A First Finite Element Solver Shared by Neutron Diffusion,Heat Transfer and Mechanics

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INTRODUCTION

Nuclear reactor cores can be deformed by thermal expansion, irradiation effects or during particular accidental transients. These deformations are likely to impact neutron transport in all reactor types. Fast neutron reactors are nevertheless particularly sensible to these effects, because of their thermal features (large temperature gradients, potentially strong temperature variations in case of accident) and the way neutrons evolve within the core (important role played by leakages in the neutron balance, weak fraction of delayed neutrons). As a consequence, in the context of the development of the fourth generation, methodologies to take into account core distortions in deterministic neutron transport codes have been developed.

These tools can aim at providing linear feedback coefficients [1, 2], or to compute the neutron flux. In this last case, the mesh used can itself be deformed [3, 4] or not [5, 6] (a geometry projection method is then needed).

In the same time, an important effort is done on multiphysics coupling techniques, mainly between neutron transport, thermohydraulics and fuel physics. The coupling between neutron transport and structural mechanics is rarely considered, simply because less needed. Nevertheless, generic lessons can be derived from this case.

In this paper, we wish to present what we believe to be a first step toward a unified finite element solver for neutron transport and thermomechanics. Using the Newton algorithm, a complete jacobian matrix, including coupling terms between finite element discretisations, is written. A very simple application is given, on a simplified view of the Godiva experiment (which was already used in [7, 8] to study the neutron transport - thermomechanics coupling). Indeed, this kind of coupling techniques is rarely considered in nuclear reactor physics, but could lead to substantial improving of calculation time and robustness.

THE COUPLED EQUATIONS

Common notations

We consider a time-dependent problem, solved with an implicit time-scheme (Each physic impacts others at current time-step). Finite elements are used for the three coupled physics, that is to say neutron transport (diffusion), heat transfer and mechanics.

Heat transfer and neutron transport share the same elementary functions, noted ξ_i . Mechanics elementary functions are noted $\underline{\xi_i}$ and are vector quantities with the same dimension than space. In general, the number of underlinings indicates the dimension of tensors (one for vectors, two for matrix).

There is no need to give more information about the finite elements used. The methodology developed here is independent of them.

The non-deformed space domain is noted Ω_0 , the current one (deformed by mechanics) is noted Ω and the last computed one (from the last Newton iteration) Ω_p .

Neutron transport

We consider the time-dependent, multigroup neutron diffusion equations, coupled with delayed neutrons. A semi-analytical solving of the delayed neutron precursor equation leads to a linear system for the next time-step neutron flux Φ:

$$A_{ne}\Phi(t) = B_{ne}. \tag{1}$$

This linear system is generally solved with Gauss-Seidel iterations over energetic groups. For the sake of simplicity, we admit here that A_{ne} and B_{ne} are built with only three kind of matrix, K, R et M :

$$(K)^g_{ij} = \int_\Omega D^g \underline{\nabla}\xi_i . \underline{\nabla}\xi_j d\Omega, \tag{2a}$$

$$(R)_{ij} = \int_\Omega \sigma \xi_i \xi_j d\Omega, \tag{2b}$$

$$(M)_{ij} = \int_\Omega \xi_i \xi_j d\Omega. \tag{2c}$$

These matrix are impacted by mechanics through Ω, which may change, and through σ and D^g, which depend on isotopic concentrations and are therefore impacted by any expansion.

On the other hand, no Doppler effect is considered here, since it is negligible in the Godiva experiment. There is therefore no direct impact of temperature change on neutron transport.

