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**JFNK PRECONDITIONING
FOR COUPLED BWR CALCULATIONS**
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ABSTRACT

In this paper, a one-dimensional Boiling Water Reactor (BWR) model in steady-state conditions is developed. The model accounts for neutron transport, fluid dynamics, heat transfer and the interdependences between the various physics. The modelling assumptions were chosen so that the physics of BWRs could be properly accounted for with an as simple as possible model. The model is thereafter used to study the effect of preconditioning when a Jacobian-Free Newton Krylov (JFNK) method is used to solve the system of equations. Preconditioning is a key aspect in any JFNK method. By clustering the eigenvalues of the system of equations, a preconditioner is expected to drastically reduce the number of iterations. Nevertheless, the design of an efficient preconditioner is a far from trivial task. Using the developed model, different preconditioning alternatives are tested. It is demonstrated that an efficient preconditioner is found to have the following characteristics: separate preconditioning of the neutron transport problem, no preconditioning of the heat transfer problem, preconditioning of the fluid dynamics problem where the cross-dependencies between the void fraction and the phasic velocities are resolved and where the pressure field is treated independently. This paper thus provides guidelines about how to develop an efficient preconditioner for coupled BWR physics.

KEYWORDS: Boiling Water Reactor, coupled calculations, Jacobian-Free Newton Krylov, preconditioning

1. INTRODUCTION

By essence, nuclear reactors represent multi-physic systems, in which different fields of physics are inter-related. In best-estimate approaches, such interdependent fields are usually restricted to the physics of neutron transport, the physics of fluid dynamics and heat transfer. The simultaneous modelling of these three fields is important both in steady-state conditions as well as in transient conditions. The addition of other fields (fuel behavior, chemistry, material physics, etc.) might also be necessary in some specific situations.

Typically, the modelling of each physics is done in a segregated manner. One code is used per field at a time, assuming that the other fields are “frozen”, and iterations are performed to resolve the interdependences until convergence on all physical fields is achieved [1]. Such a solution strategy is the result of the use of legacy codes developed for modelling each physical field separately, codes that were *à posteriori* coupled to model multi-physic problems. The main advantage of such an *à posteriori* coupling lies with the absence of internal code modification when the code is externally coupled to another software. This results in the preservation of the Verification and Validation (V&V) work for each code. Nevertheless, achieving tight convergence on all physical fields might be difficult and numerical oscillations are often encountered [2]. In addition, when considering transient calculations, the non-linearities are often never fully resolved, resulting in inconsistent coupling algorithms [1].

Other coupling methodologies were been proposed, in which the non-linearities can be fully resolved. One of the most promising approach is the so-called Jacobian-Free Newton Krylov (JFNK) method [3]. This technique gained a lot of attention in recent years for modelling multi-physic problems in nuclear engineering, as can be noticed from the number of scientific publications on this subject.

The design of a preconditioner is one of the key aspects in using the JFNK approach efficiently. The best possible preconditioner is the Jacobian of the system of equations itself, which could be estimated by numerically differentiating the set of equations with respect to each of the primary variables solved for. Even if one could use a first-order approximation for making those evaluations, a numerical Jacobian is of little use when trying to solve the set of equations in a Jacobian-free manner. Using an analytical preconditioner thus represents an interesting alternative. Nevertheless, the required efforts in developing such an analytical Jacobian are far bigger than developing the set of equations and associated models to be solved by the JFNK approach.

In addition, one of the specific features of Boiling Water Reactors (BWRs) is the presence of vapor that significantly enhances non-linear effects as compared to Pressurized Water Reactors. Although there have been some successful implementations of JFNK methods in thermal-hydraulic codes for two-phase flow systems [4-6], the modelling of coupled neutronics/thermal-hydraulics for BWRs remains largely unexplored.

The purpose of this paper is therefore twofold. First, to develop a simple enough coupled BWR model that can be used for testing e.g. a JFNK solution procedure. Thereafter, this model is used to develop and test various preconditioners, in order to identify an efficient preconditioner.

