Direct Problem of Gas Diffusion in Polar Firn

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Abstract

Simultaneous use of partial differential equations in conjunction with data analysis has proven to be an efficient way to obtain the main parameters of various phenomena in different areas, such as medical, biological, and ecological. In the ecological field, the study of climate change (including global warming) over the past centuries requires estimating different gas concentrations in the atmosphere, mainly CO2. Antarctic and Greenland Polar snow and ice constitute a unique archive of past climates and atmospheres.

The mathematical model of gas trapping in deep polar ice (firms) has been derived in [8, 11, 12, 13]. In this paper, we study the theoretical aspects of existence and uniqueness for the obtained, almost singular, parabolic partial differential equations.

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1 Introduction

Antarctic and Greenland Polar snow and ice constitute a unique archive of past climates and atmospheres. Based on a good understanding of the mechanisms controlling gas trapping in deep polar ice, and therefore of the processes of densification and pore closure in Firms (typically over the first hundred meters of the polar cap), several models have been derived as a result of the collaborations between the ICE3 team of the IGE and GIPSA Lab (24 publications [8] including 3 in Nature [11, 12, 13]).

Considering the mass conservation equations, the concentration $\rho_\alpha$ of a gas $\alpha$ in open pores satisfies an initial-value, time-dependent advection-diffusion partial differential equation on a one-space dimension segment $[0, z_F]$ with Dirichlet boundary condition at 0 and a mixed one at $z_F$, for $z \in (0, z_F)$, $t > 0$:

$$\left\{\begin{array}{l}
\frac{\partial}{\partial t}[\rho_\alpha f] + \frac{\partial}{\partial z}[\rho_\alpha f(v + w_{air})] + \rho_\alpha (r + \lambda) = \frac{\partial}{\partial z} \left[ D_\alpha \left( \frac{\partial \rho_\alpha}{\partial z} - \rho_\alpha \frac{M_\alpha g}{RT} \right) \right], \\
\rho_\alpha(0, t) = \rho_{\alpha \text{atm}}(t), \quad t > 0, \\
\frac{\partial \rho_\alpha}{\partial z}(z_F, t) - \frac{M_\alpha g}{RT} \rho_\alpha(z_F, t) = 0, \quad t > 0.
\end{array}\right. \quad (1)$$

where $D_\alpha(z)$ is the effective diffusion coefficient of the gas $\alpha$ in the Firn $(m^2/yr)$ and is given by

$$D_\alpha(z) = \left\{\begin{array}{ll}
D_{\text{eddy}}(z) + r_\alpha c_f D_{\text{CO2, air}}(z) & \text{if } z \leq z_{\text{eddy}}, \\
r_\alpha D_{\text{CO2, air}}(z) & \text{if } z > z_{\text{eddy}},
\end{array}\right. \quad (2)$$

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with \( z_{\text{eddy}} \), \( r_\alpha \), and \( c_f \) are known constants, and \( D_{\text{eddy}}(z), D_{\text{CO}_2, \text{air}}(z) \) diffusion coefficients. The constants of model, summarized in the Table 1, were obtained using data acquired from samples of ice cores (1) collected at two polar sites with different characteristics, one in Antarctica and the second in Greenland.

| \( z_F \) | the depth of the Firn |
| \( f \) | the average volume fraction in the open pores |
| \( v \) | the average descending speed in the Firn |
| \( w_{\text{air}} \) | the average speed of the air |
| \( \tau \) | the mass exchange rate between open and closed pores (/yr) |
| \( \lambda \) | the rate of radioactive decay (/yr) |
| \( M_\alpha \) | the molar mass of the gas (kg/mol) |
| \( g \) | the gravitational acceleration |
| \( R \) | the universal constant of ideal gases (J/mol/K) |
| \( T \) | the mean temperature of the Firn (K) |
| \( \rho_{\text{atm}}^0 \) | the concentration of gas in the atmosphere (mol/m\(^3\) of void space) |

Table 1: The description of the model’s parameters.

The main goal of this paper is to study the theoretical aspects of the underlying mathematical model, which is an almost singular, parabolic partial differential equations. We start in section 2 by deriving the semi-variational form of (1). Then, we prove in section 3 the existence and uniqueness of a solution to (1) by applying Lions’ Theorem (4, page 341).

Moreover, an Euler-Implicit in time and Finite Element Space discretization is proposed in section 4 that leads to a robust Direct problem algorithm. Finally, concluding remarks are given in section 5.

