Scientific Computing Final Exam

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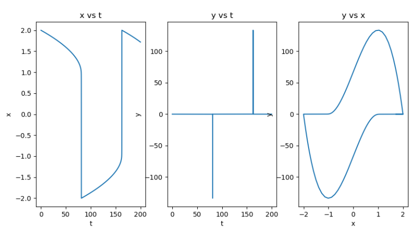
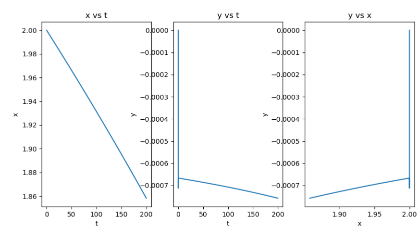
1. Code: `https://github.com/RokettoJanpu/scientific-computing-2-redux/blob/main/final%201.ipynb`

   (a) The solution for $\mu = 10^2$ is on the left and the one for $\mu = 10^3$ on the right.





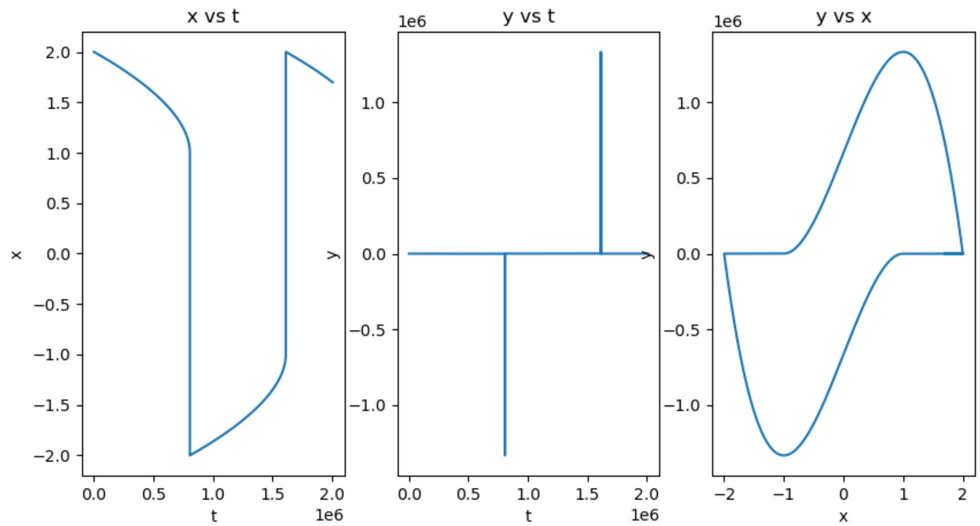
   (b) From the Butcher array, $\hat{b} = \begin{bmatrix} 1-\gamma \\ \gamma \end{bmatrix}$ and $c = \begin{bmatrix} \gamma \\ 1 \end{bmatrix}$. Pick $b := \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Then the method using b instead of $\hat{b}$ is order 1 since $b_1 + b_2 = 1$ but not order 2 since $b \cdot c = \gamma \neq \frac{1}{2}$. The error estimate is

$$e := h \sum_{q=1}^{2} (b - \hat{b})_q k_q = h(\gamma k_1 - \gamma k_2) = h\gamma(k_1 - k_2) \implies \|e\| = h\gamma \|k_1 - k_2\|$$

   The following adaptive time step algorithm repeatedly multiplies or divides the time step by 2 to get as close as possible to satisfying the step acceptance criterion.

```
err ← h*gamma*norm(k1-k2)
tol ← atol + rtol*norm([x,y])
if err < tol then
    while err < tol do
        h ← 2*h
        compute k1 and k2 using h
        err ← h*gamma*norm(k1-k2)
    end while
end if
if err > tol then
    while err > tol do
        h ← 0.5*h
        compute k1 and k2 using h
        err ← h*gamma*norm(k1-k2)
    end while
end if
```

   Using the adaptive time step algorithm for $\mu = 10^6$ and $T_{\max} = 2 \cdot 10^6$, the CPU time is 409s.



2. (a) As a preliminary, recall a "generalized" divergence theorem: for all scalars $\varphi \in C^1(\Omega, \mathbb{R})$ and vectors $F \in C^1(\Omega, \mathbb{R}^2)$,

$$\int_\Omega \boldsymbol{\nabla}\varphi \cdot F dx = -\int_O \boldsymbol{\nabla} \cdot F dx + \int_{\partial\Omega} \varphi F \cdot n ds$$

Let $P(x,y) := e^{-\beta V(x,y)} M(x,y)$. Pick $u_D \in C^2(\mathbb{R}^2)$ such that $u_D = 0$ on ∂A, $u_D = 1$ on ∂B, and $u_D = 0$ outside some neighborhood of ∂B disjoint from Γ_N (an explicit formula for u_D is given later). We obtain a BVP for $v := u - u_D$,

$$\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} v) = -\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} u_D), \quad v = 0 \text{ on } \Gamma_D := \partial A \cup \partial B, \quad \frac{\partial v}{\partial n} = 0 \text{ on } \Gamma_N$$

Now fix $w \in C^1(\Omega)$ such that $w = 0$ on Γ_D, multiply the PDE for v and integrate over Ω.

$$\int_O w\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} v) dx = -\int_O w\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} u_D) dx$$

This equation, along with the generalized divergence theorem for $\varphi := w$ and $F := P\boldsymbol{\nabla} v$, gives

$$\int_\Omega P\boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} v dx = \int_\Omega w\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} u_D) dx + \int_{\Gamma_D} wP\frac{\partial v}{\partial n} ds + \int_{\Gamma_N} wP\frac{\partial v}{\partial n} ds$$