2. DESCRIPTION OF THE COUPLED MODEL

In this Section, the models that were retained for developing a coupled numerical framework aimed at studying the performances and applicability of the JFNK method for BWR applications are presented. The incentives in the choice of the different modelling assumptions were to develop an as simple as possible set of models being still representative of the physics of BWRs. A one-dimensional axial coupled

BWR problem was thus developed in steady-state conditions. A simple enough model allows gaining physical insights into the driving mechanisms, which could remain non-trackable when using state-of-the-art modelling tools for coupled BWR physics. One of the peculiarities of the modelling of BWRs is the strong dependence of both the macroscopic cross-sections and the thermal-hydraulic correlations on the void fraction and/or the flow regimes. Special attention was thus put on preserving this feature in the modelling assumptions used.

2.1. Cross-section modelling

The macroscopic cross-sections and diffusion coefficients necessary to the neutron transport calculations were generated in advance and processed so that they could be directly used in the developed workbench. These data were created from CASMO-4E calculations [7] performed in an earlier project [8]. A two-dimensional model of a SVEA 96 BWR fuel assembly containing six fuel pins with Gadolinium oxide was considered in an infinite lattice set-up, with a critical spectrum correction to account for the effect of neutron leakage. The calculations were performed with a 70-group nuclear data library essentially based on ENDF/B-VI. Not control rod was assumed to be inserted in the fuel assembly. The calculations were performed at fresh conditions, in order to avoid the unnecessary complication of the modelling of the dependencies on history effects.

The macroscopic data were then created as functions of coolant density and fuel temperature, on a range of $[0.037 - 0.835]$ g/cm³ and $[538 - 938]$ K, respectively. Two-dimensional spline interpolation functions between the created data points were then built with respect to the coolant density and the fuel temperature. Spline extrapolations were performed when calling a coolant density value and/or a fuel temperature value outside of the ranges of the created data point values.

2.2. Neutron transport modelling

The modelling of neutron transport was performed using a low-order method based on diffusion theory. This method only resolves the first moments of the angular neutron flux, namely the scalar neutron flux and the neutron current density vector. In addition, the energy discretization was based on a two-energy group formulation. Concerning the spatial discretization of the system of equations, finite differences were used. From a neutron transport viewpoint, the solution vector is represented by

$\left[\phi_{1,1}; \dots; \phi_{1,N}; \phi_{2,1}; \dots; \phi_{2,N}; k_{eff} \right]^T$ where $\phi_{g,k}$ represents the neutron flux in energy group g and axial node k (with N being the total number of nodes in the axial direction), and k_{eff} is the effective multiplication factor of the system.

2.3. Fluid dynamics modelling

The modelling of the fluid properties was carried out using a mixture model formulation of the local conservation equations for mass, linear momentum, and enthalpy, assuming thermal equilibrium between the liquid and vapor phases and identical pressure for both phases. Some drift between the velocities of the vapor phase and of the liquid phase was allowed, using an algebraic relationship proposed by Zuber and Findlay [9] with some simplifications. The resulting model is often referred to as a four-equation model.

Additional approximations were introduced in order to keep the system of equations as simple as possible. In the momentum conservation equation, the effects of internal stresses and of their turbulent component were neglected. In the enthalpy conservation equation, the following contributions were neglected: the volumetric heat sources, the work of the forces due to phase change and pressure/stresses at the interface and at the solid walls; the kinetic energy due to mass variation in case of phase change; the viscous and turbulent dissipation terms; the effects of internal heat flux and of their turbulent component.

In the present work, it was further assumed that the coolant entered the heated channel at saturated conditions directly. The existence of the one-phase region at the bottom of BWR fuel assemblies was thus neglected, since this region is small compared to the entire length of the channel.

A simplified water table derived from the MATLAB function IAPWS-IF97.m [10] (itself essentially using the data from [11]) was created. Concerning the modelling of pressure drops due to friction, a two-phase friction factor based on the method of Lockhart-Martinelli was used [12].

For the actual correlations implemented in the drift flux model, a simplified version of the Zuber and Findlay model was developed (using some data from [12]). This simplified model can be stated as follows:

- Bubbly flow exists for a void fraction $\langle \alpha \rangle$ lying in the interval $[0; 0.15]$ for which the following correlations can be used for the Zuber and Findlay drift flux model:

$$C_0 = 1.2 \text{ and } V_{vj} = \left(1 - \langle \alpha \rangle\right)^{1.5} \times V_\infty \quad (1)$$

with

$$V_\infty = 1.53 \times \left(\sigma g \times \frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_l^2} \right)^{1/4} \quad (2)$$

in which σ represents the surface tension being equal in the present case to $0.01763 \text{ kg}\cdot\text{s}^{-2}$.

