Using ALYA in FUSION simulations

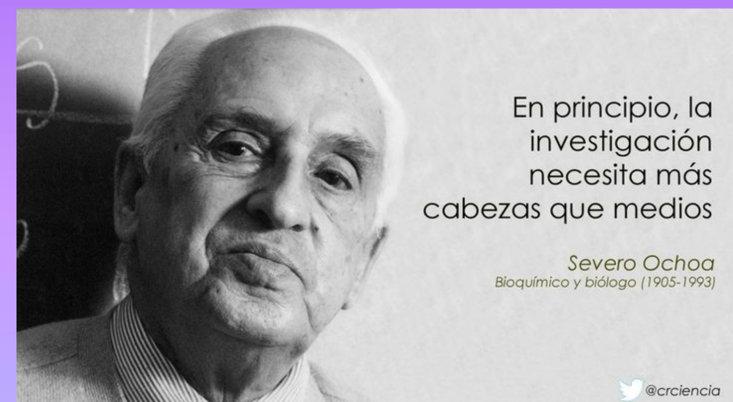
Alejandro Soba

CASE-FUSION-BSC

Background & Summary

Why?

Six month stance in BSC, in CASE- Fusion group
Under the supervision of Mervi Mantsinen



11th call **Severo Ochoa** BSC Mobility grant

What?

- Work in **ALYA**, continuing the NEUTRO module development.

- Working in a CFD project to validate **ALYA** to be used as reference code into ITER.

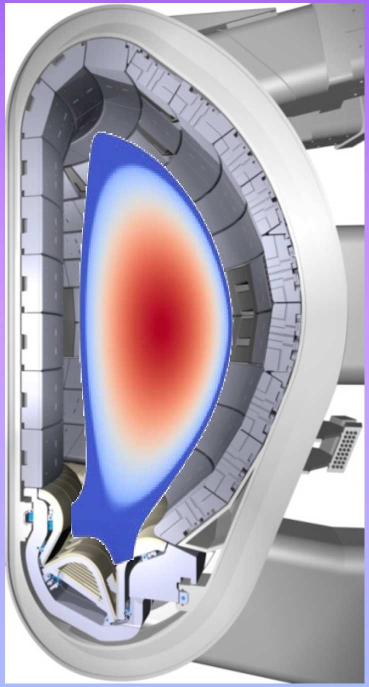
- Trying to help others developers of **ALYA** into the group.

NEUTRO module

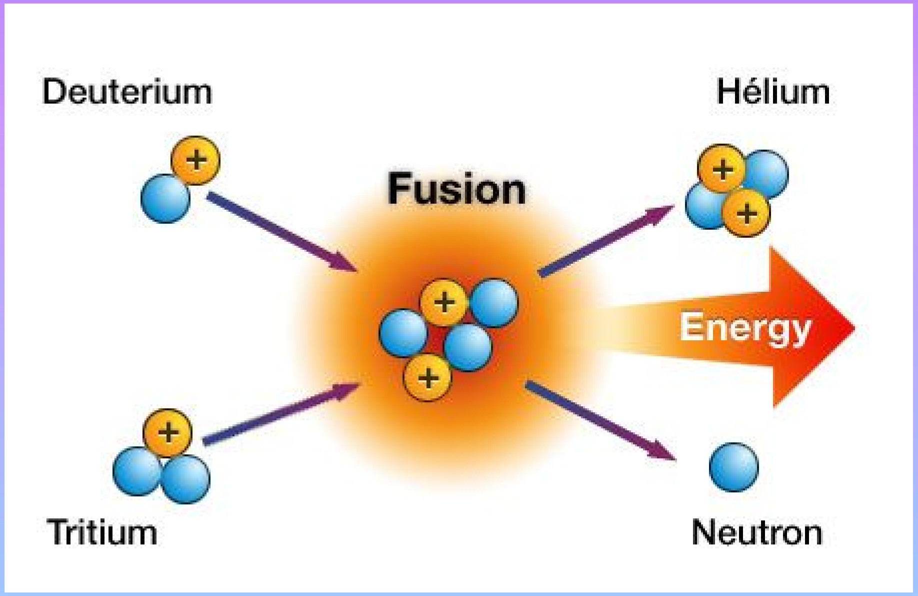
ALYA-FUSION CASE-BSC

NEUTRO Module: Contextualization

ITER: Confinement PLASMA using magnetic control



Basic Reaction



one of the consequences :::: neutrons…

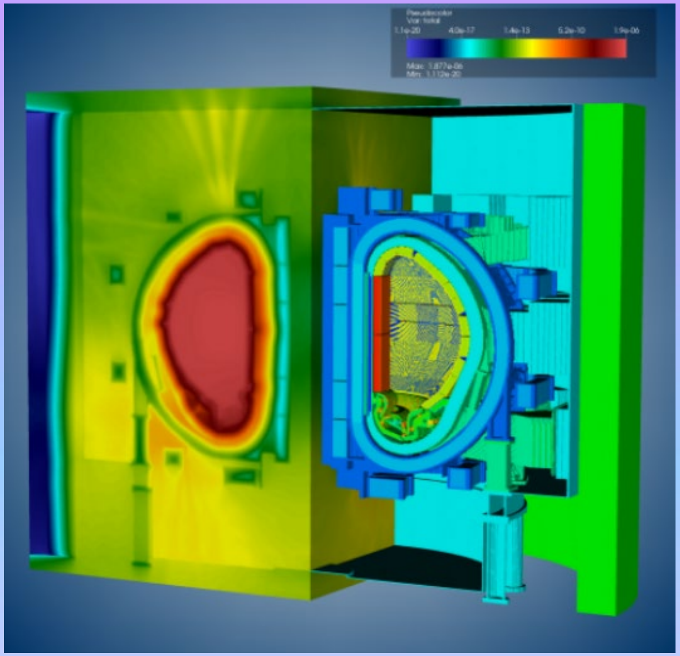
NEUTRO Module

- Fusion plasma is a source of neutrons which impinge on all material surrounding the plasma.
- Many of them will be used in the Lithium reaction in walls used to obtain T, but….

7Li + n -> 4He + T + n -2.47 MeV,
6Li + n -> 4He + T + 4.78 MeV.

- Through interaction with neutrons, materials become activated and subsequently, emit decay photons.

- Through interaction with neutrons the material will be damaged.

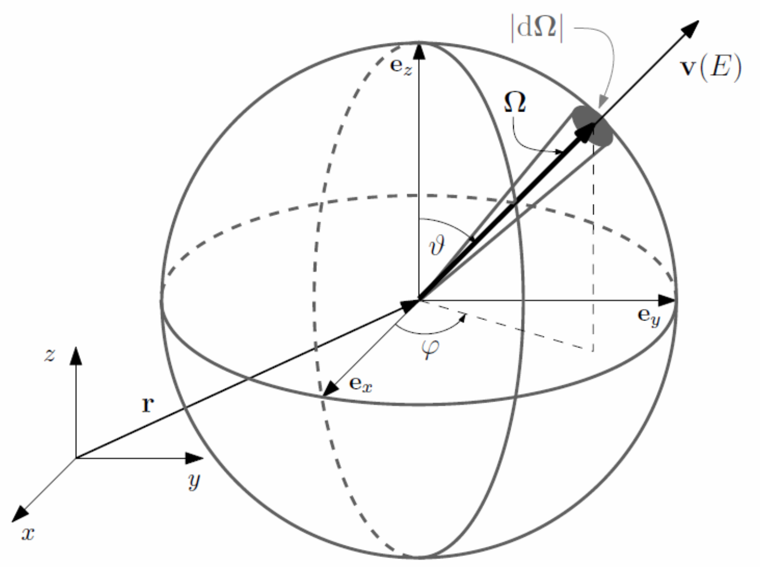


NEUTRO Module

The general stationary transport neutron equation has the form:

$$\Omega \cdot \nabla\varphi + \Sigma_t(r,E,\Omega)\varphi =$$
$$\int_0^{\infty}\int_{4\pi}\Sigma_s\left(r,E' \to E,\Omega' \to \Omega\right)\varphi d\Omega' dE' + \int_0^{\infty}\nu\Sigma_f\left(r,E' \to E,\Omega' \to \Omega\right)\varphi dE' + s(r,E,\Omega)$$

Where:
Ω: solid angle of the direction of neutron travels
E: energy of neutron.
r: general spatial variable.
φ: Function distribution of neutrons in r, E, Ω.
$\Sigma_t(r,E,\Omega)$: Total cross section.
$\nu\Sigma_f(r,E,\Omega)$: Fission cross section.
$\Sigma_s(r,E,\Omega)$: Total scattering cross section
s(r,E, Ω): External neutron source.



