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Extended Abstract

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# A biophysics problem: Computational difficulties and their solution

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In physics, different theories based on mathematical models provide very precise predictions on how systems behave. Unfortunately, it is often the case that solving the mathematical model for a particular system in order to produce a useful prediction is not feasible. This can occur, for instance, when the solution does not have a closed-form expression, or is too complicated. In such cases, numerical approximations are required. Computational physics is the subject that deals with these numerical approximations: the approximation of the solution is written as a finite (and typically large) number of simple mathematical operations (algorithm), and a computer is used to perform these operations and compute an approximated solution and respective error. Computational physics problems are in general very difficult to solve exactly. This is due to several (mathematical) reasons: lack of algebraic and/or analytic solubility, complexity, and chaos. For example, - even apparently simple problems, such as calculating the wavefunction of an electron orbiting an atom in a strong electric field (Stark effect), may require great effort to formulate a practical algorithm (if one can be found); other cruder or brute-force techniques, such as graphical methods or root finding, may be required. On the more advanced side, mathematical perturbation theory is also sometimes used (a working is shown for this particular example here).
In addition, the computational cost and computational complexity for many-body problems (and their classical counterparts) tend to grow quickly. Computational mechanics consists of computational fluid dynamics (CFD), computational solid mechanics and computational contact mechanics. One subfield at the confluence between CFD and electromagnetic modelling is computational magnetohydrodynamics. The quantum many-body problem leads naturally to the large and rapidly growing field of computational chemistry. Computational solid state physics is a very important division of computational physics dealing directly with material science. A field related to computational condensed matter is computational statistical mechanics, which deals with the simulation of models and theories (such as percolation and spin models) that are difficult to solve otherwise. Computational statistical physics makes heavy use of Monte Carlo-like methods. More broadly, (particularly through the use of agent based modeling and cellular automata) it also concerns itself with (and finds application in, through the use of its techniques) in the social sciences, network theory, and mathematical models for the propagation of disease (most notably, the SIR Model) and the spread of forest fires.
Finally, many physical systems are inherently nonlinear at best, and at worst chaotic: this means it can be difficult to ensure any numerical errors do not grow to the point of rendering the 'solution' useless. Computational biophysics are at the forefront of developing and using theoretical approaches to extend our understanding of biological processes associated with protein and nucleic acid structure, folding, misfolding and assembly, drug discovery and design and cellular processing.
The problem is in the field of controlled drug release. These authors investigate the time evolution of a spherical liposome with a semipermeable coat and containing a solution of some pharmaceutical drug, when this is immersed into a bay of a solvent. Due to the osmosis, the liposome is swelling from the initial radius R0 up to a critical value Rcat which the surrounding membrane becomes sostressed that a pore of radius rc is produced on its surface. A second stage then begins where some part of the drug content Q is released through the pore and thus the liposome is relaxed until reaching the original radius. A new cycle of the same type can begin with the only difference that now the input Q is smaller than before, and this is repeated as many times as Q is sufficient for ensuring a swelling up to Rc. As mentioned in the quoted paper, the two-stage cycle is mathematically characterized by a differential equation for R (swelling) and a system of three such equations for R, r and Q (relaxation). The numerical solution of the latter rises difficulties because this is stiff and then it asks for a high stability method. The Runge-Kutta methods are of two types, explicit and implicit. The explicit methods are easy to use but with low stability properties while vice versa holds true for the implicit methods. A method which brings the qualities of the two under the same umbrella is presented. It is of a special type in the sense that its coefficients are equation dependent, not constant, as in the standard literature on RungeKutta methods. The method is applied on the considered problem and the results confirm that the osmosis-based mechanism deserves indeed serious attention in the area of controlled drug release.

***Bottom Note:*** *This work is partly presented at 4th International Conference on Physics September 17-18, 2018, Berlin, Germany*