3CNF-SAT or 3SAT, solving in a cell, 184 3D (optical) memories branched photocycle (see sequential one-photon) comparison of bit density with other technology, 195 holographic, 203-204 multiplexing, techniques and necessity for, 211 simultaneous two-photon, 205 sequential one-photon, 205-208 erasure process, 207, 208 error analysis, 211 global erasure in prototype system, 209 reading process, 206, 207, 208 wavelengths used in data storage, 206 writing process, 206, 207-208 writing process in prototype system, 209 Acetylcholine sensor. See Biosensors, acetylcholine sensor Actuators, gel, triggered by Belousov-Zhabotinsky reaction, 72, 73 Adaptation in proteins, 8 Adaptation of system to physical dynamics (artificial evolution), 26 Adenine, binding of in a cleft, 41 Adenosine mono, di, and triphosphate (AMP, ADP, ATP) in molecular recognition, 41, 45-46, 51 ATP use in respiration process, 221-222 Aerial and satellite pictures, image processing of, 119 Alcohol sensor. See Biosensors, alcohol sensor Algorithmic complexity. See Complexity, algorithmic Allostery, 36 definition of, 44 Amino acid sensor. See Biosensor, amino acid sensor Ammonium ion (NH4⁻), 40, 41 effects of binding on pKa, 43 AND gates. See Wave gates, AND Anion recognition, 41–42 Antenna, in photoluminescence, examples of, 50 Antibiotic resistance, increased, 177 Antiport, in membrane transport, 49 Ant paradigm, 85-86 Architectures compressible, 1, 3-4, 5-6 general purpose, 4 new meaning in biological computers, 8 neuromolecular, 27-28 nonprogrammable, 3-4, 6-8 structurally programmable, 5 (see also compressible)

Arsenic-iodine reaction, used as a coupled reactiondiffusion system, 136 Associative memories, definition of, 203, See also Bacteriorhodopsin, holographic associative memories ATP. See Adenosine Autocatalysis. See Self-replication Bacteriorhodopsin associative memories (see holographic associative memories; 3D [optical] memories) comparison of size with present semiconductor elements, 193-194 energy storage use in Halobacterium salinarium, 191, 201 holographic associative memories, 203-204 (see also 3D [optical] memories) data searches, 203 entering images, 203 holographic properties, 201 photonic properties, 201–203 stability of different states of, 202-203 Behavior, complexity of. See Complexity, behavioral Belousov-Zhabotinsky reaction (system) color changes in, 115-116 history of discovery, 108 how a Belousov-Zhabotinsky reaction works, 68-69.109 pictures of temporal evolution in basic periodic process in, 110 black-and-white image processing in, 114 changes depending on different starting conditions, 111 enhancement of picture fragments in, 119 extraction of original image from low-quality data, example of, 121 half-tone pictures in, 117, 118 image processing mechanism in, 115, 116 labyrinths, 123, 127, 128, 129, 132 neural networks, similarity to processing in, 98 restoration of individual components in, 120 trigger waves in, 97, 108 trigger waves vs. circular waves, 97 wave-based logical circuit in, 74-75 as system of parallel processors, 66 Binding (vs. recognition), in catalytic cycles, 45 Biocomputers, definition of, 243 Bioelectronics. See also Molecular devices comparison with semiconductor electronics, advantages of, 192-193 control and power supply for bioelectronics, 101

Biomolecular systems and biomolecular computing basic principles of, 100-101 genetic engineering, used to improve materials, 212, 217 input of information into, 12-13, 100 output of results, 101 definition of, 92 Biosensors acetvlcholine sensor, 234 alcohol sensor, 230-231 based on microbial yeast, 241 amino acid sensor, 231 ATP sensor, 234 biochemical oxygen demand (BOD) sensor, 241 chemiluminescence-based, 234-235 enzyme-based, 229-235 fish-freshness sensor, 232-233 glucose sensor commercialization of, 227, 229 enzyme based, 229, 234 general structure of, 224-225 lifetime of, 255 reaction response, 225-226 history of, 226 immunosensor, 236-239 steric hindrance in, 237 QCM based, 236-237 using a surface plasmon resonance (SPR) device, 239 ISFET-based, 233-234 microbial sensors, 239-241 respiration-type, 240 alcohol sensor based on microbial yeast, 241 biochemical oxygen demand (BOD) sensor, 241 microfabrication of, 227, 229, 233-234 molecular recognition material in biosensor membrane, techniques of immobilization, 226-228 nucleic acid sensors, 231-232 adenosine, 231 guanine, 231 inosine, 231 xanthine, 231 saccharide sensors, 229-230 structure of, 226-227 thermistor-using sensor, 234 transducer definition of, 225 examples of, 226 tributylene sensor, 234 urea sensor, 232, 234 Bit of information storage vs. area required, trend in years, 195 Blocked cellular automata, 171-172

