Consistent accelerated schemes for nonlinear coupling problems in reactor analysis

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Abstract

Conventional coupling paradigms used nowadays to couple various physics components can be inconsistent in their treatment of the nonlinear terms. This leads to usage of smaller time steps to maintain stability and accuracy requirements, thereby increasing the CPU time. This paper aims at finding accelerated schemes that will provide accurate solution fields for coupled reactor analysis problems that are non-intrusive in-order to use existing mono-physics codes in achieving consistent coupling. These schemes were applied to both 0-D and 1-D transient problems and results obtained verify the advantages of using the predictive and accelerated schemes.

KEYWORDS: Coupled physics, reactor analysis, numerical schemes

1. Introduction

For decades, high fidelity modeling of nuclear cores has been divided into several distinct domains of physics: neutronics, which solves for the neutron population distribution; hydraulics, which solves for the moderator density and temperature fields; heat transfer, which solves for the temperature fields within the nuclear fuel. Yet, these various physics are intertwined and rely heavily on the solution field of one another. In the last decade or so, various existing mono-disciplinary codes have been coupled together in a naive "black-box" fashion, where the output of one code serves as the input of another code, thereby producing solutions that are weakly coupled. This coupling strategy, denoted hereafter as Nonlinearly Inconsistent Coupling (*NIC*) strategy, is based on an inconsistent linearization of the problem and still is the main coupling paradigm today for solving nonlinear nuclear reactor physics equations. The schematic of the "Black-box" model is shown in Fig. 1, where each physics component is solved by an independent mono-physics code and the data from one code is exchanged through message passing paradigms such as PVM or MPI. There are no iterations within a single time-step over the different physics which makes this scheme weakly coupled since the interaction and the nonlinearity due to the dependence is not fully resolved.

The fundamental inefficiency and essential drawback of this strategy is that the treatment of the nonlinear terms in the "Black-box" model is not rigourous and hence leads to a NIC scheme. For instance, the stiffness of the neutronics phenomena and the CFL condition of thermal-hydraulics requires implicit time integration be performed for numerical stability reasons.

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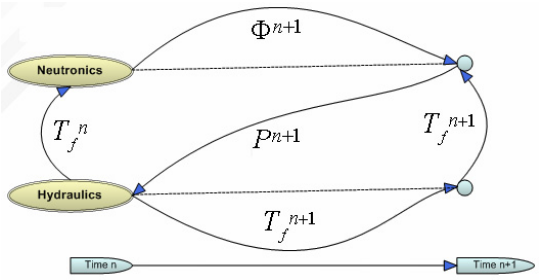
Referring to Fig. 1, the time implicit treatment of neutronics physics between t^n and t^{n+1} requires that all other physics components be known at time t^{n+1}, which is obviously not the case because neutronics physics marches forward before thermal-hydraulic physics. This inconsistent

Figure 1: Schematic of conventional "Black-box" or NIC models



treatment of the nonlinear terms wherein one or more physics solution field is lagged in time results usually in a loss of convergence order[1]. Typically to mitigate this scenario, it is required to use smaller time steps to achieve a reasonable convergence, thereby taxing the CPU and increase the overall computer calculation time.

To overcome the above drawbacks, two methodologies were derived to restore the nonlinear consistency: one is a simple and robust prediction to be performed on the exchanged data; and the second is based on Stefenssen's acceleration technique[2] for fixed-point methods[3]. Both methodologies restore the order of accuracy to a second order convergent solution while preserving the legacy of existing codes as much as possible. Hence, these modified schemes make excellent candidates for creating Nonlinearly Consistent Coupling (*NCC*) strategy, which are attractive also due to the ease in implementation in existing coupled codes.