Heat transfer

We consider the time-dependent heat transfer equation, which can be written as a linear system for the next time-step temperature $\mathcal{T}$:

$$A_{th}\mathcal{T}(t) = B_{th}, \tag{3}$$

with:

$$(A_{th})_{ij} = \frac{1}{\Delta t}\int_{\Omega_0} \rho C_p \xi_i \xi_j d\Omega_0 + \int_{\Omega_0} \lambda \nabla\xi_i \nabla\xi_j d\Omega_0, \tag{4a}$$

$$(B_{th})_i = \frac{1}{\Delta t}\int_{\Omega_0} \rho C_p \mathcal{T}(t-\Delta t)\xi_i d\Omega_0 + \int_{\Omega_0} P\xi_i d\Omega_0. \quad (4b)$$

Note that A_{th} and B_{th} are defined with Ω_0 instead of Ω. This very common simplification is known to have a very limited impact on results if distortion is small. As a consequence, heat transfer is not impacted by mechanics. However, neutron transport impacts heat transfer through the power P which is linear into the neutron flux:

$$P = \sum_{g,j} K^g \xi_j \phi_j^g. \quad (5)$$

Mechanics

For the sake of simplicity, static linear elasticity is considered here. A time-dependent equation could be used without major difficulty, but it would make the equations uselessly complicated. The considered model can be written as a linear system for the next time-step displacement U:

$$A_{me}U(t) = B_{me}, \quad (6)$$

with:

$$(A_{me})_{ij} = \int_{\Omega_0} \left(\lambda_{me} Tr(\underline{\underline{b_i}})Tr(\underline{\underline{b_j}}) + 2\mu Tr(\underline{\underline{b_i}}\cdot\underline{\underline{b_j}})\right) d\Omega_0, \quad (7a)$$

$$(B_{me})_i = \int_{\Omega_0} 3\kappa\alpha(\mathcal{T}(t) - \mathcal{T}(t=0))Tr(\underline{\underline{b_i}})d\Omega_0. \quad (7b)$$

Here again, the non-deformed space domain Ω_0 is used instead of Ω. As for heat transfer, this simplification is very common, and should not alter noticeably the results. Heat transfer impacts mechanics through the temperature $\mathcal{T}(t)$ in B_{me}. On the other hand, neutron transport has no direct feedback on mechanics.

Summary of the coupling

The coupling is summarized in Figure 1.

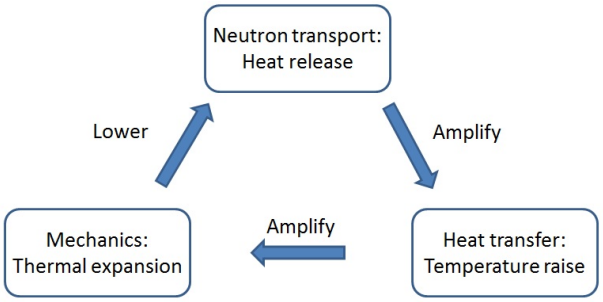

Fig. 1. Interactions between physics.

COMMON SOLVING

The Newton algorithm

Let's X be the concatenation of Φ, $\mathcal{T}$ and U. We define the global problem this way:

$$F(X) = A(X)X(t) - B(X) = 0, \quad (8)$$

with:

$$A(X) = \begin{pmatrix} A_{ne} & 0 & 0 \\ 0 & A_{th} & 0 \\ 0 & 0 & A_{me} \end{pmatrix} \text{ and } B(X) = \begin{pmatrix} B_{ne} \\ B_{th} \\ B_{me} \end{pmatrix}. \quad (9)$$

The equation (8) is not linear, as A and B depend on X. In order to solve it, we use the Newton algorithm.

The first step consists in defining the jacobian matrix J_X:

$$(J_X)_{ij} = \frac{\partial F_i}{\partial X_j} = \sum_k \frac{\partial A_{ik}}{\partial X_j} X_k + A_{ij} - \frac{\partial B_i}{\partial X_j}. \quad (10)$$

From a first guess $X^{(0)}$ of the solution, iterations are made:

- Computation of $J_{X^{(n-1)}}$ and of $F(X^{(n-1)})$,
- Solving of the linear system $J_{X^{(n-1)}}\delta X = -F(X^{(n-1)})$,
- Computation of the new approximation of X: $X^{(n)} = X^{(n-1)} + \delta X$.

Algorithm ends when $\|F(X^{(n)})\|$ is small enough.