BOD sensor. See Biosensors, biochemical oxygen demand (BOD) sensor, 241 Boolean circuit, embedded, 73–76 Borromean rings, 172 Brain, organization of, 92 Branched photocycle memory architecture. See 3D (optical) memories, sequential one-photon Branching points, 129-130, 132 Breathers. See Collision-based computing. breathers in DNA molecules as example of Brownian motion. See Brownian search Brownian search, 7 Carbon, molecular properties pertinent to molecular computation, 6-7 Carrier-mediated transport across membrane, 46-49 Cascade systems, in molecular recognition, 44 Cassette mutagenesis, 212-213, 214 Catalysis ATP hydrolysis as example of, 45–46 in Belousov-Zhabotinsky reaction, 109 link with molecular recognition, 45-46 definition of, 45 (see also Cocatalysis) Cation, recognition of. See Spherical recognition Cell, biological, using for computation, 182-184 3CNF-SAT or 3SAT, solving, 184 encoding of variables into cell, and problems with, 184 flip-flop in E. coli, 183-184 Cells, definition of in reaction-diffusion system, 102 - 103Cellular automata definition of, 66 DNA, using blocks of as, 171-172 one-dimensional, 79-80 Characterization of types of nonlinear media according to excitation characteristics, 83 Chemical computing. See also Instance machines architecture-free, 65 structured, 65 Chemical network. See Continuous-flow stirredtank reactors Chemical processors. See also Instance machines, Reaction-diffusion systems, and Belousov-Zhabotinsky reaction architecturally free processors stirred, 65 nonstirred, 65-66 structured processors, 65 Chiral receptor, 42 Chiral discrimination, 42 example of in chemical system, 54 Cilia, artificial. See Actuators, gel

Classification of nonlinear media, 83-84. See also Complexity Cleft, in molecular recognition, 35 Cocatalysis, 46-47 Collision-based computing, 73-74, 76-82 breathers in DNA molecules as example of, 77-80 collision of breather with excited impurity, 78, 79 collision of breather with impurity, 77-79 collision of two breathers, 77, 78 dynamic circuits in, 76-82 mobile excitations in molecular arrays as example, 80 - 82quasiparticles in gas-discharge systems as example, 82 sources of, 76 Complementarity, kinds of, 35 Complexation, effects of in supramolecular systems, 43-44 Complexity algorithmic, 1-4 definition of, 93-94 behavioral definition of, 93 in biological systems, 95-96 of biological systems, estimates of levels of complexity within, 95-96 computational, definition of, 93, 94-95 dynamic (see behavioral) estimation of, numeric, 94-95 examples of in biological systems, 95-96 nonlinear, and link with high computational complexity, 98-99 sources of, 8 static (see Structural complexity) structural, definition of, 93 link with behavioral complexity, 96 Compression effect on adaptability, 5 of function, 3-5 Computational complexity. See Complexity, computational Computation universality, 73, 76 Computer, deterministic, definition of, 2 Context sensitivity, 6, 12 physiochemical, 12 Continuous-flow stirred-tank reactors, 108, 137-138 Contour enhancement. See Image processing in Belousov-Zhabotinsky reaction Control complexity. See Complexity, computational Cosystems, in molecular recognition, 44

