Numerical Methods 6. Numerical solutions of partial differential equations

Vector calculus, summary

Partial differential equations and auxiliary conditions

Methods for elliptic equations

Methods for time-dependent problems

Vector calculus, summary. Differential operators

Let $u : \mathbf{R}^n \to \mathbf{R}$ be a differentiable *scalar function*, and let $E : \mathbf{R}^n \to \mathbf{R}^n$ be a differentiable *vector function*.

The **gradient** of the function u: $\operatorname{grad} u := \left(\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \ldots, \frac{\partial u}{\partial x_n} \right)$ (vector function)

The **divergence** of $E := (E_1, E_2, \ldots, E_n)$: $\operatorname{div} E := \frac{\partial E_1}{\partial x_1} + \frac{\partial E_2}{\partial x_2} + \ldots + \frac{\partial E_n}{\partial x_n}$ (scalar function)

The **rotation** of $E := (E_1, E_2, E_3)$: $\operatorname{rot} E := \left(\frac{\partial E_3}{\partial x_2} - \frac{\partial E_2}{\partial x_3}, \frac{\partial E_1}{\partial x_3} - \frac{\partial E_3}{\partial x_1}, \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2} \right)$ (vector)

The **Laplace operátor**: $\Delta u := \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \ldots + \frac{\partial^2 u}{\partial x_n^2}$ (scalar)

- $\operatorname{rot} \operatorname{grad} u \equiv 0$
- $\operatorname{div} \operatorname{rot} E \equiv \mathbf{0}$
- $\operatorname{div} \operatorname{grad} u \equiv \Delta u$
- $\operatorname{div}(E \cdot u) = (\operatorname{div} E) \cdot u + E \cdot (\operatorname{grad} u)$

Vector calculus, summary. Fundamental integral theorems

Divergence theorem of Gauss: $$\int_{\Omega} \operatorname{div} E \, d\Omega = \oint_{\Gamma} E \cdot n \, d\Gamma$$

Corollary: $$\int_{\Omega} \Delta u \, d\Omega = \oint_{\Gamma} \frac{\partial u}{\partial n} \, d\Gamma$$

Vector calculus, summary. Fundamental integral theorems

Divergence theorem of Gauss: $\int_{\Omega} \operatorname{div} E \, d\Omega = \oint_{\Gamma} E \cdot n \; d\Gamma$

Corollary: $\int_{\Omega} \Delta u \, d\Omega = \oint_{\Gamma} \frac{\partial u}{\partial n} \, d\Gamma$

$$\int_{\Omega} \Delta u \, d\Omega = \int_{\Omega} \operatorname{div} \operatorname{grad} u \, d\Omega = \oint_{\Gamma} (\operatorname{grad} u) \cdot n \, d\Gamma = \oint_{\Gamma} \frac{\partial u}{\partial n} \, d\Gamma$$

Vector calculus, summary. Fundamental integral theorems

Green's first theorem: $$\int_{\Omega} (\Delta u) v \, d\Omega = -\int_{\Omega} (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \oint_{\Gamma} \frac{\partial u}{\partial n} v \, d\Gamma$$

Vector calculus, summary. Fundamental integral theorems

Green's first theorem: $\int_\Omega (\Delta u) v \, d\Omega = -\int_\Omega (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \oint_\Gamma \frac{\partial u}{\partial n} v \, d\Gamma$

Let $E := (\operatorname{grad} u) \cdot v$, then

$$\operatorname{div} E = \operatorname{div}((\operatorname{grad} u) v) = (\operatorname{div} \operatorname{grad} u) v + (\operatorname{grad} u) \cdot (\operatorname{grad} v) = (\Delta u) v + (\operatorname{grad} u) \cdot (\operatorname{grad} v).$$

Applying the divergence theorem, we have:

$$\int_\Omega (\Delta u) v \, d\Omega = -\int_\Omega (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \int_\Omega \operatorname{div}((\operatorname{grad} u) v) \, d\Omega =$$

$$= -\int_\Omega (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \oint_\Gamma (\operatorname{grad} u) v \cdot n \, d\Gamma = -\int_\Omega (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \oint_\Gamma \frac{\partial u}{\partial n} v \, d\Gamma$$

Vector calculus, summary. Fundamental integral theorems

Green's second theorem: $$\int_{\Omega}(\Delta u)v\,d\Omega - \int_{\Omega}(\Delta v)u\,d\Omega = \oint_{\Gamma}\frac{\partial u}{\partial n}v\,d\Gamma - \oint_{\Gamma}\frac{\partial v}{\partial n}u\,d\Gamma$$

Vector calculus, summary. Fundamental integral theorems

Green's second theorem: $$\int_\Omega (\Delta u) v \, d\Omega - \int_\Omega (\Delta v) u \, d\Omega = \oint_\Gamma \frac{\partial u}{\partial n} v \, d\Gamma - \oint_\Gamma \frac{\partial v}{\partial n} u \, d\Gamma$$

According to Green's first formula:

$$\int_\Omega (\Delta u) v \, d\Omega = -\int_\Omega (\operatorname{grad} u) \cdot (\operatorname{grad} v) \, d\Omega + \oint_\Gamma \frac{\partial u}{\partial n} v \, d\Gamma$$

Swapping the roles of u and v:

$$\int_\Omega (\Delta v) u \, d\Omega = -\int_\Omega (\operatorname{grad} v) \cdot (\operatorname{grad} u) \, d\Omega + \oint_\Gamma \frac{\partial v}{\partial n} u \, d\Gamma$$

Substituting the two equations, we have the theorem.