The jacobian matrix

We give the expression of the jacobian matrix without demonstration (it will be in the final paper):

$$J_X = \begin{pmatrix} A_{ne} & 0 & C_{MN} \\ C_{NT} & A_{th} & 0 \\ 0 & C_{TM} & A_{me} \end{pmatrix}, \quad (11)$$

with

$$(C_{NT})_{ij}^g = -\int_{\Omega_0} K^g \xi_j \xi_i d\Omega_0, \quad (12a)$$

$$(C_{TM})_{ij} = -\int_{\Omega_0} 3\kappa\alpha\xi_j Tr(\underline{\underline{b_i}})d\Omega_0, \quad (12b)$$

$$(C_{MN})_{ij}^{g'\to g} = \delta_{g,g'}\sum_k \left(\frac{1}{V^g \Delta t}\int_{\Omega_p} \xi_i\xi_k Tr(\underline{\underline{b_j}})d\Omega_p\left(\phi_k^g(t) - \phi_k^g(t-\Delta t)\right) + \int_{\Omega_p} 2D_p^g (Tr(\underline{\underline{b_j}})\underline{\underline{Id}} - \underline{\underline{b_j}})\underline{\nabla}\xi_i.\underline{\nabla}\xi_k d\Omega_p\right). \quad (12c)$$

Note that C_{NT} and C_{TM} are constant. The impact of neutron transport on heat transfer, given by equations (4b) and (5), is exactly linear. This is therefore normal to find a constant bloc (C_{NT}) for this part of the jacobian. The same stands for the impact of heat transfer on mechanics (C_{TM}), given by (7b).

On the other hand, C_{MN} needs to be computed at each iteration, because of the integration over Ω_p and the presence of $\phi_k^g(t)$.

Approximations

We used two approximations in the jacobian for the following application. They are needed to simplify the computation of C_{MN}. The final result is not modified (the solved equation (8) is not modified), only the algorithm convergence speed is.

1. The first term in (12c) is simplified using:

$$\int_{\Omega_p} \bar{\xi}_i \bar{\xi}_k Tr(\underline{\underline{b}}_j) d\Omega_p \approx \delta_{i,k} \int_{\Omega_p} \bar{\xi}_i Tr(\underline{\underline{b}}_j) d\Omega_p. \qquad (13)$$

2. Ω_p is remplaced with Ω_0 in (12c).

APPLICATION

CAST3M [9], a finite element code dedicated to structural mechanics, is used for this application.

We consider a simple numerical experiment with no physical meaning: an homogeneous rectangular in 2D space. Its properties (for the three physics) are choosen arbitrary in order to reinforce the coupling.

It is divided in four rectangular meshes (we also made a one hundred meshes computation, with similar results). Elementary functions are first order polynomials. Null neutron flux and temperature bundary condition is used, and global translations and rotations are eliminated.

At $t = 0$ the system is prompt-critical, and only one time-step is computed.

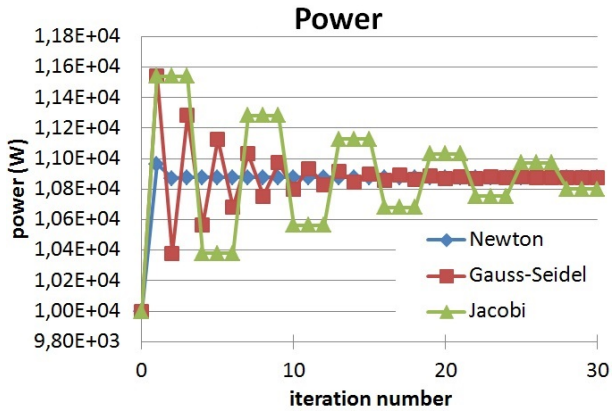

Fig. 2. Global power from different coupling techniques.

Figure 2 gives global power as function of iteration number for different coupling techniques:

- Newton: The algorithm presented in this paper;
- Gauss-Seidel: At each iteration, neutron transport is solved first, then heat transfer and finally mechanics;
- Jacobi: The three physics are solved at the same time (but independently), at each iteration.

