

Index

a

Accuracy 41
 Adams–Bashforth–Moulton 184
 Advection 555–558
 Airy function 441
 Algorithm 35, 40
 Alias 285
 Amdahl's law 228
 Analog filter 294
 Animation 374, 375, 450, 453, 514, 515, 563
 Antiferromagnet 411
 Applet 204, 210, 211
 Architecture 122, 215, 216, 220, 226, 232,
 244, 249, 254, *see also* Memory
 Arithmetic unit 219, 223
 Asymptote 344
 Attractor 343–345, 374
 – predictable 368, 370
 – strange 370
 Autocorrelation function 290–294

b

Backtracking 121, 147
 Ballistic deposition 390, 390, 391, 395, 395,
 396
 – correlated 395, 396
 Bandwidth 229
 Base 41
 Basic machine language 34, 35
 Beating 189, 190
 Beowulf 226
 Bessel function 58, 59, 61, 597
 Bias 45
 Bifurcation 343–349, 351, 352, 374, 375, 377
 – diagram 345
 – dimension of 400
 Binary number 40
 Binary point 44
 Binning 347

Bisection algorithm 142–145, 195
 Bit 40, 41
 – reversal 301
 Blue Gene 244, *see also* IBM Blue Gene
 Boltzmann distribution 148, 412
 Boolean 43
 Bound state 141, 145, 193, 194, 200, 201,
 207, 429, 431–440, 456, 591, 592, 595, 596
 Boundary condition 175, 450, 461
 Box counting 392–395, 399
 Box-Muller method 113–116
 Break command 474
 Broadcasting 244, 252
 Buffer 216
 Burgers' equation 559–561
 Bus 226
 Butterfly operation 301
 Byte 41
 – code 35, 249

c

C language 35
 Cache 216, 262, 264
 – data 262, 263
 – misses 263, 264
 – programming 262, 264, 265
 Canonical ensemble 412, 446
 Capacitor 471–474
 Catenary 501–503
 Cauchy principal value 600
 Cellular automata 400–402
 Central
 – difference 87
 – processing unit 216, 219, *see also* CPU
 – storage 216, 217
 Chaos 349, 351, 363, 368–375
 – Fourier analysis of 377
 – of pendulum 363
 – phase space 368–374

- Chi-squared measure 160
 - CISC 220, 221
 - Column-major order 125, 216
 - Command-line interpreter 34
 - Communication 231
 - time 229
 - Compiler 35
 - just-in-time 249
 - Complex number 130, 284
 - Compression 307
 - lossless 311, 333
 - PCA 333
 - wavelets 307
 - Computational
 - physics 1
 - science 1–3
 - thinking 2
 - Computer language 33
 - Control structure 36
 - Convolution 292, 294
 - Conway's Game of Life 400
 - Correlation 291, 292, 395, 396
 - auto 290, 291
 - coefficient 162
 - growth 395
 - PCA 333
 - Courant stability condition 528, 531, 560, 561
 - Course grain parallel 225
 - Covariance 162, 335
 - CPU 215–223, 230, 243, 247, 249, 263
 - design 220
 - RISC 220
 - time 221
 - Crank–Nicolson method 484, 485, 487, 490
 - Cubic spline 153, 154, *see also* Spline
 - Cumulative distribution 115
 - Curie temperature 149, 409, 412
 - Curve fitting *see* Data fitting; Data fitting
 - Cycle time 221
- d**
- Data
 - cache *see* Cache
 - compression 307
 - dependency 224
 - fitting 141, 150, 151
 - parallel 224
 - shared 230
 - stream 225
 - type 41
 - Data parallelism 239
 - Deadlock 234
 - Decay
 - exponential 82, 156
 - simulation 82
 - spontaneous 156
 - Density of states 421
 - Dependency 224
 - Deposition 390
 - ballistic 391
 - correlated ballistic 395
 - Derivative 85–88, 90, 174
 - central difference 433, 452
 - forward difference 177
 - second 155, 176, 197, 452
 - DFT 281, 293
 - Differential equation 171, 193–214
 - algorithm 177
 - boundary condition 175
 - dynamical form 175
 - Euler's rule 177
 - initial condition 175
 - order 174, 175
 - partial 174, 461, *see also* PDE
 - Runge–Kutta algorithm 179
 - type 173, 461
 - Differential equations
 - type 461
 - Differentiation 85, 86
 - Diffusion-limited aggregation 396
 - Digital 41
 - Dimension
 - array 124
 - fractional 383–386, 392–394, 399
 - Hausdorff–Besicovitch 383, 384
 - physical 124
 - scheme 125
 - Discrete Fourier transform 281, 287, 293
 - Dispersion 448, 556, 562, 563, 568, 569
 - relation 556, 562
 - Distributed memory 226
 - Domain decomposition 239
 - Double 44
 - pendulum 375–377
 - precision 44, 49
 - Drag 208, 210, *see also* friction
 - DRAM 216
 - Driving force 190
 - Duffing oscillator 379
- e**
- Eigenvalue 123, 133, 135, 175, 193, 194, 197, 201, 290, 431, 511, 591
 - Electrostatic potential 463
 - Elliptic integral 365, 366

