

Example: Partial Differential Equations

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Program construction in C++ for Scientific Computing



Introduction

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the Course

- 1 Introduction
- 2 Finite Difference Approximations
- 3 Implementation of Differential Operators
- 4 Boundary Conditions
- 5 Summary of the Course

What Do We Have

- Two simple classes for structured grids (Domain, Curvebase)
- A simple implementation of a matrix class (Matrix; don't use it for production codes!)

What Do We Want

- A class for representing grid functions
- Imposing boundary conditions
- A class for solving PDEs

Our running example will be the heat equation in 2D,

$$\frac{\partial}{\partial t} u = \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial y^2} u.$$

The Domain Class

This is what we have so far:

```
class Domain {  
    public:  
        Domain(Curvebase&, Curvebase&, Curvebase&,  
                Curvebase&);  
        void generate_grid(...);  
        // more members  
    private:  
        Curvebase *sides[4];  
        // more members  
};
```

- We will need additional members for handling grids. *Since grids do not allow any algebraic manipulation, using our `Matrix` class is not appropriate.*
- We will use C-style arrays.
- It might be more convenient to use STL containers (e.g., `vector`).

The Domain Class: Enhanced

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```
class Domain {  
    public:  
        Domain(Curvebase&, Curvebase&, Curvebase&,  
                Curvebase&) : m(0), n(0), x(nullptr),  
                               y(nullptr) {}  
        void generate_grid(int m_, int n_);  
        int xsize() { return m; }  
        int ysize() { return n; }  
        Point operator()(int i, int j);  
        bool grid_valid() { return m != 0; }  
        // more members  
    private:  
        Curvebase *sides[4];  
        int m, n;  
        double *x, *y;  
        // more members  
};
```

One Dimensional Differences 1

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- Consider a grid Ω_h ,

$$a = x_0 < x_1 < \cdots < x_{n-1} < x_m = b.$$

- Let $h_i = x_i - x_{i-1}$. Then define, for a grid function $u : \Omega_h \rightarrow \mathbb{R}$,

$$D_- u_i = \frac{u_i - u_{i-1}}{h_i}$$

$$D_+ u_i = \frac{u_{i+1} - u_i}{h_{i+1}}$$

- If u is the restriction of a smooth function onto Ω_h , these approximations are first order accurate.
- If the grid is equidistant, $D_+ D_-$ is a second order accurate approximation of $u''(x_i)$ and

$$D_+ D_- u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

One Dimensional Differences 2

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the Course

$$Du_i = \frac{u_{i+1} - u_{i-1}}{2h}$$

- First order approximation to u' on a general grid
- Second order accuracy on a constant stepsize grid

- The operators introduced above are not applicable at boundaries.
- Possibility 1: One-sided differences

$$Du_0 = \frac{3u_0 - 4u_1 + u_2}{3h}$$

$$Du_m = \frac{u_{m-2} - 4u_{m-1} + 3u_m}{3h}$$

- Possibility 2: Use ghost points

$$Du_0 = \frac{u_1 - u_{-1}}{2h}$$

$$Du_m = \frac{u_{m+1} - u_{m-1}}{2h}$$

How to get values for the ghost points?

Nonuniform Grids

- Order of approximation is determined using Taylor expansions.
- Ansatz:

$$u'(x_i) \approx a_- u(x_{i-1}) + a_0 u(x_i) + a_+ u(x_{i+1}) =: D_0 u(x_i)$$

- Taylor expansion:

$$u(x_{i-1}) = u(x_i) - h_i u'(x_i) + \frac{1}{2} h_i^2 u''(x_i) + O(h^3)$$

