Analysis and application of a non-linear consistent coupling scheme to Gen4 reactor kinetic models

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Outline

Introduction (1) - Chalmers University of Technology (a)

The research done by the Division of Nuclear Engineering at Chalmers is based on the **multi-physics nature of nuclear reactors** by taking it into account from the beginning of the modeling process.

A **D**eterministic **REA**ctor **M**odeling (**DREAM**) task force was created in 2013 in order to tackle the modeling of nuclear reactors from an innovative point of view.

The Division of Nuclear Engineering has been working in the area of Gen-IV systems.

Introduction (2) - Chalmers University of Technology (b)

The project which supports the research presented here is called the "neXt generation numerical Technique for deterministic REActor Modeling" (**XTREAM**), sponsored by the **NORTHNET** (Nordic Thermal-Hydraulic Network).

The objective is to investigate, improve and develop **numerical methods** and techniques which take the **multi-scale** and **multi-physics aspects** of nuclear reactors into account.

Introduction (3) - Fundamental ideas (a)

Detailed modeling of nuclear reactors for the whole system and at all scales is still **not feasible**.

Deterministic modeling performed today relies on the **coupling** of existing codes.

To better **understand the coupling** between neutronics (**N**) and thermal-hydraulics (**TH**) it is necessary to quantify and qualify nuclear safety parameters.

Introduction (4) - Fundamental ideas (b)

Even for scoping purposes, it is particularly desirable to have means to **perform simple but realistic simulations**.

The reactor point kinetic (**PK**) **equations** represent a **system of coupled non-linear** ordinary differential **equations** characterized as stiff and which pose significant challenges when numerical solutions are applied.

At the level of initial studies, it is still worth trying to develop improved schemes for the solution of these equations.

Introduction (5) - Fundamental ideas (c)

In this context, two cases related to Gen4 reactor types are presented.

A Sodium-cooled Fast Reactor (**SFR**) kinetic model which represents a challenge due to:

- The presence of delayed neutrons, decay heat components and its feedback reactivity.
- Its fast spectrum parameters.

A Molten Salt Reactor (**MSR**) kinetic model which includes:

- A fuel that is in solution with a molten salt, adding complications to the **PK** model.
- Additional terms in the feedback reactivity.
- The presence of moving delayed neutrons and rather complicated, though simplified, **TH** model.

Coupling techniques (1) - The fundamental problem (a)

The precise modeling of a nuclear reactor is a challenge.

Accuracy VS **Computational efficiency**

Strong non-linear coupling between neutronics (**N**) and thermal-hydraulics (**TH**).

N cross section dependence on the temperature.

TH dependence via the heat source given by fission rates.

N and **TH** characteristics of SFR and MSR which add an extra layer of complexity to the modeling.

Coupling techniques (2) - The fundamental problem (b)

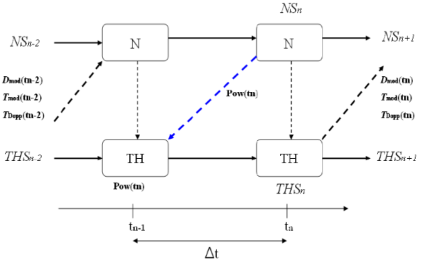
Objective of this study: To give a solid background of the methodologies used for solving the coupled physics (**N** and **TH**).

For coupling computer codes (**N** $\leftrightarrows$ **TH**) two main aspects should be considered:

- Modeling techniques.
    - Internal, external, or parallel coupling.
- Feedback management and interaction between domains.
    - Coupling through **Operator-Splitting**, implicit, etc ... techniques.

Coupling techniques (3) - Temporal coupling

- About the explicit approach, each code needs its own V&V,
- **non-linear terms** of the equations are **not fully resolved**,
- very **small time steps** usually needed to preserve accuracy.



$$NS_{t=n} = N(\Delta t, NS_{t=n-1}, THS_{t=n-1}),$$

$$THS_{t=n} = TH(\Delta t, NS_{t=n}, THS_{t=n-1}).$$

Figure: 1. Traditional Operator-Splitting (OS) coupling approach.

The unstable behavior of the **solution** is also **affected by the meshing** implemented in the models. Therefore, new fully implicit techniques are envisaged.

Coupling techniques (4) - The JFNK method (a)

Advantages of the Jacobian-Free Newton-Krylov (JFNK) method:

- Include non-linear phenomena.
- Solve the system implicitly.
- Use iterative *Krylov*-type methods requiring only the results of matrix-vector products.
- **Avoid** the sometimes very difficult and costly **evaluation of the Jacobian matrix**

Disadvantages:

- Must produce effective preconditioners.
- Convergence issues near local extrema.

