

Computational Modelling in Physics, Chemistry and Biochemistry



Molecular Modelling

Unit 3. Classic Model

Juan Torres, Univ. Politècnica Catalunya (2015)

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programs play with them and observe what happens Suitable data are generated for each example in short routines this ensuring a clear understanding of the data structure Chapter 2 includes a brief introduction to matrix algebra and its implementation in Matlab and Excel while Chapter 3 covers the theory required for the modelling of chemical processes This is followed by an introduction to linear and non linear least squares fitting each demonstrated with typical applications Finally Chapter 5 comprises a collection of several methods for model free data analyses Includes a solid introduction to the simulation of equilibrium processes and the simulation of complex kinetic processes Provides examples of routines that are easily adapted to the processes investigated by the reader Model based analysis linear and non linear regression and model free analysis are covered

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