2. Notations and problem statement

A nonlinear problem of ordinary differential equations can be formulated as follows:

$$\dot{u} = Lu + N(u) + b(t) = F(u,t) \qquad (1)$$

where u is the vector of unknowns, $\dot{u}$ represents time derivation, L is a matrix representing a linear operator, and $N(u)$ is a nonlinear vector function. L and $N(u)$ may result, say, from spatial discretization of partial differential equations. For many physical systems, the nonlinear vector function $N(u)$ may be factorized as $G(u)u$, where $G(u)$ is a matrix whose elements depend on u. Coupled neutronics / thermal-hydraulics phenomena can, of course be cast in the form of Equation 1. Let us consider an implicit time integration of Equation 1, say using a *theta*-scheme:

$$\frac{u^{n+1}-u^n}{t^{n+1}-t^n} = \theta(L^{n+1}u^{n+1}+N(u^{n+1})+b(t^{n+1}))+(1-\theta)\,(L^n u^n + N(u^n)+b(t^n)) \qquad (2)$$

In a conventional coupling paradigm, the nonlinear term $N(u^{n+1})$ would not be known but simply approximated by $N(u^n)$ which is a crude first order approximation. Hence, if both physics were solved using a second order scheme, say in our example a Crank-Nicholson scheme (θ=1/2), then the resulting overall accuracy order of the solution would only be 1 due to naive approximation for $N(u^{n+1})$ mentioned above.

3. Improved coupling strategies

3.1. Improved prediction: explicit high order treatment of nonlinear terms

A solution prediction is an idea derived from extrapolation. Instead of solving for an unknown quantity by iterative methods, it obviously makes sense to extrapolate the solution based on the history of solution and use that value as the starting point. The idea is to replace the unknown quantity $N(u^{n+1})$ by a prediction $N(u^{n+1,P})$ where the crudest prediction is $N(u^n)$ which yields $u^{n+1,P} \approx u^n + O(\Delta t)$. If each physics is integrated in time with an accuracy order of N, then the prediction should be performed with an N^{th} order accurate approximation. We will see that with the prediction of the solution by extrapolation at every time step, the order that is lost by not converging the nonlinearities, can be restored. Hence, we can have a modified Fixed Point Iteration (FPI) scheme which resembles Predictor-Corrector schemes [4] that are popularly used for solving nonlinear systems.

Prediction formulas can be derived easily using a Taylor series expansion as

$$f(x+h) = f(x) + hf'(x) + \ldots + hf^N(x) + O(h^{N+1}) \qquad (3)$$

Considering a second order accurate scheme, Equation 3 can be simplified by applying BDF, to obtain

$$f(x+h) = f(x) + (f(x) - f(x-h)) + O(h^2)$$
$$u^{n+1,p} = 2u^n - u^{n-1} + O(h^2) \qquad (4)$$

Equation 4 is a second order prediction approximation which when combined with the Crank Nicholson scheme would yield an overall second order accurate solution, an improvement from the first order accurate solution by making the inconsistent approximation. It should be obvious by now that this idea is an extension of explicit multistep methods and more terms can be used to get prediction values of higher order accuracy and subsequently corrected with consistent time discretization schemes to get overall higher orders of accuracy. This new scheme involves only minor modifications to the existing "Black-box" coupling paradigm codes but can improve and restore the overall order of accuracy. Such an improvement will allow the use of higher orders of time steps for applications in transient reactor analysis scenarios.

3.2. Accelerated fixed-point methods

Fixed-point iteration over the time step usually removes the inconsistency in the nonlinear terms, but at the cost of a certain number of iterations within the time step. For many years, mathematicians have devised many acceleration techniques to improve the speed of convergence. It should be remembered that the order of convergence does not change when acceleration techniques are used for a particular iterative scheme but the number of iterations to reach final convergence reduces significantly. There are several methods like Aitken and Chebyshev acceleration that are popularly used to reduce the number of nonlinear iterations.

For the numerical schemes and methods discussed in the preceding sections, a technique called the Aitken's Δ^2 process satisfies all the criteria. Aitken's method can be used to speed up convergence for any sequence that is linearly convergent.

Definition: Given the sequence $\{p_n\}_{n=0}^{\infty}$, we define the forward difference formula as $\Delta p_n = p_{n+1} - p_n$ for $n = 1,2,3 \ldots N$. Higher powers $\Delta^k p_n$ are defined recursively, for k≥2, by : $\Delta^k p_n = \Delta^{k-1}(\Delta p_n)$. When k=2 we have the useful formula $\Delta^2 p_n = \Delta(\Delta p_n) = (p_{n+2} - p_{n+1}) - (p_{n+1} - p_n)$ which simplifies to be $\Delta^2 p_n = p_{n+2} - 2p_{n+1} + p_n$ for $n = 2, 3, \ldots N$.

