

Computational Physics

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Editorial Note

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EDITORIAL NOTE

Computational physics is that the study and implementation of numerical analysis to unravel problems in physics that a quantitative theory already exists. Historically, computational physics was the primary application of recent computers in science, and is now a subset of computational science.

It is sometimes considered a sub discipline (or offshoot) of theoretical physics, but others consider it an intermediate branch between theoretical and experimental physics—a neighbourhood of study which supplements both theory and experiment.

Computational physics problems are generally very difficult to unravel exactly. This is often thanks to several (mathematical) reasons: lack of algebraic and/or analytic solvability, complexity, and chaos.

For example, even apparently simple problems, like calculating the wave function of an electron orbiting an atom during a strong field (Stark effect), may require great effort to formulate a practical algorithm (if one are often found); other cruder or brute-force techniques, like graphical methods or root finding, could also be required. On the more advanced side, mathematical perturbation theory is additionally 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. A macroscopic system typically features a size of the order of constituent particles, so it's somewhat of a drag. Solving quantum mechanical problems is usually of exponential order within the size of the system and for classical N-body it's of order N-squared.

Finally, many physical systems are inherently nonlinear at the best and at the worst chaotic: this suggests it is often difficult to make sure any numerical errors don't grow to the purpose of rendering the 'solution' useless.

Due to the broad class of problems computational physics deals, it's an important component of recent research in several areas of physics, namely: accelerator physics, astrophysics, hydraulics (computational fluid dynamics), lattice field theory/lattice gauge theory (especially lattice quantum chromo dynamics), physics (see plasma modelling), simulating physical systems (using e.g. molecular dynamics), engineering computer codes, protein structure prediction, weather prediction, solid state physics, soft condensed matter physics, hypervelocity impact physics etc.

Computational solid state physics, for instance, uses density functional theory to calculate properties of solids, a way almost like that employed by chemists to review molecules. Other quantities of interest in solid state physics, like the electronic band structure, magnetic properties and charge densities are often calculated by this and a number of other methods, including the Luttinger-Kohn/k.p method and ab-initio methods.

It is possible to seek out a corresponding computational branch for each major field in physics, for instance computational mechanics and computational electrodynamics. 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 magneto hydrodynamics. The quantum many-body problem leads naturally to the massive and rapidly growing field of computational chemistry.