Computational Astrophysics I: Introduction and basic concepts

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Differential equations

Types of differential equations I

One can classify differential equations regarding their

- *order*, so the degree of the highest derivative. General form of a first-order differential equation:

$$\frac{dy}{dt} = f(y,t) \tag{1}$$

for any arbitrary function f, e.g., $\frac{dy}{dt} = 2ty^8 - t^5 + \sin(y)$. A second-order differential equation has the form:

$$\frac{d^2y}{dt^2} + \lambda\frac{dy}{dt} = f(t, \frac{dy}{dt}, y) \tag{2}$$

and so on.

Types of differential equations II

Reduction

By introducing auxillary variables/functions, every higher order differential equation can be reduced to a set of *first-order* differential equations

$$y^{(m)}(x) = f(x, y(x), y^{(1)}(x), \ldots, y^{(m-1)}(x)) \tag{3}$$

introduce functions z

$$\rightarrow z_1(x) := y(x) \tag{4}$$

$$z_2(x) := y^{(1)}(x) \tag{5}$$

$$\vdots \tag{6}$$

$$z_m(x) := y^{(m-1)}(x) \tag{7}$$

$$\rightarrow z' = \begin{bmatrix} z_1' \\ \vdots \\ z_m' \end{bmatrix} = \begin{bmatrix} z_2 \\ \vdots \\ f(x, z_1, z_2, \ldots, z_m) \end{bmatrix} \tag{8}$$

Types of differential equations III

One can distinguish

- *ordinary diffential equations (ODE)*, where only one independent variable is explicitly involved (typically time or location), e.g., hydrostatic equation for $P(r)$:

$$\frac{dP}{dr} = -\rho(r)\, g(r) \tag{9}$$

- *partial differential equations (PDE)*, where derivatives with respect to at least two variables occur, e.g., Poisson equation:

$$\Delta\rho = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\rho(x,y,z) = f(x,y,z) \tag{10}$$

$\rightarrow$ The theory and (numerical) solution of PDEs is more complicated than for ODE.

Types of differential equations IV

Moreover, there are the classes of

- *linear* differential equations: only the first power of y or $d^n y/dt^n$ occurs, e.g. *wave equation*:

$$\left(\frac{1}{c^2}\frac{\partial}{\partial t} - \Delta\right) u = 0 \tag{11}$$

$\rightarrow$ special property: *law of linear superposition*, linear combinations of solutions are also solutions:

$$u_2(x,y,z,t) = a u_0(x,y,z,t) + b u_1(x,y,z,t) \tag{12}$$

$\rightarrow$ unperturbed superposition of waves

Types of differential equations V

- *nonlinear* differential equations: contain higher powers or other functions of y or $d^n y/dt^n$, e.g.:

$$\frac{d\theta^2}{dt^2} = \frac{l}{g}\sin\theta \tag{13}$$

$\rightarrow$ clear: linear combinations of solutions are not automatically solutions too, e.g.

$$\frac{dy}{dt} = \lambda y(t) - \lambda^2 y^2(t) \tag{14}$$

$$y(t) = \frac{a}{1+be^{-\lambda t}} \quad \text{one solution} \tag{15}$$

$$y_1(t) = \frac{a}{1+be^{-\lambda t}} + \frac{c}{1-de^{-\lambda t}} \quad \text{not a solution} \tag{16}$$

$\rightarrow$ nonlinear differential equations in general became feasible with the rise of computers

Boundary values I

As general solution of (ordinary) differential equation contains arbitrary constant per order, problems involving differential equations can be characterized by the type of conditions:

1. *initial* values/conditions must be given: constant for 1st order differential equation (usually time-dependent) fixed by giving $y(t)$ for some time t_0, so giving $y_0 = y(t_0)$; for 2nd order by giving additionaly $y'(t_0)$ and so on (Note, that we solve usually for $t > t_0$, but this is not a requirement), e.g., Kepler problem

$$\vec{v}(t) = \dot{\vec{r}}(t) \quad \& \quad \vec{a}(t) = \dot{\vec{v}}(t) = \vec{F}_{\mathrm{G}}(r)/m \tag{17}$$

$$x(t_0) = x_0, y(t_0) = 0; v_x(t_0) = 0, v_y(t_0) = v_{y,0} \tag{18}$$

For the initial value problem (Cauchy problem), the theorem by Picard-Lindelöf guarantees a unique solution:

