Scientific Computing Lecture 4

Differential equations (part 1)

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Part 1: Differential operator

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Differential equations

Many Physical Problems can be described with use of Differential Equations

- A differential equation is an equation for an unknown function of one or several variables that relates the values of the function itself and of its derivatives of various orders.
- **Ordinary Differential Equation:** Function has 1 independent variable.
- **Partial Differential Equation:** At least 2 independent variables.

The operator equation for differential equations is often written as:

$$D\mathbf{u} = 0,$$

where D represents both mathematical and the right-hand side (observed data); the function $\mathbf{u}$ is an unknown function to be found.

- **Ordinary differential equation (ODE):** Let $x \in \mathbb{R}^1$. ODE of the k-th order can be represented with the operator:

$$D\mathbf{u} = F\Big(x, u(x), u'(x), u''(x), ..., u^{(k)}(x)\Big).$$

- **Partial differential equation (PDE):** Let $\mathbf{x} \in \mathbb{R}^n \equiv (x_1, x_2, ..., x_n)$. PDE of the k-th order can be represented with the following operator:

$$D\mathbf{u} = F\Big(\mathbf{x}, \mathbf{u}(\mathbf{x}), \frac{\partial \mathbf{u}}{\partial x_1}, ..., \frac{\partial \mathbf{u}}{\partial x_n}, \cdots \frac{\partial^2 \mathbf{u}}{\partial x_1^2}, ..., \frac{\partial^2 \mathbf{u}}{\partial x_n^2}, \cdots \frac{\partial^{(k)} \mathbf{u}}{\partial x_1^{(k)}}, \frac{\partial^{(k)} \mathbf{u}}{\partial x_n^{(k)}}\Big).$$

- The function $F(...)$ usually satisfies the regularity conditions: measurability, differentiability, continuity etc.
- **Linear equations:** If the function F depends linearly on $\mathbf{u}$ and its derivatives, then the ODE/PDE is linear.
- **Quasi-linear equations:** the function F linearly depends on higher-order derivatives.
- **Non-linear equations:** the most complicated case. The function F depends non-linearly on higher order (and, maybe, all other) derivatives.

ODE: Problems

Ordinary Differential Equation (ODE) of p^{th} order can be written in as follows:

$$F\Big(x, u'(x), u''(x), ..., u^{(p)}(x)\Big) \equiv D\mathbf{u} = 0.$$

Rewrite it in the form:

$$u^{(p)}(x) = f(x, u, u', u'', ..., u^{(p-1)}).$$

We refer to the fact that with $u^{(k)}(x) \equiv u_k(x)$ and $u(x) = u_0(x)$, the latter equation may be represented with a system of the first-order ODEs:

$$\begin{aligned} u_k^{'}(x) &= u_{k+1}(x), \quad 0 \le k \le p-2, \\ u_{p-1}^{'}(x) &= f(x, u_0, u_1, ..., u_{p-1}), \end{aligned}$$

ODE: Three kinds of problems

By analogy, each system of differential equations of any order can be changed with equivalent system of the first-order ODE:

$$u_k^{'} = f(x, u_1, u_2, ..., u_p),$$

or, using the vector form:

$$\mathbf{u}'(x) = \mathbf{f}(x, \mathbf{u}(x)), \quad u = \{u_1, ..., u_p\}, \mathbf{f} = \{f_1, ..., f_p\}.$$

There are three kinds of problem related to the ODEs

- The Cauchy problem
- Boundary value problem
- Eigenvalues problem

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Part 2: Cauchy Problems

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ODE: The Cauchy problem

- Vector form:

$$\mathbf{u}'(x) = \mathbf{f}\big(x, \mathbf{u}(x)\big), \quad x \in [\xi, X]$$
$$\mathbf{u}(\xi) = \eta, \quad \text{or } u_k(\xi) = \eta_k, 1 \le k \le p.$$

- Or common form:

$$F\Big(x, u(x), u'(x), ..., u^{(p)}(x)\Big) \equiv D\mathbf{u} = 0.$$
$$u^{(k)}(\xi) = \eta_k, \quad 0 \le k < p$$

- The conditions may be considered as the definition of some initial point $(\xi, \eta_1, ..., \eta_p)$ for an integral curve in $(p+1$-dimensional space $(x, u_1, ..., u_p)$.

