





SCIANTIX Virtual Training - October 16, 2020

SCIANTIX: Code structure and input/output

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The SCIANTIX code

Developed at Politecnico di Milano

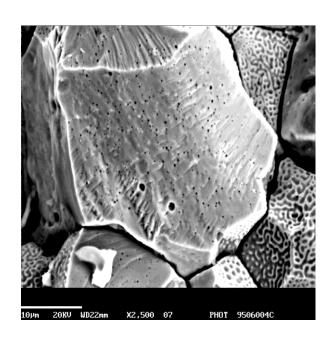
It is a OD stand-alone code, designed to be included as a mechanistic fission gas behaviour module in existing fuel performance codes

Constitutes the natural environment for the development, verification, and validation of fission gas behaviour models, and for the simulation of separate-effect test experiments

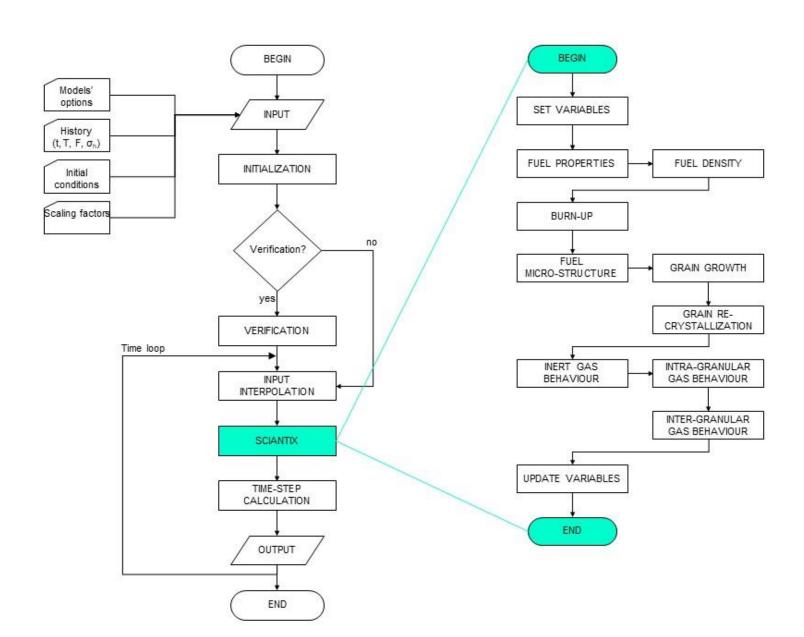
It can be <u>included in existing multiphysics</u> platforms and fuel performance codes as a <u>module</u> to evaluate fission gas release and gaseous swelling or can be <u>used as stand-alone</u>

Available as open-source software (MIT license)

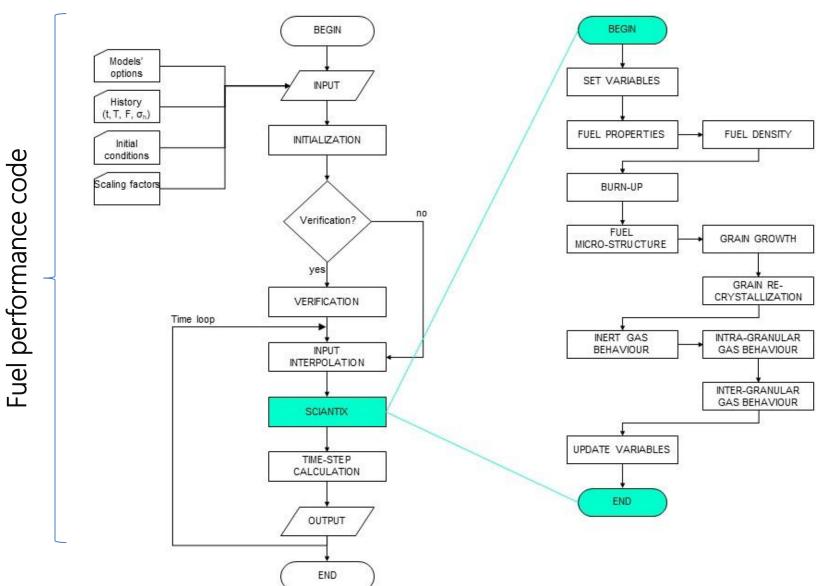




The SCIANTIX code, stand-alone



The SCIANTIX code, designed for coupling!



