Numerical Algorithms for Physics : Project List

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AA 2018-2019

Writing the Project

- In the following I will show a list of projects for this course.
- Each project should be no more than ≈ 10 pages long (excluding the code listed in the appendix).
- A .pdf file is strongly recommended.
- The document structure should consists of
  - An abstract / Introductory part where the physical problem is explained and why we need to resort to numerical integration.
  - A test section where the numerical method is validated against known analytical / reference solution.
  - A model study of the problem including plots.
  - A final summary/discussion.
  - An appendix including the code used for the project, using fixed-size fonts (a font whose letters and characters each occupy the same amount of horizontal space, e.g., Courier, Courier New, Lucida Console, Monaco, and Consolas).

Project #1: Finite Potential Well

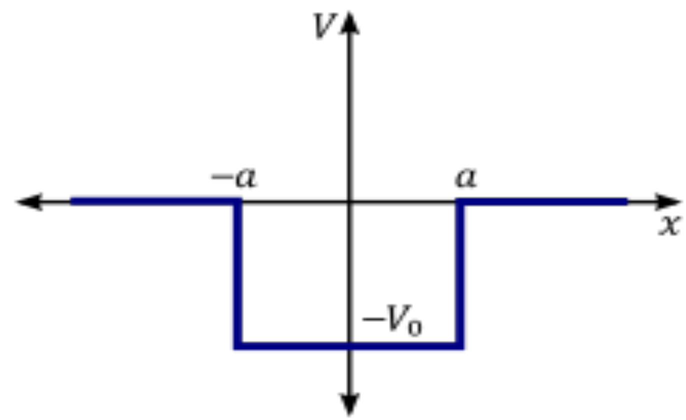
- Consider the time-independent Schrödinger equation in one dimension,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

where $\psi(x)$ is the wave function, m is the particle mass, E its energy and V(x) is the potential energy.
The probability to find the particle between x and x+dx is $\psi(x)\psi^*(x)dx = |\psi(x)|^2 dx$

- Consider the potential well given by

$$V(x) = \begin{cases} 0 & \text{for} \quad |x| > a \\ -V_0 & \text{for} \quad |x| < a \end{cases}$$



- In this case the Schrödinger equation becomes

$$\begin{cases} \dfrac{d^2\psi(x)}{dx^2} + \dfrac{2m}{\hbar^2}(E+V_0)\psi(x) = 0 & \text{for} \quad |x| < a \\ \dfrac{d^2\psi(x)}{dx^2} + \dfrac{2m}{\hbar^2}E\psi(x) = 0 & \text{for} \quad |x| > a \end{cases}$$

- Since the potential is symmetric, we assume that the wave functions have defined parity (<u>odd</u> or <u>even</u>).

Project #1: Finite Potential Well: Wavefunctions

- For an **even** wavefunction we must have

$$\psi(x) = \psi_{II}(x)) = A\cos(\alpha x) \qquad \text{for} \quad |x| < a$$
$$\psi(x) = \psi_{I,III}(x) = Be^{-\beta|x|} \qquad \text{for} \quad |x| > a$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2}(E+V_0)}\,;$$
$$\beta = \sqrt{\frac{2m}{\hbar^2}(-E)}$$

In x = a we impose continuity conditions:

$$\psi_{II}(x=a) = \psi_{III}(x=a)$$
$$\left.\frac{d\psi_{II}}{dx}\right|_{x=a} = \left.\frac{\psi_{III}}{dx}\right|_{x=a}$$

$$\longrightarrow \left\{ \begin{array}{l} A\cos(\alpha a) = Be^{-\beta a} \\ -\alpha A\sin(\alpha a) = -\beta Be^{-\beta a} \end{array} \right. \Longrightarrow \boxed{\alpha\tan(\alpha a) = \beta}$$

By solving this equation we obtain the eigenvalues *E*. Remember that *α* and *β* are functions of *E*.

- For an **odd** function, $\psi_{II}(x) = \tilde{A}\sin(\alpha x)\,, \qquad \psi_{III}(x) = \tilde{B}e^{-\beta x}$

and imposing the same continuity conditions we get

$$\boxed{\alpha\cot(\alpha a) = -\beta}$$

Project #1: Finite Potential Well: Purpose

- Compute the eigenvalues of the finite potential well.
- Use dimensionless units by introducing $\eta = \frac{E}{\hbar^2/(2ma^2)}\,, \qquad K = \frac{V_0}{\hbar^2/(2ma^2)}$
  so that the equations to be solved (in η) are:

