PARCS-SUBCHANFLOW-TRANSURANUS Multiphysics Coupling for high fidelity PWR reactor core simulation: Preliminary Results

Joaquín R. Basualdo[a], Victor Hugo Sánchez-Espinoza[a], Robert Stieglitz[a], Rafael Macián-Juan[b]

[a] Karlsruhe Institute of Technology, Institute of Neutron Physics and Reactor Technology, Herman-vom-Helmholtz-Platz-1, 76344 Eggenstein-Leopoldshafen,
[b] Technische Universität München, Lehrstuhl für Nukleartechnik, Boltzmannstraße 15, 85747 Garching bei München

1. Introduction

Traditionally, reactor core simulators use simplified models to predict the fuel temperature and thermal-hydraulic conditions in the core. To achieve better accuracy detailed models should be used to describe all different physical processes (Multiphysics approach).

Simplified solvers for the fuel temperature don't capture the material behavior under irradiation such as, swelling, cracking, pellet-clad interaction, etc. These phenomena affect properties such as fuel thermal conductivity, the fuel rod gap conductance which has an impact in the calculation of the fuel temperature. It is known that the gap conductance during reactor lifetime, depends strongly on the irradiation and power history as shown for instance in (Bielen 2015). There are only few publications about multiphysics simulations in the area of fuel behavior studies (e.g. Magedanz et al. 2015; Hales et al. 2014) and, even less containing studies of reactor core simulations (Holt et al. 2016; Holt et al. 2014).

In an evolutionary approach, at the Karlsruhe Institute for Technology (KIT), the NRC's neutronics core simulator PARCS (Downar et al. 2012) is being integrated with KIT's sub-channel code SUBCHANFLOW (SCF) (Imke, Sanchez, and Gomez-Torres 2010) and ITU's fuel behavior code TRANSURANUS (TU) (Lassman et al. 1992) into a single code, PARCS-SCF-TU. For the SCF model, each fuel assembly is represented as a single channel and, analogously, a fuel assembly in the TU model is represented as an average fuel rod. One of the objectives of this coupling is to study the impact that high fidelity solvers have on reactor core simulations. Moreover, a main objective of this coupling is the modeling of the RIA transient scenario for high burnup conditions. For this scenario, the fuel properties and fuel temperature modeling are of great importance since current simulations don't account for details of the fuel rod thermos-mechanics and subchannel thermal hydraulics. The need of this kind of calculations is an issue brought up in recent years by the CSNI (Committee on the Safety of Nuclear Installations) Working Group on Fuel Safety (OECD/NEA 2010) and a topic under discussion for regulatory authorities in many countries in Europe.

In this paper, results for the OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark core are used to compare PARCS-SCF and PARCS-SCF-TU with the PARCS standalone solution. Preliminary results are given, which show the impact of modeling the fuel temperature with a fuel behavior code considering burnup.

2. Methodology

The neutronics core simulator PARCS, the sub-channel solver SCF and the fuel behavior solver TU have been merged together into a single executable PARCS-SCF-TU. In this Multiphysics coupling, SCF replaces the simple thermal hydraulic solver of PARCS and TU replaces the fuel rod solver of SCF to compute the fuel and cladding temperature distributions.

The involved codes are written in FORTRAN using different programming styles and FORTRAN versions. The internal coupling has been developed in Microsoft Visual Studio following its convention for solutions and projects management. To maintain an organized coding and avoiding undesired callings to duplicate subroutines or variable names a modularized approach is used. The original codes are *encapsulated* in *projects* and they only interact with each other via a main project. Only in special circumstances this rule isn't followed. New coding necessary for the communication of the codes is modularized in a *project* dedicated to the coupling. All modifications to the original source code were implemented with pre-compiler directives. This allows the user to compile either only PARCS, or only PARCS-SCF or PARCS-SCF-TU depending on the used keywords.

In this coupling approach, the activation of the different solvers e.g. SCF's TH model or TU's fuel solver can be activated by the analyst independently. If SCF is activated, the options belonging to SCF can be used for the simulation. If the TU solver is invoked, then the SCF solver must be also used. In the reactor core model for PARCS-SCF-TU, each fuel assembly is represented by one neutronic node in PARCS, by one average thermal hydraulic channel in SCF and by one average fuel rod in TU. The three codes share the same axial discretization. The original PARCS input deck has been extended to control the coupled simulation and the mapping between the three different computational domains.