Vector calculus, summary. Fundamental integral theorems

Green's third theorem (in 2D):

$$u(x) = -\frac{1}{2\pi}\oint_{\Gamma}\frac{(x-y)\cdot n_y}{\| x-y \|^2}u(y)\,d\Gamma_y - \frac{1}{2\pi}\oint_{\Gamma}\log\| x-y \|\frac{\partial u(y)}{\partial n}\,d\Gamma_y + \frac{1}{2\pi}\int_{\Omega}\log\| x-y \|\,\Delta u(y)\,d\Omega_y$$

Remark: the function defined by $\boxed{V(y) := \log\| x-y \|}$ is harmonic everywhere (provided that $y \neq x$), i. e. $\Delta V \equiv 0$.

Numerical Methods 6. Numerical solutions of partial differential equations

Vector calculus, summary

Partial differential equations and auxiliary conditions

Methods for elliptic equations

Methods for time-dependent problems

Partial differential equations and auxiliary conditions

Elliptic equation: $\boxed{\Delta u = f}$ (**Poisson equation**; if $f = 0$, then **Laplace equation**)

More general elliptic equation: $\boxed{\operatorname{div} \sigma \operatorname{grad} u = f}$

Examples:

- steady-state heat flow;
- distribution of electrical potential;
- seepage through porous media;
- wind-induced flow in shallow lakes;

etc.

Convection-diffusion-reaction equation: $\boxed{\mathbf{v} \cdot \operatorname{grad} u - \operatorname{div} \sigma \operatorname{grad} u + d \cdot u = f}$

Examples:

- steady-state transport processes;
- contaminant propagation in flow/gas;

etc.

Partial differential equations and auxiliary conditions

Parabolic equation: $\boxed{\frac{\partial u}{\partial t} - D\Delta u = f}$ (**diffusion equation**)

More general parabolic equations: $\boxed{\frac{\partial u}{\partial t} - \operatorname{div} \sigma \operatorname{grad} u = f}$

Convection-diffusion equation: $\boxed{\frac{\partial u}{\partial t} + \mathbf{v} \cdot \operatorname{grad} u - \operatorname{div} \sigma \operatorname{grad} u = f}$

Examples:

- time-dependent transport processes;
- unsteady contaminant propagation in flow/gas;

etc.

Partial differential equations and auxiliary conditions

Hyperbolic equation: $\boxed{\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = f}$ (**wave equation**)

Example:

- wave propagation;

Auxiliary conditions for elliptic equations: boundary conditions

- u is prescribed along the boundary of the domain (**1. or Dirichlet boundary conditionl**)
- $\frac{\partial u}{\partial n}$ is prescribed along the boundary of the domain (**2. or Neumann boundary condition**)
- a linear combination of u and $\frac{\partial u}{\partial n}$ is prescribed along the boundary of the domain (**3. or Robin boundary condition**)

Along different pieces of the boundary, different types of boundary condition can also be defined (**mixed boundary condition**). However, at each point of the boundary, exactly one boundary condition should be prescribed.

If a part of the domain is a priori unknown, the situation is much more complicated and makes the problem nonlinear.