Now assume that the sequence $\{p_n\}_{n=0}^{\infty}$ converges linearly to the limit p and that $p_n \neq p$ for all $n \geq 0$. If there exists a real number A with $|A| < 1$ such that

$$\lim_{n\to\infty} \frac{p - p_{n+1}}{p - p_n} = A \tag{5}$$

Then the sequence $\{q_n\}_{n=0}^{\infty}$ defined by

$$q_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n} = p_n - \frac{(p_{n+1} - p_n)^2}{(p_{n+2} - 2p_{n+1} + p_n)} \tag{6}$$

converges to p faster than $\{p_n\}_{n=0}^{\infty}$, in the sense that $\lim_{n\to\infty} \left| \frac{p - q_n}{p - p_n} \right| = 0$

3.3. Steffensen's Acceleration

When Aitken's process is combined with the fixed point iteration, the resulting scheme is called Steffensen's acceleration. Starting with p_0, two steps of fixed point method are used to compute p_1 and p_2. Then Aitken's Δ^2 process is used to compute the accelerated value, q_o.

$$q_0 = p_0 - \frac{(\Delta p_0)^2}{\Delta^2 p_0} \tag{7}$$

Once q_o is calculated, $p_o = q_o$ and the whole process is repeated again. This method is very effective and is specific to Picard iterations on which we are particularly interested due to reasons based on legacy code systems.

3.4. Overcoming drawbacks in current coupling schemes

The current *NIC* schemes have several disadvantages that have been discussed before. This paper is aimed at devising methods that are robust, stable and accurate along with the flexibility to reuse existing mono-physics legacy codes as much as possible to create *a NCC* strategy.

Since current schemes perform fixed point iterations with a crude approximation, the nonlinearities are not resolved and hence the solution is only first order accurate. Now, by including prediction as in Section (3.1), or with Picard iterations, the lost order of accuracy can be regained and we can create more accurate coupling at little extra computational cost. The only change is to modify the interface between the coupling blocks and perform the appropriate extrapolation to get the predicted values.

Apart from this strategy, we will also aim to accelerate the convergence of Fixed point iterations when the nonlinearities are completely converged at each time step. The Aitken Δ^2 process is very efficient and requires storing only 2 preceding solution vectors which is trivial, given the configuration of current computers. In the results section, we will discuss the performance gain of the prediction and acceleration procedure and the amount of CPU time saved compared to the existing *NIC* models.

4. Reactor Analysis problems

Transient reactor analysis problems are excellent examples of stiff, coupled multi-physics problems [5]. The deep interaction between the neutronics / thermal-hydraulics physics makes it strongly coupled and the fast changing neutron distribution during accidents adds the stiffness to

the system. In this paper, two simple transients will be considered for a problem in 0-D and 1-D and the schemes that have been derived earlier will be applied to obtain the results.

4.1. 0-D Model

The 0-D model for the transient analysis problem of the reactor core can be subdivided into the 0-D neutronics or the Point reactor Kinetics equations (PRKE) and a 0-D thermal hydraulics given by a simple 0-D forced convection heat transfer model. The power generated in the fuel rods act as the source of heat flux and heat taken out by the coolant is the sink. A simple heat balance over the assembly gives the hydraulics equations. The fuel model is simply a 1-D radial heat conduction model consisting of a fuel pellet with gap and cladding (material conductivities and density are temperature dependent); clad-water heat exchange coefficient is computed using Dittus-Boelter correlation. A simple 0-D energy balance has been derived for a single phase liquid water moderator (heat capacity and density are temperature dependent). The 0-D model can be described as a lumped model [6] of all the physics and can be solved either as a single set of simultaneous equations or as two sets of coupled equations to obtain the solution fields.

