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# Uncertainty treatment of a coupled model of thermohydraulics and neutronics using special functions solutions

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## Abstract

This paper is a followup of the paper of Dellacherie et al. in [2], where we were able to obtain an analytic solution of a monodimensional stationary system coupling two simplified models, one solving the thermohydraulic equations, the other one solving the neutronic diffusion equation with one energy group. An approximation of the analytic solution using incomplete Jacobi elliptic integrals was derived as well as the calculation of the neutron multiplication factor  $k_{eff}$ , and we use this explicit approximation in a more general case with uncertainties on the data, which are the values of some physical functions (of the temperature  $T$ ) of the fluid characterizing the problem (namely the diffusion coefficient  $D$ , the absorption cross-section  $\Sigma_a$  and the fission cross section  $\nu\Sigma_f$ ). A thorough numerical study has been done. Using it, we demonstrate that the physical hypotheses on these function must hold for any Monte-Carlo sampling of the values, for example the values of the fission cross section must be increasing if the temperature  $T$  increases.

*Keywords:*

Ordinary differential equation, thermohydraulics, neutronics, models coupling, sensitivity analysis.

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## 1. Introduction

In this note, we recall briefly the construction of an analytic solution of the low Mach number thermohydraulic model obtained by Dellacherie et al. given in [2], detailed in [4]. In particular, the low Mach hypothesis, along with  $\rho u = D_e$  is constant, allows to rewrite the stationary internal enthalpy equation on  $z \in [0, L]$ ,  $L > 0$  being the length of the nuclear core, as

$$\rho u \frac{d}{dz} h = \mathbb{E} \Sigma_f(h) \phi(t, z) \quad (1)$$

It is coupled to the simplified neutronic model based on the diffusion approximation with one energy group

$$-\frac{d}{dz} \left[ D(h) \frac{d}{dz} \phi(z) \right] + \left[ \Sigma_a(h) - \frac{\nu \Sigma_f(h)}{k_{eff}} \right] \phi(z) = 0. \quad (2)$$

In (1) and (2), the constant  $\mathbb{E}$  is the energy released by a fission ( $\mathbb{E} > 0$  is in Joule),  $\Sigma_f(h)$  is the fission (macroscopic) cross section ( $\Sigma_f(h) > 0$  is in  $\text{m}^{-1}$ ) and  $\phi(z)$  – solution of (2) – is the scalar neutron flux

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( $\phi(z) \geq 0$  is in  $\text{m}^{-2}\cdot\text{s}^{-1}$ ). In (2),  $D(h)$  is the diffusion coefficient ( $D(h) > 0$  is in  $\text{m}$ ),  $\Sigma_a(h)$  is the absorption (macroscopic) cross section ( $\Sigma_a(h) > 0$  is in  $\text{m}^{-1}$ ) and  $\nu$  is the average number of neutron produced by a fission. At last,  $k_{eff} > 0$  is the neutron multiplication factor:  $k_{eff} \in ]0, 1[$ ,  $k_{eff} = 1$  and  $k_{eff} > 1$  means that the nuclear core is respectively subcritical, critical and supercritical.

We supplement the system (1)-(2), written for  $\phi \in C_0^2([0, L])$  (which means that  $\phi$  satisfies homogeneous Dirichlet boundary conditions  $\phi(0) = \phi(L) = 0$ )<sup>1</sup> and  $h \in C^3([0, L])$ , with the constraint  $\phi \geq 0$  on  $[0, L]$  and with the boundary conditions  $h(0) = h_e, h(L) = h_s$ . Note that the total energy released by fission of the core  $[0, L]$  is given by  $\frac{\mathbb{E}}{\nu} = D_e(h_s - h_e)$ , hence the complete set of boundary conditions yield the condition  $\int_0^L \nu \Sigma_f(h(z)) \phi(z) dz = 1$  on the flux  $\phi$ .

We constructed an analytical solution of (1)-(2) in [5], following the ideas of [4].

