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Analytic solutions of two problems of Biology and Physics using the Jacobi elliptic functions

Francois Dubois, Olivier Lafitte, Clair Poignard

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June 17th, 2022

Potential in a cell generated by a density of ions (O.L.-C. Poignard)

Coupling thermohydraulics and neutronics (O.L., F. Dubois *et al*)

Why it is interesting to have analytic formulae and special functions?

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Why it is interesting to have analytic formulae and special functions?

Special functions in this presentation

Jacobi elliptic function

$$F_m(\varphi) = \int_0^\varphi \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}}$$

Modified Jacobi elliptic function

$$K_m(\varphi) = \int_0^\varphi \sqrt{1 - m \sin^2 \theta} d\theta.$$

Solutions of $(y')^2 = R(y)$, R rational function.

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Model coupling the electrostatic potential and the distribution of ions

In Ω : ρ_k is the concentration of ions of species k , of valence z_k , ψ is the electrostatic potential, e is the charge of the proton, ε_s is the dielectric constant of the cell, k_b is the Boltzmann constant and T is the temperature:

$$\begin{cases} -\nabla_x \cdot \left(D_k \left(\nabla_x \rho_k + \frac{e z_k}{k_b T} \rho_k \nabla_x \psi \right) \right) = 0 \\ -\nabla_x \cdot (\varepsilon_s \nabla_x \psi) = e \sum_k z_k \rho_k \end{cases}$$

Inhomogeneous Dirichlet boundary condition for the potential on $\partial\Omega$ and no flux condition for each species of ions.

Reduction to a 1D model: $\Omega = [-L, L]$. Boundary conditions

- for the potential: $\psi(\pm L) = \pm\psi_D$
- for the concentration of ions: $(\rho'_k + \frac{e z_k}{k_b T} \rho_k \psi')(\pm L) = 0$.

Reduction of the model to a single ODE

For ion concentrations $\rho_k(x) = \rho_k(-L)e^{-\frac{ez_k}{k_b T}\psi(x)}$.

Electrostatic equation:

$$-\psi'' = \frac{e}{\varepsilon_s} \sum_k z_k \rho_k(-L) e^{-\frac{ez_k}{k_b T}\psi(x)}.$$

Notation $\varphi(X) = \frac{e}{k_b T}\psi(XL)$, $X \in [-1, 1]$. Equation

$$-\varphi'' = \frac{e^2 L^2}{k_b T \varepsilon_s} \sum_k z_k \rho_k(-L) e^{-z_k \varphi}.$$

Number of ions of each species given

$$n_k = \int_{-L}^L \rho_k(-L) e^{-\frac{ez_k}{k_b T}\psi(x)} dx \Leftrightarrow \rho_k(-L) = \frac{n_k}{\int_{-L}^L e^{-\frac{ez_k}{k_b T}\psi(x)} dx}.$$

Reduction to a elliptic equation

Equation: $-\varphi'' = \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k z_k \frac{e^{-z_k \varphi}}{\int_{-1}^1 e^{-z_k \varphi(X)} dX}$. Boundary conditions $\varphi(\pm 1) = \pm \varphi_D$.

Lemma

This problem has a unique solution in $H^1([-1, 1])$.

Proof: one observes that it is the Euler equation for

$$J(\varphi) = \int_{-1}^1 \frac{1}{2} [(\varphi'(X))^2 + \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k \ln(\int_{-1}^1 e^{-z_k \varphi(X)} dX)] dX.$$

$$\frac{1}{2}(\varphi')^2 - \frac{1}{2}(\varphi'(X_0))^2 = \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k \frac{e^{-z_k \varphi} - e^{-z_k \varphi(X_0)}}{\int_{-1}^1 e^{-z_k \varphi(X)} dX}. \quad (1)$$

$f(X) = e^{-\varphi(X)}$ yields $(f')^2 = (\varphi')^2 f^2 \Rightarrow (f')^2 = R(f)$, where R is a rational fraction \Rightarrow elliptic equation.