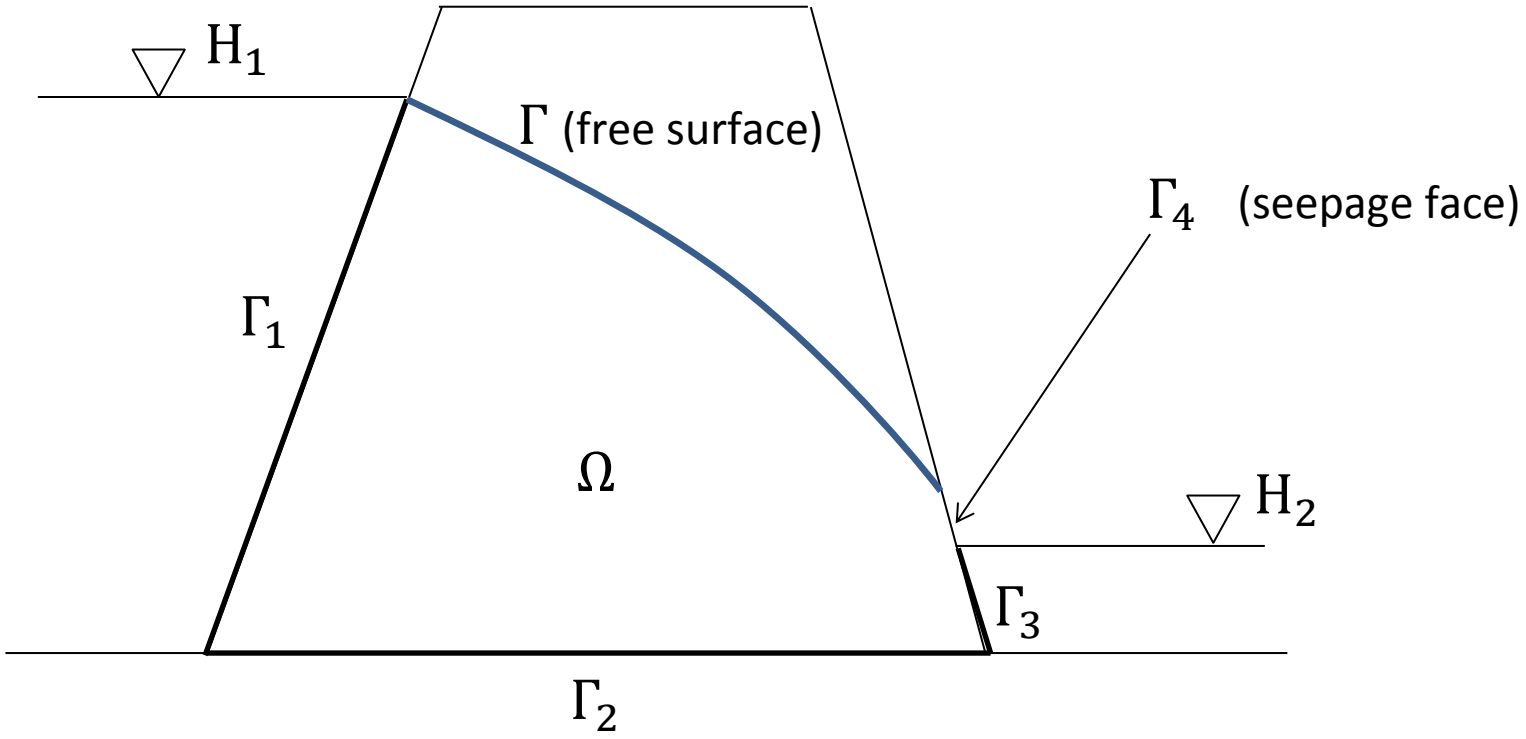
Free boundary problems

Free boundary problem - the classical dam problem

u: velocity potential: $\Delta u = 0$ in Ω

$u|_{\Gamma_1} = H_1$, $u|_{\Gamma_3} = H_2$, $u(x,y)|_{\Gamma_4} = y$ (Dirichlet conditions)
$\frac{\partial u}{\partial n}|_{\Gamma_2} = 0$ (Neumann condition),

At the free surface: $u(x,y)|_{\Gamma} = y$, **and** $\frac{\partial u}{\partial n}|_{\Gamma} = 0$



Auxiliary conditions for parabolic and hyperbolic equations: initial and boundary conditions

With respect to the spatial variables: boundary conditions (may be time-dependent)

With respect to the time variable: initial condition:

- u is prescribed at the initial moment $t = t_0$ (parabolic equations)
- u and $\frac{\partial u}{\partial t}$ are prescribed at the initial moment $t = t_0$ (hyperbolic equations)

In general, the above partial differential equations supplied with the above auxiliary conditions have a unique solution.

Numerical Methods 6. Numerical solutions of partial differential equations

Vector calculus, summary

Partial differential equations and auxiliary conditions

Methods for elliptic equations

Methods for time-dependent problems

Methods for elliptic equations
The Fourier method for the Poisson equation

Model problem: $\boxed{-\Delta u = f}$ in the rectangle $(0,a)\times(0,b)\subset \mathbf{R}^2$, $\boxed{u := 0}$ on the boundary.

Step 1: Express the function f in terms of sinusoidal Fourier series:

$$f(x,y) = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty} c_{kj} \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

The Fourier coefficients:

$$c_{kj} = \frac{4}{ab}\int_0^a\int_0^b f(x,y)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}\,dydx$$

Methods for elliptic equations
The Fourier method for the Poisson equation

Step 2: Using the same Fourier coefficients calculated in the previous step, define the following function:

$$u(x,y)=\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{c_{kj}}{\frac{k^2\pi^2}{a^2}+\frac{j^2\pi^2}{b^2}}\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

This function solves the model problem, since:

$$\Delta\left(\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}\right)=\left(\frac{\partial^2}{\partial x^2}\sin\frac{k\pi x}{a}\right)\sin\frac{j\pi y}{b}+\left(\frac{\partial^2}{\partial y^2}\sin\frac{j\pi y}{b}\right)\sin\frac{k\pi x}{a}=\left(-\frac{k^2\pi^2}{a^2}-\frac{j^2\pi^2}{b^2}\right)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

which implies

$$-\Delta u(x,y)=\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{c_{kj}}{\frac{k^2\pi^2}{a^2}+\frac{j^2\pi^2}{b^2}}\cdot\left(\frac{k^2\pi^2}{a^2}+\frac{j^2\pi^2}{b^2}\right)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}=\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}c_{kj}\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}=f(x,y)$$

Along the boundary of the rectangle, $u=0$, since at these points: $\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}=0$.