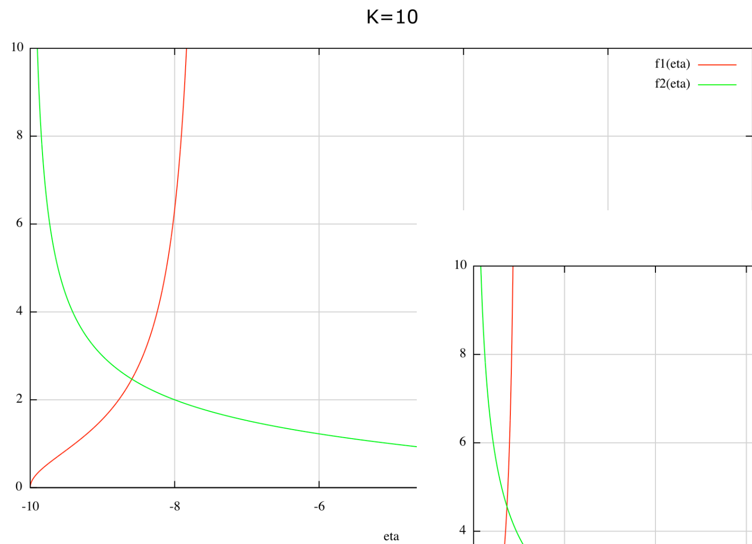
$$\begin{cases} \tan(\sqrt{\eta+K}) = \sqrt{-\frac{\eta}{\eta+K}} & \text{(even)} \\ \cot(\sqrt{\eta+K}) = -\sqrt{-\frac{\eta}{\eta+K}} & \text{(odd)} \end{cases}$$

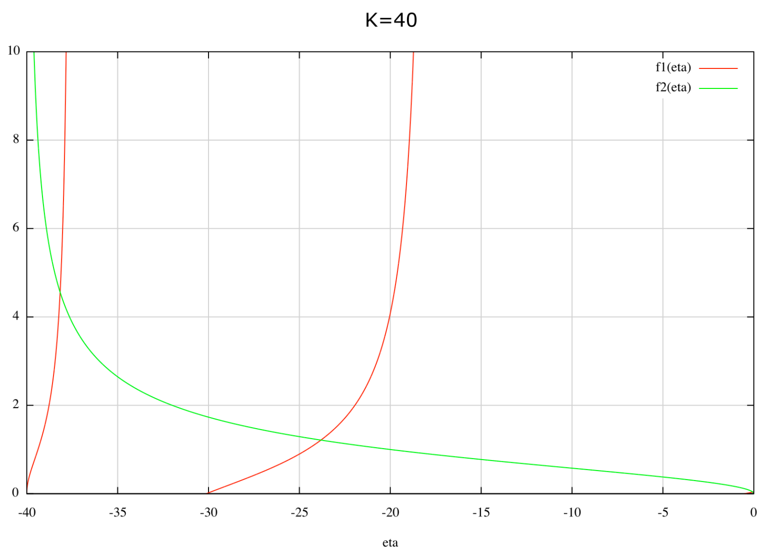
- Look for bound states which satisfy $-K < \eta < 0$ and, to avoid dealing with singularities in the tangent it is better to rewrite the equations as

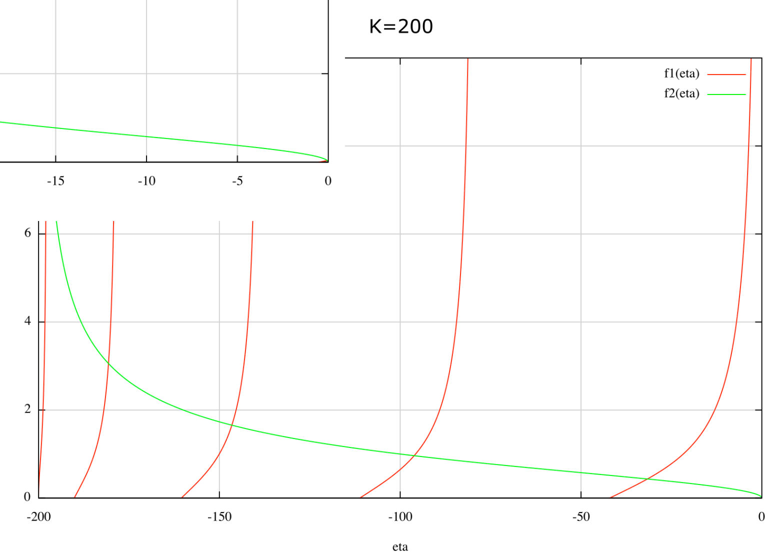
$$\begin{cases} f_e(\eta) = \sqrt{\eta+K}\sin\sqrt{\eta+K} - \sqrt{-\eta}\cos\sqrt{\eta+K} = 0 \\ f_o(\eta) = \sqrt{\eta+K}\cos\sqrt{\eta+K} + \sqrt{-\eta}\sin\sqrt{\eta+K} = 0 \end{cases}$$