The SCIANTIX code, numerical aspects

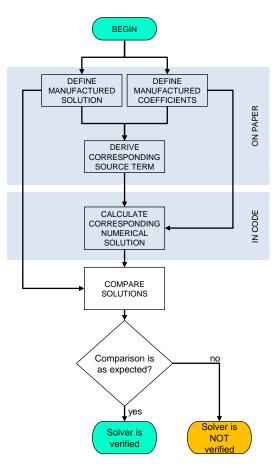
Numerical solvers (coded) independently from the "physics" allows for once and for all numerical verification

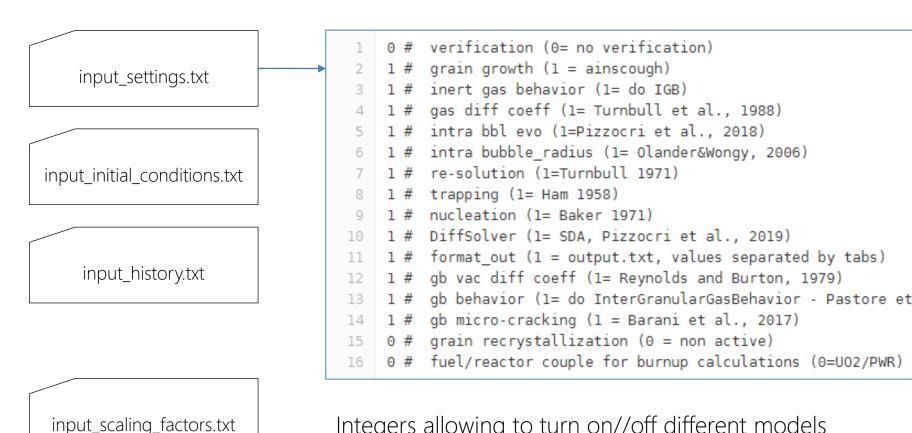
The included models are a combination of PDEs (essentially diffusion of gas along the grain) and ODEs

- Space is treated via a mesh-free spectral approach
- Time is treated with **implicit first order** scheme (backward Euler)

Computational times for the simulation of fission gas diffusion//intra-granular behaviour//inter-granular behaviour in the order of **few milliseconds per time-step**

