GEO022 – Numerical methods in Fortran
Ladislav Hanyk, KG

Annotation:
A course of numerical methods with the emphasis on their implementation in Fortran. From libraries of numerical routines through standard methods of algebra and analysis to solution of ordinary and partial differential equations. Less theory, more practice. Examples of geophysical applications.

Syllabus:
1. Real data in real computers: Storing integer and real numbers (format IEEE). Errors: classification, sources and spreading.
2. Introduction to Fortran 90: Syntactical elements, specification statements, commands and constructs. Arrays in Fortran 90, array sections, array-valued functions. Program units and structuring source codes in Fortran 90. Parallelization. On-line graphics libraries. Examples: tabulating Earth models.
3. Libraries of numerical methods: Numerical Recipes, IMSL, NAG, LAPACK, netlib aj. Orientation in libraries, calling library routines. Examples: spherical Bessel functions, algebraic matrix operations.
4. Mini-algorithms: Horner scheme. Recurrence relations and their properties. Difference schemes. Numerical derivatives. FFT. Random numbers. Searching, sorting. What not to compute. Examples: Legendre polynomials and functions.
5. Systems of linear algebraic equations. Matrix conditionality. Direct methods – Gauss elimination and factorization methods (LU factorization). Methods for systems with tridiagonal, band diagonal matrices and special matrices. Iterative methods, conjugate gradient method. Overdetermined and underdetermined systems, singular value decomposition. Matrix eigenvalues and eigenvectors – real symmetric vs. nonsymmetric matrices.
6. Approximation, basic applications: Interpolation of functions and derivatives (polynomial and rational interpolation, splines). Method of least squares. Chebyshev approximation, economization. Solution of nonlinear equations (classic methods, Newton method, combined methods). Examples: Fornberg schemes.
7. Numerical integration: Newton-Cotes formulas. Romberg integration. Gaussian quadratures. Examples: multiplication of spherical harmonic functions.
8. Systems of nonlinear algebraic equations: Linearization (Newton method). Minimalization (simplex and Powell's method, conjugate gradient methods and variable metric methods).
9. Ordinary differential equations: Initial value problems: Properties of numerical solution (local and global accuracy, convergence, stability, stiff systems). Properties of explicit and implicit schemes (Euler scheme). Runge-Kutta methods (of 2nd and 4th order, variants with adaptive stepping and for stiff systems). Extrapolation methods. Multistep methods. Boundary value problems: reduction to initial value problems, shooting methods, finite difference method, variational methods. Systems of differential and algebraic equations. Examples: Adams-Williamson equation, free oscillations of the Earth.
10. Partial differential equations: Discretization, difference schemes, properties, classification of methods. Finite difference method (difference equations, boundary conditions). Semi-discrete methods (method of lines, Rothe's method). Examples: Laplace equation, heat convection equation.

Literature:
F.S. Acton, Numerical Methods That Work, Mathematical Association of America, 1990.
U.M. Ascher, L.R. Petzold, Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, SIAM, 1998.
B. Fornberg, A Practical Guide to Pseudospectral Methods, Cambridge University Press, 1996.
M. Metcalf, J. Reid, Fortran 90/95 Explained, Oxford Science Publ., 1998.
S. Míka, Numerické metody algebry, SNTL, 1985.
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77: The Art of Scientific Computing, Second Edition, Cambridge University Press, 1996. (See also http://www.nr.com)
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing, Cambridge University Press, 1996. (See also http://www.nr.com)
V. Pretlová, J. Zahradník, Numerické metody v geofyzice I., II. (scriptum), SPN, 1978/1981.
P. Přikryl, Numerické metody matematické analýzy, SNTL, 1985.
K. Rektorys a spol., Přehled užité matematiky, Nakladatelství Prometheus, 1995.
K. Segeth, Numerický software I. (scriptum), Nakladatelství Univerzity Karlovy, 1998.
J. Segethová, Základy numerické matematiky (scriptum), Nakladatelství Univerzity Karlovy, 1998.
E. Vitásek, Numerické metody, SNTL, 1987.
V. Zahradník, Programování: Fortran 90 (scriptum), Vydavatelství ČVUT, 1996.
WWW.

PRF017 –Fortran programming
Ladislav Hanyk, KG

Annotation:
Course of programming in the Fortran language. Fortran norms 77, 90 a 95. Using compilers for Microsoft Windows, Linux and selected Unix systems. Good manners of Fortran programmers.

Syllabus:
1. Unix how-to: Users, groups, root, passwords. File system, types and properties of files, owners, rights. Processes, types and properties of processes, priority, process control. Standard shells. Basic Unix commands. Communication among users. NFS. X-Window System.
2. Introduction to Fortran: Why Fortran? History, norms and compilers of Fortran, literature on Fortran. Basic concepts. Characteristic features.
3. "FORmula TRANslation": Formatting source codes. Data types. Constants, variables, arrays, indeces. Expressions, operators, operands. Standard and statement functions. Rules for expression evaluation, priorities of operators. Cycles, statements, constructs.
4. Norm of FORTRAN 77: Type declaration, array declaration, definition of named constants, data initialization, memory sharing, retaining local variables. Assignments, goto statements, conditional statements, cycle statements, empty statement, stopping and pausing, return from a unit. Subroutines, functions, data subprograms. Actual and formal parameters.
5. Data "inside": Scoping units, global and local data. Data initialization. Passing arguments. Array storing, passing arrays between program units. Type compatibility, IEEE format. Storage sharing in practice.
6. Data "outside": Formatted and unformatted files. Sequential and direct files. Input/output statements. Format specification.
7. Text: Character data type, character substrings, character operators, standard functions for characters. Internal files.
8. Basics of Fortran 90: Free source form, syntax extensions (names, literals, operators). Type specification statements (syntax, properties and attributes of types, initialization, derived types). New statements and constructs (conditional and unbounded do, commands cycle and exit, branching construct case, named constructs). Fortran 95.
9. Arrays in Fortran 90: Actual arrays (fixed-size, allocatable and automatic arrays) and dummy arrays (assumed-shape, explicit-shape, implicit-shape nad implicit-size arrays). Indeces, index triplets, vector indeces. Conformable arrays, expressions with conformable arrays. Elemental functions, array-valued functions, logical masks, vector and matrix multiplication. Cycle with mask (where).
10. Notes on Fortran use: Compatibility of Fortran norms. Common language extensions. Obscolescent features. Optimizing compilers. Compiler configuration, metacommands. User interfaces, utilities and graphic libraries. Libraries of numerical methods. Fortran on Internet. Murphy's computer laws.

