A Computer-Assisted Proof (CAP) approach for the study of the DPCM

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1. The Diffusion Poisson Coupled Model (DPCM)

2. Rough description of a CAP approach (existence)

3. Existence of TW for the DPCM via a (first) CAP approach

4. A new CAP method based on Gegenbauer polynomials

5. Conclusions and perspectives

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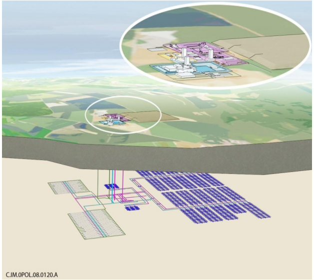
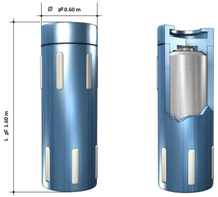
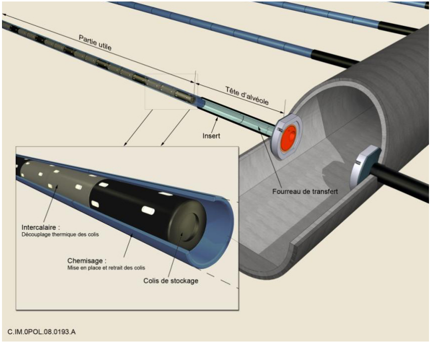
Nuclear waste repository



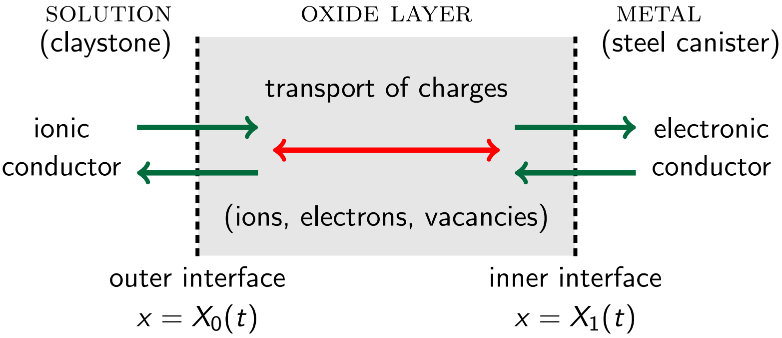


- Waste in a glass matrix, placed in a cylindrical steel canister
- Canisters placed in a micro-tunnel done in a geological layer
- Depth ≈ 500 m.



The Diffusion Coupled Model (DPCM)

❑ Bataillon *et al*, Electrochimica Acta, 2010



- → Drift-diffusion equations on the densities P, N, C
- → Poisson equation on the electrical potential Ψ
- → Nonlinear Fourier/Robin BC
- → Moving boundaries equations

The Diffusion Coupled Model (DPCM)

- Unknowns:
  - P ferric cations
  - N electrons
  - C oxygen vacancies
  - Ψ electric potential
  - X_0 and X_1 positions of the moving interfaces

- A drift-diffusion model in $[X_0(t), X_1(t)]$:

$$-\lambda^2 \partial^2_{xx} \Psi = 3P - N + 2C - 5$$

$$\begin{aligned} \partial_t P + \partial_x J_P = 0, &\quad J_P = -\partial_x P - 3P\partial_x \Psi \\ \varepsilon_N \partial_t N + \partial_x J_N = 0, &\quad J_N = -\partial_x N + N\partial_x \Psi \\ \varepsilon_C \partial_t C + \partial_x J_C = 0, &\quad J_C = -\partial_x C - 2C\partial_x \Psi \end{aligned}$$

The Diffusion Coupled Model (DPCM)

