Computational Physics and Astrophysics

Ordinary Differential Equations
Initil-value Problems

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Ordinary Differential Equations

Any arbitrary system of ordinary differential equations (ODEs) can always be re-written as a set or first-order ODEs of the form

$$\frac{d\vec{y}}{dx} = \vec{f}(\vec{y}, x)$$

For example, Newton's second law

$$\frac{d^2\vec{x}}{dt^2} = \frac{\vec{F}}{m}$$

can be re-written as

$$\begin{aligned} \frac{d\vec{x}}{dt} &= \vec{v} \\ \frac{d\vec{v}}{dt} &= \frac{\vec{F}}{m} \end{aligned}$$

Therefore, we will concentrate on methods to solve systems n ODEs of the form

$$\vec{y}' = \vec{f}(x, \vec{y})$$

in the domain $[x_0, x_N]$ where $\vec{y} = (y_1, y_2, \ldots, y_n)$ and $\vec{f} = (f_1, f_2, \ldots, f_n)$. What about the boundary conditions?

- One needs impose n boundary conditions to solve the system.
- Initial value problem: n boundary conditions are imposed at $x = x_0$, that is, $\vec{y}(x_0) = \vec{y}_0$.
- Boundary value problem: k boundary conditions are imposed at $x = x_0$, i.e. $\{y^{(i)}(x_0) = y_0^{(i)}\}_{i=1,\ldots,k}$, and m boundary conditions are imposed at $x = x_N$, i.e. $\{y^{(i)}(x_0) = y_0^{(i)}\}_{i=1,\ldots,m}$ such that $n = m + k$.
- At this point, we will focus on boundary value problems.

Single Step Methods : Euler step

- Consider the ODE $y' = f(x, y)$ with initial boundary condition $y(x_i) = y_i$.
- A possible discretization of this equation is given by

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{\bar{y} - \bar{y}_i}{x - x_i} = f(x, \bar{y}_i)$$

  where $\bar{y}$ denotes the solution to the discrete equation above and y the solution to the continuum equation $y' = f(x, y)$.
- Solving for $\bar{y}$, we get

$$\bar{y} = \bar{y}_i + (x - x_i)\, f(x_i, \bar{y}_i)$$

- Given a mesh of grid points $\{x_0, x_1, x_2, \ldots, x_N\}$ such that $h = x_{i+1} - x_i$, we can then numerically update the solution at $\bar{y}_i$ using the following rule

$$\bar{y}_{i+1} = \bar{y}_i + h\,\bar{f}_i$$

  where $\bar{f}_i \equiv f(x_i, \bar{y}_i)$.

- Recall that

$$\left[\frac{dy}{dx}\right]_i = \left[\frac{\Delta y}{\Delta x}\right]_i + \mathcal{E}_i$$

where

$$\left[\frac{\Delta y}{\Delta x}\right]_i = \frac{y_{i+1} - y_i}{h} \quad \text{and} \quad \mathcal{E}_i = -\frac{h}{2!} y_i''$$

- Therefore

$$\begin{aligned} \left[\frac{\Delta y}{\Delta x}\right]_i &= \left[\frac{dy}{dx}\right]_i + \frac{h}{2!} y_i'' \\ \frac{y_{i+1} - y_i}{h} &= f_i + \frac{h}{2!} y_i'' \\ y_{i+1} &= y_i + h\, f_i + \frac{h^2}{2!} f_i' \end{aligned}$$

- The last term is the error after each step as a consequence of using the discrete equation.

- Notice that $\bar{y}_{i+1} = \bar{y}_i + h\,\bar{f}_i$ does not have that term since $\bar{y}$ is an exact solution to the discrete equation.
- Given the error

$$\mathcal{E}_i = \frac{h^2}{2} f'_i$$

made at each step will be, after N steps, the accumulated error will be

$$\mathcal{E} = \sum_{i=0}^{N-1} \mathcal{E}_i = \frac{h^2}{2} \sum_{i=0}^{N-1} f_i \leq h^2\,N\,C = h^2 \frac{(x_N - x_0)}{h} C = h\,(x_n - x_0)\,C$$

- That is, the Euler step has an accumulated error $\mathcal{O}(h)$, i.e. first order in h.