$$u(x_{i+1}) = u(x_i) + h_{i+1} u'(x_i) + \frac{1}{2} h_{i+1}^2 u''(x_i) + O(h^3)$$

Nonuniform Grids (cont)

- Inserting into the expression for $D_0 u$, we obtain after coefficient comparison

$$a_- = \frac{-h_{i+1}}{h_i(h_i + h_{i+1})}$$

$$a_0 = \frac{h_{i+1} - h_i}{h_i h_{i+1}}$$

$$a_+ = \frac{h_i}{h_{i+1}(h_i + h_{i+1})}$$

and

$$D_0 u(x_i) - u'(x_i) = \frac{1}{6} h_i h_{i+1} u'''(x_i) + \dots$$

- For an equidistant grid, the coefficients reduce to $a_- = -1/2h$, $a_0 = 0$, $a_+ = 1/2h$.
- One sided expressions??

An Alternative Idea

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- Assume that the grid is created using a mapping $\phi : [0, 1] \rightarrow [a, b]$ with $x_i = \phi(s_i)$, $i = 0, \dots, m$ with a uniform grid

$$s_i = i\sigma, \quad \sigma = m^{-1}.$$

- Then, $du/ds = du/dx \cdot dx/ds$, and

$$u_x(x_i) \approx \frac{1}{dx(s_i)/ds} \frac{u_{i+1} - u_{i-1}}{2\sigma}$$

is a second order approximation.

And Another Idea

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- If the derivative dx/ds is not known, it can be approximated with second order accuracy by

$$\frac{dx}{ds}(s_i) \approx \frac{x_{i+1} - x_{i-1}}{2\sigma}$$

such that

$$u_x(x_i) \approx \frac{u_{i+1} - u_{i-1}}{x_{i+1} - x_{i-1}}$$

is second order accurate!

- Needed: ϕ is a smooth mapping!
- Note: *We need only two grid points in order to obtain the same order of accuracy as in the approximation in physical domain.*

Approximation of u''

Going either way, we have an approximation

$$u'(x_i) \approx D_0 u_i.$$

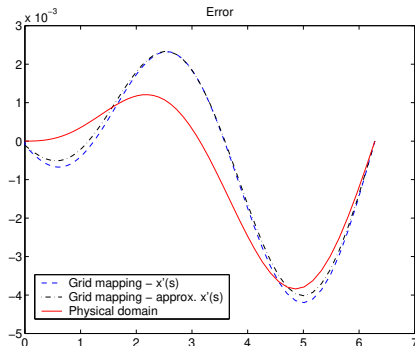
A second order approximation to the second derivative can be defined by

$$u''(x_i) \approx D_2 u_i = D_0 D_0 u_i.$$

This approximation evaluates to a five-point stencil!

Example: Comparison of Accuracy

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$$u(x) = \sin x$$

$$x(s) = 2\pi \frac{1 + \tanh(\delta(s-1)/2)}{\tanh(\delta/2)}, \quad \delta = 5$$

Hyperbolic tangent stretching, 100 gridpoints.

Conclusions

- All approximations are 2nd order accurate.
- In this simple example, approximation in physical domain is more accurate.
- The stencil (number of grid points used) is larger in physical domain for obtaining the same order of accuracy.

2D: Physical Domain

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Ansatz:

$$u_x(x_{i,j}, y_{i,j}) \approx \sum_{k,l} a_{k,l} u_{i+k,j+l}$$

Taylor expansion around $(x_{i,j}, y_{i,j})$:

$$\begin{aligned} & \sum_{k,l} a_{k,l} u_{i+k,j+l} \\ &= \sum_{k,l} a_{k,l} \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \left((x_{i+k,j+l} - x_{i,j}) \frac{\partial}{\partial x} + (y_{i+k,j+l} - y_{i,j}) \frac{\partial}{\partial y} \right)^{\nu} u \\ &= \sum_{\nu=0}^{\infty} \sum_{p=0}^{\nu} \left[\sum_{k,l} a_{k,l} \frac{1}{\nu!} \binom{\nu}{p} (x_{i+k,j+l} - x_{i,j})^p (y_{i+k,j+l} - y_{i,j})^{\nu-p} \right] \frac{\partial^p}{\partial x^p} \frac{\partial^{\nu-p}}{\partial y^{\nu-p}} u \end{aligned}$$

$D_{0,x}$ in Physical Domain

First order:

$$\sum_{k,l} a_{k,l} = 0$$

$$\sum_{k,l} a_{k,l} (x_{i+k,j+l} - x_{i,j}) = 1$$

$$\sum_{k,l} a_{k,l} (y_{i+k,j+l} - y_{i,j}) = 0$$

Second order additionally:

$$\sum_{k,l} a_{k,l} (x_{i+k,j+l} - x_{i,j})^2 = 0$$

$$\sum_{k,l} a_{k,l} (x_{i+k,j+l} - x_{i,j})(y_{i+k,j+l} - y_{i,j}) = 0$$

$$\sum_{k,l} a_{k,l} (y_{i+k,j+l} - y_{i,j})^2 = 0$$

So we expect 6 gridpoints necessary for second order accuracy!

Stencil in Reference Coordinates