Neutrons' phase space

NEUTRO Module

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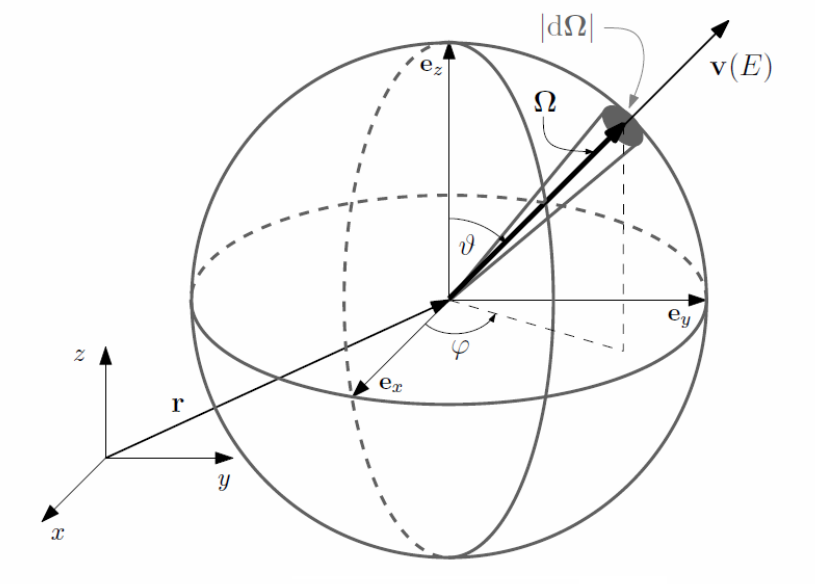

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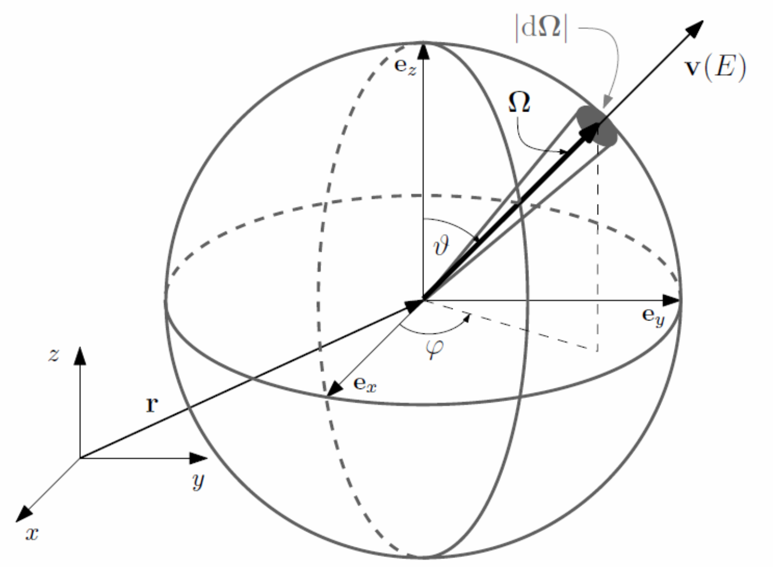

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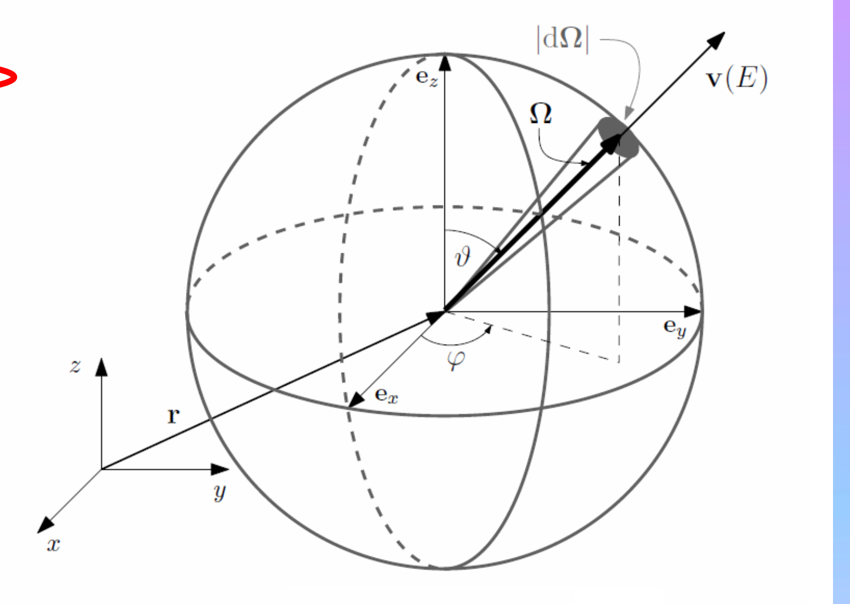
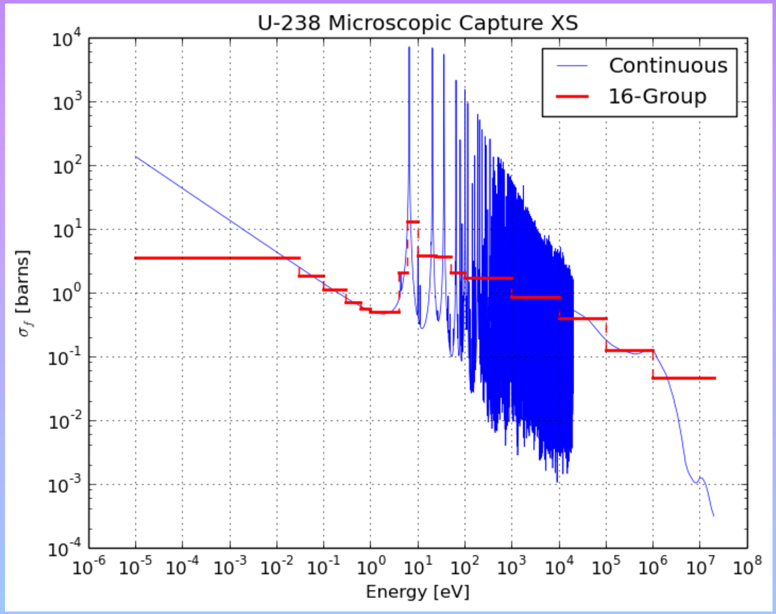


Neutrons' phase space

NEUTRO Module

Energy discretization: Multi-groups approximation using that cross sections are in many cases, soft



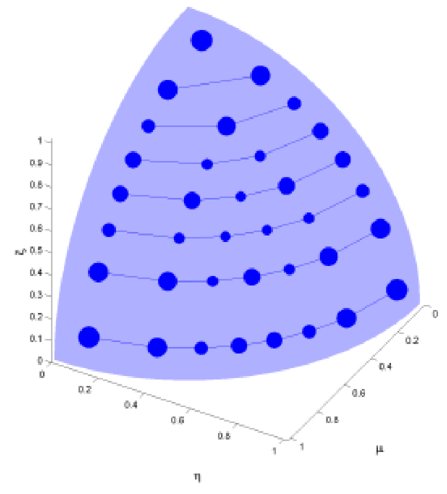
$$\Omega \cdot \nabla \varphi_g + \Sigma_t(r, E_g, \Omega)\varphi_g = \sum_{g'=1}^{G} \int_{4\pi} \Sigma_{s\,g',g}(r, \Omega' \to \Omega)\varphi_{g'} d\Omega' + s(r, E_g, \Omega)$$

$$g = 1, \dots, G$$

NEUTRO Module

Angular discretization: Discrete ordinates methods: Sn method

Idea: create cuadratures points (like in FEM) with adequate weights, in order to divide the phase space in several selected points.



Level Symmetric LS_{16} quadrature set

$$\Omega_m \cdot \nabla \varphi_{gm} + \Sigma_t(r, E_g, \Omega_m)\varphi_{gm} = \sum_{g'=1}^{G} \sum_{m'=1}^{M} \Sigma_{s\,g',g\,m',m}(r)\varphi_{g'm'} + s(r, E_g, \Omega_m)$$

$g = 1, \ldots, G$ $\quad$ $m = 1, \ldots, M$

NEUTRO Module

Scattering kernel Depending of the material, the scattering could not be isotropic, and even in those cases, the isotropic material doesn't implies not angular dependence, but invariant until rotations. That's means that scattering only depend of the product of solid angles.

$$cos(\theta) = \Omega \cdot \Omega'$$

Then we can expand the scattering kernel y Legendre polynomials (valid for one dimensional descriptions or isotropic cases)