Coupling techniques (5) - The JFNK method (b)

Solve the system through Newton iteration with,

$$F(u) = b - A(u) -> \mathit{residual}$$

$$J(u^k)\delta u^k = -F(u^k),$$

$$J(u)M^{-1}v \approx \frac{F(u + hM^{-1}v) - F(u)}{h},$$

$$u^{k+1} = u^k + \delta u^k.$$

$$\boldsymbol{J} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

Not needed !

Modeling (1) - The algorithm used (a)

The selected JFNK algorithm coded in NYES[1] MATLAB.

Algorithm 1 . Illustration of the JFNK algorithm.

```
.   call main_program
.       Generate the RESIDUAL functions
.         [input]=JFNK_INIT
.           while Newton_convergence > Newton_limit
.           [U]=NEWTON_METHOD(input)
.             [U]=KRYLOV_SUBSPACE(input)
.                 [output] = Jacobian_Vector(input): create JW
.                    [F(U)]=RESIDUALS(input)
.                 [JW] = JacobianApprox(input)
.                    Approx. JW = (residual' − residual)/ϵ
.                 call solver with (JW,RESIDUALS)
.             JFNK_CONVERGENCE: for Krylov
.             [W] = Update_Vector(output)
.                 Update U with the Krylov output W
.             JFNK_CONVERGENCE: for Newton
.           end
```

[1]The **N**eutronics and thermal-h**Y**draulic **E**quation **S**olver

Modeling (2) - The algorithm used (b)

Algorithm 2 Time advancement using the JFNK method.

```
.    POINT_KINETICS_NYES(): Initialization of the PK parameters
.    Generate the residual function
.    total time steps = total time / time step size
.    for t = 1:(total time steps)
.        Through the JFNK method:——————————————
.            [Feedback] = PERTURBATION(input/Solution)
.            [Solution] = NEWTON_METHOD(Feedback)
.        Through the typical OS approach:——————————
.            [N_output] = Neutronics(input)
.            [input] = FeedbackN2TH(N_output)
.            [TH_output] = Thermalyhydraulics(input)
.            [input] = FeedbackTH2N(TH_output)
.    end
```

The presented algorithms were used for both the SFR and MSR test cases.

SFR test case (1) - Description

- The PK with feedback model employs the standard neutron PK equations and couples them to 0D (core average) fuel heat conduction and fluid energy balance models via the reactivity function.
- Delayed neutrons and decay heat components are considered.
- An external step reactivity of $0.8 is inserted at t=*0* s and the resulting transient up to t=*5* s is calculated.

Table: 1. Modeling parameters used for the SFR test case.

Parameter	Value	Parameter	Value
Initial power (W)	1	Inlet temperature (C)	355
α_D (pcm/C)	-0.8841	Nominal power density ($\frac{W}{m^3}$)	4.77E8
α_C (pcm/C)	0.1263	Active core height (m)	0.8
Decay heat components	3	Neutron generation time (s)	1E-5
No. of delayed neutrons	6	Total no. of equations	**12**

SFR test case (2) - Setup

$$\begin{pmatrix} \frac{\partial N}{\partial t} \\ \frac{\partial C_1}{\partial t} \\ \frac{\partial C_2}{\partial t} \\ \frac{\partial C_3}{\partial t} \\ \frac{\partial C_4}{\partial t} \\ \frac{\partial C_5}{\partial t} \\ \frac{\partial C_6}{\partial t} \\ \frac{\partial w_1}{\partial t} \\ \frac{\partial w_2}{\partial t} \\ \frac{\partial w_3}{\partial t} \\ \frac{\partial T_{cool}}{\partial t} \\ \frac{\partial T_{fuel}}{\partial t} \end{pmatrix} = \begin{pmatrix} N \frac{\rho(T_{Dopp}, T_{coolant}) - \beta}{\Lambda} + \sum_{k=1}^{6} \lambda_k C_k \\ \frac{\beta_1 N}{\Lambda} - \lambda_1 C_1 \\ \frac{\beta_2 N}{\Lambda} - \lambda_2 C_2 \\ \frac{\beta_3 N}{\Lambda} - \lambda_3 C_3 \\ \frac{\beta_4 N}{\Lambda} - \lambda_4 C_4 \\ \frac{\beta_5 N}{\Lambda} - \lambda_5 C_5 \\ \frac{\beta_6 N}{\Lambda} - \lambda_6 C_6 \\ j_1 N - \lambda_1^j w_1 \\ j_2 N - \lambda_2^j w_2 \\ j_3 N - \lambda_3^j w_3 \\ \frac{Afuel (T_{fuel} - T_{cool})}{Aflow \, \rho_c C_{p,c} R} - \frac{2V(T_{cool} - T_{pool})}{H} \\ \frac{\Omega_{pow} N_{total}}{\rho_f C_{p,f}} - \frac{(T_{fuel} - T_{cool})}{\rho_f C_{p,f} R} \end{pmatrix}. \tag{1}$$

