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RELAP5-3D Conversion to FORTRAN 90

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Outline

- *Reason for Conversion*

- *Impact on Code Users*

- *Conversion Plan*

- *Details of Some Aspects of the Conversion*

- *Summary*

Reason for Conversion

- *Modernization, FORTRAN Language moves forward*
  - *Vendors only supply FORTRAN 95 compilers now*
  - *FORTRAN 2000 standard is nearing completion*
- *Take advantage of better language features*
  - *allocate, modules, derived types, etc.*
- *Simultaneously improve code development effort*
  - *Readability*
  - *Efficiency of modifying the source code*
  - *Maintainability (bug fixes, shelf-life of code, etc.)*

Impact on Code Users

- *RELAP5-3D/Ver2.0+ <u>unusable with old compilers</u>*
  - *If Operating System does not F90 libraries, even executable RELAP5-3D may not run.*
  - *Source code clients need FORTRAN 90+ compiler.*
- *<u>NO upper limit</u> on problem size, <u>when conversion done</u>.*
  - *Virtually all arrays are within FA, a fixed-size array.*
  - *After conversion, arrays will be allocated after input processing.*
- *Conversion will cause <u>changes in speed</u> and arithmetic <u>calculations</u>.*

Conversion Plan

- *Upgrade bit packing to FORTRAN 90.*

- *Convert FTB database to FORTRAN 90 modules.*

- *Convert fixed-length common blocks to modules.*

- *Convert special features*

  - *restart-plot technology, renodalization, scan-request, et cetera.*

- *Modify installation procedures, resolve platform issues.*

Details of Some Aspects of the Conversion

- *Modernization of bit-packing*

- *Use of derived type*

- *Replacement of "comdecks" with modules*

- *Array notation*

RELAP5-3D Bit Packing Overview

- *Bit packing is a data compression technique*
  - *several pieces of data are stored in a single word of memory.*
- *Special bit pack operations and tricks:*
  - *MIL-SPEC: Store, modify, and retrieve a particular datum from a compressed word.*
  - *Logical operators: for single bits.*
  - *Equivalence between reals and integers is used to apply special operator for one data type to the other.*
  - *These are used separately and in combinations.*

FORTRAN 90 Bit packing

- *Numerous, standard FORTRAN 90 bit operators*

- *Easier to read, understand, work with than MIL-SPEC and logical operators.*

- *FORTRAN 90 bit operators will replace MIL-SPEC and combined logical operators.*

Conversion of Bit Packing

- *Pervasive change will affect approximately 1400 files in the following directories:*
  - *envrl, fluids, matpro, relap, rgui, scdap*
- *Bit-packing broken into 3 major categories with about 30 subcategories or kinds*
  - *Conversion is complicated by changes in order and use of variable and arrays as arguments.*
- *A program converts one kind of bit packing in one file.*
- *One kind of conversion is performed on a group of 10 subroutines, then test cases are run.*

Derived Types

- *Derived types are user-defined data types that combine data of standard types as fields.*

- *Example: Derived type: Volume Data*
  - *Each field represents 1 array of the VOLDAT comdeck.*
  - *Field 1 is "p" (pressure); field 2 is tempg, et cetera.*
  - *Fields may have integer, logical, or even character data*

- *Array, VL, is declared to be of derived type Volume Data.*
  - *VL(k) contains all data for volume k in its fields.*
  - *VL(k)%tempg = temperature of the gas in volume k*

- *Conversion to derived types is being programmed.*

Modules

- *A FORTRAN 90 module*
  - *global data and subprograms*
  - *is accessible only to subprograms that "USE" it.*
- *Modules eliminate data overwrites due to indexing errors.*
- *Modules are have greater capabilities than comdecks.*
- *Compiled modules are "outside" the program in a separate file.*
  - *Modules can be attached to many different executable programs.*

RELAP5-3D Modules

- *Standard format: 3 Sections*
  - *Documentation: Description and Data Dictionary*
  - *Declarations (Type, dimension, access, pointer, allocatable, etc.)*
  - *Module Subroutines*
- *Conversion of a comdeck*
  - *Some of the comdecks have a very complex memory layout (e.g heat structures)*
  - *Use of derived types & pointers can reduce complexity*

RELAP5-3D Modules (continued)

- *Arrays conversion to derived types.*

- *Every subroutine that accesses a converted array has to be changed simultaneously.*

  – *Indexing with variables & arrays and referencing via FA-array makes it difficult.*

- *Method: create module with transfer routines; temporarily keep comdeck.*

  – *Convert one subroutine to access derived type*

RELAP5-3D Modules (continued)

- *Transfer from FA to module at beginning of routine; transfer back at end. Test!*

- *When every subroutine is converted, the comdeck and transfers can be eliminated.*

- *Must be done individually for each comdeck. There are about one hundred.*

- *A suite of programs is being written to perform much of the conversion automatically*

Array Notation

- *Allows operations on whole arrays or parts of them.*
- *Examples:*
  - *Vector(INDEX1:INDEX2) = 0.0*
  - *zeroes out Vector from INDEX1 to INDEX2.*
  - *A = B * C*
  - *Multiplies MxN matrices B and C to get A.*
- *Compiler is free to optimize array operations when used. Can invoke intrinsic functions.*
- *Will cause RELAP5-3D to run faster on some platforms, possibly slower on others.*

Summary

- *Conversion to FORTRAN 90 will impact users.*
  - *Requires a FORTRAN 90 compiler or beyond.*
  - *May affect calculations and speed.*
  - *Will eliminate input model size restrictions.*
  - *The restart-plot file will change.*
- *Conversion will make the source code easier to work with, reducing bugs and maintenance costs.*
- *Conversion extends usable lifetime of RELAP5-3D.*
- *Some aspects of the conversion were covered.*