FRED: Fast reactor fuel behaviour code

**Version: 1.2.0 (20241204)**

**Modifications**

**1.0.0**

Initial version

**1.0.1**

Fiel FRED\_.f90 with the old FRED code was removed

**1.1.0 (20241115)**

1. Fortran files were re-organized as follows:

- main.f90: main driver

- FRED.f90: DAE residual function, all models, Equations-of-State and auxiliary functions.

- globals.f90: declaration of all global variables

2. Restart was introduced. Now all variables and derivatives are stored in a separate rstfrd file for every timestep. The new input card allows specifying from which rstfrd to restart.

3. New criteria for the root function were introduced. The new input card allows specifying the exact times which the solver should make. To be tested.

4. MOX fuel swelling model was modified. The new input card allows specifying the multiplier for the swelling rate.

5. Material properties for stainless steel t91 were added.

6. New example of FRED input file was added.

**1.1.1 (20241127)**

A minor bug fixed in root finding routine.

**1.2.0 (20241204)**

1. Makefile is modified to generate the executable named as the version, e.g. FRED1.2.0.x

2. The functions for the burst strength, yield strength and ultimate elongation for the clad materials were added.

# Summary

Open-source Fortran code uses the SUNDIALS library for numerical modelling of base irradiation of a fast reactor fuel pin, accounting for fuel and clad heat transfer, fuel and clad stress-strain conditions, fuel and clad thermal expansion and creep, fuel swelling and fission gas release, evolution of inner gas pressure and composition as well as evolution of fuel-clad gap conductance.

Algebraic and ordinary differential equations are solved by finite-difference method on a structured r-z cylindrical mesh using the SUNDIALS library.

As the input, FRED takes time-dependent axial profile of power density assuming flat power distribution over the radius, time-dependent axial profile of clad outer temperature, as-manufactured fuel and clad dimensions, mesh specification, as well as several constants for material properties and flags to activate specific models.

The typical dataset of the calculational results includes time-dependent radial and axial maps of fuel and clad deformations, stresses, and temperatures; axial profiles of fuel-clad gap conductance, contact pressure, burnup, fuel and clad dimensions.

Available materials:

* Fuel: MOX.
* Clad: AIM1 stainless steel, T91 stainless steel.
* Bonding: helium, xenon, krypton.
* Inner gas: helium, xenon, krypton.

# Installation

First you need to install the SUNDIALS library <https://computing.llnl.gov/projects/sundials>:

1. Create INSTDIR and BUILDDIR
2. Download the last version of IDA, e.g. ida-7.0.0 archive from <https://computing.llnl.gov/projects/sundials/sundials-software> and unpack it in the BUILDDIR directory using tar -zxvf ida-7.0.0.tar.gz
3. In BUILDDIR directory perform three commands:

cmake -DCMAKE\_INSTALL\_PREFIX=/path/to/sundials/INSTDIR  
-DEXAMPLES\_INSTALL\_PATH=/path/to/sundials/INSTDIR  
-DBUILD\_FORTRAN\_MODULE\_INTERFACE=ON  
./ida-7.0.0

make

make install

Then install the code itself:

1. Download the last version of the code from github and unpack the archive.
2. In Makefile file specify the path to SUNDIALS installation directory and the path to the FORTRAN compiler (gfortran).
3. Perform make to generate executable and run: ./FRED
4. Post process the results (see Section “Postprocessing script **postprocess.py**”)

# Input file specification

The input file should have name fred.inp. It consists of cards described below.

## Comment (\*)

Asterisk \* at the first position shows that the card is a comment.

## Options (**000001**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* OPTIONS CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

000001 FGR

000001 FUEL\_CREEP

000001 FUEL\_SWEL 1.0

000001 CLAD\_CREEP

000001 FUEL\_RELOC

000001 NOMECH

Every card activates a specific model: fission gas release (FGR), fuel creep (FUEL\_CREEP), fuel swelling (FUEL\_SWEL) and a multiplier of the swelling rate (tuning factor), clad creep (CLAD\_CREEP), fuel relocation (FUEL\_RELOC). The card with the keyword NOMECH allows to switch of the whole mechanical calculations.