- Churn flow exists for a void fraction $\langle \alpha \rangle$ lying in the interval $]0.15; 0.25]$ for which the following correlations can be used for the Zuber and Findlay drift flux model:

$$C_0 = 1.2 \text{ and } V_{vj} = V_\infty \quad (3)$$

with V_∞ given by Eq. (2).

- Slug flow exists for a void fraction $\langle \alpha \rangle$ lying in the interval $]0.25; 1]$ for which the following correlations can be used for the Zuber and Findlay drift flux model:

$$C_0 = 1.2 \text{ and } V_{vj} = V_\infty \quad (4)$$

with

$$V_\infty = 0.35 \times \left(g \times \frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_l} \times D_e \right)^{1/2} \quad (5)$$

in which $D_e = 4A / P_w$ represents the equivalent hydraulic diameter.

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The model detailed above does not consider flow regimes beyond slug flows. Although this represents a major simplification compared to the actual flow regimes actually encountered in the upper part of BWR fuel assemblies, this allows to categorize the flow regimes entirely on the knowledge of the void fraction $\langle \alpha \rangle$. For the purpose of the present work, aimed at developing a simple enough model catching the features of the modelling of BWR physics, the dependence of the flow regimes on the void fraction preserves the existence of discontinuities in the use of correlations between various flow regimes (in the present case, bubbly, slug and churn flows).

The set of equations was then solved assuming a mono-directional moving fluid in the upper direction along the fuel assembly and the spatial discretization was performed using finite differences. All volume-averaged quantities were approximated by the mean between the upper and lower area-averaged quantities for each node. Using the water tables and all the correlations mentioned above, the entire set of equations was formulated using as primary unknown variables the void fraction α , the velocity of the liquid phase v_l , the velocity of the vapor phase v_v , and the pressure \hat{P} at the node interfaces. The vector of unknown quantities, thus expressed as area-averaged quantities at node interfaces can be expressed as $\left[\langle \alpha \rangle_{1+1/2}; \dots; \langle \alpha \rangle_{N+1/2}; \langle v_l \rangle_{1+1/2}; \dots; \langle v_l \rangle_{N+1/2}; \langle v_v \rangle_{1+1/2}; \dots; \langle v_v \rangle_{N+1/2}; \langle \hat{P} \rangle_{1/2}; \dots; \langle \hat{P} \rangle_{N-1/2} \right]^T$. It has to be noted that boundary conditions for the void fraction and phasic velocities are imposed at the bottom of the fuel channel, whereas the pressure is imposed at the top of the fuel channel. As can be seen in the vectorial formulation of the unknown quantities, the void fraction and phasic velocities need to be determined from the upper interface of the lowermost node to the top of the fuel channel, whereas the pressure needs to be determined from the bottom of the fuel channel to the lower interface of the uppermost node.

2.4. Heat transfer modelling

The modelling of the heat transferred from the fuel to the coolant was performed in the simplest possible manner, while preserving the physics at hand and paying attention to the necessary coupling mechanisms existing with the physics of neutron transport and of fluid dynamics. The modelling was thus carried out by analytically solving for the radial temperature profile existing in the fuel pins and in the cladding, while representing the heat transfer through the gap via an equivalent heat transfer coefficient. The radial temperature profiles were thus radially averaged to obtain radially-averaged temperatures for the fuel pellets and for the cladding, respectively. Such an averaging process was performed for each axial node of the system, so that the axial temperature profiles could be reconstructed.

In order to estimate the heat transfer coefficient between the outer cladding and the coolant, the knowledge of the outer cladding temperature is also required and solved for explicitly.

Correlations from the open literature [12, 13] were used for the heat transfer coefficients (based on Chen's correlation), the gap conductance, and the thermal conductivities of the fuel pellet and of the cladding. Since most of these correlations depend on the temperatures being searched for, the heat transfer problem is a non-linear problem. The correlations were implemented using the radially-averaged temperatures of the fuel pellet and the cladding instead of their local values. This represents an approximation which is deemed reasonable for the purpose of the present study. The vector of unknown quantities can thus be expressed as $\left[\langle T_{f,ave} \rangle_1; \dots; \langle T_{f,ave} \rangle_N; \langle T_{c,ave} \rangle_1; \dots; \langle T_{c,ave} \rangle_N; T_{w,1}; \dots; T_{w,N} \right]^T$ where the

subscripts f , c , and w denote the fuel region, the cladding region, and the outer wall of the cladding, respectively.