PARCS and SCF are coupled for steady state and transient simulations, whereas TU is coupled to PARCS-SCF for steady state simulations and the transient coupling is under development. The coupling was implemented in such a way that the original inputs of each code can be used with minimal or no modifications. Only the PARCS input includes new key commands to indicate that a coupled simulation will be performed, to choose the parameters for the coupling and to define information about the mapping.

2.1 Coupling description

A *loose,* nodal level coupling using the Operator-Splitting (OS) method (Faragó 2008) was implemented. The operator split method has the advantage of allowing the use of legacy codes with minor modifications to the original source. This is a valuable point since the validation of individual code requires big effort, making the reuse of validated tools a common practice in the nuclear field.

The PARCS-SCF-TU's iteration scheme for the steady state coupling is represented in Figure 1 and the iteration process is described hereafter:

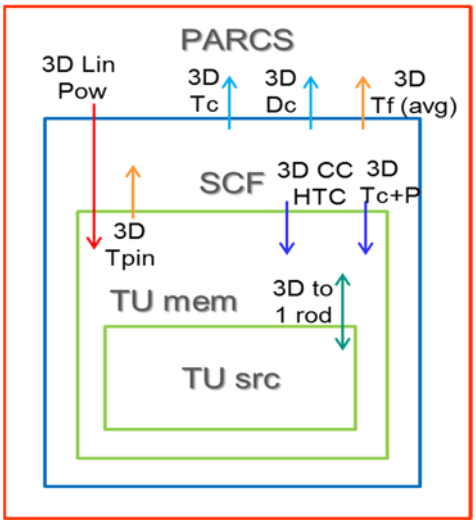


Figure 1. PARCS-SCF-TU coupling scheme for steady state simulations.

Initialization:

1) PARCS assumes flat TH conditions, and predicts 3D power distribution → pass information to TU.
2) SCF assumes initial flat power distribution and compute TH distribution → pass TH conditions to TU.
3) TU compute fuel temperature distribution (fuel and clad) for all fuel assemblies → pass information to SCF.
4) SCF computes TH conditions with given clad temperature as B.C. → pass TH information to TU.
5) Iteration loop consisting of step 3 ad 4 until convergence of fuel temperature and TH conditions is achieved.
6) SCF/TU Converges → pass fuel and coolant temperature and coolant density to PARCS.

Then, the process continues with the another iteration loop:

1) PARCS computes power with updated TH conditions: → pass power to TU.
2) TU Computes fuel assemblies → pass fuel temperature fields to SCF.
7) SCF computes TH conditions → pass information to TU.
8) Iteration loop from step 2) until convergence → when convergence criteria achieved, information is passed to PARCS.

Finally, the iterative process iterates from 1) until convergence criteria are met.

The coupling scheme for PARC-SCF transient calculation is shown in Figure 2. An explicit coupling is used in these calculations and its convergence is achieved with small time steps (Mylonakis et al. 2014).

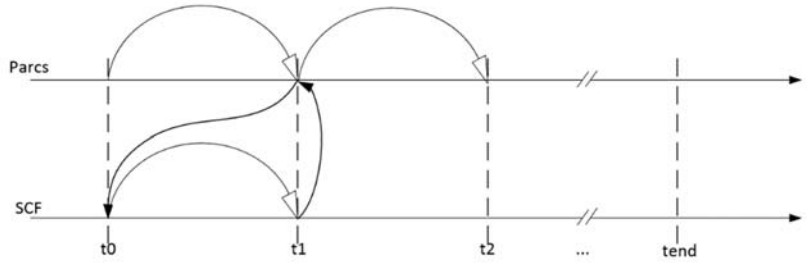


Figure 2. Time flow scheme for PARCS-SCF coupling

The transient coupling has been implemented for PARCS with SCF. The coupling with TU is under development.

3. Verification of the coupled tool

PARCS-SCF-TU is compiled into one single executable and certain options in PARCS input are enabled or disabled to run either PARCS standalone, PARCS-SCF or PARCS-SCF-TU.