Project #1: Finite Potential Well: Graphical Solution

- A graphical representation of the solution is given below:







Project #2: Realistic Projectile Motion

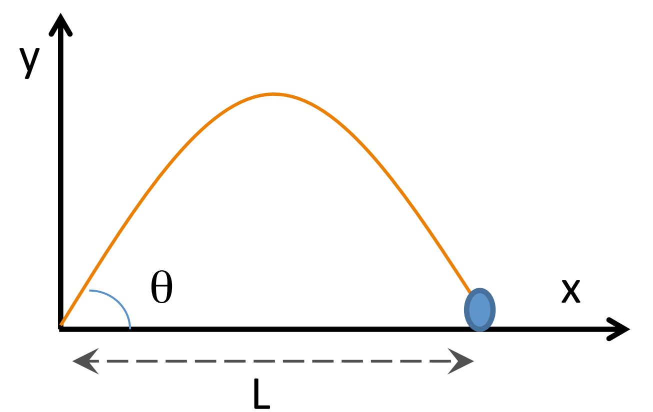
- We consider the motion of a particle subject to drag force

$$\begin{cases} \ddot{x} = F_{d,x} \\ \ddot{y} = -g + F_{d,y} \end{cases}$$

where $\vec{F}_d = -Bv\vec{v}$ is the drag force due to air resistance (for the present calculation you can use `B = 4.e-5` m^{-1}).

- This force is always opposite to velocity and therefore remember to write it in vector components.

- For a given initial velocity vo and distance L to a target, determine the angles (if any) you must orient your cannon at in order to hit the target.



Project #3: Realistic Pendulum

- Here we consider the equation of a pendulum for arbitrary amplitude and subject to damping as well as driving force:

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta - q\frac{d\theta}{dt} + F_D\sin(\Omega_D t)$$

- Here q is a measure of damping while F_D and Ω_D are the amplitude and frequency of the driving term. Transform the problem into a system of coupled 1st order ODE:

$$\begin{aligned}\frac{d\theta}{dt} &= \omega \\ \frac{d\omega}{dt} &= -(g/L)\sin\theta - q\omega + F_D\sin(\Omega_D t)\end{aligned}$$

- So that our vector of unknowns is, $Y = (\theta, \omega)$.

- With zero driving force the motion is damped.
  - With F_D = 0.5 there are two regimes:
  - An initial transient decay where the motion with angular frequency Omega is damped
  - A following phase where the pendulum settles in into a steady oscillation in response to the driving force.

Project #3: Realistic Pendulum

- The behavior changes dramatically when F_D = 1.2 since the motion is no longer simple even at long times.
- The system does not settle into a repeating steady state behavior and this is an indication of chaotic behavior.

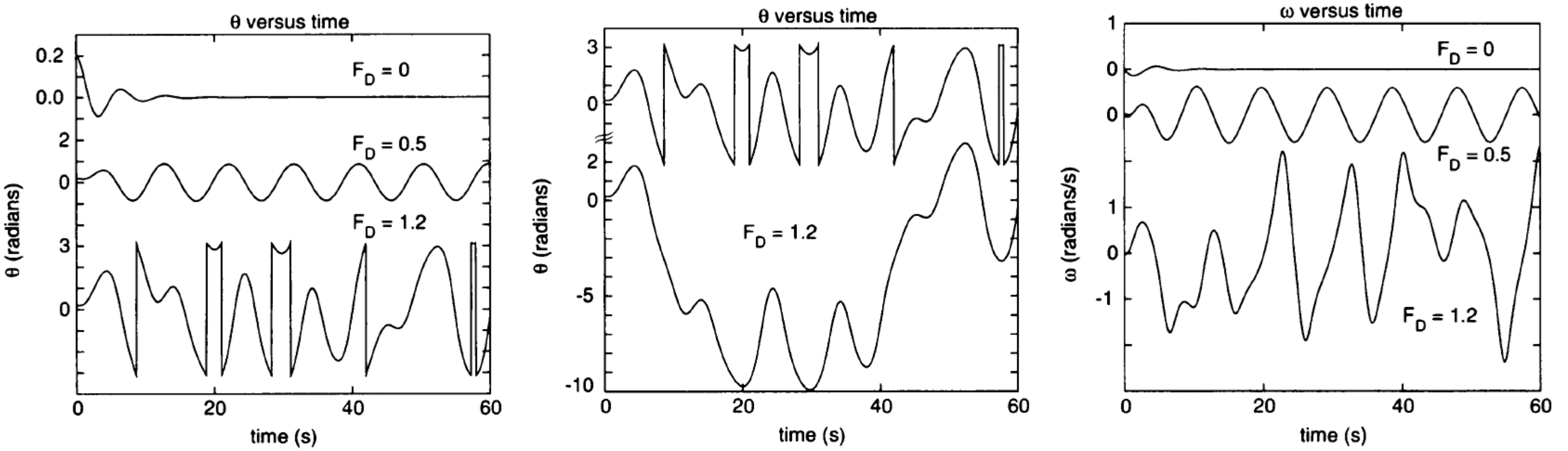
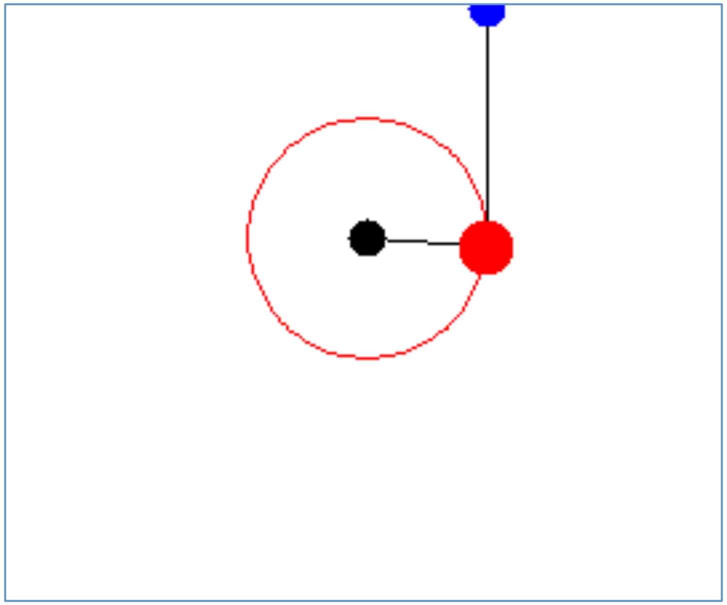