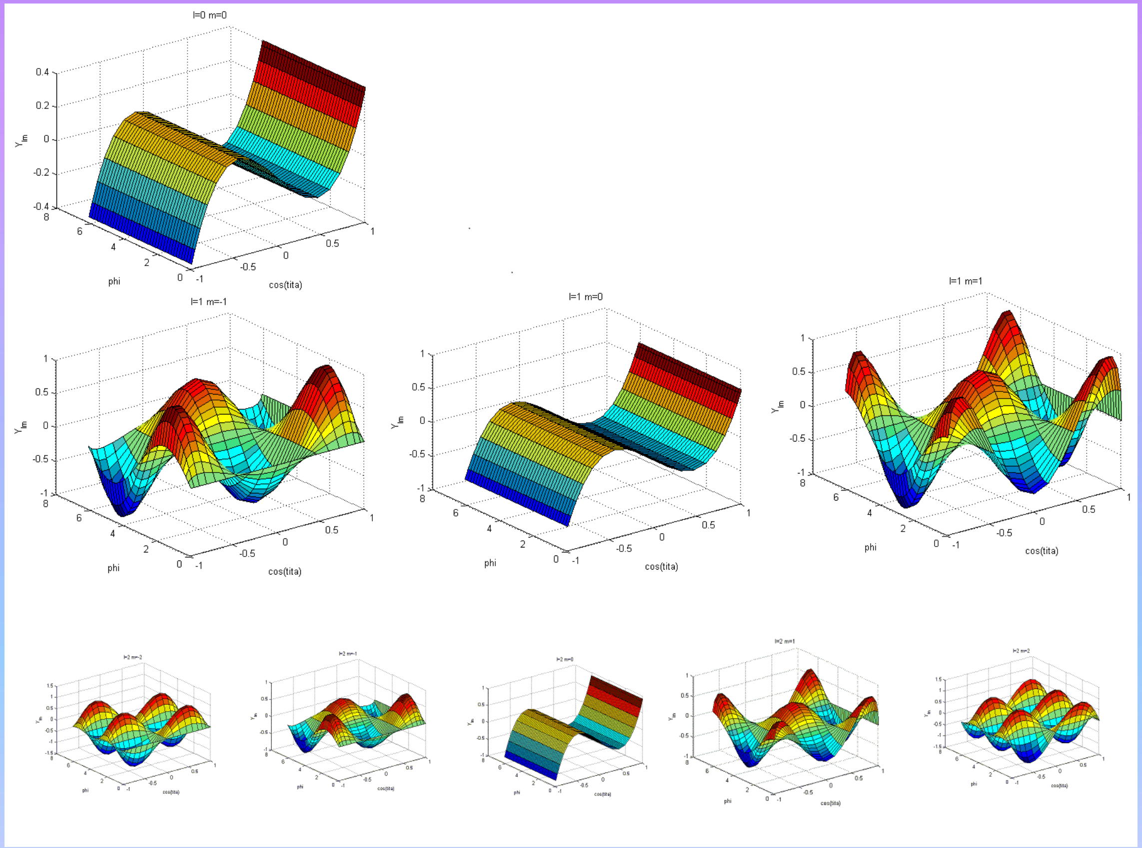
$$\Sigma_s(r.E, \cos(\theta)) = \sum_{l=0}^{L} \frac{2l+1}{4\pi} \Sigma_{sl}(r, E) P_l(\cos(\theta))$$

For general cases we use the spherical harmonics expansion

$$\mathrm{P}_l(\cos(\theta)) = \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \mathrm{Y}_\mathrm{l}^\mathrm{m}(\theta, \phi) \overline{\mathrm{Y}}_\mathrm{l}^\mathrm{m}(\theta', \phi')$$

NEUTRO Module

Scattering kernel: we use the real spherical harmonics, to avoid complex functions. At the moment only L=2 moments are programmed in ALYA, but is enough in the great majorities of cases.



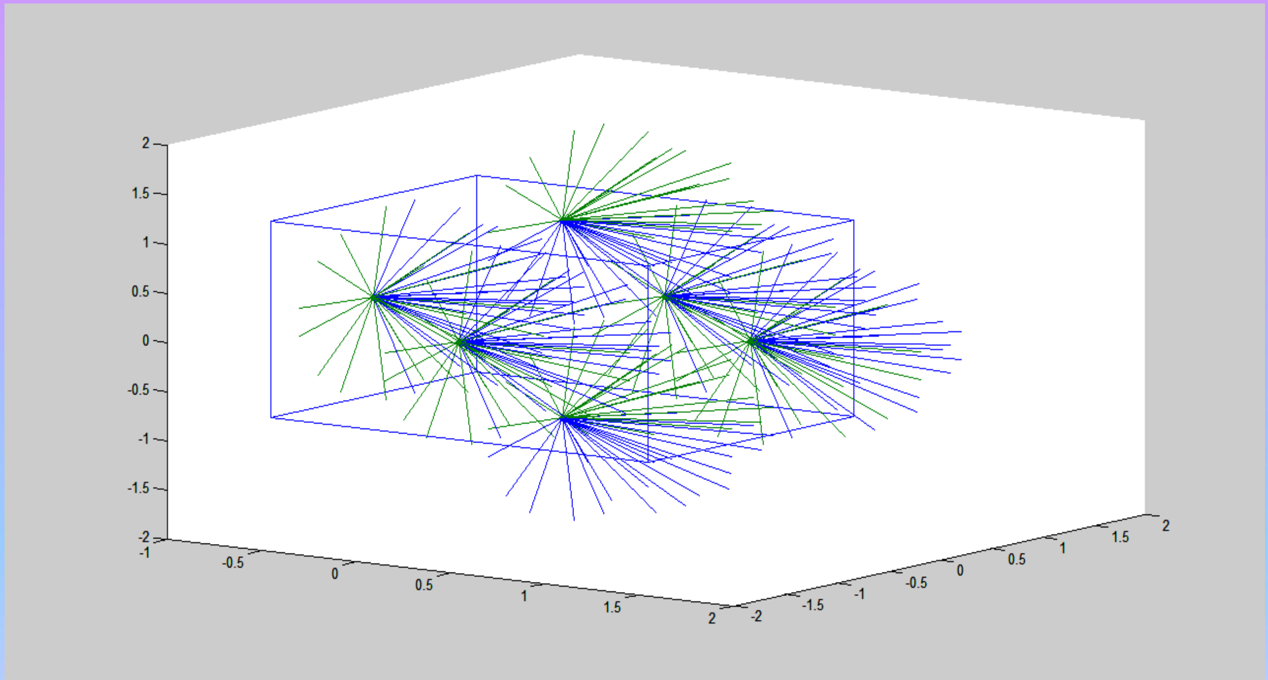
NEUTRO Module

The boundaries condition: three kinds of boundary conditions are programmed in ALYA

1) Vacuum

2) fix flux

3) Reflective B.C.

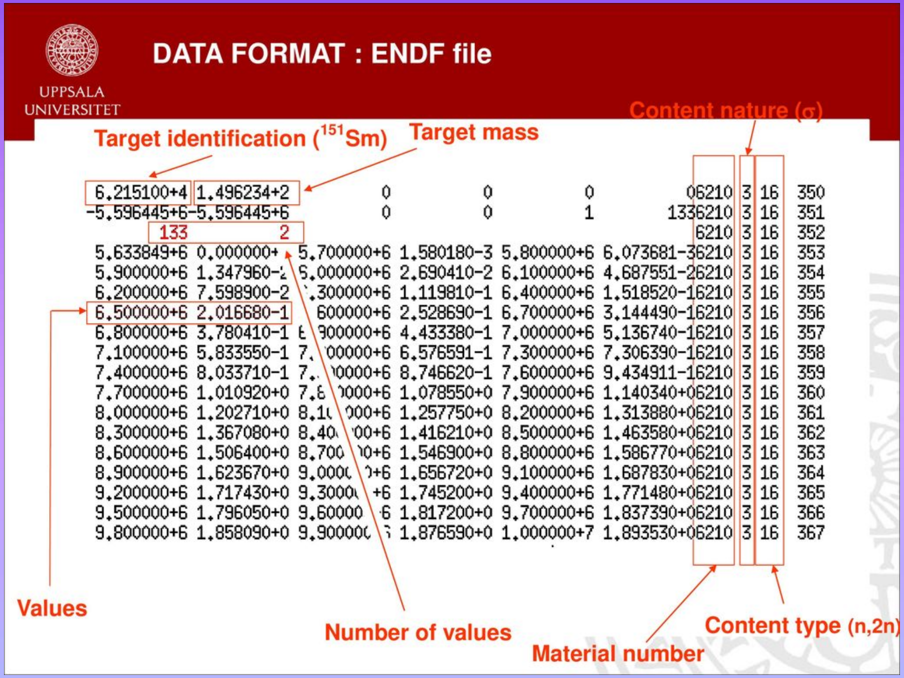


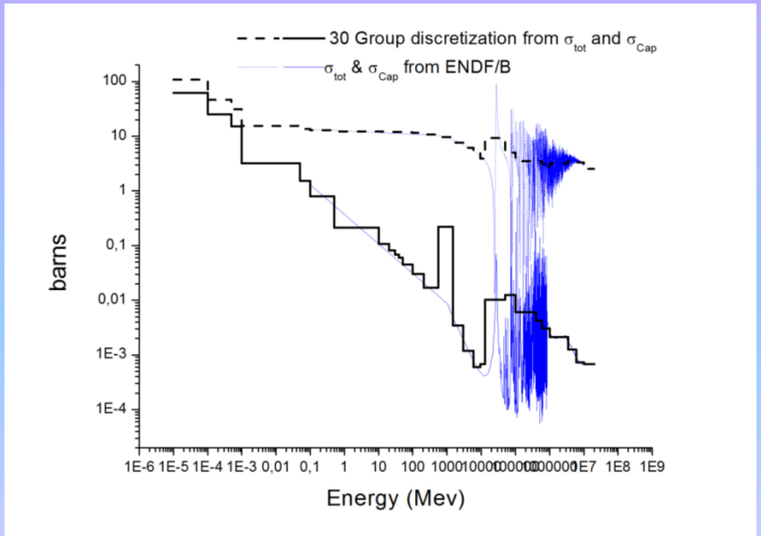
NEUTRO Module

Input Cross Sections

ENDFB **Evaluated Nuclear Data File IAEA nuclear data service**

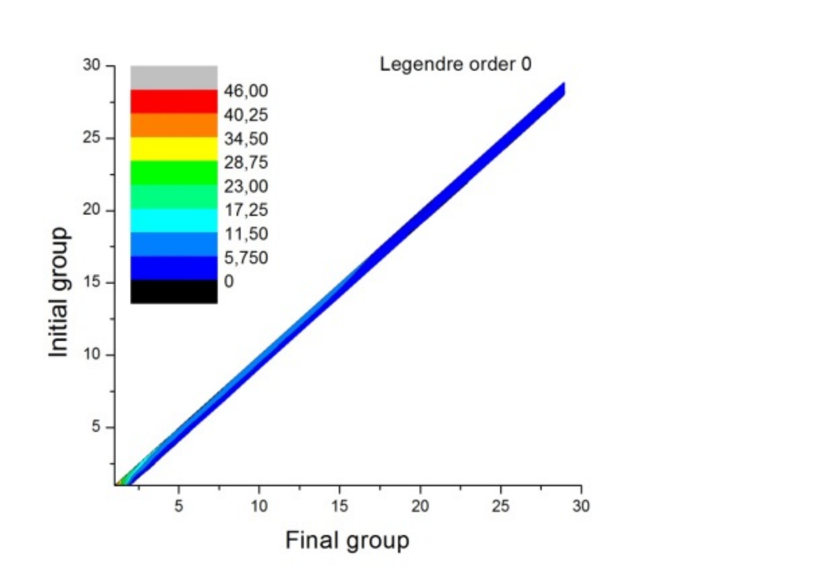
NJOY (Los Alamos national laboratory)

