

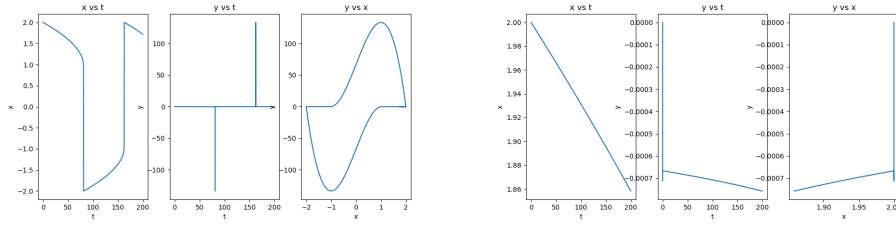
Scientific Computing Final Exam

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- 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.



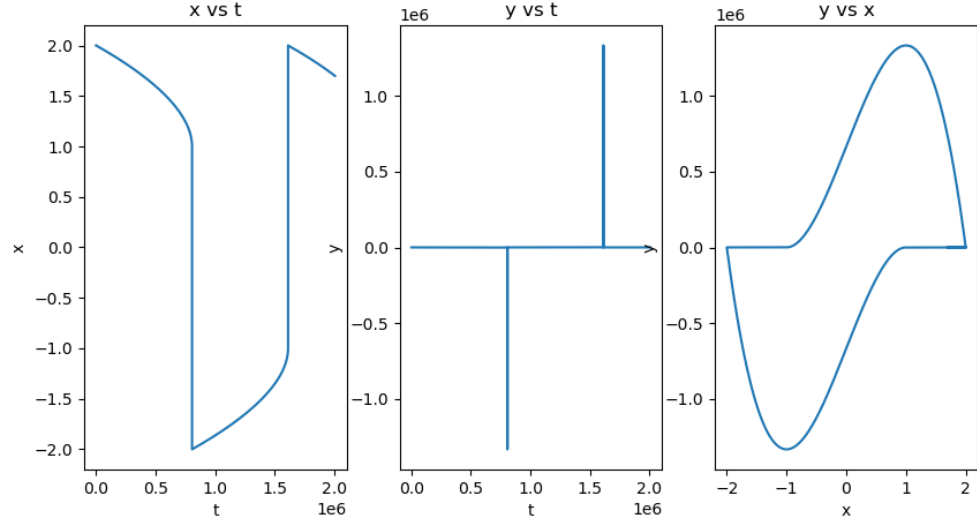
- (b) From the Butcher array, $\hat{b} = \begin{bmatrix} 1 - \gamma \\ \gamma \end{bmatrix}$ and $c = \begin{bmatrix} \gamma \\ 1 \end{bmatrix}$. Pick $b := \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Then the method using b instead of \hat{b} is order 1 since $b_1 + b_2 = 1$ but not order 2 since $b \cdot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

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

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 . We obtain a BVP for $v := u - u_D$,

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

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

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

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

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

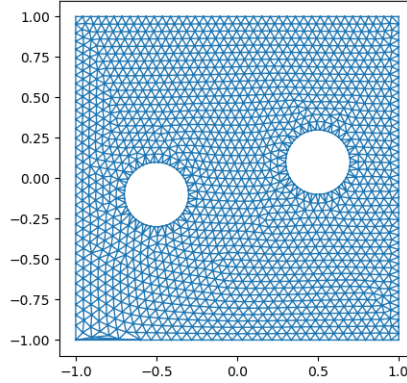
On the RHS, the second term vanishes since $w = 0$ on Γ_D , and the third term vanishes since $\frac{\partial v}{\partial n} = 0$ on Γ_N . The generalized divergence theorem for $\varphi := w$ and $F := P \nabla u_D$ gives

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

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 the integral equation formulation.

$$\int_{\Omega} \nabla w \cdot (P \nabla v) dx = - \int_{\Omega} \nabla w \cdot (P \nabla u_D) dx, \quad P(x, y) = e^{-\beta V(x, y)} M(x, y)$$

- (b) Triangulation of Ω :



