REVISITING TEMPORAL ACCURACY IN NEUTRONICS/T-H CODE COUPLING USING THE NURESIM LWR SIMULATION PLATFORM

O. Zerkak¹, I. Gajev², A. Manera¹, T. Kozlowski², A. Gommlich³, S. Zimmer⁴, S. Kliem³, N. Crouzet⁴ and M. A. Zimmermann¹

¹ Paul Scherrer Institut, Villigen PSI, Switzerland ² KTH Royal Institute of Technology, Stockholm, Sweden ³ Helmholtz-Zentrum Dresden-Rossendorf, Germany ⁴ Commissariat à l'Energie Atomique, Saclay, France

omar.zerkak@psi.ch, gajev@safety.sci.kth.se, annalisa.manera@psi.ch, tomasz@safety.sci.kth.se, a.gommlich@hzdr.de, stephanie.zimmer@cea.fr, s.kliem@hzdr.de, nicolas.crouzet@cea.fr, martin.zimmermann@psi.ch

Abstract

The first part of this paper reviews the different temporal coupling methodologies that are currently employed for the transient simulation of LWR cores. The second part shows preliminary results from the implementation of some suggested coupling improvements, including high-order corrections to the exchanged coupling fields and a dynamic time step control technique, for the simulation of an exemplary reactivity insertion transient analysed using the European NURESIM LWR simulation platform.

Keywords: Multi-physics, code coupling, temporal accuracy, thermal-hydraulics, neutron kinetics.

Introduction

The steady-state and transient analysis of a LWR core often involves the dynamic coupling of separated simulation codes, each one devoted to the solving of one of the coupled physics. Most of the existing coupled code systems apply an Operator Splitting coupling technique, where one (lead) code is iterated first to provide boundary or initial conditions to the next code and so on until the last code of the simulation system completes one overall temporal step. The accuracy of such coupling is driven by the code that uses the least accurate numerical scheme and by the accuracy in the data exchange between the codes. As a consequence, traditional OS techniques result into 1st order accuracy at most. Moreover, the non-implicit nature of this step-by-step approach imposes the use of small times steps to ensure the stability of the solution.

The objective of this paper is to identify areas for improvements of the standard Operator Splitting coupling schemes for LWR core transient analysis, but also to discuss potentially more accurate semi-implicit (iterative) schemes based on Newton methods. Moreover, first LWR transient applications of the coupling improvements made in the context of the NURISP European Project [1] are presented to illustrate the gains that can be expected in terms of accuracy versus computational efforts.

1. Improvements to code coupling techniques for LWR core simulation

Before discussing code coupling specifics, it is necessary to recall that in the special case of the simulation of LWR cores, the thermal-hydraulics (T-H) component of the problem is usually described using a spatially and time averaged two-phase model for the non-stationary mass, momentum and energy transport equations, which are neither linear nor (in general) well-posed. The ill-posedness is due to the non-hyperbolicity of the homogenized two-fluid model which can result in unphysical instabilities and thus makes the convergence properties more difficult to characterize. Among the different views that have been taken to tackle this problem [2], the most pragmatic one is to consider that non-hyperbolicity is just a natural result of the spatial homogenization procedure (loss of structural information, lack of small scale dissipative phenomena) and, since numerical diffusion introduces regularization [3], the issue of stability can be overcome by appropriate selection of the spatial discretization (numerical regularization). This is the view followed here, and all the discussions will be restricted to the case where appropriate spatial discretization is assumed.

1.1 Operator Splitting coupling methods

The Operator Splitting (OS) methods follow the "divide-and-conquer" strategy, in which the set of PDEs of the overall problem is decomposed into simpler sub-problems that can be discretized independently of each other and thus treated separately. After one time step integration on a sub-problem, the partial solution is then used as a new estimate for the boundary conditions and derivatives of the next sub-problem. OS methods can be applied even within one single set of PDEs, where the spatial derivative operator is decomposed in groups of operators that represent different individual physical phenomena. For instance, one can consider the time-dependent 1-D convection-diffusion problem shown in Figure 1.

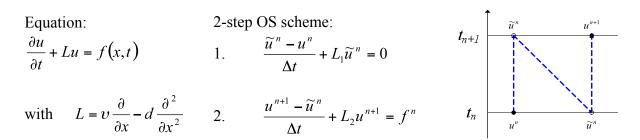


Figure 1 Operator Splitting scheme for a 1-D convection-diffusion equation.

In this case, one simple OS method would consist of decomposing the operator L into the sum of two operators $L_1 = v\partial/\partial x$ (convection term) and $L_2 = -d\partial^2/\partial x^2$ (diffusion term), and divide the discretized problem into two sequentially solved sub-problems.