The set of equations used to solve for the 0-D model is given below.

$$\frac{dP}{dt} = \frac{\rho(t) - \beta}{\Lambda} P + \lambda C \tag{8}$$

$$\frac{dC}{dt} = \frac{\beta}{\Lambda} P - \lambda C \tag{9}$$

$$(\rho C_p)_f \frac{dT_{eff}}{dt} = J_p P - (T_{eff} - T_m) / R(T_{eff}) \tag{10}$$

$$(\rho C_p)_m \frac{dT_m}{dt} = (T_{eff} - T_m) / R(T_{eff}) - 2V / H(\rho C_p)_m (T_m - T_{in}) \tag{11}$$

where P – Power, C – Precursor concentration, T_{eff} – Average fuel temperature, $R(T_{eff})$ – Overall resistance for heat conduction in fuel, T_m – Bulk moderator temperature, and β, λ, ρ, Λ – Kinetics parameters, H – the core height.

We can see from Equation 10 that the fuel temperature is coupled to Power by the power density term J_p and the dependence of the neutronics power on the fuel and moderator temperature is buried inside the reactivity term $\rho(t)$. The feedback reactivity relations used for the 0-D model are given below.

$$\rho(t) = \rho_{Doppler}(t) + \rho_{mod}(t) + \rho_{CR}(t) \tag{12}$$

The definition for the individual reactivity terms are as follows.

Doppler reactivity : $\rho_{Doppler}(t) = \alpha_{eff} (\sqrt{T_{eff}(t)} - \sqrt{T_{eff}(0)})$

Moderator reactivity : $\rho_{mod}(t) = \alpha_{\mathrm{mod}} (T_{\mathrm{m}}(t) - T_{\mathrm{m}}(0))$.

An external time dependent function for the control rod movement $\rho_{CR}(t)$. The two standard external functions used in transient analysis in this paper are step and ramp reactivity insertions.

4.2. 1-D Model

The 1-D model of the nuclear reactor core is slightly complicated than the simplified 0-D model. The neutronics in 1-D model is given by the Multi-group diffusion equation and the feedback due to Fuel and Moderator temperature causes Doppler expansion and hence directly affects the cross-section of the materials. This non-linearly couples neutronics to the other

physics. The hydraulics is given by a homogenous single phase flow model. The mass, momentum and energy balance equation along with equation of state relating pressure, enthalpy and temperature are used in calculation of the moderator properties and the bulk temperature. The non-linear heat conduction in fuel is given by a heat flux balance in the fuel pellets based on the moderator temperature and the power density in the pellet. The governing equations for different physics used in the 1-D model are given below.

Neutronics:

$$\frac{1}{\upsilon_g}\frac{\partial \phi_g}{\partial t} + \nabla.(D_g(r,t)\nabla\phi_g) + \Sigma_{t,g}(r,t)\phi_g(r,t) = \sum_{g'=1}^{G}\Sigma_{s,g'->g}(r,t)\phi_{g'}(r,t) + \chi_g\sum_{g'=1}^{G}(1-\beta_{g'})\nu\Sigma_{f,g'}(r,t)\phi_{g'}(r,t) + \sum_{k=1}^{L}\chi_{k,g}\lambda_k C_k(r,t) \quad (13)$$

$$\frac{\partial C_k(r,t)}{\partial t} = -\lambda_k C_k(r,t) + \sum_{g=1}^{G}\nu_{dk}\Sigma_{f,g}(r,t)\phi_g(r,t) \quad (14)$$

Thermal-Hydraulics: $h(z) = h_{in} + \int_0^H \frac{q'(z)}{\dot{m}}dz$, $\frac{d}{dt}(\rho_F Cp_F T) - \frac{1}{r}\frac{d}{dr}k_F(T)r\frac{dT}{dr} = q'''$ (16)

The neutronics in the model uses a Finite element method for the discretization of space and time integration is performed using the θ-scheme. The heat conduction model uses a finite difference method to solve for $T_f(r,z)$ and the effective average fuel temperature at each node along z is found out using the following formula $T_{eff}(z) = wT_f(0,z) + (1-w)T_f(R_f,z)$ where the w is the weighting parameter (usually $w = 4/9$).