Augustin-Louis Cauchy
1789-1857

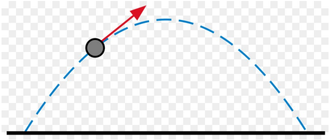
The simplest Cauchy problem

Consider a ball with mass m. Let this ball be thrown; we need to calculate its trajectory.

- m - the mass of the ball
- $\mathbf{x}(t)$ - the coordinate of the ball at the moment of time t; $\mathbf{x} \in \mathbb{R}^2$
- $\mathbf{v}(t)$ is a velocity of the ball; $\mathbf{v} \in \mathbb{R}^2$
- The governing equation:

$$\mathbf{x}'(t) = \mathbf{v}(t),$$
$$\mathbf{x}''(t) = \mathbf{g},$$

  where $\mathbf{g}$ is a gravitational acceleration.
- $\mathbf{x}(0) = \mathbf{x}_0; \mathbf{v}(0) = \mathbf{v}_0$



The simplest Cauchy problem

The solution of the problem can be easily found using simple integration:

$$\mathbf{v}(t) = Const + \int\limits_0^t \mathbf{g} d\tau = \mathbf{v}_0 + \mathbf{g}t,$$

$$\mathbf{x}(t) = Const + \int\limits_0^t \mathbf{v}(\tau) d\tau = \mathbf{x}_0 + \mathbf{v}_0 t + \mathbf{g}t^2$$

Since in our case $\mathbf{g}$ has no x-component ($\mathbf{g} = (0, -9.8)^T$), then, as we can see, the x component of the speed will be fixed. But...

- What if we have not only one body (ball)?
- What if we have air?
- What if we have other forces affecting the bodies?

Consider a number of point-bodies $B_i, i = 1, ..., N$, defined with the coordinates $x_i(t)$ at the moment of time t. Each body interacts with other bodies via the gravitation:

$$m_i \ddot{x}_i(t) = \sum_{j \neq i}^{N} G m_j m_i \frac{x_j(t) - x_i(t)}{|x_j(t) - x_i(t)|^3}, \quad 1 \leq i, j \leq N.$$

In order to state the problem, we also need to define the initial body positions with known coordinates $\tilde{x}_i$:

$$x_i(t_0) = \tilde{x}_i,$$

and the initial velocities with known velocities:

$$v_i(t_0) \equiv \dot{x}_i(t_0) = \tilde{v}_i.$$

Thus, we have the Cauchy problem.

The vector form:

$$\mathbf{u}'(x) = \mathbf{f}\big(x, \mathbf{u}(x)\big),$$
$$\mathbf{u}(\xi) = \eta, \quad \text{or } u_k(\xi) = \eta_k, 0 \le k \le p.$$

1. If the RHS $\mathbf{f}(x, \mathbf{u})$ are continuous and bounded in some neighborhood of the initial point, then the solution $\mathbf{u}(x)$ of a Cauchy problem exists (**buy may be not unique!**).
2. If the RHS additionally Lipschitz-continuous with respect to u_k, i.e. if $\exists K$:
$$|\mathbf{f}(x, \mathbf{u}_1) - \mathbf{f}(x, \mathbf{u}_2)| \le K|\mathbf{u}_1 - \mathbf{u}_2|,$$
then the solution $\mathbf{u}(x)$ of a Cauchy problem is unique and stable, i.e. the Cauchy problem is well-posed.
3. If, additionally to the conditions above, the RHS has continuous derivatives by all arguments up to q^{th} order, then the solution $\mathbf{u}(x)$ of a Cauchy problem has continuous derivatives up to order $q + 1$.

- **Exact methods:** the solution of the Cuachy problem may be represented with elementary functions. Rarely applicable even for simple equations. For example, the solution of the equation $u'(x) = x^2 + u^2(x)$ can not be presented with elementary functions (or just not reasonable).
- **Approximate methods:** the solution $\mathbf{u}(x)$ is representable as a limit of some sequence $y_n(x)$, members of which can be represented with elementary functions or with quadratures. Applicable only for relatively simple linear problems.
- **Numerical solution:** applicable for a wide class of Cauchy problems. The problem must be well-conditioned.