It is straightforward to show that this system is equivalent to following ODE on  $h$ , supplemented by the expression of  $\phi$  (the expression of  $\Psi$  is described in Lemma 2.1):

$$\begin{cases} (h')^2 = \Psi(h(z), k_{eff}), h(0) = h_e, h(L) = h_s, \\ \phi(z) = \frac{D_e}{\mathbb{E}} \frac{\sqrt{\Psi(h(z), k_{eff})}}{\nu \Sigma_f(h(z))}. \end{cases}$$

The problem is thus equivalent to<sup>2</sup> state the problem as

$$\text{find } k_{eff} \text{ such that the unique solution of } h' = \sqrt{\Psi(h(z), k_{eff}), h(0) = h_e \text{ satisfies } h(L) = h_s. \quad (3)$$

In [2], we presented a numerical method for solving this problem avoiding this ODE solving, by approximating the equation (3) by an equation which solution is a Jacobi elliptic equation (where the solution of the ODE is an incomplete Jacobi function). We use here this approximate solution to perform a sensitivity analysis on the coupling functions  $D, \Sigma_a, \Sigma_f$ .

## 2. Analytic solution and its analytic approximation

We assume in this set-up that we only know the values of  $D, \Sigma_a, \nu \Sigma_f$  at three values of the temperature (or rather the enthalpy  $h_1, h_2, h_3$ ), and that our problem is now to find a relevant approximation of the functions above in order to obtain an ODE that we can solve analytically.

Define  $X, \mathcal{Y}$  the functions of class  $C^2([h_{min}, h_{max}])$  given by

$$\left\{ \begin{array}{l} -\frac{d}{dh} \left[ D(h) \nu \Sigma_f(h) \frac{dX}{dh} \right] = \frac{\Sigma_a(h)}{\nu \Sigma_f(h)} \\ X(h_e) = X(h_s) = 0 \end{array} \right\}, \left\{ \begin{array}{l} -\frac{d}{dh} \left[ D(h) \nu \Sigma_f(h) \frac{d\mathcal{Y}}{dh} \right] = 1, \\ \mathcal{Y}(h_e) = \mathcal{Y}(h_s) = 0. \end{array} \right. \quad (4)$$

Let

$$\Psi(h, k_{eff}) = 2(\nu \Sigma_f(h))^2 \left[ X(h) - \frac{1}{k_{eff}} \mathcal{Y}(h) \right]. \quad (5)$$

<sup>1</sup>Unlike in [2], we can state this problem as a classical ODE problem.

<sup>2</sup>Note that the boundary conditions  $h'(0) = h'(L) = 0$  are built in  $\Psi$

**Lemma 2.1.** *If  $\phi, h$  are solutions of (1)-(2), with  $\phi(0) = \phi(L) = 0, h(0) = h_e, h(L) = h_s$ , then*

$$(h'(z))^2 = \Psi(h(z), k_{eff}). \quad (6)$$

*Proof.* The equation on  $\phi$  writes

$$-\frac{d}{dz}(D(h)\frac{d\phi}{dz}) + v\Sigma_f(h)\frac{d}{dh}\left[D(h)v\Sigma_f(h)\frac{dX}{dh}\right]\phi = \frac{v\Sigma_f(h)}{k_{eff}}\frac{d}{dh}\left[D(h)v\Sigma_f(h)\frac{dY}{dh}\right]\phi.$$

Replacing  $\phi$  in terms of  $h$  through  $D_e\frac{dh}{dz} = \mathbb{E}\Sigma_f(h)\phi$  yields

$$-\frac{d}{dz}(D(h)\frac{d\phi}{dz}) + \frac{D_e}{\mathbb{E}}v\frac{d}{dh}\left[D(h)v\Sigma_f(h)\frac{dX}{dh}\right]h'(z) = \frac{D_e}{\mathbb{E}}\frac{v}{k_{eff}}\frac{d}{dh}\left[D(h)v\Sigma_f(h)\frac{dY}{dh}\right]h'(z).$$

Integrating in  $z$  yields

$$-D(h)\frac{d\phi}{dz} + \frac{D_e}{\mathbb{E}}vD(h)v\Sigma_f(h)\frac{dX}{dh} = \frac{D_e}{\mathbb{E}}\frac{v}{k_{eff}}D(h)v\Sigma_f(h)\frac{dY}{dh} + C_0.$$