During the verification, several small tests cases were performed in a 3 by 3 fuel assemblies PWR minicore for steady state (PARCS-SCF and PARCS-SCF-TU) and transient (PARCS-SCF) situations observing good agreement between the codes. For the sake of brevity only results for a more complex reactor will be presented here. The OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark (Kozlowski, T and Downar 2003) was used for verification purposes. The cross sections used for the simulation are directly taken from the benchmark. Input models for SCF, PARCS and TU are derived from the benchmark specifications.

The purpose is to test the correctness of the implementation by comparing the results obtained with PARCS standalone, PARCS-SCF and PARCS-SCF-TU. The SCF model is as similar as possible to the PARCS internal thermal-hydraulics. The model of TU corresponds to a fresh UO_2 fuel pin with the geometry derived from the benchmark specifications, being the purpose of this to match the simplified model of PARCS' internal solver.

3.1 OECD/NEA and U.S. NRC PWR MOX/UO2 Core Transient Benchmark description

The benchmark PWR reactor core consist of 193 fuel assemblies arranged in a Cartesian geometry. It's composed by UO2 and MOX fuel types with different enrichments, and seven different burnup points. The necessary specifications to generate the input models are described in the benchmark (Kozlowski, T and Downar 2003).

In the benchmark, burnup is considered in the cross-section generation but not in the material properties of the fuel.

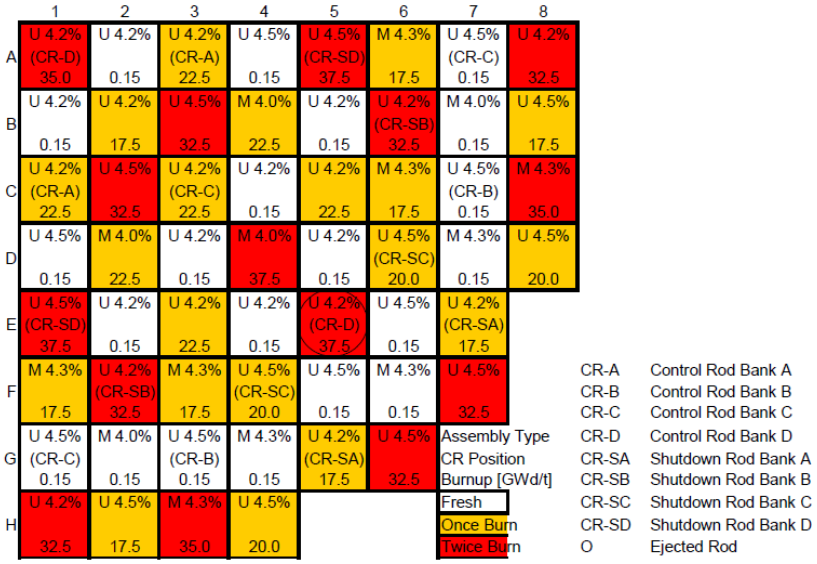


Figure 3. OECD/NEA PWR quarter-core loading pattern.

3.2 PARCS-SCF vs PARCS Standalone

The steady state and transient conditions of PARCS and SCF were tested for different configurations and exercises proposed in the benchmark, showing a good agreement in all cases. Results for the most complex cases of the OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark will be shown next.

3.2.1 Steady State Results

Table 1 shows results for the critical boron search calculation at HFP conditions with all control rods (CR) extracted with PARCS-SCF and PARCS with its simple internal thermal hydraulics model.

Table 1. Results for HFP conditions with al CR out.

	PARCS-SCF	PARCS-internal TH
Number of outer iterations	28	28
Time (sec)	124.1	18.8
Critical Boron concentration (ppm)	1693	1681
Local Tcenterline_max (°C)	1406	1560
Tcool_outlet (°C)	325.81	325.84
Tcool_inlet (°C)	286.85	

A simplified input model of SCF was done to match the PARCS internal thermal-hydraulics to check the correct implementation of SCF in the coupling. When comparing local differences for the power distribution, the maximum local difference (node to node comparison) is < 0.4% and the average power difference is < 0.04%.

3.2.2 Transient Simulation

The benchmark transient consists in the ejection of the CR with the highest worth (rod E5) in 0.1 seconds stating from HZP conditions. Figure 4 shows results for the simulation with PARCS-SCF and comparison with the rest of the benchmark participants.