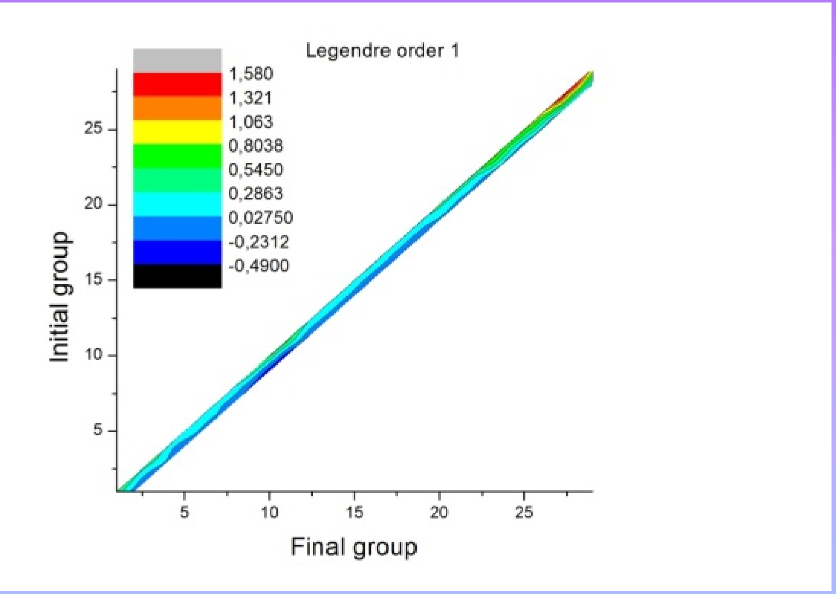




Total and capture cross section for Fe56 and respective 29 group discretization

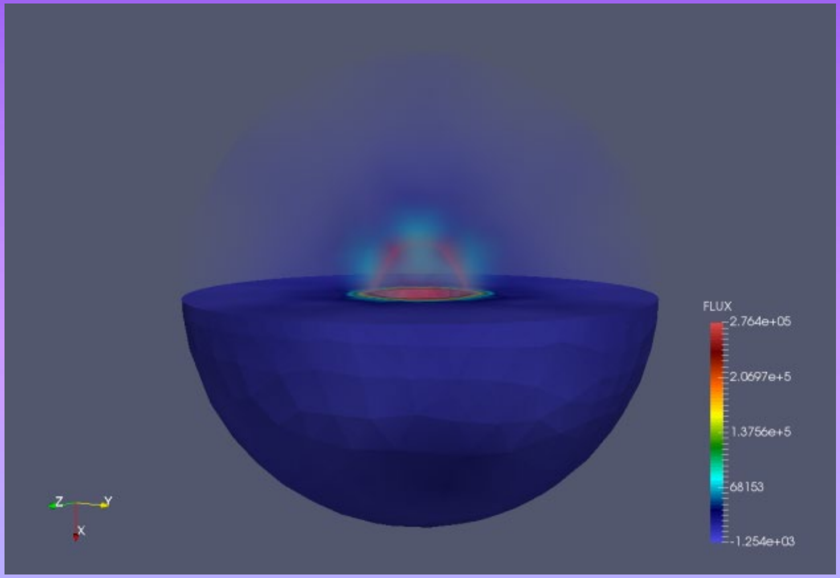
NEUTRO Module

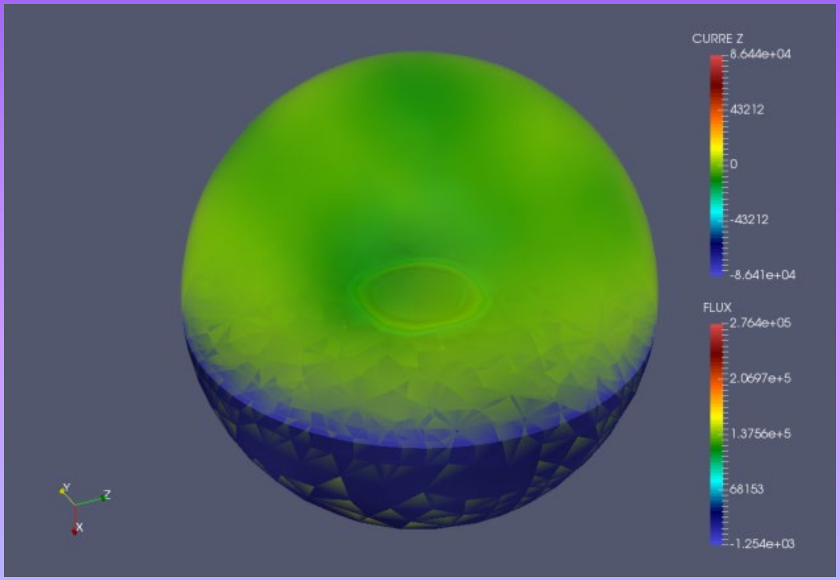




Scattering cross sections matrix for Fe56 with 29 group discretization for Legendre order L=0 and L=1.

NEUTRO Module



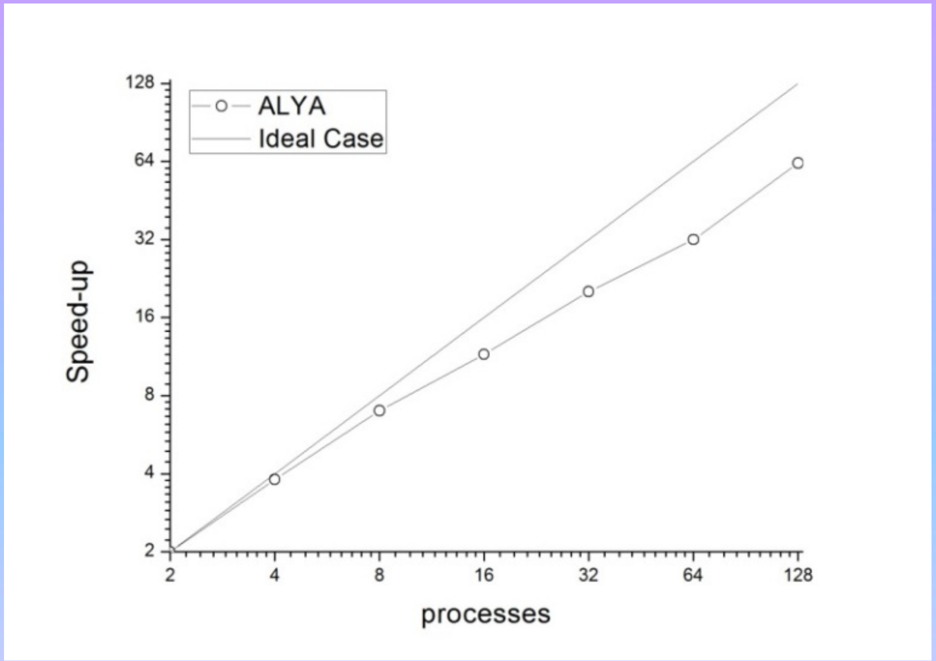


Bechmark case used to analyze NEUTRO module into ALYA code. Shielding Sphere of Fe56 with a source in the interior. Left) Total Flux, Right) Current in z direction and flux (in inferior portion)

NEUTRO Module

At the moment, all the performance analysis were made in the master thesis environment of Carles Riera. Now, adding an energy and an angular discretization, we need to solve G*M systems, over a relative simple domain. Then maybe the general domain division used until now could not be the optimal way to solve this problems.

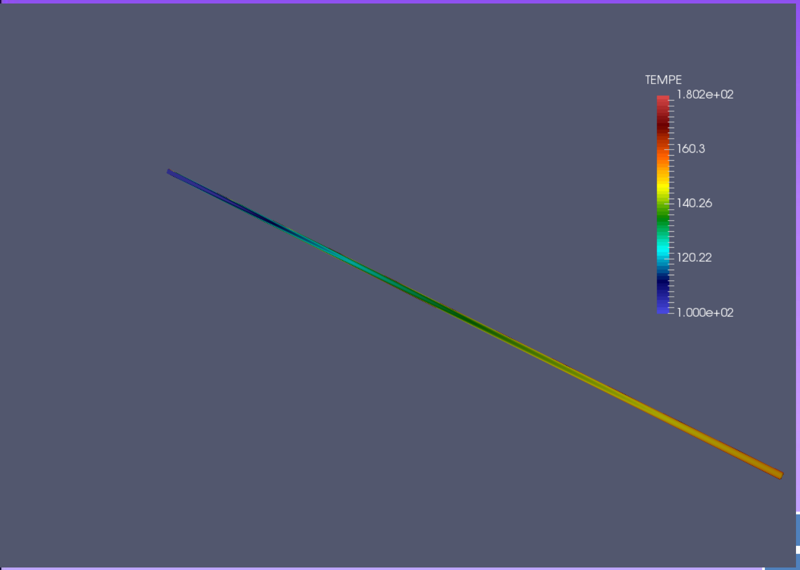
A separate equation by processor could be more efficient.

