

CONTROL OF MODELING ERRORS IN NEUTRON TRANSPORT SIMULATIONS

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Abstract. We consider in this paper the initial-boundary value problem for the 1D neutron transport equation with isotropic scattering, set in some bounded interval with entering boundary conditions. The usual parabolic scaling yields the diffusive limit. A surrogate model, coupling transport and diffusion equations, is then introduced in order to accurately assess the value of specific quantities of interest. The control of the quality of the computation, with respect to a given quantity of interest, is performed by means of a modeling error estimation method, whereas an associated algorithm enables to adapt the coupled model if necessary.

1 INTRODUCTION

In this paper, we deal with physical problems governed by the transport equation, and more specifically with problems of neutrons transport in the study and control of nuclear plants [9, 10, 14, 8]. The linear kinetic equation which is involved, sometimes referred as linear Boltzmann's equation, takes into account physical phenomena associated with particle transport, i.e. collision, absorption, and emission; its solution enables to know the density of particles with a given velocity at a given space-time coordinate. However, discretization of the transport equation in practical applications involves a huge number of degrees of freedom (since the phase space is discretized) which is out of reach for simulation tools.

Nevertheless, when the characteristic time of previously introduced transport phenomena is small compared to the one related to the domain size and particles velocity, the transport equation may be approximated with a diffusion equation. This latter equation, which can be seen as an homogenized equation at the macroscale, is therefore used wherever it is valid in the domain, leading to model reduction and affordable computations. The resulting coarse model (denoted as the surrogate model in the following) is then made of two coupled concurrent models: (i) a mesoscale model governed by the transport equation and applied in critical subregions where a fine solution is required or in which a macroscale model is not reliable; (ii) a macroscale model governed by the diffusion equation in the complementary part of the domain.

Usually, the simulation of a physical phenomenon is performed in order to get information on a set of specific quantities of interest. From the analyst's point of view, a critical issue is therefore to know whether or not the simulation model is sufficiently relevant for the assessment of these given quantities of interest. In other words, information on modeling and discretization errors is required. During the last decade, and in the Computational Mechanics community mainly, tools have been introduced in order to assess the quality of the computerized model with respect to local quantities [15, 16]. Moreover, dedicated algorithms have also been introduced in order to adapt the surrogate model up to an acceptable error level [17, 19]. In this paper, we extend these tools to the framework of neutrons transport simulated with a coupled transport/diffusion model. We consider a simple 1D transport model with isotropic scattering, and choose the pointwise neutron density as the quantity of interest.

The paper is structured as follows: after this introduction, Section 2 describes the reference transport problem; Section 3 presents the surrogate model using the diffusion approximation; in Section 4, we recall basics on modeling error estimation and extend the methodology to the framework of neutrons transport; eventually, Section 5 shows some numerical results that illustrate performances of the method.

2 Reference model

2.1 The 3D model

We consider an open bounded domain X of \mathbb{R}^3 , with boundary ∂X , populated with neutrons. Each neutron is defined by its position \mathbf{x} , and the direction \mathbf{n} of its velocity (whose modulus v is assumed to be constant). The transport equation [9] describes the evolution of a population of neutrons in this domain occupied by a medium which is in interaction with the neutrons. This equation aims at calculating the neutron phase space density, denoted by $u(\mathbf{x}, \mathbf{n}, t)$, and defined as the probable number of neutrons at position \mathbf{x} with direction \mathbf{n} at time t per unit volume per unit solid angle.

Denoting by Σ the scattering cross section i.e. the probability of collision per unit dis-

tance travelled ($\Sigma \geq 0$), and assuming that the collision process is isotropic, the transport equation consists of finding $u(\mathbf{x}, \mathbf{n}, t)$ such that [6]:

$$\frac{\partial u}{\partial t} + v\mathbf{n} \cdot \nabla_{\mathbf{x}} u = \Sigma v \left[\frac{1}{4\pi} \int_{\Omega} u' d\Omega' - u \right] = -\sigma \mathcal{S}u \quad \forall (\mathbf{x}, \mathbf{n}, t) \in X \times \Omega \times [0, T] \quad (1)$$

where $u' = u(\mathbf{x}, \mathbf{n}', t)$, $\sigma = \sigma(\mathbf{x}) := \Sigma(\mathbf{x})v$, \mathcal{S} is the scattering operator, and Ω is the unit sphere of \mathbb{R}^3 .