Methods for elliptic equations
The Fourier method for the Poisson equation

Remarks:

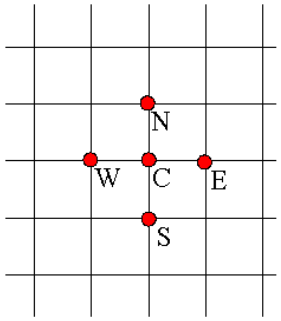
- The calculation of the Fourier coefficients as well as then evaluation of the Fourier series can be performed by using the Fast Fourier Transform (FFT) algorithm, which significantly reduces the computational complexity.

- However, the method can be applied for rectangular domains (a similar approach can be constructed for some very special domains e.g for circles).

- The method can be applied for the Poisson equation (a similar approach can be constructed for some very special elliptic equations).

Methods for elliptic equations
Finite difference methods

Model problem: $-\Delta u = f$ in a domain $\Omega \subset \mathbf{R}^2$, u is prescribed along the boundary.



Main idea: Define an equidistant grid in the domain, and approximate the derivatives by finite difference schemes.

The Laplace operator can be approximated by the **five-point central scheme**:

$$(\Delta u)_C \sim \frac{u_E - 2u_C + u_W}{h^2} + \frac{u_N - 2u_C + u_S}{h^2} = \frac{u_N + u_W + u_S + u_E - 4u_C}{h^2}$$

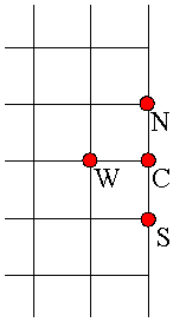
Thus, for the gridpoint C, a discrete equation can be written:

$$\boxed{4u_C - u_N - u_W - u_S - u_E = h^2 f_C}$$

This is the case for every gridpoint located in the interior of the domain. At the boundary gridpoints, u is prescribed (boundary condition).

Methods for elliptic equations
Finite difference methods

Discretization of the Neumann boundary condition $\frac{\partial u}{\partial n} = v$:



Naive solution (first-order approximation): $\boxed{\frac{\partial u_C}{\partial n} \sim \frac{u_C - u_W}{h}}$,

whence, for the boundary point *C*: $\boxed{u_C - u_W = h \cdot v_C}$

An improved (second-order) approximation: $\boxed{4u_C - 2u_W - u_N - u_S = h^2 f_C + 2hv_C}$

Methods for elliptic equations
Finite difference methods

$$u_W = u_C - \frac{\partial u_C}{\partial x} h + \frac{1}{2} \frac{\partial^2 u_C}{\partial x^2} h^2 + O(h^3), \qquad \text{and} \qquad \frac{\partial^2 u_C}{\partial x^2} = -\frac{\partial^2 u_C}{\partial y^2} - f_C, \text{ whence}$$

$$u_W = u_C - \frac{\partial u_C}{\partial x} h - \frac{1}{2} \frac{\partial^2 u_C}{\partial y^2} h^2 - \frac{1}{2} f_C h^2 + O(h^3)$$

$\frac{\partial^2 u_C}{\partial y^2}$ can be approximated by a second-order scheme: $\frac{\partial^2 u_C}{\partial y^2} = \frac{u_N - 2u_C + u_S}{h^2} + O(h^2)$:

$$u_W = u_C - \frac{\partial u_C}{\partial x} h - \frac{1}{2}(u_N - 2u_C + u_S) - \frac{1}{2} f_C h^2 + O(h^3)$$

whence:

$$\frac{\partial u_C}{\partial x} = \frac{u_C - u_W}{h} - \frac{u_N - 2u_C + u_S}{2h} - \frac{1}{2} f_C h + O(h^2)$$

Methods for elliptic equations
Finite difference methods

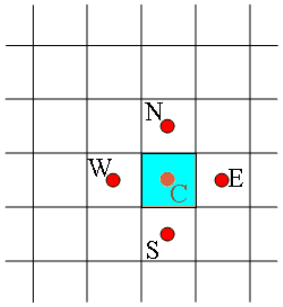
Numerical features:

- The method leads to a linear system of equations with large but **sparse** matrix.
- Direct methods: the computational cost may be extremely high..
- Simple iterative methods are generally slow.
- The approximation of the boundary is rough.

The main problem: a fast solution technique for the appearing linear system.

Methods for elliptic equations
Finite volume methods

Model problem: $-\Delta u = f$ in a domain $\Omega \subset \mathbf{R}^2$, u is prescribed along the boundary.



Main idea: Define a **cell system** in the domain and integrate the differential equation over each cell C:

$$\int_C \Delta u \, d\Omega = \int_{\Gamma_C} \frac{\partial u}{\partial n} d\Gamma_C$$

Now the integrals of the normal derivatives taken along the cell sides (the **fluxes**) are to be approximated by e.g. cell-centered difference schemes:

$$\int_C \Delta u \, d\Omega = -\int_C f \, d\Omega \sim -h^2 f_C$$

$$\int_{\Gamma_C} \frac{\partial u}{\partial n} d\Gamma_C \sim \frac{u_N - u_C}{h} h + \frac{u_W - u_C}{h} h + \frac{u_S - u_C}{h} h + \frac{u_E - u_C}{h} h = u_N + u_W + u_S + u_E - 4u_C$$

Thus, the discrete equation belonging to the cell C: $\boxed{4u_C - u_N - u_W - u_S - u_E = h^2 f_C}$,
which is valid for each cell located in the interior of the domain. For the cell sides located on the boundary, u is prescribed as a boundary condition.

