

## Index

- alternating direction implicit methods (ADI),  
*see* transient PDEs
- beam deflection, 89
- Blasius boundary layer, solution of, 76–77
- block-tridiagonal matrix
  - in elliptic PDEs, 131
  - in implicit methods for PDEs in multidimensions, 120, 127
- boundary conditions
  - Dirichlet, 117, 121, 123, 130
  - homogeneous, 89, 121, 124, 167, 169
  - mixed, 130, 131
  - Neumann, 130, 131, 168
  - non-homogeneous, 168
  - periodic, 102, 172, 173
  - radiation, Sommerfeld, 150
- boundary value problems, numerical
  - solution of, 73–79
  - direct methods, 74, 77–79
  - discrete Fourier transform methods, 191
  - Gauss–Seidel method, 140–141
  - secant method for non-linear equations, 75, 77
  - shooting method, 73–77
    - for linear equations, 74–75
  - V-cycle multigrid based on Gauss–Seidel iteration, 144–145
- Burgers equation, 153
  - fractional step method, 128–129
  - solution using discrete Fourier transform, 177–178
  - two-dimensional, 149
- CFL number, *see* convection equation
- chaotic problems, 83–85
- characteristic equation, for obtaining eigenvalues, 200
- Chebyshev polynomials
  - advantages in approximating functions, 179
  - cosine transformation, 179
  - recurrence formula, 179
- Chebyshev transform, discrete, 178–189
  - coefficients, 180
  - `cosft1`, 181
  - for differentiation, *see* differentiation, numerical
  - for integration, *see* integration, numerical
  - orthogonality, 180
  - solving linear non-constant coefficient PDEs using, 189
- chemical reaction problems, 87
- complex geometry problems and transform methods, 132
- computational prototyping, 93
- condition number, of a matrix, 199
- convection equation
  - behavior of exact solution, 98
  - CFL number, 106
  - explicit Euler
    - numerical solution example, 100
    - stability (time-step selection), 99, 105
  - fourth-order Runge–Kutta
    - numerical solution example, 100
    - stability (time-step selection), 101, 106
  - insight into physical behavior, 98, 99
  - Lax–Wendroff scheme, 148

## 204 INDEX

- convection equation (*cont.*)
  - leapfrog, stability (time-step selection), 106, 147
  - second-order Runge–Kutta, stability (time-step selection), 105
  - semi-discretization, 97
  - solution by discrete Chebyshev transform, 189, 192
  - Sommerfeld radiation condition, 150
- convection–diffusion equation, solution using
  - discrete Fourier transform, 173–174
  - finite differences, 147–149, 151, 153
  - cosine transform, discrete, 165–166, 168, 179, 180
  - `cosft1`, 166, 184, 186
  - of product of two functions, 191
  - orthogonality property, 165, 180
- Crank–Nicolson method, *see* diffusion equation, one, two, & three space dimensions
- differentiation, finite difference approximations, 12
  - accuracy
  - order, definition of, 13
  - using modified wavenumber, 16–19
- boundary schemes, selection of, 14, 20
- construction using Taylor table, 14–16, 19–20, 22
- derivation from Taylor series, 12–14
- error
  - leading term, 13
  - truncation, 13–16
- first derivative, schemes for
  - backward difference, 13, 20
  - central difference, 13, 14, 17, 20
  - first order, 13
  - forward difference, 13, 15, 20
  - fourth order, 14, 20
  - Padé, 20
  - second order, 14, 15, 17
  - third order, 20
- modified wavenumber
  - as a measure of accuracy, 16–19
  - for various finite difference schemes, 18, 25, 26
- need for non-dimensionalization, 13
- on non-uniform grids, 22–24
  - adaptive techniques, 22
- boundary layers, 22
- coordinate transformation, 22
- Padé approximations, 19, 22, 25
- second derivative, schemes for
  - central difference, 14
  - fourth order, 22
  - Padé, 22
  - second order, 14
- differentiation, numerical
  - derivative matrix operator based on discrete Chebyshev transform, 192–193
  - discrete Fourier transform, 175–178
  - Lagrange polynomial, 10–11
  - using cubic splines, 8
  - using discrete Chebyshev transform, 182–185, 192–193
- using discrete Fourier transform, periodic functions, 170–171, 175–178
  - oddball wavenumber coefficient set to zero, 170, 175
- using finite differences, *see* differentiation, finite difference approximations
  - using Lagrange polynomial, 10–11
- diffusion equation, one space dimension
  - backward Euler method, 109–110
  - stability (time-step selection), 110
- Crank–Nicolson (trapezoidal) method, 108–109
  - numerical solution example, 110
  - stability (time-step selection), 109
- Du Fort–Frankel scheme, 108, 114, 116
  - accuracy via modified equation, 114
  - numerical solution example, 114
- explicit Euler
  - accuracy via modified equation, 111–113
  - numerical solution example, 96
  - stability (time-step selection), 97, 99, 105
- insight into physical behavior, 96, 99
- leapfrog, 113
  - stability (time-step selection), 105
- semi-discretization, 94
- diffusion equation, three space dimensions
  - Douglas Rachford ADI scheme, 147
  - explicit Euler, stability, 118
  - factored form of Crank–Nicolson scheme, 123
- diffusion equation, two space dimensions
  - alternating direction implicit method (ADI), 126–128