In the next section, we shall discuss the results obtained by applying the numerical schemes that were discussed in the earlier section for both the 0-D and 1-D models of the nuclear core by simulating different accident scenarios with a step and ramp change in the external reactivity driving function.

5. Results

The θ time discretization scheme was implemented for both the 0-D and the 1-D models which allows the usage of testing two different schemes namely the Backward Euler (θ=1) and the Crank Nicholson (θ=1/2) schemes.

5.1. 0-D Model

Fig. 2 and Fig. 3 show a sample transient for a step and ramp reactivity input of about 1.2$ respectively. The feedback between neutronics and hydraulics is evident due to the power turn in the transient where the negative Doppler reactivity acts as a limiting factor and brings the power back down to a final steady state value. The figures shown below do not have any of the proposed schemes implemented but the nonlinearities in the different physics are fully converged using FPI and hence are second order accurate solutions. The figures present the relative power transient level as a function of time.

Fig. 4 shows another calculation wherein at t=250 ms, a control rod is ejected. The ramp ejection duration is 250 ms with amplitude of 1.2$. The reference computation for the transient was performed using a time step size of 0.4 ms. Three other computations were performed using a time step size of 10 ms: these computations were:

1) Conventional coupling paradigm as shown in Fig. 1,
2) Fixed-point iterations (i.e., conventional scheme iterated),
3) Explicit higher order treatment of nonlinear terms (improved prediction)

Fig. 5 shows that the conventional coupling scheme over predicts the power level by more than 10% whereas the other schemes are off by at most only 1%. Obviously, the improved prediction scheme was much cheaper than the Fixed-point method because there are no iterations over all the physics within each time step calculation. The improvement in the solution field is impressive for the improved prediction since the effort required to make the extrapolation is trivial but the effect of the modification, results in a solution closer to the reference, which was calculated with a finer time step and with full FPI convergence.

Figure 2: Step transient

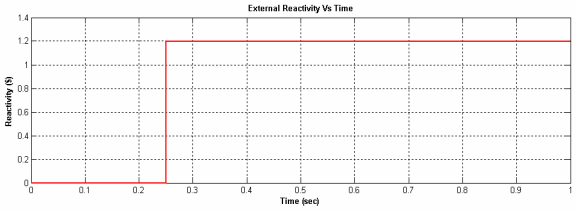
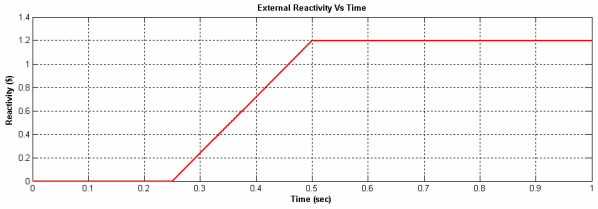