Numerical verification through the Method of Manufactured Solutions

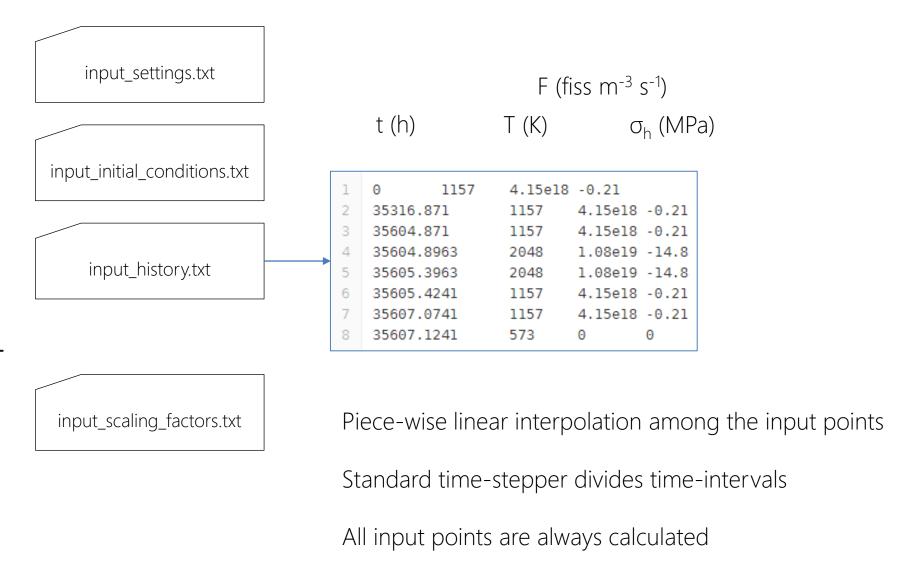


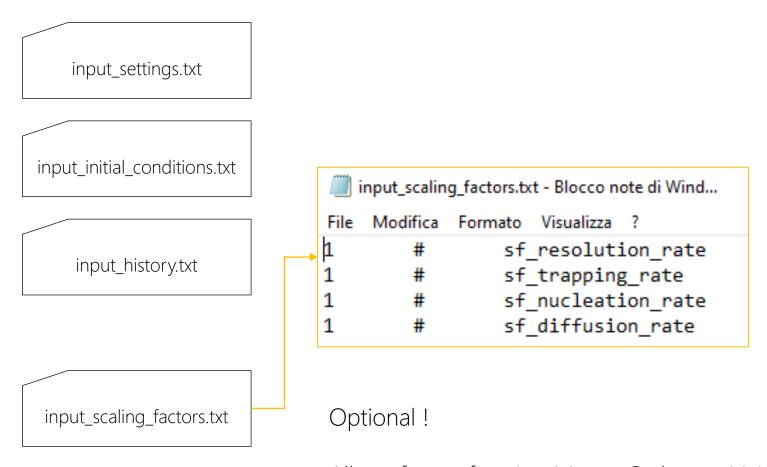


Integers allowing to turn on//off different models and to select different options for coefficients

After the "#", there is the place for a comment line

12.3e-6 # initial grain radius (m) 0 # initial Gas produced (at/m3) input_settings.txt 0 # initial Gas in grains (dissolved plus ig bubbles) (at/m3) 0 # initial Gas in solution (at/m3) 0 # initial Gas in ig bubbles (at/m3) 0 # initial Gas in gb bubbles (at/m3) 0 # initial Gas released (at/m3) input initial conditions.txt 0 # initial fuel burnup (MWd/kgU02) 8 0 # initial effective fuel burnup (MWd/kgU02) 10970 # initial fuel density (kg/m3) 10 11 2 # initial 0/M (/) 12 0 # initial He produced (every manner) (at/m3) input history.txt 0 # initial He in grains (dissolved plus ig bubbles) (at/m3) 13 14 0 # initial He in solution (at/m3) 15 0 # initial He in ig bubbles (at/m3) 0 # initial He in gb bubbles (at/m3) 16 17 0 # initial He released (at/m3) 0 3 0 0 97 # initial U234 U235 U236 U237 U238 (% of heavy atoms) content 19 20 0 0 0 input_scaling_factors.txt 21 # initial Np237 Np238 Np239 (% of heavy atoms) content 0 0 0 0 0 0 23 # initial Pu238 Pu239 Pu240 Pu241 Pu242 Pu243 (% of heavy atoms) conte 24 0 0 0 0 # initial Am241 Am242q Am242m Am243 Am244 (% of heavy atoms) content 26 0 0 0 0 # initial Cm242 Cm243 Cm244 Cm245 (% of heavy atoms) content





Allows for performing Monte Carlo sensitivity analyses by using external scripts (Matlab)