In order to scale the problem, we usually introduce the parameter ε (Knudsen's number) defined as the ratio of the average distance travelled by a neutron between two successive collisions (mean free path $\lambda = 1/\Sigma$) and a characteristic length of the problem. The transport equation (1) comes down to finding $u_\varepsilon(\mathbf{x}, \mathbf{n}, t)$ such that:

$$\varepsilon \frac{\partial u_\varepsilon}{\partial t} + v\mathbf{n} \cdot \nabla_{\mathbf{x}} u_\varepsilon = -\frac{1}{\varepsilon} \sigma \mathcal{S}u_\varepsilon \quad \forall (\mathbf{x}, \mathbf{n}, t) \in X \times \Omega \times [0, T] \quad (2)$$

On the other hand, the transport problem has initial and entering boundary conditions which respectively read:

$$u_\varepsilon(\mathbf{x}, \mathbf{n}, 0) = u_I(\mathbf{x}) \quad \forall (\mathbf{x}, \mathbf{n}) \in X \times \Omega \quad ; \quad u_\varepsilon(\mathbf{x}, \mathbf{n}, t) = u_d(\mathbf{x}, \mathbf{n}, t) \quad \forall (\mathbf{x}, \mathbf{n}) \in \Gamma_- \quad (3)$$

with u_I a given non-negative function (independent of \mathbf{n}), and $\Gamma_- = \{(\mathbf{x}, \mathbf{n}) \in \partial X \times \Omega; \boldsymbol{\nu}_{\mathbf{x}} \cdot \mathbf{n} < 0\}$, $\boldsymbol{\nu}_{\mathbf{x}}$ being the outer normal of ∂X at \mathbf{x} . Of course, $u_d = 0$ if no external source is applied.

Solving system (2)+(3) is difficult and the difficulty increases as the mean free path becomes smaller. Indeed, the operator in the transport equation acts on functions with 5 variables in the phase space $X \times \Omega$, and this operator is neither self-adjoint nor elliptic, so that general variational methods can not be used. Therefore, powerful numerical methods are required in order to get useful results.

2.2 The 1D model

In several cases, equations of transport theory can be written in 1D; this is particularly the case when considering X as an infinite 2D or 3D strip, of width L on the transversal axis x and invariant by a translation perpendicular to this axis (see [12]). The 1D problem consists of finding $u_\varepsilon(x, \mu, t)$ such that:

$$\begin{aligned} \varepsilon \frac{\partial u_\varepsilon}{\partial t} + \mu v \frac{\partial u_\varepsilon}{\partial x} + \frac{1}{\varepsilon} \sigma \mathcal{S}u_\varepsilon &= 0 \quad \forall (x, \mu, t) \in]0, L[\times]-1, 1[\times [0, T] \\ u_\varepsilon(0, \mu, t) &= u_0(\mu, t) \quad \forall \mu \geq 0 \quad ; \quad u_\varepsilon(L, \mu, t) = u_L(\mu, t) \quad \forall \mu \leq 0 \quad ; \quad u_\varepsilon(x, \mu, 0) = u_I(x) \end{aligned} \quad (4)$$

with μ the cosine of the angle between Ox and the velocity. For the neutron transport with isotropic scattering that we consider, the 1D scattering operator \mathcal{S} reads:

$$\mathcal{S}u = u - \frac{1}{2} \int_{-1}^1 u(x, \mu', t) d\mu'. \quad (5)$$

The 1D transport problem (4) can also be written under the weak form:

$$\boxed{\text{Find } u_\varepsilon(x, \mu, t) \in \mathcal{U} \text{ such that } B(u_\varepsilon, v_\varepsilon) = F(v_\varepsilon) \quad \forall v_\varepsilon \in \mathcal{V}} \quad (6)$$