- Boundary conditions:

$$\Psi - \alpha_0 \partial_x \Psi = \Delta\Psi_0^{pzc} \qquad \text{on } x = X_0(t)$$
$$\Psi + \alpha_1 \partial_x \Psi = V - \Delta\Psi_1^{pzc} \qquad \text{on } x = X_1(t)$$

$$-J_P - PX_0'(t) = r_P^0(P, \Psi) \qquad = \beta_P^0(\Psi)P - \gamma_P^0(\Psi)$$
$$J_P + PX_1'(t) = r_P^1(P, \Psi, V) \qquad = \beta_P^1(V - \Psi)P - \gamma_P^1(V - \Psi)$$

$$\beta_P^0(x) = m_P^0 e^{-3b_P^0 x} + k_P^0 e^{3a_P^0 x} \qquad \gamma_P^0(x) = m_P^0 P^m e^{-3b_P^0 x}$$
$$\beta_P^1(x) = m_P^1 e^{-3b_P^1 x} + k_P^1 e^{3a_P^1 x} \qquad \gamma_P^1(x) = k_P^1 P^m e^{3a_P^1 x}$$

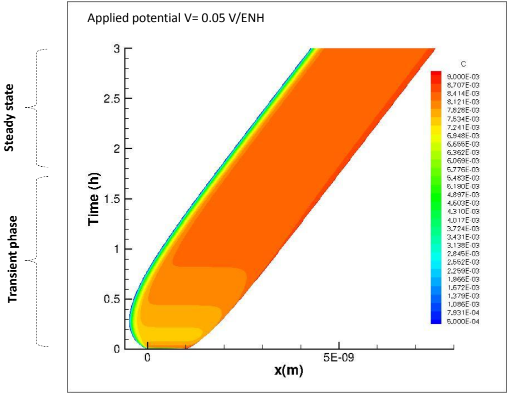
- Moving boundary equations:

$$X_0'(t) = v_d(\Psi(X_0(t)) + X_1'(t)(1 - \Pi)$$
$$X_1'(t) = -4\mu(J_C(X_1) + CX_1'(t))$$

Some results

- Existence results for a simplified model (no moving boundaries)
  - Chainais-Hillairet, Lacroix-Violet, 2012, 2015
- Convergence result of a numerical FV scheme for a simplified model (no moving boundaries)
  - Chainais-Hillairet, Colin, Lacroix-Violet, 2015
- Design of an implicit Euler in time + Finite Volume in space scheme (CALIPSO)
  - Bataillon et al, 2012

Numerical experiments: pseudo stationary state



Observations:

- → After a transient time: stationary profiles on a fixed size domain ℓ and $X_0'(t) = X_1'(t) = \delta$ a common velocity
- → Existence of pseudo stationary state if $\partial_x^2 \Psi = 0$
  - ❑ Chainais-Hilliaret, Gallouët, 2016

Two (complementary) strategies to study the DPCM

- Derive a "thermodynamically" consistent version of the DPCM
  - Merlet, Venel, Z., 2019, 2025
  - Cancès, Chainais-Hillairet, Merlet, Raimondi, Venel, 2023
  - Cancès, Chainais-Hillairet, Dupouy, 2025
  - Bataillon, Cancès, Chainais-Hillairet, Raimondi, Venel, 2026

- Apply a CAP approach in order to obtain existence results for the DPCM (or its alternative version)
  - Breden, Chainais-Hillairet, Z., 2021
  - Breden, Cadiot, Z., 2026

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Question. A CAP approach?

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Framework

- Assume that we are given a function F defined on a Banach space $\mathcal{X}$, together with an approximate zero $\bar{x}$ of F:

$$F(\bar{x}) \simeq 0.$$

Main goal

Find $r > 0$ s.t. $F(x) = 0$ for some $\|x - \bar{x}\|_{\mathcal{X}} \leq r$

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- Newton method: prove that $I - DF(\bar{x})^{-1}F$ admits a fixed point in $B_r(\bar{x})$