ODU: when the analytic solution is not reasonable

Consider the equation:

$$u'(x) = \frac{u - x}{u + x}$$

This equation can be integrated and we will find the equation for its solution:

$$\frac{1}{2} ln(x^2 + u^2) + arctg \frac{u}{x} = const.$$

However, solution of the latter equation is even more complicated than just numerical solution of the initial problem.

ODU: ill-conditioned problem example

$$u'(x) = u - x, \quad 0 \leq x \leq 100, \quad u(0) = 1.$$

The solution contains the constant being defined with the boundary condition

$$u(x; c) = 1 + x + ce^x,$$

which is equal to zero with the boundary condition $u(0) = 1$, and to $u(100) = 101$. However, even changing the boundary condition with $u(0) = 1 + 10^{-6}$ will change it to $c = 10^{-6}$, which will result in $u(100) = 2.7 \cdot 10^{37}$.

Methods of solving the Cauchy problems

- The Picard method.
- Poincare method (small parameter method).
- Runge-Kutta methods.
- Linear Multistep method.
- Implicit schemes.
- And many others...

- Numerical methods, being used with meshes.
- **Explicit methods** are commonly more accurate; there are some equations, however, which are not reasonable to solve with explicit schemes due to low stability/accuracy/performance. These equations called 'stiff equations'
  - Euler's method;
  - Runge-Kutta 4^{th} order method;
- **Implicit methods** are less accurate and somewhat slower some ODE; however, due to better stability, implicit methods are capable for wider class of problems.

The Cauchy problem:

$$u'(x) = f(x, u(x)), \quad \xi \leq x \leq X, \quad u(\xi) = \eta.$$

Let $\{x_n, 0 \leq n \leq N\}$ be some mesh covering the interval $[\xi, N]$. Using the Taylor's series for the interval $[x_n, x_{n+1}]$:

$$u_{n+1} = u_n + h_n u_n^{'} + \frac{1}{2} h_n^2 u_n^{''} + ..., \quad h_n = x_{n+1} - x_n$$

The equation states that $u'(x) = f(x, u)$. Assuming the steps h are small and ignoring higher order derivatives multiplied with $h_n^t, t > 1$, we obtain the Euler's method. The accuracy of the method is $O(max h_n)$.

The Cauchy problem:

$$u'(x) = f(x, u(x)), \quad \xi \le x \le X, \quad u(\xi) = \eta.$$

Using the same mesh, $\{u_n\}$ can be calculated as follows:

$$\begin{aligned} u_{n+1} = u_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4), \\ k_1 = f(x_n, u_n); \\ k_2 = f(x_n + \frac{h}{2}, u_n + \frac{h}{2}k_1); \\ k_3 = f(x_n + \frac{h}{2}, u_n + \frac{h}{2}k_2); \\ k_4 = f(x_n + h, y_n + hk_3). \end{aligned}$$

The accuracy of the method is $O(h^4)$.

Implicit Runge-Kutta scheme

The Cauchy problem:

$$u'(x) = f(x, u(x)), \quad \xi \le x \le X, \quad u(\xi) = \eta.$$

Using the same mesh, $\{u_n\}$ can be calculated as follows:

$$u_{n+1} = u_n + h\frac{f(x_n, u_n) + f(x_{n+1}, u_{n+1})}{2}.$$

- The latter equation might not have a solution.
- The scheme will converge only with small h, which makes the method more computationally complicated.
- We need to bound the number of iterations.

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Part 3: Boundary-Value Problems
Eigenvalue Problems

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The system of ODE:

$$u_k'(x) = f_k(x, u_1, u_2, ..., u_p), \quad 1 \leq k \leq p, \quad x \in [a, b]$$

In the Boundary Value problem, the conditions are being set both in points $x = a$ and $x = b$.

- Possible with $p \geq 2$.
- Approximate methods: Fourier-based methods, Ritz methods, Galerkin methods.
- Numerical methods: Shooting method, Finite Differences.