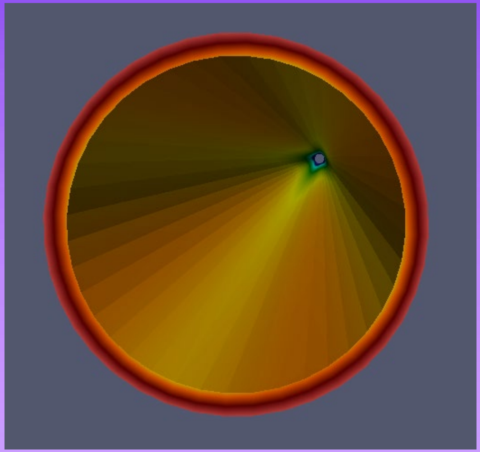


CFD codes validation for convective heat transfer. A benchmark proposed by IDOM

ALYA test

Validation of the convective heat transfer relation for a forced flux.





Correlation	Ref	Eq.	App. Range
Sieder-Tate	[2]	$Nu = 0.027Re^{0.8}Prd^{0.33333}\left(\frac{\mu}{\mu_s}\right)^{0.14}$	0.7<Prd<16700 Re>10000
Petukhov	[3]	$Nu = \frac{(f/8)RePrd}{1.07 + 12.7(f/8)^{0.5}(Prd^{0.6666} - 1)}$ $f = (1.82LogRe - 1.64)^{-2}$	0.5<Prd<2000 3000<Re<5000000
Dittus-Boelter	[4]	$Nu = 0.023Re^{0.8}Prd^{0.4}$	0.6<Prd<160 Re>10000

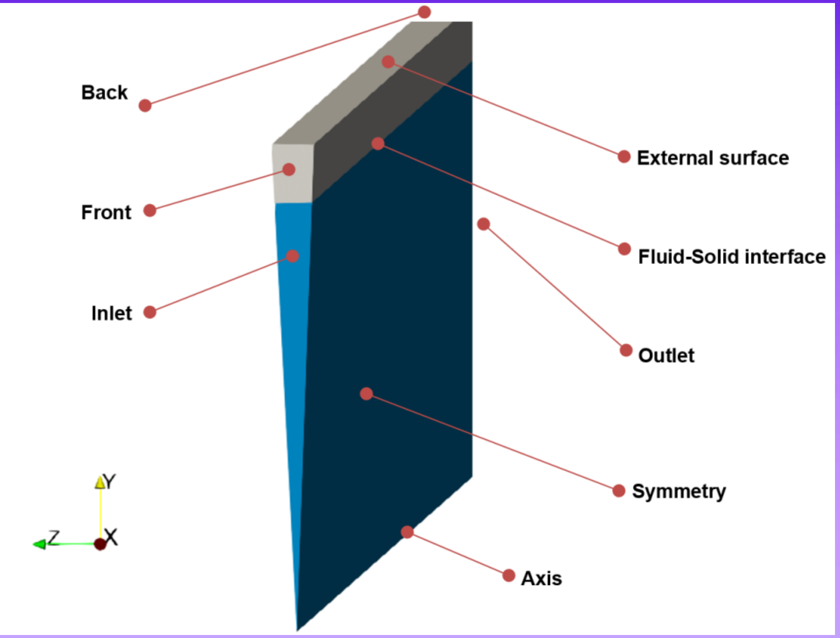
Newton law : $q'' = h(T_s - T_\infty)$ (1)

Equivalent Newton convective law for the: $\bar{q}'' = h(T_s - T_{med}) \approx h(\Delta T_{med})$ (5)

Mean logarithmic temperature difference: $\Delta T_{med} = \frac{\Delta T_{out} - \Delta T_{in}}{Log(\Delta T_{out}/\Delta T_{in})}$

Physical parameters used

Property	Water	Steel
Ref. Temper (ºC)	100.0	173.15
Ref. Press (MPa)	0.8	-
Density ρ (kg/m³)	958.8	7800
Specific Heat c_p (J/kg/K)	4214.1	500
Thermal conduct. k (W/m/K)	0.67946	16
Viscosity *ν* (kg/m/s)	0.00028193	-
Thermal exp. α (1/K)	0.00075	-



The geometry consists in a Steel tube 10.0 meters long, 0.0725 meters of diameter and 0.005 meters of width. The external temperature is 180.15 ºC. Inside the tube forces water past with different velocities in the range 0.004-4 m/seg. That's means a range from a pure laminar regimen to a totally turbulent one. 100 <Re<1,000,000

Test case as defined by IDOM

Numerical condition:

Fluid case

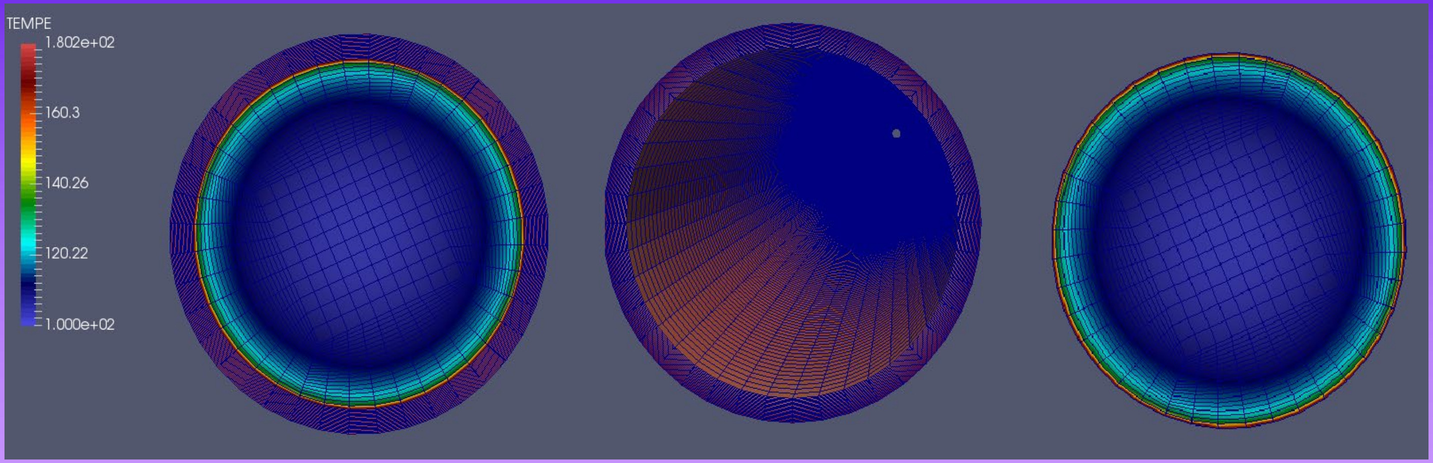
energy equation plus the incompressible convective flux
turbulence k-w with the Shear Stress Transport (SST) model
standard wall function assumption.
standard relaxation factors and Boussinesq approximation.

Solid case

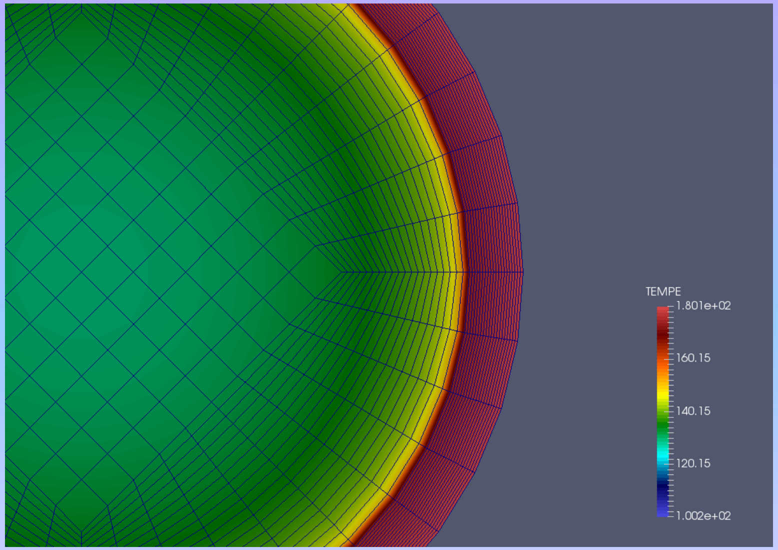
energy equation

Solid-Fluid interface coupling with the fluid into de pipe with the same assumptions mentioned above.