- Entropy 351
- Equation
 - Burgers' 559
 - differential 171, 193
 - discrete 81, 340
 - integral 591–593, 598, *see also* Integral
 - Korteweg–de Vries 563
 - motion 206, 209–211
 - Schrödinger 512
 - Van der Pool 379
- Ergodic 414
- Error 53–67, 88, 89
 - algorithmic 54, 62, 63, 96
 - approximation 54, 62, *see also* algorithmic
 - empirical 62, 100, 101
 - integration 96, 101
 - minimum 65
 - multiplicative 57
 - N-D integration 109
 - random 54
 - roundoff 51, 54, 57, 58, 62–65, 67, 71, 92, 96, 101, 106, 177, 178, 565
 - total 62, 63
 - type 54
- Euler's rule 177, 178, 180, 433, 435
- Exchange energy 410
- Executive
 - system 34
 - unit 216
- Exponential decay 80, 156
- Extinction 344
- Extrapolated difference 88

- f**
- Fast Fourier transform *see* FFT
- Feigenbaum constants 348
- Ferromagnet 411
- Fetch 222
- Feynman
 - path integrals 429–443
 - postulates 431
 - propagator 429
- FFT 284, 299–304
- Filters 294, 295
 - analog 294
 - digital 296, 327
 - sinc 297
 - windowed 296, 297
- Fine grain parallel 225, 226
- Finite
 - 2D element 547–554
 - difference 82, 467, 513, 580, 584
 - difference equation 82
 - difference time domain 525–533
 - element 537–554
- Fitting 150
 - best 151
 - global 160
 - goodness 160
 - least squares 158–160
 - linear 165
 - linear least square 160–167
 - local 160
 - Newton–Raphson 169
 - nonlinear 167
- Fixed points in maps 343, 368
- Fixed-point number 41
- Fixed-point numbers 42
- Float *see* Floating-point; Floating
- Floating-point number 41
- Floating-point numbers 42, 54
- FLOPS 186, 243
- Fluid Dynamics 555, 556, 558–560, 562–565, 575–590
- Fortran 35
 - vs Python 255
- Fourier
 - analysis 276
 - autocorrelation relation 293
 - chaos 377
 - decomposition 276
 - discrete transform 281, *see also* Discrete
 - fast transform *see* FFT
 - integral 275, 279, 280
 - PDE solution 464
 - sawtooth 279
 - series 275, 276, 279
 - short-time transform 311
 - theorem 277
 - transform 275, 279, 280
- Fractal 383–407
 - coastline 392
 - dimension 383, *see also* Dimension
 - plant 386, 387
 - Pollock painting 399
 - tree 389
- Friction 188, 189, 368, 372, 379, 576, 585
 - in oscillation 191
 - in oscillations 189
 - in waves 498–500
 - in pendulum 363–370
 - in projectile motion 208–210
- Functional integration 430–443

- g**
- Galerkin decomposition 540–543
- Game of Life 400

- Garbage 53
- Gaussian
 - distribution 113, 116
 - elimination 602
 - quadrature 92, 97, 98
 - – derivation 99
- Gibbs overshoot 279, 298
- Global array language 223
- Global optimization 219
- GPU *see* Graphical processing unit
- Granularity 225
- Graphical processing unit 266
 - programming 266–274
- Green's function 294, 429
- Grid point 99, 528, 561, 565, 596, 602
- Growth model 348, 353, 383–402
- Guest 230

- h*
- Half-wave function 278
- Hamilton's principle 429
- Hardware 215, 247–264
- Harmonics 276
- Heat bath 446
- Heat equation 477–490
- Hénon-Heiles potential 380
- High performance computing 221, 247, 264
- Hilbert transform 600
- HPC *see* High performance computing
- Huygens's principle 429
- Hyperbolic point 368