Euler Step: Propagation of Errors

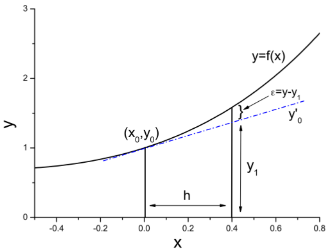
Recall that in an Euler step, the exact solution y satisfies

$$y_{n+1} = y_n + hf_n + \mathcal{E}_n$$

with $\mathcal{E}_n = h^2 f'_n/2$.

On the other hand, the numerical solution $\bar{y}$ satisfies

$$\bar{y}_{n+1} = \bar{y}_n + h\bar{f}_n$$



Define ε_n as the error at step n; that is,

$$\varepsilon_n = y_n - \bar{y}_n$$

Euler Step: Propagation of Errors

The error ε_n can re-write as

$$
\begin{aligned}
\varepsilon_n &= y_n - \bar{y}_n \\
&= y_{n-1} + h\,f(x_{n-1}, y_{n-1}) + \mathcal{E}_{n-1} - \bar{y}_{n-1} - h\,f(x_{n-1}, \bar{y}_{n-1}) \\
&= \varepsilon_{n-1} + h\,[f(x_{n-1}, y_{n-1}) - f(x_{n-1}, \omega_{n-1})] + \mathcal{E}_{n-1} \\
&= \varepsilon_{n-1} + \varepsilon_{n-1}\,h\,\frac{[f(x_{n-1}, y_{n-1}) - f(x_{n-1}, \bar{y}_{n-1})]}{y_{n-1} - \bar{y}_{n-1}} \\
&= \varepsilon_{n-1}\left[1 + h\,\frac{\partial f}{\partial y}\right]
\end{aligned}
$$

where we have neglect the higher order term $\mathcal{E}_{n-1} \propto h^2$

Therefore

$$\varepsilon_n = \varepsilon_{n-1} \left[1 + h \frac{\partial f}{\partial y} \right]$$

- Notice that the propagation of the error is linear in the step h.
- Error increases if
$$\left| 1 + h \frac{\partial f}{\partial y} \right| > 1$$
- Error decrease if
$$\left| 1 + h \frac{\partial f}{\partial y} \right| \leq 1$$
- Thus, the necessary condition for absolute convergence is
$$-\frac{2}{h} \leq \frac{\partial f}{\partial y} \leq 0$$

Convergence

- Consider the ODE of the form

$$\frac{dy}{dx} = A\,y$$

  which has as an exact solution $y = e^{Ax}$.
- According to the convergence condition for the Euler step, we need to have

$$-\frac{2}{h} < \frac{\partial f}{\partial y} = A < 0$$

- Therefore, it seems that if $A > 0$, it is not possible to use the Euler method to obtain stable and convergent solutions.
- Even in the case that $A < 0$, we need a step such that $h < 2/|A|$

Stability

- The Euler method in this case gives

$$\bar{y}_{n+1} = \bar{y}_n + h\,A\,\bar{y}_n = (1 + h\,A)\bar{y}_n$$

- Let's perturb the solution and investigate how susceptible the Euler step is to amplifying perturbations. That is consider $\bar{y}_n \to \bar{y}_n + \delta_n$ such that $\delta = C\,\xi^n$. Then

$$\begin{aligned}
\bar{y}_{n+1} + \delta_{n+1} &= (1 + hA)\,(\bar{y}_n + \delta_n) \\
&= \bar{y}_{n+1} + (1 + hA)\,\delta_n \\
&= \bar{y}_{n+1} + (1 + hA)\,\delta_n
\end{aligned}$$