Methods for elliptic equations
Finite volume methods

- The method leads to an algebraic system with large and sparse matrix. It is not easy to construct an efficient solution algorithm. However:
- Non-rectangular cells can also be applied, which makes it possible to fit the boundary in a more precise way.
- Only first-order derivatives (fluxes) have to be approximated.
- The discretization of the Neumann boundary condition is much simpler.

For instance, if the eastern side of the cell *C* fits to boundary, and here $\frac{\partial u}{\partial n} = v_E$ is prescribed, then the flux through the eastern cell side can be calculated:

$$\int_{\Gamma_C} \frac{\partial u}{\partial n} d\Gamma_C \sim \frac{u_N - u_C}{h} h + \frac{u_W - u_C}{h} h + \frac{u_S - u_C}{h} h + v_E h = u_N + u_W + u_S - 3u_C + v_E h$$

Thus, the discrete equation belonging to the cell *C* is as follows:

$$\boxed{3u_C - u_N - u_W - u_S = h^2 f_C + v_E h}$$

Methods for elliptic equations
Multigrid methods

Model problem (linear): $Au = f$
Equivalent form (suitable for iteration): $u = Bu + g$
(Generally, it is a simple Jacobi or Seidel iteration.)

Main ideas:

- multi-level discretization;
- smoothing (with Jacobi or Seidel iteration)
- improvement based on the *residual equation*:

Methods for elliptic equations
Multigrid methods

Model problem (linear): $Au = f$
Equivalent form (suitable for iteration): $u = Bu + g$
(Generally, it is a simple Jacobi or Seidel iteration.)

Main ideas:

- multi-level discretization;
- smoothing (with Jacobi or Seidel iteration)
- improvement based on the *residual equation*:

Let $\tilde{u}$ be an approximate solution of the equation $Au = f$. Then the exact solution u can be expressed in the form $u = \tilde{u} + w$, where the correction term w is the solution of the **residual equation**:

$$Aw = f - A\tilde{u}$$

If the computation of w is not exact (generally this is the case), then we obtain a new – and hopefully better – approximation of the solution.

Methods for elliptic equations
Two-grid method

Let X_H be a coarse grid with stepsize *H*, and let X_h be a fine grid with stepsize *h*.

Discretized problems: $A_h u_h = f_h$ and $A_H u_H = f_H$
Similarly: $u_h = B_h u_h + g_h$ and $u_H = B_H u_H + g_H$.

Inter-grid transfer operators: $R : X_h \to X_H$ (restriction to the coarse grid),
$P : X_H \to X_h$ (prolongation to the fine grid)

The two-grid algorithm:

- Pre-smoothing: perform $\tilde{u}_h := B_h \tilde{u}_h + g_h$ several times
- Coarse grid correction: $\tilde{u}_h := \tilde{u}_h + P w_H$, where $A_H w_H = R(f_h - A_h \tilde{u}_h)$
- Post-smoothing: perform $\tilde{u}_h := B_h \tilde{u}_h + g_h$ several times

Methods for elliptic equations
Multigrid methods

Let $X_1 \subset X_2 \subset \ldots \subset X_L$ be several grids embedded to each other (X_1 is the coarsest, X_L is the finest grid).

Discretized problems: $A_k u_k = f_k$

and similarly: $u_k = B_k u_k + g_k \quad (k = 1,2,\ldots,L)$

The inter-grid transfer operations: $R_k : X_k \to X_{k-1}$ (restrictions)

$P_k : X_{k-1} \to X_k$ (prolongations).

Methods for elliptic equations
Multigrid methods

Let $X_1 \subset X_2 \subset \ldots \subset X_L$ be several grids embedded to each other (X_1 is the coarsest, X_L is the finest grid).

Discretized problems: $A_k u_k = f_k$
and similarly: $u_k = B_k u_k + g_k \quad (k = 1,2,\ldots,L)$

The inter-grid transfer operations: $R_k : X_k \to X_{k-1}$ (restrictions)
$P_k : X_{k-1} \to X_k$ (prolongations).

Cascade method:

In the coarsest level, the discretized problem has to be solved exactly:

$$\tilde{u}_1 := A_1^{-1} f_1$$

In the finer levels, the approximate solution transferred from the coarse level is improved:

- $\tilde{u}_k := P_k \tilde{u}_{k-1}$ (transfer from the coarser level)
- $\tilde{u}_k := B_k \tilde{u}_k + g_k$ (improvement by smoothing iterations) $(k = 2,3,\ldots,L)$

Methods for elliptic equations
Multigrid methods

Let $X_1 \subset X_2 \subset ... \subset X_L$ be several grids embedded to each other (X_1 is the coarsest, X_L is the finest grid).

Discretized problems: $A_k u_k = f_k$
and similarly: $u_k = B_k u_k + g_k \quad (k = 1,2,\ldots,L)$

The inter-grid transfer operations: $R_k : X_k \to X_{k-1}$ (restrictions)
$P_k : X_{k-1} \to X_k$ (prolongations).