Mesh used



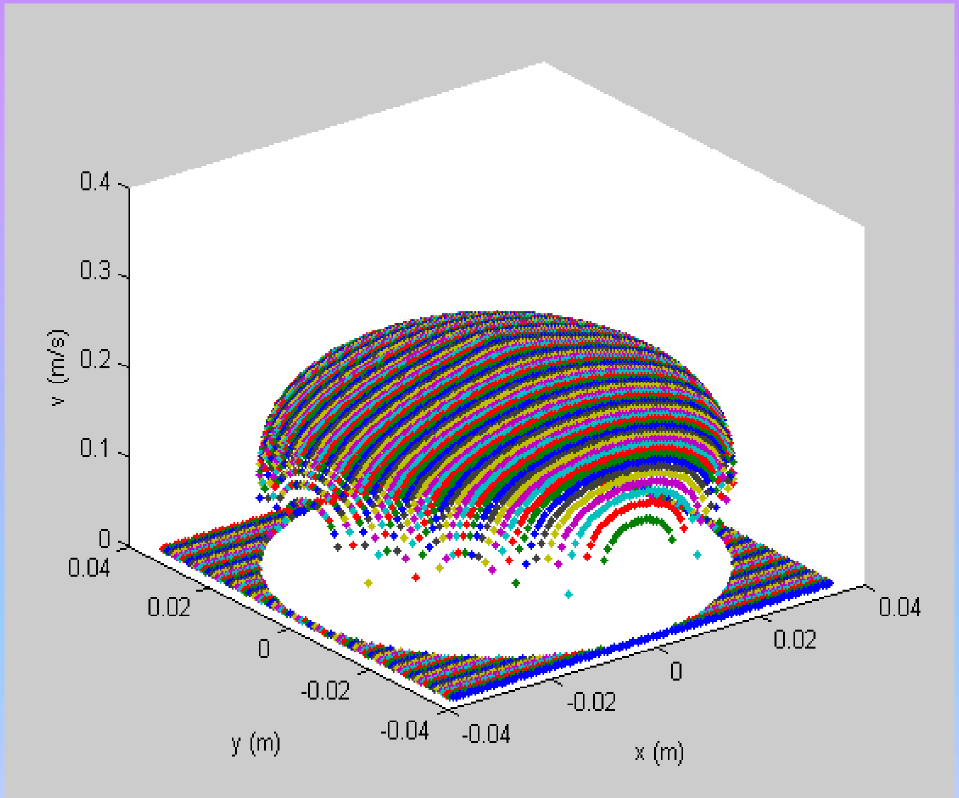
Meshes used for the coupled case. The coupled system (left), Solid steel pipe (middle), fluid (right). We use two meshes, compound of hexahedral elements one for the steel and other for the fluid
NE=1,800,000



Detail of the coupled meshes in the radio=0.03625 m.
Both meshes are coupled using the ALYA special coupling system exporting the wall temperature for the fluid and the heat flux for the solid.

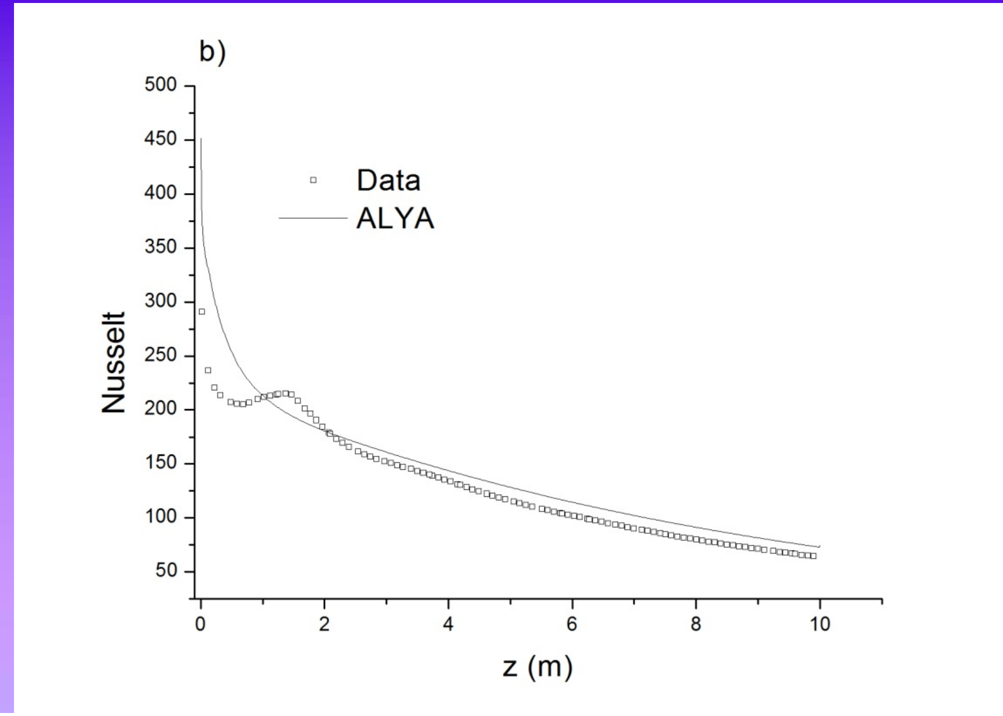
Inlet velocity inflow

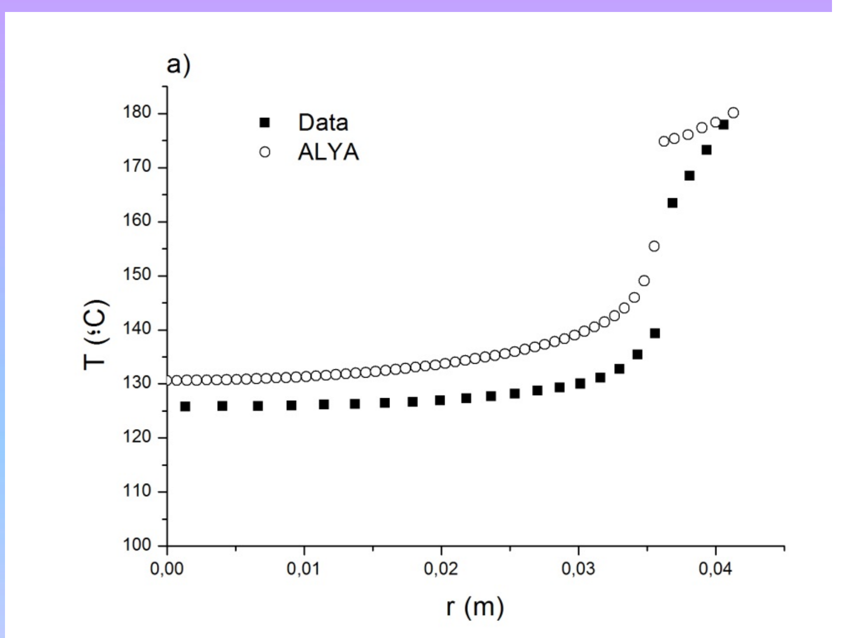
In order to improve the convergence of the model we introduce a different input shape of the velocity in the inlet zone. The function shape of a turbulent flow is forced from the initial condition as we plots in figure 3 (exemplify with the case of v=0.2 m/s)

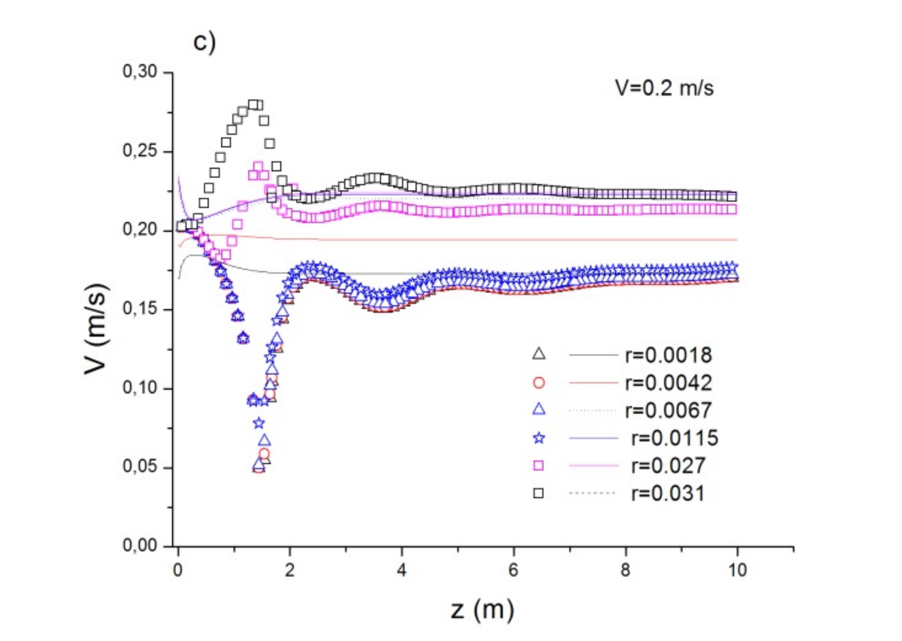


v*(1.0-(x*x+y*y)**0.5/0.03625)**(1/6)

