

Synoptic Overview on Computational Physics and its Applications

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Commentary

Received: 10-May-2022

Manuscript No. JPAP-22-65862; **Editor assigned:** 16-May-2022, Pre QC No. JPAP-22-65862(PQ); **Reviewed:** 30-May-2022, QC No. JPAP-22-65862; **Revised:** 06-June-2022, Manuscript No. JPAP-22-65862(A) **Published:** 13-June-2022,
DOI:10.4172/2320-2459.10.4.003.

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ABOUT THE STUDY

Computational physics is the study and application of numerical analysis to solve physics problems that already have a quantitative theory. Computational physics was historically the first application of modern computers in science, and it is now a subset of computational science. It is sometimes considered a sub discipline (or offshoot) of theoretical physics, but others regard it as an intermediate branch between theoretical and experimental physics—a field of study that supplements both theory and experiment. Different theories in physics based on mathematical models provide very precise predictions about how systems behave. Unfortunately, solving the mathematical model for a specific system in order to produce a useful prediction is not always possible. This can happen when the solution lacks a closed-form expression or is overly complicated. Numerical approximations are required in such cases. The subject that deals with these numerical approximations is computational physics: 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.

There is some disagreement about the place of computation within the scientific method. Some consider computer simulation to be more akin to theoretical physics; others consider it to be “computer experiments”, while still others consider it an intermediate or different branch between theoretical and experimental physics, a third way that supplements theory and experiment. While computers can be used in experiments to measure and record (and store) data, this is clearly not a computational approach. Computational physics problems are notoriously difficult to

solve precisely. This is due to a number of (mathematical) factors, including a lack of algebraic and/or analytic solvability, complexity, and chaos. For example, calculating the wave function of an electron orbiting an atom in a strong electric field (Stark effect) may require significant 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 advanced side, mathematical perturbation theory is occasionally used (a working is shown for this particular example here). Furthermore, the computational cost and complexity of many-body problems (and their classical counterparts) tend to increase rapidly. It is somewhat of a problem because a macroscopic system typically has constituent particles of the order of 10^3 in size. In general, solving quantum mechanical problems is of exponential order in terms of system size and for classical N-body problems; it is of N-squared order. Finally, many physical systems are inherently nonlinear at best and chaotic at worst: this makes it difficult to ensure that any numerical errors do not grow to the point where the 'solution' is rendered useless.

Applications

Computational physics is an essential component of modern research in a variety of fields, including accelerator physics, astrophysics, general theory of relativity (*via* numerical relativity), fluid mechanics (computational fluid dynamics), lattice field theory/lattice gauge theory (particularly lattice quantum chromo dynamics), plasma physics (see plasma modeling), and simulating physical systems (*via* molecular dynamics).

Computational solid state physics, for example, uses density functional theory to calculate solid properties, similar to how chemists study molecules. This and several other methods, including the Luttinger-Kohn/k.p method and ab-initio methods, can calculate other quantities of interest in solid state physics, such as the electronic band structure, magnetic properties, and charge densities.