NUMERICAL ANALYSIS OF COMPLEX PHENOMENA: FROM COMPUTATIONAL FLUID DYNAMICS TO COMPUTATIONAL CHEMISTRY

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Differential equations serve as powerful tools for modeling various natural phenomena, with diffusion-reaction models standing out as a versatile class within the realm of Science. While analytical solutions for these models are sporadically attainable, reliance on numerical schemes becomes essential. This presentation delves into two specific models, one arising in computational fluid dynamics (CFD) and the other in computational chemistry (CC).

One of the fundamental equations of CFD is the steady-state convection diffusion reaction equation, which is used to model the concentration of species. It can be shown that the analytical solution of such equations under appropriate assumptions satisfies the maximum principles. We want the numerical schemes to satisfy the discrete counterpart, the discrete maximum principle. Failure to do so allows the numerical solution to have layers on the boundary and the interior. Layers are narrow regions where the solution has a steep gradient. Standard numerical techniques fail to capture this property, so we have a presence over and undershoots near the layers. A solution to this problem is the use of so-called stabilization techniques. The talk's first part will examine the nonlinear stabilization techniques known as the Algebraic Flux Correction [1]. We will concentrate on the a posteriori error estimators and their interplay on grids with hanging nodes [2, 3].

The second part of the talk will deal with implicit solvation models arising in CC. Most chemical processes and virtually all biochemical processes happen in a condensed phase, where the reacting part, or generally the studied part, is embedded in an environment that usually consists of a solvent. Implicit solvation models treat the solvent as a continuum described only by a few macroscopic properties. They are computationally efficient, require fewer parameters, and are widely used in practice. In this talk, we will concentrate on the nonlinear Poisson-Boltzmann (PB) equation which is used to model the electrostatic potential. Another important aspect while modeling implicit models is the choice of the solute-solvent boundary. This talk will examine the recently proposed domain decomposition for the PB equation defined on the solvent-excluded surface (SES), [4].

References

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