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- Newton method: prove that $I - DF(\bar{x})^{-1}F$ admits a fixed point in $B_r(\bar{x})$
- Quasi-Newton method: prove that $I - AF$ admits a fixed point in $B_r(\bar{x})$ where

$$A \approx DF(\bar{x})^{-1}$$

A Newton-Kantorovich type of theorem

Let $\mathcal{X}, \mathcal{Y}$ be Banach spaces, $F : \mathcal{X} \to \mathcal{Y}$ a $\mathcal{C}^1$ function. Let $\bar{x} \in \mathcal{X}$, $A \in \mathcal{L}(\mathcal{Y}, \mathcal{X})$ injective, and assume that:

$$
\begin{aligned}
\|F(\bar{x})\|_{\mathcal{Y}} &\leq \varepsilon \\
\|A\|_{\mathcal{L}(\mathcal{Y},\mathcal{X})} &\leq \kappa \\
\|DF(x) - DF(\bar{x})\|_{\mathcal{L}(\mathcal{X},\mathcal{Y})} &\leq \omega\left(\|x - \bar{x}\|\right) \\
\|I - ADF(\bar{x})\|_{\mathcal{L}(\mathcal{X},\mathcal{X})} &\leq \delta
\end{aligned}
$$

If there exists $r > 0$ such that

$$\kappa\varepsilon + \delta r + \kappa r \omega(r) < r$$

then F has a unique zero x satisfying $\|x - \bar{x}\| \leq r$

- The constants are partially estimated by hand and partially obtained by computer (using interval arithmetic)

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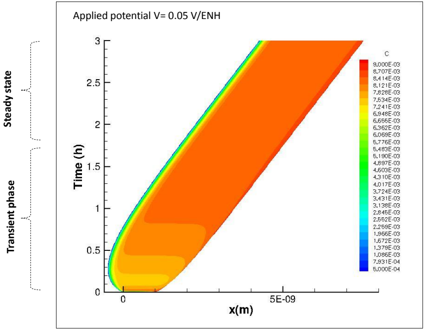
Application: the (pseudo) stationary DPCM



Main ingredients

- ➞ Rewrite the equation on a fixed domain
- ➞ Change of variable: $(X_0(t), X_1(t)) \longrightarrow (L(t), X_1(t))$
- ➞ $L(t)$ replaced by ℓ constant thickness
- ➞ $X_0'(t) = X_1'(t) = \delta$ a common velocity
- ➞ Forget the depency w.r.t. time for P, N, C and Ψ

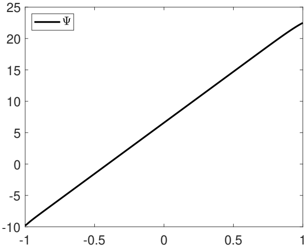
Existence of TW

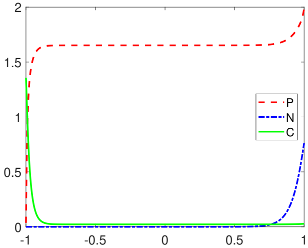
❑ Breden, Chainais-Hillairet, Z., 2021

Let $pH = 8.5$, $V_a = 0.5$ Volts. There exist analytic functions $\psi, C, N, P : [-1,1] \to \mathbb{R}$ and $\delta, \ell > 0$ pseudo stationary state satisfying

$$\sup_{[-1,1]} |\psi - \bar{\psi}| \lesssim 10^{-9}, \qquad \sup_{[-1,1]} |U - \bar{U}| \lesssim 10^{-10}$$

where $\bar{\psi}$, $\bar{C}$, $\bar{N}$ and $\bar{P}$ are explicitly known functions.





Zero finding map and Chebyshev polynomials

- $F = 0$ obtained by expanding the unknown functions as series

Zero finding map and Chebyshev polynomials

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- Bad news: BC of the DPCM do not allow to use Fourier series

Zero finding map and Chebyshev polynomials

- $F = 0$ obtained by expanding the unknown functions as series
- Bad news: BC of the DPCM do not allow to use Fourier series
- Good news: Chebyshev polynomials are well suited for BVPs
- Expand the unknown functions as

$$v = v_0 + 2\sum_{k=1}^{\infty} v_k T_k$$

where T_k is the Chebychev polynomials of the first kind, i.e.,

$$T_k(\cos(\theta)) = \cos(k\theta) \quad \forall\theta \in \mathbb{R},,\ k \in \mathbb{N}$$

