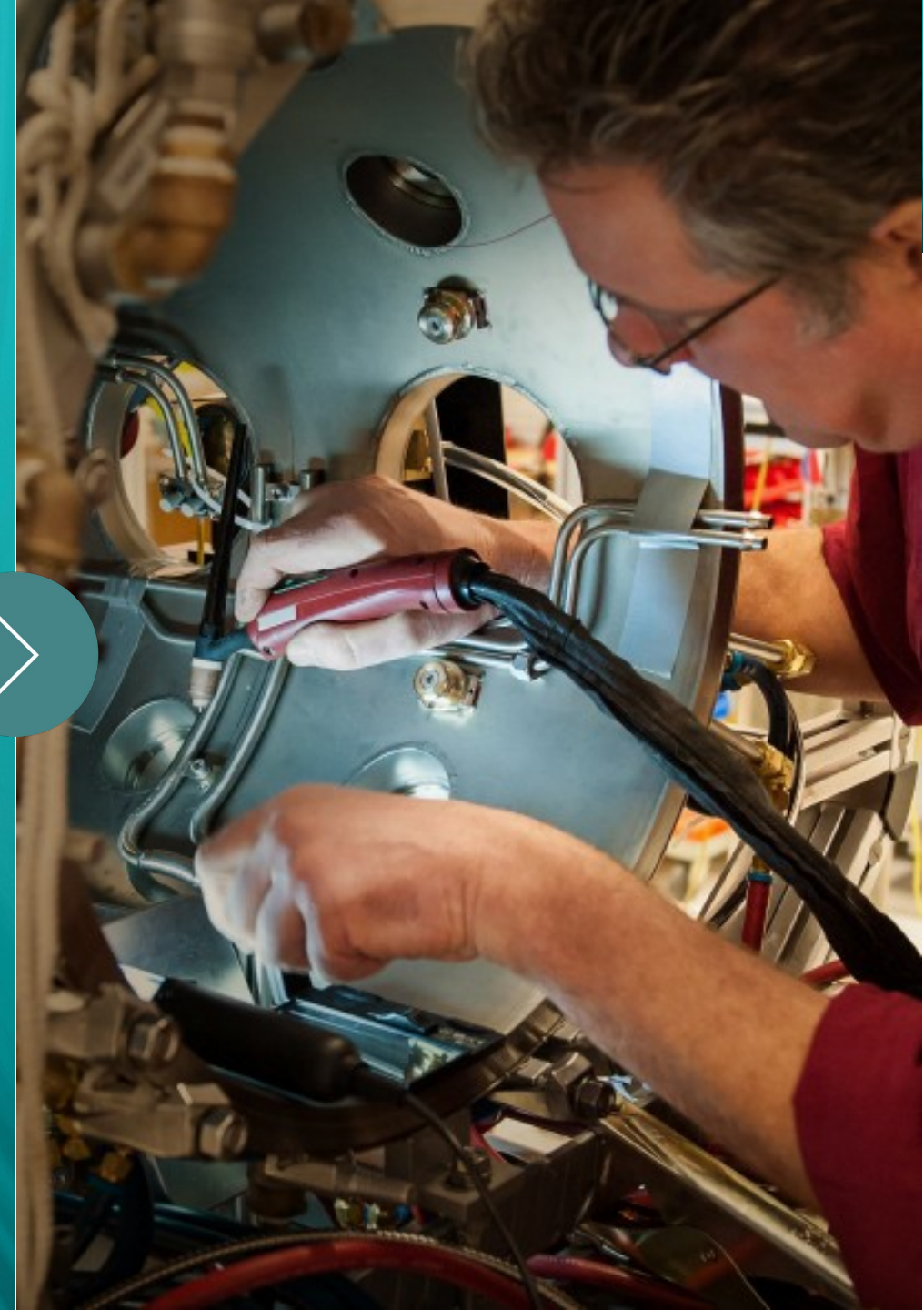# Variable Grouping

TSVV-5 Code Camp

J. Gonzalez; 21-11-2022

DIFFER

Advantages of variable grouping

Advantages of variable grouping (Conclusions from Previous Code Camp)

- Variables names should be clear.
    - When possible, they should be organized in TYPEs to improve code clarity.
    - PROCEDUREs should have a clear purpose and IN/OUT/INOUT definition for all variables.

