
    write(0,*) "Got error ", ierr, ": ", get_serr()
    ierr = 0
  endif
  call do_it(2)
  call do_it(-2)
  call do_it_again(321)
end program
```

main.f90

```
Got error          -3 : In do_it(int):
N00000
Yes! I got 2
terminate called after throwing an
instance of 'std::runtime_error'
  what():  An unhandled exception
occurred before a call to
do_it_again(int); in do_it(int): N00000
```

Array views

```
%module algorithm

%{
#include <algorithm>
%}

%include <typemaps.i>
%apply (SWIGTYPE *DATA, size_t SIZE) {
    (int* data, std::size_t size) };

%inline {
void sort(int* data, std::size_t size)
{
  std::sort(data, data + size);
}
}
```

Treat as native Fortran array

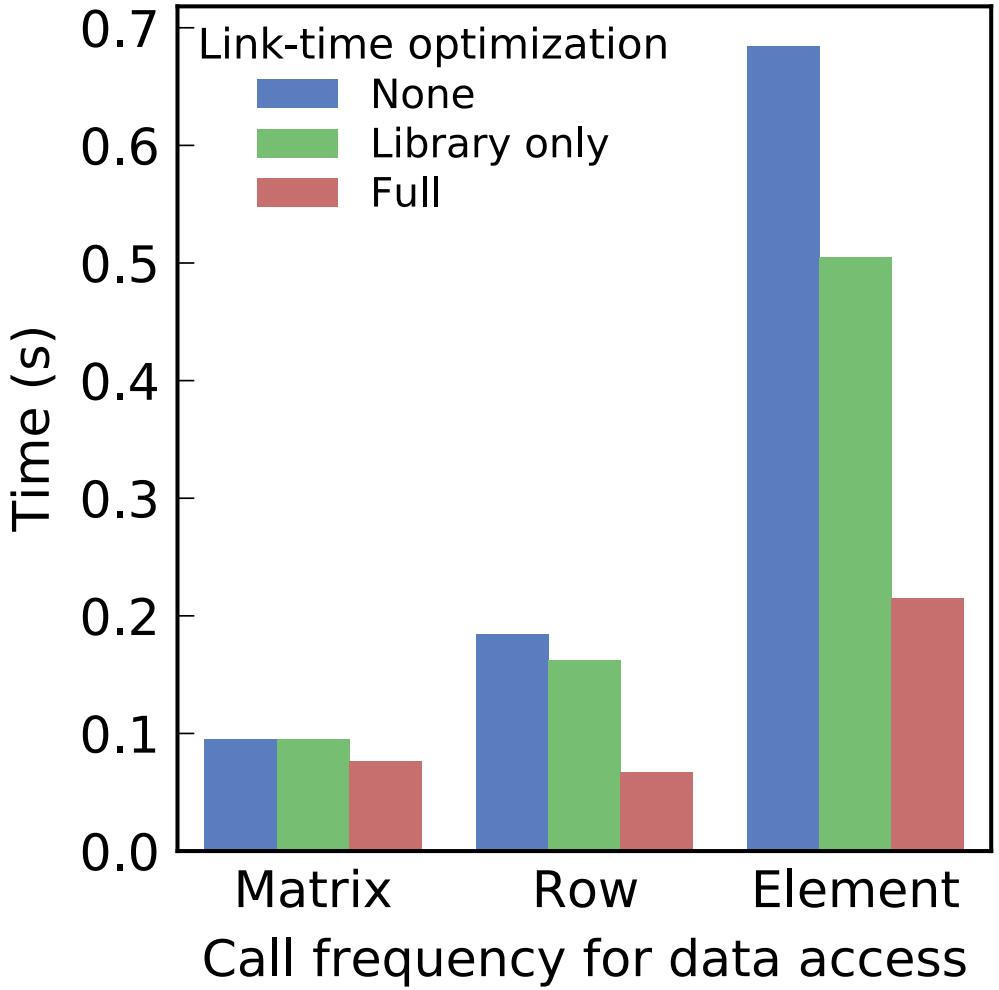
```
subroutine sort(data)
 use, intrinsic :: ISO_C_BINDING
 integer(C_INT), dimension(:), target :: data
 integer(C_INT), pointer :: farg1_view
 type(SwigArrayWrapper) :: farg1
 if (size(data) > 0) then
  farg1_view => data(1)
  farg1%data = c_loc(farg1_view)
  farg1%size = size(data)
 else
  farg1%data = c_null_ptr
  farg1%size = 0
 end if
 call swigc_sort(farg1)
end subroutine
```

