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Multigrid HowTo: A simple Multigrid solver in C++ in less than 200 lines of code

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Multigrid HowTo (Part I): A simple Multigrid solver in C++ in less than 200 lines of code

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Abstract

This short report is meant to guide multigrid beginners in order to implement their first simple multigrid solver. We choose to show a 2D Poisson solver on a structured cell-based grid that requires less than 200 lines of code. We will try to give a step-by-step introduction to multigrid from a practical point of view along this test implementation.

1 Introduction

In many areas of computation large linear or nonlinear systems have to be solved. Multigrid is one method to solve such systems that have a certain structure, e.g. that arise from the discretization of PDEs and lead to sparse and symmetric positive definite system matrices. The advantages of multigrid solvers compared to other solvers are that multigrid methods are applicable to a wide range of problems and can reach an asymptotically optimal complexity of $\mathcal{O}(N)$, where N is the number of unknowns in the system.

The multigrid principle is first mentioned by Fedorenko [8, 9] and Bakhvalov [1] and then intensively studied and pioneered by Brand [2, 3] and Hackbusch [11]. For good introductions and a comprehensive overview on multigrid methods, we, e.g., refer to [5, 19, 20, 21], for details on efficient multigrid implementations see [6, 7, 10, 12, 14, 15, 17, 18]. The MGNet Bibliography¹ collects many articles related to multigrid. In the last years multigrid has been applied to many fields, e.g., fluid mechanics, meteorology, quantum chemistry, bioelectric field computations, image processing, or computer vision.

Multigrid is not a single algorithm, but a general approach to find a solution by using several levels or resolutions. We distinguish different types of multigrid techniques depending on the meaning of a level. The *structured* or *geometric multigrid (MG)* identifies each level with a (structured) grid.

Another approach applicable to general non-uniform or unstructured grids arising, e.g., from finite element discretizations on complex domains is algebraic multigrid (AMG) [4, 16].

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¹http://www.mgnet.org/bib/mgnet.bib

AMG works directly on the algebraic system of equations and one level is just a matrix of a given size. Note that the adjacency graph of the matrix reveals the (unstructured) grid and also geometric multigrid can be written as algebraic system of equations.

In this report we try to minimize the presentation of mathematical details and refer to the literature instead [13]. Nevertheless, we have to formalize the given problem. We assume that we want to solve the partial differential equation (PDE)

$$-\Delta \boldsymbol{u} + \alpha \boldsymbol{u} = f \quad \text{in } \Omega \tag{1a}$$

$$\langle \nabla \boldsymbol{u}, \boldsymbol{n} \rangle = 0 \quad \text{on } \partial \Omega \tag{1b}$$

with (natural) Neumann boundary conditions on a rectangular domain Ω . Eq. (1) is discretized by finite differences on a structured grid what leads to a linear system

$$A^h u^h = f^h , \quad \sum_{j \in \Omega^h} a^h_{ij} u^h_j = f^h_i , i \in \Omega^h$$
 (2)

with system matrix $A^h \in \mathbb{R}^{N \times N}$, unknown vector $u^h \in \mathbb{R}^N$ and right hand side (RHS) vector $f^h \in \mathbb{R}^N$ on a discrete grid Ω^h . $n = \frac{1}{h}$ denotes the number of unknowns in x- and y-direction, and $N = n^2$ the problem size. We assume that Ω^h is a cell-based grid with mesh size $h = \frac{1}{2^i}, i \in \mathbb{N}$. In stencil notation the discretized eq. (1) reads

$$\frac{1}{h^2} \begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix} u^h + \begin{bmatrix} \alpha \end{bmatrix} u^h = f^h, \tag{3}$$

where the operator

$$A^{h} = \begin{bmatrix} 0 & -\frac{1}{h^{2}} & 0\\ -\frac{1}{h^{2}} & \frac{4}{h^{2}} + \alpha & -\frac{1}{h^{2}}\\ 0 & -\frac{1}{h^{2}} & 0 \end{bmatrix} . \tag{4}$$

In order to solve the above linear system, we apply the multigrid idea that is based on two principles:

Smoothing Property: Classical iterative methods like Gauß-Seidel (GS) are able to smooth the error after very few steps. That means the high frequency components of the error are removed well by these methods. But they have little effect on the low frequency components. Therefore, the convergence rate of classical iterative methods is good in the first few steps and decreases considerably afterwards.

