Numerical Integration of Partial Differential Equations (PDEs)

- Introduction to PDEs.
- · Semi-analytic methods to solve PDEs.
- · Introduction to Finite Differences.
- Stationary Problems, Elliptic PDEs.
- Time dependent Problems.
- Complex Problems in Solar System Research.

Stationary Problems, Elliptic PDEs.

- Example: 2D-Poisson equation.
- From differential equations to difference equations and algebraic equations.
- Relaxation methods:
 - -Jacobi and Gauss-Seidel method.
 - -Successive over-relaxation.
 - -Multigrid solvers.
- Finite Elements.

Maxwell Equations:

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \epsilon_0 \nu_0 \frac{\partial \mathbf{F}}{\partial t}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0} \rho$$

For slowly varying temporal evolution we neglect the displacement current (popular in MHD) and use the electromagnetic potentials:

$$\mathbf{B} = \nabla \times \mathbf{A}$$
$$\mathbf{E} = -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t}$$

together with the Coulomb Gauge condition:

$$\nabla \cdot \mathbf{A} = 0$$

With these definitions we get:

$$\nabla \times \nabla \times \mathbf{A} = \mu_0 \mathbf{j}$$
$$\nabla \times (-\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t}) = -\frac{\partial \nabla \times \mathbf{A}}{\partial t}$$
$$\nabla \cdot \nabla \times \mathbf{A} = 0$$
$$\nabla \cdot (-\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t}) = \frac{1}{\epsilon_0}\rho$$

We use the vector identity $\nabla \times \nabla \times \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \Delta \mathbf{A}$

$$\nabla(\nabla \cdot \mathbf{A}) - \Delta \mathbf{A} = \mu_0 \mathbf{j}$$
$$-\Delta \Phi - \frac{\partial(\nabla \cdot \mathbf{A})}{\partial t} = \frac{1}{\epsilon_0} \rho$$

Finally we use the Coulomb Gauge $\nabla \cdot \mathbf{A} = 0$ and derive Poisson equations:

$$-\Delta \mathbf{A} = \mu_0 \mathbf{j} -\Delta \mathbf{\Phi} = \frac{1}{\epsilon_0} \rho$$

Boundary value problems for elliptic PDEs: Example: Poisson Equation in 2D

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y)$$

We define short notation:

$$\begin{aligned} x_j &= x_0 + j\Delta, & j = 0, 1, ..., J & u_{j,l} \text{ for } u(x_j, y_l) \\ y_l &= y_0 + l\Delta, & l = 0, 1, ..., L & \rho_{j,l} \text{ for } \rho(x_j, y_l) \end{aligned}$$

After discretisation we get the difference equation:

$$\frac{u_{j+1,l} - 2u_{j,l} + u_{j-1,l}}{\Delta^2} + \frac{u_{j,l+1} - 2u_{j,l} + u_{j,l-1}}{\Delta^2} = \rho_{j,l}$$

 $u_{i+L+1} + u_{i-(L+1)} + u_{i+1} + u_{i-1} - 4u_i = \Delta^2 \rho_i$



Equation holds on inner points only! On the boundary we specify:

-u (Dirichlet B.C.) or-Derivative of u(von Neumann B.C.)

How to solve the difference equation? $u_{i+L+1} + u_{i-(L+1)} + u_{i+1} + u_{i-1} - 4u_i = \Delta^2 \rho_i$

We can interpret **u** as a vector and write the equation formally as an algebraic matrix equation:

$\mathbf{A} \cdot \mathbf{u} = \mathbf{b}$

- Theoretical one could solve this algebraic equation by well known algebraic equation solvers like Gauss-Jordan elimination.
- This is very unpractical, however, because A is very large and contains almost only zeros.

How large is A?

- For a very moderate 2D-grid of 100x100
 -u has 100 x 100= 10⁴ gridpoints, but
 -A has 10⁴ x 10⁴=10⁸ entries!
- For 3D-grids typically used in science application of about 300 x 300 x 300
 -u has 300³= 2.7 *10⁷ gridpoints,
 -A has (2.7 *10⁷)² =7.29*10¹⁴ entries!
 - => Memory requirement for 300-cube to store u ~100 MB, A~3Million GByte

Structure of A ?



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How to proceed?

- We have reduced our original PDE to algebraic equations (Here: system of linear equations, because we started from a linear PDE.)
- To do: Solve these equations.
- As exact Matrix solvers are of no much use we solve the equations numerically by **Relaxation methods**.