- *Multigrid cycles (MGC)*: iterative technique;
- *Full multigrid algorithm (FMG)*: non-iterative technique

Methods for elliptic equations
Multigrid methods

Recursive definition of the *multigrid cycle*:

In the coarsest level, the discretized problem has to be solved exactly:

$$\tilde{u}_1 := MGC(1, \tilde{u}_1, f_1) := A_1^{-1} f_1$$

In the finer levels:

- transfer for the previous level: $\tilde{u}_k := P_k \tilde{u}_{k-1}$
- pre-smoothing: $\tilde{u}_k := B_k u_k + g_k$ a few times
- compute the residuum: $r_k := f_k - A_k \tilde{u}_k$
- perform a multigrid cycle (only once (V-cycle) or twice (W-cycle)) for the residual equation in the next coarser level: $w_{k-1} := MGC(k-1, w_{k-1}, R_k r_k)$. The strating approximation can be zero.
- coarse grid correction: $\tilde{u}_k := \tilde{u}_k + P_k w_{k-1}$
- post-smoothing: $MGC(k, \tilde{u}_k, f_k) := B_k \tilde{u}_k + g_k$

Methods for elliptic equations
Multigrid methods

Full multigrid algorithm, recursive definition:

In the coarsest level, the discretized problem has to be solved exactly:

$$\tilde{u}_1 := FMG(1, f_1) := A_1^{-1} f_1$$

In the finer levels:

- $\tilde{u}_k := P_k(FMG(k-1, f_{k-1}))$
- $FMG(k, f_k) := MGC(k, \tilde{u}_k, f_k))$

Methods for elliptic equations
Multigrid methods

Remarks:

- The aim of the smoothing procedure is to efficiently reduce the high-frequency error components (and not to assure a fast convergence). The low-frequency error components are reduced by coarse grid correction.

- The number of the necessary arithmetic operations is proportional to the **first** power of the unknowns.

- The approach can be generalized also for nonlinear problems (Full Approximation Scheme).

Methods for elliptic equations
Variational methods, finite element methods

Model problem: $-\Delta u = f$ in a domain $\Omega \subset \mathbf{R}^2$, $u \equiv 0$ along the boundary.

Let $\varphi_1, \varphi_2, ..., \varphi_N$ be given *basis functions*, and let $\psi_1, \psi_2, ..., \psi_N$ be given *test functions*, which also vanish on the boundary.

Seek the solution in the form $u := \sum_{j=1}^{N} u_j \cdot \varphi_j$. Multiplying both sides by ψ_k and integrating over the domain:

$$\sum_{j=1}^{N} u_j \cdot \int_{\Omega} \operatorname{grad} \varphi_j \cdot \operatorname{grad} \psi_k \, d\Omega = \int_{\Omega} f \cdot \psi_k \, d\Omega \qquad (k = 1,2,...,N)$$

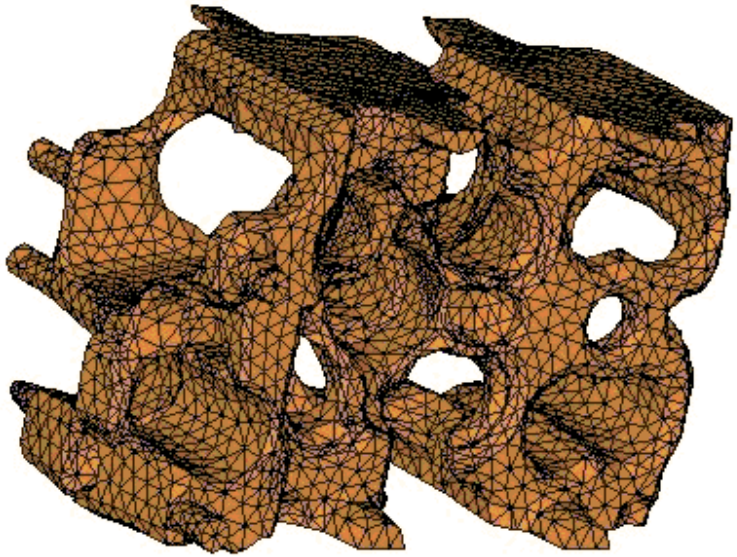
No second-order derivatives occur!

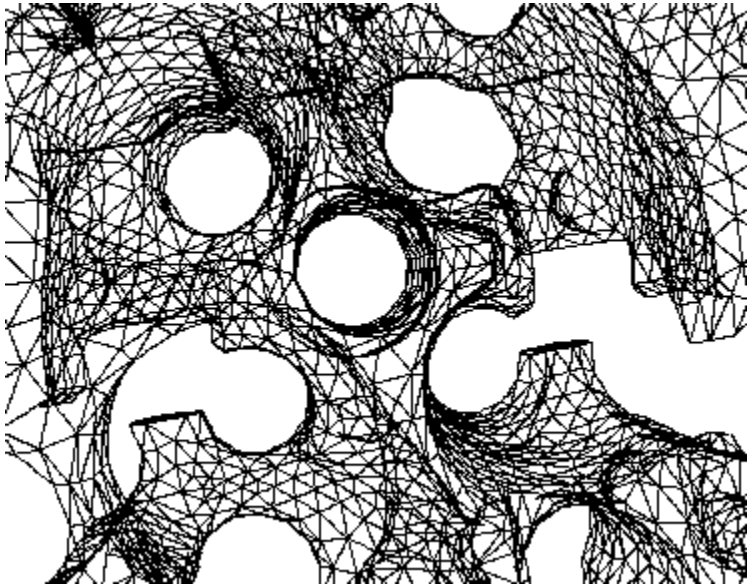
Methods for elliptic equations
Variational methods, finite element methods

