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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]:

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

$$\dots + \begin{bmatrix} r_1 & 0 & 0 \\ 0 & r_2 & 0 \\ 0 & 0 & r_3 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_x + \frac{\beta}{4} \begin{bmatrix} 4 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_y + \dots$$

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

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.

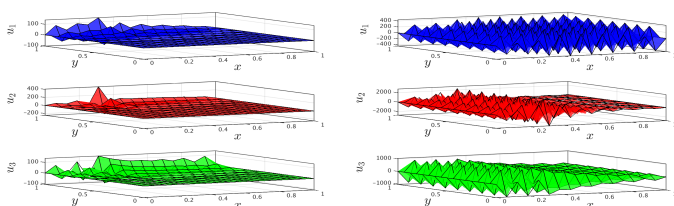


Figure 1: Classical scheme with $\delta = 10^{-2}$ and $\delta = 10^{-3}$ on a mesh made up with $n_e = 256$ elements by taking 16 divisions in each direction.

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 extends 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]:

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

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.

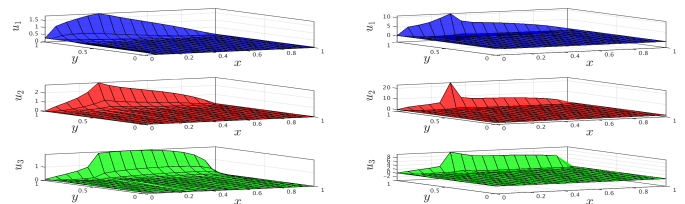


Figure 2: Stabilized scheme with $\delta = 10^{-2}$ and $\delta = 10^{-3}$ on a mesh made up with $n_e = 256$ elements by taking 16 divisions in each direction.

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

- [1] Codina R. 1998. *Comparison of some FEMs for solving the diffusion-convection-reaction equation*, Computer Methods in Applied Mechanics and Engineering, **156** 185-210.
- [2] Griboudo M. and Gaeta R. 2006. *Efficient steady-state analysis of second-order fluid stochastic Petri nets*, Performance Evaluation, **63**, 1032-1047.
- [3] Hernández H., Massart T.J., Peerlings R.H.J., and Geers M.G.D. 2015. *Towards an unconditionally stable numerical scheme for continuum dislocation transport*, Modelling and Simulation in Materials Science and Engineering, Volume 23, Number 8.
- [4] Hernández H., Massart T.J., Peerlings R.H.J., and Geers M.G.D. 2015. *A stabilization technique for coupled convection-diffusion-reaction equations*, In preparation.
- [5] Protter M.H. and Weinberger H.F. 1984. *Maximum principles in differential equations*, Springer Verlag, New-York.