Relaxation: Jacobi method



From
$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y)$$
 Carl Jacobi
1804-1851

we derived the algebraic equations:

$$u_{i+L+1} + u_{i-(L+1)} + u_{i+1} + u_{i-1} - 4u_i = \Delta^2 \rho_i$$

Assume any initial value, say $\mathbf{u}=0$ on all grid points (except the specified boundary values of course) and compute:

$$u_{j,l}^{n+1} = \frac{1}{4} \left(u_{j+1,l}^n + u_{j-1,l}^n + u_{j,l+1}^n + u_{j,l-1}^n \right) - \frac{\Delta^2}{4} \rho_{j,l}$$

Use the new values of **u** as input for the right side and repeat the iteration until **u** converges. (n: iteration step) ¹¹

Relaxation: Jacobi method

- Jacobi method converge for diagonal dominant matrices A. (diagonal entries of A larger than the others)
- This condition is usually fulfilled for Matrix equations derived from finite differencing. (Tridiagonal block matrix: Most entries in A are zeros!)
- Jacobi method converges (but slowly) and can be used in principle, but maybe we can improve it?
- For practice: Method should converge fast!

Gauss Seidel method

- Similar as Jacobi method.
- Difference: Use on the right-hand site already the new (and assumed to be better) approximation uⁿ⁺¹, as soon as known.



C.F. Gauss 1777-1855

$$u_{j,l}^{n+1} = \frac{1}{4} \left(u_{j+1,l}^n + u_{j-1,l}^{n+1} + u_{j,l+1}^n + u_{j,l-1}^{n+1} \right) - \frac{\Delta^2}{4} \rho_{j,l}$$

How fast do the methods converge?

To solve: $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ We split A as: $\mathbf{A} = \mathbf{L} + \mathbf{D} + \mathbf{U}$ Lower Diagonal Upper Triangle Elements Triangle

For the **r**th iteration step of the Jacobi method we get:

$$\mathbf{D} \cdot \mathbf{x}^{(r)} = -(\mathbf{L} + \mathbf{U}) \cdot \mathbf{x}^{(r-1)} + \mathbf{b}$$

How fast do the methods converge?

We have to investigate the iteration matrix

$$-\mathbf{D}^{-1} \cdot (\mathbf{L} + \mathbf{U})$$

Eigenvalues of iteration matrix define how fast residual are suppressed. Slowest decaying Eigenmode (largest factor) defines convergence rate. => Spectral radius ρ_s of relaxation operator. $0 < \rho_s < 1$

How many iteration steps r are needed to reduces the overall error by a factor of 10^{-p} ?

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How many iteration steps \mathbf{r} are needed to reduces the overall error by a factor of 10^{-p} ?

In general:
$$r \approx \frac{p \ln 10}{(-\ln \rho_s)}$$

For a J x J grid and Dirichlet B.C. one gets:



Can we do better?

 $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ $\mathbf{A} = \mathbf{L} + \mathbf{D} + \mathbf{U}$

Gauss Seidel (L + D) $\cdot \mathbf{x}^{(r)} = -\mathbf{U} \cdot \mathbf{x}^{(r-1)} + \mathbf{b}$

Can be rewritten as:

$$\mathbf{x}^{(r)} = \mathbf{x}^{(r-1)} - (\mathbf{L} + \mathbf{D})^{-1} \cdot \underbrace{[(\mathbf{L} + \mathbf{D} + \mathbf{U}) \cdot \mathbf{x}^{(r-1)} - \mathbf{b}]}_{\text{residual vector } \xi^{(r-1)}}$$

Successive Overrelaxation (SOR)

$$\mathbf{x}^{(r)} = \mathbf{x}^{(r-1)} - (\mathbf{L} + \mathbf{D})^{-1} \cdot \xi^{(r-1)}$$

Now we overcorrect the residual error by

$$\mathbf{x}^{(r)} = \mathbf{x}^{(r-1)} - \underbrace{\boldsymbol{\omega}}_{\text{overrelaxation}} \mathbf{L} + \mathbf{D})^{-1} \cdot \boldsymbol{\xi}^{(r-1)}$$

Method is only convergent for 0<w<2. (for w<1 we have underrelaxation) Aim: Find optimal overrelaxation parameter. Often done empirically.

Successive Overrelaxation (SOR)

For the optimal overrelaxation parameter w the number of iteration steps to reduce the error by 10^{-p} are:

$$r \simeq \frac{pJ\ln 10}{2\pi} \simeq \frac{1}{3}pJ$$

Number of iteration steps increases only linear with the number of mesh points **J** for SOR method. For Jacobi and Gauss Seidel it was $\sim J^2$

Successive Overrelaxation (SOR)

- SOR method only more effective when overrelaxation parameter w is close it's optimum.
- Some analytic methods exist to estimate optimum w, but often one has to find it empirically.
- Unfortunately the optimum value w does not depend only on the PDE, but also on the grid resolution.
- The optimum asymptotic w is not necessarily a good initial choice.
- Chebyshev acceleration changes w during iteration.