- Plug the series expansions + identify $\Rightarrow F(\boldsymbol{X}) = 0$
- Approximate zero obtained by "truncating" F

Chebyshev polynomials and derivative

Let U_n denotes a Chebyshev polynomials of the second kind, then

$$T_n' = nU_{n-1} \quad \text{and} \quad U_n' = \left((n+1)T_{n+1} - xU_n(x)\right)/(x^2-1)$$

Lemma

Let u, $v : [-1,1] \to \mathbb{R}$, $\mathcal{C}^1$ functions with $u'(x) = v(x)$ for all $x \in (-1,1)$. Then, there Chebyshev coefficients ("of first kind") satisfying

$$u_k + \frac{v_{k+1} - v_{k-1}}{2k} = 0 \quad \forall k \geq 1$$

To define $F = 0$, rewrite the stationary DPCM as a system of first order equations and use the above lemma

- Add more equations
- Structure of the initial differential operators lost

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Gegenbauer polynomials of order $k \in \mathbb{N}$

$(G_n^{(k)})_{n\in\mathbb{N}}$ are orthogonal polynomials on $[-1, 1]$ for the weight

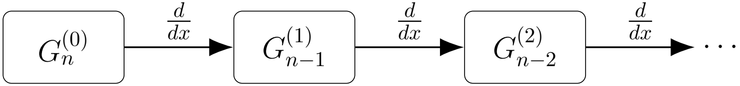
$$\omega_k = (1 - x^2)^{k-\frac{1}{2}} \quad \text{for } k \in \mathbb{N} \quad \text{and} \quad G_n^{(0)} = T_n,\ G_n^{(1)} = U_n$$

- Change of basis formula

$$G_n^{(k)} = \begin{cases} \frac{1}{2}\left(G_n^{(1)} - G_{n-2}^{(1)}\right) & \text{if } k = 0 \\ \frac{k}{n+k}\left(G_n^{(k+1)} - G_{n-2}^{(k+1)}\right) & \text{if } k \in \mathbb{N} \end{cases}$$

- Let $\mathcal{C}_k$ the change of basis operator from $(G_n^{(k)})$ to $(G_n^{k+1})_n$
- If $k \leq m$, let $\mathcal{C}_{k,m} = \mathcal{C}_{m-1}\mathcal{C}_{m-2}\ldots\mathcal{C}_{k+1}\mathcal{C}_k$

Differential and boundary operators in coefficient spaces



Differential and boundary operators in coefficient spaces

$$(\mathcal{D}_k U)_n := \begin{cases} 2^k\, k!\, U_k & \text{if } n = 0 \\ (n+k)\, 2^{k-1}\, (k-1)!\, U_{n+k} & \text{if } n \in \mathbb{N}^* \end{cases}$$

$\mathcal{D}_k$ not diagonal. Define $(\Sigma U)_n = U_{n-1}$ if $n \geq 1$, 0 otherwise

- $\Sigma^k \mathcal{D}_k$ diagonal
- First k rows of $\Sigma^k \mathcal{D}_k$ are empty (space for BC)
- $\Sigma^k \mathcal{D}_k$ explicitly invertible

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- $\Sigma^k \mathcal{D}_k$ explicitly invertible

For all $k \in \mathbb{N}$, values $(\partial_x^j G_n^{(k)}(\pm 1))$ explicitly known

- Consider a BVP with $2m$ linear BC, e.g.,

$$\text{(BC)} \qquad \sum_{j=1}^{2m-1} \beta^{\pm}_{j,i}\, \partial_x^j v(\pm 1) = 0 \quad i \in \{1, \ldots, m\}$$

- Yields op. $\mathcal{B}$ with first $2m$ rows "full", remaining rows empty

Expression of BVPs in coefficient spaces

$$(-1)^{m+1}\partial_x^{2m} v + Q(v) = 0 \quad x \in (-1,1) \quad \text{and (BC)}$$