```
program main
  use, intrinsic :: ISO_C_BINDING
  use algorithm, only : sort
  implicit none
  integer(C_INT), dimension(6) &
    :: test_int  = (/ 3, -1, 7, 3, 1, 5 /)

  call sort(test_int)
  write (*,*) test_int
end program
```

Performance considerations

- Small overhead for each wrapped function call
- Link-time optimization can mitigate
- Test problem: toy numerical library with CRS matrix class
- Results: sparse matrix–vector multiply for 3000×3000 Laplacian
  (average of 40 runs)

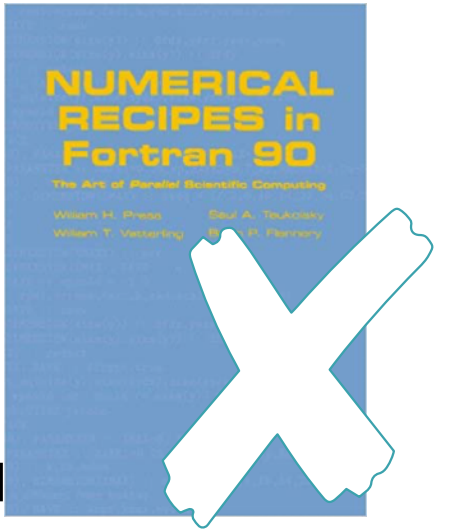


Data credit: Andrey Prokopenko

Strategies

How to add new capabilities that “should be” library functions to your Fortran app

- Wait for standards committee…
  then wait for compiler implementors
- Roll your own (e.g. numerical recipes)
- Fortran package ecosystem/fortran (FPM)*
- Contribute Fortran interfaces to C++ libraries
- Transition toward C++ by writing new C++ classes and u
  to couple to existing Fortran codebase



Adding Fortran interfaces to your C++ library

- Expose low-level C++ objects: Fortran user code looks like C++
- Write thin high-level C++ wrappers for targeted capabilities
- Target idiomatic usage for Fortran apps

Idiomatic Fortran

- Accept arrays rather than scalars or iterators as function inputs
- Return "status values" as optional argument of `subroutine` rather than result value of `function`
- Indexing convention: first element of an array is 1, possibly use 0 to indicate "not found"
- Use native Fortran types where possible rather than C types

SWIG+Fortran assists with all the above

Challenges

- Tension between Fortran/C “static” nature and increasingly dynamic C++ capabilities
  - Kokkos relies on lambdas and compile-time detection of backend
  - Numerous C++11 libraries are interface-only with extensive templating, `auto` keyword, initializer lists, etc.
  - Explicit compile-time interface needed to bind C++ and Fortran
- SWIG-generated interface must be configuration-independent

Example libraries

Flibcpp: Fortran bindings for C++ standard library

- Speed and reliability of C++ standard library
- Trivial installation and downstream usage
- App development requires only idiomatic Fortran
- Sort/search/set, sets, vectors, strings, PRNGs, …
- Callbacks for sorting too!

```
use flc_algorithm, only : argsort
implicit none
integer, dimension(5) :: iarr = [ 2, 5, -2, 3, -10000]
integer(C_INT), dimension(5) :: idx

call argsort(iarr, idx)
! This line prints a sorted array:
write(*,*) iarr(idx)
```

```
use flc_random, only : Engine, normal_distribution
real(C_DOUBLE), dimension(20) :: arr
type(Engine) :: rng

rng = Engine()
call normal_distribution(8.0d0, 2.0d0, rng, arr)
```

https://github.com/swig-fortran/flibcpp

ForTrilinos

- Includes low-level Tpetra/ Teuchos objects **and** high-level solver interfaces
- Inversion-of-control for Fortran implementations of operators