First application: the electroneutral case for two species of ions $z_k = \pm 1$

Notation $n_+ = n_- = n$ and introduce $\alpha = \frac{e^2 L n}{k_b T \epsilon_s}$. Equation

$$-\varphi'' = \alpha \left[\frac{e^{-\varphi}}{\int_{-1}^1 e^{-\varphi(X)} dX} - \frac{e^{\varphi}}{\int_{-1}^1 e^{\varphi(X)} dX} \right].$$

One proves φ odd. Thanks to

$\int_{-1}^1 e^{-\varphi(X)} dX = \int_{-1}^1 e^{\varphi(X)} dX = 2 \int_0^1 e^{-\varphi(X)} dX$, reduce the equation on $(0, 1)$ to

$$(f')^2 = 2f^2 \alpha \frac{f+f^{-1}-2K}{\int_{-1}^1 e^{-\varphi(X)} dX} = \beta f(f^2 - 2Kf + 1),$$

$$\beta = \frac{2\alpha}{\int_{-1}^1 e^{-\varphi(X)} dX}, \quad K = 1 - \frac{(\varphi'(0))^2}{2\beta} < 1, \quad f(0) = 1, \quad f(1) = e^{-\varphi_D}.$$

$$\int_1^{e^{-\varphi(X)}} \frac{df}{\sqrt{f(f^2 - 2Kf + 1)}} = \sqrt{\beta} X. \quad (2)$$

Equations for determining β and K :

$$\int_1^{e^{-\varphi_D}} \frac{df}{\sqrt{f(f^2 - 2Kf + 1)}} = \sqrt{\beta}, \quad \int_1^{e^{-\varphi_D}} \frac{fdf}{\sqrt{f(f^2 - 2Kf + 1)}} = \frac{\alpha}{\sqrt{\beta}}.$$

Expression of the solution

Case $K < -1$. Polynomial $f(f + q)(f + \frac{1}{q})$, $q > 1$. New unknown

$$\sin^2 \varphi = \frac{e^{-\varphi(X)}}{e^{-\varphi(X)} + \frac{1}{q}}, \text{ new variable } \sin^2 \theta = \frac{f}{f + \frac{1}{q}} = 1 - \frac{1}{q} \frac{1}{f + \frac{1}{q}},$$

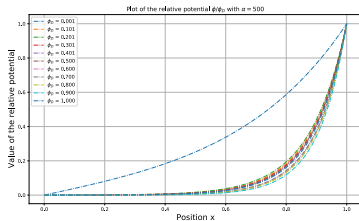
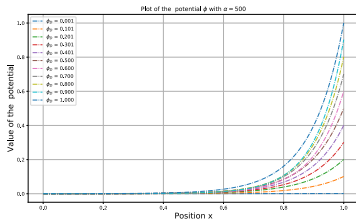
$$2 \sin \theta \cos \theta d\theta = \frac{1}{q} \frac{df}{(f + \frac{1}{q})^2}, \quad \cos^2 \theta = \frac{1}{q} \frac{1}{(f + \frac{1}{q})^2},$$

$$f(f + q)(f + \frac{1}{q}) = \frac{1}{q^2} \frac{\sin^2 \theta}{\cos^6 \theta} (q + (\frac{1}{q} - q) \sin^2 \theta).$$

With $m = 1 - \frac{1}{q^2}$

$$\frac{df}{\sqrt{f(f + q)(f + \frac{1}{q})}} = \frac{2}{\sqrt{q}} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}},$$

$$F_m(\arcsin \sqrt{\frac{e^{-\varphi(X)}}{e^{-\varphi(X)} + \frac{1}{q}}}) - F_m(\arcsin \sqrt{\frac{1}{1 + \frac{1}{q}}}) = \sqrt{\beta} X \quad (3)$$



Boundary layer on the potential near the charged interface.
The potential in the Gouy-Chapman-Stern is described exactly.

Second application: the non electroneutral case for two species of ions $z_k = \pm 1$

With $\varphi_D = 0$, $n_+ \neq n_-$, **one proves that** the function φ is even, has its maximum (or its minimum) at $X = 0$ according to the sign of $n_+ - n_-$. Equation ($f_0 = e^{-\varphi(0)} := e^{-\varphi_0}$)

$$(f')^2 = 2\alpha f^2 \left[\beta_- \left(\frac{1}{f} - \frac{1}{f_0} \right) + \beta_+ (f - f_0) \right],$$

with $\beta_- = \frac{n_-}{\int_{-1}^1 f(X) dX}$, $\beta_+ = \frac{n_+}{\int_{-1}^1 f^{-1}(X) dX}$. Need three equations fo

f_0, β_-, β_+ . Introduce $f_1 = \frac{\beta_+}{\beta_- f_0}$. Equation

$$(f')^2 = 2\alpha \beta_+ f_0^{-1} f (f - f_0) (f - f_1) = K^2 f (f - f_0) (f - f_1).$$

Two cases: $f_1 < f_0$ (f_0 is the point of minimum of f) or $f_1 > f_0$ (f_0 is the point of maximum of f).