Now in the context of the steady-state and transient simulation of LWR, the multi-physics problem involves the temporal coupling of separated codes. In this case, the OS method is applied to the extent that one code would correspond to one sub-problem (e.g. PARCS/RELAP5 [4], CRONOS2/FLICA4 [5], SIMULA/COBRA and SIMULA/RELAP5 [6], SIMULATE-3K/TRACE [7]). The main advantage of this approach is that only limited modifications to the individual codes are needed to implement the coupling scheme. On the other hand, the resulting order of temporal accuracy of the scheme cannot be higher than one, mainly because of the 1st order transfer of non-linearities resulting from the explicit exchange of the coupling terms. This can bring about

numerical instability, and the convergence of the solution requires the use of relatively small time steps, resulting in a large CPU time use.

1.1.1 <u>Leapfrogging time grids</u>

These methods consist of advancing the coupled sub-problems (or physics) in a leapfrog manner on different staggered time grids, as shown in the example in Figure 2. Taking a simple example of a set of two coupled PDEs $\{u' = f(u,v); v' = g(u,v)\}$, a θ -scheme employed on these time grids for u and v would yield the set of coupled equations shown on the left part of the figure. Thus, selecting $\theta_1 = \theta_2 = 1/2$, the resulting coupled scheme would mimic the Crank-Nicolson scheme, which is 2^{nd} order accurate.

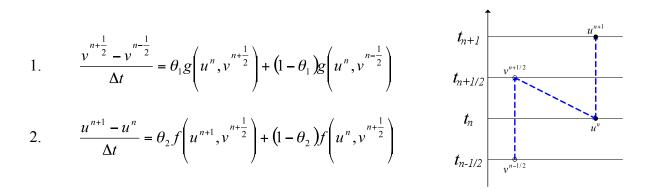


Figure 2 Operator splitting scheme using leapfrogging time grids

A similar method was used for a coupled N-K/T-H LWR transient problem in [6]. In this case, the 3-D power and thermal-hydraulics fields were computed on leapfrogging time grids using the codes SIMULA and RELAP5, respectively. Moreover, to provide the scheme with additional stability, the exchanged T-H fields were extrapolated in time over one N-K half-time step to achieve approximately 1st-order implicit treatment of the feedback variables in the N-K calculation. Unfortunately, no convergence study was provided so that it was not possible to know the improvement resulting from this technique.

1.1.2 <u>Higher-order treatment of the coupled variables</u>

In order to correct for the inaccurate transfer of non-linearities, one possibility is to use higher order estimates of the coupled non-linear terms. This approach was described in [8] where it was shown that two codes employing 2^{nd} order accurate temporal schemes can have their temporal coupling degraded to 1^{st} order accuracy if a standard OS method is employed. To correct for this problem higher-order corrections to the coupled variables were suggested. Thus, considering an exchanged variable u, instead of transferring u^{n-1} to the coupled code for the execution of the time step n, one option is to devise a higher-order linearization \tilde{u}^n that will be used as a surrogate for the implicit non-linear coupled terms, for example:

$$\widetilde{u}^{n} = u^{n-1} + \left(u^{n-1} - u^{n-2}\right) + O(\Delta t^{2}) \tag{1}$$

This brings about a more accurate estimate for u^n and thus helps restore the order of accuracy that was lost when transferring u^{n-1} . Note that this approximation is still explicit and the stability of the coupled scheme would still be conditional.

1.2 Semi-implicit coupling methods

1.2.1 Fixed-Point-Iterations

Another way to solve for the loss of non-linearity in the data exchange procedure is to introduce an additional Fixed Point Iteration (FPI) loop in the scheme. The non-linearities would be then implicitly solved, within a given tolerance specified by the user. Additional stability would be also expected, but at the cost of additional computation effort due to the iteration loop. One solution to reduce the number of iterations is to use acceleration techniques such as the Aitken Δ^2 technique [8] that uses information from the two previous FPI iterations to derive a more accurate estimate of the next *i*-th iteration of the FPI:

$$\widetilde{u}^{n,i} = u^{n,i-2} - \frac{\left(\Delta u^{n,i-2}\right)^{n}}{\Delta^{2} u^{n,i-2}}$$
 (2.1) with
$$\begin{cases} \Delta u^{n,i-2} = u^{n,i-1} - u^{n,i-2} \\ \Delta^{2} u^{n,i-2} = u^{n,i} - 2u^{n,i-1} + u^{n,i-2} \end{cases}$$
 (2.2)

This technique can be applied after the first two iterations of the fixed-point problem and, together with an OS technique, can restore the accuracy order of the coupled scheme with very little modifications to the coupled codes. These different coupling improvements were applied to a reduced-order model of a PWR reactor core (1-D time-dependent T-H model coupled with time-dependent point kinetics or 1-D neutron kinetics models, alternatively) [8]. The results show a clear benefit of these methods in terms of accuracy improvement and it would be worth evaluating the merits of these techniques when using higher-resolution codes and for larger LWR problems.