- equivalence to factored form of
  - Crank–Nicolson scheme, 127
- implementation of boundary conditions, 127
  - Crank–Nicolson scheme, 118–121
  - explicit Euler, 116–118
    - stability, 117
  - factored form of Crank–Nicolson scheme, 121–126
    - implementation of boundary conditions, 123
    - neglecting the cross terms, 122
    - numerical solution example, 124
    - stability, 125
  - locally one dimensional scheme (LOD), 129
    - steady state, 124, 138
- Du Fort–Frankel method, *see* diffusion equation, one space dimension
  
- eigenvalues and eigenvectors, 200–201
  - and convergence of iterative methods, 134, 136, 137, 139
- and decoupling of systems of ODEs, 47, 55, 96
- and matrix diagonalization, 47, 96, 134, 201
  - and stiff systems of ODEs, 70, 95
  - characteristic equation, 200
  - QR* algorithm, 200
  - spectral radius, 133
- elliptic PDEs, 129
  - boundary conditions for, 130
  - examples of, 130
  - numerical solution of, *see* partial differential equations
  - occurrence of, 129
- equilibrium problems, *see* elliptic PDEs
  
- finite difference approximations,
  - see* differentiation, finite difference approximations
- Fourier series (transform), discrete, 158–178
  - fast Fourier transform (FFT), 159, 175, 179
  - for differentiation, *see* differentiation, numerical
  - forward transform, 159
  - in higher dimensions, 162
  - inverse transform, 159
  
- of product of two functions, 163–164
  - aliasing error, 163
  - convolution sum, 163
- of real functions, 160
  - realft*, 161, 171, 173
  - orthogonality property, 159
  - solving linear constant coefficient PDEs using, 172–174
  - solving nonlinear PDEs using, 177–178
- Fourier series, continuous, 157
  
- Gauss elimination, 132, 136, 158, 167, 198
  - backward substitution, 198
  - forward sweep, 198
  - LU* decomposition, 136, 198, 200
  - operations counts, 200
  - pivoting, 199
  - round-off error, 198
  - scaling, 199
- Gauss quadrature, *see* integration
- Gauss–Seidel method, *see* iterative methods
- grid resolution, 17
  
- heat equation, *see* diffusion equation
- Helmholtz equation, 130
- Hermite polynomials
  - and Gauss quadrature, 40
  
- index notation, for discrete equations, 122, 123, 134
- initial value problems, numerical solution of, 43–73
  - accuracy vs. stability, 51
  - Adams–Bashforth method, 66–68, 129
  - amplification factor, 47, 52, 54, 61
  - amplitude error, 55, 56, 62, 64, 66, 68, 101
  - definition of, 52–53
  - error analysis, 51–53
- Euler method, 44, 47–49, 52, 55, 56, 61, 62, 65, 67–70, 97, 99, 100, 102, 105, 107, 111, 116, 117, 126, 127, 177, 189
- explicit methods, 45
- function evaluations, number of, 63–65
- implicit (backward) Euler method, 50–52, 54–56, 109, 110, 126, 127
- implicit methods, 45, 50, 51, 54, 56, 71
  - linearization for, 57–58, 72–73