On the RHS, the second term vanishes since $w = 0$ on Γ_D, and the third term vanishes since $\frac{\partial v}{\partial n} = 0$ on Γ_N. The generalized divergence theorem for $\varphi := w$ and $F := P\boldsymbol{\nabla} u_D$ gives

$$\int_\Omega P\boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} u_D dx = -\int_\Omega w\boldsymbol{\nabla} \cdot (P\boldsymbol{\nabla} u_D) dx + \int_{\Gamma_D} wP\frac{\partial u_D}{\partial n} ds + \int_{\Gamma_N} wP\frac{\partial u_D}{\partial n} ds$$

On the RHS, the second term vanishes since $w = 0$ on Γ_D, and the third term vanishes since $u_D = 0$ on Γ_N. Combining the last two equations gives

$$\int_\Omega P\boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} v dx = -\int_\Omega P\boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} u_D dx$$

This is the integral equation formulation for all solutions to the BVP for v and for all $w \in C^1(\Omega)$. The standard mollifier on $\mathbb{R}^2$ is

$$\eta(x) := \begin{cases} C \exp\left(\frac{1}{\|x\|^2 - 1}\right), & \|x\| < 1 \\ 0, & \|x\| \geq 1 \end{cases}$$

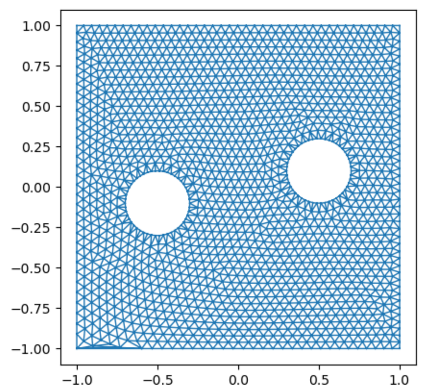
with C such that $\int_{\mathbb{R}^2} \eta dx = 1$. The family of mollifiers for $\epsilon > 0$ is

$$\eta_\epsilon(x) := \frac{1}{\epsilon^2} \eta \left(\frac{x}{\epsilon} \right)$$

Note that the support of η_ϵ is the open ball with center $(0,0)$ and radius ϵ. Pick u_D to be a mollifier which equals 1 on ∂B and vanishes at points more than 0.1 away from ∂B.

$$u_D(x) := \frac{1}{\eta_{0.3}(0.2, 0)} \eta_{0.3}(x - (0.5, 0.1))$$

(b) Triangulation of Ω:



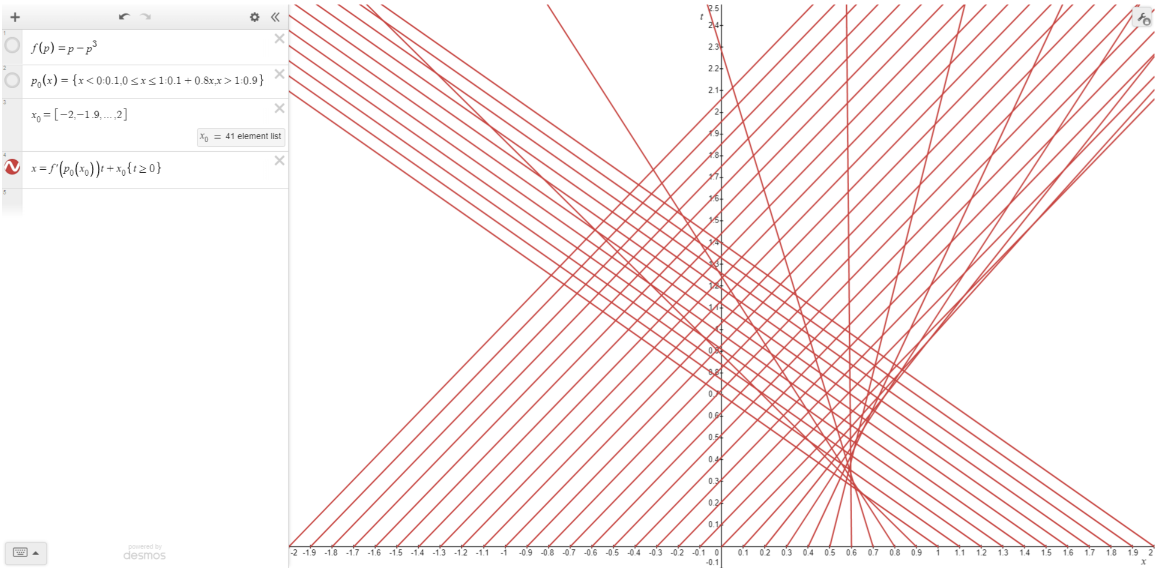
3. (a) Rewrite the PDE as

$$\rho_t + [f(\rho)]_x = 0, \quad f(\rho) := \rho v(\rho) = \rho - \rho^3$$

Characteristics are given by

$$x(t) = f'(\rho_0(x_0))t + x_0, \quad f'(\rho) = 1 - 3\rho^2$$

They are plotted below.



(b) The breaking time, when the first shock occurs, is

$$T_b = -\left[\min_z f''(\rho_0(z))\rho_0'(z)\right]^{-1} \approx 0.231$$

The equation for ρ_0 gives $\rho_L = 0.1$ and $\rho_R = 0.9$, so the eventual shock speed is

$$s = \frac{f(\rho_L) - f(\rho_R)}{\rho_L - \rho_R} = 0.09$$