Numerical stabilization for multidimensional coupled convection-diffusion-reaction equations

Applications to continuum dislocation transport

PROEFSCHRIFT

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A mis padres Mónico y María Elena
A mis hermanas Ana y Carmen

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Abstract

Partial differential equations having diffusive, convective and reactive terms appear naturally in the modeling of a large variety of processes of practical interest in several branches of science such as biology, chemistry, economics, physics, physiology and materials science. Moreover, in some instances several species or components interact with each other requiring to solve strongly coupled systems of convection-diffusion-reaction equations. Of special interest for us is the numerical treatment of the advection dominated continuum dislocation transport equations used to describe the plastic behavior of crystalline materials.

Analytical solutions for such equations are extremely scarce and practically limited to linear equations with homogeneous coefficients and simple initial and boundary conditions. Therefore, resorting to numerical approximations is the most affordable and often the only viable strategy to deal with such models. However, when classical numerical methods are used to approximate the solutions of such equations, even in the simplest one dimensional case in the steady state regime for a single equation, instabilities in the form of node to node spurious oscillations are found when the convective or reactive terms dominate over the diffusive term.

To address such issues, stabilization techniques have been developed over the years in order to handle such transport equations by numerical means, overcoming the stability difficulties. However, such stabilization techniques are most often suited for particular problems. Additionally, no extensive work has been carried out for systems of coupled equations. The reason for this immaturity is the lack of a maximum principle when going from a single transport equation towards systems of coupled equations.

The main aim of this work is to present a stabilization technique for systems of coupled multidimensional convection-diffusion-reaction equations based on coefficient perturbations. These perturbations are optimally chosen in such a way that certain compatibility conditions analogous to a maximum principle are satisfied. Once the computed perturbations are injected in the classical Bubnov-Galerkin finite element method, they provide smooth and stable numerical approximations.

Such a stabilization technique is first developed for the single one-dimensional convection-diffusion-reaction equation. Rigorous proof of its effectiveness in rendering unconditionally stable numerical approximations with respect to the space discretization is provided for the convection-diffusion case via the fulfillment of the discrete maximum principle. It is also demonstrated and confirmed by numerical assessments that the stabilized solution is consistent with the discretized partial differential equation, since it converges to the classical Bubnov-Galerkin solution if the mesh Péclet number is small enough. The corresponding proofs for the diffusion-reaction and the general convection-diffusion-reaction cases can be obtained in a similar manner. Furthermore, it is demonstrated that this stabilization technique is applicable irrespective of whether the advective or the divergence form is used for the spatial discretization, making it highly flexible and general. Subsequently the stabilization technique is extended to the one-dimensional multiple equations case by using the superposition principle, a well-known strategy used when solving non-homogeneous second order ordinary differential equations. Finally, the stabilization technique is applied to mutually perpendicular spatial dimensions in order to deal with multidimensional problems.

Applications to several prototypical linear coupled systems of partial differential equations, of interest in several scientific disciplines, are presented. Subsequently the stabilization technique is applied to the continuum dislocation transport equations, involving their non-linearity, their strongly coupled character and the special boundary conditions used in this context; a combination of additional difficulties which most traditional stabilization techniques are unable to deal with. The proposed stabilization scheme has been successfully applied to these equations. Its effectiveness in stabilizing the classical Bubnov-Galerkin scheme and being consistent with the discretized partial differential equation are both demonstrated in the numerical simulations performed. Such effectiveness remains unaffected when different types of dislocation transport models with constant or variable length scales are used.

These results allow envisioning the use of the developed technique for simulating systems of strongly coupled convection-diffusion-reaction equations with an affordable computational effort. In particular, the above mentioned crystal plasticity models can now be handled with reasonable computation times without the use of extraordinary computational power, but still being able to render accurate and physically meaningful numerical approximations.

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