NUMERISCHE METHODEN IN DER PHYSIK
Second exercise WS 2013/2014   C

Numerical evaluation of a linear system of inhomogeneous equations with sparse coefficient matrices by means of the Gauss-Seidel method

Presentation of the method: Script chapter 2.7 (German script)

For this exercise the following software will be provided on the homepage of this course:

```
gausei.c    nrutil.c    elektr_Linse_1.dat    to    elektr_Linse_5.dat
```

Headline of the GAUSEI procedure:

```
void gausei(int n, int ndiag, int s[], double **diag,double f[],
            int tmax, double w, int irel, double gen, double loes[],
            int *t, int *error)
```

To make your start up with the programming language C a bit easier, a commented listing of a main program (named e.g. *gstest.c*), which calls the given routine *gausei.c*, can be found in the following lines:

```c
#include <stdio.h>       // input/output functions etc.
#include <math.h>        // mathematical functions and constants

#include "nrutil.c"      // utility programs for dynamic memory
                         // management from the Numerical Recipes C

#include "gausei.c"      // including the Gauss-Seidel program
                         // from the script
// Headline of the Gauss-Seidel program:
// void gausei(int n, int ndiag, int s[], double **diag,double f[],
//             int tmax, double w, int irel, double gen, double loes[],
//             int *t, int *error);



int main(void)                  // beginning of the main program
{
   int ord, ndiag, tmax, irel, t, error;   // def. of scalars
   double w, gen;
```

```c
    int *s;                         // def. of one- and twodim. fields
    double **diag, *f, *loes;

// input of the number of linear equations (ord) and the number
// of diagonals (ndiag):
    ord=...;
    ndiag=...;
// memory allocation for the one- and twodim. fields by the
// NRUTIL programs  ivector, dmatrix and dvector:
    s= ivector(1,ndiag);
    diag=dmatrix(1,ord,1,ndiag);
    f=dvector(1,ord);
    loes=dvector(1,ord);

// input of the relative position of the diagonals:
    s[1]=...; s[2]=...; ...

// input of the values of the diagonals:
    diag[...][...]=...; ...

// input of the inhomogeneous vector:
    f[1]=...; f[2]=...; ...

// definition of the GAUSEI parameters:
    tmax=5000;
    w=1.0;
    irel=0;
    gen=1.e-6;

// Calling of the procedure GAUSEI. It has to be considered, that the
// scalar parameters "t" and "error" are not assigned as values, but
// as address. So the data transfer is bidirectional (from MAIN to GAUSEI
// and from GAUSEI to MAIN):
    gausei(ord, ndiag, s, diag, f, tmax, w, irel, gen, loes, &t, &error);

// output of the results of the procedure GAUSEI:
    if(error==1) printf("ERROR in GAUSEI !\n");
    else {
      printf("Solution vector:   %11.8f   %11.8f\n",loes[1],loes[2]);
      printf("Number of Iterations needed = %4i\n", t);
    }
    return (0);
}
```

Building an executable file (named e.g. *gstest.exe*) with the command

```
gcc  -o gstest.exe  gstest.c -lm
```

Application of the Gauss-Seidel method for solving the Laplace equation in two dimensions by means of the finite difference method.

Note: The following exercise is basically taken from the book: E.W. Schmid, G. Spitz und W. Lösch, *Theoretische Physik mit dem Personal Computer*, Springer-Verlag Berlin, 1987, Kap. 9

Physical problem:
The problem considered here comes from electrostatics: The following figure shows a strongly simplified *electric lense*, as nowadays still found in electron optics:
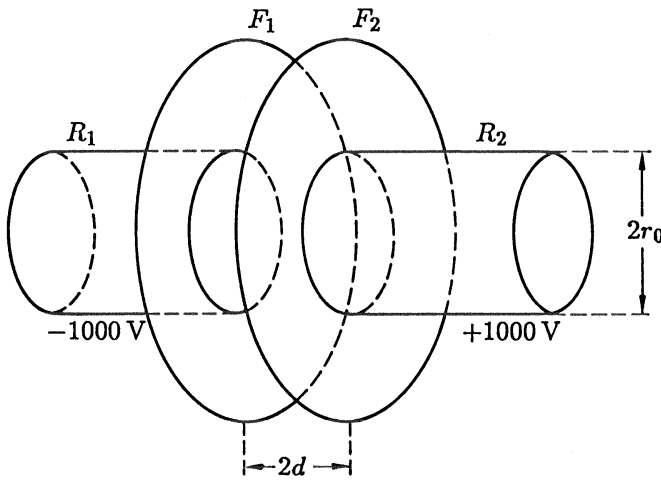

Fig. 1: Schema of an electric lense.

