### **Modernizing OpenRadioss**

Modernizing OpenRadioss: A Journey Through Three Decades of Fortran Evolution



Olivier Wienholtz, Director Software Development <u>olivier@altair.com</u>, co-Author & Speaker

Laurent Berenguer, Lead Software Developer HPC <a href="mailto:lberenguer@altair.com">lberenguer@altair.com</a>, co-Author

Marian Bulla, Director OpenRadioss Community bulla@altair.com, co-Author

#### Altair Radioss – Proven Crash & Impact Simulation Software

**Consumer Goods & Automotive & Rail Aero & Defense** Manufacturing

#### OpenRadioss – The Open-Source Version of Radioss

Democratize explicit dynamics, build active community and accelerate innovation

#### Introduced 3 years ago

#### OpenRadioss.org



#### Fast growing adoption since then

- 16000+ binary downloads
- 4000+ commits / 14 active contributors
- 400+ discussion topics on forum
- Social Media: LinkedIn, YouTube, webinars, ...
- Steering committee / Users Days

#### https://github.com/OpenRadioss/OpenRadioss





#### **R&D Collaborations & Partnerships**





Hardware & Software Providers



























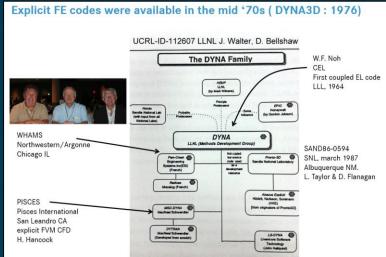


#### Radioss / OpenRadioss

Project started mid 80s with roots in the 70th

**Today: High performance Parallel code** 

- Compute intensive Solver
  - Code translates Mathematical equations
  - Self-written algorithms / few calls to Numerical libraries (Blas/Lapack)
- Highly Optimized and vectorized code
- Massive parallel Solvers
  - SMP / OpenMP
  - DMP / MPI
- Portable Solver
  - X86 Linux and Windows
  - ARM64 Linux



- 2 millions lines of Fortran code
  - ~ 90% Fortran77 Fixed Format files
  - ~ 10% Fortran90 Free Format files
  - Fortran 90/95 Types for Data structures
- Some C/C++ modules mainly for I/O applications
- Interface to Python for User Code (functions)



#### **OpenRadioss**

#### We continue to use Fortran because

- A lot of working legacy code
- Accessible for our typical contributors: Mechanical Engineer, Matlab background
- Consistent and high performant with only a few guidelines
- Proven reliability and maturity

#### **But C++ contributions are also welcome**

#### **Design Constraints**

- Performance: High Solver efficiency & parallel performance
- Portability: ARM64, X86-64, Linux, Windows, Compilers (GCC/Gfortran, ArmFlang, AOCC, Intel OneAPI)
- **Bitwise reproducibility:** Whatever Parallel run modus: MPI x OpenMP configurations Reduce Optimizations: avoid use of Multiply-Add (FMA) assembly instructions





#### **Modernization?**

#### **Ongoing efforts for more than 30 Years**

- Improve code structure to adapt parallelism needs
- Work on main data structures

#### **Prior to OpenRadioss**

- Makefile with self-made dependency creation tool (use of Cygwin on Windows)
- F77 Fixed Format
- F77 Common blocks, Some equivalences, Common variables in Modules
- OpenMP Threadprivate variables in commons
- C preprocessor directives #ifdef for system specific code
- Need of code modernization



#### Modernization strategy: gradual improvements

#### **Data structures**

Group arrays and variables in user defined types: reduce argument list in routine call

#### **New files / subroutines : Guidelines from fortran-lang.org** (with minor caveats)

- Free-form file format, Fortran 95 + selected recent features
  - C/Fortran interface : iso\_c\_bindings
  - Intrinsic functions etc...
- ➤ New subroutines → module
  - Forces explicit interface and compile time errors when argument mismatch
- ▶ Limit C preprocessor usage: #define → parameter



#### Modernization strategy: gradual improvements Legacy files: Start refactoring

- > Equivalences have been removed.
- > OpenMP Threadprivate variables in common blocs has been removed
- Remove COMMON BLOCK : in progress
  - Common Blocks defined in include files & shared in multiple routines
  - Move them in meaningful types with appropriate arrays
  - Some common variables are parameters : transform them into parameters
- Rewrite Fortran fixed routines in Fortran Free format

#### **Executable generation:**

#### **Porting to CMake**

- Simplification of build process: Few 100. lines of CMake wrt. Thousands Makefile
- Windows native build with Ninja (no need for Cygwin/MSYS2 or equiv. layer)
- Automatic dependency checker instead of handmade dependency checker.
- Less duplication because of the variety of compilers
- fpm (Fortran Package Manager) was not mature enough (lacks mutli-language capabilities)





# Executable generation: Code Quality / Avoiding bugs

# ¥

#### **Gfortran: Needed for Open sourcing Radioss**

- Use of Gfortran capabilities with address sanitizer:
  - Find earlier memory related bugs / report to developer is faster
- GCC plugin for minimal static analysis
  - argument mismatch on legacy files + other minor checks
- Several Gfortran warnings transformed into errors
  - Uninitialized variables : -Werror=maybe-uninitialized