3. JFNK PRECONDITIONING

3.1. Understanding the structure of the preconditioner

If one assembles the vector of the primary variables in the following manner:

$$\mathbf{x} = [\mathbf{x}^{NK}; \mathbf{x}^{FLUID}; \mathbf{x}^{TEMP}]^T \quad (6)$$

with

$$\mathbf{x}^{NK} = [\phi_{1,1}; \dots; \phi_{1,N}; \phi_{2,1}; \dots; \phi_{2,N}; k_{eff}] \quad (7)$$

$$\mathbf{x}^{FLUID} = \left[\{\underline{\alpha}\}_{1+1/2}; \dots; \{\underline{\alpha}\}_{N+1/2}; \{v_l\}_{1+1/2}; \dots; \{v_l\}_{N+1/2}; \{v_v\}_{1+1/2}; \dots; \{v_v\}_{N+1/2}; \{\hat{P}\}_{1/2}; \dots; \{\hat{P}\}_{N-1/2} \right] \quad (8)$$

$$\mathbf{x}^{TEMP} = \left[\langle T_{f,ave} \rangle_1; \dots; \langle T_{f,ave} \rangle_N; \langle T_{c,ave} \rangle_1; \dots; \langle T_{c,ave} \rangle_N; T_{w,1}; \dots; T_{w,N} \right] \quad (9)$$

the structure of the resulting Jacobian looks as depicted in Fig. 1. The Jacobian represented in this figure was estimated by first-order differentiating each of the balance equations with respect to each of the chosen primary variables.

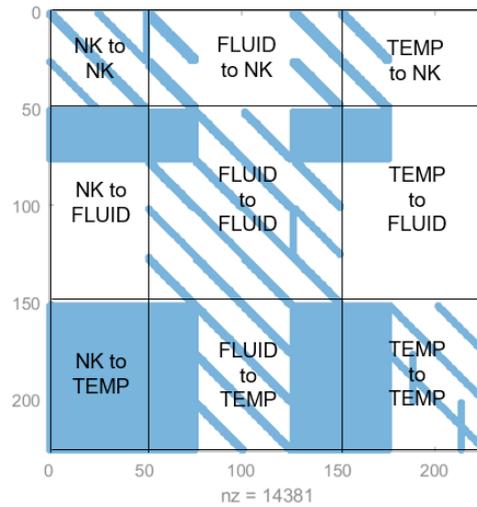


Fig. 1. Structure of the Jacobian

The Jacobian is essentially a sparse matrix. It is made of three main diagonal blocks and six off-diagonal blocks. The diagonal blocks essentially represent each of the mono-physics problems: “NK to NK” for neutron transport; “FLUID to FLUID” for fluid dynamics; and “TEMP to TEMP” for heat transfer. The off-diagonal blocks represent the coupling existing between the various physics: “NK to FLUID” and “FLUID to NK” for the coupling from neutron transport to fluid dynamics and vice versa, respectively; “NK to TEMP” and “TEMP to NK” for the coupling from neutron transport to heat transfer and vice versa, respectively; and “FLUID to TEMP” and “TEMP to FLUID” for the coupling from fluid dynamics to heat transfer and vice versa, respectively.

Although the Jacobian is primarily a sparse matrix, some dense blocks also appear in the Jacobian. They come from the normalization of the power density to a fixed power level for the entire channel. Each primary variable perturbing the estimation of the power density in one axial node has thus an effect on the entire length of the heated channel.

3.2. Effect of partial preconditioning

Although mostly sparse, the estimation of each on the non-zero terms of the Jacobian in an analytical manner represents a major effort, far bigger than developing a JFNK solution strategy itself and formulating the corresponding residuals.

The essence of preconditioning is to change the condition number of the system being solved. The effect of the preconditioning is to efficiently cluster the eigenvalues of the problem. Because of the multi-physics nature of the problem at hand, it is very likely that some of the eigenvalues are already clustered. A preconditioning related to these eigenvalues is thus unnecessary.