A cylindrical metal pipe with the radius r_0 is interrupted by a flange F_1, F_2. The flange and the perforated plates F_1, F_2 form a plate capacitor with the distance $2d$, and the two pipes R_1, R_2 are connected to the plates. On the right side of the construction a voltage of 1000 V is applied and on the left side a voltage of -1000 V. Now we are interested in the distribution of the potential Φ in the pipes and between the capacitor plates.

The spatial distribution of the Potential $\Phi(\mathbf{r})$ is described by one of the most important differential equation in theoretical physics, the *Laplace equation*:

$$\Delta \, \Phi(\mathbf{r}) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Phi(x, y, z) = 0 \qquad (1)$$

The boundary conditions of the problem determine the potential on the surface of the region where the equation (1) is to be solved.

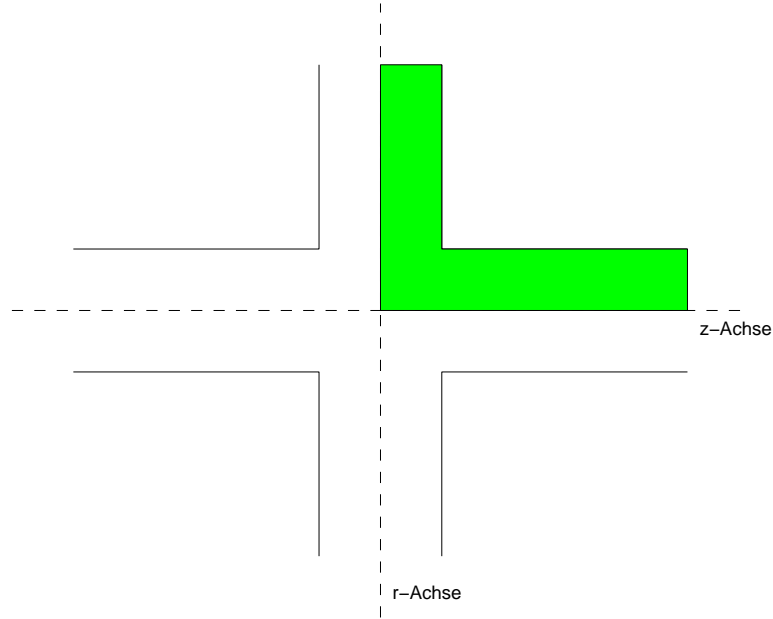For a better understanding of the following approach, a profile of fig. 1, is shown in the next figure:

Fig. 2: Profile of the electric lense.
The region where the Laplace equation should be solved, is shaded green.

From fig. 1 and fig. 2 follows:

- Due to the geometrical form of the electrical lense it is reasonable to use cylindrical coordinates (z,r,φ) instead of Cartesian coordinates (x,y,z). In this coordinate system the Laplace equation reads

$$\Delta\Phi = \frac{\partial^2\Phi}{\partial z^2} + \frac{1}{r}\frac{\partial\Phi}{\partial r} + \frac{\partial^2\Phi}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\varphi^2} = 0 \quad (r > 0)\,. \tag{2}$$

- Concerning the simple geometry of the problem it is obvious, that the solution of the differential equation (2) has to have cylindrical symmetry around the z-axis. This means that

$$\Phi(\mathbf{r}) = \Phi(z, r, \varphi) = \Phi(z, r) \tag{3}$$

has to hold. The Laplace equation is thus reduced to:

$$\Delta\Phi = \frac{\partial^2\Phi}{\partial z^2} + \frac{1}{r}\frac{\partial\Phi}{\partial r} + \frac{\partial^2\Phi}{\partial r^2} = 0 \quad (r > 0)\,. \tag{4}$$