Figure 3: Ramp transient



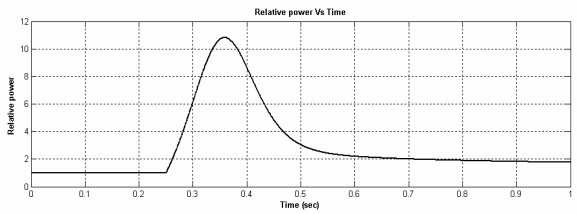


Figure 4: Comparison between schemes

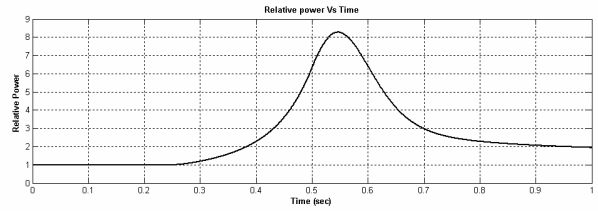
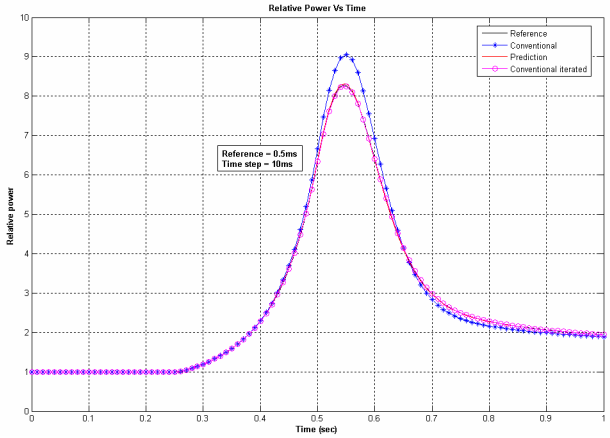
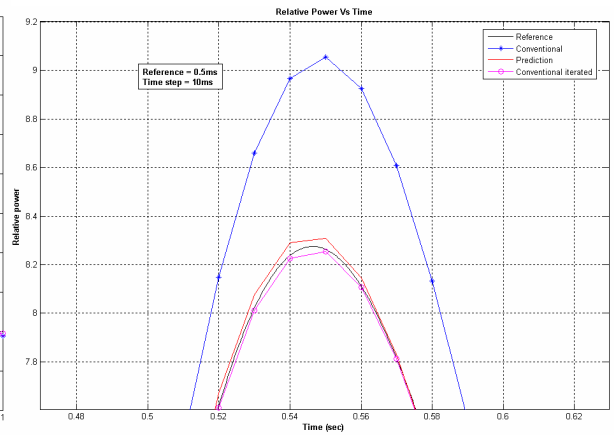


Figure 5: Enlarged at power peak





Based on the calculations, the number of fixed-point iterations/time step is plotted in Fig. 6 for different values of time steps and for each of the schemes mentioned above. It is evident from the figure that using either solution prediction or acceleration definitely improves the number of fixed point iterations. Even though using only prediction does not yield considerable reduction in number of iterations, the synergistic effects of using both acceleration and prediction provides a reduction of more than 30% in the number of iterations per time step. On a large time scale, the total reduction in CPU time can then be 3 fold since on an average, only one third of iterations are needed to fully converge the nonlinearities between the different physics. Also from Fig. 6, it

is clear that the usage of acceleration for finer time steps yields no perceptible improvement due to the fact that only fewer iterations are needed to converge nonlinearities while acceleration for coarser time steps results in a considerably faster convergence, still retaining the order of accuracy.

Apart from measuring the improvement in the CPU time for the predictive methods, it is also clear that the predictive methods will restore the lost order of accuracy for the coupled transient scenario even without outer FPI. To analyze this, a ramp transient, similar to the one plotted in Fig. 3 was simulated and the orders of accuracy of the various different schemes was found out. Fig. 7 presents the accuracy order obtained for the three aforementioned schemes: (1) conventional coupling, (2) fixed-point iterations, (3) explicit high order treatment of nonlinear terms (improved prediction). The time step sizes used varied from 0.8 ms to 100 ms.

The conventional coupling scheme only yields first order accuracy, whereas fixed-point iterations and improved prediction both yields second-order accuracy: these schemes are therefore nonlinearly consistent and yield the expected higher accuracy order. It is obvious that the improvement in number of iterations by Steffensen's acceleration technique does not change the order accuracy. But the solution prediction method improved the conventional first order solution to yield a second order accurate solution with a simple extrapolation based on the previous history of the solution.

