

Scientific Computing

Lecture 3

Differential equations

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Differential equations

- ▶ Differential operator
- ▶ Cauchy problems
- ▶ Boundary-value problems
- ▶ Eigenvalue problems
- ▶ Partial differential equations of the first order
- ▶ Classification of second order PDEs

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Part 1: Differential operator

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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 model and the right-hand side; the function \mathbf{u} is an unknown function to be found.

Examples

- Ordinary differential equation:

$$\frac{d\mathbf{u}}{dx} = f(x) \Leftrightarrow D \equiv \frac{d}{dx} - f(x).$$

- Partial differential equation (Poisson equation, 2D):

$$\Delta\mathbf{u} = -f(\mathbf{u}, x, y); \quad \Delta\mathbf{u} = \frac{\partial^2\mathbf{u}}{\partial x^2} + \frac{\partial^2\mathbf{u}}{\partial y^2}; \quad D\mathbf{u} \equiv \Delta\mathbf{u} + f(\mathbf{u}, x, y)$$

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

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

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

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

- ▶ The function $F(\dots)$ 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.

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

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

Solve the equation above with respect to higher order derivative $u^{(p)}$ to express it via all other derivatives:

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

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:

$$u_{k+1}(x) = u'_k(x), \quad 0 \leq k \leq p-2,$$

$$u'_p(x) = f(x, u_0, u_1, \dots, u_{p-1}),$$

ODE: Three kinds of problems

Let $\mathbf{u} = \{u_0, \dots, u_p\}$, and $\mathbf{f} = \{f_1, \dots, f_p\}$ By analogy, each system of differential equations of any order can be changed with equivalent system of the first-order ODE:

$$u'_k = f(x, u_0, u_1, \dots, u_p),$$

Or, the vector form of the system above:

$$\mathbf{u}'(x) = \mathbf{f}(x, \mathbf{u}(x)), \quad \mathbf{u} = \{u_0, \dots, u_p\}, \mathbf{f} = \{f_1, \dots, f_p\}.$$

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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- Vector form:

$$\begin{aligned} \mathbf{u}'(x) &= \mathbf{f}(x, \mathbf{u}(x)), \quad x \in [\xi, X] \\ \mathbf{u}(\xi) &= \boldsymbol{\eta}, \quad \text{or } u_k(\xi) = \eta_k, \quad 1 \leq k \leq p. \end{aligned}$$

- Or common form:

$$\begin{aligned} F\left(x, u(x), u'(x), \dots, u^{(p)}(x)\right) &\equiv D\mathbf{u} = 0. \\ u^{(k)}(\xi) &= \eta_k, \quad 0 \leq k < p \end{aligned}$$

- The conditions may be considered as the definition of some initial point $(\xi, \eta_0, \dots, \eta_{p-1})$ for an integral curve in $(p+1)$ -dimensional space (x, u_0, \dots, u_p) .



Augustin-Louis Cauchy
1789-1857

The simplest Cauchy problem

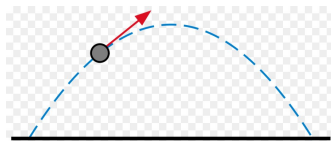
Consider a ball with mass m . Let this ball be thrown; we need to calculate its trajectory.

- ▶ m - the mass of the ball
- ▶ $\mathbf{x} \in L_2(\mathbb{R}^2) \times L_2(\mathbb{R}^2)$
- ▶ $\mathbf{v} \in L_2(\mathbb{R}^2) \times L_2(\mathbb{R}^2)$
- ▶ The governing equation:

$$\begin{aligned}\mathbf{x}''(t) &= \mathbf{g}, \\ \mathbf{x}'(t) &= \mathbf{v}(t),\end{aligned}$$

where \mathbf{g} is a gravitational acceleration.

- ▶ Initial conditions:
 $\mathbf{x}(0) = \mathbf{x}_0; \mathbf{x}'(0) \equiv \mathbf{v}(0) = \mathbf{v}_0$



The simplest Cauchy problem

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

$$\mathbf{v}(t) = \text{Const} + \int_0^t \mathbf{g} d\tau = \mathbf{v}_0 + \mathbf{g}t,$$

$$\mathbf{x}(t) = \text{Const} + \int_0^t \mathbf{v}(\tau) d\tau = \mathbf{x}_0 + \mathbf{v}_0 t + \mathbf{g}t^2$$

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?