where \mathcal{U} , \mathcal{V} , B , and F are defined consistently (cf. [4]). In practice, (4) (or (6)) is numerically solved by means of a specific discretization in each dimension: P elements in the space domain $[0, L]$, N time steps in the time domain $[0, T]$, and K angular steps in the angular domain $[-\pi, 0]$. Using a finite differences algorithm, the discretized problem provides for an approximate solution $u_\varepsilon^{(p,k,n)}$, with $(p, k, n) \in [1, P+1] \times [1, K+1] \times [1, N+1]$.

3 The surrogate model

3.1 Diffusive limit for the transport equation

For media which have a large size compared to the characteristic lengths of the transport equation (mean free path for instance), we can obtain an approximate solution of the transport equation by means of a diffusion equation whose coefficients are derived from those of the transport equation. This is the diffusion approximation [9, 12], in which \mathbf{x} and t are the only variables, so that information about the direction \mathbf{n} of the neutrons velocity is lost.

Let us recall that mathematically speaking, one introduces a scaling parameter ε which is related to the mean free path of the particles, such that the scattering cross section is of order Σ/ε and the mean time between collisions is of order ε . We are thus led in the 1D case to the scaled system (4). Denoting the neutron density $\rho_\varepsilon(x, t) = \int_{-1}^1 u_\varepsilon(x, \mu, t) d\mu$ and the neutron current $j_\varepsilon(x, t) = \frac{1}{\varepsilon} \int_{-1}^1 \mu v u_\varepsilon(x, \mu, t) d\mu$, the two following equations can be deduced from (4):

$$\begin{aligned} \frac{\partial \rho_\varepsilon}{\partial t} + \frac{\partial j_\varepsilon}{\partial x} &= 0 && \left(\text{obtained from } \frac{1}{\varepsilon} \int_{-1}^1 \bullet d\mu \right) \\ \varepsilon^2 \frac{\partial j_\varepsilon}{\partial t} + v \frac{\partial}{\partial x} \int_{-1}^1 \mu^2 u_\varepsilon(x, \mu, t) d\mu + \sigma(x) j_\varepsilon &= 0 && \left(\text{obtained from } \int_{-1}^1 \bullet \mu d\mu \right) \end{aligned} \quad (7)$$

where \bullet stands for the 1D transport equation. Combining equations in (7), we get:

$$\frac{\partial \rho_\varepsilon}{\partial t} - \frac{\partial}{\partial x} \left[\frac{1}{\sigma(x)} \left(\varepsilon^2 \frac{\partial j_\varepsilon}{\partial t} + v \frac{\partial}{\partial x} \int_{-1}^1 \mu^2 u_\varepsilon(x, \mu, t) d\mu \right) \right] = 0. \quad (8)$$

When parameter ε is sufficiently small, the neutron angular density $u_\varepsilon(x, t)$ (and consequently $\rho_\varepsilon(x, t)$) can then be correctly approximated with its *diffusive limit*, i.e. the solution $\hat{u}(x, t)$ of the following heat equation (see [12, 6, 3, 13, 11, 20]):

$$\frac{\partial \hat{u}}{\partial t} - \frac{\partial}{\partial x} \left[\frac{2}{3\Sigma(x)} \frac{\partial \hat{u}}{\partial x} \right] = 0. \quad (9)$$

It is associated with the initial condition $\hat{u}(x, 0) = u_I(x)$. As regards boundary conditions for the diffusive limit, an accurate (order 2) approximation of the transport model is provided by the use of Robin boundary conditions [6]. These mixed boundary conditions consider that when applying homogeneous Dirichlet boundary conditions (on the microscale transport model), the neutron density actually goes to zero at some distance from the outer boundary of the macroscale diffusion model. The distance d at which it drops off to zero is called the *extrapolation length* [7]; it is related to the mean free path λ by a coefficient Λ ($d = \Lambda\lambda$) obtained by means of the conservative Milne problem, which is a stationary problem defined in a semi-infinite domain. In our case, $\Lambda \approx 0,7104$ [5].