Figure 6: Efficiency of acceleration

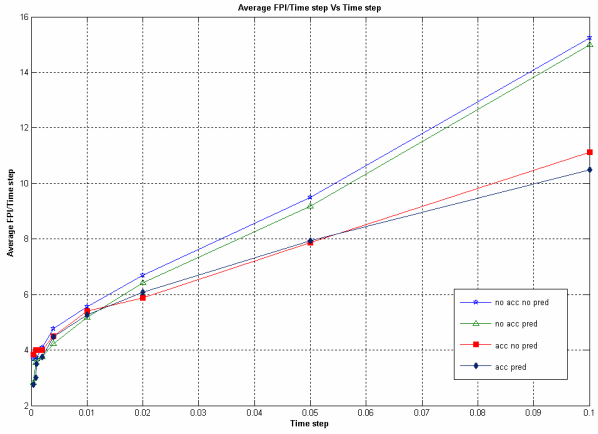
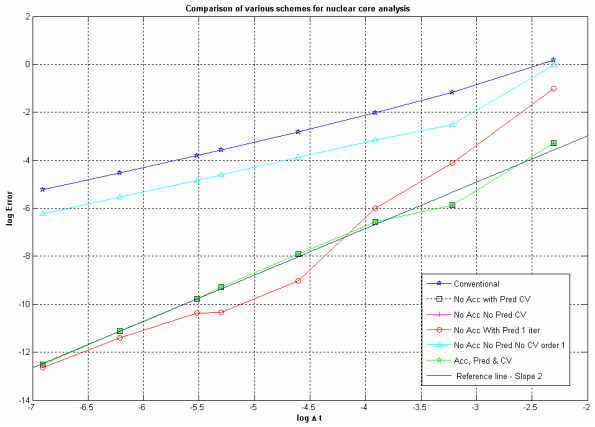


Figure 7: Order of accuracy for schemes



Based on the results obtained for the 0-D model, a solution prediction was implemented for the 1-D model but the Steffensen's acceleration was not implemented due to the reason that the gain in acceleration for FPI is much less compared to the gain in CPU time by using prediction alone with no FPI over all the physics. The results obtained for the 1-D model are given in the next section.

5.2. 1-D Model

In the 1-D model, it is important to discretize the spatial variable thoroughly in order to eliminate the loss of order of convergence in the time integration due to a spatially un-converged or weak solution. Hence, 100 meshes were used to calculate the solution over a total height of 400cm in all the following cases.

For the 1-D model, the homogenous reactivity addition is simulated by changing the thermal fission cross-section as a function of time, similar to the external reactivity function in the 0-D model. It is also imperative to note that the $1/v$ values for the chosen material as a function of

energy groups are {.5456853E-07, .2491910E-05} sec/m which results in a very small generation time (Λ), making the coupled system very stiff.

Multi-parameterized cross-section data was obtained from NEA [7] for Rod ejection benchmark problems and were used for simulating all 1-D transients. The 2 group cross-section set provides the necessary data as a function of fuel temperature (T_{eff}) and moderator density (ρ_{mod}). For feedback calculations, the cross-section was linearly interpolated between the table points using solution fields from hydraulics physics.

5.2.1. Fully coupled system

Before testing the fully coupled system, the order of convergence for each of the individual 1-D physics without feedback from the other physics was tested and the results yield the expected convergence rates i.e., second-order accurate solution for CN scheme. The results for coupled physics analysis in 1-D in this section are for a 2-energy group, 1-delayed group, homogenous medium with a reactivity insertion of 1.2$. This experimental run for the transient was performed for the ramp reactivity insertion with feedback for a total of 50 ms. The order of convergence was also found out for different schemes and have been plotted and shown in Fig. 8.

Fig. 8 shows that the results for the 1-D model are consistent with the 0-D model. The coupled system solution without FPI or prediction (conventional) yields a first order accurate solution for all the variables similar to the results shown in Fig. 7.

Figure 8: Accuracy order: No FPI

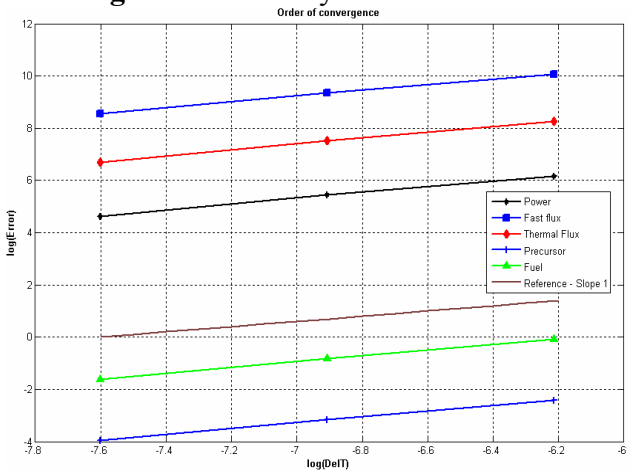
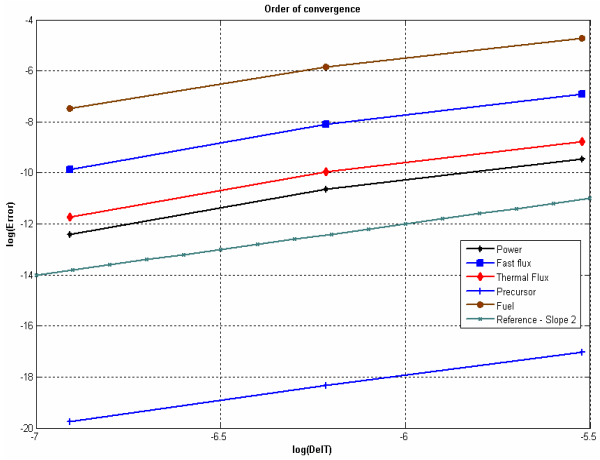


