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MATH 7422: Numerical Partial Differential Equations March 5, 2023

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Project 1

Study the ozone photo-chemistry problem. This is a stiff ODE. The following chemical reaction is from atmospheric science. The reaction involves oxygen(O), nitrogen oxides(NO, NO_2), and (O_3):

$$NO_2 + h\nu \xrightarrow{k_1} NO + O$$

$$O + O_2 \xrightarrow{k_2} O_3$$

$$NO + O_3 \xrightarrow{k_2} O_2 + NO_2$$

Here, $h\nu$ denotes a photo of solar radiation. Let $c_1, ..., c_4$ be the concentrations of O, NO, NO₂ and O₃, respectively. The reaction system is

$$\dot{c}_1 = k_1 c_3 - k_2 c_1
\dot{c}_2 = k_1 c_3 - k_3 c_2 c_4
\dot{c}_3 = k_3 c_2 c_4 - k_1 c_3
\dot{c}_4 = k_2 c_1 - k_3 c_2 c_4$$

The numerical reaction rates are

$$k_1 = 10^{-2} max[0, sin(2\pi t/t_d)]s^{-1}, t_d$$
 the length of 1 day,
 $k_2 = 10^5 s^{-1}, k_3 = 10^{-16} cm^3 molecule^{-1} s^{-1}$

The initial concentration at sunrise is

$$(c_1, c_2, c_3, c_4) = (0, 0, 5 \times 10^{11}, 8 \times 10^{11}) molecules/cm^3$$

Find the concentration in the next two days. Plot your answers.

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