- Thus

$$\begin{aligned}
\delta_{n+1} &= (1 + hA)\,\delta_n \\
C\,\xi^{n+1} &= (1 + hA)\,C\,\xi^n \\
\xi &= (1 + hA)
\end{aligned}$$

- To keep the perturbations under control, one needs to have $|\xi| \leq 1$. That is, $|1 + hA| \leq 1$, which implies again $-2/h < A < 0$

This is a form of a predictor - corrector method

$$
\begin{aligned}
\text{1st step :} \quad \hat{y}^* &= y_n + h\,f_n + O(h^2) \\
\text{2nd step :} \quad y_{n+1} &= y_n + \frac{f}{2}\left(f_n + f^*\right) + O(h^3)
\end{aligned}
$$

where $f^* = f(x_n, y^*)$

Can you explain the smaller error?

Runge - Kutta Methods

Given the ODE

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

A possible prescription to update the solution from y_n to y_{n+1} is

$$y_{n+1} = y_n + a\,k_1 + b\,k_2$$

with

$$\begin{aligned} k_1 &= h\,f(x_n, y_n) && (2)\\ k_2 &= h\,f(x_n + p\,h, y_n + q\,k_1) && (3) \end{aligned}$$

where $\{a, b, p, q\}$ are constants to be determined which lead to a second order method.

Runge - Kutta Method: 2nd Order

Let's derive the values of the parameters $\{a, b, p, q\}$. The constants will be found by comparing the ansatz $y_{n+1} = y_n + a\,k_1 + b\,k_2$ with the Taylor expansion

$$y_{n+1} = y_n + h\,f_n + \frac{h^2}{2}\left(\frac{df}{dx}\right)_n + O(h^3)$$

and we notice that

$$\begin{aligned}\frac{df}{dx} &= \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} \\ &= \frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\end{aligned}$$

thus

$$y_{n+1} = y_n + h\,f_n + \frac{h^2}{2}\left[\left(\frac{\partial f}{\partial x}\right)_n + f_n\left(\frac{\partial f}{\partial y}\right)_n\right]$$

On the other hand, from

$$\begin{aligned} y_{n+1} &= = y_n + a\,k_1 + b\,k_2 \\ &= y_n + a\,h\,f_n + b\,h\,f\,(x_n + p\,h, y_n + q\,h\,f_n) \end{aligned}$$

we Taylor expand

$$f\,(x_n + p\,h, y_n + q\,h\,f_n) \quad = \quad f_n + p\,h\left(\frac{\partial f}{\partial x}\right)_n + q\,h\,f_n\left(\frac{\partial f}{\partial y}\right)_n + \cdots$$

Therefore

$$y_{n+1} = y_n + h\,(a+b)\,f_n + h^2\left[p\,b\left(\frac{\partial f}{\partial x}\right)_n + q\,b\,f_n\left(\frac{\partial f}{\partial y}\right)_n\right]$$

Comparing this equation with

$$y_{n+1} = y_n + h\,f_n + \frac{h^2}{2}\left[\left(\frac{\partial f}{\partial x}\right)_n + f_n\left(\frac{\partial f}{\partial y}\right)_n\right]$$

we get that

$$a + b = 1, \qquad p \cdot b = \frac{1}{2} \quad \text{and} \quad q \cdot b = \frac{1}{2}$$

- Case $b = 1/2$: Thus $a = 1/2$ and $p = q = 1$. Notice that in this case the first step is $t_n + h$. This version of RK is also called the *Improved Euler or Euler-Heun Method*.

$$
\begin{aligned}
y_{n+1} &= y_n + \frac{1}{2}(k_1 + k_2) \\
k_1 &= h\, f\,(x_n, y_n) \\
k_2 &= h\, f\,(x_n + h, y_n + k_1)
\end{aligned}
$$