Boundary value problem

- Simulation of loaded string.

$$u''(x) = -f(x), \quad a \leq x \leq b, u(a) = u(b) = 0,$$

  where $f(x)$ is a deforming force.
- Ballistic trajectory in space:

$$\mathbf{x}''(t) = \mathbf{g}, \quad \mathbf{x}(a) = \mathbf{x}_a, \mathbf{x}(b) = \mathbf{x}_b, |\mathbf{x}'(t)| = v_0.$$

Shooting method

Consider the second order ODE:

$$u''(x) = f\left(x, u(x), u'(x)\right), \quad u(a) = u_a, u(b) = u_b.$$

Instead, we are looking for a parametrized solution $u(x, d)$:

$$u''(x) = f\left(x, u(x), u'(x)\right), \quad u(a) = u_a, u'(a) = d.$$

If we find d such that $u(b; d) = u_b$, than the problem is solved. Thus:

The boundary value problem is being reduced to the set of Cauchy problems

If the equation is linear: $f(x,u,u') = p(x)u'(x) + q(x)u(x) + r(x)$, then

$$u(x) = u_{(1)}(x) + \frac{u_b - u_{(1)}(b)}{u_{(2)}(b)} u_{(2)}(x),$$

where $u_{(1)}$ and $u_{(2)}$ are the solutions of the following problems respectively:

$$u''_{(1)}(x) = f(x, u_{(1)}, u'_{(1)}), \quad u_{(1)}(a) = u_a, u_{(1)}(a) = 0,$$
$$u''_{(2)}(x) = f(x, u_{(2)}, u'_{(2)}), \quad u_{(2)}(a) = u_a, u_{(2)}(a) = 1,$$

If the problem is non-linear, than we have to iterate in order to find a proper parameter d.

The Galerkin method

Consider the equation:

$$A(u(x)) = f(x), \quad a \le x \le b, u(a) = u_a, u(b) = u_b.$$

- Approximate the function $u(x) \approx y_n(x) = \varphi_0(x) + \sum_{k=1}^{n} c_k \varphi_k(x)$, where the continuous function $\varphi_0(x)$ satisfies the boundary conditions: $\varphi_0(a) = u_a, \varphi_0(b) = u_b$;
  the functions $\varphi_k(x), 1 \le k < \infty$ are linearly independent and vanish at points a and b: $\varphi_k(a) = \varphi_k(b) = 0$.
- The algebraic system of equations for the coefficients c_k:

$$\int_a^b \Big(A\big(y_n(x)\big) - f(x) \Big) \varphi_k(x) dx = 0, \quad 1 \le k \le n$$

- After definition of the coefficients c_k, we construct the approximate solution of the BV problem.

The Eigenvalue problem:

$$\mathbf{u}'(x) = \mathbf{f}(x, \mathbf{u}; \lambda_r, r = 1, ..., q);$$
$$\mathbf{u} = \{u_1, u_2, ..., u_p\}, \quad \mathbf{f} = \{f_1, f_2, ..., f_p\}.$$

- Need to find both u_k and λ_r.
- Additional (boundary) conditions needed: $p + q$.
- The solution: u_k and λ_r - eigenfunctions and eigenvalues.
- λ_k is also called **spectrum**.

The wave (D'Alembert) equation:

$$\left(\Delta - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right)u = 0, \quad a \le x \le b, u(a) = 0; \quad u(b) = 0.$$

Assume the solution can be presented in a form $u(x,t) = y(x) \cdot exp(i\omega t)$. After substitution to the equation above, we obtain the following ODE:

$$\frac{d}{dx}\left(p(x)\frac{dy(x)}{dx}\right) = -k^2 q(x) y(x), \quad y(a) = 0, y(b) = 0.$$

where $k = \omega/v$ is a wavenumber, ω - its frequency, and v is the speed.

The Shooting method

Ignoring the right boundary condition, we have the Cauchy problem

$$\frac{d}{dx}\left(p(x)\frac{dy(x)}{dx}\right) = -k^2 q(x)y(x), \quad y(a) = 0$$

the solution of which $y(x;k)$ depends on the values of the parameter k.
The eigenvalues may be found then by finding the minimum of the function:

$$f(k) = f(1;k).$$

Here the parameter k represents the proper (eigen) frequency of the string.

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Part 4: Partial differential equations of the first order
Partial differential equations of the second order

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Partial differential equations of the first order

The Partial differential equation of the first order:

$$D\mathbf{u} = F\left(\mathbf{x}, \mathbf{u}, \frac{\partial \mathbf{u}}{\partial x_1}, ..., \frac{\partial \mathbf{u}}{\partial x_n}\right)$$

- N-body problem (Hamilton's equations)
- The Hopf equation.
- Eikonal equation.
- Molecular dynamics method.