Generalization of SOR-method.

Finite difference schemes from 2D-elliptic PDEs have the form:

 $a_{j,l}u_{j+1,l} + b_{j,l}u_{j-1,l} + c_{j,l}u_{j,l+1} + d_{j,l}u_{j,l-1} + e_{j,l}u_{j,l} = f_{j,l}u_{j,l-1} + e_{j,l}u_{j,l} = f_{j,l}u_{j,l-1} + e_{j,l}u_{j,l-1} + e_{j,l}u_{j,l-1$

a = b = c = d = 1, e = -4 for our example

We iterate for the solution by

$$u^*_{j,l} = \frac{1}{e_{j,l}} \left(f_{j,l} - a_{j,l} u_{j+1,l} - b_{j,l} u_{j-1,l} - c_{j,l} u_{j,l+1} - d_{j,l} u_{j,l-1} \right)$$

and get:

$$u_{j,l}^{\text{new}} = \omega u^*_{j,l} + (1-\omega)u_{j,l}^{\text{old}}$$

Generalization to 3D is straight forward $\frac{1}{21}$

Summary: Relaxation methods

- Choose an initial solution u⁰ (usually zeros)
 Relax for u^{new} from u^{old} (Jacobi, GS, SOR)
 Are u^{old} and u^{new} identical within some tolerance level?
 If No continue, If yes solution is found.
- 4.) $u^{old} = u^{new}$ and go to step 2.)

Iterate only where u is unknown!!

-Dirichlet B.C.: **u** remains unchanged on boundaries.

-von Neumann: compute **U** from grad(u)=known at each iteration step before 2.) [Ghost cells or one-sided derivatives] ²²

Computing time for relaxation methods

- For a J x J 2D-PDE the number of iteration steps is ~J² (Jacobi GS) or ~J (SOR)
- But: Each iteration step takes $\sim J^2$
- Total computing time: $\sim J^4$ (Jacobi, Gauss Seidel) $\sim J^3$ (SOR-method)
- Computing time depends also on other factors: -required accuracy
 - -computational implementation
 - -IDL is much slower as C or Fortran
 - -Hardware and parallelization

How fast are errors smoothed out?



Show: demo_laplace.pro

This IDL program shows how fast or slow Errors of different wave-length are relaxed for Jacobi, Gauss-Seidel and SOR for the homogenous Laplace-equation.

How fast are errors smoothed out? We use Gauss-Seidel 40x40 box and investigate a **high frequency (k=10)** disturbance.



Converged (Error <10⁻⁶) after **24** iteration steps)

How fast are errors smoothed out? We use Gauss-Seidel 40x40 box and investigate a **low frequency (k=1)** disturbance.



Converged (Error <10⁻⁶) after **747** iteration steps)

How fast are errors smoothed out? We use **Gauss-Seidel** on JxJ boxes and investigate number of steps to converge for different frequencies

k	1	10	20	40
J				
40	747	24	13	11
80	2615	67	26	14
160	8800	216	72	28

Gauss-Seidel method is very good smoother!

How fast are errors smoothed out? Same test with SOR method

k	1	10	20	40
J				
40	81	109	112	119
80	213	141	146	152
160	844	173	179	189

SOR is a faster solver, but NOT good smoother!

How fast are errors smoothed out? (Gauss-Seidel)

- High frequency errors are smoothed out fast.
- Low frequency errors take very long to vanish.
- But the long frequency errors are reduced faster on low resolution grids.
- Can we use this property to speed up the relaxation?
- Yes! The answer is **Multigrid**.

Multigrid Methods

- Aim: Be even better (faster) then the SOR-method.
- From experience we know that any relaxation methods smoothes out errors fast on small length scales, but very slowly on large scales.
- Idea: compute solution on grids with reduced spatial resolution.
- Interpolate to finer grids.
- Need to swap between grids in a consistent way.