In the following, the effect of partially conditioning the actual problem using a numerically-evaluated Jacobian is investigated, so that it is possible to identify the parts of the system of equations that need to be preconditioned. For that purpose, the eigenvalues of the system are determined. If such eigenvalues are not clustered, a preconditioning related to these eigenvalues is thus tested using the corresponding parts of the Jacobian.

In Fig. 2, the effect of block-preconditioning each of the mono-physics problems is investigated, i.e. neglecting the cross-dependencies between the various physics. The eigenvalues of the actual Jacobian are represented on the left figure, together with the eigenvalues of each of the mono-physics problem. It can be noticed that only the eigenvalues related to fluid dynamics and neutron transport are not clustered. The middle figure gives the eigenvalues when the neutron transport, the fluid dynamics, and the heat transfer problems are separately preconditioned and when only neutron transport and the fluid dynamics problems are preconditioned. As can be seen, the effect of neglecting the preconditioning of the heat transfer problem seems to be negligible. This can also be noticed on the right figure, where the residuals are plotted as functions of the iteration number. Using a mono-physics block preconditioning greatly improves the convergence rate compared to non-preconditioning at all (for which the condition number is about 3.70×10^8). Nevertheless, not preconditioning the heat transfer problem does not seem to have any significant effect on the convergence rate. The condition numbers with heat transfer preconditioning included is 1.72×10^6 , whereas it is 1.68×10^6 when excluded.

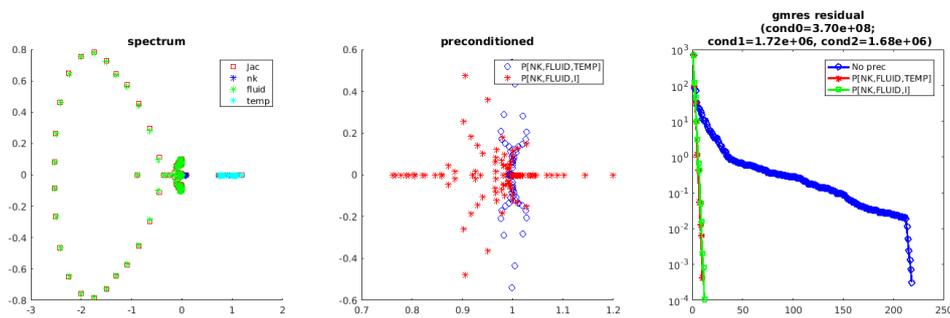


Fig. 2. Effect of preconditioning each of the physics separately.

It can thus be concluded that, in order to develop an efficient preconditioner, it is sufficient to only precondition the neutron transport problem and the fluid dynamics problem separately, without taking the cross-dependencies between any mono-physics solver into account.

Although the design of a preconditioner for the neutron transport problem does not represent a major undertaking, due to the essentially linear nature of the governing equations, the design of a preconditioner for the fluid dynamics problem constitutes a challenge. This is due to the fact that the fluid dynamics problem is a strongly non-linear problem containing many interdependencies between the primary variables. In the following, we will investigate whether all the cross-dependencies need to be retained for efficiently preconditioning the fluid dynamics problem.

Fig. 3 investigates the effect of preconditioning each of the primary variables separately in the fluid dynamics solver. As can be seen on the left figure, the eigenvalues associated to the void fraction, the liquid velocity, the vapor velocity, and the pressure are not clustered. Applying a mono-variable preconditioning leads to clustered eigenvalues, as seen in the middle figure. When looking at the convergence rate without preconditioning (with a condition number of 7.86×10^3) and with preconditioning (with a condition number of 7.51×10^3), one notices that a mono-variable preconditioning for the fluid dynamics solver increases the convergence rate, but as can be seen on the left figure, some other important eigenvalues in the actual Jacobian do not seem to be captured by a mono-variable preconditioner. This means that resolving some of the cross-dependencies seems necessary.