## 2 Semi-Variational Formulation

Let \( T = \{ \phi \in H^1(0, z_F) \mid \phi(0) = 0 \} \) then (1) is given in variational form by (3) where \( \rho_{\text{atm}}^o \) is denoted by \( \rho \). Using integration by parts with respect to \( z \), in addition to the initial and boundary conditions, and \( \phi(0) = 0 \), then equation (3) is reduced to (5)

\[
\langle \langle f \rho \rangle, \phi \rangle_2 + \langle \langle f \rho F \rangle, \phi \rangle_2 + \langle \rho G, \phi \rangle_2 = \langle \langle D_\alpha (\rho z - \rho M_\alpha), \phi \rangle \rangle_2 
\]

(3)

\[
f \langle \rho_t, \phi \rangle + \int f \langle \rho F \rangle = f \langle \rho z, \phi \rangle_2 + \langle \rho G, \phi \rangle_2 = \langle \rho D_\alpha (\rho z - \rho M_\alpha), \phi \rangle_2 - \langle \rho F (\rho z, \phi \rangle_2 + \langle \rho G, \phi \rangle_2 
\]

(4)

\[
f \langle \rho_t, \phi \rangle + f \langle \rho \rangle(z_F) - f \langle \rho z, \phi \rangle_2 + \langle \rho G, \phi \rangle_2 = -\langle \rho D_\alpha (\rho z - \rho M_\alpha), \phi \rangle_2
\]

(5)

where \( f > 0, M_\alpha = \frac{M_\alpha g}{RT} > 0, G = \tau + \lambda > 0 \) and \( F = v + w_{\text{air}} > 0 \) are constants. Let the bilinear form

\[
A(\rho, \phi) = \frac{G}{f} \langle \rho, \phi \rangle_2 + \int \langle D_\alpha \rho z, \phi \rangle_2 + f \langle \rho \rangle(z_F) \rho(z_F, t) - f \langle \rho z, \phi \rangle_2 - \frac{M_\alpha}{f} \langle \rho D_\alpha, \phi \rangle_2
\]

(6)

then, (5) becomes

\[
\langle \rho_t, \phi \rangle + A(\rho, \phi) = 0
\]

(7)

Seek \( \rho : [t_0, T] \times [0, z_F] \to \mathbb{R} \) such that for all \( t > t_0 \) and \( \rho(., t) \in T + \{ \rho_{\text{atm}}^o \} \)

\[
\begin{cases}
\langle \rho_t, \phi \rangle + A(\rho, \phi) = 0 \\
\rho(z, t_0) = \bar{\rho}(z)
\end{cases}
\]

(8)

where \( \bar{\rho}(z) \) is a smooth function, \( \rho(z, -\infty) = 0 \), and \( t_0 = 0 \).
3 Proof of Existence and uniqueness

To deal with the issue of existence and uniqueness, we use Lions theorem (?) that we state in section (3.1). Then, we apply it to our problem in section (3.2).

3.1 Statement of Lions Theorem ([4], page 341)

Theorem 3.1. Let \( V \) and \( H \) be 2 Hilbert spaces satisfying:

\[
V \subset H \subset V^* \quad (\text{the dual of } V),
\]

(9)

with the injection from \( V \) to \( H \) is dense and continuous.

Assuming a bilinear form \( a(\cdot, \cdot) : V \times V \to \mathbb{R} \) satisfies

\[
\begin{align*}
|a(v, w)| & \leq M \|v\|_V \|w\|_V, \\
|a(v, v)| & \geq c \|v\|_V^2 - \hat{c} \|v\|_H^2
\end{align*}
\]

(10)

then for \( u_0 \in H \) and \( F(t) \in L^2(0, T; V^*) \), the initial value problem

\[
\begin{align*}
\langle u_t, v \rangle_2 + a(u(t), v) &= \langle F(t), v \rangle, \\
u(0) &= u_0
\end{align*}
\]

(11)

admits a unique solution \( u \), satisfying:

\[
\begin{align*}
u & \in L^2(0, T; V) \cap C([0, T]; H), \\
\frac{du}{dt} & \in L^2(0, T; V^*)
\end{align*}
\]

(12)

3.2 Application of Lions Theorem to (8)

To define the Hilbert spaces \( H \) and \( V \), we first make a change of variable:

Let: \( \tilde{\rho}(\cdot, t) = \rho(\cdot, t) - \rho^{\text{atm}}(t) \)

(13)

Then \( \text{(8)} \) becomes:

\[
\begin{align*}
\langle (\tilde{\rho} + \rho^{\text{atm}}(t))_t, \phi \rangle_2 + A((\tilde{\rho} + \rho^{\text{atm}}(t)), \phi) &= 0, \\
\tilde{\rho}(0) &= \overline{\rho}(z) - \rho^{\text{atm}}(0)
\end{align*}
\]

i.e.,

\[
\begin{align*}
\langle \rho_t, \phi \rangle_2 + A(\rho, \phi) &= -\langle \rho^{\text{atm}}(t)_t, \phi \rangle_2 - A(\rho^{\text{atm}}(t), \phi) \\
\tilde{\rho}(0) &= \overline{\rho}(z) - \rho^{\text{atm}}(0)
\end{align*}
\]