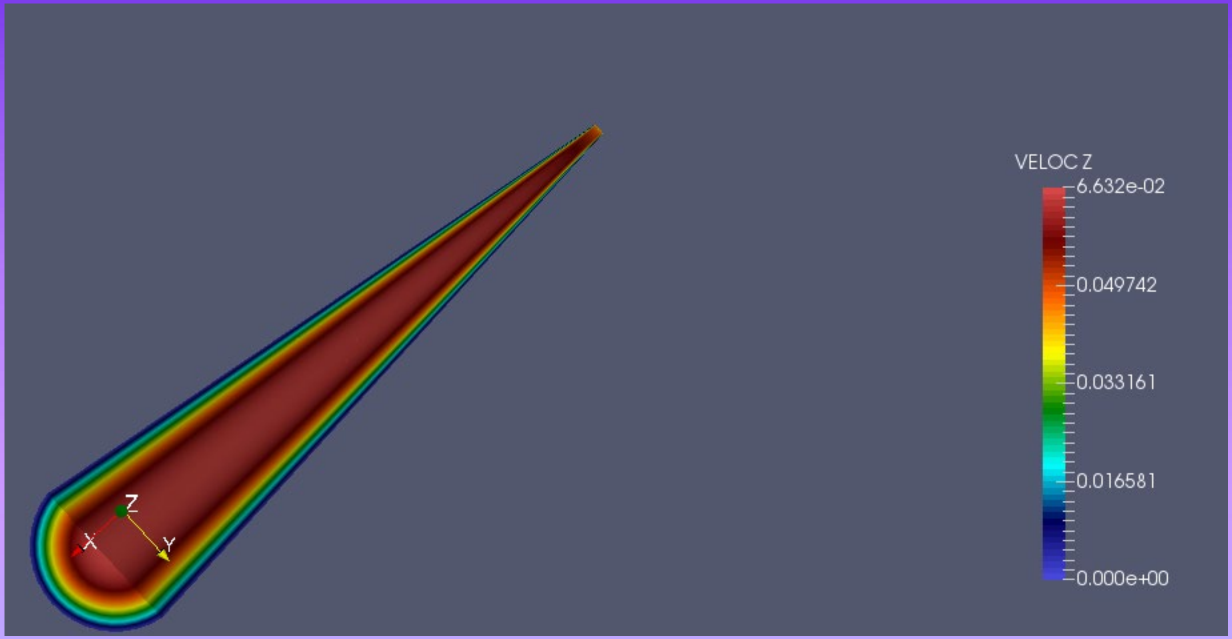
Comparison for velocity 0.2 m/s

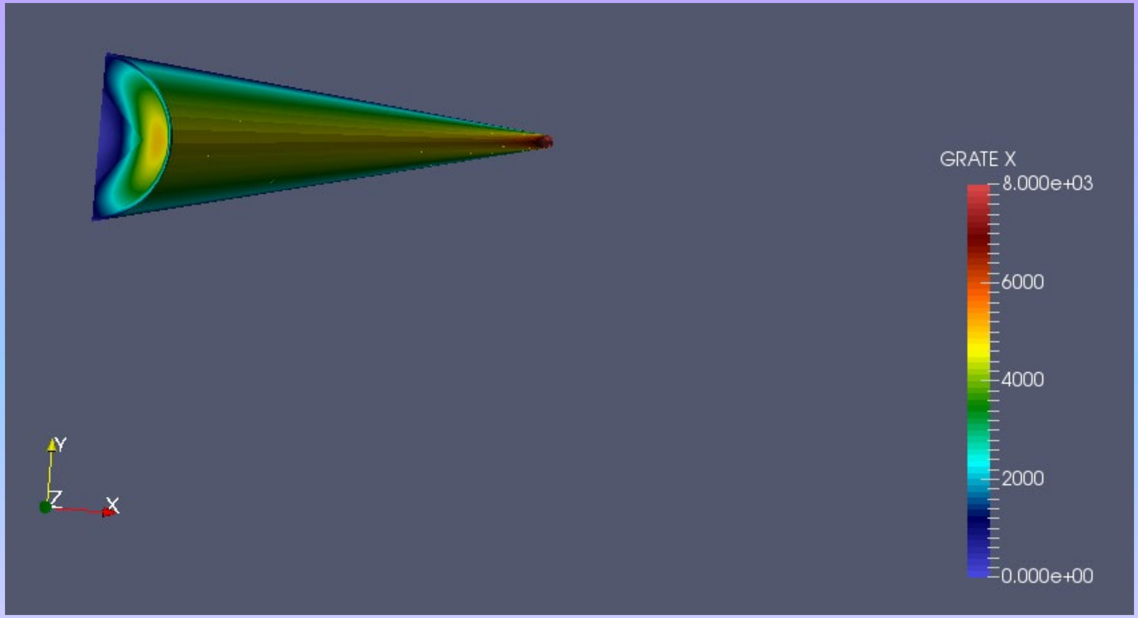




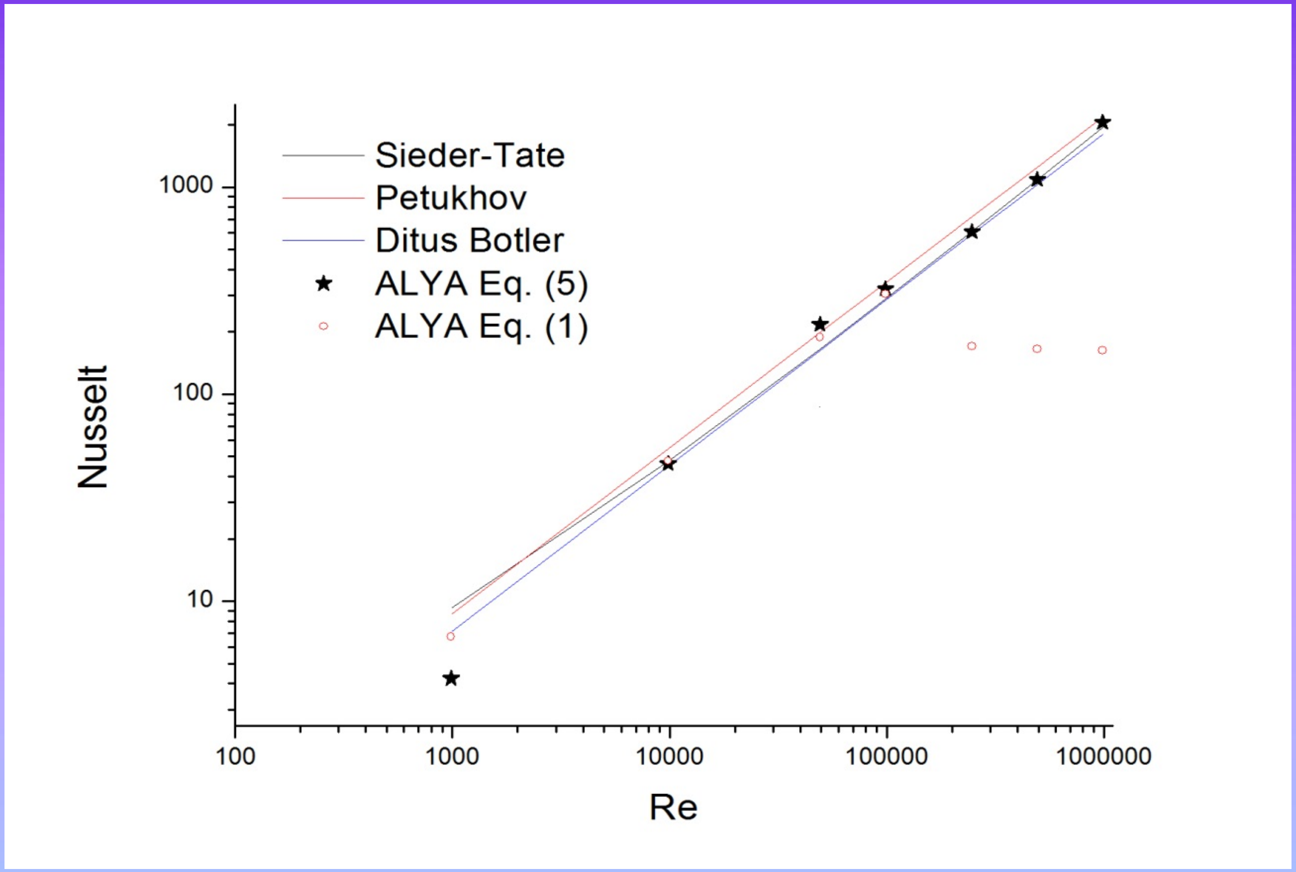


Velocity and temperature gradient



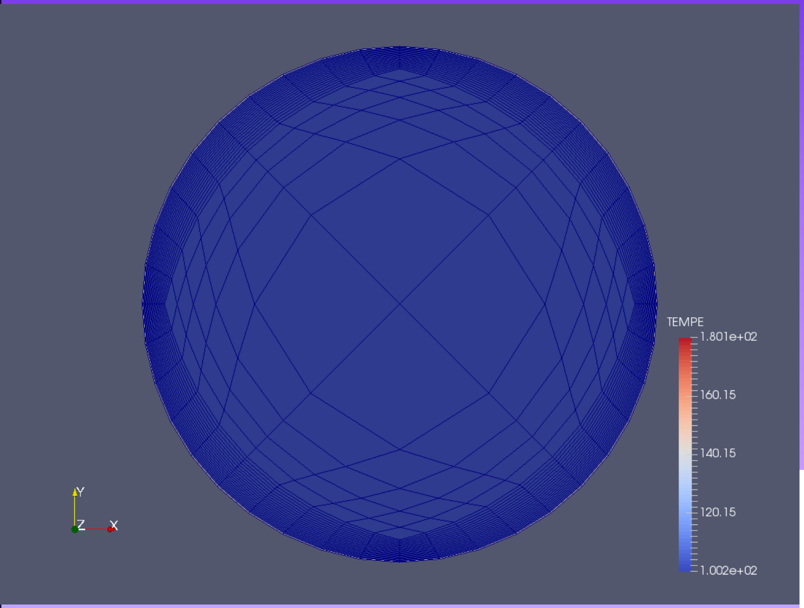


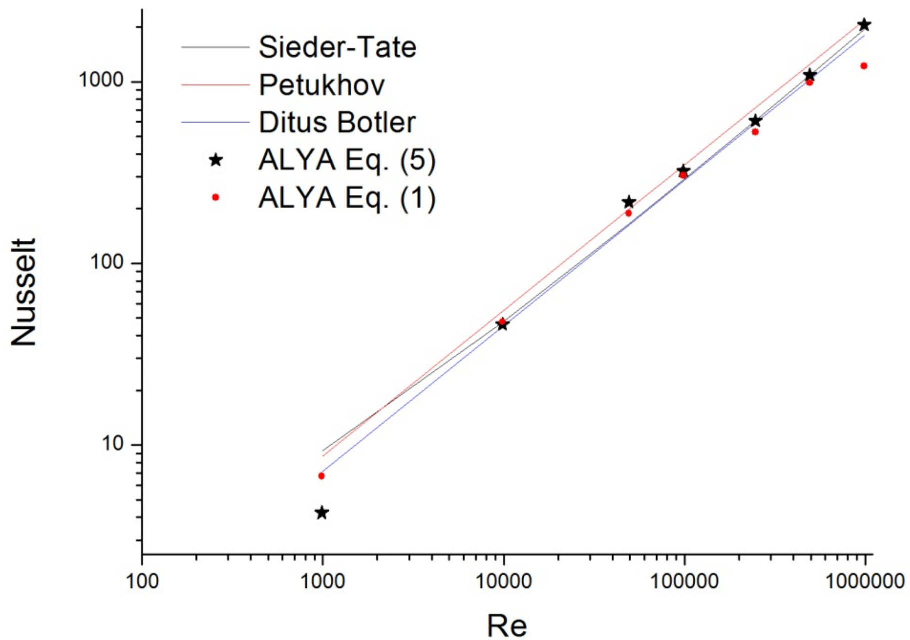
Convective heat transfer relation for a forced flux.



- Good results using Equivalent Newton Law (expected)
- Good results using Newton Law for v<1 m/s
- Working in better meshes for capture boundary layer physics (elements <1e-6 m)

Modify Mesh: logarithmic improve and divide=1





Resources used for this simple test!

NORD3: 25600 hs. (aprox.)

MN4:

19 Apr 19	26 Apr 19 (*)	3 May 19(*)	10 May 19
71774	398949	516821	81149

Total: 1068802 horas/CPU

(*) Top user en CASE

MAGNET module

ALYA-FUSION CASE-BSC

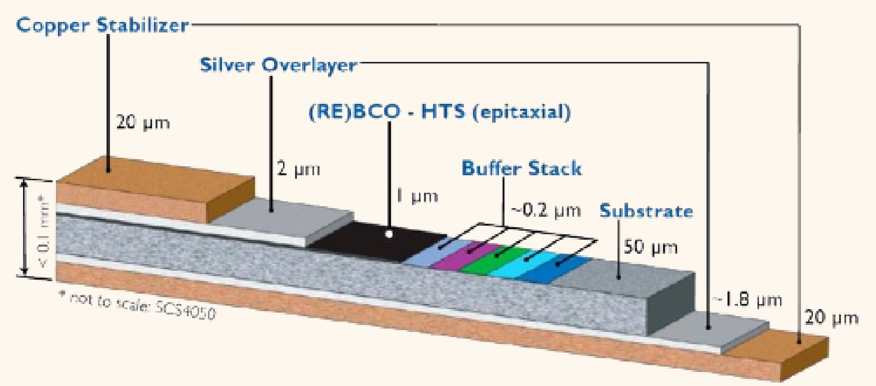
MAGNET Module

•Electromagnetic Model for High Temperature Superconductors (HTS) enable higher magnetic fields and current densities and thereby a reduction of overall sizes and running costs due to lower heat load in the cryogenic system.

•Usual HTS wires composites: ReBCO. **Rare-earth barium copper oxide**

•This superconductors have the potential to carry a few hundreds of amperes in stronger magnetic fields at low temperatures.

•Since 30 to100 kA are needed to power the large magnets u fusion reactors, high current cables with several tens of super conductions wires must be assembled.



A single REBCO tape (*SuperPower 2G HTS Wire*). Several tapes can be assembled following different layouts (Conductor On Round Core, Roebel conductor, stacked tapes) to form cables with high current capability.

MAGNET Module

The H-Formulation of Maxwell's equations

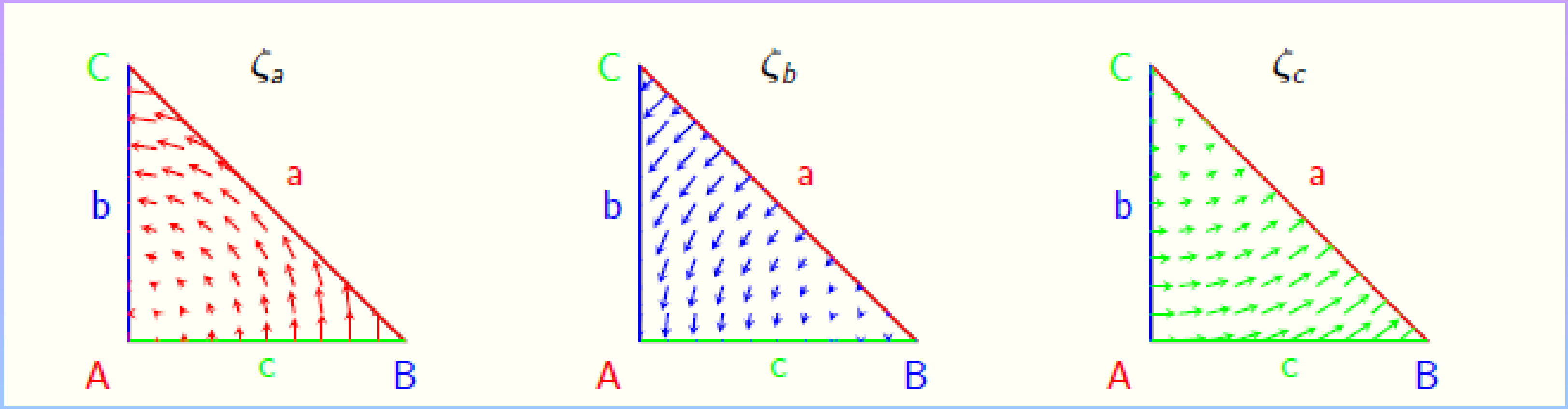
$$
\begin{aligned}
&\partial_t(\mu\mathbf{H}) + \nabla \times (\rho\nabla \times \mathbf{H}) = 0 && \text{in } \Omega \times (0, T],\\
&\mathbf{n} \times \mathbf{H} = \mathbf{g}_D && \text{on } \Gamma_D \times (0, T],\\
&\mathbf{n} \times (\rho\nabla \times \mathbf{H}) = \mathbf{g}_N && \text{on } \Gamma_N \times (0, T],\\