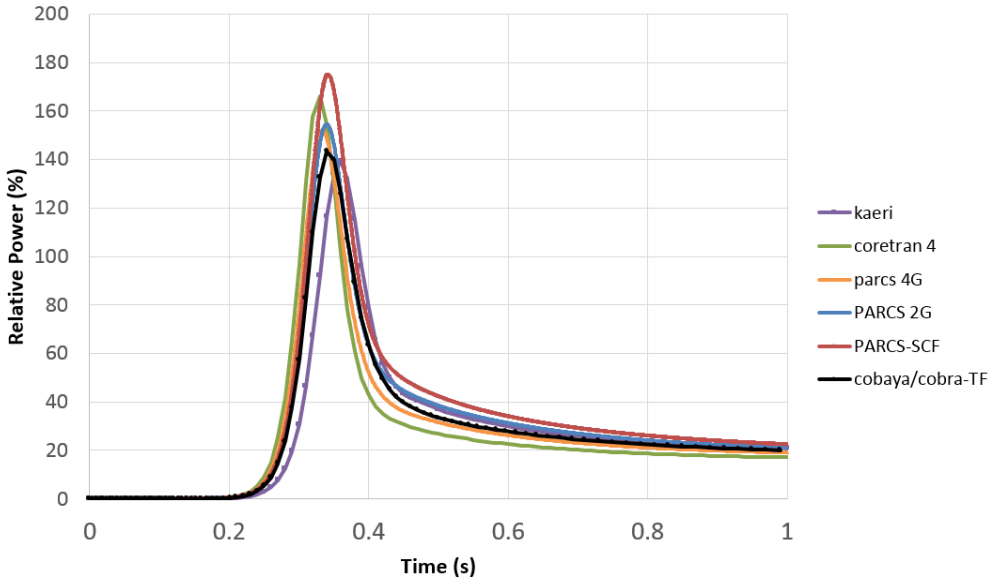
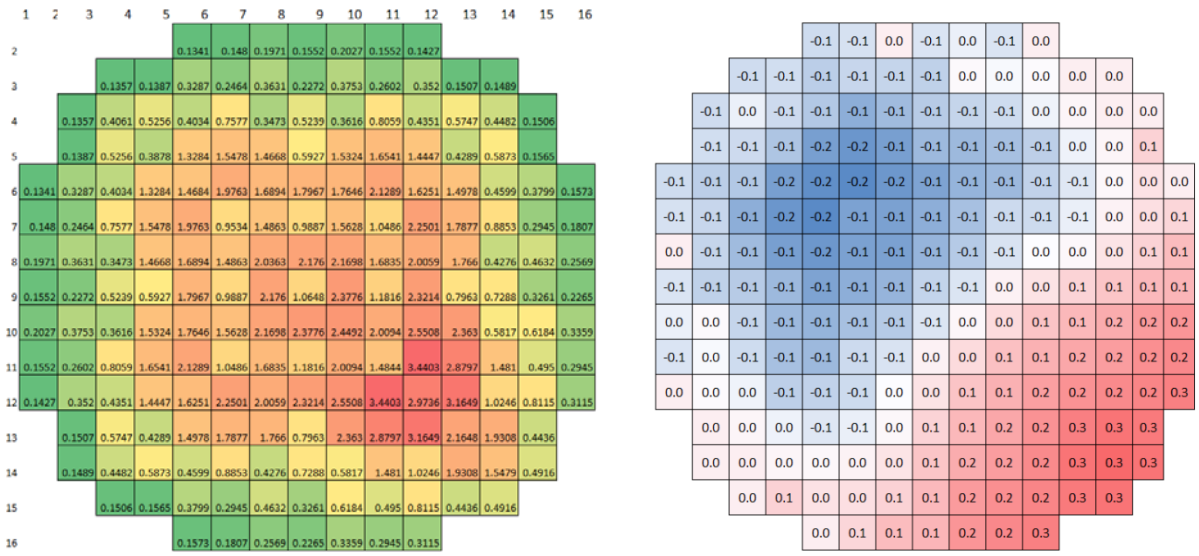


Figure 4. Power evolution for the OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark computed with PARCS-SCF and compared against other benchmark participants.



a) PARCS-SCF axially integrated power at power peak time.

b) PARCS-SCF vs PARCS standalone relative power difference at power peak time.