1.2.2 Newton methods

Different variants of coupling techniques based on the Newton method do exist. The Jacobian-Free Newton-Krylov methods (JFNK) are based on a global approach, where a Newton method is applied to a residual equation res(u) = 0 of the full set of multi-physic PDEs, and in which each Newton step is solved iteratively using a linear decomposition on a Krylov vector basis. An overview of this group of methods can be found in [9], where the fundamentals of the Newton method and Krylov method are presented. One of the main advantages of the JFNK methods is that they do not require computing the Jacobian of the overall system. But a proper pre-conditioning and an optimal set of parameters (tolerances, directional derivative parameters) are required to ensure robust and rapid convergence.

In the context of LWR core analysis, a mono-block JFNK method with physics based preconditioning was proposed for the solution of the 1-D six-equation two-phase flow model coupled to a 2-D nonlinear heat conduction model [10]. Called implicitly balanced solution, it consists of nesting a fast but inaccurate solution method (Operator Split Semi-Implicit, or OSSI) as a preconditioner of a more accurate JFNK method in order to provide a solution method which is both fast and accurate. The system used to assess the method was a simplified version of a nuclear reactor. In [11], the closure models determining the interfacial area, the liquid and vapor wall areas, the interfacial drag and heat transfer coefficients were all made functions of the void fraction. This

increased the level of non-linearity of the problem and one important result of these studies was to show how the JFNK methods could help increase the accuracy of the solution but also that the quality of the non-linear two-phase flow closure relations could affect the performance of the JFNK methods.

Another group of JFNK methods, referred to as Approximate Block Newton (ABN) methods, is based on a less intrusive approach seeking modularity and simpler implementation, where the different solvers of the coupling can be preserved as black-boxes, and thus offers the advantage to readily inherit from the development and the validation work made on existing simulation codes. The base idea is to derive a Newton method based not on the original equation set, but on the solvers of each sub-problem. The main quality of the ABN methods is to break the large system into smaller blocks, which results in inverting a matrix that is smaller than in a mono-block JFNK method. Different variants of this approach have been developed, and one can get an excellent overview in [12].

2. First applications using the NURESIM platform

2.1 The NURESIM platform

The NURESIM reactor simulation platform has been developed as a part of the eponym Integrated European Union Project that was completed in 2008. Besides promoting a significant research and development program on advanced high-fidelity methods in LWR core physics and core thermal-hydraulics, the NURESIM project was also aiming at the integration of existing and well established scientific codes on one common Multi-physics software infrastructure based on the SALOME software [13]. The first version of the platform was released in 2008 (NURESIM V1) and is now further developed as part of the Multi-physics subproject of the current NURISP European Union Project. On this platform, the solvers are based on pre-existing simulation codes that can be embedded as individual components and can be exchanging information through a limited set of interfaces and be operated using generic functionalities.

The FLICA4 v1.10.13 two-phase flow sub-channel code is integrated in the platform, as well as several core physics simulation codes including CRONOS v2.9, DYN3D v3.3 and COBAYA3. At the current level of development, these three later codes can be dynamically coupled to FLICA4 in a "black-box" mode, with the possibility of using different and non-congruent meshing schemes thanks to a three-dimensional spatial interpolation library (INTERP2.5D) [14]. As part of these developments, several stationary and transient test cases corresponding to different Light Water Reactor types (PWR, BWR and VVER), and at different scales of simulation (from pin-level/sub-channel level to fuel assembly/fuel channel level for full core simulation) were analyzed to test and validate the different tools that are developed as part of the NURISP project (see first NURESIM applications using SALOME in [15], [16]).

2.2 Rod ejection accident for a PWR mini-core

A PWR mini-core test case was selected to assess the developments discussed in the section 1.1. The mini-core is a hypothetical core [17] consisting of a square array of 9 typical 17x17 fuel assemblies, with a nominal power density similar to a generic PWR (~11 MW thermal power per

fuel assembly). The model was derived from the specifications of the OECD/NEA and U.S. NRC PWR MOX/UO2 benchmark [18].