&\mathbf{H}(t = 0, \mathbf{x}) = \mathbf{H}_0(\mathbf{x}), && \text{in } \Omega,
\end{aligned}
$$

H is the magnetic field intensity, μ is the magnetic permeability, ρ is teh electrical resistivity given for a power law, where Ec=1μ V/cm Jc(H) is experimental data

$$
\rho_{HTS} = \frac{E_c}{J_c}\left(\frac{\|\nabla \times \mathbf{H}\|}{J_c}\right)^{n-1}
$$

MAGNET Module

The Edge Finite Element Method (EFEM) is the common approach in the field of numerical modeling for applied superconductivity. Unlike nodal FEM, in edge FEM the degrees of freedom (DoF) are assigned to the mesh edges.



The edge element guaranteed for a field H(x) continuity of tangential components and divergence nule.

MAGNET Module

- Multi physics simulation of HTS devices: Critical current also depends on the temperature and the strain

- Electromagnetic, Thermal and Mechanical problems are coupled!

- Thermal and Hydraulic problems are coupled! Helium dynamics during quench are governed by compressible NS equations.

- Electromagnetic calculations in HTS are very time-consuming due to the highly non-linear behavior of superconductors, even for rather simple problems as the ones showed above.

A first standalone serial prototype has been successfully tested against analytical models

Final Remarks

•IN general, NEUTRO and MAGNET are in development.

• NEUTRO provides a good and simple approximation for particular problems, related to ITER demands. We can obtain a fast tool with more and more physics added in future.

•With the increase in precision and quality of the simulations, the FUSION CASE groups will we need more and more ALYA (more and more HPC simulations). That's mean more and more interaction with the different people of CASE. Both examples shows these necessities.

•A proof of concept was the CFD test, we need to require the expertise of several professional from CASE.

•Maybe, (a suggestion) general ALYA course need to be prepared and impose to the CASE new incorporations in the future.

•Finally: Acknowledgments.

Using ALYA in FUSION simulations

Many Thanks!

CASE-FUSION-BSC