Joint ICTP-IAEA Workshop on Open-Source Nuclear Codes for Reactor Analysis (smr 3865)

Group 2

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Open∇FOAM

Exercise 1

Exercise 1: Assignments

- The provided startingCase contains everything done on Monday, except that in GeN-Foam we do not use fvOptions, but the phaseProperties file. And of course the controlDict is different.
- So, up to you to set them! Try to replicate the simulation we did on Monday for fluid-dynamics only (no energy solution, no neutronics, no thermal-mechanics). Run it for 10 seconds. To simulate the pump, you will need a momentum source set to -300000 $kg/m^2/s^2$ in z direction.
- Compare it with the case done Monday.

Exercise 1: Tips

- Always try to open your case in paraFoam. What do you notice compared to Monday?
- To learn how to set a momentum source for a pump, try to browse the documentation or the tutorials. The "grep -ir pump" command in the terminal can be helpful. Or, you can ask chatGPT to create a linux command to specifically search for the keyword "pump" in files named "phaseProperties" in Tutorials
- Always take a look at fvSchemes, fvSolution. They define how a numerical solution is obtained.
- Be careful with the time-step setting(s) in controlDict

Exercise 1 – Setting the case

- constant/fluidRegion/phaseProperties:

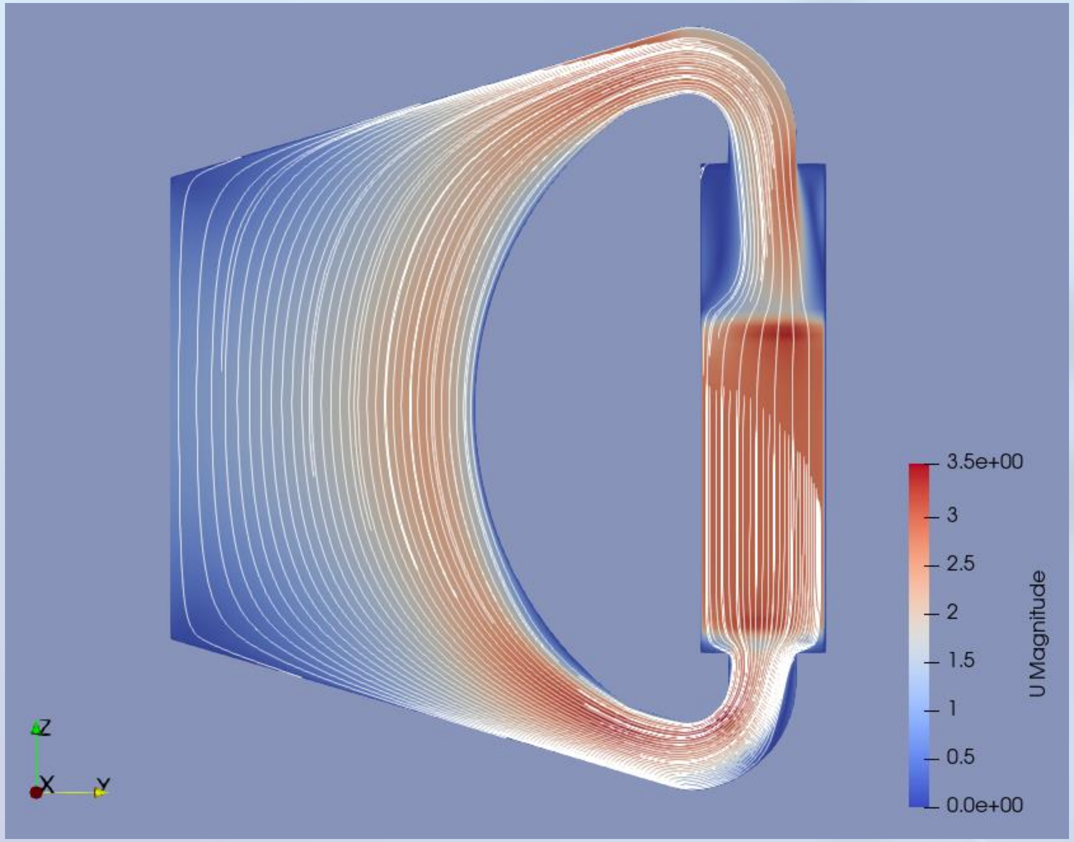
```
"pump“
{
    volumeFraction      0;
    Dh                  1;
    momentumSource      (0  0  -300000);
}
```

- system/controlDict;

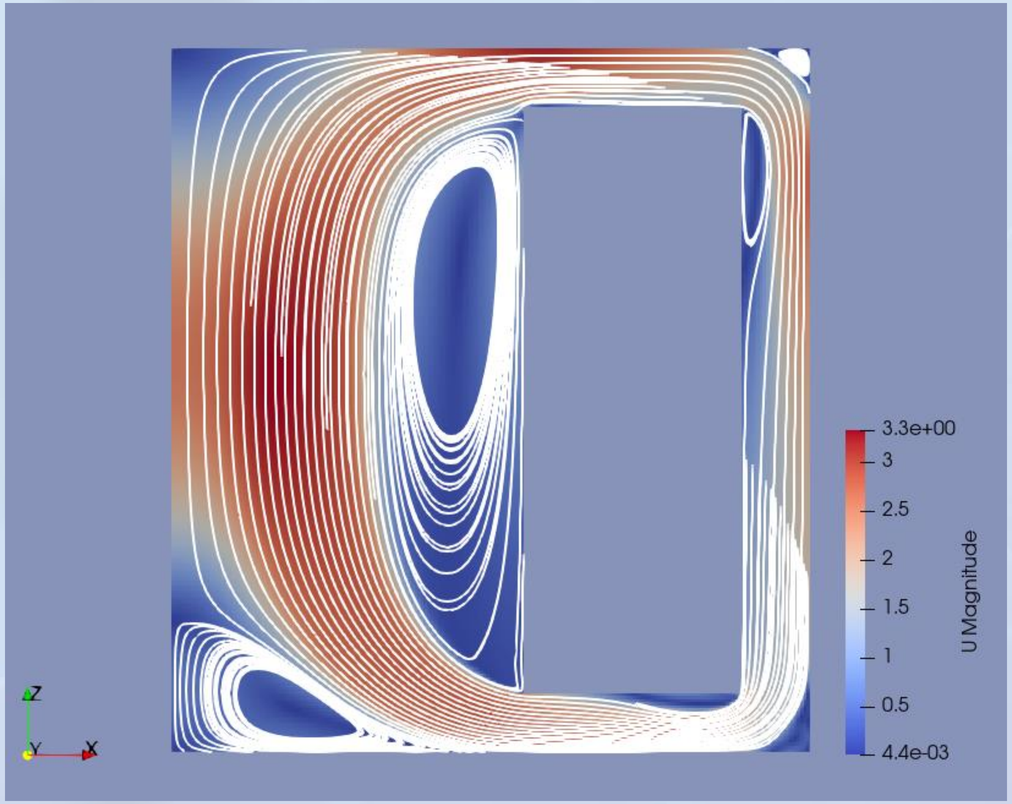
```
endTime      20;
deltaT       1e-3;
solveFluidMechanics true;
adjustTimeStep  true;
```

Exercise 1 - Results

GeN-Foam



Monday's exercise - simpleFoam



L. Cattoni et al., Multiphysics Topology Optimization with Application to Molten Salt Fast Reactor, NENE 2021

Exercise 2

Exercise 2: Assignments

- Starting from the previous case (copy-paste it, and keep the previous), clean up the time steps and set up a GeN-Foam case to be able to solve for diffusion-based neutronics. The nuclearData* files and the mesh are provided in the "inputs" folder. We want the power of the reactor to be 20MW.
- Spend some time trying to understand the nuclearData* files. How many energy groups? How many precursors groups? How are cross-sections parameterized?
- Try to solve for neutronics only, eigenvalue, from time zero. Use both Dirichlet (zero) and Neumann (zero) BC.
- Try to visualize the distribution of power/flux and of precursors groups 0 and 7, and look at keff.

Exercise 2: Tips

- GeN-Foam allows using a defaultFlux field to initialize initial and boundary conditions for all the energy groups.
- Why 20MW when the MSFR should be 3GW?
- Be careful about the boundary conditions for the fluxes.
- Think about the meaning of doing "time-steps" in an eigenvalue calculation. What are, in fact, the time steps? Do we need to adjust time steps?

Exercise 2 – Setting the case

- Starting from the previous case
- Copy nuclear data to constant/neutroRegion
- system/controlDict;

```
endTime        10;
deltaT         1e-1;
solveFluidMechanics false;
solveNeutronics true;
adjustTimeStep  false;
liquidFuel      true;
```

- 0/neutroRegion/defaultFlux + defaultFlux2:

```
front   {   type   wedge;   }
back    {   type   wedge;   }
"(bottomwall|topwall|reflector|hx)"   {   type   fixedValue;   value   uniform 0;   }
```

- 0/uniform/reactorState:

```
pTarget    20.0e+06;
```

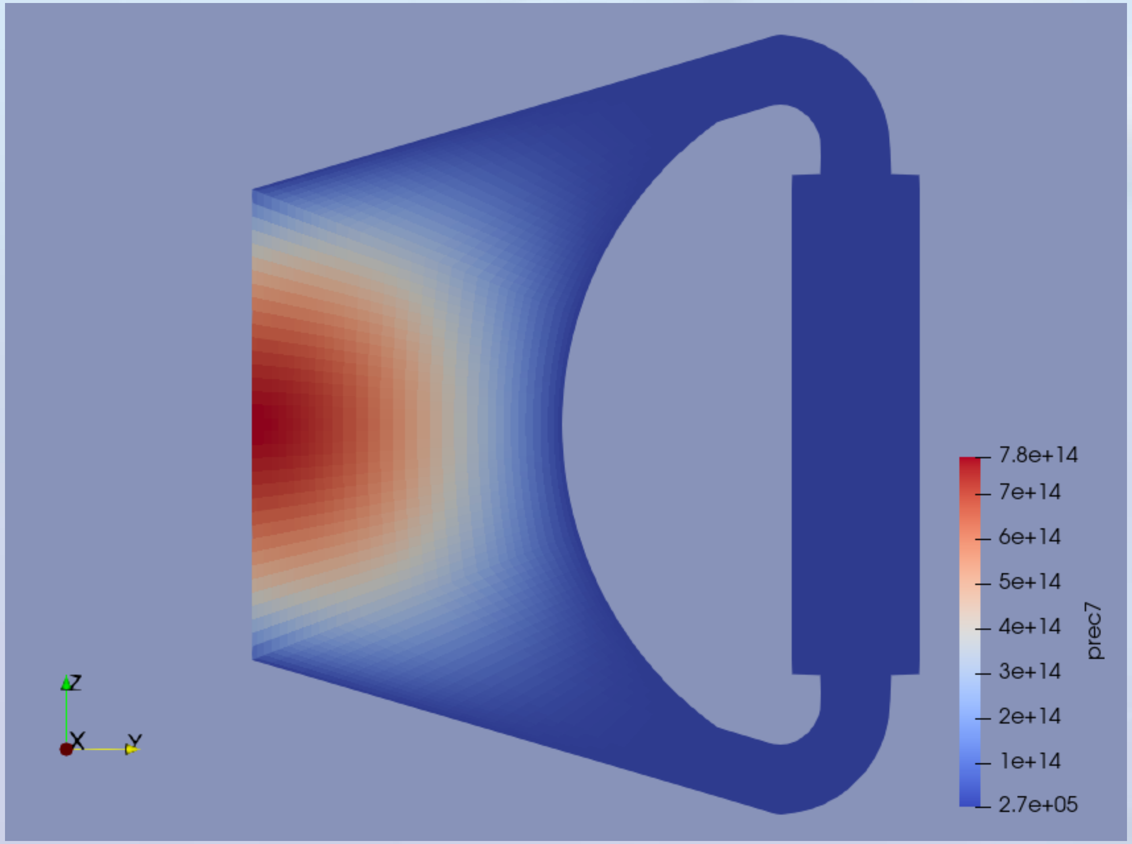
- Constant/neutroRegion/neutronicsProperties:

```
eigenvalueNeutronics    true;
```