The transient scenario is a rod ejection accident while the mini-core is stable at 10 % of its nominal power. As a result of the fast and large reactivity insertion, very rapid variations of power and fuel temperatures take place during this transient, which is perfectly suited for the purpose of evaluating the accuracy vs. CPU merits of the developed temporal coupling schemes. Moreover, the small size of the problem allows for the computation of a solution using a very small time-step that can be used as a reasonable surrogate for the exact reference solution to evaluate the convergence errors.

2.2.1 Transient evolution

The mini-core steady-state and rod ejection transient were simulated using DYN3D coupled with FLICA4 in SALOME. The time evolutions of the core power and the T-H variables obtained using different time-steps are shown in Figure 3.

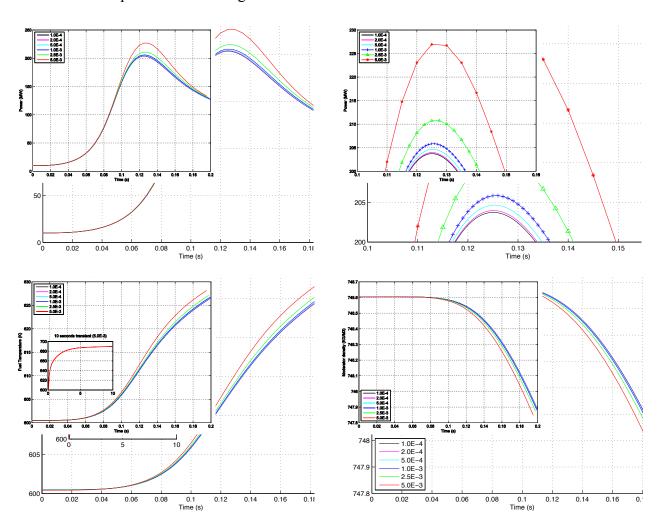


Figure 3 Maximum power and fuel temperatures and minimum moderator density evolutions.

The control rods cluster is ejected at 0 ms and reaches the top of the core active region after 100 ms. As a result of the reactivity insertion (420 pcm) the core power increases rapidly and heats up the fuel which in turn introduces negative reactivity through the Doppler temperature effect. The resulting power peak is reached after 125 ms and the power begins to decrease. One can see that the

moderator density is also affected by the increased heat generation but to a much lesser extent than the fuel temperature, which will asymptotically increase up to the stationary temperature commensurate with the new equilibrium power level (as pointed up in the bottom left part of Figure 3, where the fuel temperature evolution from an extended 10 s long simulation is shown). The most important coupling fields for this transient are the power density and the fuel temperature distribution. The sensitivity study to the time-stepping strategy will therefore be focused on these variables.

2.2.2 <u>Time-stepping strategies</u>

The simulation codes DYN3D and FLICA4 are implemented in SALOME in a "black-box" mode, which means that they can execute one time step when requested by the calculation scheme and provide a new set of results (coupling fields) that is made available to the other codes of the coupling through the Memory Data Exchange Model (MEDMEM) of the platform. Within this coupling framework few strategies could be investigated:

- Fully explicit coupling
- Staggered and leapfrogging time-stepping
- Time-extrapolation of the coupling fields

Figure 4 illustrates some variants of these strategies. The first example on the left corresponds to a fully explicit coupling scheme between the physics in the sense that each code executes temporal advancement of the solution using coupling information from the current point in time exclusively. The second example is the traditional OS scheme where the physics are advanced one after the other following a staggered scheme. Here, the N-K solution leads the T-H solution, therefore the N-K code is provided with explicit coupling fields, while the lagging T-H employs power densities that are predicted at the end of the time-step. This brings about some limited implicitness into the T-H component of the scheme.

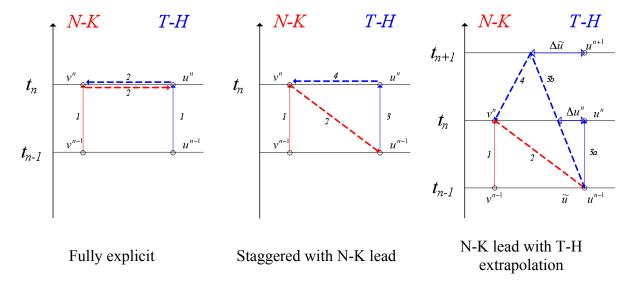


Figure 4 Explicit and semi-implicit coupling strategies

The scheme on the right part of Figure 4 supplements the staggered scheme with a time extrapolation of the lagged coupling fields (here the T-H). The idea behind the time-extrapolation

technique is to provide additional implicitness to the solution of the leading code (there the N-K) by predicting the T-H coupling fields at the next temporal point from their values at the current and previous temporal points. In this work, the following extrapolation scheme was used:

$$\widetilde{u}^{n+1} = u^n + \Delta \widetilde{u} = u^n + \gamma \left(\frac{t_{n+1} - t_n}{t_n - t_{n-1}} \right) \left(u^n - u^{n-1} \right)$$
(3)