- Likewise one can easily see, that the above equation only has to be solved *for the shaded region in fig. 1.* Symmetry considerations lead to the relations

$$\Phi(-z, r) = -\Phi(z, r)\,, \tag{5}$$

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and
$$\Phi(z, -r) = \Phi(z, r) \,. \tag{6}$$

<u>Note:</u> This relations of course does not mean that the length of the radial vector (r) can be negative. It only expresses that the distribution of the potential Φ in fig. 2 has to be mirror symmetrical with respect to the z-axis.

Now an important point follows: From the mathematical point of view, this boundary <u>value</u> <u>problem</u> (4) has a unique solution, only if the behavior of the solution $\Phi(z, r)$ is specified on the <u>whole</u> margin of the (shaded) integration region. To discuss this problem in more detail, we look at the integration region of fig. 2 once again in more detail:
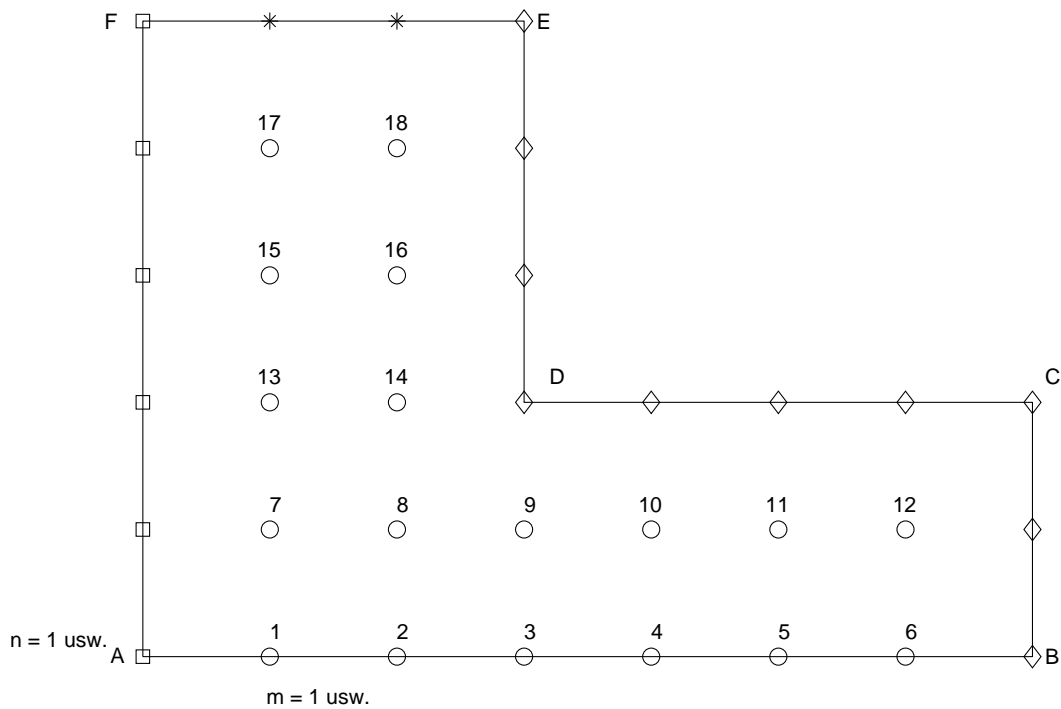

Fig. 3: The base region of the problem "electrical lense". The horizontal axis is the z-axis, the vertical axis is the r-axis. The points on the boundary of the base region can be read as follows:
diamonds = boundary condition (BC) (1.), (2.); squares = BC (3.); stars = BC (4.).
The (numbered) circles show the so-called "inner points". The potential values of these points have to be calculated by the solution of the Laplace equation. They form a <u>quadratic</u> <u>control</u> <u>network</u> where the points on the z-axis satisfy the symmetry condition (5.).