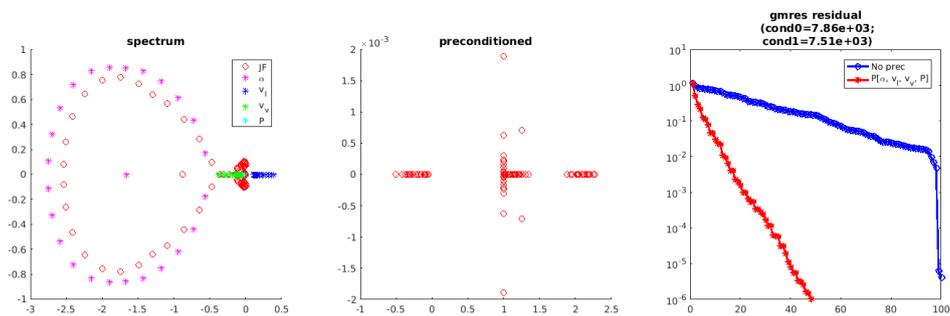


Fig. 3. Effect of preconditioning each of the fluid primary variables separately.

Several possibilities for resolving in the fluid dynamics the cross-dependencies between the primary variables were investigated:

- Void fraction and pressure treated separately, but interdependencies between phasic velocities taken into account – see Fig. 4.
- Interdependencies between the phasic velocities taken into account and interdependencies between void fraction and pressure taken into account – see Fig. 5.
- Void fraction treated separately and interdependencies between phasic velocities and pressure taken into account – see Fig. 6.
- Interdependencies between void fraction and phasic velocities taken into account and pressure treated separately – see Fig. 7.

For each of the figures, the eigenvalues of the actual Jacobian are given on the left, together with the eigenvalues associated to the corresponding hypotheses (a, b, c or d). The eigenvalues of the preconditioned systems for each of the hypotheses are represented in the middle figures, whereas the convergence rate is depicted on the right figures. As can be seen in these figures, the three first alternatives lead to identical results, with no major improvement in convergence rate compared to a mono-variable preconditioning (given in Fig. 3). This can also be noticed with the corresponding condition numbers: 9.55×10^3 for case a, 9.55×10^3 for case b, and 9.56×10^3 for case c.

On the other hand, the last preconditioner taking the cross-dependencies between the void fraction and the phasic velocities into account and accounting for pressure separately leads to much higher convergence rate with less than 10 iterations required. This can also be seen in the condition number being greatly reduced to 3.68. An examination of the eigenvalues estimated assuming cross-dependencies between the void fraction and the phasic velocities and pressure treated separately also demonstrates a perfect match between those eigenvalues and the eigenvalues of the actual full Jacobian. It is also interesting to notice that this result is in accordance with how fluid dynamics calculations are typically carried out in system codes (i.e. not relying on JFNK approaches): the void fraction and phasic velocities are solved together, assuming a given pressure distribution. Pressure is then updated and the process is repeated until convergence.

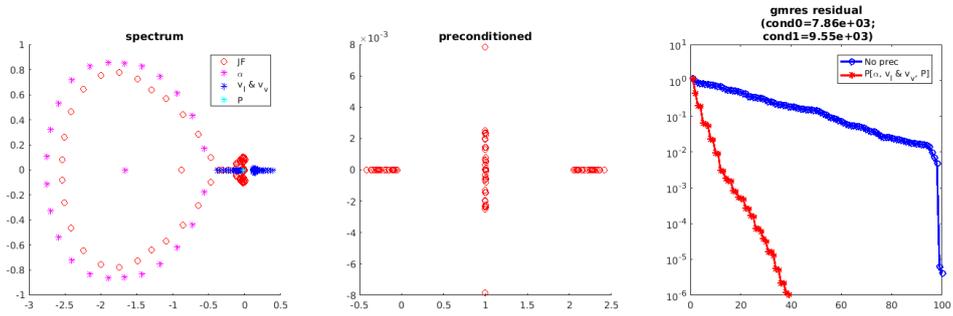


Fig. 4. Effect of preconditioning the void fraction and pressure separately and the phasic velocities together.