N-body problem

Consider a number of point-bodies $B_i, i = 1, \dots, N$, 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.

Solution of the Cauchy problem

The vector form:

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

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 (**but might be not unique!**).
2. If the RHS additionally Lipschitz-continuous with respect to u_k , i.e. if $\exists K$:

$$|\mathbf{f}(x, \mathbf{u}_1) - \mathbf{f}(x, \mathbf{u}_2)| \leq K|\mathbf{u}_1 - \mathbf{u}_2|,$$

then the solution $\mathbf{u}(x)$ of a Cauchy problem is unique (**but might be not stable!**)

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 Cauchy 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 $u(x)$ 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.

Consider the equation:

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

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

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

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

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

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 4th 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 Euler's method

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 $[x_n, x_{n+1}]$:

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

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 $O(\max h_n)$.

4th order Runge-Kutta scheme

The Cauchy problem:

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

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

$$u_{n+1} = u_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

$$k_1 = f(x_n, u_n);$$

$$k_2 = f\left(x_n + \frac{h}{2}, u_n + \frac{h}{2}k_1\right);$$

$$k_3 = f\left(x_n + \frac{h}{2}, u_n + \frac{h}{2}k_2\right);$$

$$k_4 = f(x_n + h, u_n + hk_3).$$

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

The Cauchy problem:

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

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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Lecture 4

Part 3: Boundary-Value Problems

Eigenvalue Problems

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The system of ODE:

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

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.

- Simulation of loaded string (static deflection).

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

where $f(x)$ is a deforming force.

- Ballistic trajectory in space:

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

Consider the second order ODE:

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

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

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

If we find d such that $u(b; d) = u_b$, then 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:

$$\begin{aligned}u_1''(x) &= f(x, u_1, u_1'), & u_1(a) &= u_a, u_1'(a) = 0, \\u_2''(x) &= f(x, u_2, u_2') - r(x), & u_2(a) &= 0, u_2'(a) = 1,\end{aligned}$$

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:

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

- 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 $\varphi_k(x), 1 \leq k < \infty$ 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 :

$$\int_a^b \left(A(y_n(x)) - f(x) \right) \varphi_k(x) dx = 0, \quad 1 \leq k \leq n$$

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

The Eigenvalue problem:

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

- ▶ 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:

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

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.

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 changing the parameter k until the right boundary value be satisfied. 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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The Partial differential equation of the first order:

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

- ▶ 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:

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

The Molecular Dynamics (MD) method

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:

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

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 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:

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

The operator L is called the Principle Part and being defined with the matrix:

$$L\mathbf{u} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n1} & \dots & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_1} & \frac{\partial^2 \mathbf{u}}{\partial x_2 \partial x_1} & \dots & \frac{\partial^2 \mathbf{u}}{\partial x_n \partial x_1} \\ \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_2} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_n} & \dots & \dots & \frac{\partial^2 \mathbf{u}}{\partial x_n \partial x_n} \end{pmatrix} = A_L H^T.$$

Here the matrix H is a **Hessian**.

We are able to find the eigenvalues λ of the matrix A_L :

$$A_L \mathbf{v} = \lambda \mathbf{v}$$

- ▶ Suppose we have found several eigenvalues λ_i .
- ▶ **Elliptic equation:** $\lambda_i > 0$ or $\lambda_i < 0$ for $\forall i$.
All-positive or all-negative eigenvalues
- ▶ **Parabolic equation:** $\exists k : \lambda_k = 0$ while $\lambda_i > 0$ or $\lambda_i < 0$ for $\forall i \neq k$. There is only one zero eigenvalue while all others have the same sign.
- ▶ **Hyperbolic equation:** $\exists k : \lambda_k > 0$ while $\lambda_i < 0 \forall i \neq k$ OR $\exists k : \lambda_k < 0$ while $\lambda_i > 0 \forall i \neq k$
The signs of eigenvalues are the same excepting one of them, which is non-zero and has contrary sign.

The equation

$$L\mathbf{u} + F(\dots) = 0 \quad (1)$$

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.