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Remember:

- Let Φ to a (smooth) one-to-one mapping $\Phi : [0, 1]^2 \rightarrow \Omega$.
- For given m, n , a uniform grid on $[0, 1]^2$ can be defined by:

$$\begin{aligned}\xi_i &= ih_1, & h_1 &= 1/m, & i &= 0, \dots, m, \\ \eta_j &= jh_2, & h_2 &= 1/n, & j &= 0, \dots, n.\end{aligned}$$

- A strucured grid on Ω can then simply be obtained via

$$x_{ij} = \Phi_x(\xi_i, \eta_j), \quad y_{ij} = \Phi_y(\xi_i, \eta_j), \quad i = 0, \dots, m, j = 0, \dots, n.$$

Reference Coordinates (cont)

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- Using the chain rule of differentiation, we obtain

$$\frac{\partial u(x, y)}{\partial \xi} = \frac{\partial u}{\partial x} \cdot \frac{\partial \Phi_x}{\partial \xi} + \frac{\partial u}{\partial y} \cdot \frac{\partial \Phi_y}{\partial \xi}$$

$$\frac{\partial u(x, y)}{\partial \eta} = \frac{\partial u}{\partial x} \cdot \frac{\partial \Phi_x}{\partial \eta} + \frac{\partial u}{\partial y} \cdot \frac{\partial \Phi_y}{\partial \eta}$$

Since the transformation Φ_x, Φ_y is known, this is a linear system for the partial derivatives $\partial u / \partial x, \partial u / \partial y$.

- Let

$$J = \begin{pmatrix} \frac{\partial \Phi_x}{\partial \xi} & \frac{\partial \Phi_y}{\partial \xi} \\ \frac{\partial \Phi_x}{\partial \eta} & \frac{\partial \Phi_y}{\partial \eta} \end{pmatrix}$$

Then

$$\frac{\partial u}{\partial x} = \frac{1}{\det J} \left(\frac{\partial u}{\partial \xi} \cdot \frac{\partial \Phi_y}{\partial \eta} - \frac{\partial u}{\partial \eta} \cdot \frac{\partial \Phi_y}{\partial \xi} \right)$$

$$\frac{\partial u}{\partial y} = \frac{1}{\det J} \left(\frac{\partial u}{\partial \eta} \cdot \frac{\partial \Phi_x}{\partial \xi} - \frac{\partial u}{\partial \xi} \cdot \frac{\partial \Phi_x}{\partial \eta} \right)$$

Reference Coordinates (cont)

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- The derivatives with respect to reference coordinates can be approximated by standard stencils (4-point stencil).
- Once all partial derivatives w_r, t_ξ have been evaluated, the necessary partial derivatives $w_r, t_{x,y}$ can be computed.

Class for Grid Functions: Requirements

- (Scalar) grid functions are defined on grids.
- We are using structured grids as represented in the class `Domain`.
- Operations allowed with grid functions:
 - Addition, multiplication by a scalar (they form a vector space)
 - Pointwise multiplication (together, this becomes a commutative algebra)
 - Differentiation (e.g., by finite differences)
 - Computation of norms
 - Integration (? maybe)

Further Considerations

- In the two-dimensional case, many of these operations are already implemented in the `Matrix` class!
- However, some operations are not meaningful for grid functions, e.g., matrix-matrix multiplication.
- A grid functions lives only on a specific grid:
 - Shall the grid be part of an object?
 - Many grid functions share the same grid!
 - Algebraic manipulations are only defined for grid functions living on the same grid

Remember: The Matrix Class

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```
class Matrix {
    int m, n; // should be size_t
    double *A;
public:
    Matrix(int m_ = 0, int n_ = 0) : m(m_), n(n_),
                                   A(nullptr) {
        if (m*n > 0) {
            A = new double[m*n];
            std::fill(A,A+m*n,0.0);
        }
    }
    // etc
};
```