- initial value problems (*cont.*)
  - leapfrog method, 65–66, 68, 105–107, 113, 128
  - model problem for stability and accuracy, 46
  - solution by various methods, 47, 50–52, 54, 61, 63, 65, 67
  - multi-step methods, 45, 65–68
  - spurious roots for, 66, 67
  - ODE solvers, 71
    - `lsode`, 71
    - `ode23s`, 71
    - `ODEPACK`, 71n
    - `stifbs`, 71
    - with adaptive time-step, 71
  - order of accuracy
    - from the amplification factor, 52
    - of various methods, 44, 59
  - phase error, 52–53, 55, 56, 62, 64, 68
  - predictor–corrector, 60
  - Runge–Kutta methods, 44, 59–65
    - fourth order, 62, 101, 105–107, 173
    - second order, 59, 105
    - third order, 108
  - stability analysis, 45–47
    - of various methods, 47–51, 54, 57, 61, 63, 66–67, 70
  - stability diagrams, 48, 63, 68, 101, 105, 174
  - system of ODEs, 69–73
    - Jacobian matrix, 73
    - linearization of implicit methods for, 72–73
    - model problem for, 69
    - stiff, 69–73, 87, 88, 94, 95, 108
  - Taylor series methods, 43, 44
  - trapezoidal method, 53–58, 72, 108–110, 118, 129
  - linearized, 58
  - integral equation
    - Fredholm, 41
    - Volterra, 41
  - integration, numerical, 27
    - adaptive quadrature, 34–37
    - error tolerance, 34, 36
    - `odeint`, 42
    - `quad8`, 42
    - error analysis, 28–31
    - function evaluations, number of, 34, 40–42
    - Gauss quadrature, 37–41, 180
    - `gauher`, 40
    - `gauleg`, 39
    - Gauss–Hermite quadrature, 40
    - Gauss–Legendre quadrature, 39, 186
    - weights, 39, 40
  - midpoint rule, 29–31
  - order of accuracy of the approximations, 29–31, 33, 35
  - rectangle rule, 29–31
  - Richardson extrapolation, 32–34, 36
  - Romberg integration, 32–34
    - error tolerance, 33
  - Simpson’s rule, 28, 31–33, 35, 37, 39, 186
  - trapezoidal rule, 27, 29–32, 34, 36, 37
    - with end-correction, 31
  - truncation error of the approximations, 30–32, 35, 36
  - using discrete Chebyshev transform, 185–186
  - interpolation, 1–11
    - applications of, 1
    - cubic spline, 4–8
      - end-conditions, 6–7
      - formula, 6
      - natural, 6
      - spline, 7
      - tension, 8
    - cubic spline vs. Lagrange polynomial, 7
  - Lagrange polynomial, 1–4
    - formula, 2
    - piecewise, 4, 10
    - `polint`, 8
    - uniqueness of, 2n
    - wandering problem for high order, 2–4
  - use of least squares, 1
  - iterative methods for linear algebraic systems, 132–146, *see also* Poisson equation
  - acceleration parameter, 137
  - convergence
    - acceleration, 136, 137, 139, 143
    - criterion, 133
    - spectral radius, 133
    - Gauss–Seidel, 135–136, 139–141, 144, 146
    - convergence, 136
  - multigrid acceleration, *see* multigrid acceleration for linear algebraic systems 93
  - point Jacobi, 133–135, 139
    - convergence, 134
  - pre-conditioning, 139

- successive over relaxation (SOR),  
136–139
- convergence, 137
- relaxation parameter, 137
- Jacobi method, *see* iterative methods
- kidney, three tube model problem, 88
- Lagrange polynomial, 1–4
  - and Gauss quadrature, 37
  - in differentiation, *see* differentiation, numerical
  - in interpolation, *see* interpolation
- Laplace equation, 130, 155
- Legendre polynomial
  - and Gauss quadrature, 38, 186
- linear algebra, review of, 195–201
- linear independence, 196
- LU* decomposition, *see* Gauss elimination
- MATLAB functions, 42, 71, 82, 84, 85, 87, 88
- matrix, 196–197
  - anti-symmetric, 100, 196
  - banded, 78, 94, 120, 129, 131, 177, 196, 200
  - block-tridiagonal, *see* block-tridiagonal matrix
  - condition number, 199
  - determinant, 197, 200
  - diagonalization, 47, 96, 99, 134, 201
  - identity, 196
  - ill-conditioned, 199
  - inverse, 196
  - LU* decomposition, *see* Gauss elimination
  - multiplication with a matrix, 196
    - operations counts, 199
  - multiplication with a vector, 196
    - operations counts, 199
  - norm, *see* norm 199
  - pentadiagonal, 78, 131, 197
  - power, 70, 201
  - similar matrices, 201
  - singular, 196, 197, 199, 200
  - skew-symmetric, 100, 196
  - sparse, 132
  - symmetric, 96, 135, 196, 201
  - transpose, 196
  - tridiagonal, *see* tridiagonal system (matrix)
  - modified wavenumber
    - for various finite difference schemes, *see* differentiation, finite difference approximations
    - in stability analysis, *see* stability analysis for transient PDEs
  - multigrid acceleration for linear algebraic systems, 139–146
    - algorithm, 143
    - full multigrid cycle (FMC), 143
    - key concept, 141
    - prolongation, 143, 144
    - residual, 139, 140
      - equation, 140
    - restriction, 143, 144
    - V cycle, 143, 144, 146
    - W cycle, 143
  - norm
    - matrix, 135, 199
    - vector, 135, 195, 199
  - Numerical Recipes* subroutines, 7, 8, 39, 40, 42, 71, 82, 85, 87, 88, 161, 166, 169, 171, 173, 181, 184, 186
  - operations counts, 199–200
    - for Gauss elimination, 200
    - for matrix operations, 199
  - operator notation, for discrete equations, 121, 127
  - ordinary differential equation (ODE),  
numerical solution of, 43
    - boundary value problems, *see* boundary value problems, numerical solution of
    - initial value problems, *see* initial value problems, numerical solution of
  - orthogonality
    - of polynomials, 40
  - partial differential equation (PDE),  
numerical solution of
  - equilibrium problems (elliptic PDEs)
    - discrete Fourier transform methods, 172–173
  - discrete sine transform combined with finite difference methods, 166–170