Figure 3.4: Left: behavior of θ as a function of time for our driven, damped, nonlinear pendulum, for several different values of the driving force. The vertical "jumps" in θ occur when the angle is reset so as to keep it in the range $-\pi$ to $+\pi$; they do not correspond to discontinuities in $\theta(t)$. Center: behavior of $\theta(t)$ for $F_D = 1.2$ with and without these "resets." Right: corresponding behavior of the angular velocity of the pendulum, ω. The parameters for the calculation were $q = 1/2$, $\ell = g = 9.8$, $\Omega_D = 2/3$, and $dt = 0.04$, all in SI. The initial conditions were $\theta(0) = 0.2$ and $\omega(0) = 0$.

Project #4: the Double Pendulum

- A double pendulum consists of one pendulum attached to another. It is an example of a simple physical system which can exhibit chaotic behavior.

- Consider a double bob pendulum with masses m_1 and m_2 attached by rigid massless wires of lengths L_1 and L_2. Further, let the angles the two wires make with the vertical be denoted θ_1 and θ_2.



- The position of the two masses are given by

$$x_1 = L_1 \sin \theta_1 \qquad x_2 = x_1 + L_2 \sin \theta_2$$

$$y_1 = -L_1 \cos \theta_1 \qquad y_2 = y_1 - L_2 \cos \theta_2$$

Project #4: the Double Pendulum

- After some tedious algebra, the equations of motion can be written as:

$$\theta_1'' = \frac{-g\,(2\,m_1 + m_2)\sin\theta_1 - m_2\,g\,\sin(\theta_1 - 2\,\theta_2) - 2\,\sin(\theta_1 - \theta_2)\,m_2\,(\theta_2'^2\,L_2 + \theta_1'^2\,L_1\cos(\theta_1 - \theta_2))}{L_1\,(2\,m_1 + m_2 - m_2\cos(2\,\theta_1 - 2\,\theta_2))}$$