- i*
- IBM Blue Gene 243, 244
- IEEE floating-point 41–44
- Importance sampling 111
- Initial condition 175
- Input/Output (I/O) 37
- Instruction
 - stack 216
 - stream 225
- Integral equation 592–605
- Integration 85, 91–116
 - error 96, 101
 - from splines 155
 - Gaussian quadrature 97
 - mapping point 98
 - mean value 105
 - Monte Carlo 104–116
 - multi-dimensional 108
 - rejection techniques for 104
 - scaling 99
 - Simpson's rule 94–97
 - spline 155
 - trapezoid rule 92–97
 - variance reduction 110
 - von Neumann rejection 112
- Integro-differential equation 592
- Intermittency 344
- Interpolation
 - Lagrange 151–153
 - spline 154
- Interpreter 35
- Inverse matrix 123, 133, 134, 328
- Ising model 409–428
 - 2D 413, 420

- j*
- Jacobi method 469
- Jacobian matrix 121
- Just-in-time compiler 249

- k*
- Kernel 34, 429
- Korteweg–de Vries equation 563

- l*
- Lag time 291
- Lagrange interpolation 151–153
- Language
 - compiled 35
 - computer 33
 - high-level 34
 - interpreted 35
 - Python 8
- Languages
 - BASIC 35
 - compiled 35
- Laplace's equation 463–554, 583
- Latency 216, 229, 244
- Lattice computation 409, 432, 433, 440
- Lattice point *see* Grid point
- Lax–Wendroff algorithm 560, 561, 561
- Leap frog *see* Time stepping
- Least-squares fitting 159, 160
- Length of coastline 391
- Lifetime 156
- Limit cycle 368, 369
- Linear
 - algebra 122, 132, 162
 - congruent method 70
 - least square fitting 160
 - regression 160, 161
 - superposition 174
- Linux 34
- Lippmann–Schwinger equation 598

- Load 35
 - balancing 230
 - module 35
- Logistic map 339–348
- Loop unrolling 258, 262
- Lorenz attractor 379
- Lotka–Volterra model 354–362
- Lyapunov coefficients 349–351

- m**
- Machine
 - number 42, 54
 - precision 49
- Magnetic material 148, 409–428
- Mantissa 42
- Master and slave 234
- Matplotlib 17–26
- Matrix 117–139
 - column-major order 125
 - computing 124
 - diagonalization 124
 - equation 598
 - inversion 121, 123, 602–605
 - storage 216
 - subroutine library 134
 - tri-diagonal 487
- Maxwell’s Equations 525–533
- Mayavi 26–30
- Mean value theorem 105
- Memory 215, 216, 219, 247, 254
 - architecture 122, 216
 - conflict 228, 248
 - distributed 226
 - page 125
 - virtual 218, 219, 222
- Message passing 225–227, 231, 233, 234
- Metropolis algorithm 409, 413–416, 420, 432
- Microcanonical ensemble 412, 446
- Microcode 220
- Miller’s device 60
- MIMD 225–227, 231
- Mode locking 190, 369, 372
- Molecular dynamics 445–459
- Momentum space 591–605
- Monte Carlo
 - error in 109
 - integration 104–116
 - simulation 58, 69, 75, 104–116, 397, 409, 414, 436, 446, 449
 - technique 69, 80
- Multiple-core processor 221
- Multiresolution analysis 322
- Multitasking 219, 230, 232

- n**
- NAN 47
- Navier–Stokes equation 556, 576–583
- Newton–Cotes methods 92
- Newton–Raphson 119, 147
 - algorithm 145, 203
 - with backtracking 147
- Node 154, 225
- Noise 402
 - Perlin 403
 - reduction 290, 291, 298
- Nonlinear
 - dynamics 339–363
 - limit cycle 369
 - map 341, 348, 349
 - ODE 174
 - oscillation *see* Oscillation
- Nonlocal potentials 591, 592, 597, 598
- Nonstationary signal 307
- Normal
 - distribution 116
 - mode expansion 276, 277, 464, 493
 - number 44
- Number
 - binary 40
 - complex 130
 - fixed-point 41, 42
 - floating-point 41, 42
 - hexadecimal 41
 - IEEE 44
 - machine 42
 - normal 44
 - octal 41
 - range of 40
 - representation of 40
 - subnormal 44
 - uniform 73
- Numerov method 197, 197, 198
- NumPy 127–137
 - optimization 251
- Nyquist criterion 286
- Nyquist–Shannon interpolation 297