Coarse Grid Principle: It is well known that a smooth function on a fine grid can be approximated satisfactorily on a grid with less discretization points, whereas oscillating functions would disappear. Furthermore, a procedure on a coarse grid is less expensive than on a fine grid. The idea is now to approximate the low frequency error components on a coarse grid.

The usual multigrid efficiency is achieved through the combination of two iterations, the smoother, or relaxation, and the coarse grid correction. Here, the smoother reduces the high frequency error components first, and then the low frequency error components are approximated on coarser grids, interpolated back to the finer grids and eliminated there. This leads to recursive algorithms which traverse between fine and coarse grids in the grid hierarchy. Two successive grid levels Ω^h and Ω^H with fine mesh size h and coarse mesh size H = 2h are shown in fig. 1.

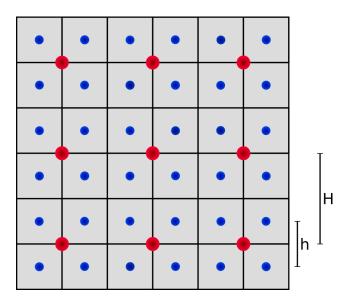


Figure 1: Grid in 2D with cell-centered coarsening. Small (blue) circles denote fine grid points, big (red) circles coarse grid points.

One multigrid iteration, here the so-called V-cycle, is summarized in algorithm 1. Note that in general the operator A^h has to be computed on each grid level, for our simple test problem the coarse operator is

$$A^{H} = \begin{bmatrix} 0 & -\frac{1}{H^{2}} & 0\\ -\frac{1}{H^{2}} & \frac{4}{H^{2}} + \alpha & -\frac{1}{H^{2}}\\ 0 & -\frac{1}{H^{2}} & 0 \end{bmatrix} .$$
 (5)

By nested iteration, the multigrid algorithm can be extended to Full Multigrid (FMG) shown in fig. 2. This means that we combine an unidirectional multilevel approach with a V-cycle and start on each level l with an interpolated initial guess computed on level l-1. Since ultimately only a small number of relaxation steps independent of the number of unknowns must be performed on each level, multigrid can reach an asymptotically optimal complexity $\mathcal{O}(N)$ [19]. The meaning of the signs and arrows in fig. 2 is explained in the following:

 \bullet exact solution on the coarsest grid: \square

```
Algorithm 1 Recursive V-cycle: u_h^{(k+1)} = V_h(u_h^{(k)}, A^h, f^h, \nu_1, \nu_2)
```

- 1: if coarsest level then
- solve $A^h u^h = f^h$ exactly or by many smoothing iterations
- $\bar{u}_h^{(k)} = \mathcal{S}_h^{\nu_1}(u_h^{(k)}, A^h, f^h) \; /\!/ \; pre\text{-smoothing}$
- $r^{h} = f^{h} A^{h} \bar{u}_{h}^{(k)} // compute \ residual$
- $r^H = \mathcal{I}_h^H r^h // restrict residual$
- $e^{H} = V_{H}(0, A^{H}, r^{H}, \nu_{1}, \nu_{2}) // recursion$ 7:
- $e^h = \mathcal{I}_H^h e^H // interpolate error$
- $\tilde{u}_h^{(k)} = \bar{u}_h^{(k)} + e^h // coarse \ grid \ correction$ $u_h^{(k+1)} = \mathcal{S}_h^{\nu_2}(\tilde{u}_h^{(k)}, A^h, f^h) // post-smoothing$
- 11: end if

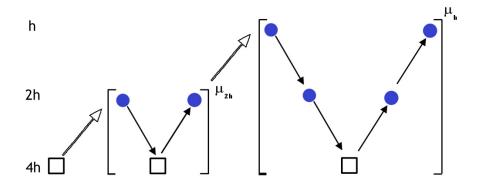


Figure 2: FMG algorithm (with V-cycles).

- prolongation of a coarse grid solution from coarse to fine grid:
- a small number (typically 1-3) of iteration steps, e.g., of GS method, called smoothing steps, on a fine grid applied to the current solution:
- restriction of fine grid residual to coarse grid:
- prolongation of coarse grid correction to fine grid and adding it to the corresponding previous fine grid approximation: /
- the corresponding procedure is applied μ_h times, e.g., once for a V-cycle.