Multiplying by  $\frac{\phi(z)}{D(h(z))} := \frac{D_e}{\mathbb{E}D\Sigma_f(h)}h'(z)$  yields

$$-\phi\frac{d\phi}{dz} + \left(\frac{D_e}{\mathbb{E}}\right)^2v^2\frac{dX}{dh}h' = \left(\frac{D_e}{\mathbb{E}}\right)^2\frac{v^2}{k_{eff}}\frac{dY}{dh}h' + \frac{D_e}{\mathbb{E}}\frac{C_0}{D(h)\Sigma_f(h)}h'.$$

Integration from 0 to  $L$  yields  $C_0 = 0$  thanks to  $X(h_e) = Y(h_e) = 0, \phi(0) = \phi(L) = 0$  and  $X(h_s) = Y(h_s) = \phi(L) = 0$ . Hence one has

$$\left(\frac{D_e}{\mathbb{E}}\right)^2v^2X(h(z)) - \left(\frac{D_e}{\mathbb{E}}\right)^2\frac{v^2}{k_{eff}}Y(h(z)) = \frac{1}{2}(\phi(z))^2.$$

This proves Lemma 2.1. □

### 3. Interpolation

#### 3.1. The Jacobi equation

We assume that the quantities  $D, \Sigma_a, v\Sigma_f$  are only known at three values of the enthalpy  $h$ , namely  $h_1 < h_2 < h_3$ . We want to obtain a good approximation of  $D, \Sigma_a, v\Sigma_f$ . The first idea would be to interpolate  $D, \Sigma_a, v\Sigma_f$  and to solve the equation. However  $\Psi$  would be a polynomial of degree 6 or a rational fraction. The first step that we shall deal with is to use an analytic transformations in order to reduce the problem as follows:

1. we consider the polynomial  $\frac{1}{v\Sigma_f(h)D(h)}$ , of degree 2, of value  $\frac{1}{v\Sigma_f^i D^i}$  at each point  $(h_1, h_2, h_3)$ .
2. we consider the change of variable, depending on  $h_e, h_s$  as well, introducing  $u(h) = \int_0^h \frac{ds}{v\Sigma_f(s)D(s)}$

$$x(h) = -1 + 2\frac{u(h) - u(h_e)}{u(h_s) - u(h_e)}. \quad (7)$$

This provides a list of points  $-1 < x_1 < x_2 < x_3 < 1$ , associated with  $h_e < h_1 < h_2 < h_3 < h_s$ .

3. We derive the quantities  $X$  and  $Y$  such that

$$-\frac{d^2Y}{dx^2} = D\nu\Sigma_f(h(x)), -\frac{d^2X}{dx^2} = D\Sigma_a(h(x)), X(-1) = X(1) = Y(-1) = Y(1) = 0. \quad (8)$$

For example, from (??) one deduces  $-\frac{d^2X}{dx^2} = \left(\frac{u(h_s)-u(h_e)}{2}\right)^2(D\Sigma_a)(h)$ . We then derive an approximate analytical solution through the following

1. interpolate<sup>3</sup> the quantities  $D\nu\Sigma_f$  and  $D\Sigma_a$  as functions of  $x$  (using the values at  $x_1, x_2, x_3$ ). Note that these two functions are dimensionless, as well as  $x$ .
2. compute  $a_X, b_X, a_Y, b_Y$  such that, in the space  $V = \{x(1-x)(ax+b), (a,b) \in \mathbb{R}^2\}$ ,  $X$  (resp.  $Y$ ) is the solution of the variational problem (8)

3. state the approximate ODE as  $\frac{dx}{dz} = \sqrt{x(1-x) \left[ \left( a_X - \frac{a_Y}{k_{eff}} \right) x + \left( b_X - \frac{b_Y}{k_{eff}} \right) \right]}$ , which is equivalent to the

Jacobi equation of parameter  $m(k_{eff}) = -\frac{a_X - \frac{a_Y}{k_{eff}}}{b_X - \frac{b_Y}{k_{eff}}}$ :

$$\phi'(z) = \left( b_X - \frac{b_Y}{k_{eff}} \right)^{\frac{1}{2}} \sqrt{1 - m(k_{eff}) \sin^2 \phi(z)}.$$