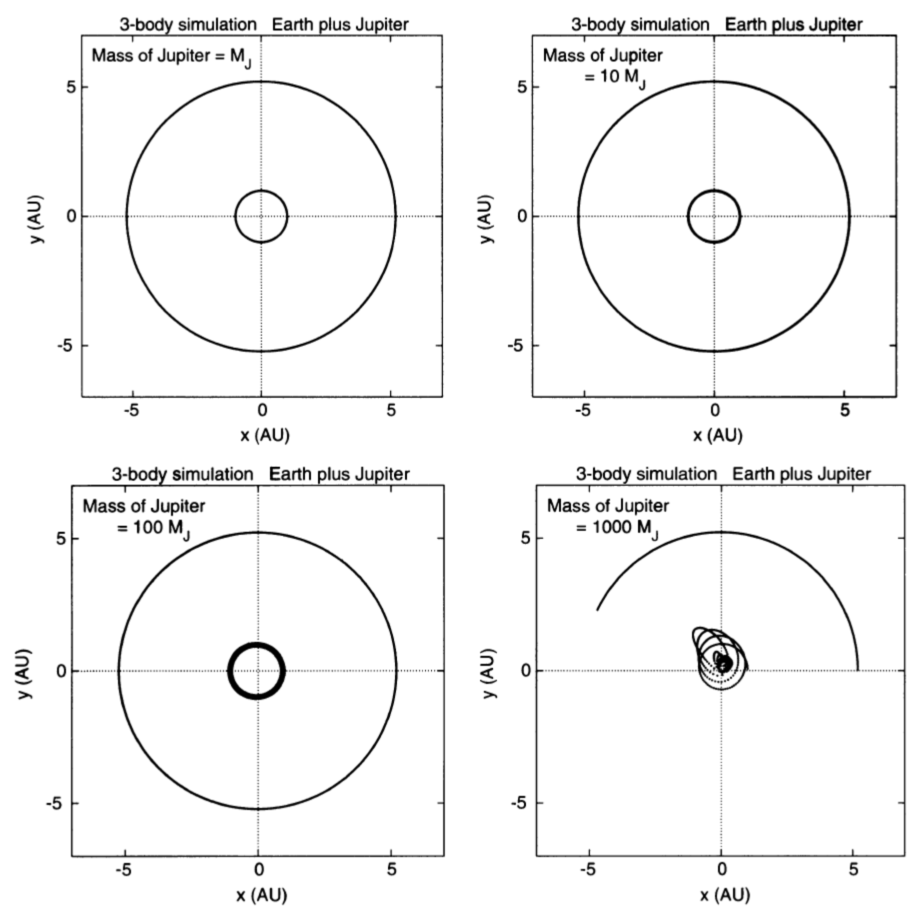
$$\theta_2'' = \frac{2\,\sin(\theta_1 - \theta_2)\,(\theta_1'^2\,L_1\,(m_1 + m_2) + g(m_1 + m_2)\cos\theta_1 + \theta_2'^2\,L_2\,m_2\cos(\theta_1 - \theta_2))}{L_2\,(2\,m_1 + m_2 - m_2\cos(2\,\theta_1 - 2\,\theta_2))}$$

- Using $m_1 = m_2$ and $L_1 = L_2$, study the double pendulum motion by direct integration of the equations of motion.

- Try to address the following issues:
  - Is energy conserved ?
  - Can you determine a range of initial condition that leads the system to chaos ?
  - Does the pendulum flip ?

Project #5: Three-body problem

- Consider the simplest three-body problem given by the earth, the Sun and Jupiter.
- We know that without Jupiter, the Earth's orbit is stable and does not change in time.
- Our objective is to quantify how much effect the gravitational field of Jupiter has on Earth's motion.
- Change the Jupiter mass by a factor of 10, 100 and 1000: do you start seeing an effect ?



Project #6: Lane-Emden Equation

- In astrophysics, the **Lane–Emden equation is a dimensionless** form of Poisson's equation for the gravitational potential of a Newtonian self-gravitating, spherically symmetric, polytropic fluid. It is named after astrophysicists Jonathan Homer Lane and Robert Emden.
- A spherically symmetric star in hydrostatic equilibrium must obey the hydrostatic balance equation

$$\frac{dP}{dr} = -\rho \frac{GM_r}{r^2}$$ where mass is related to density by $$\frac{dM_r}{dr} = 4\pi r^2 \rho$$

- Assuming an adiabatic "quasi-static" change of state of the gas following:

$$P = K\rho^\gamma = K\rho^{(n+1)/n},$$

one can rewrite the previous equation as

$$\boxed{\frac{1}{\xi^2}\frac{d}{d\xi}\left(\xi^2 \frac{d\theta}{d\xi}\right) = -\theta^n\ .}$$

This is the Lane-Emden equation.

- The equation is written in terms of dimensionless variable defined by

$$\rho = \rho_c\, \theta^n$$

$$\begin{aligned} r &= a\,\xi \\ a &= \left[(n+1)\,\frac{K}{4\pi\, G}\,\rho_c^{(1-n)/n}\right]^{1/2} \\ &= \left[(n+1)\,\frac{K}{4\pi\, G}\right]^{1/2} \rho_c^{(1-n)/2n}, \end{aligned}$$

Project #6: Lane-Emden Equation

- Exact solutions to the Lane-Emden exist for n=0,1,5 (see e.g., wikipedia) but otherwise numerical integration must be used.
- *Boundary conditions*: to get a unique solution to the Lane-Emden Equation, we need to specify two boundary conditions for this 2nd order ODE. A realistic model cannot have a 'cusp' at the origin which means that

$$\begin{aligned} \theta = 1 \quad &\text{at} \quad \xi = 0 \\ \frac{d\theta}{d\xi} = 0 \quad &\text{at} \quad \xi = 0 \end{aligned}$$