Multigrid Methods

We want to solve the linear elliptic PDE

$$\mathcal{L}u = f$$
 discretized we get $\mathcal{L}_h u_h = f_h$

If \widetilde{u}_h is an approximation and u_h the exact solution we have an error of: $v_h = u_h - \widetilde{u}_h$

The residual or defect $d_h = \mathcal{L}_h \widetilde{u}_h - f_h$

and for the error $\mathcal{L}_h v_h = -d_h$

Multigrid methods

Any iteration methods now uses a simplified operator (e.g. Jacobi: diagonal part only, GS: lower triangle) to find error or correction: $\widehat{\mathcal{L}}_h \widehat{v}_h = -d_h$

and the next approximation $\widetilde{u}_h^{\mathrm{new}} = \widetilde{u}_h + \widehat{v}_h$

Now we take a different approach. We do not simplify the operator, but approximate \mathcal{L}_h on a coarser grid H=2h by

$$\mathcal{L}_H v_H = -d_H$$

which will be easier to solve, because of lower dimension.

Multigrid Methods

We need an restriction operator to compute the residual on the coarser grid:

$$d_H = \mathcal{R}d_h$$

And after we find the solution \tilde{v}_H on the coarser grid a prolongation operator to interpolate to the finer grid:

$$\widetilde{v}_h = \mathcal{P}\widetilde{v}_H$$

Finally we update:

$$\widetilde{u}_h^{\rm new} = \widetilde{u}_h + \widetilde{v}_h$$

Multigrid Methods



Prolongation (coarse to fine)

$$\begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & 1 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{bmatrix}$$



Restriction (fine to coarse)

$$\begin{bmatrix} \frac{1}{16} & \frac{1}{8} & \frac{1}{16} \\ \frac{1}{8} & \frac{1}{4} & \frac{1}{8} \\ \frac{1}{16} & \frac{1}{8} & \frac{1}{16} \end{bmatrix}$$

Coarse grid correction

One coarse-grid correction step in a 2-level Multigrid scheme contains:

- Compute defect on fine grid.
- Restrict defect to coarse grid.
- Solve correction exactly on coarse grid.
- Prolongate (interpolate) correction to fine grid.
- Update next approximation.

2-level Multigrid scheme

- Pre-smoothing: Apply some relaxation steps (usually with Gauss-Seidel method) on fine grid.
- Coarse grid correction.
- Post-smoothing: Relax some steps again on the fine grid to the updated solution.

- -High frequency defects are smoothed out fast on the fine grid.
- Low frequency defects (which took very long to relax on fine grid) are taken care by on coarse grid.

N-level Multigrid scheme

- Generalization of 2-level multigrid method.
- Instead of solving the equation on 2. grid exactly we approximate it on an even coarser grid.
- Very easy to solve on coarsest grid.
- Different possibilities cycles are possible:
 - -V-cycle
 - -W-cycle
 - -Full multigrid
- Hint: Do not use the SOR-method for smoothing (but Gauss-Seidel). Overrelaxation in SOR-methods destroys the high-frequency smoothing.

V-cycle for 3 levels









Full Multigrid cycles Start on coarsest grid



Multigrid and Full Multigrid

- Multigrid methods speed up the convergence of relaxation scheme.
- Number of cycles needed does not depend on grid size. (computing time for each cycle does of course)
- Way more demanding in programming afford.
- Multigrid computes only defect on coarser grid, but Full Multigrid (FMG) provides solution of the PDE on all grids.
- FMG can be generalized for nonlinear PDEs, Full Approximation Storage Algorithm (FAS). Discussion is outside scope of this lecture.

Summary: Relaxation Methods

- Methods are well suited to solve Matrix equations derived from finite difference representation of elliptic PDEs.
- Classic methods are easy to program and suitable not to large numerical grids. Computing time increases rapidly with grid size.
- Multigrid methods are much faster for large grids and should be first choice.
- Computational implementation of Multigrid Methods is way more demanding.

Alternatives to solve Matrix Equations derived from PDEs

- **Direct Matrix solvers:** Only for very small 2D-Problems or as exact solver on coarsest Multigrid.
- Fast Fourier Transform Methods (FFT): Suitable for linear PDEs with constant coefficients. Original FFT assumes periodic boundary conditions. Fourier series solutions look somewhat similar as what we got from separation of variables.
- Krylov subspace methods: Zoo of algorithms for sparse matrix solvers, e.g. Conjugate Gradient Method (CG).



Exercise: 2D-Poisson equation

lecture_poisson2d_draft.pro

This is a draft IDL-program to solve the Poisson-equation for provide charge distribution.

Task: implement Jacobi, Gauss-Seidel and SOR-method. Find optimal relaxation parameter for SOR-method.



Elliptic PDEs Summary

- Discretized differential equations lead to difference equations and **algebraic equations**.
- System of coupled equations is way to large for direct solvers. => Use **Relaxation methods.**
- **Gauss-Seidel** and **SOR**-method are in particular suitable to solve algebraic equations derived from elliptic PDEs.
- Fastest solvers are based on **Multigrid** methods.

