MTH 655, Winter 2013, LAB2

The goal of this assignment is to explore applications problems in $N \geq 1$ dimensions where Newton's iteration has substantial difficulties. For each problem we provide the applications background and then we present the mathematical model and the problem to be solved. The challenges come from real life !

TURN IN 1,2, and 4.

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1. *The potential equation in semiconductor modeling has the form*

$$-\nabla \cdot (\epsilon \nabla \phi) + q(p - n - C) = 0 \tag{1}$$

where ϕ is the potential, p, n are the concentrations of holes and electrons, respectively, and ϵ, C are constants of permittivity and doping. This equation is coupled to separate equations written for the transport of p, and n, and is supplied with appropriate boundary (and, if relevant), also initial conditions.

In thermal equilibrium, with no current $\nabla \phi = 0$, one can write

$$p = N_v e^{\beta(\phi - \chi)} e^{-\beta E_g}, \quad n = N_c e^{-\beta(\phi - \chi)} \tag{2}$$

where N_v, N_c, E_g, χ are given. Then we solve ϕ the equation $p - n - C = 0$ so that (1) holds.

(i) **Extra:** Show that this is equivalent to solving for an auxiliary variable $z = e^{\beta(\phi - \chi)}$, where $\beta = 38.7$, $\chi = 4.05$, the equation

$$Az - \frac{B}{z} - C = 0 \tag{3}$$

with a suitably chosen A, B.

(ii) **Propose** a suitable method for solving (3) when A, B are some positive constants. Reformulate it so it can be solved for z with Newton's method, fixed point, or as a quadratic equation. Test it when $A = B = C = 1$. Compare with `fzero`, and `roots`, if you wish.

(iii) Now consider realistic values of $A = 2.74, B = 2.82e19$, and C ranges from $1e2$ up to $1e19$. Test the same methods as in (ii). Pay attention to the values of z and of ϕ. **Explain** where the difficulties are coming from and which of the methods you used seems to be most robust.

References: Markovich, The Stationary Semiconductor Device Equations. Problem courtesy of David Foster, OSU Physics

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2. *Equation of state (EOS) is a relationship of type $f(P, V, T) = 0$ binding the pressure P, (molar) volume V, and temperature T of a gas or liquid. In the simplest form for ideal gas we have $\frac{PV}{T} = R$ where R is the ideal gas constant. Since most gases are not ideal, one uses more accurate relationships. For example, van der Walls EOS for carbon dioxide is given as*

$$P = \frac{RT}{V - b} - \frac{a}{V^2} \tag{4}$$

(i) In order to understand the difficulties to follow in (ii), plot this function for $V \in [0.06, 0.6]$ and $T = 280[K]$ and $T = 380[K]$ when the constants for CO_2 in appropriate units are

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R = 8.314e-2; %% [bar L/mol K]
a = 3.64;     %% L^2 bar/mol^2
b = 0.04;     %% L/mol
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Explain where solvers may have difficulties. [**Enjoy** more plots for T between $280, 380$. The non-monotone behavior is actually not physical, but it shows regions of phase change between gas and liquid. You can ask me about it if interested !]

(ii) Now, for $T = 380$, given $P = 100$, find the corresponding V by Newton's method. [The answer is $V \approx 0.22$]. You can compare with `fzero`, if you wish. **Explore** various initial guesses ... In general, an initial guess can be taken from the ideal gas law. Repeat for $P = 200$.

(iii) More challenging, of course, is the case $T = 280$. Try $P = 100$, and $P = 40$. **Discuss** the pitfalls and your remedies.

References: Smith, Van Ness, Abbott, "Introduction to Chemical Engineering Thermodynamics", Sixt Edition, McGraw-Hill, 2001, Chap.3

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3. **Explore:** Implement Newton's method for the problem in class where $x \in \mathbb{R}^2, F : \mathbb{R}^2 \mapsto \mathbb{R}^2$, and

$$F(x) = (x_1^2 - x_2 + \alpha, -x_1 + x_2^2 + \alpha)^T = (0,0)^T. \tag{5}$$

Test your method first for $\alpha = 0$ solving with $x_0 = (2,2)^T$ and/or $x_0 = (1/3, 1/3)^T$. What about $x_0 = (3,0)^T$? Keep track of your guesses on a plot.

This example (from Ortega/Rheinboldt) will be later implemented in Fortran so make sure you have a good handle on the solution.

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4. *Find chemical equilibria in a chemical reaction involving water and carbon dioxide, in a coalbed fed with gas stream contain air and steam. [In the reaction and model the oxygen component is eliminated].*

$$C + CO_2 \mapsto 2CO \tag{6}$$

$$H_2 + C \mapsto H_2 + CO \tag{7}$$

In equilibrium the mole fractions of the components are given by

$$y_{H_2} := \frac{\epsilon_b}{3.38 + \epsilon_a + \epsilon_b}, \; y_{CO} := \frac{2\epsilon_a + \epsilon_b}{3.38 + \epsilon_a + \epsilon_b}, \; y_{H_2O} := \frac{1 - \epsilon_b}{3.38 + \epsilon_a + \epsilon_b}, \; y_{CO_2} := \frac{0.5 - \epsilon_a}{3.38 + \epsilon_a + \epsilon_b}, \tag{8}$$

and the auxiliary variables $-0.5 \le \epsilon_a \le 0.5, 0 \le \epsilon_b \le 1$ satisfy the system

$$K_a = 20 \tfrac{(2\epsilon_a + \epsilon_b)^2}{(0.5 - \epsilon_a)(3.38 + \epsilon_a + \epsilon_b)} \tag{9}$$

$$K_b = 20 \tfrac{\epsilon_b(2\epsilon_a + \epsilon_b)}{(1 - \epsilon_b)(3.38 + \epsilon_a + \epsilon_b)} \tag{10}$$

Given K_a, K_b, the system (9)–(10) needs to be solved for ϵ_a, ϵ_b from which one can determine the "y" values for the components from (8).

(i) In particular, at $T = 1,400[k]$, we have $K_a = 584.85, K_b = 268.76$ and one obtains $\epsilon_a = 0.4739, \epsilon_b = 0.9713$.

(ii) **Set-up** fixed-point solver for this problem. Confirm the solution in (i). (A good starting point is $(0, 0.5)$).

(iii) **Implement and test** Newton (or Newton-like) and solve for ϵ_a, ϵ_b when $K_a = 11.405, K_b = 11.219$.(Solution is around 0.12, 0.71). Note that fixed point iteration in (ii) may have trouble converging already for $K_a = 20, K_b = 20$, while the secant method with $h = 1e - 4$ should converge fast. **How fast ?**

Adapted from Smith, Van Ness, Abbott, "Introduction to Chemical Engineering Thermodynamics", Sixt Edition, McGraw-Hill, 2001, Chap.13