- (c) Assuming the notation of FEM, let $\{\tau_k\}_{k=1}^{N_{\text{tri}}}$ be the above triangulation of Ω , let $w = \eta_i$ for $i \in I_{\text{free}}$, and write $v = \sum_{j \in I_{\text{free}}} v_j \eta_j$. The LHS of the integral formulation becomes

$$\sum_{j \in I_{\text{free}}} \left[\sum_{k=1}^{N_{\text{tri}}} \underbrace{\int_{\tau_k} \nabla \eta_i \cdot (P \nabla \eta_j) dx}_{A_{ij}} \right] v_j$$

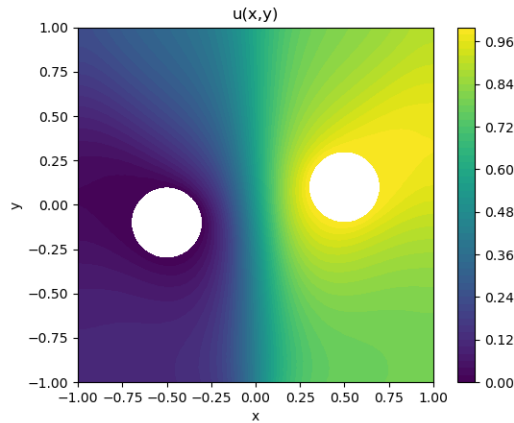
The stiffness matrix entries A_{ij} can be found by modifying the `stima3` function in `FEM_TPT.py`,

$$0.5 DGP(v_{\text{mid}}) G^T$$

where $P(v_{\text{mid}})$ is the function P evaluated at the midpoint of the triangle τ_k , and

$$D = \begin{bmatrix} 1 & 1 & 1 \\ x_i & x_{i+1} & x_{i+2} \\ y_i & y_{i+1} & y_{i+2} \end{bmatrix}, \quad G = \begin{bmatrix} (\nabla \eta_i)^T \\ (\nabla \eta_{i+1})^T \\ (\nabla \eta_{i+2})^T \end{bmatrix}$$

Below is the FEM solution.



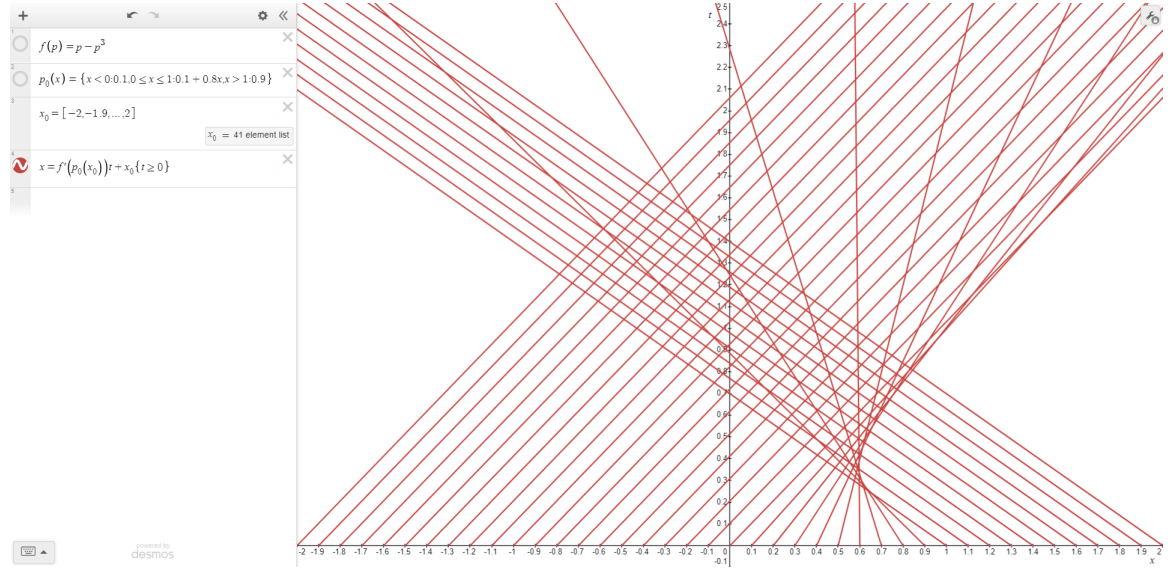
3. (a) Rewrite the PDE as

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

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

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