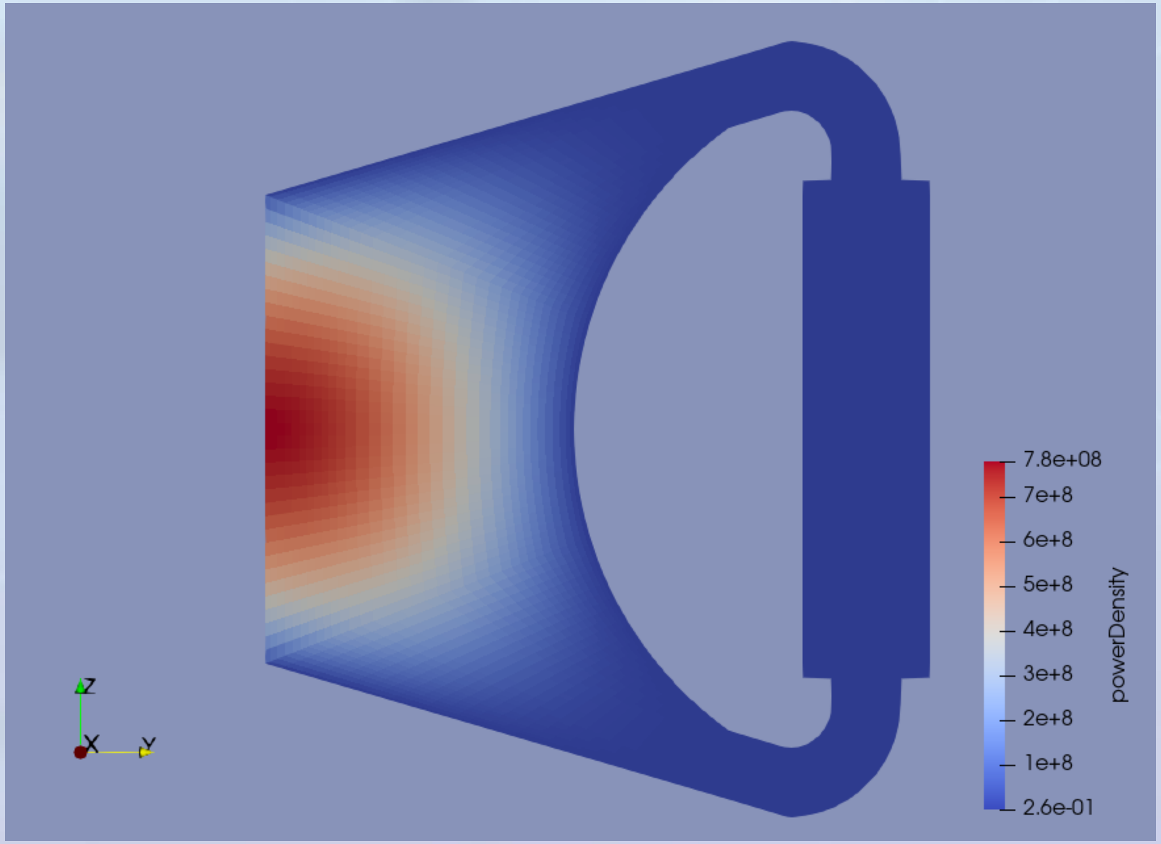
Exercise 2 - Results

kEff = 0.94390716

Precursor 7



Power density



Exercise 3

Exercise 3: Assignments

- Now we want to see if the velocity field has an influence on neutronics.
- Try to run a coupled solution of fluid-dynamics and eigenvalue neutronics
- Try to plot the distribution of power/flux and of precursors groups 0 and 7 and compare with the previous exercise. What do you notice?
- Try also to look at the keff for the 2 cases. How does it change?

Exercise 3: Tips

- What is changing physically for neutronics compared to previous case?
- Is there something that we are solving now, and that we were not solving for before? Do we need new initial and boundary conditions?
- It might also be worthwhile looking at fvSchemes in neutronics in some details this time. Is there a scheme that is always bounded? Maybe it is worth using it for $div(phi\_, precStar\_)$:)
- Can we start from a good guess for the fluid dynamics and limit the computational time? (Do we have a one-way or two-way coupling?)

Exercise 3 – Setting the case

- Starting from previous case
- Copying results from Exercise 1 ($lastTimeStep/fluidRegion) to 0/fluidRegion
- system/controlDict;

```
deltaT        1e-3;
solveFluidMechanics true;
solveNeutronics true;
adjustTimeStep  true;
```

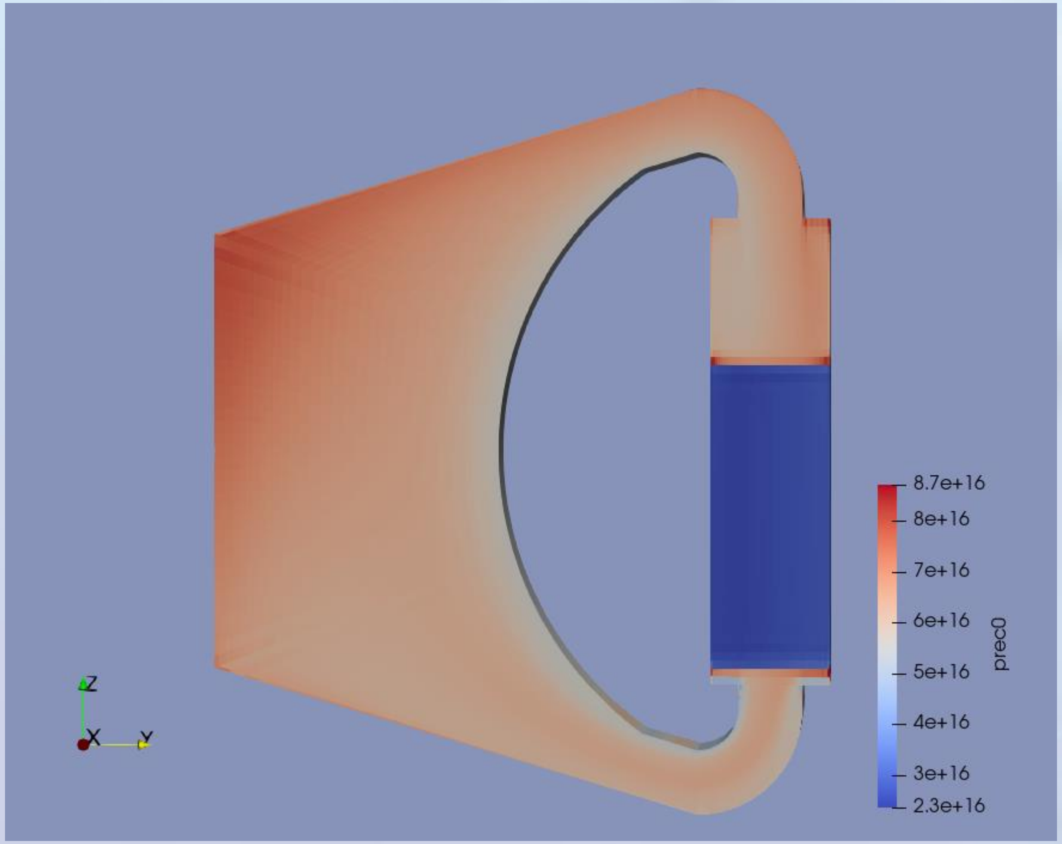
- System/neutroRegion/fvSchemes:

```
divSchemes
{
    default        Gauss linear;
    "div(facePhi_,angularFlux_)"   Gauss upwind;
    "div(phi_,precStar_)"   Gauss upwind;
}
```

