FRED: Fast reactor fuel behaviour code

Version: 1.4.0 (20250422)

Modifications

1.0.0
Initial version

1.0.1
File 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.

1.3.0 (20250123)
1. Clad plastic deformation model added. To be checked, validated, and improved.
2. The bug with yield strength properties of the material t91 fixed (yield strength was undefined for temperatures above 600 K).

1.4.0 (20250422)
1. Card for Zirconium content in U-Pu-Zr alloy fuel added (Options card 000001 ZR_CONTENT 0.1).
2. Cards for relative and absolute tolerances added:
   - btol, etol, ftol, htol, gtol, stol, ttol variables added to global.f90 for absolute tolerances for burnup (MWd/kg), strain (-), fission gas (mol), gap conductance (W/m2K), gap (m), stress (MPa), temperature (K)
   - card 000001 Options are extended for relative tolerance rtol and 7 absolute tolerances as described above (see options card description in the manual for keywords and default values).

1. 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.

2. 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`**”)

3. 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
000001       ZR_CONTENT       0.1
000001       RTOL             1.0E-8
000001       ATOL_BURNUP      1.0E-4
000001       ATOL_STRAIN      1.0E-6
000001       ATOL_FISGAS      1.0E-7
000001       ATOL_GAPCON      1.0E-4
000001       ATOL_GAPWID      1.0E-6
000001       ATOL_STRESS      1.0E-4
000001       ATOL_TEMPER      1.0E-6
```

Every card has a keyword and some of the cards has numerical values:

- `FGR` activates the fission gas release model (default: the model is off);
- `FUEL_CREEP` activates the fuel creep model (default: the model is off);
- `FUEL_SWEL` activates the fuel swelling model (default: the model is off) and specifies a multiplier of the swelling rate (tuning factor, default: 1.0);
- `CLAD_CREEP` activates the clad creep model (default: the model is off);
- `FUEL_RELOC` activates the fuel relocation model (default: the model is off);
- `NOMECH` allows to switch of the whole mechanical calculations (default: the fuel mechanics is on);
- `ZR_CONTENT` specifies the Zirconium weight fraction in U-Pu-Zr metallic fuel (default 0.1);
- `RTOL` specifies relative tolerance, one value for all equations (default: 1.0E-8);
- `ATOL_BURNUP` specifies absolute tolerance for burnup (MWd/kgHM) (default: 1.0E-4);
- `ATOL_STRAIN` specifies absolute tolerance for strain (m/m) (default: 1.0E-6);
- `ATOL_FISGAS` specifies absolute tolerance for fission gas amount (mol) (default: 1.0E-7);
- `ATOL_GAPCON` specifies absolute tolerance for gap conductance (W/m2K) (default: 1.0E-6);
- `ATOL_GAPWID` specifies absolute tolerance for gap width (m) (default: 1.0E-6);
- `ATOL_STRESS` specifies absolute tolerance for stress (MPa) (default: 1.0E-4);
- `ATOL_TEMPER` specifies absolute tolerance for temperature (K) (default: 1.0E-6).

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/m^3), 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 (m^3).

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/m^3) 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.

4. 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
---	
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
---	
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
---	
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
...
```

5. 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
```