3.2 Coupling between transport and diffusion models

When simulating transport models, a classical model reduction method consists in replacing the transport equation by the diffusion equation in parts of the domain where this latter equation is relevant. The practical importance of such a procedure is to enable one to approximate the transport problem by using a suitable (and computable) approximation provided by a tractable coupled problem. Here, we introduce the diffusive limit model in order to obtain a surrogate model of the transport model, as in [18, 21, 22]. The domain $X =]0, L[$ is divided into two parts $X_t =]0, a[$ and $X_d =]a, L[$ ($0 < a < L$). Assuming that in X_t the diffusion theory gives a poor approximation of the neutron phase space density, the proposed method consists of coupling two models: (i) the transport model used in X_t ; (ii) its diffusion approximation used in X_d . These two models are only coupled by their boundary conditions at $x = a$. The coupled problem thus reads: find the solution pair $(\tilde{u}_\varepsilon, \hat{u})$, with $\tilde{u}_\varepsilon(x, \mu, t)$ (resp. $\hat{u}(x, t)$) defined in X_t (resp. X_d), such that:

$$\begin{aligned} \varepsilon \frac{\partial \tilde{u}_\varepsilon}{\partial t} + \mu v \frac{\partial \tilde{u}_\varepsilon}{\partial x} &= -\frac{1}{\varepsilon} \sigma \mathcal{S} \tilde{u}_\varepsilon \quad \text{in } X_t \times [-1, 1] \times [0, T] \\ \tilde{u}_\varepsilon(0, \mu, t) &= u_0(\mu, t) \quad \forall \mu \geq 0 \quad ; \quad \tilde{u}_\varepsilon(a, \mu, t) = \hat{u}(a, t) \quad \forall \mu \leq 0 \end{aligned}$$

$$\begin{aligned} \frac{\partial \hat{u}}{\partial t} - \frac{\partial}{\partial x} \left(\frac{2}{3\Sigma(x)} \frac{\partial \hat{u}}{\partial x} \right) &= 0 \quad \text{in } X_d \times [0, T] \\ \hat{u}(a, t) - \frac{\Lambda \varepsilon}{\Sigma(a)} \frac{\partial \hat{u}}{\partial x}(a, t) &= 2 \int_0^1 \tilde{u}_\varepsilon(a, \mu', t) \mu' d\mu' \\ \hat{u}(L, t) + \frac{\Lambda \varepsilon}{\Sigma(L)} \frac{\partial \hat{u}}{\partial x}(L, t) &= 2 \int_{-1}^0 u_L(\mu', t) |\mu'| d\mu'. \end{aligned} \quad (10)$$

with initial conditions $\tilde{u}_\varepsilon(x, \mu, 0) = \hat{u}(x, 0) = u_I(x)$.

The model (10) coupling transport and diffusion models is denoted as the surrogate model. It can be written under the weak form:

$$\boxed{\text{Find } (\tilde{u}_\varepsilon, \hat{u}) \in \mathcal{U}_c \text{ such that } B_0((\tilde{u}_\varepsilon, \hat{u}), (\tilde{v}_\varepsilon, \hat{v})) = F_0(\tilde{v}_\varepsilon, \hat{v}) \quad \forall (\tilde{v}_\varepsilon, \hat{v}) \in \mathcal{V}_c,} \quad (11)$$

where \mathcal{U}_c , \mathcal{V}_c , B_0 , and F_0 are coherently chosen (cf. [4]).

4 Modeling error estimation and model adaptation

In this section, we introduce the methodology used to assess discretization and modeling errors that occur in numerical simulations. In our case, it will be specifically used to control the quality of the surrogate model that couples transport and diffusion equations. The error estimates and adaptive control procedures it enables to derive are targeted to specific quantities of interest and are thus referred to as *goal-oriented*. The development of such numerical tools has been the object of numerous works in recent years [15, 16, 1, 19].