- Removal of SAVE statements.

- Switch to Frotran Free Format.

- Possible points of action:

- Initial particle properties

- Geometry (generic unstructured grid)

- MODCOL

Application case: MODCLF and MODCOL

What is MODLCF

- MODCLF(IR) = NMLKJ contains information on how many parameters are used in a cross-section or energy-rate fit:

  - 1: 8th-order polynomial of $\ln(\sigma_v \text{ or } \delta_E)$ vs. $\ln(T)$ (H.2)

  - 2: double polynomial of $\ln(\sigma_v \text{ or } \delta_E)$ vs. $\ln(T)$ and $\ln(e0)$ (projectile energy).
    Can only be partially precalculated as projectile energy is only available during flight of particle.

  - 3: double polynomial of $\ln(\sigma_v \text{ or } \delta_E)$ vs. $\ln(T)$ and $\ln(ne)$

- For other rates (potential and momentum rate) no options are available.

- Value assigned in file-handling/slreac.f

Integration of MODCLF into REACDAT

- New INTEGER per dataset in REACDAT with the same meaning as MODCLF (1, 2 or 3 depending of type) to indicate which variables are being used for the fitting.

- MODCLF can be entirely removed.

- Not it is responsible of each dataset to contain information about the fitting variables.
  - More possibilities to expand and adapt to multiple datasets.

Structure of MODCOL

- Petra did an amazing work compiling the different values of MODCOL and how they are used.

- MODCOL(ICT,I2,irxx) is a 3D array organized as:
  - ICT: Reaction type
  - I2: Reaction Data
  - irxx: local reaction index

- The value of MODCOL depends on the reaction type.

- Different values for "Default reactions".

ICT	Reaction Type
ICT = 1	EI
ICT = 2	DS (out)
ICT = 3	CX
ICT = 4	PI
ICT = 5	EL
ICT = 6	RC
ICT = 7	PH

I2	Reaction data
I2 = 0	Potential (H.0)
I2 = 1	Cross section (H.1)
I2 = 2	Rate coefficient (H.2, H.3, H.4)
I2 = 3	Momentum averaged rate coefficient (H.5, H.6, H.7)
I2 = 4	Energy averaged rate coefficient (H.8, H.9, H.10)

Function of MODCOL

- MODCOL has to main functions:

  - MODCOL(ICT,1,irxx) relates the local reaction index irxx of type ICT

  - MODCOL(ICT,2,irxx) and MODCOL(ICT,4,irxx) (in combination with MODCLF) indicate the type of collision rate and energy rate.

- The meaning of MODCOL, particularly for I2 = 2 and I2 = 4, changes for each reaction type.

New way to represent the information in MODCOL

- Relation between local and global reaction index:
  - New integer arrays per reaction type (EI, CX, PI…) that link the local index (array index) to the global reaction index.
  - Clear function and name.

- Information about collision and energy rate:
  - New TYPE per reaction type that includes a number of INTEGERs that determine the parameters to be used in the fit (one, two variables...).
  - Flexible to cover every all reaction types.
  - It can be easily documented in each TYPE definition with comments.
  - Easy to extend for new values.

Conclusions

Conclusions

- The information in MODCLF and MODCOL is confused, not documented and not easy to modify or extend.

- The goal is to separate the multiple functions of these arrays and put them in new variables with focused functions.

- Most of the information of MODCOL and MODCLF will be stored in REACDAT now.

  - Addition of new arrays to relate local with global reaction indexes.

- This will improve code readability, documentation and even memory access.

- Transformation of obscure arrays into variables with meaning.

Thank you for your attention

J. Gonzalez | TSVV-5 Code Camp 2022

DIFFER

Text

- Text