Finite Element Method (FEM)





Arbitrary shaped boundaries are difficult to implement in finite difference methods. Alternative: Finite Elements, popular in particular to solve PDEs in engineering/structural mechanics.

Finite Elements





FEM covers the space with finite elements (in 2D often triangles, in 3D tetrahedra). The elements **do not need** to have the same size and shape. This allows to use a higher resolution where needed. ⁴⁷

Variational formulation: 1D example

P1 :
$$\begin{cases} u'' = f \text{ in } (0,1), \\ u(0) = u(1) = 0, \end{cases}$$

If u fulfills P1 and v(x) is an arbitrary function which vanishes on the boundary:

 $\int_{0}^{1} f(x)v(x) dx = \int_{0}^{1} u''(x)v(x) dx \text{ Partial integration of right side}$ $= u'(x)v(x)|_{0}^{1} - \int_{0}^{1} u'(x)v'(x) dx$ $= -\int_{0}^{1} u'(x)v'(x) dx = -\phi(u, v). \text{ Weak formulation}$ of the PDE

Solution of weak problem and original PDE are identical.

Variational formulation: 2D example
P2 :
$$\begin{cases} u_{xx} + u_{yy} = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial \Omega, \end{cases}$$
 Poisson equation

For an arbitrary function v the PDE can again be formulated in weak form (using Greens theorem):

$$\int_{\Omega} f v \, ds = - \int_{\Omega} \nabla u \cdot \nabla v \, ds = -\phi(u, v),$$

If we find a solution for the weak problem, we solved our (strong form) original PDE. Order of derivatives is reduced in weak form, which is helpful to treat discontinuities.

Shape function v

- How to choose the function v ?
- v must be at least once differentiable.
- For FEM-approach one takes polynomials or in lowest order **piecewise linear functions**:







Basis of functions for v

We choose piecewise linear functions which are one at a particular grid-point and zero at all other grid-points (triangle or tent-function)

$$v_k(x) = \begin{cases} \frac{x - x_{k-1}}{x_k - x_{k-1}} & \text{if } x \in [x_{k-1}, x_k], \\ \frac{x_{k+1} - x}{x_{k+1} - x_k} & \text{if } x \in [x_k, x_{k+1}], \\ 0 & \text{otherwise,} \end{cases}$$

We get function value and derivative by interpolation.

Basic tent-function (blue) and superposition to piecewise linear function (red)

×2

Х.,

Xa

x_=0

x₅=1

 X_4

Basis of functions for v

• For such base-functions almost all integrals in the form: D 2D

$$\langle v_j, v_k \rangle = \int_0^1 v_j v_k \, dx \qquad \qquad \int_\Omega v_j v_k \, ds$$

$$\phi(v_j, v_k) = \int_0^1 v'_j v'_k \, dx \qquad \qquad \int_\Omega \nabla v_j \cdot \nabla v_k \, ds$$

are zero. Only integrals of elements sharing grid points (edges of triangles in 2D) are non-zero.

From FEM to matrix form

Let's try to describe the unknown function u(x) and the known f(x) with these basis functions:

$$u(x) = \sum_{k=1}^{n} u_k v_k(x) \quad f(x) = \sum_{k=1}^{n} f_k v_k(x)$$

Aim: Find the parameters u_k ! This will be the solution in FEM-approach.

How to find this solution? Insert this approaches for u and f into the weak formulation of the PDE.

From FEM to matrix form



which leads to a system of equations which has to be resolved for u_k .

We can write in matrix form:

$-L\mathbf{u} = M\mathbf{f}$

This sparse matrix system can be solved with the method we studied for finite differences.

Lets remember all steps:
P2 :
$$\begin{cases} u_{xx} + u_{yy} = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$
Original PDE (strong form)

$$\int_{\Omega} fv \, ds = -\int_{\Omega} \nabla u \cdot \nabla v \, ds = -\phi(u, v), \quad \text{PDE in weak form} \\ \sum_{k=1}^{n} u_{k} \phi(v_{k}, v_{j}) = \sum_{k=1}^{n} f_{k} \int v_{k} v_{j} \quad \text{PDE in discretized form} \end{cases}$$

Solve corresponding sparse Matrix system: => Solution of PDE in FEM-approach.



Finite Element Method Summary

- Finite Elements are an alternative to finite differences. Good for complicated boundaries.
- PDE is solved in weak form.
- More flexible as finite differences, but also more complicated to implement in code.
- Setting up the optimal grid can be tricky. (Some research groups only work on this.)