Coupled reaction-diffusion systems. See also Belousov-Zhabotinsky systems chlorite-iodine reaction, used as a coupled reaction-diffusion system, 134-135 efficiency of recalling patterns in actual system, 138 finite-state machines, 135 Hopfield-type neural networks, implementing, 135 - 136recognition capabilities of, 133-138 Turing machine, implementing, 135 Crown ether, as example of effects of complexation, 43 Cryptate, 37, 43 CSTR. See Continuous-flow stirred-tank reactors Data encryption standard (DES). See DNA computation, algorithms Detecting bisector point between two points of a plane, 67 Deterministic computer, definition of, 2 Diffusion length, diffusion coefficient in reactiondiffusion systems, 103 Directed evolution, 216-217 Discrete Voronoi diagram, 67-68 DNA breather waves in, 77-80 excitons as equivalents of, 80-81 gates in. 77-80 using blocks of as cellular automata, 171-172 DNA computing, 244 advantages of, 157 algorithms and problems (see also Gene scrambling; RNA editing; Cell computation) 3SAT problem, 167 solving in a cell, 184 addition of two non-negative numbers, 168-171 Boolean circuit, finding all inputs, 163-165 Borromean rings for computation, 172 cellular automata in, 171-172 data encryption standard (DES), 175-176 dynamic programming problems, 176 generate-and-test algorithms, 163-167 graph connectivity problem, 176 Hamiltonian Path Problem, 153-156, 180, 181-182 Knight's problem, 166-167 matrix multiplication, 174-175 maximal clique problem, 165 programmed chain reactions (algorithms) 168-175 programmed mutagenesis, 172-173 sources of error (see sources of error) sticker representation, 165-166

DNA computing (cont.) time necessary, 156 whiplash PCR, 173-174 comparison with silicon, 167 sources of error, 177-180 DNA ligation, enhanced, 46, 47 DNA manipulation, 172-173 RNA editing being similar, 182 tools used and definitions, 158-161, 212-215 amplify, 161 anneal, 159 append, 161 cassette mutagenesis, 212-213, 214 cut, 159 destroy, 159 ligate, 159 mark, 161 melt, 159 merge, 160 mismatched primer mutagenesis, 213, 215 polymerase extension, 159 programmed mutagenesis, 172-173, 182 reverse chirality, 160, 174 separate by length, 160 separate by subsequence, 161 staggered extension process (StEP) 217 unmark, 161 Dynamic complexity. See Behavioral complexity Electron transport path in respiratory chain, 222 Endoreceptor, 35 Endorecognition, 37 Enzyme networks, 22, 23 Enzyme sensors. See Biosensors, enzyme-based Enzymes effects of medium on, 36 as examples of molecular recognition, 45 Error filter, self-assembly as example of, 52 Errors, in DNA computation, sources of, 177-180 Evolutionary adaptability, and structural programmability, 5-6 Evolvable hardware, and reaction diffusion materials, 84-85 Excitable medium, excitation waves, 64 characterization of different types of medium, 83-84 Exciton, definition in Scheibe aggregate, 80 analogies to DNA breather gates, 80-81 Exclusive-or. See XOR Exoreceptor, 35, 37-38 Fish-freshness sensor. See Biosensors, fish-freshness

sensor

FKN model, 113, 117 Flip-flop in E. coli, 183-184 Fluidics, 28 Fourier transform holographic (FTH) associative memory, 204. See also Bacteriorhodopsin, holographic associative memories Gene, using as inverter, 183 flip-flop, using genes to construct in E. coli, 183-184 Generate-and-test algorithms, in DNA computing, 158, 163-167 Gene scrambling, 181-182 Genetic engineering (DNA) explanation of, 212 mutations in, 212 Genetic engineering of proteins for device applications, 212-217 Grass-fire transformation, 68. See also Prairie-fire transformation Half-tone picture image processing. See Image processing in Belousov-Zhabotinsky systems Hamiltonian Path Problem (HPP), 153 Heat bath, as source of complexity, 7-8 Hebbian rule, 136-137 Helicates, 54-56 assembly as example of molecular programming, 56 Holographic associative memories using bacteriorhodopsin, 203-204 Homogeneous neural networks, equations describing, 99 Hybridization. See DNA manipulation, tools used and definitions, anneal Hydrogen bonding, in molecular recognition, 40 Image processing, simulated, of reaction-diffusion systems, 139-141 contour enhancement, 139-140 skeletonization, 139-140 Image processing in chemical light-sensitive media, history of, 112-113 Image processing in Belousov-Zhabotinsky systems alternation of negative and positive images, 110 in black-and-white images, 114–117 contour enhancement, 110, 118 disappearance of small features of the picture, 110 enhancement of picture fragments in, 118, 119 half-tone pictures, 117-121 overlapping components, 120 restoration of image with defects, 116, 120 satellite images, 119 skeletonization, 116