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1. In the region C→D→E the potential has a constant value V_0

$$\Phi(C \to D \to E) = V_0 \,.$$

2. If the pipes are long enough, the inner potential at the end will change only marginally. This means that the end of the pipe can be locked with a metal plate, which leads to the boundary condition

$$\Phi(B \to C) = V_0 \,.$$

3. As regards the distribution of the potential between the cylindrical plates, it is obvious that on the plane of symmetry perpendicular to the z-axis at $z=0$ the potentials on the left and right side compensate each other. So the boundary condition is

$$\Phi(A \to F) = 0 \,.$$

4. Now the boundary condition on the upper margin between point F ($\Phi = 0$) and point E ($\Phi = V_0$) is still missing. As a good approximation a *linear* gradient of the potential between the capacitor plates can be expected.

$$\Phi(F \to E) = V_0 \cdot z$$

5. The values along the z-axis have to be considered in more detail, as this is not a margin of the base region, but a symmetry axis. Due to the $1/r$ singularity of the z-axis, the Laplace equation cannot be evaluated in cylindrical coordinates (4). It has to be written in Cartesian coordinates (1):

$$\Phi(-x, 0, z) = \Phi(x, 0, z) \quad \text{and} \quad \Phi(0, -y, z) = \Phi(0, y, z)$$

The numerical exercise is to solve the DE (2) by considering the boundary conditions described on this page. For this the *finite difference method* is frequently used. Thereby a control network is constructed in the base region and this network defines the (inner and outer) grid points. It is obvious that this discretization of a continuous problem introduces a methodological error and furthermore it is clear that the methodological error is reduced by increasing the point density in the base region, i.e. by rising the number of grid points.

For a correct graphical display of the potential values obtained, it is necessary to know the position of each (inner) grid point in the base region. For this the following convention is employed:

- An index n is assigned to each row of the grid points starting with the lowest row (along the z-axis) which gets the index $n = 1$.

- An index m is assigned to each column of the grid points starting with the column to the very left which gets the index $m = 1$.

Now the quantity $m_{max}(n)$ is defined, which gives the number of inner grid points for the n-th row:

$$m_{max} = \begin{cases} m_a & \text{for} & 1 \le n \le n_a \\ m_b & \text{for} & n_a < n \le n_a + n_b \end{cases} , \tag{7}$$

where the 4 parameters mean:

n_a number of "long" rows   ($n_a = 2$ in fig. 3),

m_a points per "long" row   ($m_a = 6$ in fig. 3),

n_b number of "short" rows   ($n_b = 3$ in fig. 3),

m_b points per "short" row   ($m_b = 2$ in fig. 3),

the <u>total</u> <u>number</u> of inner grid points N_{tot} is:

$$N_{tot} = n_a \, m_a + n_b \, m_b . \tag{8}$$

The approximate calculation of the solution of the DE (4) at the N_{tot} grid points by considering the boundary conditions defined on page 6 employs - as already mentioned - the "finite difference method". Though the DE including the boundary conditions is converted into a *system of inhomogeneous, linear equations*.

For this exercise I will make it easier for you by giving you the already "complete" system of linear, inhomogeneous equations which arises out of the Laplace equation. Such a system has e.g. for the point distribution seen in fig. 3 the following characteristic structure:

```
+ +            +                                    +
+ + +            +                                  +
  + + +            +                                +
    + + +            +                              +
      + + +            +                            +
        + +              +                          +
+            + +            +                        +
  +          + + +            +                      +
    +          + + +                                +
      +          + + +                              +
        +          + + +                            +
          +          + +                            +
            +              + + +                     +
              +            + +    +                  +
                +            + + +                   +
                  + + +          +                   +
                    +    + +                         +
                      + + +                          +
```

Independently of the parameters n_a, m_a, n_b and m_b, the coefficient matrix is always formed by 7 diagonals:

$$s[1] \quad s[2] \quad s[3] \quad s[4] \quad s[5] \quad s[6] \quad s[7]$$

The definition of the integer field s can be seen in the script, section 2.7.3 (German script). At this point it should only be remarked, that the way of numbering the diagonals does not matter! It is only important <u>where</u> the diagonals can be found in the coefficient matrix. The relative positions (relating to the main diagonal) depend on the parameters n_a, m_a, n_b and m_b; The main diagonal always has to be fully occupied (this means one of the s values has to be zero) and there always has to be a first lower (s=-1) and a first upper (s=1) diagonal.