(14)

with:

\[
\begin{align*}
A(\tilde{\rho}, \phi) &= \frac{1}{f} \langle \mathcal{G} \langle \tilde{\rho}, \phi \rangle_2 + \langle D_\alpha \tilde{\rho}_z - M_\alpha \tilde{\rho} D_\alpha, \phi_z \rangle_2 \rangle + \mathcal{F}(\phi(z_F) \tilde{\rho}(z_F, t) - \langle \rho, \phi_z \rangle_2) \\
A(\rho^{\text{atm}}(t), \phi) &= \rho^{\text{atm}}(t) \left( \frac{G}{f} \langle 1, \phi \rangle_2 + \mathcal{F}(\phi(z_F) - \mathcal{F}(1, \phi_z)_2 - \frac{M_\alpha}{f} \langle D_\alpha, \phi_z \rangle_2 \right)
\end{align*}
\]

(15)

Then, to be in line with Theorem 3.1, we let:

- \( u = \tilde{\rho} \)
- \( F(t, \phi) = -\langle (\rho^{\text{atm}}(t))_t, \phi \rangle_2 - A(\rho^{\text{atm}}(t), \phi) \), which for every \( t \) is a linear form in \( \phi \).
- \( u_0 = \overline{\rho}(z) - \rho^{\text{atm}}(0) \)

3
Thus \((8)\) can be stated as follows:

\[
\begin{aligned}
(u_t, \phi)_2 + A(u(t), \phi) &= F(t, \phi) \\
(\alpha, \psi)_{1,\alpha,d} &= 0
\end{aligned}
\]  

(16)

Assuming \(D_\alpha \in C[0, L]\), we define the Hilbert space

\[
H^{1,\alpha} = \{ v \in H^1 \mid \|v\|_{H^{1,\alpha}^2} < \infty \}
\]

with the following inner product and norm

\[
\langle v, w \rangle_{H^{1,\alpha}^1} = \langle D_\alpha v_z, w_z \rangle_2 + \langle v, w \rangle_2
\]

(17)

\[
\|v\|^2_{H^{1,\alpha}^1} = \left\| D^{1/2}_\alpha v_z \right\|^2_2 + \|v\|^2_2.
\]

(18)

Note that the injection of \(H^{1,\alpha} \) in \(H^1\) is continuous with:

\[
\|v\|^2_{H^{1,\alpha}^1} \leq q_{\alpha,\infty} \|v\|^2_{H^1}, \text{ where } q_{\alpha,\infty} = \max\{1, \|D_\alpha\|_\infty\}
\]

Lemma 3.2. Assumming \(1/D^{1/2}_\alpha \in L^2(0, z_F)\) with:

\[
q_\alpha = \left\| 1/D^{1/2}_\alpha \right\|_2 = \left( \int_0^{z_F} \frac{1}{D_\alpha(z)} \, dz \right)^{1/2} < \infty.
\]

(19)

then \(\{v \in H^{1,\alpha} \mid v(0) = 0\}\) is a closed subspace of \(H^{1,\alpha}\) and therefore itself a Hilbert space.

Proof. Let \(\{v_n\} \in H^{1,\alpha}_{\alpha,d}\) be a converging sequence with \(v\) its limit point, and let \(\{v'_n\} \in L^2(0, z_F)\) be a uniformly converging sequence. We need to show that \(v \in H^{1,\alpha}_{\alpha,d}\), i.e. \(v \in L^2(0, z_F), v' \in L^2(0, z_F)\) and \(v(0) = 0\). Since \(\{v_n\} \in H^{1,\alpha}_{\alpha,d}\), then \(v_n \in L^2(0, z_F), v'_n \in L^2(0, z_F)\) and \(v_n(0) = 0\) for all \(n\).

Moreover, \(\lim_{n \to \infty} v_n = v\) and \(v' = (\lim_{n \to \infty} v'_n)' = \lim_{n \to \infty} v''_n\). Thus \(v \in L^2(0, z_F)\) and \(v' \in L^2(0, z_F)\).

It remains to prove that \(v(0) = 0\) where \(\lim_{n \to \infty} \|v - v_n\|_{H^{1,\alpha}} = 0\).

\[
v(z) - v(0) = \int_0^{z} v'(s) \, ds
\]

\[
v_n(z) - v_n(0) = \int_0^{z} v'_n(s) \, ds
\]

\[
-v(0) = v_n(z) - v(z) + \int_0^{z} v'(s) - v'_n(s) \, ds
\]

\[
|v(0)| \leq |v_n(z) - v(z)| + \int_0^{z} |v'(s) - v'_n(s)| \, ds
\]

Note that

\[
\int_0^{z} |v'(s) - v'_n(s)| \, ds = \int_0^{z_F} \frac{D^{1/2}_\alpha}{D^{1/2}_\alpha} |v'(s) - v'_n(s)| \, ds = \left( \int_0^{z_F} \frac{D^{1/2}_\alpha}{D^{1/2}_\alpha} |v'(s) - v'_n(s)| \, ds \right)^{1/2} \leq q_\alpha \|v(z) - v_n(z)\|_{H^{1,\alpha}}
\]