4.1 Definition of the error on a quantity of interest

We assume we are interested in a specific feature of the solution u_ε , i.e. a quantity of interest denoted $Q(u_\varepsilon)$. The functional Q can generally be written under the global form:

$$Q(u_\varepsilon) = \int_0^T \int_{-1}^1 \int_0^L g(x, \mu, t) u_\varepsilon(x, \mu, t) dx d\mu dt \quad (12)$$

where g is called the *extraction function* or *extractor*.

In practical cases, u_ε is unreachable and the quantity of interest Q is approximated from a coupled problem (cf. (11)) of the form:

$$\boxed{\text{Find } u_0 \in \mathcal{U}_0 \subset \mathcal{U} \text{ such that } B_0(u_0, v_0) = F_0(v_0) \quad \forall v_0 \in \mathcal{V}_0 \subset \mathcal{V}} \quad (13)$$

with $u_0(x, \mu, t) = \tilde{u}_\varepsilon(x, \mu, t)$ in X_t and $u_0(x, \mu, t) = \hat{u}(x, t)$ in X_d . The modeling error in the quantity of interest Q we aim at assessing thus reads:

$$\mathcal{E}_{mod} = Q(u_\varepsilon) - Q(u_0). \quad (14)$$

4.2 Adjoint problem and goal-oriented error estimation

In [2], an optimal control approach is proposed in order to deal with errors on Q ; it is based on a constrained minimization framework and leads to an adjoint problem. In our case, B and Q are respectively bilinear and linear functionals so that this adjoint problem reduces to:

$$\boxed{\text{Find } p_\varepsilon \in \mathcal{V} \text{ such that } B(v_\varepsilon, p_\varepsilon) = Q(v_\varepsilon) \quad \forall v_\varepsilon \in \mathcal{V}} \quad (15)$$

Physically speaking, adjoint problem (15) is a transport problem similar to (4), except that it is reverse in time (with zero final conditions), has homogeneous outgoing boundary conditions, and is loaded by a source term represented by extractor g . It reads in its strong form:

$$\begin{aligned} -\varepsilon \frac{\partial p_\varepsilon}{\partial t} - \mu v \frac{\partial p_\varepsilon}{\partial x} + \frac{1}{\varepsilon} \sigma \mathcal{S} p_\varepsilon &= g(x, \mu, t) \quad \forall (x, \mu, t) \in]0, L[\times [-1, 1] \times [0, T] \\ p_\varepsilon(0, \mu, t) &= 0 \quad \forall \mu \leq 0 \quad ; \quad p_\varepsilon(L, \mu, t) = 0 \quad \forall \mu \geq 0 \quad ; \quad p_\varepsilon(x, \mu, T) = 0 \end{aligned} \quad (16)$$

Again, the adjoint problem is usually not tractable and needs to be replaced by a coupled problem of the form:

$$\boxed{\text{Find } p_0 \in \bar{\mathcal{V}}_0 \text{ such that } \bar{B}_0(v_0, p_0) = Q(v_0) \quad \forall v_0 \in \bar{\mathcal{V}}_0} \quad (17)$$

where \bar{B}_0 and $\bar{\mathcal{V}}_0$ are similar to B_0 and \mathcal{V}_0 except that domain X_t in which the transport model is conserved is taken a bit larger. In practice, the interface between the concurrent coupled models is placed at $x = \bar{a} := a + \Delta a$, with $\Delta a > 0$.

We can now define the following residual functionals, associated with reference and adjoint problems respectively:

$$\mathcal{R}(u_0, v) := F(v) - B(u_0, v) \quad ; \quad \bar{\mathcal{R}}(p_0, v) := Q(v) - B(v, p_0). \quad (18)$$

They represent the degree to which u_0 and p_0 fail to satisfy reference and adjoint problems (6) and (15).