- Case $b = 1$: Thus $a = 0$ and $p = q = 1/2$. This is also called the *Modified Euler Method*. Notice that the first step is $t_n + h/2$.

$$
\begin{aligned}
y_{n+1} &= y_n + k_2 \\
k_1 &= h\, f\,(x_n, y_n) \\
k_2 &= h\, f\,(x_n + h/2, y_n + k_1/2)
\end{aligned}
$$

4th order Runge - Kutta Method

If we repeat the same procedure, comparing $y_{n+1} = y_n + a\,k_1 + b\,k_2 + c\,k_3 + d\,k_4$ to the corresponding Taylor series up to $O(h^4)$, we will get a system of 11 equations with 13 unknowns. Then with the appropriate choice of two of them, we come to a recurrence relation of the form :

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

where

$$\begin{aligned}
k_1 &= h\,f\,(x_n, y_n) \\
k_2 &= h\,f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \\
k_3 &= h\,f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right) \\
k_4 &= h\,f\,(x_n + h, y_n + k_3)
\end{aligned}$$

The local error is $0(h^5)$ and the global error $0(h^4)$.

Runge - Kutta - Fehlberg Method

$$
\begin{aligned}
k_1 &= h f\left(x_n, y_n\right) \\
k_2 &= h f\left(x_n + \frac{1}{4}h, y_n + \frac{1}{4}k_1\right) \\
k_3 &= h f\left(x_n + \frac{3}{8}h, y_n + \frac{3}{32}k_1 + \frac{9}{32}k_2\right) \\
k_4 &= h f\left(x_n + \frac{12}{13}h, y_n + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3\right) \\
k_5 &= h f\left(x_n + h, y_n + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4\right) \\
k_6 &= h f\left(x_n + \frac{1}{2}h, y_n - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5\right)
\end{aligned}
$$

A step with local error is $O(h^5)$ is obtained with

$$y_{n+1} = y_n + \left(\frac{25}{216} k_1 + \frac{1408}{2565} k_3 + \frac{2197}{4104} k_4 - \frac{1}{5} k_5 \right)$$

A step with local error is $O(h^6)$ is obtained with

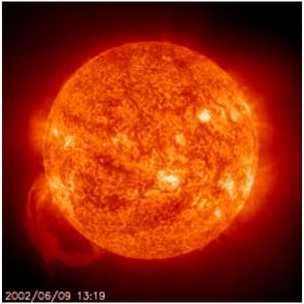
$$y_{n+1} = y_n + \left(\frac{16}{135} k_1 + \frac{6656}{12825} k_3 + \frac{28561}{56430} k_4 - \frac{9}{50} k_5 + \frac{2}{55} k_6 \right)$$

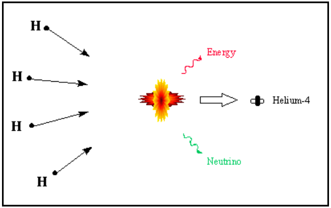
Project: Stellar Structure Models

The main physical processes that determine the structure of stars are:

- Gravity
- Internal Thermal Pressure
- Hydrostatic Equilibrium

We will assume that the star is isolated, static and spherically symmetric. Therefore, the problem is time-independent, and all the variables depend only on the distance from the center of the star.





Hydrostatic Equilibrium

Density:

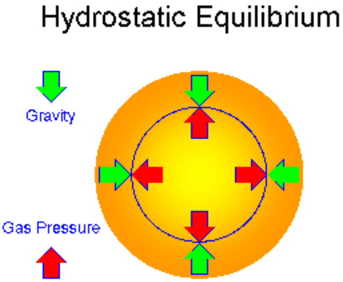
$$\rho = \frac{dm}{dV}$$

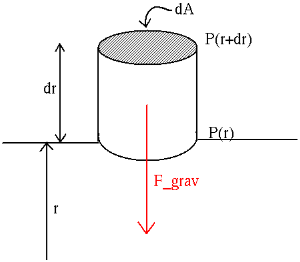
but

$$dV = dA\,dr = 4\,\pi\,r^2\,dr$$

therefore

$$\rho = \frac{1}{4\,\pi\,r^2}\frac{dm}{dr} \quad \text{or} \quad \frac{dm}{dr} = 4\,\pi\,r^2\rho$$