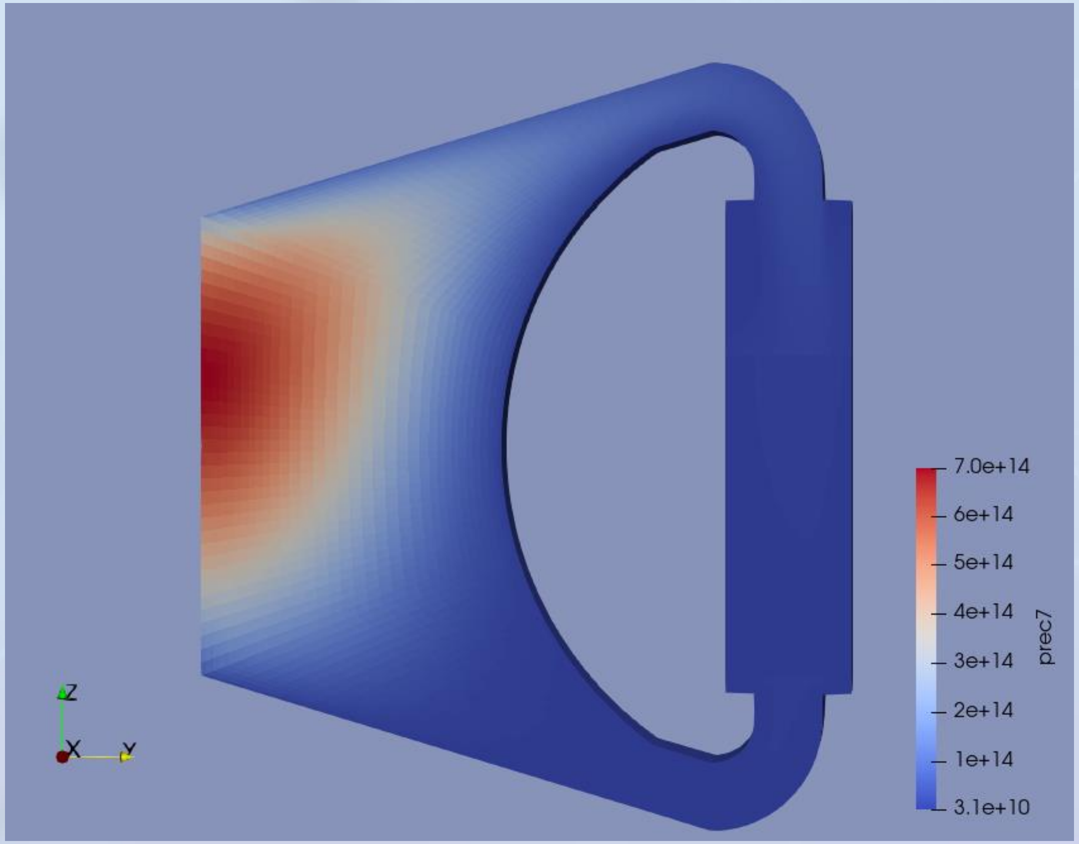
Exercise 3 - Results

kEff = 0.94196475

Precursor 0



Precursor 7



Exercise 4

Exercise 4: Assignments

- Now we want to add the solution for energy.
- Copy-paste the previous case.
- Try to solve also for temperatures till the achievement of a steady-state. Assume that fluid-dynamics is not affected by temperature. Is that really the case?
- You'll need a heat exchanger to evacuate the heat produced by the neutronics. Assume an average temperature on the secondary side of 900K and a volumetric area of 200 m^{-1}.
- Try to plot prec7 and temperature and think about differences and similarities, and where they came from.
- How does keff change compared to a case without solution of temperature? Can you tell why?

Exercise 4: Tips

- A simple way to emulate a heat exchanger is a fixed-temperature sub-scale structure.
- In GeN-Foam, sub-scale structures with special properties are called "powerModels."
- What boundary conditions do we use for temperature?
- Is this one-way or two-way coupling?
- Do we need to solve for fluid-dynamics again?
- Can we (do we need to) keep the neutronics solution as eigenvalue?
- Three (physical) minutes should be enough for the reactor to get to an approximate steady state.
- Avoid excessive writing of results to disk.

Exercise 4 – Setting the case

- Starting from previous case
- system/controlDict;

```
endTime     180;
deltaT      1e-1;
writeInterval    10;
solveFluidMechanics false;
    solveEnergy             true;
solveNeutronics true;
adjustTimeStep  false;
```

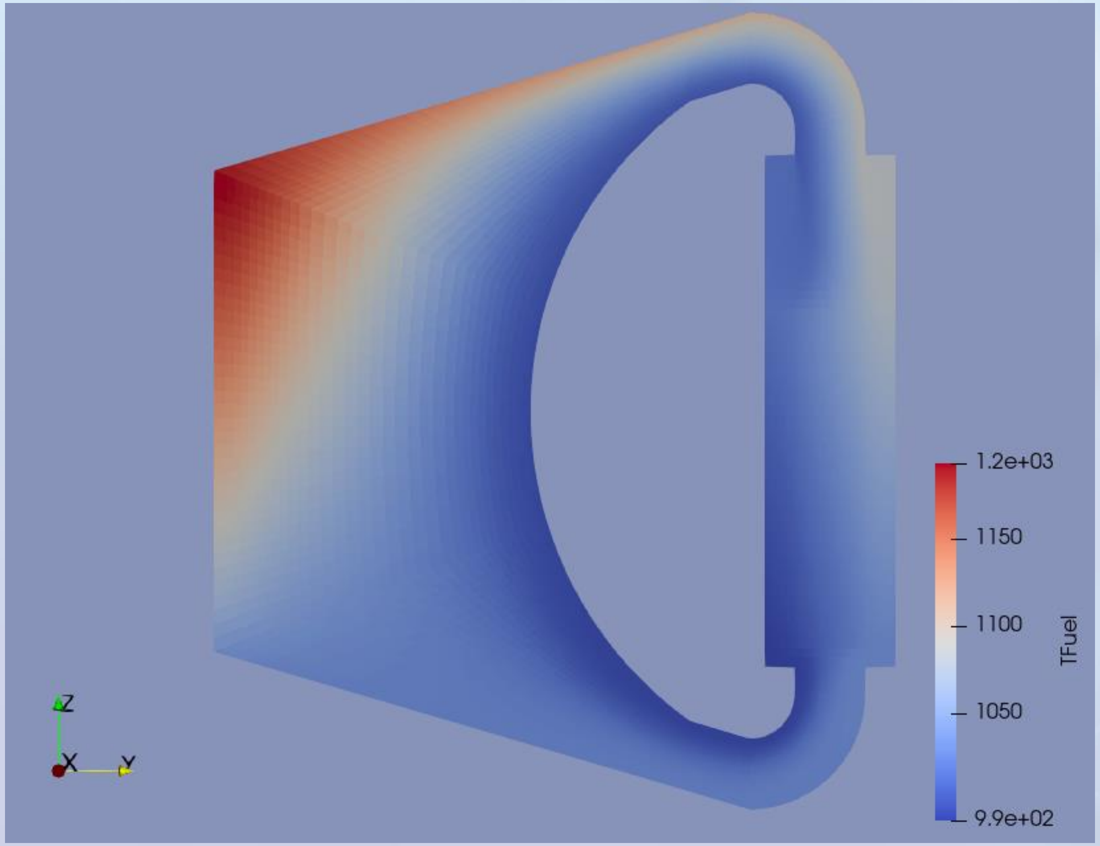
- Constant/fluidRegion/phaseProperties:

```
"hx“
 {
        volumeFraction     0.6;
        Dh                 0.01;
        powerModel
        {       type          fixedTemperature;
                volumetricArea  200;
                T             900;
        }  }
}
```

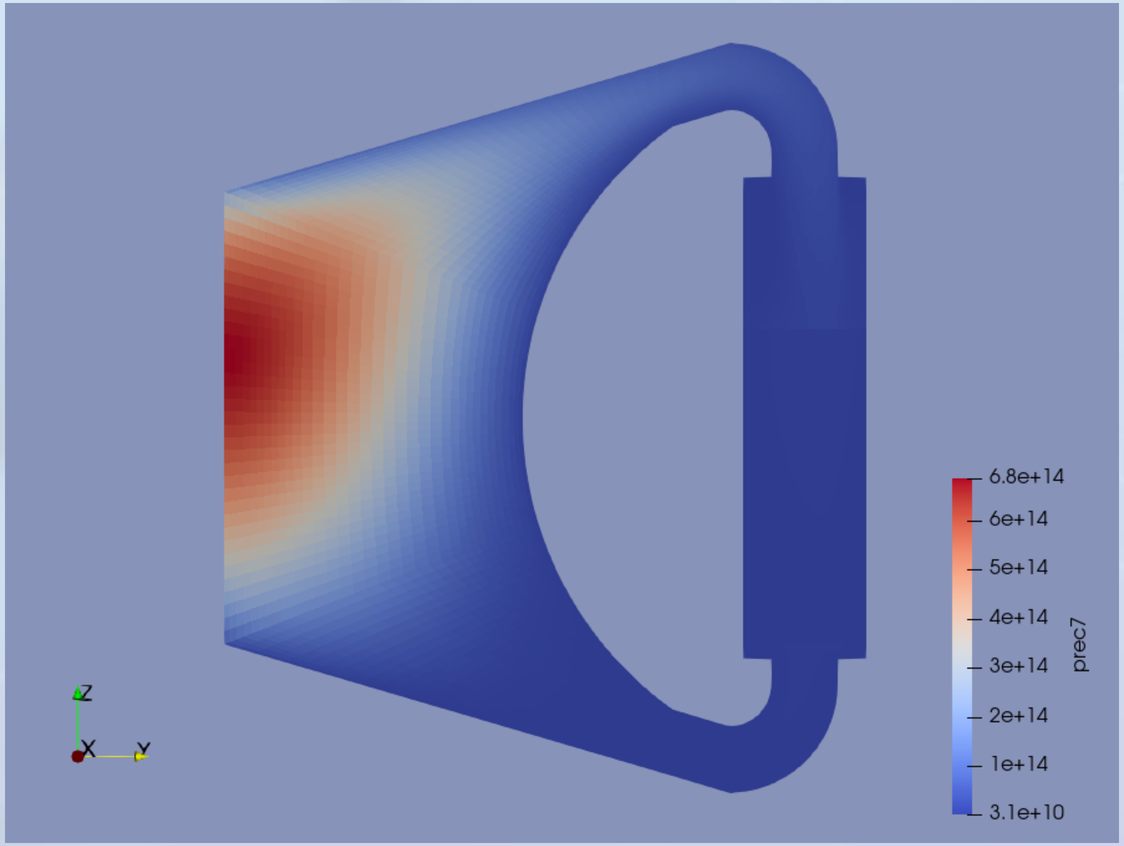
Exercise 4 - Results

kEff = 0.92740091 (in previous exercise 0.94196475)