- Because $\rho \approx \theta^n$, only $\theta \geq 0$ can be realistic: this defines the surface of the polytrope is defined as the radius at which θ first becomes zero (or quite small). This is designated as ξ_s, so

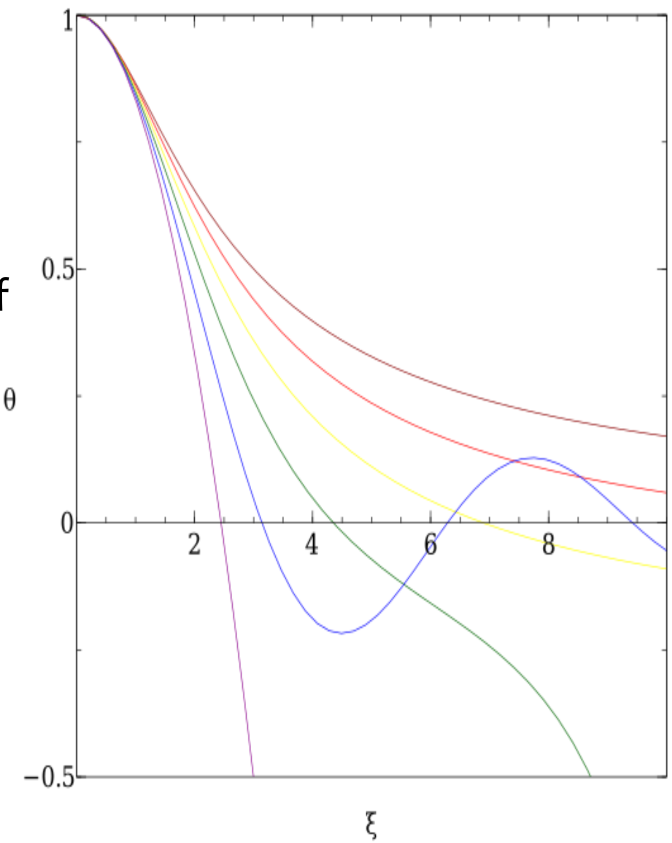
$$R = a\,\xi_s \ .$$

- If the surface seems to be approaching infinity in size, (e.g. for n = 5) the code should stop the integration.
- Note that, at the beginning, an indefinite value of $1/\xi * d\theta/d\xi$ exists. This is solved by expanding θ as

$$\theta = 1 - \frac{1}{6}\xi^2 + \frac{n}{120}\xi^4 + \cdots$$

Project #6: Lane-Emden Equation

- Solve the Lane-Emden equations for different values of n = 0, 1, 3/2, 3.
- Verify (when possible) against analytical solution (e.g. n = 1 → $\theta = \sin\xi / \xi$).
- Find the radius of the different polytropes and make plot of the density in units of the central density.



- For white dwarfs with high densities, the equation of state is well approximated by a polytropic equation of state with index n = 3. The constant K in the polytropic equation of state then is

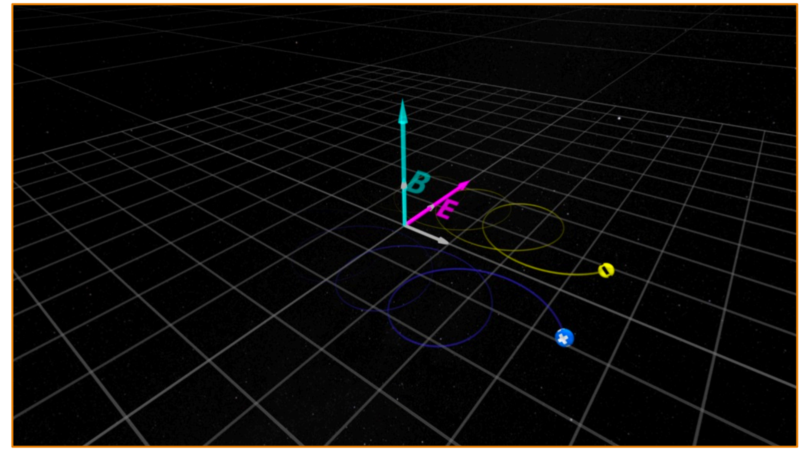
$$K = \frac{3^{1/3}\pi^{2/3}}{2^{4/3}4}\frac{\hbar c}{m_p^{4/3}},$$

- What is the mass of a high density white dwarf? If you have done everything
- right, you will have rediscovered the Chandrasekhar Mass!

Project #7: Particle(s) in EM Fields

- Study the motion of one or more (non-relativistic) particles in a fixed electromagnetic field:

$$\frac{d\vec{v}}{dt} = \frac{e}{m}\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$$



- The previous equation is written in the c.g.s sytem (widely used in astrophysics) but dimensionless units are recommended.