Implementation of Grid Functions

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```
class GFkt {  
    private:  
        Matrix u;  
        Domain *grid;  
    public:  
        GFkt(Domain *grid_) : u(grid_>xsize()+1,  
                                grid_>ysize()+1), grid(grid_) {}  
        GFkt(const GFkt& U) : u(U.u), grid(U.grid) {}  
        GFkt& operator=(const GFkt& U);  
        GFkt operator+(const GFkt& U) const;  
        GFkt operator*(const GFkt& U) const;  
    // etc  
};
```

A Sample Implementation

```
GFkt GFkt::operator+(const GFkt& U) const {
    if (grid == U.grid) { // defined on the same grid?
        GFkt tmp(grid);
        tmp.u = u+U.u; // Matrix::operator+()
        return tmp;
    }
    else error();
}

GFkt GFkt::operator*(const GFkt& U) const {
    if (grid == U.grid) { // defined on the same grid?
        GFkt tmp(grid);
        for (int j = 0; j <= grid.ysize(); j++)
            for (int i = 0; i <= grid.xsize(); i++)
                tmp.u(i,j) = u(i,j)*U.u(i,j);
        return tmp;
    }
    else error();
}
```

A Problem And Its Solution

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- The grid is handled by the caller.
- In the above implementation, the caller may delete the grid such that all objects referring to it have a dangling pointer!
- In C++ 11 there is a solution: smart pointers
- Smart pointers belong to the C++ library, include file: `memory`

Smart Pointers

- There are two types of them: `shared_ptr` and `unique_ptr`.
- Both classes are in fact template classes: The template argument is a typename.
- *`shared_ptr` uses a reference count: As soon as the reference count reaches 0, the dynamic object will be destroyed. But not earlier!*
- This way, all resources will be freed (including dynamic memory).
- *C-type pointers and smart pointers cannot be mixed!* There is always an **explicit type cast** necessary! Recommendation: Avoid mixing.

Smart Pointers (cont)

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- Create a smart pointer, initialize it to 0 (nullptr):

```
shared_ptr<class> p1;
```

- The equivalent of new:

```
shared_ptr<class> p2 = make_shared<class>(args);
```

- The following statement is in error:

```
shared_ptr<class> p3 = new class(args); // Error!
```

- But this works:

```
shared_ptr<class> p3 =  
    shared_ptr<class>(new class(args));
```

- There is no equivalent of delete needed.

A Better Implementation of GFkt

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```

class GFkt {
private:
    Matrix u;
    shared_ptr<Domain> grid;
public:
    GFkt(shared_ptr<Domain> grid_) :
        u(grid_->xsize()+1,grid_->ysize()+1),
        grid(grid_) {}
    GFkt(const GFkt& U) : u(U.u), grid(U.grid) {}
    // etc
};

```

Notes:

- *We assume silently that, once a grid has been generated, it will never be changed!*
- It is most probably a good idea to use shared pointers in Domain, too:

```
shared_ptr<Curvebase> sides[4];
```