Numerical features:

- The method results in a system with large but **sparse** matrix (provided that the basis and test functions are properly chosen; practically their support should be small).
- Direct solution techniques lead to extremely high computational cost.
- The boundary can be approximated in a sufficiently exact way.
- However, the definition of a sufficiently fine element structure is a quite difficult subtask.

Methods for elliptic equations
Variational methods, finite element methods





Methods for elliptic equations
The boundary element method

Model problem: $\Delta U = f$ in a domain $\Omega \subset \mathbf{R}^2$, supplied with mixed boundary conditions:

U is prescribed in a part Γ_1 of the boundary;

along the remaining part Γ_2 of the boundary, the normal derivative $\partial U / \partial n$ is prescribed.

Third Green's formula: denote by $u := U|_\Gamma$, $v := \frac{\partial U}{\partial n}|_\Gamma$, then in every *inner z* point of Ω:

$$U(z) = -\frac{1}{2\pi}\int_\Gamma \frac{(z-y)\cdot n_y}{\| z-y \|^2} u(y)\, d\Gamma_y - \frac{1}{2\pi}\int_\Gamma \log \| z-y \| \cdot v(y)\, d\Gamma_y + \frac{1}{2\pi}\int_\Omega \log \| z-y \| \cdot f(y)\, d\Omega_y$$

The terms in the righ-hand side: *double layer potential*, *single layer potential*, and *logarithmic potential*.

Main idea: Let $x \in \Gamma$ be e point of the **boundary**. Letting $z \to x$, compute the limit of both sides. Thus, we obtain an *integral* equation, in which the unknown functions (u and v) are defined on the boundary.

The logarithmic and the single layer potentials are continuous functions (with respect to z).

If u is continuous, then the double layer potential has a jump at the boundary, moreover:

$$\lim_{z \to x} \oint_{\Gamma} \frac{(z-y)\cdot n_y}{\| z-y \|^2} u(y)\, d\Gamma_y = \oint_{\Gamma} \frac{(x-y)\cdot n_y}{\| x-y \|^2} u(y)\, d\Gamma_y - u(x)\cdot(2\pi - \alpha(x))$$

where $\alpha(x)$ is the inner angle of the boundary at the boundary point x.

The boundary element method

The boundary functions *u* and *v* satisfy the following **boundary integral equation**:

$$\alpha u + Ku - Rv = -Lf$$

where

$$(Ku)(x) := \oint_{\Gamma} \frac{(x-y)\cdot n_y}{\| x-y \|^2} u(y)\, d\Gamma_y,$$

$$(Rv)(x) := \oint_{\Gamma} \log \| x-y \|\, v(y)\, d\Gamma_y, \qquad (Lf)(x) := \int_{\Omega} \log \| x-y \|\, f(y)\, d\Omega_y$$

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Indeed, performing the limit $z \to x$, we obtain:

$$u(x) = -\frac{1}{2\pi} \oint_{\Gamma} \frac{(x-y)\cdot n_y}{\| x-y \|^2} u(y)\, d\Gamma_y + \frac{1}{2\pi} u(x)\cdot(2\pi - \alpha(x)) - \frac{1}{2\pi} \oint_{\Gamma} \log \| x-y \|\, v(y)\, d\Gamma_y +$$

$$+ \frac{1}{2\pi} \int_{\Omega} \log \| x-y \|\, f(y)\, d\Omega_y$$

and hence the boundary integral equation follows.

Numerical solution of the boundary integral equation by collocation

Let $\varphi_1, \varphi_2, ..., \varphi_N$ be given boundary functions, and let $x_1, x_2, ... x_N$ be given boundary points (*collocation points* hereafter). The simplest choice: the boundary is divided into N parts by some boundary points, and φ_k is defined as the characteristic function of the kth part, i.e. φ_k is identically equal to 1 on the kth part and zero elsewhere. The kth collocation point can be defined as the midpoint of the kth part.

Now let us seek the functions u and v as a linear combination of these functions:

$$u \sim \sum_{j=1}^{N} u_j \varphi_j, \quad v \sim \sum_{j=1}^{N} v_j \varphi_j$$

Substituting these expressions into the boundary integral equation and requiring the equality at the collocation points $x_1, x_2, ... x_N$, we obtain a linear system of equations for the coefficients:

$$\alpha_k u_k + \sum_{j=1}^{N} K_{kj} u_j - \sum_{j=1}^{N} R_{kj} v_j = -Lf(x_k) \qquad (K_{kj} := (K\varphi_j)(x_k), \quad R_{kj} := (R\varphi_j)(x_k))$$

$(k = 1,2,...,N)$. This system consists of N equations. The boundary conditions give additional N equations.