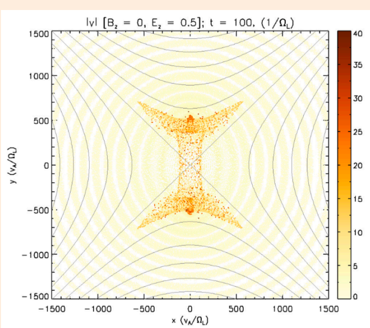
- The equation of motion (possibly) involves propagation in all 3 direction (x,y,z).

- The electric and magnetic field vector are given externally and particles do not interact with each other.

- The project involves direct integration of the equation of motion using RK-type integrators and/or the generalization of symplectic integration scheme to the case of velocity-dependent force (the Boris algorithm is the progenitor of such schemes).

Project #7: Particle(s) in EM Fields

- Provide a project with at least three different cases. A suggestion is given here:

Case	***N_{part}***	***E***	***B***	***Notes***
Simple gyration	1	(0,0,0)	(0,0,1)	Consider both perpendicular and parallel propagation. Check your results with analytical formula.
ExB drift	1	(0,E,0) with E < 1	(0,0,1)	Consider propagation along y-direction: what motion do you see ? Does the particle accelerate ? Explain.
X point 	10^3	(0,0,1/2)	(y/L, x/L,0) $L=10^3$.	Place particles uniformly in the square domain $[-L,L]^2$ and initialize particle velocity to 0.1 using randomly numbers distributed angles. Describe your results: - What kind of motion is observed ? - Do particles accelerate ? Where ?

Project #8: Physics of Partially Ionized Hydrogen

- In a variety of astrpphysical scenarios (protoplanetary disks, interstellar medium, stellar interiors, supernovae, etc…) the internal energy of the plasma is subject to radiative cooling due to a variety of processes, including bremmstrahlung, collisional ionization and excitation, etc…
- For a uniform gas distribution (no spatial variation) and assuming a partially ionized hydrogen gas, this equation may be simplified and written as

$$\frac{d(\rho e)}{dt} = -n_e n \Lambda(T)$$

where $\Lambda(n,T)$ is the cooling function, n_e is the number of electrons, n is the hydrogen number density.

- The gas internal energy includes a standard kinetic term plus the ionization energy (neutral atoms have a potential energy that is lower than that of ions by an amount χ_0= 13.6 eV).

$$\rho e = \frac{3}{2} n k_B T + \chi_0 n x(T)$$

- Here x(T) is the ionization fraction, defined by $x = \frac{n_e}{n}$

Project #8: Physics of Partially Ionized Hydrogen

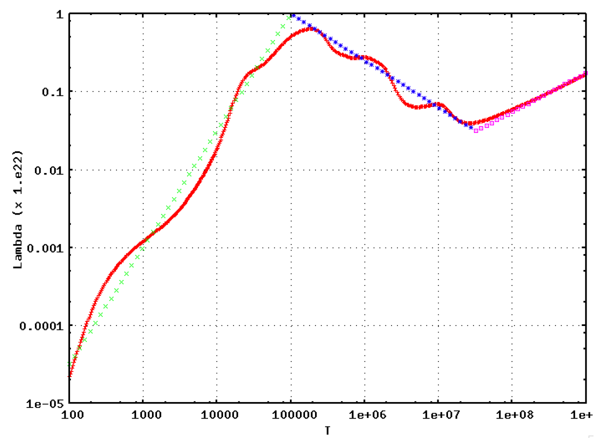
- In dilute gases (as it is the case for several astrophysical environments such as the interstellar medium or a proto-planetary disk), the degree of ionization x can be computed using Collisional excitation equilibrium (CIE), according to which

$$\boxed{x = \frac{c_r(T)}{c_i(T) + c_r(T)}, \qquad \text{where} \quad c_r = \frac{2.6 \cdot 10^{-11}}{\sqrt{T}}, \quad c_i = \frac{1.08 \cdot 10^{-8}\sqrt{T}}{\chi_0^2} \exp\left(-\alpha/T\right)}$$

where $\alpha = 157890.0$, while $\chi_0 = 13.6$.

- The cooling function is usually tabulated but, as a very crude approximation, we can use the following empirical relation:

$$\boxed{\Lambda(T) = \begin{cases} C\left(\frac{T}{T_M}\right)^{3/2} & \text{for} \quad 10^2 \lesssim T \lesssim T_M \\ C\left(\frac{T}{T_M}\right)^{-0.6} & \text{for} \quad T_M \lesssim T \lesssim T_B \\ C\left(\frac{T_B}{T_M}\right)^{-0.6}\left(\frac{T}{T_B}\right)^{1/2} & \text{for} \quad T \gtrsim T_B \end{cases}}$$



where $C = 10^{-22}$ erg/(cm^3 s).