(20)

Integrate (20) with respect to \(z\) from 0 to \(z_F\), then

\[
z_F |v(0)| \leq \int_0^{z_F} |v_n(z) - v(z)| \, dz + z_F q_\alpha \|v(z) - v_n(z)\|_{H^{1,\alpha}}
\]

\[
\leq z_F \|v_n - v\|_2 + z_F \|v - v_n\|_{H^{1,\alpha}} \left\| 1/D^{1/2}_\alpha \right\|_2
\]

(21)

Hence:

\[
|v(0) - v_n(0)| \leq (1 + q_\alpha) \|v(z) - v_n(z)\|_{H^{1,\alpha}}
\]

\[
\lim_{n \to \infty} |v(0)| \leq (1 + q_\alpha) \lim_{n \to \infty} \|v - v_n\|_{H^{1,\alpha}} = 0
\]

Thus \(v(0) = 0\). \(\square\)
In the sequel, we prove a more general estimate in $H^1_\alpha$. Specifically, one obtains the following result.

**Lemma 3.3.** Under the assumption of Lemma 3.2, one has:

$$H^1_\alpha \subset C[0, z_F] \text{ with } \|v\|_\infty \leq (1 + 2q_\alpha) \|v\|_{H^1_\alpha}, \quad \forall v \in H^1_\alpha.$$ 

*Proof.* Using the identity $v(z) = v(0) + \int_0^z v'(x) \, dx$, for $z \in [0, z_F]$, then

$$|v(z)| \leq |v(0)| + \int_0^z |v'(x)| \, dx,$$

and therefore on the basis of arguments that lead to (20) and (21), one has:

$$\int_0^z |v'(x)| \, dx \leq q_\alpha \left\| D^{1/2}_\alpha u' \right\|_2 \leq q_\alpha \|v\|_{H^1_\alpha}$$

$$|v(0)| \leq |v(z)| + \int_0^z |v'(x)| \, dx \leq |v(z)| + q_\alpha \|v\|_{H^1_\alpha}$$

$$\left\langle \left| v(0) \right|, \frac{1}{z_F} \right\rangle_2 = |v(0)| \leq \left\langle \left| v \right|, \frac{1}{z_F} \right\rangle_2 + q_\alpha \|v\|_{H^1_\alpha} \leq \|v\|_2 + q_\alpha \|v\|_{H^1_\alpha} \leq (1 + q_\alpha) \|v\|_{H^1_\alpha}$$

Hence,

$$|v(z)| \leq |v(0)| + \int_0^z |v'(x)| \, dx \leq (1 + q_\alpha) \|v\|_{H^1_\alpha} + q_\alpha \|v\|_{H^1_\alpha} \leq (1 + 2q_\alpha) \|v\|_{H^1_\alpha}.$$

\[ (22) \]

To prove existence and uniqueness, we are now in a position to use on (16) Lions Theorem (3.1) from Brezis (Theorem 10.9.). Specifically we let:

$$H = L^2(0, z_F) \text{ and } V = H^1_{\alpha,d}(0, z_F).$$

Naturally,

$$V \subset H \subset V^* \quad (V^*, \text{ the dual of } V).$$

with continuous injection from $V$ into $H$. Three results are needed:

1. **Bi-continuity of $A(\cdot, \cdot)$:**

$$\forall v, \phi \in H^1_\alpha : \ |A(v, \phi)| \leq C \|v\|_{H^1_\alpha} \cdot \|\phi\|_{H^1_\alpha},$$

2. **Weak coercivity of $A(\cdot, \cdot)$ on $H^1_{\alpha,d}$:**

$$\forall v \in H^1_{\alpha,d} : A(v, v) \geq C_0 \|v\|_{H^1_\alpha}^2 - C_2 \|v\|_2^2.$$

3. **The existence of $f(t) \in V$, such that: $F(t, \phi) = \langle f(t), \phi \rangle_{H^1_\alpha}, \forall t, \forall \phi \in H^1_\alpha.$**

where $C, C_0$ and $C_1$ are positive constants independent of $v$ and $w$. Let

$$G_f = \frac{G}{f_1} ; \quad f_1 = \frac{1}{f} ; \quad M_{\alpha,f} = \frac{M_\alpha}{f}$$

Then, $A(v, \phi) = G_f \langle v, \phi \rangle_2 + f_1 \langle D_\alpha v_z, \phi_z \rangle_2 + F \langle \phi(z_F) v(z_F) - F \langle v, \phi_z \rangle_2 - M_{\alpha,f} \langle vD_\alpha, \phi_z \rangle_2$

1. **We start by checking the bi-continuity of $A(\cdot, \cdot)$.**

Given that:

(a) $\langle v, \phi \rangle_2 \leq \|v\|_2 \cdot \|\phi\|_2 \leq \|v\|_{H^1_\alpha} \cdot \|\phi\|_{H^1_\alpha}$
We turn now to the coercivity of $A(\cdot, \cdot)$ on $H_{\alpha,d}^1$. Let $v \in H_{\alpha,d}^1$.
$$A(v, v) = G_f \langle v, v \rangle_2 + f_1 \langle D_\alpha v, v \rangle_2 + F(v, z_F) - F(v, z_F) - M_\alpha, f \langle D_\alpha v, v \rangle_2$$

Then:

(a) $G_f \langle v, v \rangle_2 + f_1 \langle D_\alpha v, v \rangle_2 \geq \min \{G_f, f_1\} \|v\|_{H_{\alpha}^1}$.

(b) $F(v, z_F) \geq 0$ since $F \geq 0$.

(c) Using Cauchy-Schwartz inequality $\langle v, v \rangle_2 \leq \|v\|_2 \cdot \|v\|_2$ we have
$$- \langle v, v \rangle_2 \geq - \|v\|_2 \cdot \|v\|_2 \geq - \frac{1}{\|D_\alpha^{1/2}v\|_2} \|D_\alpha^{1/2}v\|_2 \cdot \|v\|_2$$

(d) Similarly, $\langle D_\alpha v, v \rangle_2 \leq \|D_\alpha^{1/2}v\|_2 \cdot \|D_\alpha^{1/2}v\|_2 \leq \|D_\alpha^{1/2}v\|_2 \cdot \|D_\alpha^{1/2}v\|_2 \cdot \|v\|_2$.

This implies that for $\Gamma = \frac{F}{\|D_\alpha^{1/2}v\|_2} + M_\alpha, f \|D_\alpha^{1/2}v\|_2 > 0$
$$A(v, v) \geq \min \{G_f, f_1\} \|v\|_{H_{\alpha}^1} + \Gamma \|D_\alpha^{1/2}v\|_2 \cdot \|v\|_2$$

Using the geometric inequality: $ab \leq \frac{\epsilon}{2} a^2 + \frac{1}{2\epsilon} b^2$, for all $\epsilon > 0$, then
$$\|D_\alpha^{1/2}v\|_2 \cdot \|v\|_2 \leq \frac{\epsilon}{2} \|D_\alpha^{1/2}v\|_2^2 + \frac{1}{2\epsilon} \|v\|_2 \leq \frac{\epsilon}{2} \|v\|_{H_{\alpha}^1}^2 + \frac{1}{2\epsilon} \|v\|_2^2$$

and one obtains:
$$A(v, v) \geq \left[ \min \{G_f, f_1\} - \frac{\epsilon}{2} \right] \|v\|_{H_{\alpha}^1}^2 + \frac{\Gamma}{2\epsilon} \|v\|_2^2$$

Thus choosing $\epsilon > 0$ such that:
$$C_{0,\epsilon} = \min \{G_f, f_1\} - \frac{\epsilon}{2} = \min \{G_f, f_1\} - \frac{\epsilon}{2} \left( \left[ \frac{F}{\|D_\alpha^{1/2}v\|_2} + M_\alpha, f \|D_\alpha^{1/2}v\|_2 \right] \right) \geq 0$$

and
$$C_{1,\epsilon} = \frac{1}{2\epsilon} \Gamma = \frac{F}{2\epsilon} \frac{1}{\|D_\alpha^{1/2}v\|_2} + M_\alpha, f \|D_\alpha^{1/2}v\|_2 \geq 0$$

validates the weak coercivity.
3. Last point to prove is the existence of a function $f^*(t) \in L^2(0, T; V)$, such that:

$$F(t, \phi) = -\langle (\rho_{\text{atm}}^\alpha(t))_t, \phi \rangle_2 - A(\rho_{\text{atm}}^\alpha(t), \phi) = \langle f^*(t), \phi \rangle_{H^1_{\alpha}}, \forall \phi \in H^1_{\alpha}.$$  

Using the bi-continuity of $A(., .)$

$$|A(\rho_{\text{atm}}^\alpha(t), \phi)| \leq C \|\rho_{\text{atm}}^\alpha(t)\|_{H^1_{\alpha}} \|\phi\|_{H^1_{\alpha}} = C z_F^{1/2} |\rho_{\text{atm}}^\alpha(t)| \|\phi\|_{H^1_{\alpha}}$$

and Cauchy-Schwarz inequality on the inner product $<., .>$,

$$|\langle (\rho_{\text{atm}}^\alpha(t))_t, \phi \rangle_2| \leq \|\rho_{\text{atm}}^\alpha(t)\|_2 \|\phi\|_2 \leq z_F^{1/2} |\rho_{\text{atm}}^\alpha(t)| \|\phi\|_{H^1_{\alpha}}$$

one has:

$$|F(t, \phi)| \leq z_F^{1/2} \left[ |(\rho_{\text{atm}}^\alpha(t)| + C|\rho_{\text{atm}}^\alpha| \right] \|\phi\|_{H^1_{\alpha}} \leq \hat{C} \|\phi\|_{H^1_{\alpha}}, \quad \forall t, \forall \phi \in H^1_{\alpha} \quad (29)$$

where $\hat{C} = z_F^{1/2} \max\{1, C\} \|\rho_{\text{atm}}^\alpha\|_{1, \infty} > 0$ and $\|\rho_{\text{atm}}^\alpha\|_{1, \infty} = \max_t \left[ |(\rho_{\text{atm}}^\alpha(t)| + |\rho_{\text{atm}}^\alpha| \right]$  

**Lemma 3.4.** $F(t, \phi)$ is linear and continuous on $H^1_{\alpha}$, i.e. $F(t, \cdot) \in (H^1_{\alpha})^* \subset V^*$ for all $t$.

**Proof.** $F(t, \phi)$ is linear in $\phi$ by the linearity of the $L^2$ inner product and the bilinear form $A(\rho, \phi)$. As for the continuity of $F(t, \phi)$ in $H^1_{\alpha}$, let $\phi_n \in H^1_{\alpha}$ be a sequence converging to $\phi$, i.e.

$$\lim_{n \to \infty} \phi_n = \phi,$$

then, by (29)

$$|F(t, \phi_n) - F(t, \phi)| = |F(t, \phi_n - \phi)| \leq \hat{C} \|\phi_n - \phi\|_{H^1_{\alpha}}.$$  

Taking the limit as $n$ goes to infinity implies $\lim_{n \to \infty} |F(t, \phi_n) - F(t, \phi)| = 0$.

Thus, $\lim_{n \to \infty} F(t, \phi_n) = F(t, \phi)$.

By the Riesz-Frêchet representation and Lemma (3.4), there exists $f^*(t) \in V$ such that $\forall t$ and $\forall \phi \in H^1_{\alpha}$,

$$F(t, \phi) = \langle f^*(t), \phi \rangle_{H^1_{\alpha}}.$$  

Thus, by isometry, $\|f^*(t)\|_{H^1_{\alpha}} = \|F(t, \phi)\|_{V^*} = \sup_{\phi \in V} |F(t, \phi)| \leq \hat{C}$

Then, $f^*(t) \in L^2(0, T; V)$ since

$$\int_0^T \|f^*(t)\|^2_{H^1_{\alpha}} dt \leq T \hat{C}^2.$$

### 4 Discretization

We start first by discretizing the problem in time using Finite Difference Euler-Implicit scheme, followed by space discretization using Finite Element.

#### 4.1 Euler-Implicit Time Discretization

By integrating (3) over the temporal interval $[t, t + \Delta t]$, with $0 \leq t \leq T_{\text{end}} - \Delta t$, one reaches the following $L^2$ integral formulation:

$$\begin{align*}
\left\{ \begin{array}{l}
\langle \rho(z, t + \Delta t) - \rho(z, t), \phi \rangle_2 = -\int_t^{t+\Delta t} A(\rho(z, s), \phi(z))ds \\
\rho(z, t_0) = \mathcal{P}(z)
\end{array} \right.
\end{align*} \quad (30)$$
Such formulation is well-suited for semi and full discretization of the original system

For the full discretization of the Firn equation, the term \( \int_t^{t+\Delta t} A(\rho(z, s), \phi(z))ds \) is first discretized using an implicit right rectangular rule:

\[
\int_t^{t+\Delta t} A(\rho(z, s), \phi(z))ds = \Delta t \ A(\rho(z, t + \Delta t), \phi(z))
\]

leading to the following fully implicit scheme in time.

\[
\left\{ \begin{array}{l}
\langle \rho(z, t + \Delta t) - \rho(z, t), \phi \rangle_2 = -\Delta t \ A(\rho(z, t + \Delta t), \phi(z)) \\
\rho(z, t_0) = \rho(z) 
\end{array} \right. \tag{31}
\]

### 4.2 Finite Element Space Discretization

Let \( \mathcal{N} = \{ z_i \mid i = 1, 2, \ldots, n \} \) be the set of nodes based on the partition of \((0, z_F)\) with

\[
0 = z_1 < z_2 < \ldots < z_n = z_F
\]

and \( \mathcal{E} = \{ E_j = [z_j, z_{j+1}] \mid j = 1, 2, \ldots, n-1 \} \) the resulting set of elements.