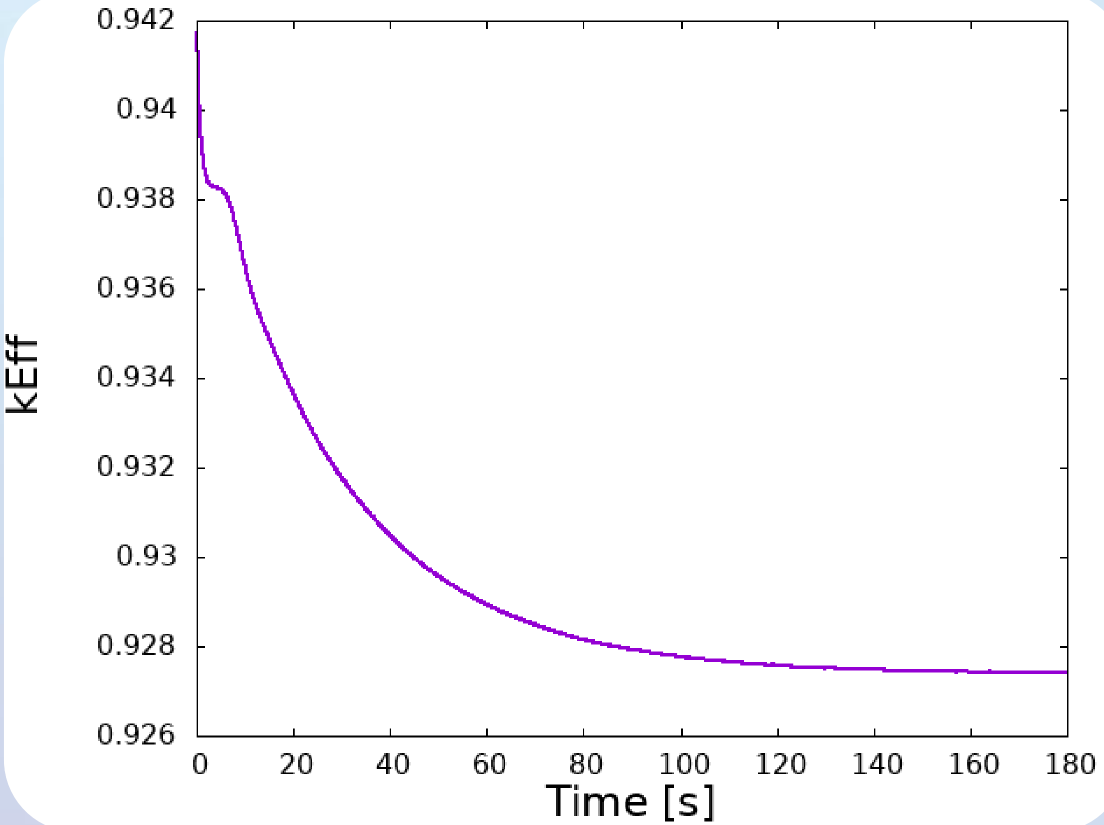
T(fuel)

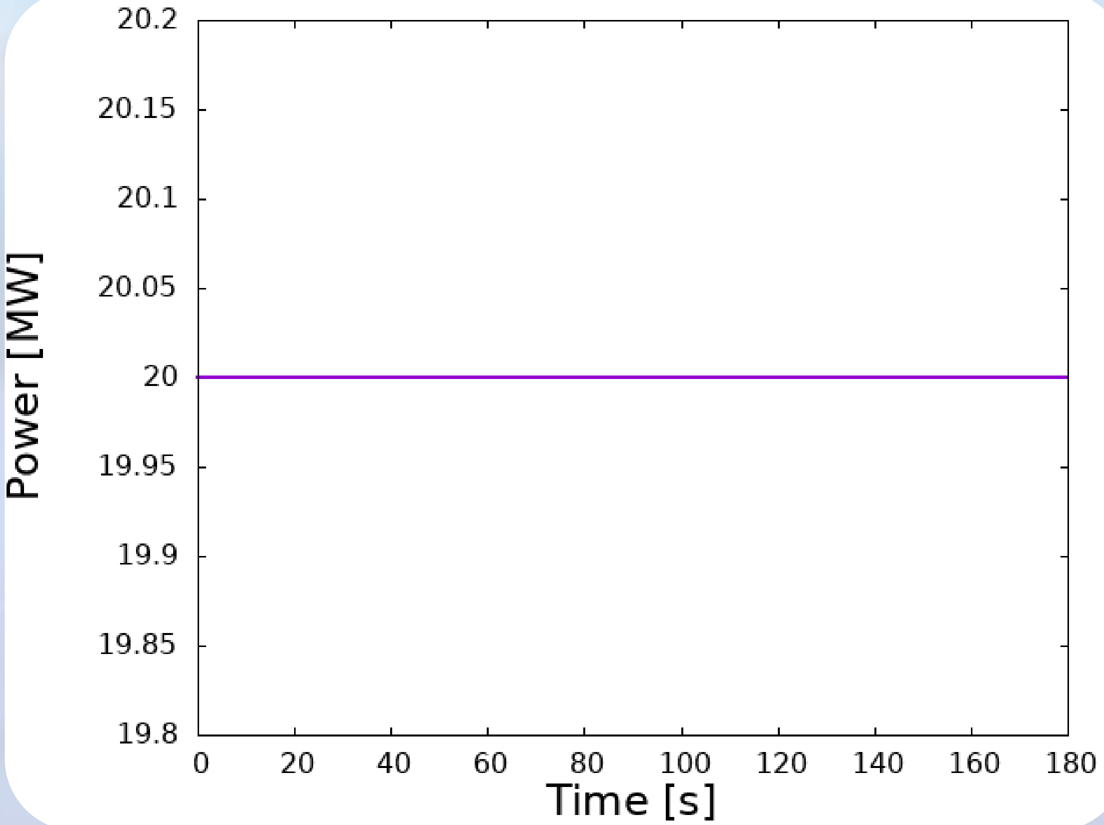


Precursor 7



Exercise 4 - Results





Exercise 5

Exercise 5: Assignments

- Now we want to study the transient behavior of the reactor.
- Starting from the steady state of Exercise 4, run a transient with an increase of 30 pcm in reactivity.
- Analyze the results (you can read from the log, use paraview, or use the GeN-Foam.dat file).

Exercise 5: Tips

- Note that diffusion solvers usually require a keff to run a transient (do you know why?). GeN-Foam stores it in reactorState and use the value from previous simulation if available. Or you can give the value you prefer.
- What dictionary do we need to change to set the neutronics to transient?
- It could be useful to start tightening up the coupling. Where can we find this option? In which dictionary numerical things usually are in OpenFOAM? Is this related to a specific physics or not?
- Always be careful about initial time step. This is not adjusted by OpenFOAM.

Exercise 5 – Setting the case

- Starting from previous case (Exercise 4)
- system/controlDict:

  deltaT 1e-3;

  solveFluidMechanics true;

  solveEnergy true;

  solveNeutronics true;

  adjustTimeStep true;

- system/fvSolution;

  tightlyCoupled true;

- constant/neutroRegion/neutronicsProperties:

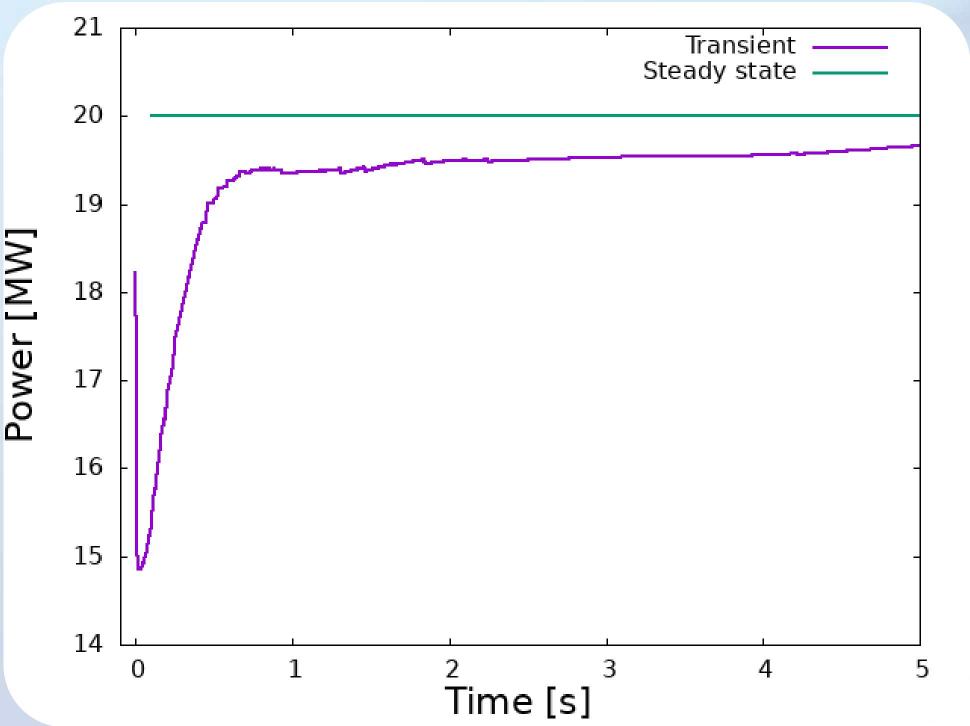
  eigenvalueNeutronics false;