Solution ($0 < f_1 < f_0$, $m_0 f_0 = f_1$)

$$K|X| = \int_{f_0}^{e^{-\varphi(X)}} \frac{df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}$$

Conditions for the three constants ($K^2 f_0 = 2\alpha\beta_+$):

$$\begin{cases} K = \int_{f_0}^1 \frac{df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}, \\ Kn_+ = 2\beta_+ \int_{f_0}^1 \frac{f df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}, \\ Kn_- = 2\beta_- \int_{f_0}^1 \frac{df}{f \sqrt{f(f-f_0)(f-m_0 f_0)}}. \end{cases}$$

Change of variable in the integral $\sin^2 \varphi = \frac{f-f_0}{f-m_0 f_0}$

$$K|X| = 2(1-m_0)f_0^{\frac{1}{2}} F_{m_0}(\arcsin \sqrt{\frac{e^{-\varphi(X)} - f_0}{e^{-\varphi(X)} - m_0 f_0}}). \quad (4)$$

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The coupled 1d model

Diffusion equation for the neutrons: density of probability $\Phi(z, t)$ of neutrons in $[0, L]$ at time t (h : enthalpy (temperature), V : velocity of neutrons)

$$\frac{1}{V} \partial_t \Phi - \partial_z (D(h) \partial_z \Phi) + \Sigma_a(h) \Phi = \Sigma_f(h) \Phi$$

Boundary conditions: $\Phi(0, t) = 0, \Phi(L, t) = 0$. Condition on the density $\int_0^L \Phi(z, 0) dz = 1$.

Classical analysis: $\Phi(z, t) = e^{t\tau} \varphi(z)$. Sign of τ important.

Equation on φ

$$-\frac{d}{dz} (D(h) \frac{d\varphi}{dz}) + \Sigma_a(h) \varphi = (\Sigma_f(h) - \frac{\tau}{V}) \varphi$$

Definition $k_{eff} = \frac{\Sigma_f(h)}{\Sigma_f(h) - \frac{\tau}{V}}$. Eigenvalue problem:

$$\begin{cases} -\frac{d}{dz} (D(h) \frac{d\varphi}{dz}) + \Sigma_a(h) \varphi = \frac{\Sigma_f(h)}{k_{eff}} \varphi, \\ \varphi(0) = \varphi(L) = 0. \end{cases}$$

Coupled with the production of enthalpy $h' = Q \Sigma_f(h) \varphi$.

Coupled problem and its integration

$$\text{Nonlinear system} \begin{cases} -\frac{d}{dz}(D(h)\frac{d\varphi}{dz}) + \Sigma_a(h)\varphi = \frac{\Sigma_f(h)}{k_{eff}}\varphi, \\ h' = Q\Sigma_f(h)\varphi, \\ \varphi(0) = \varphi(L) = 0, \\ h(0) = h_e, h(L) = h_s. \end{cases}$$

Four boundary conditions, problem of order 3: yields $k_{eff} := \lambda^{-1}$.

Exact integration

$$-\frac{d}{dz}(D(h)\frac{d\varphi}{dz}) + \left(\frac{\Sigma_a(h)}{\Sigma_f(h)} - \lambda\right)\frac{h'}{Q} = 0$$

$$-D(h)\frac{d\varphi}{dz} + \frac{F(h) - \lambda h + C_0}{Q} = 0$$

$$-\frac{d\varphi}{dz}\varphi + \frac{F(h) - \lambda h + C_0}{\Sigma_f(h)D(h)Q^2}h' = 0$$

Finally (with $X(h_e) = X(h_s) = Y(h_e) = Y(h_s) = 0$)

$$-Q^2\frac{\varphi^2}{2} + X(h) - \lambda Y(h) = 0 \Rightarrow (h')^2 = R(h). \quad (5)$$

When Σ_a, Σ_f and D are known only at given points

$h_i, 1 \leq i \leq p$, R is a rational fraction: elliptic integrals again.

Coupled problem and its integration

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First example: $X(h) \simeq (h - h_e)(h_s - h)(a_X h + b_X)$,
 $Y(h) \simeq (h - h_e)(h_s - h)(a_Y h + b_Y)$.