- o**
- Object
 - code 35
- Octal number 41
- ODE 171, 173–186, 197, 198
 - second order 206, 209
- ODExc
 - second order 209
- One cycle population 343
- Operand 216
- Operating system 34

- Optimization 61, 122, 186, 247–249, 255, 258, 262, 264
- Oscillation
 - anharmonic 172, 187, 276, 277
 - damped 189
 - double pendulum 376
 - driven 190
 - electromagnetic 526
 - Fourier analysis of 275
 - from error 151, 153, 298, 466
 - harmonic 186, 187, 276, 277
 - in phase space 368
 - isochronous 186, 187
 - nonlinear 171–214, 275
 - of pendulum 381
 - population 342, 360
 - quantum 431, 437
- Over relaxation *see* Relaxation
- Overdetermined 123
- Overflow 41, 42, 47, 48
- Overhead 229, 231, 250

- P**
- Padding of signal 286
- Page 125, 217
 - fault 219
- Parallel computing 215, 223, 236, 244
 - granularity 225
 - master, slave 234
 - message passing 231
 - perfect 232
 - performance 227
 - pipeline 232
 - programming 232
 - strategy 230
 - subroutines 226, 230
 - synchronous 232
 - type 224
- Partial differential equation 461, *see also* PDE
- Path integration 409, 429–443
- PDE 174, 461–463, 477, 491, 511, 525, 537, 578–590
 - elliptic 463
 - explicit solution 513
 - hyperbolic 491
 - implicit solution 513
 - nonlinear 563
 - parabolic 462, 477, 478
 - type 461
 - weak form of 539
- Pendulum 375, 377
 - analytic solution 364, 365
 - bifurcation diagram 374
 - chaotic 363, 372, 375
 - coupled 567
- Performance *see* Tuning
- Period doubling 343, *see also* Bifurcation
- Periodic boundary condition 450
- Perlin noise 402–407
- Phantom bit 44
- Phase space 355, 367–374, 377, 378, 567
- Phase transition 409
- Phase-space 368
- Pipelined CPU 219, 222
- Planetary motion 211–214
- Plot 13
 - surface 471
- Poisson's equation 463, 464, 467–469, 538
- Population dynamics 340–343, 345, 347, 348, 353–362
- Potential
 - delta shell 595
 - Lennard–Jones 446
 - momentum space 595
- Pov-Ray 404
- Power
 - PCA 333
 - residue method 70
 - spectrum 280, 292, 293, 378
- Precision 53
 - empirical 50
 - machine 49, 50
 - test 188
- Predator–prey model 353–362
- Predictor–corrector method 184
- Principal
 - components analysis 332–337
 - value 600
 - value integral 600
- Problem
 - by subject 4–8
 - solving paradigm 3
- Programming 35, 37
 - design 36
 - for virtual memory 219
 - parallel 232
 - reproducible 36
 - structured 36, 37
- Projectile motion 203, 208–210
- Propagator 434
- Protein folding 79
- Pseudocode 35, 37, 52
- Pseudorandom *see* Random numbers
- Pulsions 572
- Pyramid scheme 323

- Python
 - algebraic tools 31
 - arrays 126–134
 - Canopy 12
 - distribution 12
 - I/O 39
 - language 8
 - library 9–13
 - linear algebra 132
 - list 126
 - package 9–13
 - reference 8
 - virtual machine 249
 - Visual package 14
 - vs Fortran 255

- q**
- Quadrature 91
- Quantum 142
 - bouncer 441
 - mechanics 197
 - scattering 597

- r**
- Race condition 234
- Radioactive decay 80
- Radix 42
- RAM 125, 216, 217, 219, 248, 263, 264
- Random 69
 - generator 70, 113, 348
 - linear congruent 70
 - nonuniform 111, 114
 - number 63, 69–75, 348, 386
 - pseudo 70
 - self-avoiding walk 79
 - sequence 69, 70, 72
 - test 73–75
 - walk 75–79, 396, 397
- Ray tracing 404
- Recursion 58–61
- Register 49, 216, 264
 - working 49
- Rejection technique 104, 111, 113, 415
- Relaxation 469, 469, 470, 470, 474, 580–590
- Resonance 150, 167, 189, 190, 372
 - nonlinear 189
- Reynolds number 585
- RISC 220, 221, 244
- rkN 178–182, 185, 206
- Romberg extrapolation 103
- Root mean square 75–77, 459
- Roundoff errors 54
- Row-major order 125
- Runge–Kutta 178–182, 186