The \( \mathbb{P}_1 \) finite element subspace \( X_N \) of \( H^1(0, z_F) \) is given by:

\[
X_n = \{ v \in C(0, z_F)|v \text{ restricted to } E_j \in \mathbb{P}_1, \ j = 1, 2, \ldots, n-1 \} \subset H^1(0, z_F),
\]

For that purpose, we let \( B_n = \{ \varphi_i | i = 1, 2, \ldots, n \} \) be a finite element basis of functions with compact support in \((0, z_F)\), i.e.,

\[
\forall v_n \in X_n : v_n(z) = \sum_{i=1}^{n} V_i \varphi_i(z), \ V_i = v_n(z_i),
\]

where \( \varphi_1(z) = \begin{cases} \frac{z_2 - z}{z_2 - z_1}, & z_1 \leq z \leq z_2 \\ \frac{z_1 - z}{z_2 - z_1}, & \text{else} \end{cases} \)

\( \varphi_2(z) = \begin{cases} \frac{z - z_{n-1}}{z_n - z_{n-1}}, & z_{n-1} \leq z \leq z_n \\ 0, & \text{else} \end{cases} \)

and \( \varphi_i(z) = \begin{cases} \frac{z - z_{i-1}}{z_i - z_{i-1}}, & z_{i-1} \leq z \leq z_i \\ \frac{z_{i+1} - z_i}{z_{i+1} - z_i}, & z_i \leq z \leq z_{i+1} \text{ for } i = 2, \ldots, n-1. \\ 0, & \text{else} \end{cases} \)

We obtain the following fully implicit Computational Model.

Given \( \rho_n(t) \in X_n \), one seeks \( \rho_n(t + \Delta t) \in X_n \), such that:

\[
\left\{ \begin{array}{l}
\langle \rho_n(t + \Delta t) - \rho_n(t), \phi \rangle_2 = -\Delta t A(\rho_n(t + \Delta t), \phi) \\
\rho_n(t_0) = \rho(t)
\end{array} \right. \tag{32}
\]

where

\[
\rho_n(t) = \rho_n^{atm}(t) \varphi_1(z) + \sum_{i=2}^{n} \rho(z_i, t) \varphi_i(z),
\]

\[
\rho_{nz}(t) = \rho_n^{atm}(t) \varphi'_1(z) + \sum_{i=2}^{n} \rho(z_i, t) \varphi'_i(z),
\]

\[
\varphi'_1(z) = \begin{cases} \frac{1}{z_i - z_{i-1}}, & z_{i-1} \leq z \leq z_i \\ \frac{1}{z_{i+1} - z_i}, & z_i \leq z \leq z_{i+1} \text{ for } i = 2, \ldots, n-1 \\ 0, & \text{else} \end{cases}
\]

\[
\varphi'_2(z) = \begin{cases} \frac{-1}{z_2 - z_1}, & z_1 \leq z \leq z_2 \\ \frac{-1}{z_n - z_{n-1}}, & z_{n-1} \leq z \leq z_n \\ 0, & \text{else} \end{cases}
\]

\[
\varphi'_n(z) = \begin{cases} \frac{1}{z_n - z_{n-1}}, & z_{n-1} \leq z \leq z_n \\ 0, & \text{else} \end{cases}
\]
Then (32) can be simplified as follows

\[
\sum_{i=2}^{n} \langle (\rho(z_i, t + \Delta t) - \rho(z_i, t)) \varphi_i, \phi \rangle_2 = - \langle (\rho_{\text{atm}}^\alpha(t + \Delta t) - \rho_{\text{atm}}^\alpha(t)) \varphi_1, \phi \rangle_2 - \Delta tA(\rho_{\text{atm}}^\alpha(t + \Delta t) \varphi_1, \phi)
\]

\[
\Delta tA \left( \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \varphi_i, \phi \right) + \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \langle \varphi_i, \phi \rangle_2 = - \Delta tA(\rho_{\text{atm}}^\alpha(t + \Delta t) \varphi_1, \phi) + \sum_{i=2}^{n} \rho(z_i, t) \langle \varphi_i, \phi \rangle_2 - \rho_{\text{atm}}^\alpha(t + \Delta t) - \rho_{\text{atm}}^\alpha(t) \langle \varphi_1, \phi \rangle_2
\]

(33)

Let \( \phi = \varphi_j \) for \( j = 2, \ldots, n \) in (33) and define the vector \( \Lambda(t) = [\rho(z_2, t), \rho(z_3, t), \ldots, \rho(z_n, t)]^T \) of length \( n-1 \), then (33) can be written in Matrix form

\[
\begin{align*}
\begin{bmatrix} M + \Delta t \left( \frac{G}{f} M + \frac{1}{f} S - K - \frac{M_a}{A} A + B \right) & \Lambda(t + \Delta t) \\
\Lambda(0) &= \Lambda \end{bmatrix} & = M \Lambda(t) - v_1(t) - \Delta t v_3(t) \\
\end{align*}
\]

(34)

by noting that for \( j = 2, \ldots, n \):

- \( \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \langle \varphi_i, \varphi_j \rangle_2 \) is equivalent to \( MA(t + \Delta t) \) where \( M \) is the \( (n-1) \times (n-1) \) Mass matrix whose entries are \( M_{i,j} = \langle \varphi_{i+1}, \varphi_{j+1} \rangle_2 \) for \( i, j = 1, 2, \ldots, n-1 \).