In [16], a general relation is established between the modeling error in the quantity of interest and the residual functionals. In our case, it merely reads:

$$\mathcal{E}_{mod} = Q(u_\varepsilon) - Q(u_0) = \mathcal{R}(u_0, p_\varepsilon) = \mathcal{R}(u_0, p_0) + \mathcal{R}(u_0, \varepsilon_0) \quad (19)$$

where $\varepsilon_0 = p_\varepsilon - p_0$ is the error on the adjoint solution. Assuming that this error is small, a good estimate of the modeling error on Q is $\mathcal{E}_{mod} \approx \mathcal{R}(u_0, p_0)$.

4.3 Goal-oriented model adaptation

When using a surrogate model, it is fundamental to be able to adapt this surrogate model if necessary. In our case, assuming the discretization error can be neglected, the adaptation of the surrogate model consists in enlarging the region X_t in which the transport model lies, up to obtaining a sufficiently accurate value for the quantity Q .

Therefore, we come up with an adaptive greedy algorithm that aims at controlling the modeling error \mathcal{E}_{mod} within some preset error tolerance γ_{tol} . This is achieved by generating a sequence of surrogate problems with solutions (u_0^k, p_0^k) so that for some integer k_0 , the modeling error satisfies:

$$|Q(u_\varepsilon) - Q(u_0^{k_0})| \leq \gamma_{tol} \quad (20)$$

At each iteration, the goal is to reduce the global quantity $\mathcal{R}(u_0, p_0)$ by locally enriching the surrogate model, i.e. by locally switching on the transport model in the subregions where the diffusion model is not accurate enough. This is made possible by observing that the residual term $\mathcal{R}(u_0, p_0)$ is defined globally over the whole domain and can be decomposed into local contributions η_c defined over predefined subdomains (here finite elements of the mesh used to discretize the diffusion model in space). Finally, prescribing a user-defined parameter γ_a such that $0 < \gamma_a < 1$, the subdomains with contributions η_c can be switched from the diffusion model to the transport model whenever $\eta_c > \gamma_a \max_c \eta_c$.

The proposed algorithm, denoted *Goals Algorithm*, reads as follows:

1. Specify error tolerance γ_{tol} and refinement parameter γ_a .
2. Solve the primal surrogate problem for u_0 .
3. Solve the adjoint surrogate problem for p_0 .
4. Compute $\eta_{\text{est}} = \mathcal{R}(u_0, p_0)$. If

$$\left| \frac{\eta_{\text{est}}}{Q(u_0)} \right| < \gamma_{\text{tol}}$$
 then stop. Otherwise, continue to step 5.
5. Decompose the residual term $\mathcal{R}(u_0, p_0)$ into contributions η_c over predefined subdomains (can be chosen as the elements for the discretization of the diffusion model).
6. Switch subdomain with contribution η_c to transport model if $\eta_c > \gamma_a \max_c \eta_c$, and go to step 2.

Figure 1: Greedy algorithm for goal-oriented error estimation and control of modeling error.

5 Numerical results

In the following experiments, we consider a 1D diffusion problem over a time-space domain $]0, L[\times]0, T[$, with $L = 5$ and $T = 2$. Moreover, we choose $\varepsilon = 5 \cdot 10^{-2}$ and $v = 1$. On the other hand, we take zero initial conditions ($u_I(x, t) = 0$) and the following boundary conditions:

$$u_0(\mu, t) = 1 \quad \forall (\mu, t) \in [0, 1] \times [0, T] \quad ; \quad u_L(\mu, t) = 0 \quad \forall (\mu, t) \in [-1, 0] \times [0, T] \quad (21)$$

We consider a piecewise linear evolution for $\Sigma(x)$ (see Fig.2):

$$\Sigma(x) = \begin{cases} \varepsilon & \text{for } x \in [0, 2]; \\ \varepsilon + (x - 2)(1 - \varepsilon) & \text{for } x \in [2, 3]; \\ 1 & \text{for } x \in [3, 5]. \end{cases} \quad (22)$$

Therefore, $\Sigma/\varepsilon = 1$ in the transparent part of the domain.