- s**
- Sampling 104, 281, 414
 - importance 111
- Sawtooth function 278
- Scalability 236–239
- Scattering 597, 604
- Schrödinger equation 197, 203, 512, 517, 591–605
 - time dependent 511
- Searching 141–148, 169, 195, 196, *see also*
 - Trial and error
- Section size 222
- Secular equation 123
- Seed 71
- Seeds 342, 344
- Self
 - affine connection 386, 387
 - affinity 389
 - limiting 379
 - similar 347, 385, 386
- Separatrix 188, 366, 567
- Serial computing 225, 228, 230, 231
- Series summation 51
- Shannon Entropy 351
- Shell 34
- Shock wave 555, 556, 559–563
- Sierpiński gasket 383–386, 402
- Sign bit 46, 47
- Signal processing 290
- Significant figure (part) 55
- SIMD 225
- Simpson's rule 94, 95
- Simulation 69
- Sinc filter 286, 296
- Sine-Gordon equation 570, 571
- Single precision 44, 49
- Singular integral 599
- SISD 225
- Slave 234
- SMP 221, 223
- Soliton 555–574
 - crossing 567
 - KdeV 564
 - ring 572
 - sine-Gordon 571
 - water wave 563
- Spline 154
 - cubic 153
 - natural 155
- Spontaneous decay 80–84, 156, 158, 159, 162, 340
- SRAM 216
- Stable state 344

- Statistical mechanics 412, 413, 445–449
 - Stochastic 80
 - Storage 222
 - Strange attractor 370
 - Stride 252, 263, 265
 - Subnormal number 44
 - Subroutine 35
 - library/package 122, 132–134
 - Subscript 125, *see also* Dimension
 - scheme 125
 - Subtask 230
 - Subtractive cancelation 55–57, 60, 66, 85, 86, 156, 162, 177, 186, 599
 - Successive over-relaxation *see* Relaxation
 - Supercomputer 215, 244
 - Swap space 216, 218, 219
 - Symmetric processor *see* SMP
- t**
- Task 224, 230, 231
 - Texture 402
 - Thermodynamics 409–428, 436, 446, 449
 - Three body problem 211
 - Time delay 207
 - Time stepping 477, 479–481, 491, 494–496, 513–515, 558, 560, 560, 561, 561
 - Top-down programming 38
 - Transient 190, 344, 347, 374, 375
 - Trapezoid rule 92–94
 - Trial and error 120, 121, 141–143, 159, 160, 167, 168, 175, 195, 196, 198–203, 414, 415, 436, 442, 474, 539
 - Trivial solution 123, 594
 - Tuning *see* Optimization
 - Two cycle 343
 - Two's complement 42, 49
- u**
- Uncertainty principle 309, 310
 - Underflow 42, 47, 48
 - Uniform
 - distribution 70, 72–75, 99, 115, 348
 - sequence 70, 73
 - sequences 70
 - test 73–75
 - weight 115
 - Unix 34
- v**
- Van der Pool equation 379
 - Variance 110, 161, 335
 - reduction 110, 414
 - Vector 132, 222, 475
 - field 525
 - Vector processor 222
 - Vectorization 252
 - Velocity-Verlet algorithm 452
 - Verlet algorithm 452
 - Virtual machine 249
 - Virtual memory 125, 217–219, 222, 248, 250, 251
 - Viscosity 576, 585
 - Visualization 13–30, 347
 - of vector 475
 - Volume rendering 13
 - von Neumann
 - rejection 111, 112, 415
 - stability assessment 456, 474, 481, 482, 484, 487, 490, 495–497, 528, 529
 - Vorticity 582–589
 - VPython 14–17
- w**
- Wang–Landau Sampling (WLS) 420–428
 - Wave
 - electromagnetic 491, 511, 525–533
 - equation 491–503
 - function 431, 437, 597, 604
 - on catenary 501–503
 - on string 491–503
 - packet 279, 280, 491, 511–518
 - shallow water 563
 - Wavelet 307–332
 - basis 313
 - continuous 316
 - Daubechies 327
 - discrete transform (DWT) 318, 330
 - multiresolution analysis 322, 323
 - pyramid scheme 323
 - transform 313
 - Weak form of PDE 539
 - Windows 34
 - Word length 41
 - Working set size 248