The N-body problem: potential energy

As we wrote before:

$$m_i \ddot{\mathbf{x}}_i = \sum_{j \neq i}^{N} G m_i m_j \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|^3}, \quad 1 \leq i, j \leq N.$$

$$\mathbf{x}_i(t_0) = \tilde{\mathbf{x}}_i,$$

$$\mathbf{v}_i(t_0) \equiv \dot{\mathbf{x}}_i(t_0) = \tilde{\mathbf{v}}_i.$$

The equation, can be formulated in terms of the potential energy:

$$m_i \ddot{x}_i = \sum_{j \neq i}^{N} G m_i m_j \frac{x_j - x_i}{|x_j - x_i|^3} = -\frac{\partial U}{\partial \mathbf{x}_i},$$

where $U(\mathbf{x})$ is self-potential energy:

$$U = -\sum_{1 \leq i < j \leq n} \frac{G m_i m_j}{|\mathbf{x}_j - \mathbf{x}_i|^3}.$$

Defining the momentum $\mathbf{p} = m_i \frac{d\mathbf{x}_i}{dt} \Rightarrow$ Hamilton's equations.

Microcanonical ensemble: the system is isolated from changes in moles (N), volume (V), and energy (E): adiabatic process with no heat exchange.

Newton's law of motion:

$$
\begin{aligned}
F(X) = -\nabla U(X) &= M\dot{V}(t) \\
V(t) &= \dot{X}(t).
\end{aligned}
$$

Here:

- X are the particle coordinates.
- $U(X)$ is a potential energy of the system (comes from pair or many-body potentials).
- M - mass of particles.
- V - velocities of particles.

The Eikonal

- The eikonal equation:

$$|\nabla u(\mathbf{x})| = \frac{1}{f(\mathbf{x})}, \quad f(\mathbf{x}) > 0, \mathbf{x} \in \Omega, u(\mathbf{x})|_{\partial\Omega} = q(\mathbf{x});$$

- In electrostatics:

$$\mathbf{E} = -\nabla V,$$

where V is electric potential, and $\mathbf{E}$ is an electric field.

- In fluid dynamics:

$$\mathbf{v} = \nabla \varphi,$$

where v is potential flow velocity, and φ is a potential.

2^{nd} order PDEs

Partial differential equations of second order

Most of PDE-driven problems can be described with PDEs of second order. The differential operator D can be represented as follows:

$$D\mathbf{u} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(\mathbf{x})\frac{\partial^2 \mathbf{u}}{\partial x_i \partial x_j} + F\left(\mathbf{x}, \mathbf{u}, \frac{\partial \mathbf{u}}{\partial x_1}, ..., \frac{\partial \mathbf{u}}{\partial x_n}\right) \equiv L\mathbf{u} + F(...).$$

The operator L is called the Principle Part. In dependence on it, the equations can be classified as:

- Elliptic equations;
- Parabolic equations;
- Hyperbolic and Ultrahyperbolic equations.

The equation

$$L\mathbf{u} + F(\ldots) = 0 \tag{1}$$

is considered elliptic if the coefficient matrix $\{a_{ij}\}$ has all-positive or all-negative eigenvalues.

- The solution is as smooth as the coefficients and boundary conditions allow.
- Well suited to describe static (for example, equilibrium states).
- Less suitable for dynamic processes.

Parabolic equations

The equation

$$L\mathbf{u} + F(...) = 0 \tag{2}$$

is considered parabolic if the coefficient matrix $\{a_{ij}\}$ has one zero eigenvalue, while all others have the same sign (positive or negative)

- May be represented in form $u_t = -L\mathbf{u}$, where $\mathbf{u}$ is an elliptic operator.
- Are well suited to describe the smoothly evolving processes such diffusion or heat transfers.
- The solution is generally smoother than the initial value.

The equation

$$Lu + F(...) = 0 \tag{3}$$

is considered parabolic if the coefficient matrix $\{a_{ij}\}$ has eigenvalues, the signs of which are the same excepting one of them, which is non-zero and has contrary sign.

- May be represented with elliptic operator: $L\mathbf{u} - a^2 \frac{\partial^2 \mathbf{u}}{\partial t^2} = F(...)$, where L is an elliptic operator.
- Hyperbolic equations solutions retain discontinuities of initial data.
- Well-suited to describe wave processes.

Thank you for your attention!