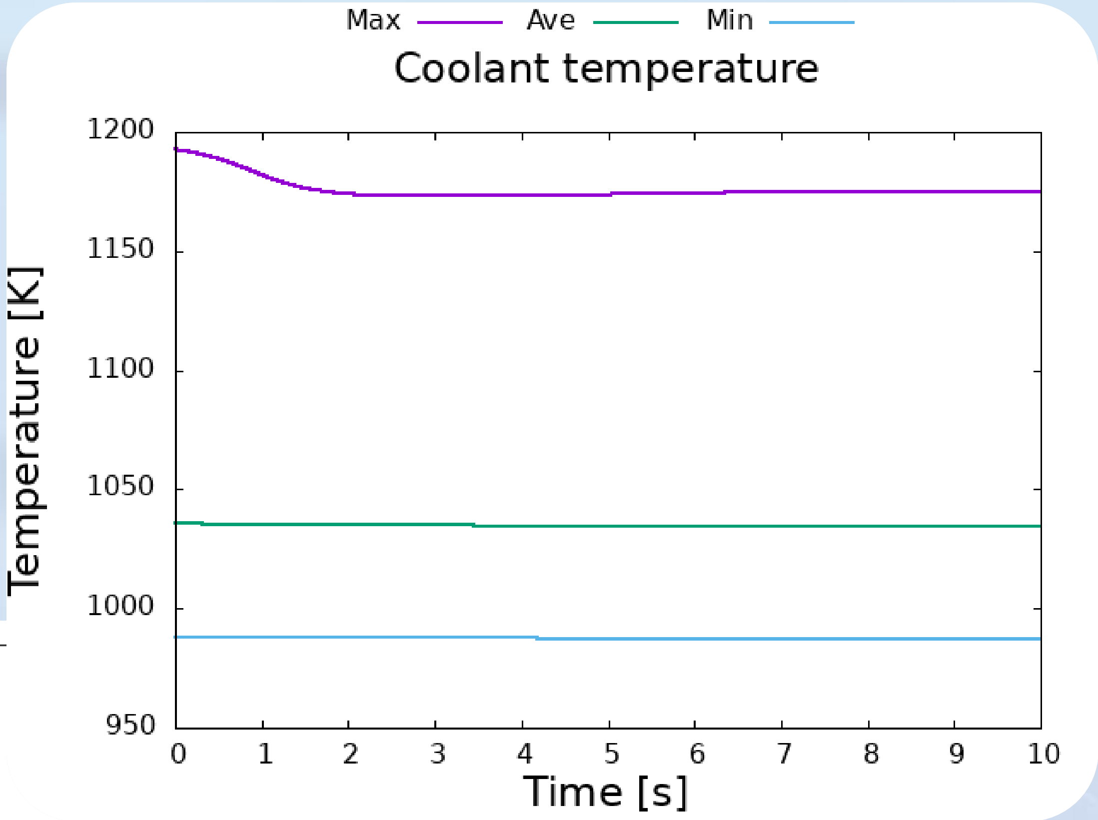
$$\Delta k_{eff} = \frac{1}{1-\rho}$$

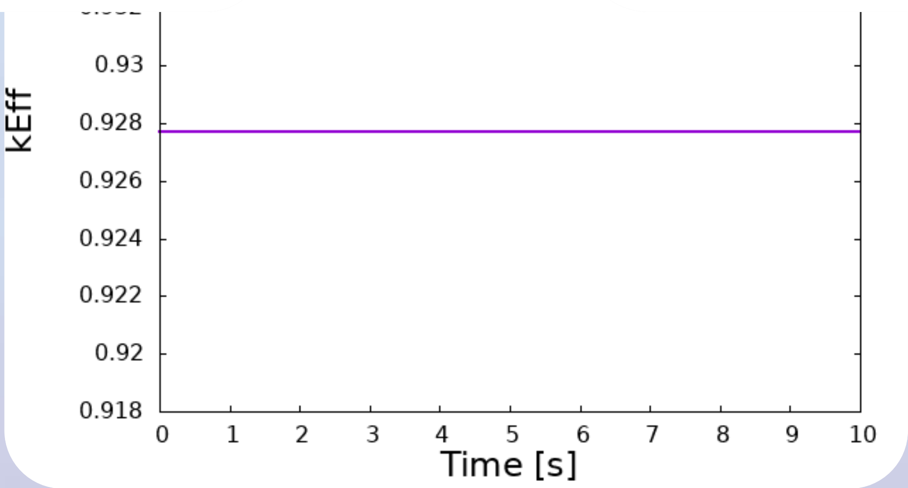
- 0/uniform/reactorState:

  keff 0.927701; // 0.92740091

Exercise 5 - Results







Exercise 6

Exercise 6: Assignments

- Starting from the case of Exercise 4, run a transient with an exponential reduction in the pump momentum source with a time constant of 5 seconds, for 10 seconds. After 10 seconds, the reduction stops. But keep the transient going for 20 seconds.
- Analyze the results.

Exercise 6: Tips

- How to impose a change in the momentum source? Always look at the documentation, source code, tutorials, etc. And do not forget the grep.

Exercise 6 – Setting the case

- Starting from previous Exercise 4
- system/controlDict:

  endTime 25;

  deltaT 1e-3;

  solveFluidMechanics true;

  solveEnergy true;

  solveNeutronics true;

  adjustTimeStep true;

- constant/neutroRegion/neutronicsProperties:

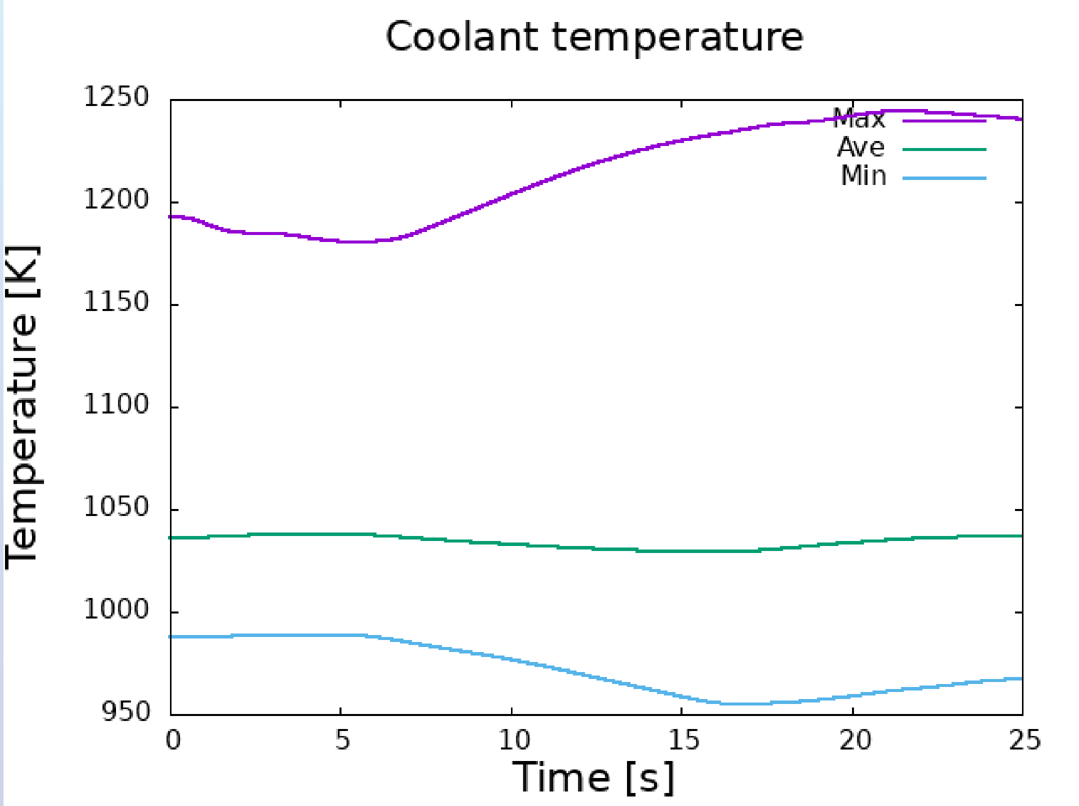
  eigenvalueNeutronics false;

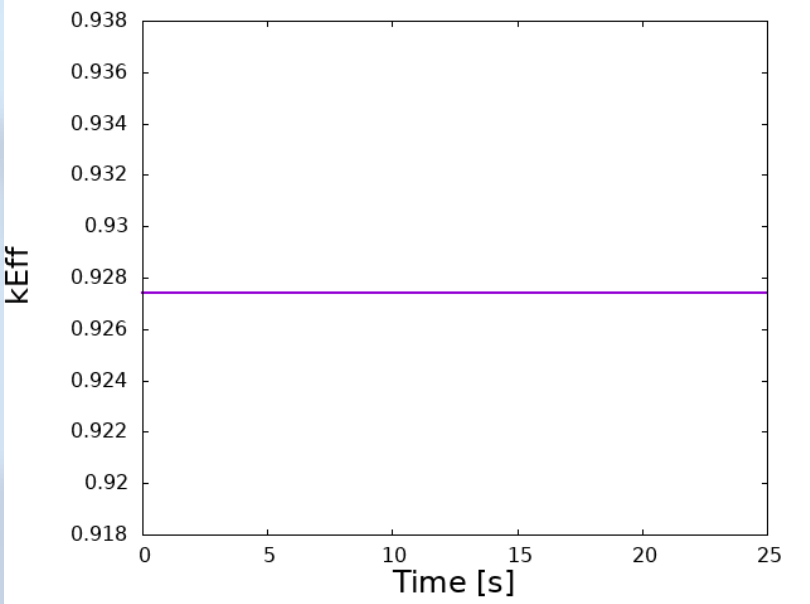
- constant/fluidRegion/phaseProperties:

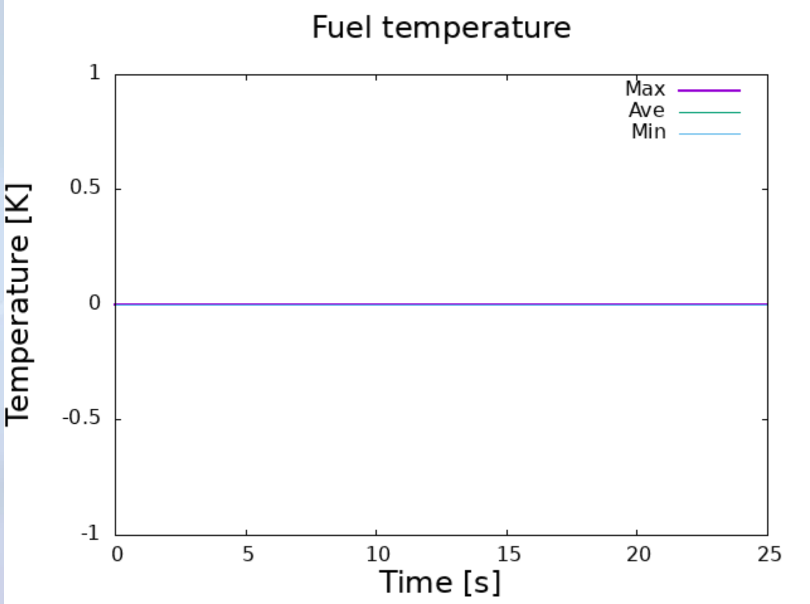
```
Valid Function1 types :

25
(
coded
constant
cosine
csvFile
expression
functionObjectTrigger
functionObjectValue
halfCosineRamp
inputValueMapper
linearRamp
none
one
polynomial
quadraticRamp
quarterCosineRamp
quarterSineRamp
sample
scale
sine
square
step
table
tableFile
uniform
zero
)
```

```
"pump"
{
    volumeFraction      0;
    Dh                  1;
    momentumSource      (0 0 -300000);

    momentumSourceTimeProfile
    {
        type                                table;

        //- Time after which the time table is applied
        startTime                           5;

        //- Left column is time elapsed since the startTime defined
        //  above
        table       table
        (
            (   0   1   )
            (   1   0.818730753    )
            (   2   0.670320046    )
            (   3   0.548811636    )
            (   4   0.449328964    )
            (   5   0.367879441    )
            (   6   0.301194212    )
            (   7   0.246596964    )
            (   8   0.201896518    )
            (   9   0.165298888    )
            (   10  0.135335283    )
        );
    }
}
```