Literature:
L. Petrlík, Jemný úvod do systému Unix, Nakladatelství KOPP, 1995.
J. Hřebíček a kol., FORTRAN 77 a vědeckotechnické výpočty, Academia, 1989.
M. Metcalf, J. Reid, Fortran 90/95 Explained, Oxford Science Publ., 1998.
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77: The Art of Scientific Computing, Second Edition, Cambridge University Press, 1996. (See also http://www.nr.com)
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing, Cambridge University Press, 1996. (See also http://www.nr.com)
V. Zahradník, Programování: Fortran 90 (scriptum), Vydavatelství ČVUT, 1996.
User manuals (MS Fortran PowerStation, HP-UX Fortran).
WWW.

PRF018 – Computers in geophysical practice
Ladislav Hanyk, KG

Annotation:
Course of using computing facilities for students of geophysics. Understanding hardware, operating systems of Microsoft, Unix systems and computer networks. Introduction to the Fortran language and libraries of numerical routines. Software for visualization and typesetting.

Syllabus:
1. Understanding hardware: personal computers, Unix workstations, peripherials (printers, scanners, streamers, CD recorders, ZIP drives, modems).
2. Understanding operating systems: Unix (HP-UX, Linux) and MS Windows: basic concepts, commands, utilities (archiving and compressing, code page conversion).
3. Local area networks: shared disks and printers, access to shared resources, system and user communication (telnet, ssh, ftp, scp, NFS, system X-Window).
4. Computational software: compilers of Fortran 77, 90 and 95 for HP-UX, Linux and MS Windows, libraries of numerical methods (Numerical Recipes, IMSL, NAG, LAPACK, Internet sources). Optimizing compilers, compiler configuration.
5. Graphic and visualization software: data visualization in 1, 2 and 3 dimensions (Gnuplot, Grapher, Surfer, IDL, GMT, Amira).
6. Preparation of typographically valuable texts: TeX and LaTeX. Structuring source files. Selected keywords. Writing mathematical expressions. Import of graphics. Conversion to PDF and HTML.

Literature:
L. Petrlík, Jemný úvod do systému Unix, Nakladatelství KOPP, 1995.
Linux: Dokumentační projekt, Computer Press, 1998.
D. Gilly et al., UNIX in a Nutshell, O'Reilly & Assoc.,1994.
J. Hřebíček a kol., FORTRAN 77 a vědeckotechnické výpočty, Academia, 1989.
L. Lamport, LaTeX: A Document Preparation System, User's Guide and Reference Manual, Addison-Wesley Publ., 1994.
M. Metcalf, J. Reid, Fortran 90/95 Explained, Oxford Science Publ., 1998.
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77: The Art of Scientific Computing, Second Edition, Cambridge University Press, 1996. (See also http://www.nr.com)
J. Rybička: LaTeX pro začátečníky, Konvoj, 1995.
V. Zahradník, Programování: Fortran 90 (scriptum), Vydavatelství ČVUT, 1996.
User manuals (MS Fortran PowerStation, HP-UX Fortran, IDL).
WWW.

PRF039 – Fortran 90 and parallel programming
Ladislav Hanyk, KG

Annotation:
Course of programming in Fortran 90/95. Fortran features supporting data parallelism. Parallel algorithms. Compilers and numerical libraries for Microsoft Windows and Unix.

Syllabus:
1. Recapitulation of Fortran 77.
2. Basics of Fortran 90: Formatting source codes, syntactical elements, specification, statements, constructs; compatibility of Fortran norms, obscolescent features.
3. Arrays in Fortran 90: Actual arrays (fixed-size, allocatable and automatic arrays) and dummy arrays (assumed-shape, explicit-shape, implicit-shape nad implicit-size arrays). Indeces, index triplets, vector indeces. Conformable arrays, expressions with conformable arrays. Elemental functions, array-valued functions, logical masks, vector and matrix multiplication. Cycle with mask (where).
4. More on Fortran 90: modules, program unit interfaces, data sharing; internal subprograms; direct and indirect recursion; optional arguments; pointers and targets; new standard functions.
5. Fortran 95: more parallelization (forall construct, pure and elemental subprograms). Perspectives of Fortran standards.
6. Compilers of Fortran 90-95: MS PowerStation, Digital/Compaq, Fortran 90 for HP-UX, Absoft and Portland for Linux; compilers of supercomputers; optimalization levels, optimizing preprocessors, numerical libraries bundled with compilers.
7. Parallel programming: using standard Fortran 90, parallel versions of standard constructs; parallel versions of basic algorithms (linear recurrence, cyclic reduction, linear algebraic equations with tridiagonal matrices, FFT).

Literature:
M. Metcalf, J. Reid, Fortran 90/95 Explained, Oxford Science Publ., 1998.
W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing, Cambridge University Press, 1996. (See also http://www.nr.com)
V. Zahradník, Programování: Fortran 90 (scriptum), Vydavatelství ČVUT, 1996.
WWW.