SHALLOW WATER EQUATIONS WITH CHEMICAL TRANSPORT

Janusz A. Pudykiewicz, Environment Canada, RPN, e-mail: Janusz.Pudykiewicz@ec.gc.ca

The main requirements for the accurate numerical technique for solving the fully coupled system of atmospheric dynamics and chemistry include stability for stiff systems, monotonicity, mass conservation, small numerical diffusion, and flexibility with respect to the selection of horizontal discretization. The selection of the optimum method satisfying all these requirements is not easy and it requires extensive studies of both analytical and numerical nature. The majority of these studies could be accomplished analyzing a relatively simple set of shallow water equations coupled to a set of reaction-advection-diffusion equations

$$\frac{\partial \mathbf{v}}{\partial t} + (\zeta + f)(\mathbf{k} \times \mathbf{v}) = -\nabla\left(gh + \frac{\mathbf{vv}}{2}\right) \tag{1}$$

$$\frac{\partial h^{\star}}{\partial t} + \nabla(h^{\star}\mathbf{v}) = 0. \tag{2}$$

$$\frac{\partial \varphi^k}{\partial t} = -\nabla \mathbf{v}\varphi^k + \nabla \mathbf{K}\nabla\varphi^k + F_c^k(\varphi^1, \ldots, \varphi^{N_s}), \tag{3}$$

where $\mathbf{v}$ is the velocity field on the sphere, ζ is the vertical component of vorticity, f is the Coriolis parameter, $h^{\star}$ is the geopotential height, h_s is the surface height, $\mathbf{k}$ is the unit vector normal to the sphere, and g is the gravity acceleration, φ^k is the kth scalar field; $k = 1, \ldots, N_s$, N_s is number of scalar fields, $\mathbf{K}$ is the diffusion tensor, and F_c^k are the functions describing the interactions between scalar fields. In a general case, F_c^k can be written as $\alpha_{klm}\varphi^l\varphi^m + \beta_{kl}\varphi^l$, where α_{klm} and β_{kl} are the kinetic coefficients. The system of equations (1)-(3) is discretized on a geodesic icosahedral grid (Fig. 3) using a finite volume method developed originally for scalar conservation laws (Pudykiewicz, 2006). The methodology employed is based on the concept of semidiscretization; first the operators on the right hand sides of (1)-(3) are approximated and then, the resulting set of the Ordinary Differential Equations (ODEs) is solved using the appropriate time stepping algorithm. Depending on the stiffness of the system, the time integration is performed either with the 4th order Runge-Kutta scheme or with the Rosenbrock solver. The performance of the numerical technique for the coupled set of equations (1)-(3) is assessed using the initial conditions defining the Rossby-Haurwitz wave number 12 (Williamson et al., 1991) with the chemistry described by the Brusselator system (Prigogine and Lefever, 1968). This experimental setting is interesting from the point of view of the interaction of dynamics and chemistry because the tracer filamentation by the Rossby wave (Pierrehumbert, 1991) is coupled in a complex manner with the nonlinear chemistry. The chemical terms on the right hand side of (3) used in the study can be described as

$$F_c^1 = k_1 a - (k_4 + k_2 b)\varphi^1 + k_3(\varphi^1)^2\varphi^2 \tag{4}$$

$$F_c^2 = k_2 b\varphi^1 - k_3(\varphi^1)^2\varphi^2 \tag{5}$$

The parameters of the chemical system were selected as follows: $\mu_1 = 0.7 \times 10^5 [\text{sec}^{-1}]$, $\mu_2 = 2\mu_1$, $k_i = 1.16 \times 10^{-5}[\text{sec}^{-1}]$ (for $i = 1, .., 4$), $a = 2$, $b = 5$. The main property of the reaction-diffusion system with such parameters is the tendency to develop patterns in form of the stripes and belts. The effect of the interaction of the pattern formation with the stretching and folding of the material surfaces by the evolving unstable Rossby wave is depicted in Figs. 4-6 (initial conditions for φ^1 is shown in Fig. 1; $\varphi^2 = \varphi^1 + ((b/a) - a)$). The main conclusion from the experiment investigating numerical solver in a complex setting of a fully interactive scheme involving nonlinear dynamics and chemistry is that the system is able to develop fine structures resulting both from chemistry (pattern formation) and dynamics (filamentation) without numerical noise. Despite the very fine structures of the tracer filaments, the advected chemical tracer fields remained positive definite during the prolonged numerical integration of (1)-(3) on icosahedral geodesic grid.