#### Intel OneAPI

Check bounds and other debug capabilities



#### **Benefits**

#### Code is easier to read and maintain!

- Lower the entry barrier for new contributors
  - More modern code style is more appealing for our external (non Altair) contributors
  - Code becomes more readable
  - Reduce routines argument list make reading more comprehensive.
- Reduce development time: Less time spent in structural tasks
  - With newly created types : adding members is easier than modifying call tree.
- Working with LLMs gives better results
- Better Code review by LLM (GitHub CoPilot)
  - Better result with GitHub Co-Pilot review & Pull Request summary
- Iso\_c\_bindings: cleaner and easier to maintain C/C++ interface



#### **Benefits**

#### Less C processor directives and Fortran Free format:

Compatibility with FORTITUDE

#### Improved Code quality on contributions with GCC/Gfortran features

- Compile time error (modules+gcc plugin) / Asan catch on non-regression tests
- Gfortran Warnings moved to errors: Several catches per Week!
   Examples: 2/3 catches on uninitialized variables

```
Error: 'z14' may be used uninitialized [-Werror=maybe-uninitialized]
/home/lberenguer/OpenRadioss/engine/source/boundary_conditions/bcs_nrf.F90:140:36:

140 | real(kind=WP) :: X14,Y14,Z14 !< [N1N4] vector
```





#### Restricts usage of

#### Intent(in|out|inout)

- Easy to forget.
- Bug when in a call stack: INTENT(IN) or OUT and variable is modified
- Different behavior depending on compiler (Gfortran/IntelOneAPI)

# Legacy Routine 1 INTEGER,INTENT(IN) :: A Legacy Routine 2 INTEGER :: A Legacy Routine 2 INTEGER, INTENT(INOUT) :: A A=A+1

#### **Arrays of user-defined type:**

#### Nice to write, but:

- Poor performance: Memory access, Compute loop may not vectorize
- Memory overhead
- Opposite is preferred : Types of Arrays



#### Restricts usage of

#### **Pointers: performance degradation**

- Can be partially mitigated with CONTIGUOUS
- Different behavior depending on compiler (Gfortran/IntelOneAPI)

```
module compute_head_mod subroutine compute_head(arrays,n,ibegin)
```

integer, intent(in) :: n,ibegin
type(my\_type), intent(inout), TARGET :: arrays
real(8), dimension(:), pointer, CONTIGUOUS :: acc

acc => array%in%hierarchy%of%struct
call compute(acc)

end subroutine compute\_head
end module compute\_head\_mod

#### MPI: keep #include "mpif.h" instead of use mpi module

- No module compatibility between 2 Gfortran versions
   Installed OpenMPI on Linux may no be built with used Gfortran compiler
- Encapsulate MPI calls in routines to limit C preprocessor usage
  - Kind of homemade mpi module



#### Restricts usage of

#### **Polymorphism:** One OpenRadioss option uses polymorphism

- Syntax can be confusing for our mechanical contributors,
- Experienced bugs or unexpected behave on some compilers: ifort (now deprecated), armflang.

```
class(base), allocatable :: arr(:)
integer :: status
allocate(extended :: arr(3))
select type (assoc => arr)
    type is (extended)
    ! ok
    write(6,*) allocated(arr)
end select
select type (arr)
    type is (extended)
    ! compilation error:
    write(6,*) allocated(arr)
end select
```

```
t1%id = 1
t2%id = 2
ptr => t1
select type (ptr)
    type is (extended)
    ptr => t2
end select
print *, "After: ptr%id =", ptr%id !1
ptr => t1
select type (assoc => ptr)
    type is (extended)
    ptr => t2
end select
print *, "After: ptr%id =", ptr%id !2
```

Slow down performance: Comparison with C++ (C++ de-virtualize & is ~4x faster)

#### **Blog on polymorphism by Steeve Lionel**

https://stevelionel.com/drfortran/2020/06/30/doctor-fortran-in-not-my-type

#### Issues & forums on Stackoverflow

https://stackoverflow.com/questions/26068020/error-if-selector-expression-in-select-type-is-not-a-named-variable-associate





## Conclusion: OpenRadioss will remain Fortran based program! But Code Modernization is a need for us.

#### **Pragmatic approach: Need drives the refactoring**

- Rewrite/Refactor legacy code to F95 free format when working on projects
- Adopt new feature only when clear benefits

#### Still a long journey ahead

~ 10 % of our Fortran code base is modernized

#### Workforce shortage mitigation

- Simple computational kernels, so that non-expert can contribute: "Basic Fortran"
- Open to C++ contribution thanks to iso\_c\_bindings



#### **Wishlist**

#### Simple generic programming for basic types

- lot of code duplication can be avoided
- Today's workarounds (Parametrized derived types PDTs, Fypp) not satisfactory

#### ISO C binding: Better String / character handling

ISO C bindings not ideal for Character:

- Silent truncation / garbage
- Array of strings (typically one string per line of a file)