Obtain a_X, a_Y, b_X, b_Y by projection of solutions of certain ODEs.

$$(h')^2 = \mu^2 (h - h_e)(h_s - h)((a_X - \lambda a_Y)h + (b_X - \lambda b_Y)).$$

New unknown $h(z) = h_e + (h_s - h_e) \sin^2 \theta(z)$, $\theta(0) = 0, \theta(L) = \frac{\pi}{2}$:

$$(\theta'(z))^2 = \frac{\mu^2}{4} [(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y) + (a_X - \lambda a_Y)(h_s - h_e) \sin^2 \theta(z)].$$

Define $m(\lambda) = -\frac{(a_X - \lambda a_Y)(h_s - h_e)}{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)}$. Equality

$$\int_0^{\theta(z)} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}} = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} z. \quad (6)$$

Equation for determining λ :

$$F_{m(\lambda)}\left(\frac{\pi}{2}\right) = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} L.$$

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$$F_{m(\lambda)}\left(\frac{\pi}{2}\right) = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} L.$$

Second example (joint work with F. Dubois):

$$D = 1, \Sigma_a = 1, \Sigma_f \text{ known at three values } h_1, h_2, h_3$$

Possible choice of solutions for the coupled problem

1. Σ_f interpolation polynomial of degree 2 $\rightarrow Y$ polynomial of degree four \rightarrow elliptic function as solutions (see A-S formulae 17.4.41 to 17.4.57), after transformation of the polynomial to $(t^2 - a^2)(b^2 - t^2)$ or $(a^2 - t^2)(t^2 + b^2)$ by homographic transform of the roots of Y into $\pm a, \pm b$ or $\pm a, \pm ib$.
2. Σ_f continuous, piecewise linear on intervals $[h_e, h_1], [h_1, h_2], [h_2, h_3], [h_3, h_s] \rightarrow Y \in C^1$ piecewise cubic polynomial h piecewise an inverse incomplete elliptic function.

In the first case, equation on λ of the form $F_{m(\lambda)}(g(\lambda)) = L$.

In the second case, one has a more complicated equation.

Main result for applications: the values of λ are quite different, though the solutions are extremely similar.

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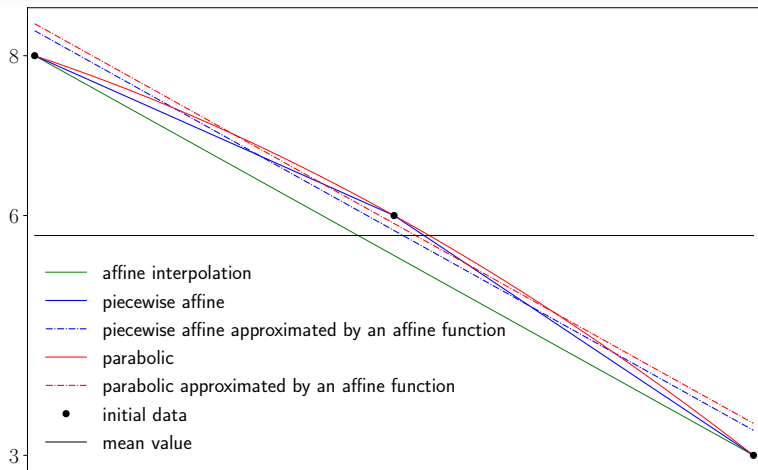


Figure: Function $h \mapsto \Sigma(h)$.

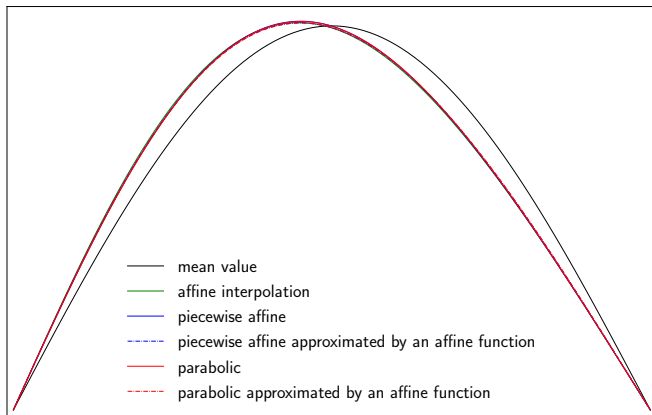
φ and λ 

Figure: Functions $z \mapsto \varphi(z) : \lambda$:
1.01722, 1.07373, 1.0043, 1.01991, 1, 01507.

Contents

Potential in a cell generated by a density of ions (O.L.-C. Poignard)

Coupling thermohydraulics and neutronics (O.L., F. Dubois *et al*)

Why it is interesting to have analytic formulae and special functions?

Why does one need analytic formulae?

- Quick and accurate calculations and graphical representation thanks to the presence of the special functions in packages.
- In the study of the potential inside a cell: link with models of exchanges of ions: dependency in terms of L and of φ_D or of number of ions.
- Uncertainty and sensitivity analysis (one has a dependency on parameters, n and L in the case of the first problem, n_-, n_+, L in the case of the second problem, given values of $D(h), \Sigma_a(h), \Sigma_f(h)$ in the third problem)