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(Theory); 3.1.1 Model for Disaster: Subtractive Cancellation; 3.1.2 Subtractive Cancellation Exercises; 3.1.3 Round-off Errors; 3.1.4 Round-off Error Accumulation; 3.2 Error in Bessel Functions (Problem); 3.2.1 Numerical Recursion (Method); 3.2.2 Implementation and Assessment: Recursion Relations; 3.3 Experimental Error Investigation; 3.3.1 Error Assessment; 4 Monte Carlo: Randomness, Walks, and Decays; 4.1 Deterministic Randomness; 4.2 Random Sequences (Theory); 4.2.1 Random-Number Generation (Algorithm)
4.2.2 Implementation: Random Sequences 4.2.3 Assessing Randomness and Uniformity; 4.3 Random Walks (Problem); 4.3.1 Random-Walk Simulation; 4.3.2 Implementation: Random Walk; 4.4 Extension: Protein Folding and Self-Avoiding Random Walks; 4.5 Spontaneous Decay (Problem); 4.5.1 Discrete Decay (Model); 4.5.2 Continuous Decay (Model); 4.5.3 Decay Simulation with Geiger Counter Sound; 4.6 Decay Implementation and Visualization; 5 Differentiation and Integration; 5.1 Differentiation; 5.2 Forward Difference (Algorithm); 5.3 Central Difference (Algorithm); 5.4 Extrapolated Difference (Algorithm)
5.5 Error Assessment 5.6 Second Derivatives (Problem); 5.6.1 Second-Derivative Assessment; 5.7 Integration; 5.8 Quadrature as Box Counting (Math); 5.9 Algorithm: Trapezoid Rule; 5.10 Algorithm: Simpson's Rule; 5.11 Integration Error (Assessment); 5.12 Algorithm: Gaussian Quadrature; 5.12.1 Mapping Integration Points; 5.12.2 Gaussian Points Derivation; 5.12.3 Integration Error Assessment; 5.13 Higher Order Rules (Algorithm); 5.14 Monte Carlo Integration by Stone Throwing (Problem); 5.14.1 Stone Throwing Implementation; 5.15 Mean Value Integration (Theory and Math); 5.16 Integration Exercises
5.17 Multidimensional Monte Carlo Integration (Problem)

Sommario/riassunto

The use of computation and simulation has become an essential part of the scientific process. Being able to transform a theory into an algorithm requires significant theoretical insight, detailed physical and mathematical understanding, and a working level of competency in programming. This upper-division text provides an unusually broad survey of the topics of modern computational physics from a multidisciplinary, computational science point of view. Its philosophy is rooted in learning by doing (assisted by many model programs), with new scientific materials as well as with the Python program