Implementation of $D_{0,x}$

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```
GFkt GFkt::D0x() const {  
    GFkt tmp(grid);  
    if (grid->grid_valid()) {  
        // generate derivative in tmp  
        // according to one of the possibilities above  
    }  
    return tmp;  
}
```

- The function $D_{0,y}$ can be implemented similarly.
- In order to reduce overhead, it might be a good idea to implement even

```
void GFkt::D0xy(GFkt *dx, GFkt *dy) const;
```

Boundary Conditions

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Name	Prescribed	Interpretation
Dirichlet	u	Fixed temperature
Neumann	$\partial u / \partial n$	Energy flow
Robin (mixed)	$\partial u / \partial n + f(u)$	Temperature dependent flow
Periodic		

Boundary conditions have a crucial impact on the solution.

What are Boundary Conditions?

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- ① The mathematician's point of view:

domain
+ differential equation
+ boundary conditions

- ② The physicist's point of view:

differential equation	→	physics
domain	→	space
boundary conditions	→	influence of outer world

- ③ The software engineer's point of view:

differential equation	→	expression of differentials
domain	→	grid
boundary conditions	→	what??

Object-Oriented Representation

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- As part of the PDE
 - mathematical interpretation
 - requires high-level representation of equation and discretization
 - difficult to obtain efficiency
- As part of the grid function
 - mathematically correct
 - no class for PDEs needed
 - convenient for explicit time-stepping
- As part of the operator (e.g., D_0)
 - convenient for implicit and explicit methods
 - can be difficult to implement
 - may encounter mathematical contradictions if used wrongly

Associate boundary conditions with grid functions:

```
class Solution {  
    public:  
        Solution(Domain *D) : sol(D) {}  
        ~Solution();  
        void timesteps(double dt, int nsteps);  
        void init(); // Set initial condition  
        void print();  
    private:  
        GFkt sol;  
        void impose_bc();  
};
```

`impose_bc()` will be called in `timesteps()` for imposing the boundary conditions.

- The proposed implementation is questionable because the boundary conditions and timestepping are “hardwired”.

- It is better to have a *class* for boundary conditions:

```
class BCtype {  
    public:  
        BCtype(GFkt& u, int boundary_id);  
        virtual void impose(GFkt& u) = 0;  
};
```

- The actual definition of the boundary condition takes place in derived classes.
- This way, several boundaries can share the same condition (e.g., homogeneous Dirichlet conditions).
- Classes can be derived for Dirichlet, Neumann, Robin boundary conditions.

Example Implementation

Assumptions:

- The grid has four distinct edges (as ours in the previous Domain class).
- Each edge is associated with one boundary condition, only.

Then:

```
class Solution {  
    public:  
        Solution(Domain *D) : sol(D) {}  
        ~Solution();  
        void print();  
    private:  
        GFkt sol;  
        shared_ptr<BCtype> bcs[4];  
        virtual void init() = 0;  
        virtual void bc() = 0;  
};
```

We have separated: the grid, the equation, the initial conditions, and the boundary conditions.

Time Stepping

For the heat equation in 2D, we can implement the explicit Euler method now:

```
Solution u(&d);  
u.init();  
for (int step=0; step < maxsteps; step++) {  
    u += dt*(u.D2x()+u.D2y());  
    t += dt;  
    u.bc();  
}
```

(Provided the missing functions are implemented along the lines provided before)

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the Course

- Finite difference approximations on structured grids.
- Smart pointers
- Implementation strategies for differential operators, boundary conditions, and time steppers.

Course Summary

C++

- Basic elements of C++
- Abstract data types, C++ classes
- Constructors, destructors, memory management, copy, move
- Operator overloading
- Inheritance, abstract classes
- Templates, STL
- I/O

Scientific Computing

- Structured grids, differential operators, boundary conditions
- Implementation strategies and their C++ tools
- Efficient programming
- Scientific libraries