Exercise 6 - Results

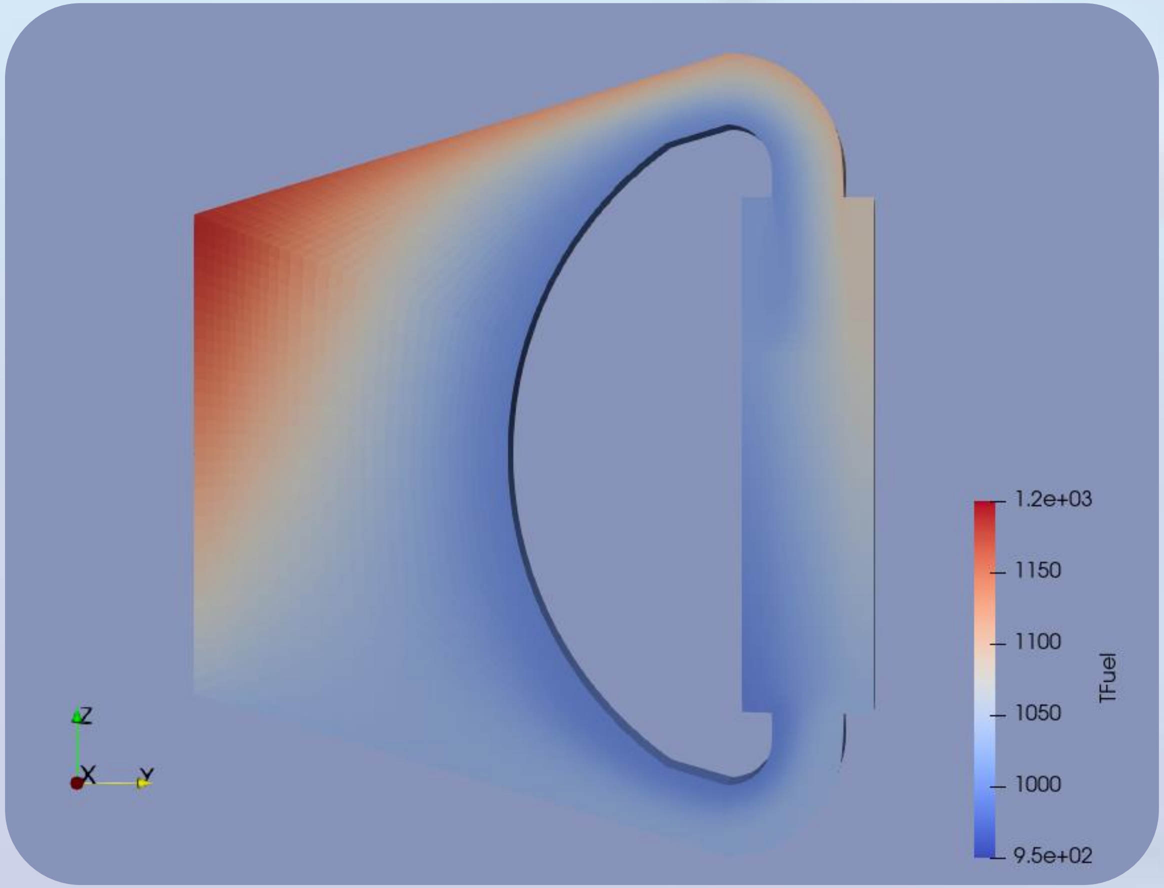




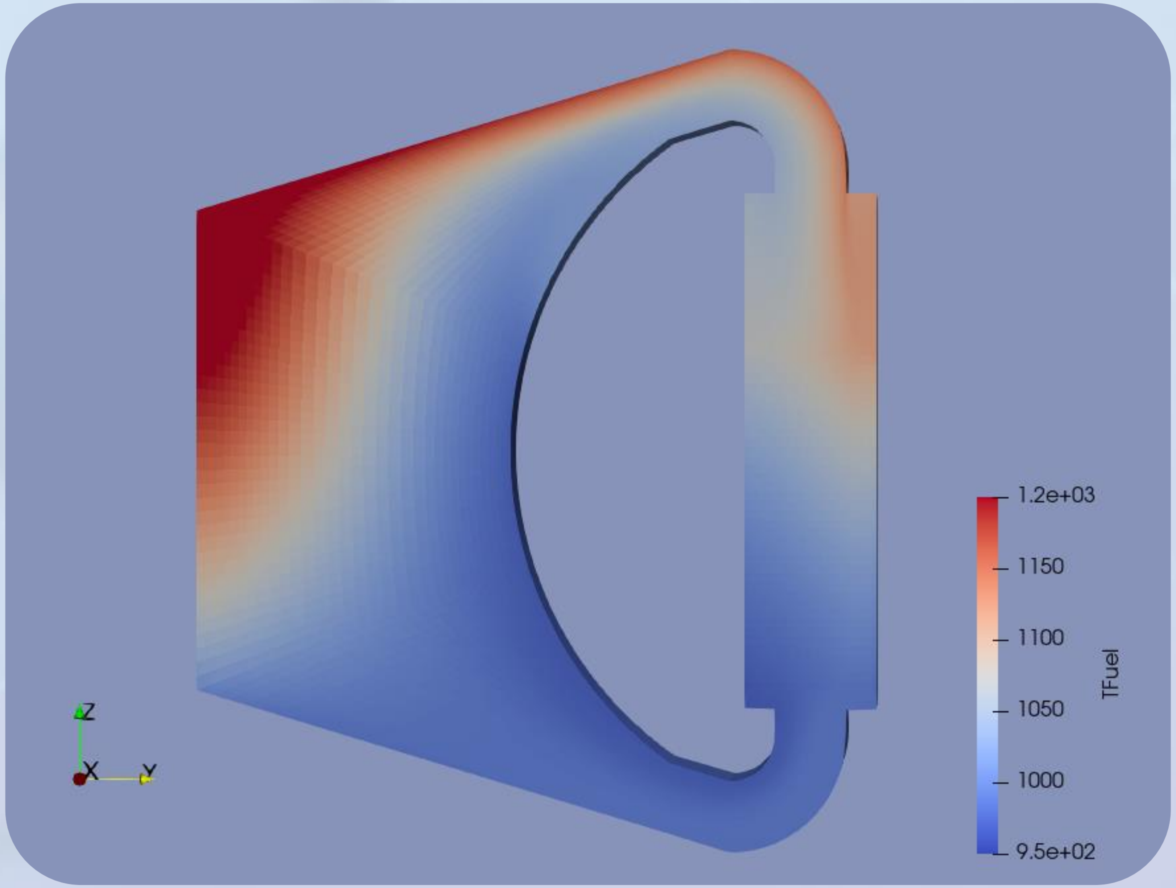


Exercise 6 - Results

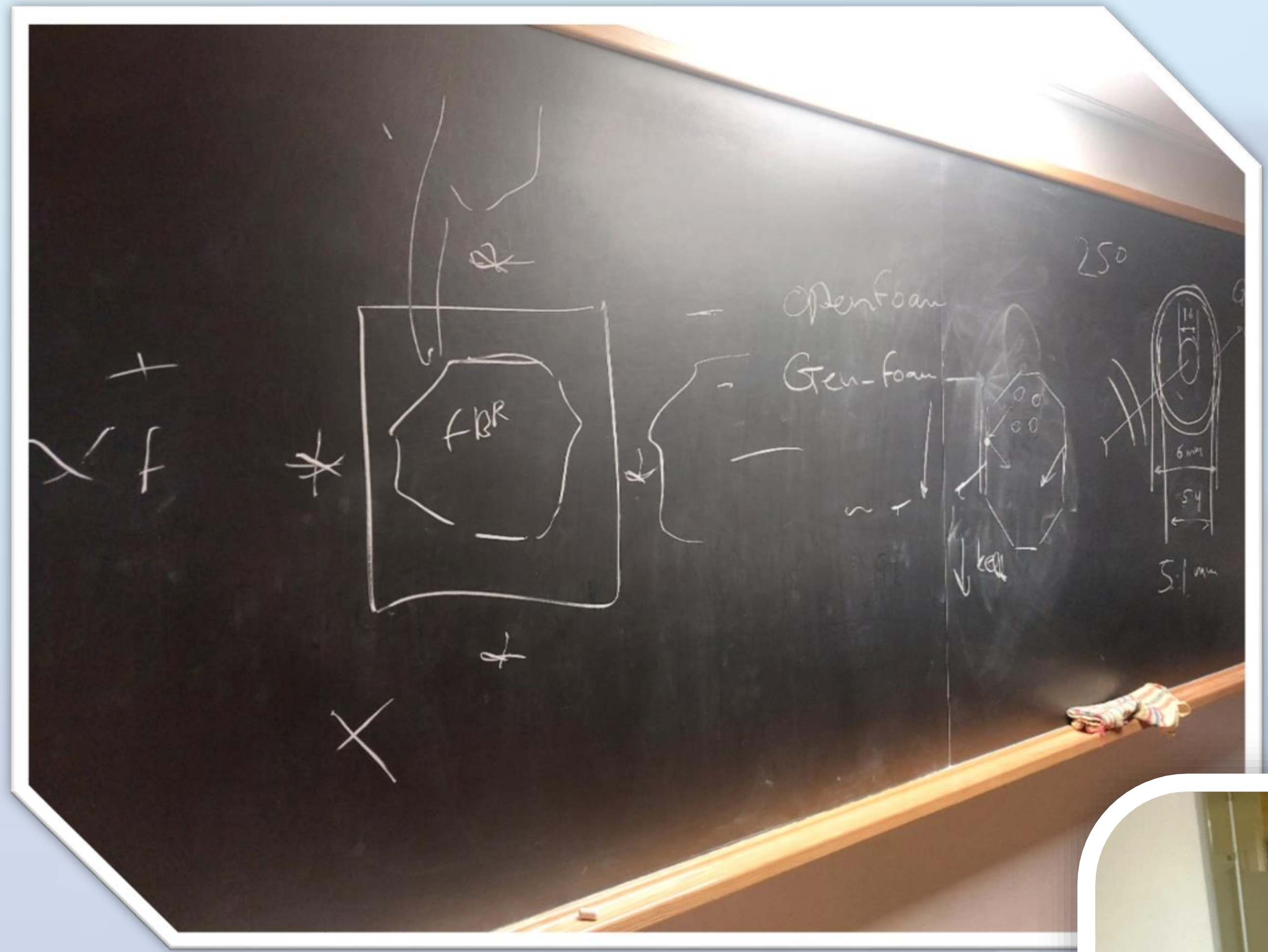
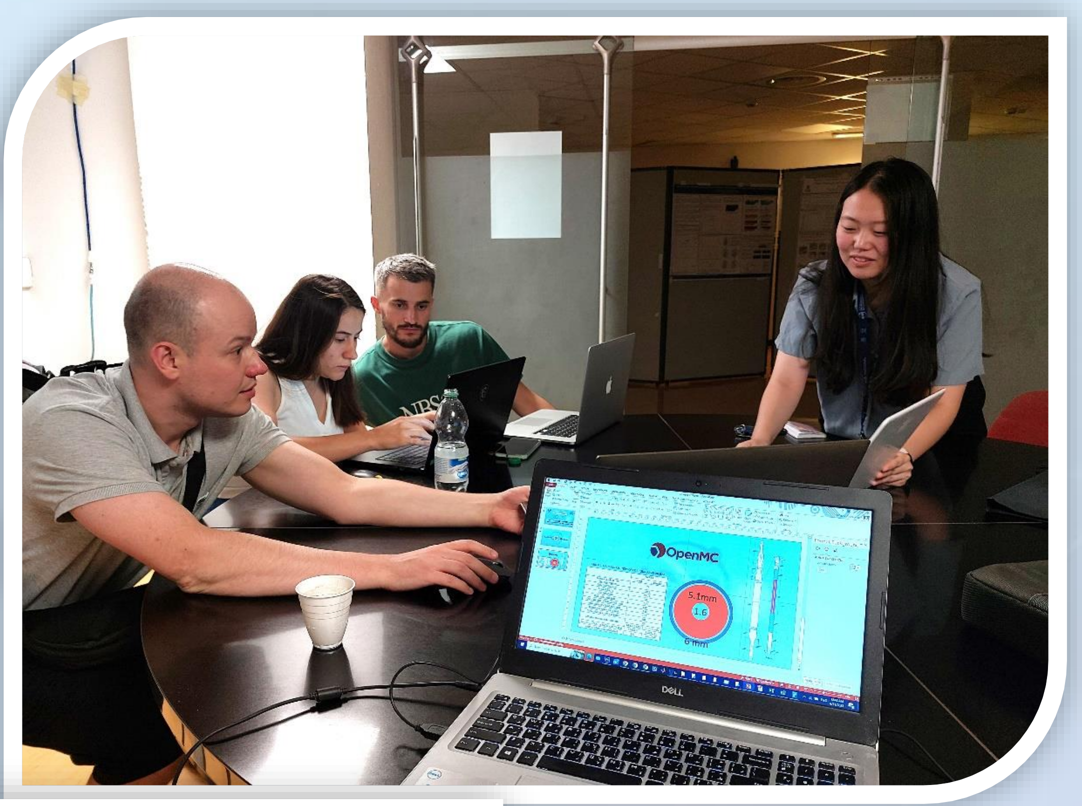
T(fuel) @ t = 0 s