In the basis $(G_n^{(0)})$, we search a zero $V = (V_k)_{k\in\mathbb{N}}$ of F with

$$F(V) = \underbrace{\left(\Sigma^{2m}\mathcal{D}_{2m} + \mathcal{B}\right)}_{\mathcal{L}:=} V + \Sigma^{2m} C_{0,2m} \quad \underbrace{\mathcal{Q}(V)}_{Q(v) \text{ in } (G_n^{(0)})}$$

If $\mathcal{L}$ invertible we can equivalently rewrite F as

$$F(V) = V + \mathcal{L}^{-1}\Sigma^{2m} C_{0,2m}\, \mathcal{Q}(V)$$

- We recover a Fourier like approach
- $\mathcal{L}$ invertible $\Leftrightarrow$ finite matrix $\pi^{\leq 2m-1}\,\mathcal{B}\,\pi^{\leq 2m-1}$ invertible

$$\mathcal{L} = \left(\begin{array}{c|c} \pi^{\leq 2m-1}\,\mathcal{B}\,\pi^{\leq 2m-1} & \pi^{\leq 2m-1}\,\mathcal{B}\,\pi^{>2m-1} \\ \hline 0 & \pi^{>2m-1}(-1)^{m+1}\Sigma^{2m}\mathcal{D}_{2m}\,\pi^{>2m-1} \end{array}\right)$$

- Can be checked and computed (rigorously) on a computer

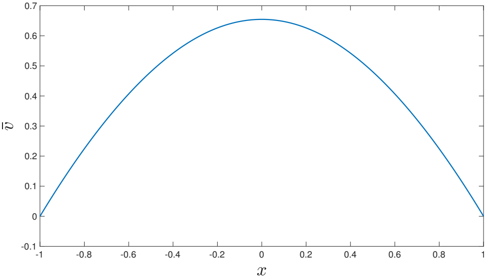
Example $m = 1$, $Q(v) = v^2 + 1$, homo. Dirichlet BC

❑ Breden, Cadiot, Z., 2026

There exists a smooth (stable) steady state $\tilde{v}$ such that

$$\max\left\{\|\tilde{v} - \bar{v}\|_\infty,\ \|\partial_x^2 \tilde{v} - \partial_x^2 \bar{v}\|_\infty\right\} \leq 10^{-14}$$

$\bar{v}$ is explicitly known and is an approximated zero of the system



Second example: Kuramoto-Sivashinsky (KS) equation

$$\begin{cases} \partial_t v = -\partial_x^4 v - \alpha\,\partial_x^2 v - \alpha\, v\,\partial_x v \\ \partial_x v(t,-1) = \partial_x v(t,1) = \partial_x^3 v(t,-1) = \partial_x^3 v(t,1) = 0, \ \ v \text{ odd} \end{cases}$$

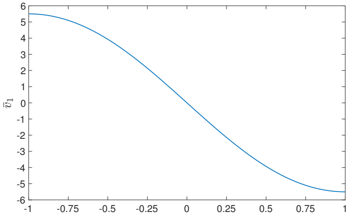
❑ Breden, Cadiot, Z., 2026

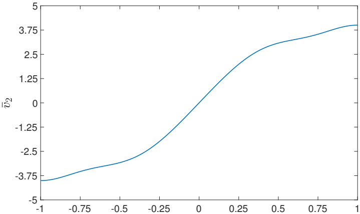
For $\alpha = 1$ and $\alpha = 100$, there exist two smooth (unstable) steady states $\tilde{v}_1$ and $\tilde{v}_2$ of KS with

$$\max\left\{\|\tilde{v}_1 - \bar{v}_1\|_\infty,\ \|\partial_x^4 \tilde{v}_1 - \partial_x^4 \bar{v}_1\|_\infty\right\} \le 1.28 \times 10^{-12}$$

$$\max\left\{\|\tilde{v}_2 - \bar{v}_2\|_\infty,\ \|\partial_x^4 \tilde{v}_2 - \partial_x^4 \bar{v}_2\|_\infty\right\} \le 3.92 \times 10^{-9}$$