### 3.2. Exact Solution

We choose to evaluate the length when  $k_{eff} = 1$ , using the equation

$$L = (b_X - b_Y)^{-\frac{1}{2}} \int_0^{\frac{\pi}{2}} \frac{d\phi}{\sqrt{1 - m(1) \sin^2 \phi}}. \quad (9)$$

There are many possible ways to solve the problem for  $\phi$ . In our computations we use the implementation with the Finite elements method, because of time efficiency. This is very helpful when using the MC sampling methods that require in general many samples. In this section, we test the validity of the approximation. For that matter, we computed using exact integration the solution  $\phi$  by solving the ODEs for  $X$  and  $Y$  4 and equation 5. The MATLAB symbolic package was used for all computations, the Dirichlet boundary conditions were computed up to the tenth order. To compute the length  $L_{exact}$  we used instead a trapezoidal method for integral approximations, using the interval  $[-1 + \varepsilon, 1 - \varepsilon]$  with  $\varepsilon = 5 \times 10^{-7}$  instead of  $[-1, 1]$  since  $Y - X \searrow 0$  and thus the inverse diverges in the boundaries. It is possible to compute reciprocally  $k_{eff}$  for some known value of  $L$ , however it comes to solving an inverse problem using newton method, which is more complicated given the incomplete Jacobi integral.

We show only five entries in the table for the sake of illustration. Looking at the variation of the norm, we can see that the error never exceeds 2%. The approximation of the length  $L$  is also valid with an error of  $3 \sim 4\%$ .

## 4. Analysis of sensitivity with respect to $\nu\Sigma_f$

In all this section, we consider  $\Sigma_a^i$  and  $D^i$  to be constant real values. For all numerical applications, we use  $(T_1, T_2, T_3) = (585.15, 597.15, 617.15)$ ,  $T_e = 559.15$  and  $T_s = 633.15$ . We use also  $(\Sigma_a^1, \Sigma_a^2, \Sigma_a^3) = (0.05089, 0.04989, 0.04779)$ ;  $(D_1, D_2, D_3) = (0.24799, 0.24899, 0.25198)$  and  $\nu = 2.453679$

<sup>3</sup>We can interpolate  $D\nu\Sigma_f$  or  $\frac{1}{D\nu\Sigma_f}$

$L_{exact}$	$L_{FE}$	ratio in %
42.2133	43.7919	0.8951
39.9453	41.9850	1.1525
40.7945	42.1138	0.7568
38.0065	40.7060	1.6543
41.1522	43.9041	1.4408

Table 1: The values  $L_{exact}$ ,  $L_{FE}$  and  $ratio = \frac{\|\phi_{exact} - \phi_{FE}\|_1}{\|\phi_{exact}\|_1}$  in %, for some random samples using  $\Sigma_f^1 \sim N(0.054, (1.35 \times 10^{-4})^2)$ ,  $\Sigma_f^2 \sim N(0.0516, (1.3 \times 10^{-4})^2)$  and  $\Sigma_f^3 \sim N(0.0482, (1.2 \times 10^{-4})^2)$

#### 4.1. Model with Gaussian distribution

- At first try, we made the assumption that the three values of  $\nu\Sigma_f$  come from the same distribution with variance large enough,  $\nu\Sigma_f^i \sim N(\Sigma_f^{i*}, \sigma^2)$  given  $\sigma \approx 10^{-2}$ . As abuse of notation we use  $\Sigma_f^i$  instead of  $\nu\Sigma_f^i$ , since  $\nu$  is constant. This approach tends to be wrong, as numerically the solution is no longer well defined  $\mathcal{Y} - \mathcal{X} < 0$ .
- Since the values should be sparse, we assume that the three values  $\nu\Sigma_f^i$  are random variables from three different Gaussians  $\nu\Sigma_f^i \sim N(\Sigma_f^{i*}, \sigma_i^2)$ . This actually solves partially the problem, as it only remains to tune effectively the  $\sigma_i^2$  for  $i = 1, 2, 3$  to make the problem mathematically solvable i.e.  $\mathcal{Y} - \mathcal{X} \geq 0$ .