T(fuel) @ t = 20 s



OpenMC


FBR
OpenFoam
Gen-foam
250

OpenMC
DELL

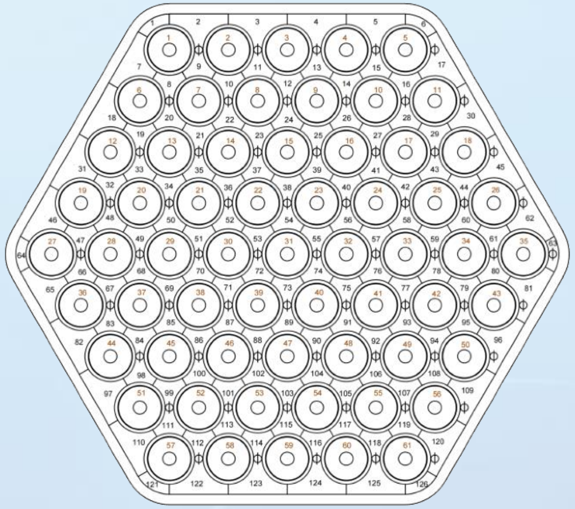
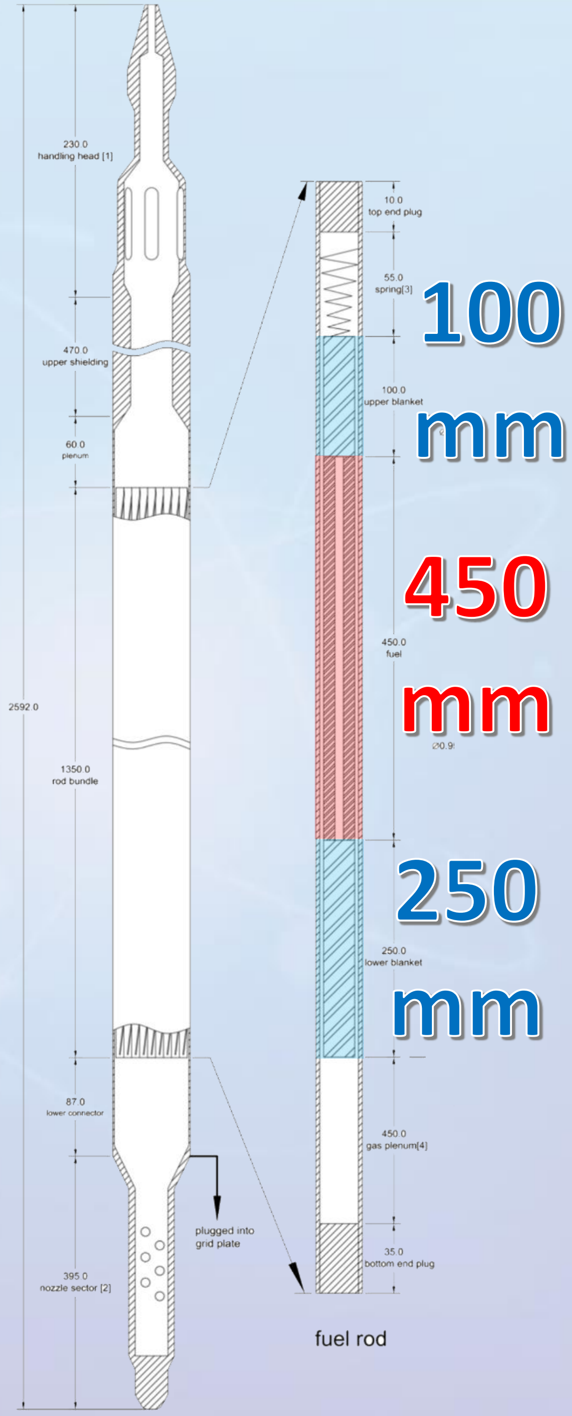



TABLE 9. MAIN PARAMETERS OF CORE SUB-ASSEMBLIES*

	Fuel SA	
	Fuel	Blanket
Number of SAs in core (operation loading)	79	
Length of SA [mm]	2592	
Mass of SA [kg]	29~31	
Number of rods	61	
Rod lattice pitch [mm]	6.95	
Outer diameter of rod/cladding [mm]	6.00	
Inner diameter of cladding [mm]	5.40	
Diameter of spacer wire [mm]	0.95	
Screw pitch of spacer wire [mm]	100	
Effective material and enrichment	UO_2	
	64.4±0.5 wt%	0.3~0.72 wt%
Total mass of UO_2 or B_4C in each SA [kg]	5.30±0.13	1.28/3.23(1)
Length of effective material [mm]	450	100/250(2)



Two cases

20 C°

Inputs
Materials
Geometries
Setting

250 C°

$$A_i = A_{i,1} \cdot f_{i,1} + \ldots\ldots + A_{i,n} \cdot f_{i,n}$$

$$\rho_i = \rho_j \cdot w\%_i$$

$$ND_i = \frac{\rho_i}{A_i} \cdot N_{Avo}$$

$$ND_{i,1} = ND_i \cdot f_{i,1}$$

ISOTOPIC COMPOSITION OF STEEL MATERIALS (15-15TI)

Elem.	Rel. mass, w%	Isot	Natural abundance, %	ND, #/barn・cm	
				20 °C	250 °C
Fe	64.24	Fe-54	0.05845	3.2138E-03	3.2006E-03
		Fe-56	0.91754	5.0450E-02	5.0242E-02
		Fe-57	0.02119	1.1651E-03	1.1603E-03
		Fe-58	0.00282	1.5505E-04	1.5442E-04
Cr	16.25	Cr-50	0.04345	6.4906E-04	6.4639E-04
		Cr-52	0.83789	1.2517E-02	1.2465E-02
		Cr-53	0.09501	1.4193E-03	1.4134E-03
		Cr-54	0.02365	3.5329E-04	3.5183E-04
Ni	14.75	Ni-58	0.68077	8.1775E-03	8.1437E-03
		Ni-60	0.26223	3.1499E-03	3.1369E-03
		Ni-61	0.011399	1.3693E-04	1.3636E-04
		Ni-62	0.036346	4.3659E-04	4.3479E-04
		Ni-64	0.009255	1.1117E-04	1.1071E-04
Mo	2.2	Mo-92	0.1453	1.5923E-04	1.5857E-04
		Mo-94	0.0915	1.0027E-04	9.9856E-05
		Mo-95	0.1584	1.7358E-04	1.7287E-04
		Mo-96	0.1667	1.8268E-04	1.8192E-04
		Mo-97	0.096	1.0520E-04	1.0477E-04
		Mo-98	0.2439	2.6728E-04	2.6617E-04
		Mo-100	0.0982	1.0761E-04	1.0717E-04
Mn	1.5	Mn-55	1	1.3051E-03	1.2997E-03
C	0.06	C-12	0.9893	2.3622E-04	2.3525E-04
		C-13	0.0107	2.5549E-06	2.5444E-06
Ti	0.35	Ti-46	0.0825	2.8834E-05	2.8715E-05
		Ti-47	0.0744	2.6003E-05	2.5896E-05
		Ti-48	0.7372	2.5765E-04	2.5659E-04
		Ti-49	0.0541	1.8908E-05	1.8830E-05
		Ti-50	0.0518	1.8104E-05	1.8030E-05
Si	0.45	Si-28	0.92223	7.0629E-04	7.0338E-04
		Si-29	0.04685	3.5880E-05	3.5732E-05
		Si-30	0.03092	2.3680E-05	2.3583E-05
V	0.2	V-50	0.0025	4.6915E-07	4.6722E-07

