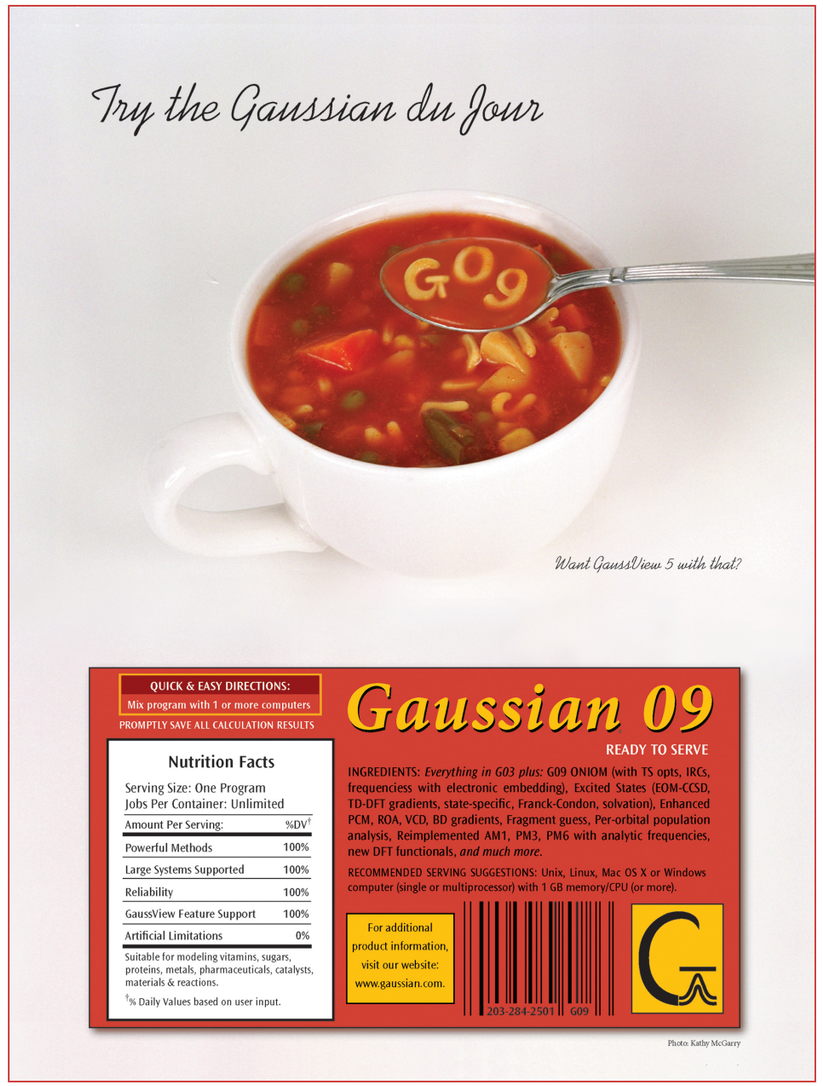
Computational Chemistry

The theoretical basis of quantum chemistry was developed throughout the early 20th Century. Yet it was not until the use of programmable computers became widespread in the latter half of the century that most chemists had access to sophisticated computational tools. Software was developed that simplified the calculation processes and made them accessible to non-specialist researchers. Historically notable is the software package *Gaussian*, first released in 1970 and still in use today.

Chemistry is often viewed as a subject rooted in the practical: a 1957 A-level syllabus states that "the study of chemistry should be based on experiment". Is this still true today?



Above: A 2009 print advert for Gaussian 09.