#### 4.2. Sobol Indices

##### 4.2.1. Model with Uniform distribution

In order to perform the classic Sobol indices method we have to modify the assumption [7] about the distribution of  $\nu\Sigma_f$ . The table 2 shows a comparison between the effect of the uniform and Gaussian distribution on the  $\sigma(L)$  and  $\sigma(\|\phi\|_\infty)$ .

$\sigma_1$	$\sigma_{Unif}(\ \phi\ _\infty)$	$\sigma_{Norm}(\ \phi\ _\infty)$	$\sigma_1$	$\sigma_{Unif}(L)$	$\sigma_{Norm}(L)$
$10^{-6}$	191,67784	191,9331751	$10^{-6}$	0.8935738035	0.8647311592
$10^{-5}$	199,4398211	197,4510773	$10^{-5}$	0.9061758807	0.9265941107
$10^{-4}$	253,3425816	280,1592573	$10^{-4}$	0.997735197	1.051759978
$10^{-3}$	1812,816971	2148,394222	$10^{-3}$	5.588457635	8.663453029
$10^{-2}$	4061,028384	4560,977406	$10^{-2}$	18.52307413	19.23950532

Table 2: Effect of different scales of variation  $\sigma_1$  on the output considering the uniform and normal distributions as prior for  $\Sigma_f$  using 400 samples for each case

We deduce from the values of the output deviations that the uniform distribution performs as well as the normal distribution for small scale deviations (the case that is actually interesting for our study).

##### 4.2.2. Sobol Indices $S_1, S_2$ and $S_3$

For our estimations, we use the Python SALib library that generates low-discrepancy sequence using Saltelli's extension of the Sobol sequence [7, 8], and compute the Sobol sensitivity analysis.

The Table 3 provides the computed first order and total order Sobol indices  $S_1^1, S_2^1$  and  $S_3^1$  and  $S_1^T, S_2^T$  and  $S_3^T$  with respect to the output L. We conclude that:

- The model is not sensitive w.r.t. the variable  $\Sigma_f^2$ .
- Independence : We have  $S_1 + S_2 + S_3 \approx 99.5\%$  which means that the interaction effect can be neglected. Therefore, the variables  $\Sigma_f^1$  and  $\Sigma_f^3$  are independent.

Sobol Index	$\Sigma_f^1$	$\Sigma_f^2$	$\Sigma_f^3$
First order	0.2944	0.0365	0.6685
Bootstrap $CI_1$	0.0402	0.0174	0.0671
Total order	0.2929	0.0372	0.6731
Bootstrap $CI_T$	0.0241	0.0032	0.0491

Table 3: Computed first order Sobol indices  $S_1^1, S_2^1, S_3^1$  and total order indices  $S_1^T, S_2^T$  and  $S_3^T$  using  $\Sigma_f^1, \Sigma_f^2$  and  $\Sigma_f^3$  following from uniform distribution as priors, along with their bootstrap confidence quantiles at level 95%

#### 4.3. Parameter estimation $\sigma_1$

In this section, we show the effect of the parameter  $\sigma_1$  on the model. We keep  $\sigma_{2,3} \approx 10^{-4}$  constant. Same relationships can be induced for  $\sigma_3$ . We take  $\Sigma_f^{1*} = 0.054, \Sigma_f^{2*} = 0.0516, \Sigma_f^{3*} = 0.0482$ .

We track the behavior of the variance of  $\|\phi\|_\infty$  and L, by varying the deviation  $\sigma_1$  in the interval  $[1 \times 10^{-4}, 10 \times 10^{-4}]$  and  $[1 \times 10^{-4}, 5 \times 10^{-4}]$  respectively. We generate for each value of  $\sigma_1$  200 samples, and analyse the deviation of the outputs.