The scheme uses a coefficient γ to control the level of extrapolation from 0 (no extrapolation) to 1 (coupling field extrapolated up to the end of the time step). Moreover, by including the ratio of the current time-step to the previous one, the extrapolation accommodates the use of variable time-steps, which is necessary for time-step optimization techniques. Also, as discussed in [8], this type of extrapolation should allow correcting for the loss of non-linearity information inherent to the traditional OS coupling techniques.

The different time-stepping schemes were implemented in the coupling procedure of SALOME and a sensitivity study to the time-step size was executed for each scheme. The accuracy in the power and fuel temperature peaks predictions are shown in Figure 5 (since the fuel temperature is not to reach any extremum for this scenario, the maximum value was taken at the end of the transient, i.e. at t = 200 ms).

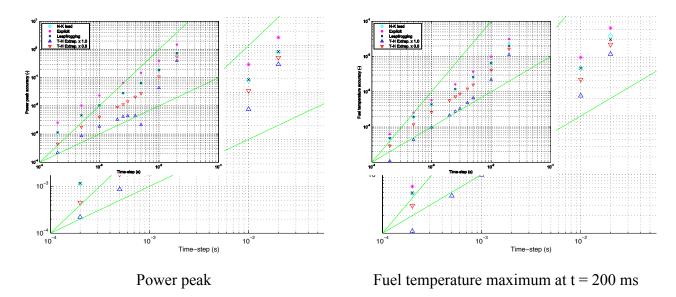


Figure 5 Simulation accuracy.

The accuracy shown for each coupling scheme in the figure corresponds to the relative error compared to the reference solution obtained with the minimum time-step of 0.1 ms. As expected the fully explicit method, where both physics use coupling information from the current time point, leads to the least accurate N-K and T-H solutions. Then, one can see how the staggering and the leapfrogging of the scheme with leading N-K slightly increase the accuracy. When supplemented with a time extrapolation of the lagged T-H solution, the N-K lead scheme accuracy is more substantially improved. For time-steps smaller than 3 ms the power peak accuracy can be increased by a factor 10 between the explicit coupling scheme and the most accurate N-K lead scheme with full T-H interpolation.

One can also see how the extrapolation coefficient γ affects the accuracy of the coupling scheme. For y = 1, the power accuracy curve shows a slight oddity for time-steps between 3 ms and 10 ms. This marks the transition of the convergence of the solution from positive error to negative error. This is shown in Figure 6, which zooms on the power evolutions using different time-steps for $\gamma =$ 0.5 and $\gamma = 1$, respectively. On the left part of the figure, for $\gamma = 0.5$, the convergence proceeds downward to the reference power peak as a function of the time-step refinement, similarly to all other coupling schemes that were tested in this study. But for y = 1, the power peak is underestimated for $\Delta t < 5$ ms, and the asymptotic convergence proceeds then upward to the reference solution. The T-H extrapolation within one time-step somehow under-predicts the fuel temperature increase and hence the Doppler feedback during the initial rise of the temperatures and power, since a linear extrapolation cannot match an exponential evolution. But when the power and temperature evolution slows down around the time of power maximum, the opposite effect is obtained and the Doppler feedback within one time-step is over-predicted by the linear extrapolation. For the larger time-steps, the former effect is more important but for sufficiently small time-step, the latter becomes dominant. Nevertheless, in both cases the accuracy is significantly improved by the extrapolation technique.

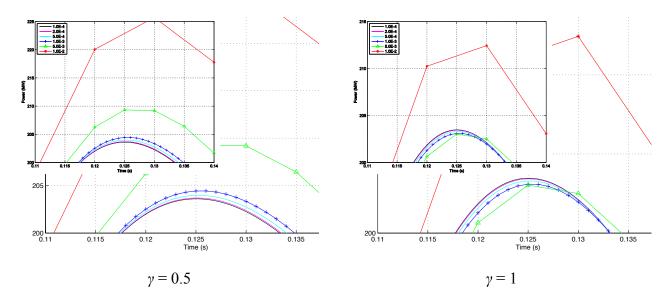


Figure 6 Core power evolutions using the NK-Lead scheme with T-H extrapolation.