$$\rho(T_{fuel}, T_{cool}) = \rho_{ext.} + \alpha_D (T_{fuel} - T_{f,0}) + \alpha_C (T_{cool} - T_{c,0}). \tag{2}$$

SFR test case (3) - Results (a)

Table: 2. Preliminary results obtained for the SFR test case.

	Power Max.(-)	Time Peak(s)	T_{fuel} Max.(C)	$T_{coolant}$ Max.(C)	tstep used (s)	time CPU(s)	ϵ
Ref. [2]	4.070	0.095	790.00	600.0	0.0004	-	-
NYES	4.668	0.039	813.90	517.7	0.001	9.5	-
JFNK1	4.639	0.040	813.87	517.7	0.001	31.95	E-3
JFNK2	4.638	0.040	813.87	517.7	0.001	31.78	E-5
JFNK3	4.638	0.040	813.90	517.7	0.001	67.06	VAR
JFNK4	4.658	0.040	813.70	517.7	0.010	2.88	E-5
JFNK5	4.925	0.050	813.70	517.6	0.050	1.034	E-5
JFNK6	4.659	0.040	813.70	517.7	0.010	2.863	E-5

The traditional OS coupling followed by NYES has been valiadated against Housiadas, 2002 [8].

[2] The reference problem is based on [3].

SFR test case (4) - Results (b)

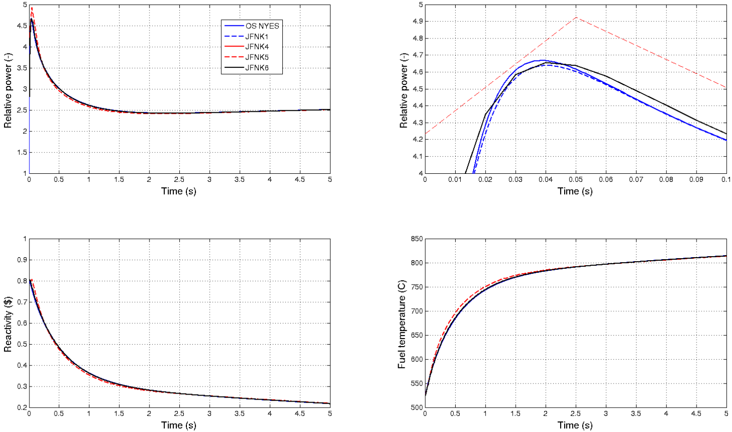


Figure: 2. Fast reactor step case. Top left: power transient; top right: power transient zoom; bottom left: total reactivity in $; bottom right: fuel temperature transient.

MSR test case (1) - Description (a)

- The PK model takes one spatial dimension into account, differences in the radial direction are neglected.
- Delayed neutrons and fission source profiles are included.
- The model is divided in three components: the core, the heat exchanger and the pipes around.
- An external step reactivity of \$1.23 is inserted at t=*0* s and the resulting transient up to t=*4* s is calculated.

Table: 3. Modeling parameters used for the MSR test case.

Parameter	Value	Parameter	Value
Initial Neutron density	1E11	Inlet temperature (C)	566.85
α_D (pcm/C)	-1.45E-5	Core areas (m^2)	0.409
Discretized elements	40	Heat exchanger area (m^2)	0.3005
Core fission source	sine	Neutron generation time (s)	3.48E-4
No. of delayed neutrons	6	Total no. of equations	**282**

MSR test case (2) - Description (b)

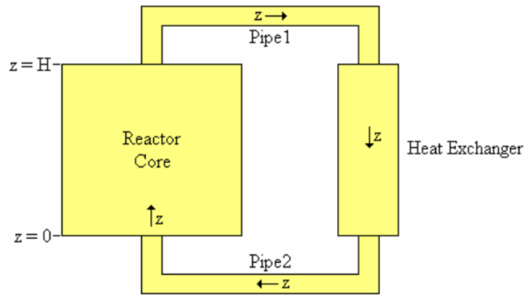


Figure: 3. Simplified to scale vertical scheme of the MSR system [3].