OpenMC

Two cases

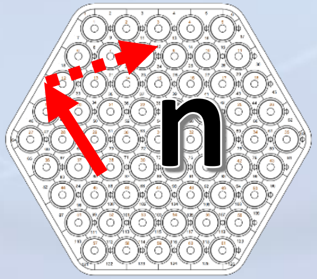
20 C°

~~1000~~ 5000

~~120~~ 300

~~20~~ 50

Inputs
Materials
Geometries
Setting



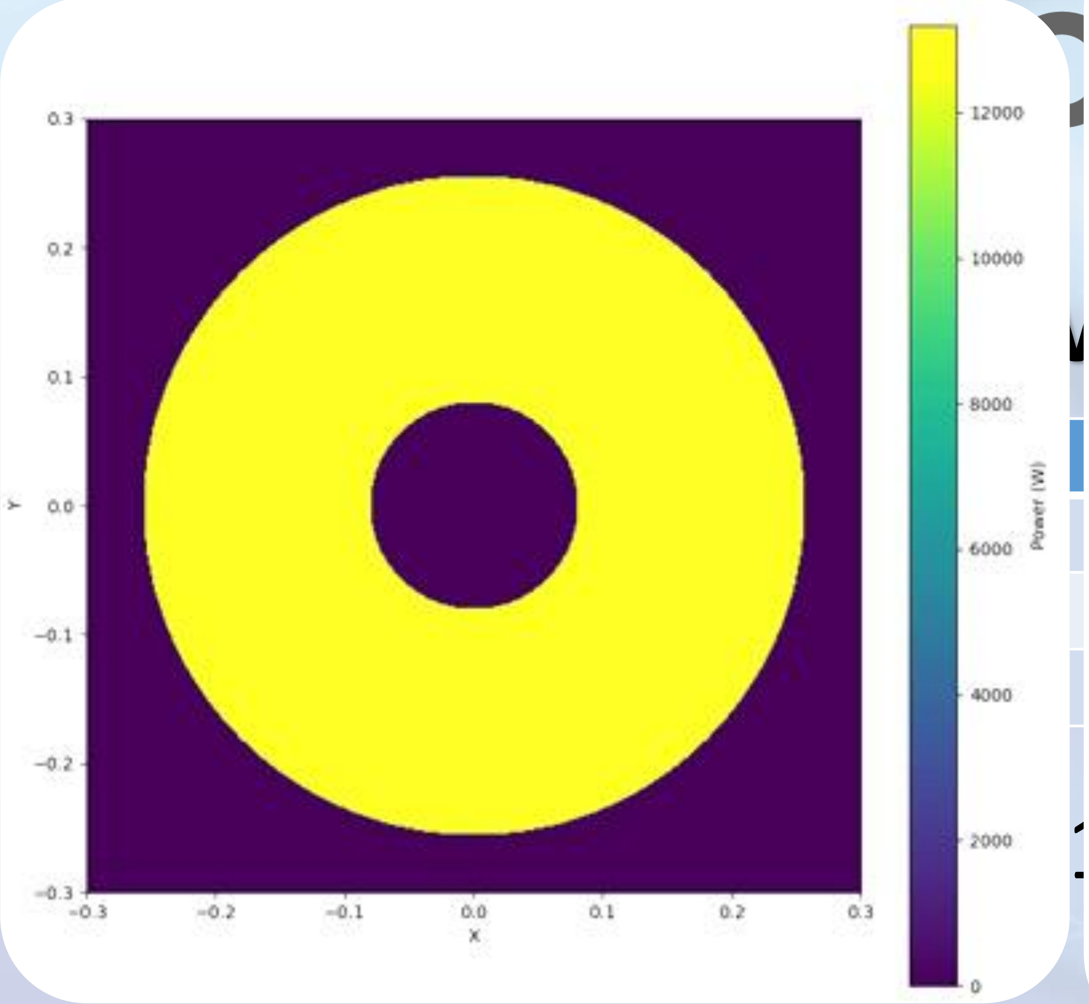
Reflection BC

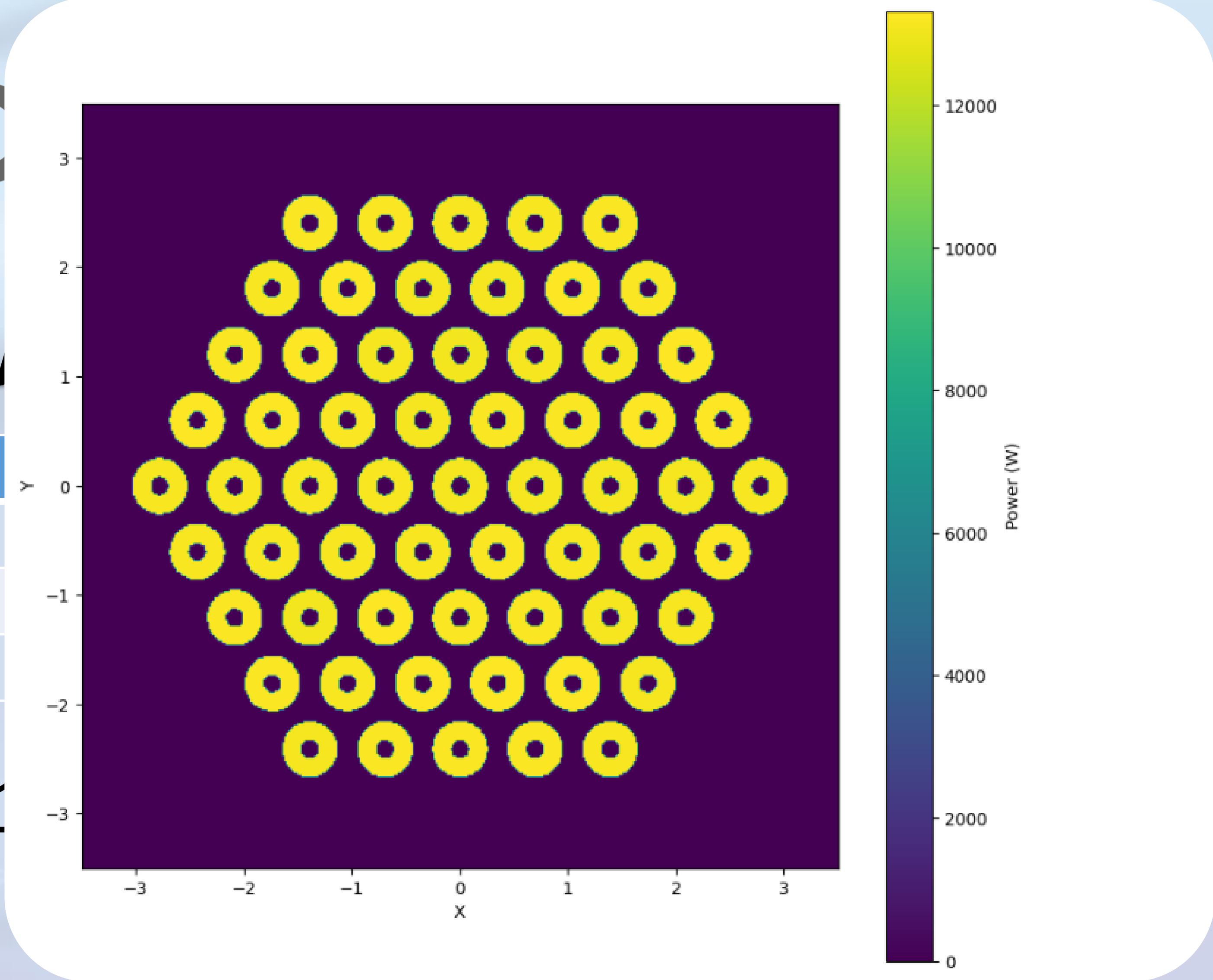
250 C°

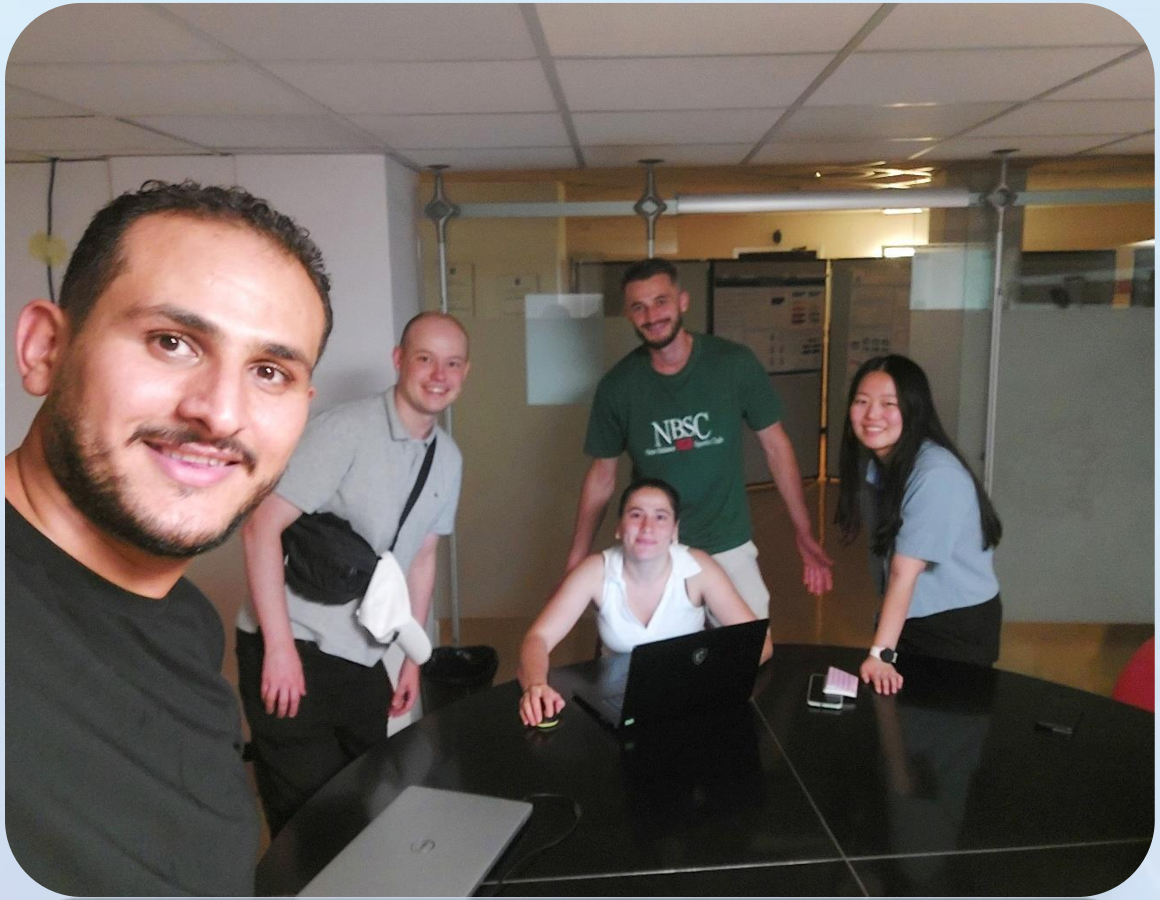
k_{eff}

Power

FA & Pin


0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
Y
−0.3 −0.2 −0.1 0.0 0.1 0.2 0.3
X
12000
10000
8000
6000
4000
2000
0
Power (W)


3
2
1
0
−1
−2
−3
Y
−3 −2 −1 0 1 2 3
X
12000
10000
8000
6000
4000
2000
0
Power (W)



Thank you for your attention