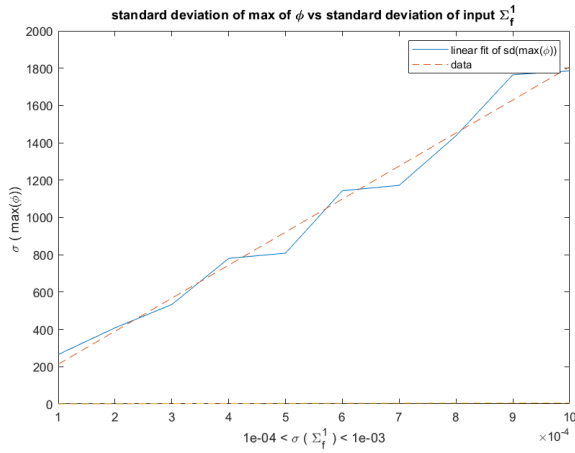


Figure 1:  $\sigma(\|\phi\|_\infty)$  vs  $\sigma_1$

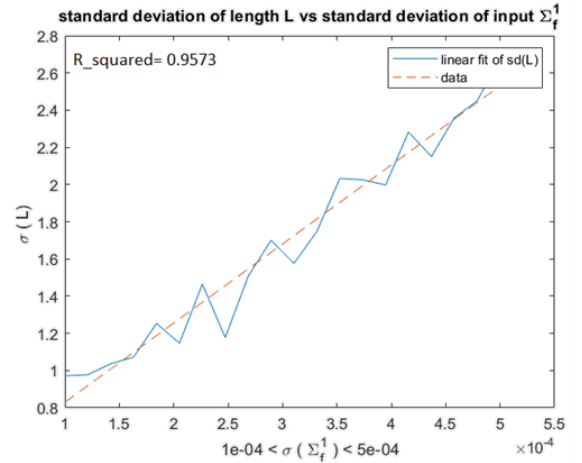


Figure 2:  $\sigma(L)$  vs  $\sigma_1$

From figures 1 and 2, we claim at level of certainty of 95% that both outputs' deviations are linearly correlated with  $\sigma_1$  having  $R_\phi^2 = 0.9811, R_L^2 = 0.9573$ , and we can write:

$$\begin{aligned} \sigma(\|\phi\|_\infty) &= \alpha_\infty \sigma_{1,3} + \beta_\infty \\ \sigma(L) &= \alpha_L \sigma_{1,3} + \beta_L, \end{aligned} \tag{10}$$

## 5. Analysis of the mean parameter $\Sigma_f^{i*}$

In all the previous sections we focused on the stability with respect to the deviation  $\sigma$  small (scale errors ( $10^{-5}$ )). In this section we will analyze the effect of the mean value of the parameters, we can interpret this analysis as of large scale errors ( $10^{-2}$ ). We use  $\sigma_{1,2,3} = 10^{-4}$ .

### 5.1. Activation point

Since we have a physical monotony condition on the values  $\Sigma_f^i$ , there is no solution for  $\Sigma_f^1 < \Sigma_f^2$ , but it remains not sufficient. To study these *activation points*  $\Sigma_f^{i,act}$ , we keep the deviation very small  $\sigma \approx 10^{-6}$  and vary  $\Sigma_f^{1*}$ . From figure 3-left/right resp. we claim at level 98% the following equality:

$$\begin{aligned}\Sigma_f^{1,act} &= 0.020798 + 0.60713\Sigma_f^{2*} \\ \Sigma_f^{3,act} &= \Sigma_f^{2*} - 0.00298\end{aligned}\tag{11}$$

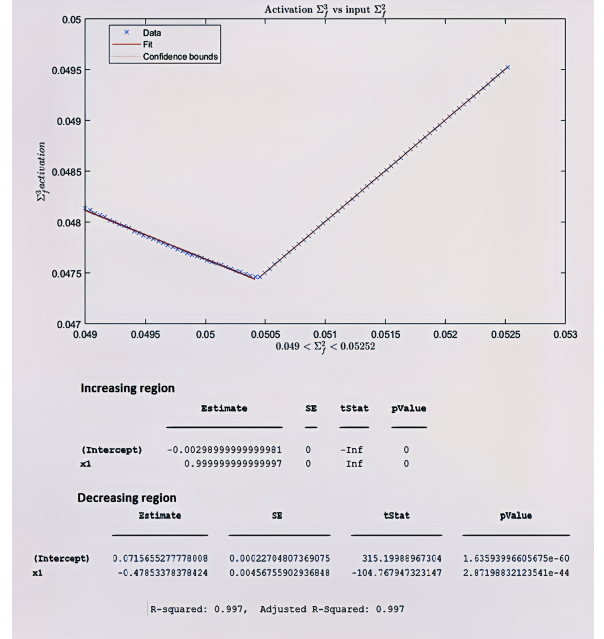
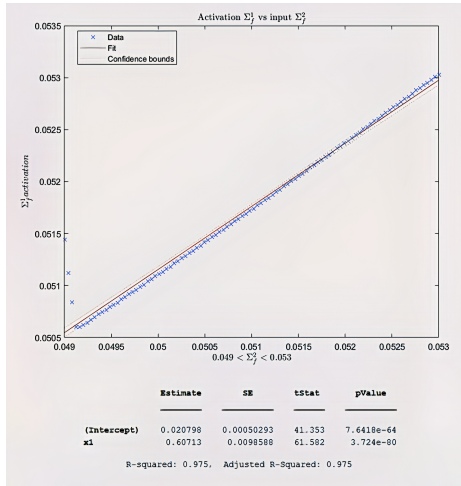