Figure 5. UO2/MOX PWR Benchmark axially integrated power distribution - Comparison of PARCS-SCF vs PARCS standalone solutions.

Figure 4 shows the total power evolution, the peak time width agrees with the PARCS standalone result. PARCS-SCF predicts a higher peak. Figure 5 shows the

axially integrated power distribution at peak time and a comparison of PARCS-SCF against PARCS standalone solution, the relative differences are < 0.3% in all cases.

3.3 PARCS-SCF-TU Results

To test the implementation of PARCS-SCF-TU the OEDC/NEA benchmark core was used. The standalone case at HFP conditions is presented. For each fuel assembly, the average fuel rod modeled with TU corresponds to a fresh fuel, to be consistent with the models of PARCS standalone and PARCS-SCF which use material properties corresponding to fresh UO2 fuel. Comparisons against PARCS-SCF and PARCS standalone solver are presented in

Table 2 and Table 3.

Table 2. Results for the boron concentration and relative and absolute differences in the power distribution.

	Critical Boron conc.	Runtime (s)	Power		
			Max. diff (%)	Avg. diff pow	Abs. avg. diff
PARCS standalone	1681.11	19.0	1.16	0.09	0.49
PARCS-SCF	1693.82	92.5	0.73	-0.05	0.28
PARCS-SCF-TU	1679.21	7206.2	Ref.	Ref.	Ref.

Table 3. Centerline and Fuel average temperature comparisons.

	Centerline Temperature (ºC)			Fuel avg. Temperature (ºC)		
	Max diff (%)	Avg. diff	Abs. avg. diff	Max diff (%)	Avg. diff	Abs. avg. diff
PARCS standalone	10.0	6.3	6.4	4.9	1.2	2.6
PARCS-SCF	6.8	3.4	3.4	6.8	4.9	4.9
PARCS-SCF-TU	Ref.	Ref.	Ref.	Ref.	Ref	Ref.

The most significant comparison is the one against PARCS-SCF since the same TH solver is used and the differences come only from the different fuel temperature solver. Differences of less than 7% are found for the centerline temperature, with an average difference of 3.4%. For the average fuel temperature, the maximum difference is 6.8% with an average of 4.9%. The temperatures predicted by TU are higher.

The calls to TU's solver increase greatly the computational time. There are 2 main reasons for this, the first is that TU's solver must read TU's input every time the solver is called which generates a big overhead for TU's calculations. The second is that TU's solver is more time consuming than the simplified solver of SCF for the fuel temperature since it describes the thermo-mechanics including fission gas release in a more accurate manner than SCF. TU solvers one FA at a time, so a parallel implementation for TU is being considered to speed up the calculations.

3.3.1 PARCS-SCF-TU: Burnup consideration in fuel properties

One of the advantages of having coupled TU with PARCS-SCF is the possibility to simulate the burnup dependent fuel material properties and the behavior of irradiated fuel. In the benchmark PWR core, the fuels have 7 defined burnup points. These burnups are considered in the cross-section generation process, but they are not considered in the material properties (such as the gap conductance) when computing the radial fuel temperature (in an average pin).

A steady state calculation for the benchmark PWR core was performed with PARCS-SCF-TU for 2 cases: The first case considering fresh uranium in the TU model, the second case considering the corresponding burnup condition of each fuel in the TU model. The rest of the parameters in the model of PARCS, SCF and TU remain the same.

Figure 6 shows a comparison of the fuel centerline temperature for calculations with PARCS-SCF-TU for three different fuels with different burnup. As it is expected the difference between both solutions (with and without BU considerations in TU's input model) grow higher as the burnup goes up.