```
module myoperators
  use forteuchos
  use fortpetra
  implicit none

  type, extends(ForTpetraOperator) &
      :: TriDiagOperator
    type(TpetraMap) :: row_map, col_map, &
      domain_map, range_map
  contains
    procedure :: apply => my_apply
    procedure :: getDomainMap &
      => my_getDomainMap
    procedure :: getRangeMap &
      => my_getRangeMap
    procedure :: release &
      => delete_TriDiagOperator
  end type
  interface TriDiagOperator
    procedure new_TriDiagOperator
  end interface
  ! ...
end module
```

ForTrilinos coauthor:
Andrey Prokopenko

Flibhpc: Thrust/OpenACC/MPI

- Uses SWIG to integrate `acc_deviceptr/C_DEVPTR` with Thrust `device_ptr<T>` to pass
- MPI integration (convert F77/90-style MPI integers into C `MPI_Comm` objects)

Sneak peek

```
program test_thrustacc
  use flhpc, only :: sort
  implicit none
  integer, parameter :: n = 32768
  integer :: i
  real, dimension(:), allocatable :: a

  ! Generate N uniform numbers on [0,1)
  allocate(a(n))
  call random_number(a)

  !$acc data copy(a)
    !$acc kernels
      do i = 1,n
        a(i) = a(i) * 10 + i
      end do
    !$acc end kernels
    call sort(a)
  !$acc end data
  write(*,*) sum(a)
end program
```

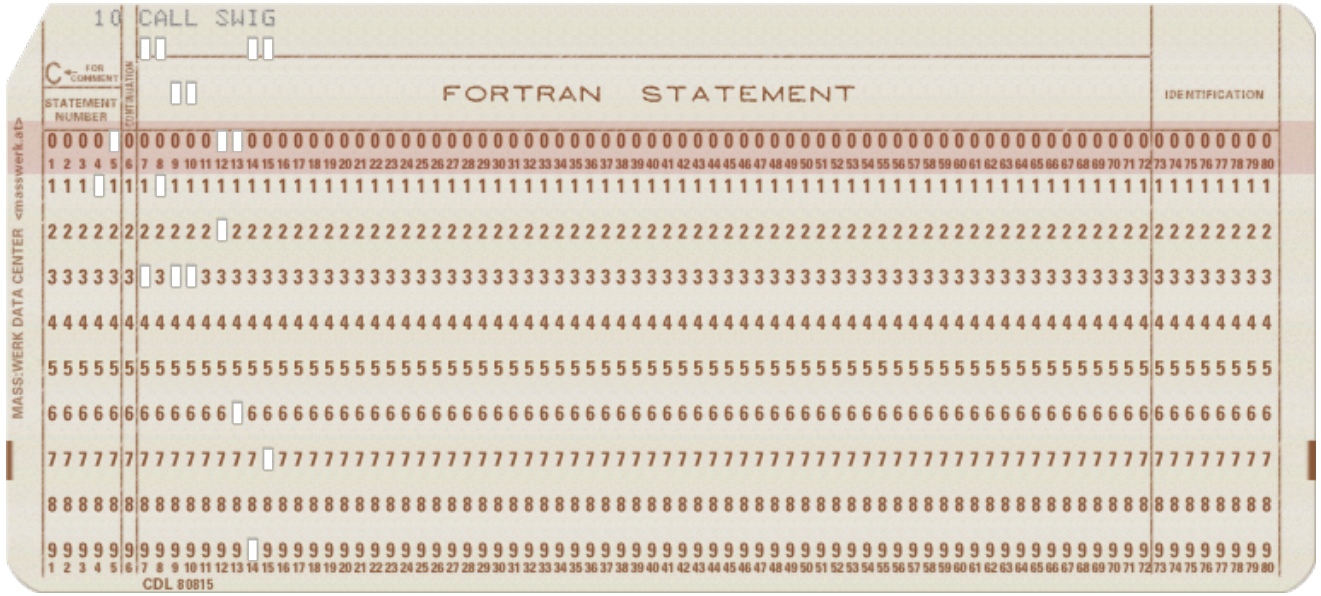
Other ECP codes using SWIG+Fortran

- SUNDIALS
- TASMANIAN
- DTK
- STRUMPACK
- SCALE

Summary

- Exascale era is another driver for inter-language operability
- Coupling can be driven by apps *and/or* libraries
- SWIG+Fortran produces robust, idiomatic glue code
- New library bindings can give a taste of C++ capabilities to Fortran codes

	Github	Spack	E4S
SWIG+Fortran	✓	✓	✓
ForTrilinos	✓	✓	✓
Flibcpp	✓	✓	
Flibhpc	✓		



https://github.com/swig-fortran

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