## Initial temperature (**000002**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* INITIAL TEMPERATURE CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno tem0

000002 668.0

At time zero all temperatures are set equal to the initial temperature (K) specified by this card.

## Axial division (**000003**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* INITIAL AXIAL DIVISION CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno dz0 nz

000003 0.05 17

The code uses a uniform axial nodalization. The axial division card specified the height of the axial layers (m) and the number of the axial layers.

## Fixed time (**000004**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* FIXED TIME CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno ftime

000004 86400.0

The user can instruct the solver to reach exact times (up to 50 cards).

## Fuel (**100001**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* FUEL CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno fmat fden pucont rfi rfo ruff stoch nf

100001 mox 10410. 0.45 1.0E-3 2.71E-3 3.0E-6 2.0 22

The card specifies the fuel material (only mox is available for the current version), as-fabricated fuel density (kg/m3), plutonium weight fraction (kg/kg), inner and outer radii of the fuel pellet (m), fuel outer surface roughness (m), initial stoichiometry of the fuel, and number of the radial nodes.

## Gap (**100002**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* GAP CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno gmat dgap pin vpl

100002 he 115.0E-6 0.1 1.455E-5

The card specifies the gap material (only he is available for the current version), as-fabricated fuel-clad gap width (m), as-fabricated inner gas pressure (MPa), and gas plenum volume (m3).

## Clad (**100003**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* CLADDING CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno cmat rco roc0 rufc nc

100003 aim1 3.275E-3 7900. 1.0E-6 3

The card specifies the cladding material (aim1 , which is 15-15Ti stainless steel, and t91 stainlesse steel are available for the current version), as-fabricated outer clad radius (m) and density (kg/m3), as well as number of radial nodes in the cladding.

## Time (**200000**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* TIME CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno tend dtout hmax

200000 3.494398E8 86400. 3600.

The card specifies the final time (s), output time step (s) and maximum time step (s).

## Clad outer temperature vs time table (**200001**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* CLAD OUTER TEMPERATURE VS TIME TABLE

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno time tc01 tc02 tc03 tc04 tc05 tc06

200001 0.0 668.0 668.0 668.0 668.0 668.0 668.0

200001 3600.0 660.75 674.50 686.00 698.25 711.70 725.80

Up to 50 cards can be used to specify the evolution of the axial profile of outer cladding temperature (K) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the clad outer temperature should be equal to the initial temperature specified in card **000002**.

## Power density vs time table (**200002**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* POWER DENSITY CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno time(s) qv1 qv2 qv3 qv4 qv5 qv6

200002 0.0 0.0 0.0 0.0 0.0 0.0 0.0

200002 3600. 1.11095E9 1.26272E9 1.40308E9 1.54105E9 1.63463E9 1.70308E9

Up to 50 cards can be used to specify the evolution of the axial profile of power density (W/m3) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the power density should be equal to zero.

## Fuel creep rate law constants (**200003**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* FUEL CREEP RATE LAW CONSTANTS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno C1 C2 C3

200003 1.0E-39 1.0 0.0

The card specifies three constants used in the creep rate law: ECR = C1 \* SIG\*\*C2 \* exp(-C3/(R\*T)), where SIG is the stress (MPa), R the universal gas constant (J/mol-K) and T the temperature (K).

## Fuel stoichiometry vs fuel burnup table (**200004**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* FUEL STOICHIOMETRY VS BURNUP

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno bup stoich

200004 0.0 2.0

200004 100. 2.0

Up to 50 cards can be used to specify the dependence of fuel stoichiometry (-) on burnup (MWd/kg).

## Coolant pressure (**200005**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* COOLANT PRESSURE CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno press

200005 0.2

The card specifies the coolant pressure (MPa) assumed constant. This is boundary condition.

## Gas plenum temperature vs time table (**200006**)

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\* GAS PLENUM TEMPERATURE VS TIME TABLE

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7----

\*crdno time tple

500001 0.0 668.0

500001 3600. 660.75

Up to 50 cards can be used to specify the evolution of plenum temperature (K) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the gas plenum temperature should be equal to the initial temperature specified in card **000002**.