$\bar{v}_1$ and $\bar{v}_2$ are approximated zeros of the stationary KS





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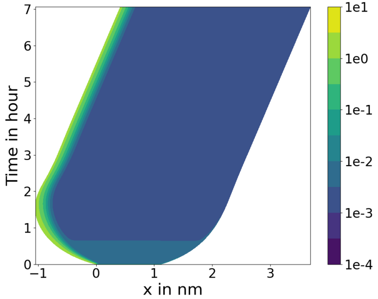
Conclusions and perspectives

Conclusions:

- First existence results for the DPCM
- Development of a new CAP method based on Gegenbauer polynomials to study existence and stability of some semi-linear BVPs

Perspectives:

- Study the existence and stability/instability of TW for the new version of the DPCM



- Extensions of the new CAP method

❏ Bataillon et al, 2026

Stability of zeros of $F(v) = (-1)^{m+1}\partial_x^{2m} v + Q(v)$

Let $\tilde{v}$ be a zero of F, $\lambda \in \mathbb{C}$ associated to a non-trivial solution v of

(GEig) $\qquad DF(\tilde{v})\, v = \lambda\, v \quad$ and $\quad$ (BC)

λ is stable if $\Re(\lambda) < 0$, unstable if $\Re(\lambda) > 0$

Main objectives:

- We aim to rigorously enclose the spectrum of $DF(\tilde{v})$

Main problem:

- Generalized eigenvalue pb. in coefficient spaces, because of λv

$$B\, V = \lambda\, \Sigma^{2m}\, C_{0,2m}\, V$$

Enclosure of the spectrum via Gershgorin disks

- Recast (GEig) as a standard eigenvalue pb.

$$u = (-1)^{m+1} \left(\partial_x^{2m}\right)^{-1} u \quad \Rightarrow DF(\tilde{U})^{-1}\mathcal{L}^{-1} U = \lambda^{-1} U$$

- $DF(\tilde{U})^{-1}\mathcal{L}^{-1}$ compact operator $\Rightarrow$ eigenvalues $\rightarrow 0$
- Gershgorin argument $\Rightarrow$ sign of real part of λ "small"
- for λ big (in modulus), we only need to know the sign of $\Re(\lambda)$
- This is done thanks to some a priori bounds on the spectrum

$$\exists \lambda_{\max} > 0 \text{ such that if } \Re(\lambda) > 0 \text{ then } |\lambda| < \lambda_{\max}$$

In practice, we (pseudo-)diagonalize $DF(\tilde{U})^{-1}\mathcal{L}^{-1}$ and compute the N first Gershgorin disks

- $n_u \in \{0, \ldots, N\}$ disks in $\{z \in \mathbb{C} : \Re(z) > 0\}$
- $N + 1 - n_u$ disks located in $\{z \in \mathbb{C} : \Re(z) < 0\}$
- The remaining disks are included in $B_{\lambda_{\max}^{-1}}(0)$ with $\Re(\lambda) < 0$

Application: $F(v) = \partial_x^2 v + v^2 + 1 = 0$, homo. Dirichlet BC

Any eigenvalue λ associated to the eigenvalue of $DF(\tilde{v})$ satisfies

$$\lambda \leq 1.43 = \lambda_{\text{max}}$$

Besides

$$\Re\left(\cup_{n\leq 30} B_{r_n}\left[(DF(\tilde{U})^{-1}\mathcal{L}^{-1})_{n,n}\right]\right) \subset [-0.75, 1.08 \times 10^{-4}]$$

and $r_n \leq 4.6 \times 10^{-3}$ for $n > 30$. The Spectrum of $DF(\tilde{U})^{-1}\mathcal{L}^{-1}$ in

$$[-0.75, 4.6 \times 10^{-3}]$$

However, nonnegative eigenvalue of $DF(\tilde{U})^{-1}\mathcal{L}^{-1}$ bigger than $1/1.43$. But, as $4.6 \times 10^{-3} < \frac{1}{1.43}$, all the eigenvalues of $DF(\tilde{U})^{-1}\mathcal{L}^{-1}$ must be contained in $[-0.75, 0)$

- This implies that $\tilde{v}$ is stable!