Figure 5 also hints at an interesting result on the order of accuracy of the different coupling schemes (the two solid green lines show the slopes corresponding to 1^{st} and 2^{nd} order accuracies). Looking at the slopes of the curves, one can see that for all the coupling schemes the asymptotical trend is close to 1^{st} order accuracy. This result is consistent with the temporal accuracy that can be expected from the two codes employed for this study. In DYN3D, the two-group neutron nodal diffusion equations are integrated using an implicit finite difference temporal scheme together with an exponential transformation of the flux [20], which is represented in each node i by:

$$\Phi_g^i(r,t) = \exp\left[\Omega^{i,k}(t-t'+\Delta t)\right]\Phi_g^{ii}(r,t') \qquad \text{with } t-\Delta t \le t' \le t$$
(4)

The flux at the beginning of a time-step is updated with the value of the slowly varying component of the flux (Φ') obtained from the previous temporal integration, and $\Omega^{i,k}$ is updated after each iteration k of the iterative solution method from the logarithmic variation of the node-averaged

The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14 Toronto, Ontario, Canada, September 25-30, 2011

fluxes between the beginning and the end of the time step. The implicit (Backward Euler) temporal difference scheme adopted in DYN3D reads:

$$\frac{d\Phi_{g}^{i}(r,t)}{dt} \approx \frac{1}{\Delta t} \left[\left(1 + \Omega^{i} \Delta t \right) \Phi_{g}^{i}(r,t) - \exp\left(\Omega^{i} \Delta t \right) \Phi_{g}^{i}(r,t - \Delta t) \right]$$
(5)

Therefore, assuming constant value of Ω^i over the integration time-step, the consistency error $\delta\Phi$ of the scheme can be derived by difference with a backward Taylor expansion in time of the flux:

$$\delta\Phi = \left(\frac{d\Phi_g^i(r,t)}{dt} - \frac{\partial\Phi}{\partial t}\right)\Delta t = -\left[\frac{\partial^2\Phi'}{\partial t^2}\frac{\Delta t^2}{2} + O(\Delta t^3)\right]\exp(\Omega^i\Delta t) = -\frac{\partial^2\Phi'}{\partial t^2}\frac{\Delta t^2}{2} + O(\Delta t^3)$$
(6)

Thus, even though Φ' should be slowly varying with time, the truncation error is locally 2^{nd} order (i.e. within one time step) and therefore the accuracy will be further decreased after integration over multiple time-steps, so that the expected accuracy at the time of power peak should be lower than 2.

More importantly, in FLICA4, the temporal integration scheme for the heat transfer equation in the fuel rods uses a 1st order Backward Euler method, with the thermal properties of the materials (e.g. heat conductivity, heat capacity) calculated from the temperatures at the beginning of the time step [20]. Thus, with the given order of accuracy of the two employed codes, the different coupling schemes could only improve the convergence rate of the solution but not increase the order of accuracy. Nevertheless, this type of non-intrusive strategy to improve the coupling accuracy remains of interest when a full "black-box" coupling mode is to be adopted, and will be further evaluated for the coupling of higher-resolution codes that are being integrated in the NURESIM platform.

2.2.3 <u>Time-step optimization</u>

The improvement in the accuracy of a coupled scheme allows for the use of larger time-steps (provided sufficient stability is ensured), and opens the opportunity to employ time-step optimization techniques to reduce the computation effort. One strategy consists of adjusting the overall time step to the dynamic scales of the different physics involved in the simulation. The idea is to make the time step smaller when the solution is changing rapidly and to increase the time step when the solution is "steady like" [21]. The time step is controlled by the following equation:

$$\Delta t_n = \eta_{dyn} \min_{x,i,j} \left[\frac{2}{x_{i,j}^n + x_{i,j}^n} \left(\frac{x_{i,j}^n - x_{i,f}^{n-1}}{\Delta t^{n-1}} \right)^{-1} \right]$$
 (7)

where x represents the exchange variables of the problem (total power, power distribution, fuel temperature, moderator temperature, and moderator density), i and j the mesh identifiers, and η_{dyn} a user specified coefficient ($\eta_{dyn} \le 1$). In this work, a parameter r_{dyn} was implemented to keep the time step increase lower than a user defined percentage, in order to ensure reasonable time step variations when reaching peaks and inflection points in the time evolution of the exchange variables.