Existence and uniqueness of the solution for the initial value problem

$$y' = f(y, x), \quad y(x_0) = y_0 \tag{19}$$

If f is continuous on the stripe $S := \{(x, y)|a \leq x \leq b, y \in \mathbb{R}^n\}$ with finite a, b and a constant L, such that

$$||f(x, y_1) - f(x, y_2)|| \leq L||y_1 - y_2|| \tag{20}$$

for all $x \in [a, b]$ and for all $y_1, y_2 \in \mathbb{R}^n$ (Lipschitz continuous), then exists for all $x_0 \in [a, b]$ and for all $y_0 \in \mathbb{R}^n$ a unique function $y(x)$ for $x \in [a, b]$ with

1. $y(x)$ is continuous and continuously differentiable for $x \in [a, b]$;
2. $y'(x) = f(x, y(x))$ for $x \in [a, b]$;
3. $y(x_0) = y_0$

Note that the Lipschitz condition (bounded slope) of $f(y,x)$ is required for uniqueness, e.g., $y'(x) = \sqrt{|x|}$ with $y(0) = 0$ is fulfilled by $y_1(x) \equiv 0$ and also by $y_2(x) = \frac{x^2}{4}$, that is because $f'(y,x) = \frac{1}{\sqrt{|x|}}$ and hence $\lim_{x\to 0} f' = \infty$.

Without Lipschitz condition the *Peano existence theorem* guarantees at least the existence of a solution.

Proof concept

Integrating Eq. (19) gives a fixed point equation:

$$y(x) - y(x_0) = \int_{x_0}^{x} f(s, y(s))ds \tag{21}$$

with Picard-Lindelöf iteration

$$\phi_0(x) = y_0 \quad \text{and} \quad \phi_{k+1} = y_0 + \int_{x_0}^{x} f(s, \phi_k(s))ds \tag{22}$$

Example: Picard iteration

For the Cauchy problem

$$y'(x) = 1 + y(x)^2, \quad y(x_0) = y(0) = 0 \tag{23}$$

$$\phi_0(x) = 0 \tag{24}$$

$$\phi_1(x) = 0 + \int_0^x (1 + 0^2) ds = x \tag{25}$$

$$\phi_2(x) = 0 + \int_0^x (1 + s^2) ds = x + \frac{1}{3}x^3 \tag{26}$$

→ Taylor series expansion of $y(x) = \tan(x)$

so following *Banach fixed point theorem* ϕ_k converges uniquely to the solution $y(x)$. The existence of $y(x)$ (Peano) is proven by constructing a piecewise continuous function with help of the Euler method (polygonal curve) that converges uniformly for $\Delta x \rightarrow 0$.

Boundary values V

2. *boundary* values/conditions can be given, (additionally to initial conditions) to restrict further the solutions, i.e., constrain it to fixed values at the boundaries of the solution space, usually for 2nd order differential equation

$$u''(x) = f(u, u', x) \tag{27}$$

where u or u' is given at boundaries, by transformation, e.g.,

$$x' = (x - x_1)/(x_2 - x_1) \tag{28}$$

at $x = 0$ and $x = 1$. Then $\rightarrow$ 4 possible types of boundary conditions

1. $u(0) = u_0$ and $u(1) = u_1$
2. $u(0) = u_0$ and $u'(1) = v_1$
3. $u'(0) = v_0$ and $u(1) = u_1$
4. $u'(0) = v_0$ and $u'(1) = v_1$

Boundary values VI

Usually: reduce to set of 1st order differential equations and start integration with given $u(0)$ *and* $u'(0)$. But for boundary-value problem: only $u(0)$ ***or*** $u'(0)$ given, $\rightarrow$ not sufficient for any initial-value algorithm

Example: Boundary values

First two equations of stellar structure (e.g., for white dwarf)

$$\frac{\partial r}{\partial m} = \frac{1}{4\pi r^2 \rho} \quad \text{mass continuity} \tag{29}$$

$$\frac{\partial P}{\partial m} = -\frac{G\,M}{4\pi r^4} \quad \text{hydrostatic equilibrium} \tag{30}$$

+ equation of state $P(\rho)$ (e.g., ideal gas $P = RT\rho/\mu$), and boundary values

$$\text{center} \quad m = 0 : r = 0 \tag{31}$$

$$\text{surface} \quad m = M : \rho = 0 \rightarrow P = 0 \tag{32}$$

$\rightarrow$ solve for $r(m)$, specifically for $R_* = r(m = M_*)$

Boundary values VII

3. *eigenvalue problems:* solution for selected parameters (λ) in the equations; usually even more complicated and solution not always exist, sometimes *trial-and-error search* necessary. E.g.,

$$u'' = f(u, u', x, \lambda) \tag{33}$$

for eigenvalue λ plus a set of boundary conditions. Eigenvalue λ can only have some selected values for valid solution.