The boundary element method
Numerical features

- The (approximate) solution of the boundary integral equation requires boundary points only. A discretization of the domain is not necessary.

- After discretizing the boundary integral equation, the size of the resulting system of equations is much smaller than in the case of finite differences. However, the matrix of the system is densely populated, generally nonsymmetric, and sometimes it is ill-conditioned.

- The multigrid technique can also be applied here, and reduces the computational cost further.

Methods for elliptic equations
The method of fundamental solutions

Mode problem: $\Delta U = 0$ in a domain $\Omega \subset \mathbf{R}^2$ supplied with mixed boundary conditions:

U is prescribed along a part Γ_1 of the boundary;

along the remaining part Γ_2 of the boundary, the normal derivative $\partial U / \partial n$ is prescribed;

Let $\tilde{x}_1, \tilde{x}_2, ..., \tilde{x}_N$ be predefined exterior points (*source points*);
Let $x_1, x_2, ..., x_M \in \Gamma_1, \quad x_{M+1}, x_{M+2}, ..., x_N \in \Gamma_2$ be predefined *boundary collocation points*.
Consider the function

$$\Phi(x) := \frac{1}{2\pi} \log \| x \| \quad \text{(fundamental solution), then } \Delta\Phi = 0 \quad (x \neq \mathbf{0})$$

Let us look for the solution in the following form:

$$U(x) := \sum_{j=1}^{N} \alpha_j \Phi(x - \tilde{x}_j)$$

The a priori unknown coefficients can be calculated by enforcing the boundary conditions.

Methods for elliptic equations
The method of fundamental solutions

$$U(x) := \sum_{j=1}^{N} \alpha_j \Phi(x - \tilde{x}_j)$$

The a priori unknown coefficients can be calculated by enforcing the boundary conditions:

$$\sum_{j=1}^{N} \alpha_j \Phi(x_k - \tilde{x}_j) = U(x_k) \qquad (k = 1,2,\ldots,M)$$

$$\sum_{j=1}^{N} \alpha_j \frac{\partial \Phi}{\partial n_k}(x_k - \tilde{x}_j) = \frac{\partial U}{\partial n_k}(x_k) \qquad (k = M+1, M+2,\ldots,N)$$

The method of fundamental solutions
Numerical features

- The method needs boundary collocation points and some external source points only. Neither domain nor boundary discretization (by e. g. grid or element structures) is required.

- It can be programmed in an extremely simple way.

- The matrix of the resulting system is fully populated and non-symmetric in general.

- In many cases, the matrix of the system is extremely ill-conditioned. The greater the distance of the source points from the boundary, the higher the condition number of the matrix.

Numerical Methods 6. Numerical solutions of partial differential equations

Vector calculus, summary

Partial differential equations and auxiliary conditions

Methods for elliptic equations

Methods for time-dependent problems

Methods for time-dependent problems
Fourier's method

Model problem: $\dfrac{\partial u}{\partial t} - D\Delta u = f$ in the rectangle $(0,a)\times(0,b)\subset \mathbf{R}^2$

Boundary condition: $u = 0$ along the boundary (for every $t > 0$).

Initial condition: $u(0,x,y) = u_0(x,y)$.

Step 1: Express the function f in terms of sinusoidal Fourier series for every $t > 0$:

$$f(t,x,y) = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty} c_{kj}(t)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

Step 2: Express also the initial condition in terms of sinusoidal Fourier series:

$$u_0(x,y) = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty} a_{kj}\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

Step 3: Look for the solution in the form of a sinusoidal Fourier series with temporarily unknown, time-dependent Fourier coefficients:

$$u(t,x,y) = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty} u_{kj}(t)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

Methods for time-dependent problems
Fourier's method

Substituting the above form of u into the differential equation:

$$\frac{\partial u}{\partial t} - D\Delta u = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\left(u'_{kj}(t) + D(\frac{k^2\pi^2}{a^2} + \frac{j^2\pi^2}{b^2})u_{kj}(t) \right)\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}$$

The function u satisfies the original problem, if the Fourier coefficient functions u_{kj} satisfy the following ordinary differential equations and initial conditions:

$$\boxed{\begin{aligned} &u'_{kj}(t) + D(\frac{k^2\pi^2}{a^2} + \frac{j^2\pi^2}{b^2})u_{kj}(t) = c_{kj}(t) \\ &u_{kj}(0) = a_{kj} \end{aligned}}$$

As a special case, if the functions c_{kj} are constant (i.e. the function f does not depend on t), then:

$$u_{kj}(t) = \frac{c_{kj}}{D\cdot\lambda_{kj}} + \left(a_{kj} - \frac{c_{kj}}{D\cdot\lambda_{kj}} \right)e^{-D\cdot t\cdot\lambda_{kj}} \qquad \left(\lambda_{kj} := \frac{k^2\pi^2}{a^2} + \frac{j^2\pi^2}{b^2} \right)$$

The effect of the initial condition rapidly decays, and the solution tends to the solution of the Poisson equation $\boxed{-D\Delta u = f}$ (supplied with homogeneous boundary conditions).