Hydrostatic Equilibrium

Notice that the mass enclosed within a radius r is

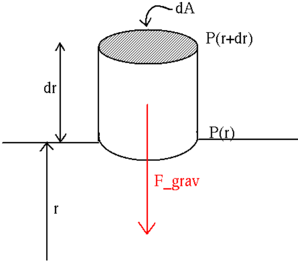
$$m(r) = \int_0^r \rho\, dV = \int_0^r 4\,\pi\,\bar{r}^2\,\rho\, d\bar{r}$$

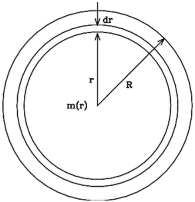
The external force dF_g of the enclosed mass $m(r)$ on the mass element dm is

$$dF_g = -\frac{G\,m\,dm}{r^2}$$

The external force dF_p from the gas pressure on dm

$$\begin{aligned} dF_p &= -\left[P(r+dr) - P(r)\right] dA \\ &= -\frac{\left[P(r+dr) - P(r)\right]}{dr}\, dr\, dA \\ &= -\frac{dP}{dr}\, dV \end{aligned}$$





Hydrostatic Equilibrium

The condition for equilibrium is then $dF_g + dF_p = 0$. Thus,

$$\begin{aligned}
\frac{dP}{dr}dV &= -\frac{G\,m\,dm}{r^2} \\
\frac{dP}{dr} &= \frac{G\,m}{r^2}\frac{dm}{dV} \\
&= -\frac{G\,m}{r^2}\rho
\end{aligned}$$

In summary

$$\begin{aligned}
\frac{dm}{dr} &= 4\,\pi\,r^2\rho \\
\frac{dP}{dr} &= -\frac{G\,m}{r^2}\rho
\end{aligned}$$

for the physical quantities: mass (m), density (ρ) and pressure (P).

Equation of State

We have two equations for three unknowns. We need to provide an addition equation to close the system: Equation of State (EOS) That is, $P = P(\rho)$.

Usually, we use the EOS to eliminate the pressure from the equations. That is,

$$
\begin{aligned}
\frac{dP}{dr} &= -\frac{G\,m}{r^2}\rho \\
\frac{dP}{d\rho}\frac{d\rho}{dr} &= -\frac{G\,m}{r^2}\rho \\
\frac{d\rho}{dr} &= -\frac{G\,m}{r^2}\rho\left(\frac{dP}{d\rho}\right)^{-1}
\end{aligned}
$$

Boundary Conditions

Stellar Model Equations

$$\begin{aligned} \frac{dm}{dr} &= 4\,\pi\,r^2\rho \\ \frac{d\rho}{dr} &= -\frac{G\,m}{r^2}\rho\left(\frac{dP}{d\rho}\right)^{-1} \end{aligned}$$

- At $r = 0$, that is at the center of the star, $m = 0$ and $\rho = \rho_c$
- At $r = R$, that is at the surface of the star, $m = M$ and $\rho = 0$

We cannot impose all four conditions at the same time since we only have two equations.