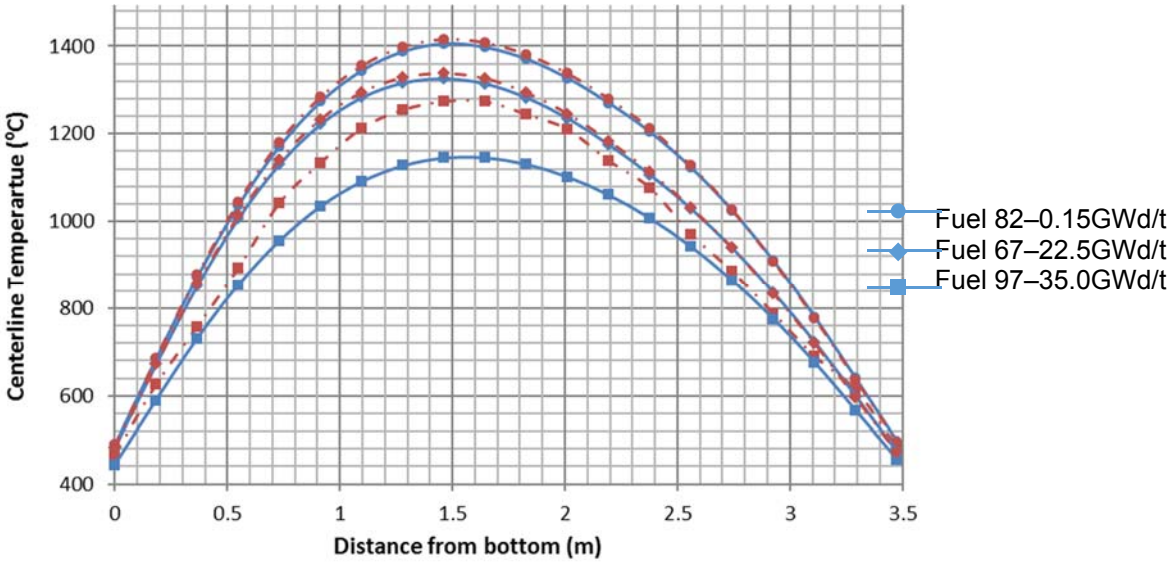


Figure 6. Centerline fuel temperature. Results considering No Burnup (blue) vs considering Burnup (red) at different burnup points.

4. Discussion

In the comparison for the PARCS-SCF-TU calculation with burnup considerations, it is observed that there is a considerable influence of the burnup in the fuel temperature distribution. Figure shows that the higher the burnup, the higher the differences in the fuel temperature when comparing to cases w/o burnup. Differences for the fuel centerline temperature rising up to 130 ºC when comparing results considering the burnup history of the fuels or not doing so in TU input. These differences show that there is a considerably impact when having taken into account fuel BU history in material properties and suggest that further analyses should be done in this direction.

A good agreement has been found in the steady state and transient comparisons of PARCS-SCF against PARCS standalone solution showing a correct implementation of the coupling.

The comparison of the PARCS-SCF results against the ones of the benchmark participants shows a good agreement.

Regarding the comparison of PARCS-SCF against PARCS standalone for the transient simulation a small over peak can be observed in PARCS-SCF which can be explained because of the different models for fuel rod properties. Whereas the peak time and the width of the peak are the same as expected since (as explained by the adiabatic Nordheim-Fuchs model) they depend on the inserted reactivity and the precursors constant which are the same in both cases. PARCS-SCF-TU results have been compared against PARCS-SCF and PARCS standalone using fresh fuel condition in TU model. Local comparisons for the fuel average, and fuel centerline temperature, show a good agreement between the solutions confirming the correct implementation of the coupling approach.

Finally, it should be noted that the calculation time of PARCS-SCF-TU increased considerably since the TU-solver must be called as many time as the number of fuel assemblies during each SCF SOR-iteration. It means 193 calls of TU-solver times approximately 10-15 SOR iterations per PARCS inner iterations (~30). So far, no optimization of the numerical methods to accelerate convergence have been implemented and implementations like the predictor-corrector method is in the plans for future improvements.

5. Conclusions and Outlook

The consideration of burnup history in fuel properties in PARCS-SCF-TU has shown significant differences in fuel temperature prediction as expected. The code-to-code comparison demonstrated the correct implementation of the coupling.

The implementation of a predictor-corrector method to accelerate the convergence on the fuel temperature, along with a parallel implementation are planned to be implemented for the PARCS-SCF-TU code to speed up the calculation. The development of PARCS-SCF-TU for transient simulations is underway and it will pave the way for the analysis of RIA-scenarios and high burnup fuels.

6. Acknowledgments

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