Image processing in nonstirred chemical processors, 65. See also Image processing in Belousov-Zhabotinsky systems Immunosensor. See Biosensors, immunosensor Instance machine, reaction-diffusion processor as example of, 101 Intramolecular cavity, 35 In vitro evolution, 157-158 comparison with in vivo, 182 (see also Directed evolution) In vivo evolution, 157. See also Cell, biological, using for computation Knight's problem, in DNA computing, 166-167 λ parameter, Langton, 84 Labyrinths branching points in, 129-130, 132 determination of pathway turning points, 131 finding shortest paths in, 121-133 Labyrinth path tracing effects of background uniformity on, 125-126 effects of branching points on wave propagation, 129-130.132 efficiency of algorithm, 131-133 examples of labyrinths with different complexity, 123 image storage of, 124-125 organizing the wave-spreading process, 125-126 procedure for finding shortest paths, 127, 130-133 Langmuir-Blodgett film (LB film) as self-assembling entity, 53, 198 used as rectifier, 242 Life, Conway's Game of, in connection with collision-based computing, 76 Light-induced phase waves, produced by nonuniform background, 126 Linear recognition of molecules, 42-43 Lock-and-key, 7, 35 Logical gates, constructed using reaction-diffusion materials, 74-76 McCulloch and Pitts neuron, 91, 136 Macrobicyclic structures, 37, 39, 41, 42 Macro-micro interface, 10-12. See also Micromacro interface Macrotricyclic structures, 37, 40 Macrocyclic/macropolycyclic structures, definition of. 37 Maximal clique problem, using DNA computing, 165

Medium, effects on molecular recognition, 36

Membrane transport. See Carrier-mediated transport

Micelles, as self-organizing entities, 52-53 Microbial sensors. See Biosensors, microbial sensors Mitochondria, role in respiration and ATP generation, 222-223 Micro-macro interface, 101. See also Macro-micro interface Molecular computers, definition of, xii Molecular devices, 241-243 maximum frequency of operation, 196 Molecular electronics. See also Molecular devices estimate of reliability, 199-200 Molecular gates, 242 switching speeds, 196-197 Molecular memories, comparison with other information storage devices, 195, 197 Molecular recognition, definition of, xv, 32 Molecular systems, self-organization of as example of molecular computation, 56-58 Molecular switch, 242 Moore's law, 191 Multiple recognition, in molecular recognition, 44 Mutations vs. compressibility of algorithm, 5 NAG (N-acetylglucosamine), in linear recognition, 43 Negative image enhancement, 119 Negative (molecular) recognition, 35 Neural networks. See also Belousov-Zhabotinsky system chemically implemented, example of, 136-138 with lateral connections, 103-104 shunting on-center off-surround feedback networks, analogy with reaction-diffusion systems, 106 with sigmoidal feedback, signal processing of, 104 - 105Neutral molecules, in molecular recognition, 40-41 Nonlinear chemical medium, in reaction-diffusion system, 64. See also Belousov-Zhabotinsky system Nonstirred reagent layer, 66 NP-complete. See Hamiltonian Path Problem; Maximal clique problem One-dimensional breather machines. See Cellular automata, one-dimensional; DNA, breather waves in Optical memories. See 3D (optical) memories Organic synthesis used in nanoscale engineering, 197 - 198