The equation

$$L\mathbf{u} + F(\dots) = 0 \quad (2)$$

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

$$L\mathbf{u} + F(\dots) = 0 \quad (3)$$

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

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Part 5: Example 1.

Cauchy problem for an elliptic PDE

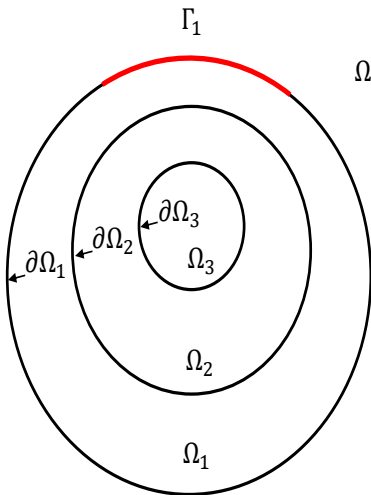
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The EEG Cauchy problem (Data mapping): the domain



► Notations:

- $\Omega \subset \mathbb{R}^3$ - the whole domain.
- $\Omega_k, k = 1, \dots, N_\Omega - 1$ - the outer 'sourceless' domains
($\sigma(\Omega_k) = \sigma_k = \text{const}$).
- Ω_{N_Ω} - the inner domain containing sources ($\sigma(\Omega_{N_\Omega}) = \sigma_{N_\Omega} = \text{const}$)
- The accessible part of the boundary

$$\Gamma_k = \begin{cases} \Gamma_1, & k = 1 \\ \partial\Omega_k, & k \geq 2. \end{cases}$$

- The rest of the boundary: Π_k .

► Assumptions:

- Current density volumetric distribution is non-zero only in the inner domain:
 $\mathbf{J} : \text{supp}(\mathbf{J}) \in \Omega_{N_\Omega}$
- Conductivities:
 $\sigma_k \ll \sigma_{N_\Omega}, k = 1, \dots, N_\Omega - 1.$

Data mapping: the Cauchy problem

Assume the function $u(\mathbf{x})$, $\mathbf{x} \in \Pi_1 \subset \partial\Omega_1$ to be known. Find the function $U(\mathbf{x})$, $\mathbf{x} \in \Omega_1$, such that:

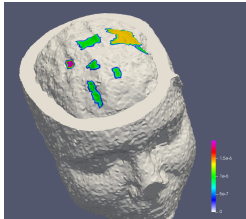
$$\begin{aligned}\Delta U &= 0, & \mathbf{x} \in \Omega_1; \\ U(\mathbf{x}) &= u(\mathbf{x}), & \mathbf{x} \in \Gamma_1; \\ \frac{\partial U}{\partial \mathbf{n}}(\mathbf{x}) &= g(\mathbf{x}), & \mathbf{x} \in \Gamma_1,\end{aligned}$$

where

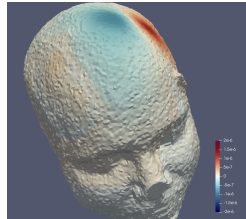
$$g(\mathbf{x}) = \begin{cases} 0, & \Gamma_1 \subset \partial\Omega, \\ \frac{\sigma_1}{\sigma_2} \mathbf{n} \cdot \nabla U(\mathbf{x}), & \Gamma_1 \subset \partial\Omega_2. \end{cases}$$

Whenever the function $U(\mathbf{x})$ is found at every point $\mathbf{x} \in \Omega_1$, we obviously have the potential on the rest of a boundary $\Pi_1 = \partial\Omega_1 \setminus \Gamma_1$.

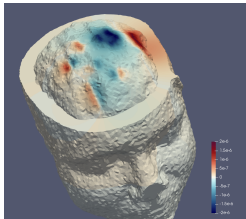
Numerical results: regular currents



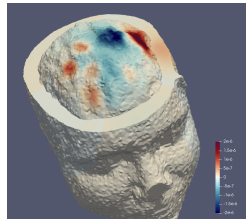
The sources



Potential on the scalp

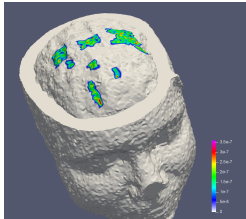


Real potential (brain)