# Output file **outfrd**

The main output file is the ASCII file generated at every output time step with the name outfrdXXXXXXXXXXXX, where XXXXXXXXXXXX is the time step number. The file contains the following information:

time (s) Current time

time (d) Current time

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rof0 (kg/m3) Initial fuel density

fggen (cm3) Volume of generated fission gas

fgrel (cm3) Volume of released fission gas

fgrel (%) Fission gas release, i.e. released-to-generated fission gas ratio

gpres (MPa) Inner gas pressure

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z (m) Coordinates of the axial nodes

tfin (C) Axial profile of the inner fuel temperature

tfout (C) Axial profile of the outer fuel temperature

tcin (C) Axial profile of the inner cladding temperature

tcout (C) Axial profile of the outer cladding temperature

rfi (m) Axial profile of the inner fuel radius

rfo (m) Axial profile of the outer fuel radius

rci (m) Axial profile of the inner cladding radius

rco (m) Axial profile of the outer cladding radius

dzf (m) Axial profile of the axial fuel layer heights

dzc (m) Axial profile of the axial cladding layer heights

reloc (-) Axial profile of fuel relocation in fractions of the initial gap

qv (W/m3) Axial profile of power density

ql (W/cm) Axial profile of linear heat generation rate

ql2 (W/cm) Axial profile of linear heat generation rate with account for axial strain

bup (MWd/kg) Axial profile of fuel burnup

gap (m) Axial profile of fuel-clad gap

gapth (m) Axial profile of fuel-clad gap with accommodation distance and fuel relocations

hgap (W/m2K) Axial profile of fuel-clad gap conductance

hgap1 (W/m2K) Axial profile of the conduction component of fuel-clad gap conductance

hgap2 (W/m2K) Axial profile of the radiation component of fuel-clad gap conductance

hgap3 (W/m2K) Axial profile of the contact component of fuel-clad gap conductance

ajump (m) Axial profile of the accommodation distance of fuel-clad gap

gask (W/m-K) Axial profile of the fuel-clad gap conductance

pfc (MPa) Axial profile of the fuel-clad contact pressure

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r (m) Coordinates of the radial nodes

temperature (C) iz: 1 Radial profile of temperature

...

sig h (MPa) iz: 1 Radial profile of hoop stress for every axial level

...

sig r (MPa) iz: 1 Radial profile of radial stress for every axial level

...

sig z (MPa) iz: 1 Radial profile of axial stress for every axial level

...

eps h total (%) iz: 1 Radial profile of hoop total strain for every axial level

...

eps r total (%) iz: 1 Radial profile of radial total strain for every axial level

...

eps z total (%) iz: 1 Radial profile of axial total strain for every axial level

...

eps h creep (%) iz: 1 Radial profile of hoop creep strain for every axial level

...

eps r creep (%) iz: 1 Radial profile of radial creep strain for every axial level

...

eps z creep (%) iz: 1 Radial profile of axial creep strain for every axial level

...

eps thermal lin (%) iz: 1 Radial profile of linear thermal expansion strain for every axial level

...

eps swell vol (%) iz: 1 Radial profile of volumetric swelling strain for every axial level

...

# Postprocessing script **postprocess.py**

For postprocessing:

1. Create virtual environment:

python3 -m venv venv\_fred

2. Activate it:

source venv\_fred/bin/activate

3. Update pip

pip install --upgrade pip

4. Install libraries:

python -m pip install python-pptx

python -m pip install -U matplotlib

5. Run the script:

python postprocess.py

The script reads the output files outfrd which should be in the working directory and creates two PowerPoint files: plot-bup.pptx and plots-time.pptx. The first contains the plots of key variables as a function of time and the second one—as a function of burnup.

At the beginning of the script the user should provide three values which are explained by the comments:

#axial level for output

jz = 8

#number of fuel radial nodes

nf = 22

#number of clad radial nodes

nc = 3