execution.txt

input_check.txt

output.txt

Output can be dumped at different time-steps

Ctrl + A

Ctrl + C

Ctrl + V in Excel ©

```
Time (h)
                                                                         Hydrostatic stress (MPa)
                      Temperature (K) Fission rate (fiss/m3-s)
     0
             1157
                      4.15e+018
                                       -0.21
                                               1.23e-005
                                                                                                   Θ
     35.3169 1157
                      4.15e+018
                                               1.22998e-005
                                                                1.5829e+023
                                                                                  1.57354e+023
                                       -0.21
                                                                                                   2.6
     70.6337 1157
                      4.15e+018
                                       -0.21
                                               1.22995e-005
                                                                3.1658e+023
                                                                                  3.14044e+023
     105.951 1157
                      4.15e+018
                                       -0.21
                                               1.22993e-005
                                                                4.74871e+023
                                                                                  4.7015e+023
                                                                                                   3.8
                                                                                                   5.2
     141.267 1157
                      4.15e+018
                                       -0.21
                                               1.22991e-005
                                                                6.33161e+023
                                                                                  6.25677e+023
     176.584 1157
                      4.15e+018
                                       -0.21
                                               1.22988e-005
                                                                7.91451e+023
                                                                                 7.80717e+023
     211.901 1157
                                               1.22986e-005
                                                                9.49741e+023
                                                                                  9.35338e+023
                      4.15e+018
                                       -0.21
                                                                                                   9.2
     247.218 1157
                      4.15e+018
                                       -0.21
                                               1.22984e-005
                                                                1.10803e+024
                                                                                 1.08959e+024
     282.535 1157
                      4.15e+018
                                       -0.21
                                               1.22981e-005
                                                                1.26632e+024
                                                                                  1.24353e+024
     317.852 1157
                      4.15e+018
                                       -0.21
                                               1.22979e-005
                                                                1.42461e+024
                                                                                  1.39717e+024
                                                                                                   1.1
     353.169 1157
                      4.15e+018
                                       -0.21
                                               1.22977e-005
                                                                1.5829e+024
                                                                                 1.55056e+024
                                                                                                   1.3
     388.486 1157
                      4.15e+018
                                       -0.21
                                               1.22974e-005
                                                                1.74119e+024
                                                                                  1.70373e+024
14
     423.802 1157
                      4.15e+018
                                       -0.21
                                               1.22972e-005
                                                                1.89948e+024
                                                                                  1.85668e+024
15
     459.119 1157
                      4.15e+018
                                       -0.21
                                               1.2297e-005
                                                                2.05777e+024
                                                                                  2.00945e+024
     494.436 1157
                                                                                                  1.8
                      4.15e+018
                                       -0.21
                                               1.22968e-005
                                                                2.21606e+024
                                                                                  2.16204e+024
                      4.15e+018
     529.753 1157
                                       -0.21
                                               1.22965e-005
                                                                2.37435e+024
                                                                                                   1.9
                                                                                  2.31448e+024
     565.07 1157
                      4.15e+018
                                       -0.21
                                               1.22963e-005
                                                                2.53264e+024
                                                                                  2.46677e+024
                                                                                                   2.6
     600.387 1157
                      4.15e+018
                                       -0.21
                                               1.22961e-005
                                                                2.69093e+024
                                                                                 2.61892e+024
                                                                                                   2.2
20
     635.704 1157
                                       -0.21
                                                                                                   2.3
                      4.15e+018
                                               1.22958e-005
                                                                2.84922e+024
                                                                                  2.77094e+024
21
     671.021 1157
                      4.15e+018
                                       -0.21
                                               1.22956e-005
                                                                3.00751e+024
                                                                                  2.92284e+024
22
     706.337 1157
                      4.15e+018
                                       -0.21
                                               1.22954e-005
                                                                3.1658e+024
                                                                                  3.07463e+024
                                                                                                   2.6
23
     741.654 1157
                      4.15e+018
                                       -0.21
                                               1.22951e-005
                                                                3.32409e+024
                                                                                  3.2263e+024
                                                                                                   2.7
     776.971 1157
24
                      4.15e+018
                                       -0.21
                                               1.22949e-005
                                                                3.48238e+024
                                                                                  3.37786e+024
                                                                                                   2.8
     812.288 1157
                      4.15e+018
                                       -0.21
                                               1.22947e-005
                                                                3.64067e+024
                                                                                  3.52932e+024
                                                                                                   3.6
     847.605 1157
                      4.15e+018
                                       -0.21
                                               1.22944e-005
                                                                3.79897e+024
                                                                                  3.68068e+024
                                                                                                   3.1
27
     882.922 1157
                      4.15e+018
                                       -0.21
                                               1.22942e-005
                                                                3.95726e+024
                                                                                  3.83194e+024
                                                                                                   3.2
     918.239 1157
                      4.15e+018
                                       -0.21
                                               1.2294e-005
                                                                4.11555e+024
                                                                                  3.9831e+024
                                                                                                   3.3
29
     953.556 1157
                                               1.22937e-005
                      4.15e+018
                                       -0.21
                                                                4.27384e+024
                                                                                  4.13417e+024
                                                                                                   3.6
     988.872 1157
                      4.15e+018
                                       -0.21
                                               1.22935e-005
                                                                4.43213e+024
                                                                                  4.28515e+024
```

The SCIANTIX code, coupling with FPCs TRANSURANUS & GERMINAL & OFFBEAT

SCIANTIX INPUT
Settings
Initial conditions
(Scaling factors)

Interface binding C++ and F95 code (<u>independent of further SCIANTIX development!</u>) (2 *.C and 2 *.f95) developed for the coupling with TRANSURANUS

SCIANTIX and FPC are <u>compiled together</u>, generating one single executable

- Easier to handle for present users of FPCs
- No need for major modification to FPC input//output
- Strategy is tailored for each FPC