- similarly \( \sum_{i=2}^{n} \rho(z_i, t) \langle \varphi_i, \varphi_j \rangle_2 \) is equivalent to \( M \Lambda(t) \).

- \( (\rho_{\text{atm}}^\alpha(t + \Delta t) - \rho_{\text{atm}}^\alpha(t)) \langle \varphi_1, \varphi_j \rangle_2 \) is equivalent to the vector \( v_1(t) = (\rho_{\text{atm}}^\alpha(t + \Delta t) - \rho_{\text{atm}}^\alpha(t)) \langle \varphi_1, \varphi_2 \rangle_2 e_1 \) of length \( n-1 \), where \( e_1 = [1, 0, \ldots, 0]^T \).

- \( A \left( \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \varphi_i, \varphi_j \right) = \frac{G}{f} \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \langle \varphi_i, \varphi_j \rangle_2 + \frac{1}{f} \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \langle D_\alpha \varphi_i', \varphi_j' \rangle_2 \\
- \sum_{i=2}^{n} \mathcal{F} \rho(z_i, t + \Delta t) \langle \varphi_i, \varphi_j' \rangle_2 - \frac{M_a}{f} \sum_{i=2}^{n} \rho(z_i, t + \Delta t) \langle D_\alpha \varphi_i, \varphi_j' \rangle_2 \right)

\]

is equivalent to

\[
\left( \frac{G}{f} M + \frac{1}{f} S - K - \frac{M_a}{A} A + B \right) \Lambda(t + \Delta t) + v_2(t + \Delta t) = \left( \frac{G}{f} M + \frac{1}{f} S - K - \frac{M_a}{A} A + B \right) \Lambda(t + \Delta t)
\]

where \( v_2(t + \Delta t) = \mathcal{F} \rho(z_F, t + \Delta t) e_{n-1} = B \Lambda(t + \Delta t) \) is an \( (n-1) \times 1 \) vector of zeros except the last entry, \( B \) is an \( (n-1) \times (n-1) \) zero matrix with \( B(n-1, n-1) = \mathcal{F} \) and \( S, K, A \) are \( (n-1) \times (n-1) \) matrices whose entries for \( i, j = 1, \ldots, n-1 \) are respectively

\[
S_{i,j} = \langle D_\alpha \varphi_{i+1}', \varphi_{j+1}' \rangle_2, \quad K_{i,j} = \mathcal{F} \langle \varphi_{i+1}', \varphi_{j+1} \rangle_2, \quad A_{i,j} = \langle D_\alpha \varphi_{i+1}', \varphi_{j+1} \rangle_2.
\]

- \( A (\rho_{\text{atm}}^\alpha(t + \Delta t) \varphi_1, \varphi_j) = \rho_{\text{atm}}^\alpha(t + \Delta t) \left[ \frac{G}{f} \langle \varphi_1, \varphi_j \rangle_2 + \frac{1}{2} \langle D_\alpha \varphi_1', \varphi_j' \rangle_2 - \mathcal{F} \langle \varphi_1, \varphi_j' \rangle_2 - \frac{M_a}{f} \langle D_\alpha \varphi_1, \varphi_j' \rangle_2 \right] 

\]

is equivalent to the \( (n-1) \times 1 \) vector

\[
v_3(t) = \rho_{\text{atm}}^\alpha(t + \Delta t) \left[ \frac{G}{f} \langle \varphi_1, \varphi_2 \rangle_2 + \frac{1}{2} \langle D_\alpha \varphi_1', \varphi_2' \rangle_2 - \mathcal{F} \langle \varphi_1, \varphi_2' \rangle_2 - \frac{M_a}{f} \langle D_\alpha \varphi_1, \varphi_2' \rangle_2 \right] e_1
\]

System (34) can be expressed in a compact form by

\[
\begin{align*}
\begin{bmatrix} M + \Delta tC \end{bmatrix} \Lambda(t + \Delta t) & = M \Lambda(t) - v_b \Lambda(0) = \Lambda
\end{align*}
\]

(35)

where \( C = \frac{G}{f} M + \frac{1}{f} S - K - \frac{M_a}{A} A + B \) and \( \Delta t b = v_1(t) + \Delta t v_3(t) \), i.e. \( b = \frac{1}{\Delta t} v_1(t) + v_3(t) \).

Moreover, system (35) is solved iteratively given \( \Lambda(0) \), where at each time step a system of linear equations has to be solved using iterative methods such as Krylov Subspace methods.
5 Conclusion

In this paper, we studied theoretical and computational aspects of the Firn direct problem. This lays the ground for constructing a robust inverse problem algorithm that should extract past history diffusion coefficients of different gases of interest for understanding climate changes, and which will be the content of a forthcoming work.

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