Note: More details about the models such as material properties, fission profiles, volumes, and neutronic parameters among others, can be given upon request [4].

[3]Figure courtesy of G. Auwerda [5]

[4]Contact M. Calleja: calleja@chalmers.se

MSR test case (3) - Description (c)

$$\frac{\partial N(t)}{\partial t} = \frac{\rho(T) + \rho_{ext}(T) - \beta}{\Lambda} N(t) + \lambda_i \frac{\int_0^H A(z)C(z,t)_i \phi(z)dz}{\int_0^H f(z)\phi(z)dz}, \quad (3)$$

$$\frac{\partial C(z,t)_i}{\partial t} = \frac{\beta_i f(z)}{\Lambda A(z)} N(t) - \lambda_i C(z,t)_i - \frac{\partial g(z,t)C(z,t)_i}{\partial z A(z)}, \quad (4)$$

$$\rho^{n+1} = \alpha_{avg}(\Sigma_j f_j T_j^{n+1} - T_0), \quad (5)$$

$$(\rho C_p)_{total}(z)\frac{\partial T(z,t)}{\partial t} = \frac{p_{fiss} f(z)}{\Lambda \nu A(z)} N(t) - (\rho C_p)_{fuel} \frac{\partial g(z,t)}{\partial A(z)} T(z,t) - \frac{h(z)O(z)}{A(z)}(T(z,t) - T_{he}), \quad (6)$$

where,

$$(\rho C_p)_{total} = \begin{cases} (\rho C_p)_{fuel} + C_{p,graphite} M_{graphite}/V_{fuelincore}, inside - core, \\ (\rho C_p)_{fuel}, outside - core. \end{cases}$$

MSR test case (4) - Results (a)

Table: 4. Preliminary results obtained for the MSR test case.

Parameter	JFNK1	JFNK2	JFNK3
Max. Power (-)	26.92	26.64	26.72
Time at peak (s)	3.85	3.20	3.18
Mixture outlet temp. (C)	575.80	580.70	581.20
Time step (s)	0.05	0.01	0.001
CPU time (s)	8.72	18.08	157.68

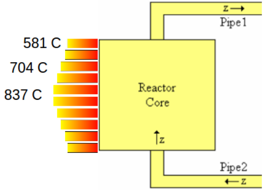


Figure: 4. Cross sectional view of the system and core temperature prediction at the end of the transient.

MSR test case (5) - Results (b)

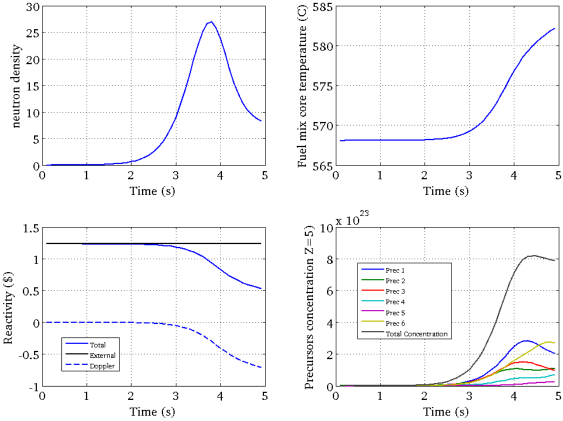


Figure: 5. MSR transient evolution for step reactivity using the JFNK2 [5] method.

[5] Refere to previous slide.

Conclusions (1)

Due to the tight coupling between neutronics and thermal-hydraulics, there is a **strong need to improve the numerical algorithms** used to solve the coupled equations.

The Jacobian-Free Newton-Krylov method seems to be a very complete and **practical algorithm** that could be implemented to any type of reactor system.

The differences found between the presented results and the reference for the SFR case, are mostly attributed to the **discrepancies between** the neutronic and thermal-hydraulic **parameters used**.

Conclusions (2) - Outlook

The NYES MATLAB **code** represents **a versatile tool** for exploring advanced numerical schemes for coupling between neutronics and thermal-hydraulics.

The process proposed in the X-TREAM project is valuable and will lead to a **better understanding of the solution** methodology in terms of JFNK.

Evaluation of the behavior of different solvers should be envisaged.

Acceleration techniques and preconditioners should be analyzed, followed by an increase in the dimensions of the model.

References

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