## 208 INDEX

- partial differential equation (PDE) (*cont.*)
  - finite difference methods, direct, 132
  - finite difference methods, iterative,
    - see* iterative methods
  - transient problems
    - discrete Chebyshev transform methods, 189, 192
    - discrete Fourier transform methods, 173–174, 177–178
    - finite difference methods, *see* transient PDEs, finite difference solutions
  - pendulum, 80
    - double, 81
  - pivot, 198, 199
- Poisson equation
  - discrete Fourier transform method, numerical solution example, 172
  - discrete sine transform method, 166–170
    - numerical solution example, 169
  - discretization, 130
    - implementation of boundary conditions, 131
  - Gauss–Seidel scheme, 136
    - eigenvalues and convergence, 136
    - numerical solution example, 138
  - multigrid, V cycle
    - numerical solution example, 146
  - point Jacobi scheme, 134
    - eigenvalues and accuracy, 135
    - eigenvalues and convergence, 134
    - numerical solution example, 138
  - successive over relaxation SOR scheme
    - eigenvalues and convergence, 137
    - numerical solution example, 138
- QR* algorithm, 200
- quadrature, *see* integration
- Richardson extrapolation, 32
  - in numerical differentiation, 42
  - in numerical integration, *see* integration
- secant method
  - in shooting method for boundary value problems, 75
- shear layer, compressible, 89
- shooting method, *see* boundary value problems
- sine transform, discrete, 166
- sinf*, 166, 169
- solving finite differenced Poisson equation using, 167–170
- SOR, *see* iterative methods
- spline, cubic, *see* interpolation
- stability analysis for ODEs, *see* initial value problems, numerical solution of
- stability analysis for transient PDEs
- matrix, 94–101
  - advantages, 101
- modified wavenumber, 103–109, 117, 118, 125
  - advantages, 103, 105
  - domain of applicability, 108
- von Neumann, 101–103, 105, 109, 125
  - domain of applicability, 103
- stencil, 14
- successive over relaxation scheme,
  - see* iterative methods
- system of linear algebraic equations, 198–199
  - condition number, 199
  - ill-conditioned, 1, 199
  - round-off error, 198–199
  - solution by Gauss elimination, *see* Gauss elimination
  - solution by iterations, *see* iterative methods
  - tridiagonal, *see* tridiagonal system (matrix)
- system of ODEs
  - decoupling, 47, 55, 96
  - numerical solution, *see* initial value problems 73
  - resulting from high-order ODEs, 43, 46, 55, 76, 80, 81, 89–91
  - resulting from semi-discretization of PDEs, 94, 98, 100
  - stiff, *see* system of ODEs *under* initial value problems
- transient PDEs, finite difference solutions, 93–129, *see also* diffusion, convection, convection–diffusion, & Burgers equations
  - accuracy via modified equation, 111–113
  - explicit methods, 97–108, 116–118, 173, 177, 189
  - implicit methods, 108–111, 118–120
    - alternating direction implicit (ADI) methods, 126–128

- factored (split) schemes, 120–126
  - fractional step methods, 128–129
  - in three space dimensions, 123, 147
  - in two space dimensions, 116–129
  - inconsistent scheme, 113–116
  - locally one dimensional (LOD) schemes, 129
- semi-discretization, 94
  - stability analysis (time-step selection),
    - see* stability analysis for transient PDEs
- trapezoidal
  - method for ODEs and PDEs, *see* initial value problems
  - rule for integration, *see* integration
- tridiagonal system (matrix), 94, 98, 197, 200
  - eigenvalues of, 95
  - in ADI schemes, 126
- in boundary value problems, 78
  - in cubic spline interpolation, 6, 8
  - in factored schemes, 122
  - in finite-differenced Poisson equation, 168
  - in implicit methods for PDEs, 108, 110
  - in Padé schemes, 20
- vector, 195–196
  - column, 195
  - inner (scalar) product, 195
  - norm, *see* norm
  - row, 195
- vortex dynamics problem, 84
- wave equation, *see* convection equation
  - wavenumber, 17, 140
  - modified, *see* modified wavenumber