The elements of the main diagonal have the values -4 or -6 and they are in absolute values <u>much</u> bigger than the absolute values of the other diagonals. This means that the rule of thumb stated in the script on page 46 for the convergence of the iterative Gauss-Seidel method is full filled very well for the given problem!

The inhomogeneous vector appears additionally, it contains information about the boundary conditions.

As mentioned at the beginning, I have prepared for you five systems of linear equations, each with 7 diagonals of the coefficient matrix and the corresponding inhomogeneous vector, for the following parameters:

File name	n_a	m_a	n_b	m_b	N_{tot}	V_0 (Volt)	Occupation (%)
elektr_Linse_1	2	6	3	2	18	1000.0	38.9
elektr_Linse_2	8	27	12	11	348	1000.0	2.0
elektr_Linse_3	8	27	12	5	276	1000.0	2.5
elektr_Linse_4	8	27	12	2	240	1000.0	2.9
elektr_Linse_5	16	55	24	5	1000	1000.0	0.7

The occupation describes the amount of memory needed for the sparse matrix compared to the amount that would be needed to save the whole matrix.

The associated relative positions of the seven diagonals of the coefficient matrices are:

File name	$s(1)$	$s(2)$	$s(3)$	$s(4)$	$s(5)$	$s(6)$	$s(7)$
elektr_Linse_1	0	+1	+6	-1	-6	+2	-2
elektr_Linse_2	0	+1	+27	-1	-27	+11	-11
elektr_Linse_3	0	+1	+27	-1	-27	+5	-5
elektr_Linse_4	0	+1	+27	-1	-27	+2	-2
elektr_Linse_5	0	+1	+55	-1	-55	+5	-5

The according data can be found in the files

```
elektr_Linse_1.dat     elektr_Linse_2.dat  .....  elektr_Linse_5.dat
```

Those files are structured in the following way:

```
na   ma   nb   mb
Ntot
s(1)  s(2)  s(3)  s(4)  s(5)  s(6)  s(7)   inhom.vector
.
.
 line by line 8 data entries
.
.
```

Task 1

- Test the Gauss-Seidel program *gausei.c* for the Laplace problem *elektr_Linse_1* (18 inner nodes). Use for the simulation ω=1.0 and GEN(abs)=10^{-6}.

  If you print the 18 values of the potential field Φ line by line, you should get the result:

  ```
  332.55  665.73     0.00     0.00     0.00     0.00
  330.81  663.30     0.00     0.00     0.00     0.00
  326.34  654.86     0.00     0.00     0.00     0.00
  315.96  618.66  874.16  957.73  985.83  995.68
  311.38  604.41  840.49  941.87  979.82  993.76
  ```

Start with the second task if and only if you get exactly the above test values!

Task 2

- For the following calculations evaluate the Laplace problem *elektr_Linse_5* (1000 inner nodes), again with an accuracy of GEN(abs)=10^{-6}.

  Calculate this problem for different relaxation parameters ω in the range of $1 \leq \omega < 2$ and plot the number of required iteration steps as a function of ω in a diagram.

  How many iteration steps are needed at $\omega = 1.0$?
  Which value has the optimum ω (with an accuracy of 2 significant places after the decimal point)?
  How many iteration steps does *gausei.c* need at this ω_{opt}?

- Now you have to extend the existing Gauss-Seidel program by implementing an automatic ω optimization (see German script equation (2.26) and (2.27)). As a value for t_0 take 50.

  What is the value of ω_{ideal} that is reached by your extended program and how many iteration steps does the program need to solve the Laplace problem *elektr_Linse_5*?

Task 3

- After those numerical tests, calculate the distribution of the potential for the series of data sets *elektr_Linse_2.dat*, *elektr_Linse_3.dat*, *elektr_Linse_4.dat* and *elektr_Linse_5.dat*.

- Concerning the graphical presentation of the calculated distribution of the potential by so called contour plots, you can find some important comments in the text file

  `en_lense_contourplot.txt`

- Discuss the results phenomenologically.