Figure 9: Accuracy order: Prediction



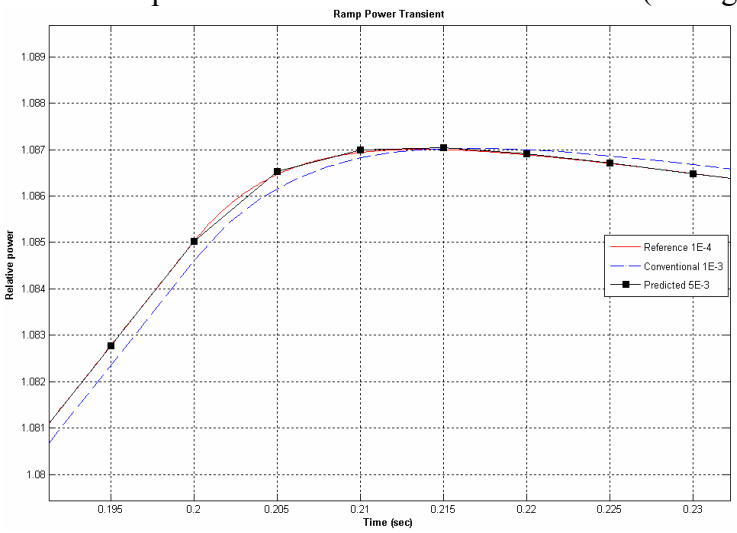
If we perform FPI over the system, all the nonlinearities will be resolved completely and the order of convergence will be restored. But this is very expensive for even a 1-D model since the number of matrix inversions and floating point operations limit the number of iterations that can be performed to avoid the influence of round-off errors. Instead, to save both CPU time and to get an accurate solution, a prediction is performed and tested for the 1-D model, with all the other parameters remaining the same.

Fig. 9 presents the improvement in the order of convergence of the coupled system for all the solution fields using the simple prediction scheme. Again, the 1-D model yields results that agree with the ones from the 0-D model for the transient analysis of the coupled reactor core.

Before concluding with the advantages of solution prediction, it is also important to compare the transient solution improvement for a higher time step compared to the one without prediction or FPI. Fig. 10 presents this data and it is evident that the predicted solution is closer to the

reference than the solution from the conventional scheme, eventhough the prediction time step is higher than the conventional solution time step by a factor of 5.

Figure 10: Comparison of Conventional Vs Predicted (Enlarged)



6. Conclusions

Conventional coupling paradigms used nowadays to couple various physics components can be inconsistent in their treatment of the nonlinear terms. This can lead to decreased accuracy order, which in turn forces the use of extremely small time steps. Simple methods such as the improved prediction based on an explicit higher order treatment of nonlinear terms, can restore the accuracy order. Such methods require very little code modification and, therefore, preserve the legacy of mono-disciplinary codes used today in coupled simulations. Transient simulations in a nuclear reactor core were performed for a 0-D and 1-D model to obtain higher order accurate solutions for all the involved variables in the reactor system. The results presented in the paper validate the use of such intelligent approximations to calculate accurate solution fields with minor modifications in the interface or the driver of the multi-physics coupled "Black-box" model.

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