2 Implementation

In this section we present a implementation of a FMG solver for problem (1) in the domain $\Omega = [0, 1]^2$ in 2D. Be aware that this is not the only way to implement multigrid. Our goal is just to show one way how it can be done for teaching purposes and not to do it very efficiently.

2.1 Prerequisites

In order to use our code you need to have a simple Array class

```
template < class T > class Array;
```

that has a member

```
T* data;
```

to store the grid data in an onedimensional array. It is accessed by an overloaded operator

```
inline T& operator()(int i,int j)
{
   return data[i*ncols + j];
}
```

In addition to that we make use of the helper functions nrows() and ncols() to obtain the size of the grid in each dimension and the function $resize(int\ i,int\ j)$ for allocating memory for the grid. The member function $initrandom\ (\ 0,1\)$ initializes the values on each grid point by a random number between 0 and 1.

2.2 Main Solver Routine

Next you find the main program in C++.

```
#include "Array.h"

double alpha = double ( 0.0001 );

// grid level factor 1/h^2
double *invh2;

int main ( int argc, char** argv )
{
    if ( argc != 5 )
        {
        cout << "Args: unrowsuncolsulevelsucycles" << endl;
        exit ( 0 );
    }

    int nrows = atoi ( argv[1] );
    int ncols = atoi ( argv[2] );
    int nlevels = atoi ( argv[3] );
    int iters = atoi ( argv[4] );</pre>
```

```
// Solution and right hand side on each level
Array < double > * Sol = new Array < double > [nlevels];
Array < double > * RHS = new Array < double > [nlevels];
// add 1 ghost layer in each direction
int sizeadd = 2;
invh2 = new double[nlevels];
// allocate memory on each grid level
for ( int i = 0; i < nlevels; i++ )
{
        Sol[i].resize ( nrows+sizeadd, ncols+sizeadd );
        RHS[i].resize ( nrows+sizeadd,ncols+sizeadd );
        nrows= ( nrows/2 );
        ncols= ( ncols/2 );
        invh2[i] = double (1.0)
                    / ( pow ( double ( 4.0 ),i ) );
}
// initialize solution and right hand side
Sol[nlevels-1].initrandom ( 0,1 );
Sol[0] = 1;
// simply set f = 0 to obtain the solution u = 0
RHS[0] = 0;
// restrict right hand side to all coarse grids
for ( int i = 1; i < nlevels; i++ )
        Restrict ( RHS[i-1],RHS[i] );
// compute normalized starting residual
double res_0 = residual ( 0,Sol,RHS );
cout << "Starting_residual:_" << res_0 << endl;
// call FMG solver
cout << "Residual_{\square}after_{\square}FMG_{\square}iteration:_{\square}" <<
     FMG_Solver(Sol, RHS, nlevels, iters, res_0)
     << endl;
```

```
delete [] invh2;
delete [] Sol;
delete [] RHS;

return 0;
}
```

After reading the command line arguments, the number of grid points in x- and y- direction, the number of multigrid levels and the number of multigrid V-cycles to perform, the memory for solution and right hand side on each grid level is allocated and both are initialized. Note that the coarser levels become smaller by a factor of 2 in each direction per additional grid level. For the treatment of Neumann boundary conditions, we add one additional layer of so-called ghost cells around each grid. The lines

initialize the factor $\frac{1}{h^2}$ on each level, where we assume h=1 on the finest level.

Before and after each iteration we compute the residual $r^h = f^h - A^h u^h$ in order to measure the accuracy of the current solution and use it as a stopping criterion. For typical multigrid efficiency the residual reduction per V-cycle, that is the convergence rate, should as a rule of thumb be around 0.1, i.e. the residual is reduced by one order of magnitude per multigrid cycle. Note that this factor is different for different problems and depends e.g. on the number of smoothing steps. If we do a complete FMG iteration the remaining error should be in the range of the discretization error, thus the problem is solved as accurate as possible for a given mesh size.