Figure 3: left: the distribution of  $\Sigma_f^{1,act}$  given different entries  $\Sigma_f^{2*} \in [0.049, 0.053]$  and its fitted linear regression with  $\Sigma_f^3 = 0.048$ , right: the distribution of  $\Sigma_f^{3,act}$  given different entries  $\Sigma_f^{2*} \in [0.049, \Sigma_f^{1,act}]$  and its fitted linear regression, with  $\Sigma_f^1 = 0.054$

These activation constraints (11) replace the monotony condition with a necessary and sufficient condition.

### 5.2. Stability w.r.t. $\Sigma_f^1$

In this section we consider the effect of the entry  $\Sigma_f^1$  on the stability of the solution. To quantify, we will take into consideration three parameters: The **norm**  $L^1([-1, 1])$  of the solution  $\phi$ , the length  $L$  and the parameter  $m$ .



From figure 4, we can see that the monotony condition  $\Sigma_f^1 > \Sigma_f^2$  corresponds to the condition  $m > 1$  with equality at  $m = 1$ . At the right of  $\Sigma_f^{1,act}$ , the linear form  $K\phi = \|\phi\|_1$  is continuous and concave. It is worth mentioning that the solutions never touch, i.e.  $\Sigma_f^{1,a} \neq \Sigma_f^{1,b} \implies \phi(\Sigma_f^{1,a}) - \phi(\Sigma_f^{1,b})$  has a constant sign. Finally, we can define a reciprocal map  $(L, \|\phi\|_1) \mapsto \Sigma_f^1$ , as the value of the norm  $\|\phi\|_1$  will pinpoint to two

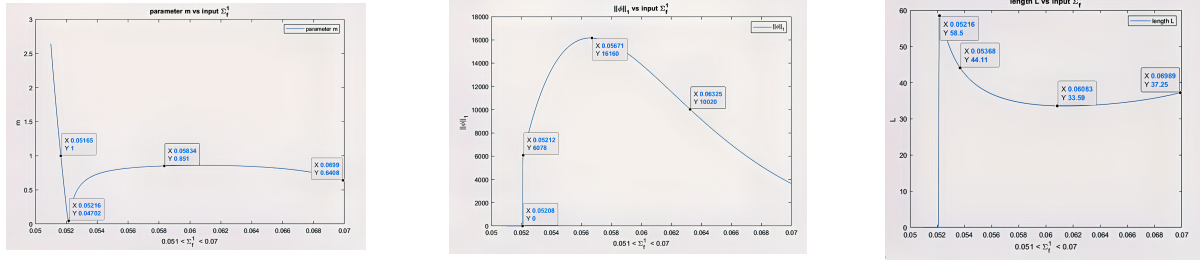


Figure 4: the evolution of the three parameters  $m$ ,  $\|\phi\|_1$  and length  $L$  with respect to the entry  $\Sigma_f^1 \in [0.05, 0.07]$

different points and the length  $L$  allows to decide the side.

It is worth mentioning that when  $\Sigma_f^1$  grows bigger, none of the variables are well controlled, in fact in the neighborhood of  $\Sigma_f^1 = 0.1$  solutions do no longer exist and  $m \nearrow 3$ . It is not a realistic error approximation, and therefore not subject of the study.

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