Physical Properties Preserving Algorithms

Shengxin Zhu

Oxford Centre for Collaborative and Applied Mathematics, Mathematical Institute, 24-29 St Giles', Oxford, OX1 3LB, U.K.

Solutions to real-word applications, especially those challenging ones governed by time dependent coupled nonlinear PDEs , have to preserve certain physical constraints. Solutions to a certain class of problems have to satisfy some conservation law according to the underlying principles of physics. Numerical methods for conservation laws were, are and will be one of the main realm in scientific computing. Still, non-physical solutions which satisfy the underlying numerical conservation law often appear for many challenging problems. For example, positivity is a desirable property when simulating advection of physical positive quantities such as density, temperature, probabilities, or particle distribution functions. This is particularly important in the presence of shocks, blobs, and other steep-gradient features. Such phenomenons arises from several challenging applications like fusion plasma, drift-wave turbulence, neutral fluid turbulence, multi-physics biomedical systems and other general Hamilton systems. Simulating such phenomenons not only need supercomputing but also super sophisticated and super customized numerical schemes.

When solving those challenging, time dependent nonlinear coupled systems, one has to synthesize many techniques. Each of these techniques works very well for some model problems designed for the underlying steps, whereas it may fail when collaborating with other techniques for a whole project. It is much easier for some talent researchers to design many powerful methods for each individual part, especially for some tricky toy problems designed for the part. While "best" plus "best" can fail. For example, some monotonicity preserving time discretization schemes don't work well with certain spatial positivity preserving schemes. Even if all the mathematical schemes are all totally rights, it is very often the underlying schemes are tremendously difficulty to fully utilize the capability of supercomputers due to some issues not concerned by mathematicians.

Challenging problems which need supercomputing are usually needed to be considered as whole projects integrating several disciplines rather than to be split /abstracted into several isolated parts. Physical properties preserving algorithms should be viewed as such a long run integrated project.

The challenging of the problems lies both in numerical schemes and in the underlying data structures which often require consideration on load balance.

References

[1] H. An and Z. Mo. Iteration process of JFNK method and physical constraints. *Chinese Journal of Computational Physics*, 25(5), 2012.

[2] Ophélie Angélini, Clément Chavant, Eric Chénier, and Robert Eymard. A finite volume scheme for diffusion problems on general meshes applying monotony constraints. *SIAM Journal on Numerical Analysis*, 47(6):4193–4213, 2010.

[3] KB Nakshatrala and AJ Valocchi. Non-negative mixed finite element formulations for a tensorial diffusion equation. *Journal of Computational Physics*, 228(18):6726–6752, 2009.

Email address: shengxin.zhu@maths.ox.ac.uk (Shengxin Zhu)

URL: https://www.maths.ox.ac.uk/contact/details/zhus (Shengxin Zhu)

Preprint submitted to ExMath13 *May 7, 2013*

[4] J. L. Peterson and G. W. Hammett. Positivity Preservation and Advection Algorithms with Applications to Edge Plasma Turbulence. *SIAM J. Sci. Comput.*, 35(3):B576–B605, 2013.

[5] Z. Sheng, J. Yue, and G. Yuan. Monotone finite volume schemes of nonequilibrium radiation diffusion equations on distorted meshes. *SIAM Journal on Scientific Computing*, 31(4):2915–2934, 2009.

[6] W. Tang, G. Yuan, Z. Shen, and J. Chen. Positivity preserving time step for lagrange method. *Chinese Journal of Computational Physics*, 25(5), 2012.

[7] Y. Yao and G. Yuan. Enforcing positivity with conservation for nine-point scheme of nonlinear diffusion equations. *Comput. Methods Appl. Mech. Engrg.*, 223/224:161–172, 2012.

[8] G. Yuan and Z. Sheng. Monotone finite volume schemes for diffusion equations on polygonal meshes. *Journal of computational physics*, 227(12):6288–6312, 2008.