Project #8: Physics of Partially Ionized Hydrogen

- Assuming an initial temperature of T = 10^6 K and a cloud of constant density n = 1 cm^{-3}, solve the internal energy equation

$$\frac{d(\rho e)}{dt} = -n_e n \Lambda(T)$$

- Note that at each step, the temperature must be found from the internal energy by inverting the expression for the internal energy:

$$\rho e = \frac{3}{2} n k_B T + \chi_0 n x(T)$$

where n (the gas number density) is fixed throughout the evolution.

A root finding algorithm must be used.

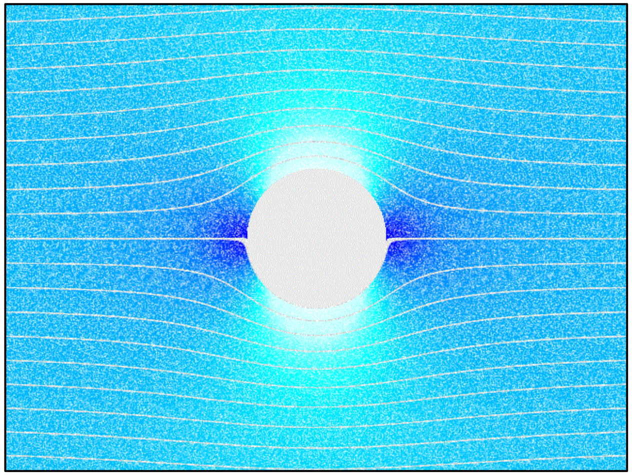
- Stop when you reach T ≈ 10^3 K.

- Produce a plot of the temperature as a function of time.

Project #9: Potential flow around cylinder

- The potential flow around a circular cylinder is a classical solution for the equations of an inviscid, incompressible fluid flow.
- Far from the cylinder, the flow is unidirectional and uniform.
- The flow is incompressible and has no vorticity :

$$\nabla \cdot \vec{V} = \nabla \times \vec{V} = 0$$



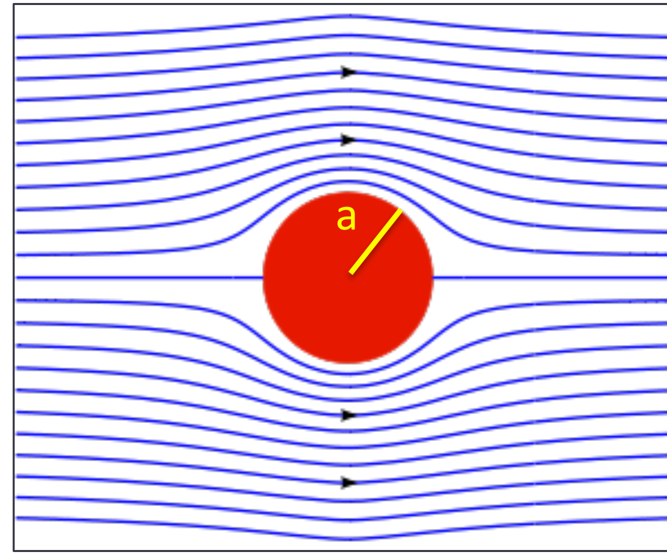
so that its velocity can thus be written

1. as the gradient of a potential: $\vec{V} = \nabla \phi$
2. using the stream function: $\vec{V} = \nabla \psi \times \hat{k}$

- Both the velocity potential and the stream functions satisfy the Laplace equation:

$$\boxed{\nabla^2 \phi = \nabla^2 \psi = 0}$$

Project #9: Potential flow around cylinder



- Solve the problem in polar coordinates *(r,ϑ)*

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \phi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 \phi}{\partial \theta^2}=0$$

- Discretized the previous equation on a domain defined by $a \le r \le 5a$, $0 \le \vartheta \le 2\pi$ *[or similar, set a=1]*

- Use the exact solution (simple) to prescribe the boundary conditions.

$$\begin{cases} \phi(r,\theta) & = & U\left(r+\frac{a^2}{r}\right)\cos\theta \\ \psi(r,\theta) & = & U\left(r-\frac{a^2}{r}\right)\sin\theta \end{cases}$$

- Or a combination or Dirichlet + Neumann b.c.

- Compute error.

Project #10: Poisson Equation in Axial symmetry

- Three dimensional problems with axial symmetry can be treated using cylindrical coordinates (r,z).

- Generalize the iterative algorithms presented in Ch. 10 to to solve the Poisson equation in 2D cylindrical coordinates

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial\varphi}{\partial r}\right) + \frac{\partial^2\varphi}{\partial z^2} + S(r,z) = 0$$

- Apply the resulting discretization to a number of problems such as:
  - Uniformly charged disk
  - Uniformly charged ring
  - Dipole field (assume charges are distributed on a finite size spheres).

- Compare results with known analytical solutions on the axis.