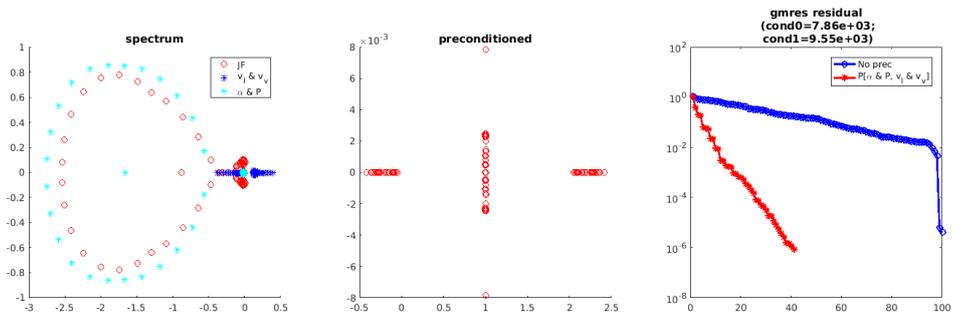


Fig. 5. Effect of preconditioning the void fraction and pressure together and the phasic velocities together.

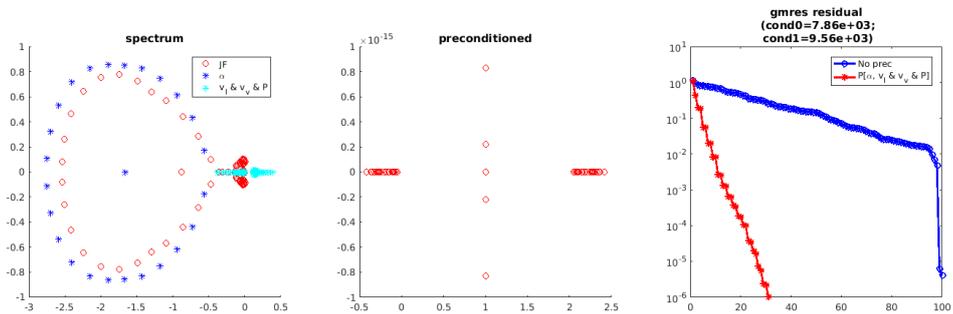


Fig. 6. Effect of preconditioning the void fraction separately and the phasic velocities and pressure together.

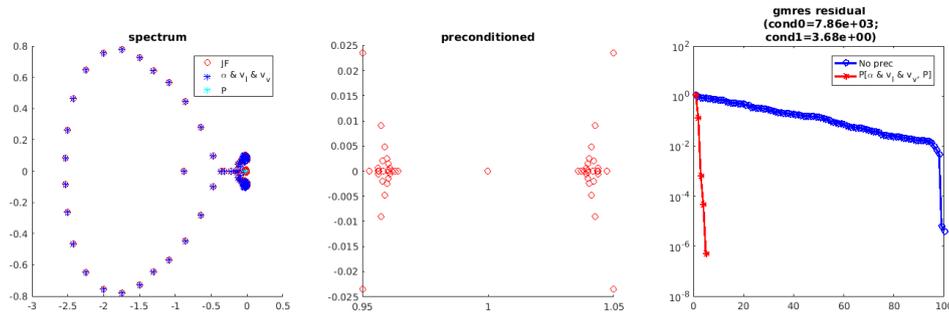


Fig. 7. Effect of preconditioning the void fraction and phasic velocities together and the pressure separately.

One can then conclude that an efficient preconditioner for a monolithic JFNK approach should be designed as follows:

- Preconditioning of the neutron transport solver separately.
- No preconditioning of the heat transfer solver.
- Preconditioning of the fluid dynamics solver separately, with the cross-dependencies between the void fraction and the phasic velocities taken into account.

4. CONCLUSIONS AND DISCUSSION

Preconditioning is a key feature when applying a JFNK method. The essence of preconditioning is to cluster the eigenvalues of the system of equations being solved, thus resulting in higher convergence rates. For the coupled model used in this study, it was found that the neutron transport model can be preconditioned separately and that no preconditioning is required for the heat transfer problem. For the fluid dynamics problem, the pressure field can be preconditioned separately, whereas the cross-dependencies between void fraction and phasic velocities need to be resolved in the preconditioner.

Although in the present model it was found that the structure of the preconditioner could be greatly simplified, preconditioning is specific to the system of equations being solved. It would be highly desirable to test whether the findings of this work are still applicable to much more sophisticated and complex models, based e.g. on three-dimensional tools using more sophisticated models simulating the interdependence of the various physics in a monolithic manner.

It should also be emphasized that even though this study indicates how to greatly simplify the preconditioner while maintaining good convergence properties, the development of a corresponding preconditioner not relying on a numerical evaluation of the partial Jacobian remains.

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