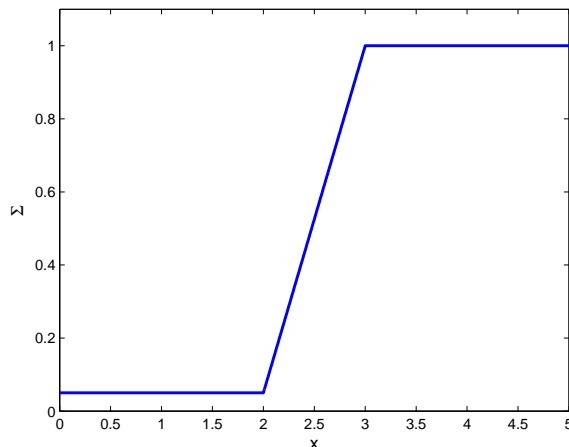


Figure 2: Evolution of the scattering cross section Σ over the space domain.

Theoretically, the diffusion limit is valid at each time-space point where: (i) the mean free path is very small compared to the characteristic size of the domain; (ii) the considered space point is far from the boundaries where data have high gradients. We thus intend that the diffusion model is valid in the left-hand side of the domain in our case. In the following, the interface between transport and diffusion models is initially placed at $a = 2$.

Even though, in practical applications, larger time steps Δt and space steps Δx are used for the discretization of the diffusion model, we use here the same values as for the discretization of the transport model. For this last model, the CFL condition reads $\Delta t < \varepsilon \Delta x$. Furthermore, in order to represent the scattering phenomenon correctly, the time step should verify $\Delta t \ll \frac{\varepsilon^2}{\sigma}$ and as regards the diffusion model, the stability condition reads $\Delta t < \frac{\Sigma \Delta x^2}{2}$. In the following, we thus choose $\Delta x = 5 \cdot 10^{-2}$ and $\Delta t = 2 \cdot 10^{-5}$.

We choose as a quantity of interest the neutron density at a given space-time point $(x_0, t_0) \in]0, L[\times]0, T]$, which leads to the extractor $g(x, t) = \delta_{x_0}(x) \delta_{t_0}(t)$. In the following, we take $x_0 = 1.5$ and $t_0 = 1.8$.

We represent in Fig. 3 (resp. Fig. 4) the quasi-exact solution of the reference (resp. adjoint) problem, obtained by means of an overkill computation.

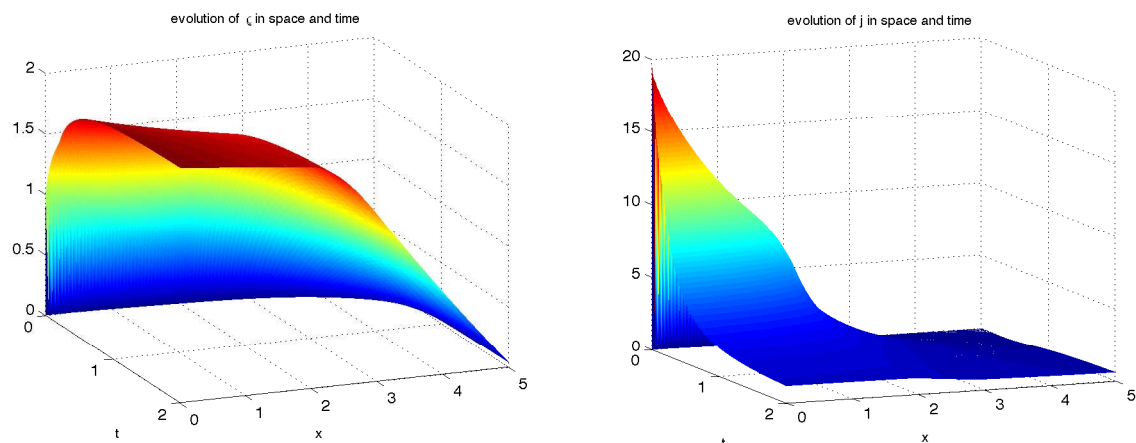


Figure 3: Quasi-exact solution of the reference problem: ρ_ε (left), j_ε (right).