Sensitivity study has been performed on the parameter η_{dyn} for the fully explicit scheme, the N-K lead scheme with and without T-H extrapolation, and for two different levels of extrapolations (0.5 and 1.0). The variation of the η_{dyn} is responsible for the acceleration of the time step decrease. The lower this coefficient is, the faster the time step decreases, and the larger the total calculation time is. Results are presented in Figure 7 for the total power accuracy and the fuel temperature accuracy as a function of the speed-up of the calculation time (which corresponds to the calculation time of the most refined solution using a time step of 0.1 ms divided by the actual calculation time). The difference in the two sets of plots is the coefficient r_{dyn} , on the left side the calculations were performed with 10% maximum change, and on the right side with 20%.

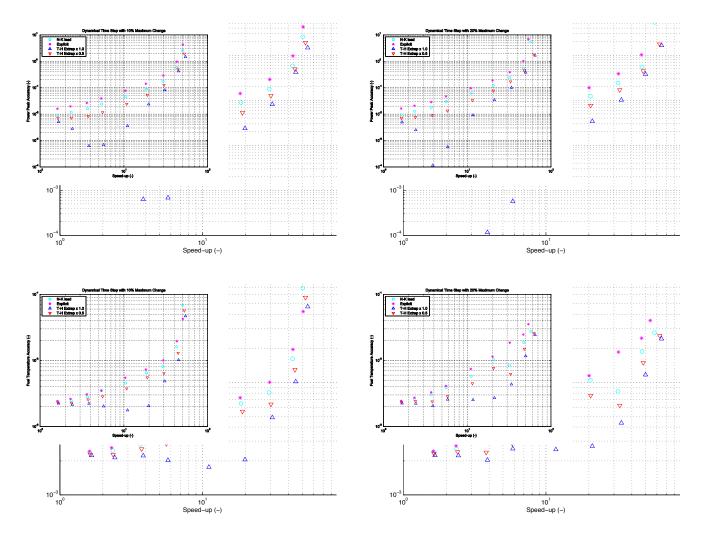


Figure 7 Time-step optimization results.

One can see that for the same level of accuracy in the total power, the N-K lead scheme calculation is about 2 times faster than the fully explicit scheme calculation. Most importantly, the extrapolation scheme with extrapolation level of 1.0 accelerates much faster to the reference solution but one can notice in this scheme that after reaching a level of 5.E-3, the accuracy trend starts to fluctuate. This is due to the transition of the convergence behaviour explained in Section 2.2.2 (see also Figure 6). Nevertheless, the results show that one could obtain a solution of the same accuracy with the extrapolation method five times faster than the fully explicit scheme.

For the fuel temperature, which is the thermal-hydraulics parameter that gives most of the feedback to the N-K in this transient, one can notice the same trend. The fuel temperature converges much faster to the reference with the extrapolation method rather than with the explicit and N-K lead schemes.

3. Conclusion

When selecting a dynamic coupling methodology for LWR core analysis, one should first define what type of improvement should be sought after in priority, be it the convergence, the computation efficiency, the implementation effort or even the modularity.

The OS methods correspond to the lowest implementation effort. However, these methods suffer from poor accuracy in the exchange of variables that can lead to a "bottle neck" effect limiting the accuracy of the overall solution. One possible remedy to this issue is to correct for the nonlinearities in the exchanged variables between the solvers, as was shown with the mini-core rod ejection analysis using the DYN3D/FLICA4 coupled codes in SALOME. Another one would be to implement a FPI method, which should provide additional stability to the solution but at the expense of a significant increase of the computation effort, although this could be somewhat mitigated by convergence acceleration techniques. More advanced methods based on the Newton method were briefly mentioned. One particularly interesting variant is the ABN method, whose main quality is to keep the modularity between the solvers by employing them as a "black-box" within the coupling scheme, and will be investigated in more details in a future work.

Another important aspect of the multi-physics analysis of LWR core transient is the need for efficient time-step control in order to optimize the computation effort. Here, a time-step control algorithm driven by the dynamical time scales of the coupled problem was implemented and tested. And, as illustrated by the mini-core control rods ejection example, significant savings in computation effort were obtained without sacrificing the accuracy of the key results.

Acknowledgment

This work was funded by the European Commission through the NURISP Collaborative Project (Grant Agreement Number: 232124).

4. References

- [1] B. Chanaron, C. Ahnert, D. Bestion, M. Zimmermann, Dan Cacuci and N. Crouzet, "The European Project NURISP for Nuclear Reactor Simulation", Transactions of the American Nuclear Society, 2010, vol. 103, pp. 671-672.
- [2] T.N. Dinh, R.R. Nourgaliev and T.G. Theofanous, "Understanding the ill-posed two-fluid model", Proceedings of the 10th Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-10), Seoul, Korea, 2003 October 5-9.
- [3] H. Pokharma, M. Mori, and V.H. Ransom, "Regularization of two-phase flow models: A comparison of numerical and differential approaches," Journal of Computational Physics, 134, 1997, pp. 282-295.