E.g., Schrödinger equation for particle confined in a potential:
eigenfunctions $\rightarrow$ wavefunction ϕ_k;
eigenvalues $\rightarrow$ discrete energies $E_k \rightarrow \hat{H}\phi_k = E_k\phi_k$

Boundary values VIII

Eigenvalue problem: Stationary elastic waves

Displacement $u(x)$ by

$$u'' = -k^2 u \tag{34}$$

Allowed values of wavevector $k = \omega/c \rightarrow$ eigenvalues of the problem
both ends fixed: $u(0) = u(1) = 0$ or one end fixed, other end free: $u(0) = 0$ and $u'(1) = 0$.
Fortunately, analytical solutions:

$$u_n(x) = \sqrt{2}\sin(k_n x) \quad \& \quad k_n = n\pi \quad n = \pm 1, \pm 2, \ldots \tag{35}$$

Moreover, complete solution of longitudinal waves along elastic rod: linear combination of *all* eigenfunctions with their initial solutions (fixing c_n)

$$u(x,t) = \sum_{n=-\infty}^{\infty} c_n u_n(x) e^{in\pi ct} \tag{36}$$

Simple method for *boundary-value* and *eigenvalue* problems: shooting method (origin from artillery), cf. Pang (1997)
e.g., for boundary-value problem $u'' = f(u, u', x)$ with $y_1 \equiv u$ and $y_2 \equiv u'$

$$\frac{dy_1}{dx} = y_2 \tag{37}$$

$$\frac{dy_2}{dx} = f(y_1, y_2, x) \tag{38}$$

plus boundary conditions, e.g., $u(0) = y_1(0) = u_0$ and $u(1) = y_1(1) = u_1$.
Idea: introduce adjustable parameter δ, so that we have an initial value problem. E.g., $u'(0) = \delta \rightarrow$ together with given $u(0) = u_0$; integrate for given intial values up to $x = 1$ with result $u(1) = u_\delta(1)$, so that

$$F(\delta) = u_\delta(1) - u_1 \stackrel{!}{=} 0 \tag{39}$$

$\rightarrow$ use root search algorithm to determine (approximative) δ

Shooting method for boundary value problem (Stoer & Bulirsch 2005)

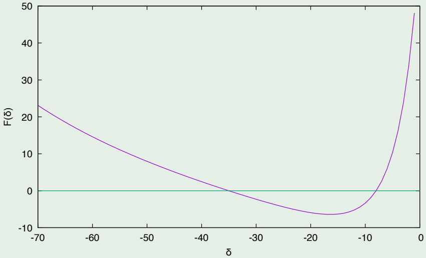
$$u''(x) = \frac{3}{2}u^2, \quad u(0) = 4, \quad u(1) = 1 \tag{40}$$

$$\text{set } y_1 \equiv u \text{ and } y_2 \equiv u' \quad y_1(0) = 4, \quad y_2(0) = \delta = -1, \ldots - 70 \tag{41}$$

$$\rightarrow y_{1,k+1} = y_{1,k} + \Delta x \cdot y_{2,k} \tag{42}$$

$$y_{2,k+1} = y_{2,k} + \Delta x \cdot 3./2. * y_{1,k}^2 \tag{43}$$

plot $F(\delta) = y_{1,n} - u(1)$, roots give missing initial values $u'(0)$



The shooting method III

Similarly, for given

- $u'(0) = v_0$ and $u(1) = u_1 \to u(0) = \delta$, find root of $F(\delta) = u_\delta(1) - u_1$
- $u'(0) = v_0$ and $u'(1) = v_1 \to F(\delta) = u'_\delta(1) - v_1$

Moreover, for eigenvalue problem:

- if $u(0) = u_0$ and $u(1) = u_1$ given, start integration with $u'(0) = \delta$ with small δ
- search root $F(\lambda) = u_\lambda(1) - u_1 \to$ approximated eigenvalue λ and eigenvector from normalized solution $u_\lambda(x) \to \delta$ automatically modified to be correct $u'(0)$ through normalization of eigenfunctions

Direct solution of 2nd order ODE I

Although, always possible $\rightarrow$ reduce 2nd order ODE to set of coupled 1st order ODEs, however, sometimes direct solution has advantages

Example: Radiative Transfer Equation

For the 1d case:

$$\frac{dI^{\pm}}{d\tau} = \pm(S - I^{\pm}), \quad d\tau = \kappa dz \tag{44}$$

with inward $(-)$ and outward $(+)$ intensities $I = dE/d\Omega\, dA\, dt\, d\nu$, optical depth τ and source function $S = \eta/\kappa$.
Introducing Feautrier variables (Schuster 1905; Feautrier 1964):

$$u = \frac{1}{2}(I^{+} + I^{-}) \quad \text{(intensity-like)} \tag{45}$$

$$v = \frac{1}{2}(I^{+} - I^{-}) \quad \text{(flux-like)} \tag{46}$$

Direct solution of 2nd order ODE II

we get system of two coupled 1st order ODE:

$$\frac{du}{d\tau} = v \quad \text{and} \quad \frac{dv}{d\tau} = u - S \tag{47}$$

or, combining them:

$$\frac{d^2u}{d\tau^2} = u - S \tag{48}$$

discretization on a τ grid (τ_i) with numerical derivatives (see below):

$$\left.\frac{d^2u}{d\tau^2}\right|_{\tau_i} \approx \frac{\left.\frac{du}{d\tau}\right|_{\tau_{i+1/2}} - \left.\frac{du}{d\tau}\right|_{\tau_{i-1/2}}}{\tau_{i+1/2} - \tau_{i-1/2}} \approx \frac{\frac{u_{i+1}-u_i}{\tau_{i+1}-\tau_i} - \frac{u_i-u_{i-1}}{\tau_i-\tau_{i-1}}}{\frac{1}{2}(\tau_{i+1} - \tau_i) - \frac{1}{2}(\tau_i - \tau_{i-1})} \tag{49}$$

$\rightarrow$ set of linear equations for u_i for $i = 2, \ldots, i_{\max} - 1$:

$$-A_i u_{i-1} + B_i u_i - C_i u_{i+1} = S_i \tag{50}$$

with the coefficients

$$A_i = \left(\frac{1}{2}(\tau_{i+1} - \tau_{i-1})(\tau_i - \tau_{i-1})\right)^{-1} \tag{51}$$

$$C_i = \left(\frac{1}{2}(\tau_{i+1} - \tau_{i-1})(\tau_{i+1} - \tau_i)\right)^{-1} \tag{52}$$

$$B_i = 1 + A_i + C_i \tag{53}$$

Direct solution of 2nd order ODE IV

$\rightarrow$ tridiagonal matrix, efficiently solvable by standard linear algebra solvers (e.g., Gauß-Seidel elimination)

$$\begin{bmatrix} B_1 & -C_1 & & & & \\ -A_2 & B_2 & -C_2 & & & \\ \cdots & & & & & \\ & & -A_i & B_i & -C_i & \\ \cdots & & & & & \\ & & & & B_{i_{\max}} & -C_{i_{\max}} \end{bmatrix} \circ \begin{bmatrix} u_1 \\ u_2 \\ \cdots \\ u_i \\ \cdots \\ u_{i_{\max}} \end{bmatrix} = \begin{bmatrix} W_1 \\ W_2 \\ \cdots \\ W_i \\ \cdots \\ W_{i_{\max}} \end{bmatrix} \tag{54}$$

Note: $W_i = S_i$ exept for $i = 1$ and $i_{\max} \rightarrow$ boundary conditions

Advantage of Feautrier scheme

- direct solution of 2nd order ODE saves memory
- at large optical depths $I^+ \approx I^- \rightarrow$ radiative flux $\sim I^+ - I^-$ inaccurate because of roundoff error, Feautrier scheme uses instead averaged quantities u, v for higher accuracy ($\rightarrow$ stability in an iterative scheme for $S(I), \tau(I)$)

Literature I

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