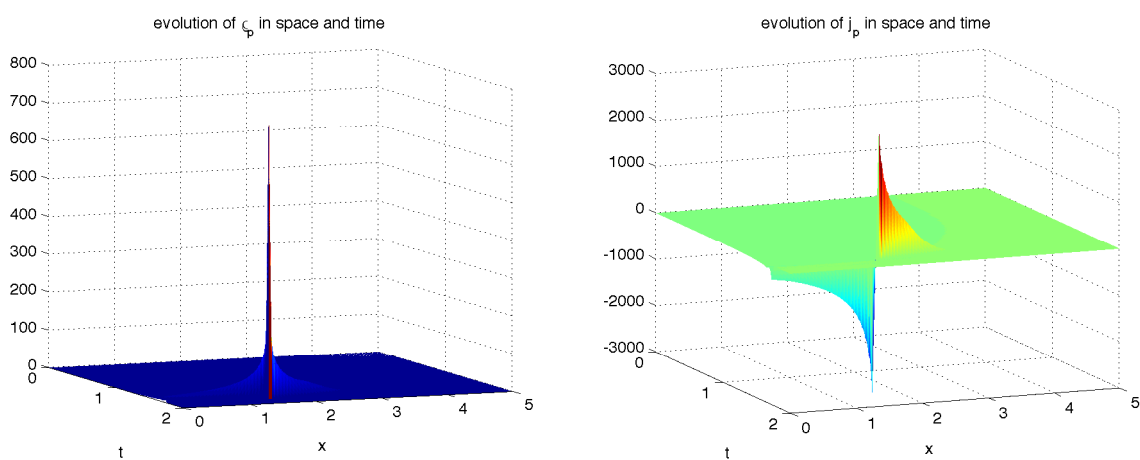


Figure 4: Quasi-exact solution of the adjoint problem: ρ_ε^p (left), j_ε^p (right).

We give in Fig. 5 the approximate solution ρ_0 (neutron density obtained by means of the coupled model with interface at $a = 2$) as well as the contributions to the error estimate $\mathcal{R}(u_0, p_0)$ over the space domain $[0, L]$.

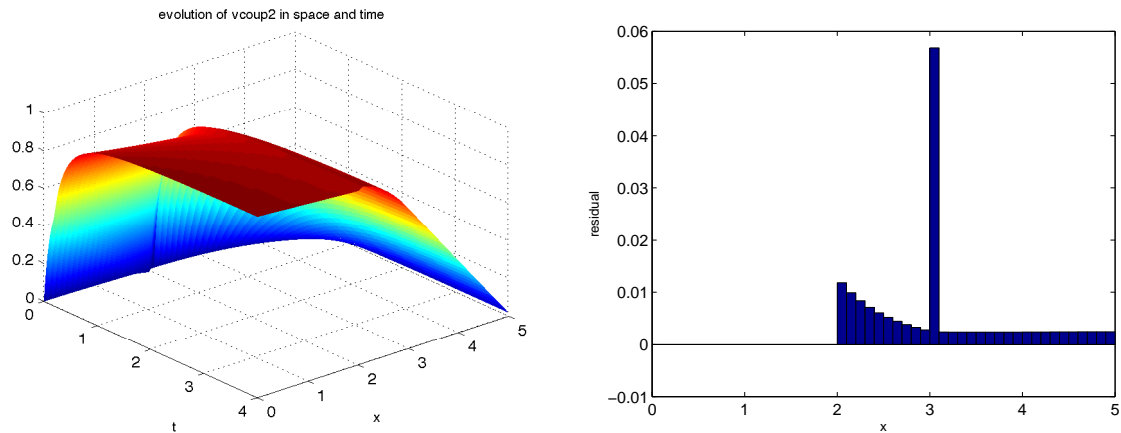


Figure 5: Approximate solution ρ_0 (left), and contributions to the error estimate (right).

After five iterations in the Goals Algorithm, we obtain a relative estimated error lower than 5% for Q , with a surrogate model whose interface is placed at $a = 3.8$.

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