One can see on Figure 2 that the Newton algorithm is faster than the others. Power computed by the Jacobi algorithm is modified only every three iterations because of the circularity of the coupling.

Discrepancy between current global power and converged one (after 50 Newton iterations) is plotted in Figure 3. It confirms that the Newton algorithm is the fastest one by far. The ratio of minimal discrepancy to initial global power value is about 10^{-14}, the numerical noise level.

Note that the convergence of our "Newton" algorithm is linear (whereas actual Newton algorithm convergence should be quadratic). This is due to the two approximations we made in the jacobian computation.

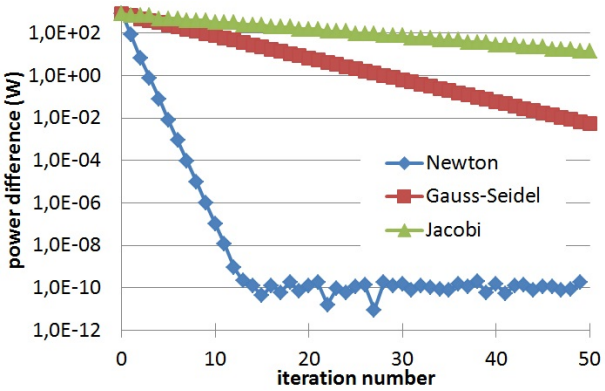

Fig. 3. Discrepancy with converge global power for different coupling techniques.

CONCLUSION

We give in this paper the exact form of the jacobian matrix for a coupling between finite element modeling of multigroup neutron diffusion, heat transfer and linear mechanics. This approach is not dependent on the application case considered or the finite element type used.

A simple application case shows that it does converge faster (in terms of iteration number) than common multisolver coupling techniques. A better robustness is also expected. It would be premature to conclude now on calculation time, work still needs to be done on the linear system solving.

The process was simplified here by the use of the same discretisation for every physics: use of the finite element method, with the same elementary functions, on the same mesh and with the same time-step. This is not required by the method. If discretisations differ, an additional step is needed, similar to a projection or a variable change. It can be taken into account in the jacobian matrix.

Future work should be undertaken to remove the two approximations we made in the jacobian computation, in order to numericaly prove the exactness of our jacobian matrix.

We wish this work to inspire development of new innovative coupling solvers.

NOMENCLATURE

α thermal expansion coefficient

Δt	Time-step length
λ	Heat conductivity
$\lambda_{me}, \mu, \kappa$	Lamé parameters, $\kappa = \lambda_{me} + (2/3)\mu$
$\mathcal{T}$	Discretized form of the temperature
Ω	Current space domain
Ω_0	Non-deformed space domain
Ω_p	Previous Newton iteration space domain
Φ	Discretized form of the neutron flux
ϕ_j^g	Scalar component of Φ
ρC_p	Volumic heat capacity
σ	A macroscopic cross-section
$\underline{\xi_i}$	Elementary function for mechanics
$\underline{\underline{b_j}}$	$= \frac{1}{2}\left(\underline{\underline{\nabla \xi_j}} + \underline{\underline{\nabla \xi_j}}^t\right)$ (elementary strain)
ξ_i	Elementary function for heat transfer and neutron transport
A	Global matrix with A_{ne}, A_{th} and A_{me} on the diagonal
A_{me}	Matrix of the mechanics problem
A_{ne}	Matrix of the neutron diffusion problem
A_{th}	Matrix of the heat transfer problem
B	Concatenation of B_{ne}, B_{th} and B_{me}
B_{me}	Right hand side of the mechanics problem
B_{ne}	Right hand side of the neutron diffusion problem
B_{th}	Right hand side of the heat transfer problem
D^g	Diffusion coefficient of group g
D_p^g	Diffusion coefficient of group g over Ω_p
F	$= AX - B$
K^g	Power production cross-section
P	Volumic power
U	Discretized form of the displacement
V^g	Speed of neutrons of group g
X	Concatenation of Φ, $\mathcal{T}$ and U

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