- [4] D.A. Barber, R.M. Miller, H.G. Joo, and J.T. Downar, "Application of a generalized interface module to the coupling of spatial kinetics and thermal-hydraulics codes" Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-9) San Francisco, California, October 3 8, 1999.
- [5] E. Royer and I. Toumi, "CATHARE-CRONOS-FLICA coupling with ISAS: A powerful tool for nuclear studies", ICONE-6 Meeting, San Diego, California, USA, 1998.
- [6] J.M. Aragonés, C. Ahnert, O. Cabellos, N. García-Herranz, and V. Aragonés-Ahnert, "Methods and results for the MSLB NEA benchmark using SIMTRAN and RELAP 5", Nuclear technology, Vol. 146, pp. 29-40, 2004.
- [7] K. Nikitin, J. Judd, G.M. Grandi, A. Manera, and H. Ferroukhi, "Peach Bottom 2 Turbine Trip 2 simulation by TRACE/S3K coupled code", PHYSOR 2010 Advances in Reactor Physics to Power the Nuclear renaissance, Pittsburgh, Pennsylvania, May 9-14, 2010.
- [8] J.C. Ragusa and V.S. Mahadevan, "Consistent and accurate schemes for coupled neutronics thermal-hydraulics reactor analysis", Nuclear Engineering and Design 239, 2009, pp. 566–579.
- [9] D.A. Knoll and D.E. Keyes, "Jacobian-free Newton-Krylov methods: a survey of approaches and applications", Journal of Computational Physics 193 (2004) 357-397.
- [10] V.A. Mousseau, "Implicitly balanced solution of the two-phase flow equations coupled to nonlinear heat conduction", Journal of Computational Physics 200 (2004) 104–132.
- [11] V.A. Mousseau, "A fully implicitly hybrid solution method for a two-phase thermal-hydraulic model", Journal of Heat Transfer Vol. 127 531–539, May 2005.
- [12] A. Yeckel, L. Lun and J.J. Derby, "An approximate block Newton method for coupled iterations of nonlinear solvers: Theory and conjugate heat transfer applications", Journal of Computational Physics 228, 2009, pp. 8566-8588.
- [13] "SALOME: The Open Source Integration Platform for Numerical Simulation", http://www.salome-platform.org.
- [14] O. Zerkak, P. Coddington, N. Crouzet, E. Royer, J. Jimenez and D. Cuervo, "LWR multiphysics developments and applications within the framework of the NURESIM European Project", Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), 15-19 April 2007, Monterey, CA, USA, American Nuclear Society, LaGrange Park, IL (2007).
- [15] E. Royer, N. Crouzet, "Validation of NURESIM SP3 on VVER-1000 reactor", NURESIM Platform for Nuclear Reactor Simulation (Contract Number: NUCTECH-2004-3.4.3.1-1), Deliverable D3.2.1, April 2008.
- [16] J. Jimenez, D. Cuervo, N. Crouzet, and J. Roy, "COBAYA3 Integration within the SALOME Platform", NURESIM Platform for Nuclear Reactor Simulation (Contract Number: NUCTECH-2004-3.4.3.1-1), Deliverable D3.4, December 2008.
- [17] S. Kliem, S. Mittag, A. Gommlich, P. Apanasevich, "Definition of a PWR boron dilution benchmark", NURISP NUclear Reactor Integrated Simulation Project (Contract Number: 232124), Deliverable D3.1.2.2, Revision 3, February 2011.

The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14 Toronto, Ontario, Canada, September 25-30, 2011

- [18] T. Kozlowski, T.J. Downar, "OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark. Final report", NEA/NSC/DOC(2006)20 (January 2007).
- [19] U. Grundmann, U. Rohde, S. Mittag and S. Kliem, "DYN3D Version 3.2. Description of Models and Methods", Forschungzentrum Rossendorf (August 2005).
- [20] J. Grimoud, "FLICA4 (Version 1.0), Manuel de référence, Modules de conduction de la chaleur en géométrie cylindrique monodimensionnelle", Technical Report DMT/93-034 SERMA/LETR/93-1467, CEA (1993).
- [21] V.A. Mousseau, "A fully implicit, second order in time, simulation of a nuclear reactor core", Proceedings of ICONE 14 International Conference on Nuclear Engineering, Miami, Florida, USA, July 17-20, 2006