Typically, one pick the conditions at $r = 0$ and integrates out to the surface, stoping when the density becomes $\rho \leq 0$

Polytropes

- We will model the star as a polytrope with an EOS give by $P = K\,\rho^{\Gamma}$, also written as $P = K\,\rho^{(n+1)/n}$ with n called the polytropic index; thus, $\Gamma = (n+1)/n$
- For stars like the Sun supported by radiation pressure, $\Gamma = 4/3, n = 3$. For stars like white dwarfs supported by degenerate pressure $\Gamma = 5/3, n = 3/2$
- With this EOS, we can rewrite

$$\frac{dP}{d\rho} = K\,\Gamma\,\rho^{\Gamma-1}$$

- Notice that we need to have $\Gamma \leq 2$ so $d\rho/dr$ is finite when $\rho = 0$ at $r = R$

A more careful calculation of the EOS yields

$$\begin{aligned}
\frac{dP}{d\rho} &= \frac{Y_e\, c^2\, m_e}{m_p}\gamma(x) \quad \text{where} \\
\gamma(x) &= \frac{x^2}{3\,(1+x^2)^{1/2}} \quad \text{with} \\
x &\equiv \frac{\rho}{\rho_0}
\end{aligned}$$

Above

$$\begin{aligned}
Y_e &= \text{electron per nucleon} \\
m_e &= \text{electron mass} \\
m_p &= \text{proton mass} \\
\rho_0 &= \frac{m_p\, n_0}{Y_e} \\
n_0 &= \frac{8\,\pi}{3}\frac{m_e^3\, c^3}{h^3}
\end{aligned}$$

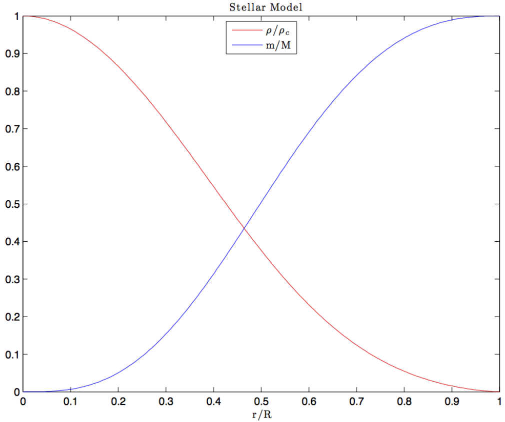
For relativistic stars, in which one need to use General Relativity instead of Newtonian gravity, the system of equations become

$$
\begin{aligned}
\frac{dm}{dr} &= 4\,\pi\, r^2 \rho \\
\frac{d\rho}{dr} &= -\frac{(\rho + P)\,(m + 4\,\pi\, r^3\, P)}{r(r - 2\, m)} \left(\frac{dP}{d\rho}\right)^{-1}
\end{aligned}
$$

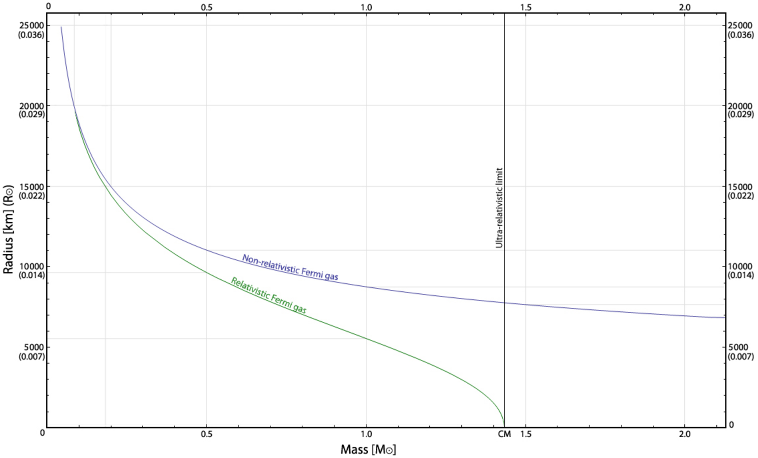
in units in which $c = G = 1$.
The Newtonian limit is recovered when

$$
r \gg 2\, m \quad \rho \gg P \quad m/(4\,\pi\, r^3) \gg P
$$

White-dwarf case



White-dwarf mass-radius relationship



Notice that in the relativistic case, there is a maximum mass that a WD could have $\sim 1.44\ M_\odot$. This is the so-called Chandrasekhar mass limit.