2.3 FMG Solver

In the following we show the FMG Solver routine. It implements fig. 2 and its core part is the V-cycle call.

```
for ( int i = 0; i < iters; i++ )
          {
            res_old = res;
            VCycle ( lev,Sol,RHS,nprae,npost,ncoarse,nlevels );
            // compute residual as accuracy measure
            res = residual ( lev,Sol, RHS );
            cout << "FMG_level:_" << lev << "_cycle:_"
                 << i << "uresidual:u" << res
                 << "uresidualureduction:u" << res_0/res
                 << "uconvergenceufactor:u"
                 << res/res_old << endl;
          }
          // if not finest level interpolate current solution
          if (lev > 0)
            interpolate ( Sol[lev-1], Sol[lev], lev );
        }
        return res;
}
```

The V-cycle itself is the most time consuming part in the multigrid solver and within the V-cycle, the smoother takes usually most of the time.

```
// compute and restrict the residual
Restrict_Residual ( lev, Sol, RHS );

// initialize the coarse solution to zero
Sol[lev+1] = 0;

VCycle ( lev+1,Sol,RHS,nprae,npost,ncoarse,nlevels );

// interpolate error and correct fine solution
interpolate_correct ( Sol[lev], Sol[lev+1], lev+1 );

// do some postsmoothing steps
for ( int i = 0; i < npost; i++ )
    GaussSeidel ( lev, Sol, RHS );
}</pre>
```

Note that on the coarsest grid also a direct solver can be used.

2.4 Gauss-Seidel Smoother

Since most of the time is spent in the smoother, it should be implemented efficiently. Nevertheless, we present a straightforward implementation for simplicity. The core routine solves eq. (3) by looping over all grid points in the domain and fixing all unknowns except the current grid point. Therefore the problem reduces to the solution of an equation with only one unknown what can be done very easily.

In order to treat the Neumann boundary conditions we explicitly copy the solution from the boundary into the ghost layers.

```
void treatboundary ( int lev, Array <double >* Sol )
{
        // treat left and right boundary
        for ( int i=0; i<Sol[lev].nrows(); i++ )</pre>
        {
                Sol[lev] (i,0) = Sol[lev] (i,1);
                Sol[lev] (i,Sol[lev].ncols()-1) =
                         Sol[lev] ( i,Sol[lev].ncols()-2 );
        }
        // treat upper and lower boundary
        for ( int j=0; j<Sol[lev].ncols(); j++ )</pre>
        {
                Sol[lev] (0,j) = Sol[lev] (1,j);
                Sol[lev] (Sol[lev].nrows()-1,j) =
                          Sol[lev] (Sol[lev].nrows()-2,j);
        }
}
```

2.5 Residual and Restriction Routines

The residual is computed in the L_2 norm by

```
double residual ( int lev,Array < double > * Sol,Array < double > * RHS )
{
```

with

```
#define RES(i,j) (RHS[lev](i,j) + invh2[lev]*(Sol[lev](i+1,j)
+ Sol[lev](i,j+1) + Sol[lev](i,j-1)
+ Sol[lev](i-1,j) )
- (4.0*invh2[lev] + alpha)*Sol[lev](i,j))
```

what corresponds to $f^h - A^h u^h$ at a given grid point (i, j). Next the grid transfers are printed. Within the FMG algorithm we need a simple restriction routine one a fine grid into a coarse one. The value of a coarse grid point is computed by a weighted sum of the surrounding fine grid points, this can be written in stencil notation by

$$\mathcal{I}_h^H = \frac{1}{4} \begin{bmatrix} 1 & 1 \\ & \cdot \\ 1 & 1 \end{bmatrix}.$$
(6)

```
fine ( fi, fj-1 ) + fine ( fi-1, fj-1 ) );
}
}
```

During the V-cycle we have to compute the residual and to restrict it to the next coarser grid level. This is done together in one routine.

```
void Restrict_Residual ( int lev, Array < double > * Sol,
                          Array < double >* RHS )
{
        // loop over coarse grid points
        for ( int i=1; i<RHS[lev+1].nrows()-1; i++ )
        {
          int fi = 2*i;
          for ( int j=1; j<RHS[lev+1].ncols()-1; j++ )
          {
            int fj = 2*j;
            RHS[lev+1] ( i,j ) = double ( 0.25 ) *
                  (RES(fi, fj) + RES(fi-1, fj) +
                   RES( fi, fj-1 ) + RES( fi-1, fj-1 ));
          }
        }
}
```