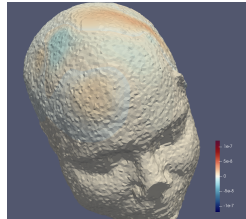


Reconstruction result

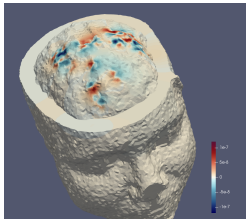
Numerical results: Random currents in each point



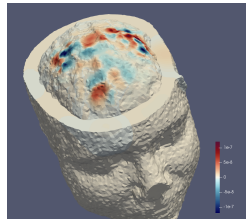
The sources



Potential on the scalp



Real potential (brain)



Reconstruction result

Scientific Computing

Lecture 3

Part 5: Example 2.

Cauchy problem for the parabolic PDE

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The quasilinear heat transfer equation (statement of 1D Forward Problem (simulation))

$$\begin{aligned}u_t &= u_{xx} + aS(u) + F(x, t), & (x, t) &\in [0, 1]^2, \\u(x, 0) &= f(x), \\u(0, t) &= g(t), \\u(1, t) &= p(t).\end{aligned}$$

The ill-posed Cauchy problem for heat transfer

The ill-posed Cauchy problem for heat transfer equation.

Suppose both initial condition $f(x)$ and the left boundary condition $g(t)$ to be unknown, and the function $q(t) = \partial u / \partial x(1, t)$ to be known:

$$\begin{aligned} u_t &= u_{xx} + aS(u) + F(x, t), & (x, t) &\in [0, 1]^2, \\ u(1, t) &= p(t), & \frac{\partial u}{\partial x}(1, t) &= q(t). \end{aligned}$$

Find $u(x, t)$.

The problem is non-linear (quasi-linear), which leads that the cost functional has local minima

Coefficient problem for a heat-transfer equation

Let $\Omega \subset \mathbb{R}^n$ be some domain, $\partial\Omega$ - its boundary, and $\Gamma \subset \partial\Omega$ is some part of this boundary. Consider the problem:

$$\begin{aligned}u_t &= \Delta u + a(\mathbf{x})u, \quad \mathbf{x} \in \Omega \\ u(\mathbf{x})|_{\Gamma} &= p(\mathbf{x}); \quad \partial_n u(\mathbf{x})|_{\Gamma} = q(x)\end{aligned}$$

Assuming $u(\mathbf{x}) > 0, \mathbf{x} \in \Omega$ introduce the notation $v = \ln(u)$ (so that $u = e^v$). Thus,

$$v_t u = u \Delta v + u (\nabla v)^2 + a(\mathbf{x})u, \quad v|_{\Gamma} = \ln(p).$$

Dividing the equation by u , we obtain:

$$v_t = \Delta v + (\nabla v)^2 + a(\mathbf{x}).$$

Now, differentiating the latter equation on t , we just exclude the coefficient $a(x)$!

Thank you for your attention!

QUESTIONS

Questions (Lec 3)

- ▶ Write down the forms of differential operator for Ordinary Differential Equation and for Partial Differential Equation. Explain the difference between them.
- ▶ Explain the meaning of terms: Linear differential equation, Quasi-linear differential equation, Non-linear differential equation. Provide examples of these equations.
- ▶ How the ODE of k^{th} order can be replaced with a system of ODE of the first order?
- ▶ List three kinds of problems for differential equations. Explain each of them in a few words.
- ▶ What is the Cauchy problem? Describe it with an example.
- ▶ What is the boundary value problem? Describe it with an example.
- ▶ What is the eigenvalue problem? Describe it with an example.
- ▶ When the Cauchy problem is well-posed?
- ▶ List three general approaches for solution of the Cauchy problem. Explain in few words advantages and disadvantages of them.
- ▶ What is explicit and implicit schemes for solving the Cauchy problem? Explain advantages and disadvantages for all of them.
- ▶ Explain the idea of Euler's method.
- ▶ Explain the idea of Shooting method.
- ▶ Write at least three real-world examples of problems leading to the partial differential equations of the first order. Analyze your examples in terms of linearity.
- ▶ Can the Cauchy problem be stated for the partial differential equation? If yes, give an example of it.
- ▶ Describe the main idea of statement of N-body problem.
- ▶ Describe the main idea of the Molecular dynamics method.