Quantum effects in molecular devices, 196-197 effects on reliability, 199-200

Palladium processor, as example of chemical computer doing image processing, 68-69 logical gates implemented with, 75-76 Particle guns, 81 PCR. See Polymerase chain reaction Percolation thresholds, using reaction-diffusion to investigate, 141 Phase waves, velocity of, 125 Photonic molecular devices, 49-51 Plane subdivision, using chemical processor for, 67 - 68Pocket, in molecular recognition, 35 Polymerase chain reaction (PCR), 160, 161, 162 sources of error in, 178 used in construction of site-specific mutations, 212-213 Polymer matrices use of in encapsulating enzymes in biosensors, 228 - 229use of in reaction-diffusion systems, 142-144 Positive image enhancement, 119 Positive (molecular) recognition, 35 Prairie fire transformation, 111. See also Grass-fire transformation Problem size, xiv, 94–95 Programmed chain reaction, 168-171 Programmed mutagenesis. See DNA computing, algorithms Reaction-diffusion processors cells of, as primitive processors, 102-103 definition of, 64 Reaction-diffusion paradigm, as possible explanation of human behavior, 85-87 as example of non-von Neumann system, 92 Reaction-diffusion systems. See also Belousov-Zhabotinsky reaction arsenic-iodide system, 136 chlorite-iodine system, 134-138 equivalence to neural networks, 104, 106, 107 human brain, analogy with, 147–148 simulations of, 138-141 Receptor, definition of, 34 Reliability of molecular electronics, estimation of, 199 - 201Respiration process, energy liberation in, 221–222 River quality monitoring using microbial sensors, 241 RNA editing, in cells, 181–182 Robots, reaction-diffusion system used as unconventional controller for, 70-72 artificial cilia, 72-73 coupling with nonstandard actuators, 71-72 light-seeking, explanation of using diffusion waves as controller for, 71

Saccharide sensors. See Biosensors, saccharide sensors Satellite pictures, image processing of, 119 Scheibe aggregates, 80 Scroll waves, 145 Segmentation of image, 116 Self-assembly, 52-56 of self-sorting helicates, 54-55 Self-organization, in molecular systems, 52 Self-replication in molecular systems, 58 Sequential one-photon memory. See 3D (optical) memories, sequential one-photon Shortest path in a labyrinth, using Belousov-Zhabotinsky reaction to determine, 121-133 Signal amplification, in chiral system, 54 Simulations, of reaction-diffusion systems, 85-87, 138 - 141Simultaneous two-photon memory. See 3D (optical) memories, simultaneous two photon Single-molecular bit, possibility of, 200-201 Skeletonization of image using chemical computers, 68-70, 116 Spherical recognition, molecular, 38-39 size discrimination in, 38 Spiral waves, 145 Spots on the skin of a cat, image restoration of, 120-121 Staggered extension process (StEP) in DNA manipulation, 217 Static results from a Belousov-Zhabotinsky reaction, using precipitate in skeletonizing, 69 Stationary circuit, examples of chemical-based logical gates kinetic, 74 waves in excitable media, 75 Stirred-tank reactors. See Continuous-flow stirred tank reactors Structural complexity. See Complexity, structural Substrate, definition of, 34 Symport, in membrane transport, 49 Tetrahedral recognition, molecular, 40 Thermodynamics, and molecular computation, 56-58 Thermodynamic limits on computation, xiv Three-dimensional memory. See 3D (optical) memories Time, needed in carrying out DNA computing, 156 Time, needed to carry wave through labyrinth, 128 Trade-off principle, xiii-xv, 4-5, 146-147 Tree graphs, tracing paths in, 122, 123, 127-128 Trigger waves in reaction-diffusion systems, velocity of, 125

Urea sensor. See Biosensors, urea sensor

Index

Valinomycin, as example of macrocycle, 38, 39
Very long range energy transfer (VLRET), 50 in Scheibe aggregates, 80
Von Neumann versus non-von Neumann computing, 91–93
Voronoi cell, definition of, 67
Voronoi diagram, 85, 86 calculation of using chemical computers, 67–68 pictures of, 69, 70
Wave gates, examples of, 75–76 AND gates, 75 XOR gates, 75

Whiplash PCR. See DNA computing, algorithms and problems, whiplash PCR

XOR, implementation in chemical computing systems, 14–18, 75–76