2.6 Interpolation Routines

For the transfer from a coarse to a fine grid we use a simple constant cell-based interpolation, where the value of each coarse grid point is just distributed to its fine neighbors, written in stencil notation

$$\mathcal{I}_H^h = \begin{bmatrix} 1 & 1 \\ & \cdot \\ 1 & 1 \end{bmatrix}.$$
(7)

```
void interpolate ( Array < double > & uf, Array < double > & uc, int 1 )
{
          double v;

          // loop over coarse grid points
          for ( int i=1; i < uc.nrows()-1; i++ )
          {</pre>
```

```
int fi = 2*i;
for ( int j=1; j < uc.ncols()-1; j++ )
{
    int fj = 2*j;
    v = uc ( i, j );

    uf ( fi, fj ) = v;
    uf ( fi-1, fj ) = v;
    uf ( fi, fj-1 ) = v;
    uf ( fi-1, fj-1 ) = v;
}
}</pre>
```

The interpolation of the approximated error from the coarse grid and the correction of the current solution is again done in a single routine.

```
void interpolate_correct ( Array < double > & uf,
                            Array < double > & uc, int 1 )
{
        double v;
        // loop over coarse grid points
        for ( int i=1; i <uc.nrows()-1; i++ )
        {
                 int fi = 2*i;
                 for ( int j=1; j < uc.ncols()-1; j++ )
                         int fj = 2*j;
                         v = uc (i,j);
                         uf (fi,fj) += v;
                         uf (fi-1,fj) += v;
                         uf (fi,fj-1) += v;
                         uf (fi-1,fj-1) += v;
                 }
        }
}
```

3 Costs and Test Run

In this section we want to provide some insight on the performance of the code. First we summarize the costs for the multigrid solver parts in table 1.

Table 1: Costs per unknown on one grid level: read and write accesses, number of integer operations and number of floating point operations.

part	read	write	Ops	FOps
smoother	5	1	4	6
$restrict_residual$	0.25	6	5.5	10
$interpolate_correct$	0.25	1	1.5	1
residual	6	1	4	11

From a run of the solver with parameters

$./{\tt FMGSolverSimple2D}\ 1024\ 1024\ 11\ 2$

we obtain the timing plots shown in fig. 3 and fig. 4 that are visualized by kcachegrind. The data are produced by $valgrind^2$.

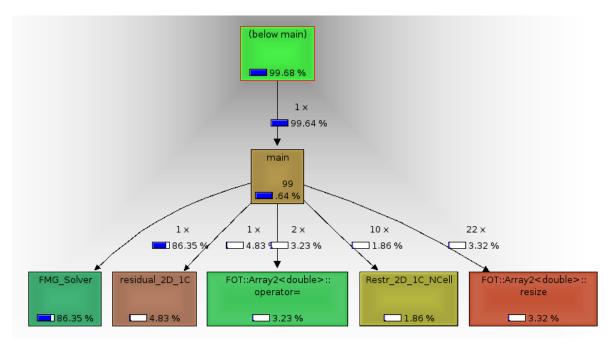


Figure 3: CPU time (in percentage) and number of calls for each routine called directly from the main routine.

²http://valgrind.org/

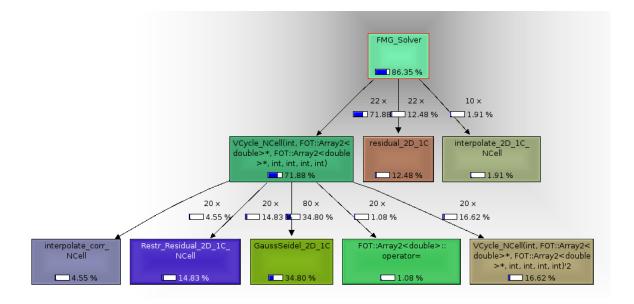


Figure 4: CPU time (in percentage) and number of calls for parts of the FMG algorithm.

4 Conclusion and Outlook

Next we will extend our multigrid solver step by step in order to treat e.g. 3D problems, handle different boundary conditions, use node-based grids, and parallelize the code.

In addition to that we plan to set up a website to download the multigrid code and present some sample applications for multigrid in image processing.

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