A stabilization technique for coupled convection-diffusion-reaction equations: multidimensional extension

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A stabilization technique for coupled convection-diffusion-reaction equations

Multidimensional extension

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Motivation

A variety of phenomena of scientific interest can be described by the **Convection-Diffusion-Reaction** equation:

$$\rho\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(\delta\frac{\partial u}{\partial x} - \beta u\right) + \gamma u = f.$$

Moreover, interactions among different transported quantities can be modeled by using **coupled** CDR equations. Some of the branches of science where such systems arise are:

- **Bio-mechanics**: bone poro-elasticity, vaccine delivery.
- **Computer science**: Petri nets, optimization.
- **Ecology, epidemiology, neuroscience, physiology**.
- **Economics, finance, stock market behavior**.
- **Fluid dynamics**: multiphase-flows, turbulence.
- **Transport phenomena**: combustion, electro-analytical chemistry.
- **Mechanics of materials**: **Continuum dislocation transport**.

Exact solutions are available in extremely few cases making **numerical approximation** the most affordable strategy to deal with them.

Numerical example

Consider the following system of equations of interest in Petri nets systems simulation [2]:

$$-\frac{\delta}{2}\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\end{bmatrix}_{xx} - \frac{\delta}{2}\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\end{bmatrix}_{yy} + \cdots$$

$$\cdots + \begin{bmatrix}r_1&0&0\\0&r_2&0\\0&0&r_3\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\end{bmatrix}_{x} + \frac{\beta}{4}\begin{bmatrix}4&2&1\\2&4&2\\1&2&4\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\end{bmatrix}_{y} + \cdots$$

$$\cdots + \begin{bmatrix}2\alpha_1&-2\alpha_1&0\\-\alpha_2&\alpha_1+\alpha_2&-\alpha_1\\0&-2\alpha_2&2\alpha_2\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\end{bmatrix} = \begin{bmatrix}f_1(x,y)\\f_2(x,y)\\f_3(x,y)\end{bmatrix}.$$

After discretizing this system using the **classical Bubnov-Galerkin** FEM, numerical approximations plagued with **spurious oscillations** are obtained as can be observed in Figure 1.

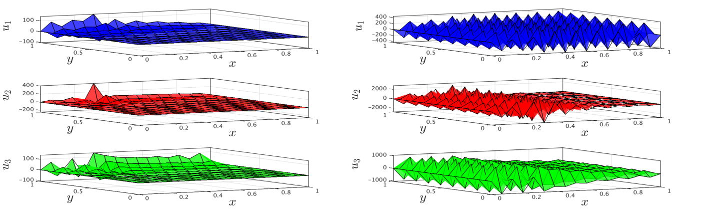

Figure 1: **Classical** scheme with $\delta = 10^{-2}$and $\delta = 10^{-3}$ on a mesh made up with $n_e = 256$ elements by taking 16 divisions in each direction.

Stabilization via perturbation

Several **stabilization techniques** have been developed to handle such transport equations by numerical means [1]. Recently, a new **perturbation-based** stabilization technique was proposed with dislocation transport as the main focus [3].

Yet, not extensive work has been done for systems of coupled equations. The reason of such immaturity is the lack of a **maximum principle** when going from a single transport equation towards systems of coupled equations [5].

The main goal of this communication is to present a stabilization technique for a system of **multiple dimensional coupled** CDR equations based on coefficient perturbations. This methodology extents the approach for a single equation [3] which in turn has been extended to a general 1D system of coupled equations to multiple dimensions [4]:

$$\rho_{pq}u_{q,t} - \left(\delta_{ijpq}u_{q,j} - \beta_{ipq}u_q\right)_{,i} + \gamma_{pq}u_q = f_p.$$

These perturbations are optimally chosen in such a way that certain **compatibility conditions** analogous to a maximum principle are satisfied in each direction. Once the computed perturbations are injected in the classical Bubnov-Galerkin FEM, they render **smooth and stable** numerical approximations.

Numerical assessment

Figure 2 shows the results obtained when the stabilization technique has been applied to the previously shown system.

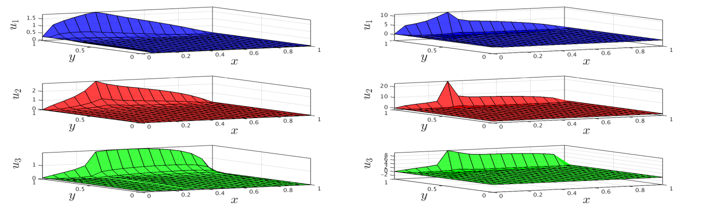

Figure 2: **Stabilized** scheme with $\delta = 10^{-2}$and $\delta = 10^{-3}$ on a mesh made up with $n_e = 256$ elements by taking 16 divisions in each direction.

This time the numerical approximations are non-negative, smooth, and free of wiggles.

Conclusions

These results allow envisioning the use of the developed technique to simulate multi-dimensional dislocation transport in crystalline materials with an affordable computational effort. Also a thorough analysis of the stabilization technique is the further work to be carried out.

References

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