REFERENCES

[1] Pierrehumbert R. T., 1991: Chaotic Mixing of Tracer and Vorticity by Modulated Traveling Rossby Waves. *Geophysical and Astrophysical Fluid Dynamics*, **58**, 285-320.

[2] Prigogine I. and R. Lefever, 1968: Symmetry-Breaking Instabilities in Dissipative Systems. *J. Chem. Phys.*, **48**, 1695-1700.

[3] Pudykiewicz J., 2006: Numerical solution of the reaction–advection–diffusion equation on the sphere. *J. Comp. Phys.*, **213**, 358.

[4] Williamson D. L., J. B. Drake, J. J. Hack, R. Jakob, and P. N. Shwartzrauber, 1992: A Standard Test Set for Numerical Approximations to the Shallow Water Equations in Spherical Geometry. *J. Comp. Phys.*, **102**, 211.
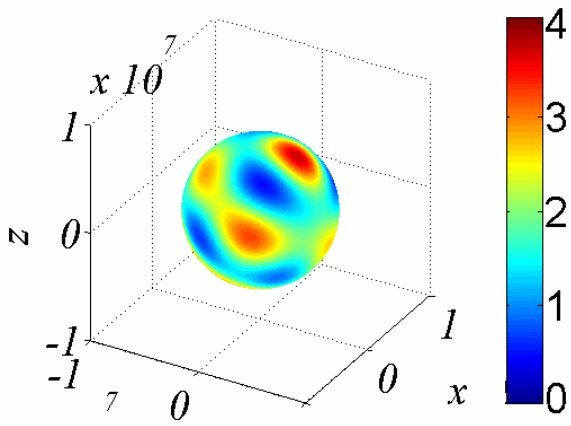
Fig. 1 The initial condition for the first chemical field
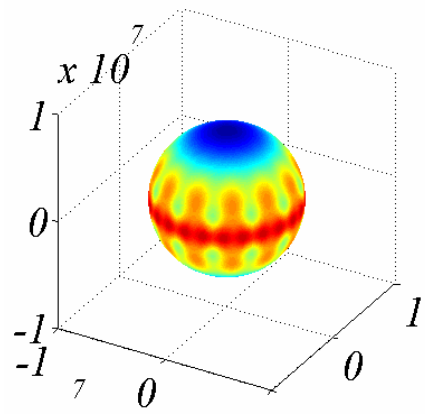

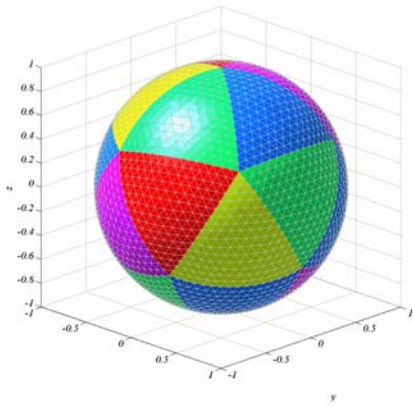Fig. 2 The geopotential field after 24 hrs.

Fig. 3 The geodesic grid obtained after 4 divisions of the original icosahedron; calculation shown in Figs. 4-6 were performed on grid obtained after 6 divisions
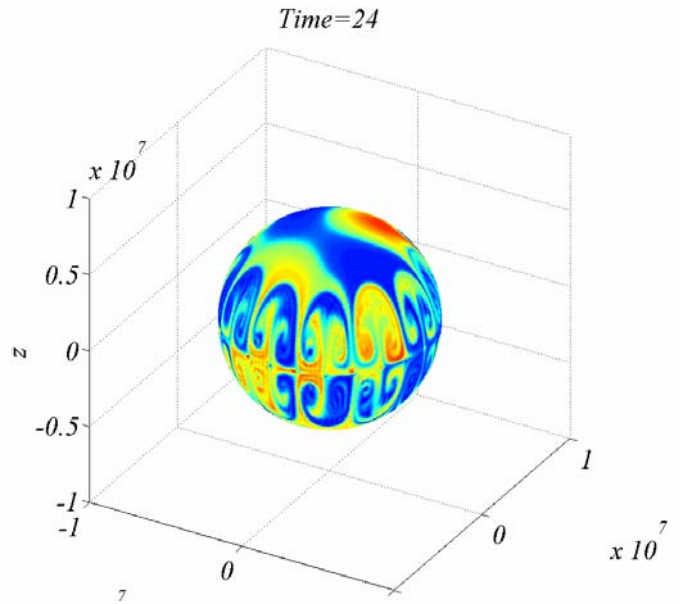

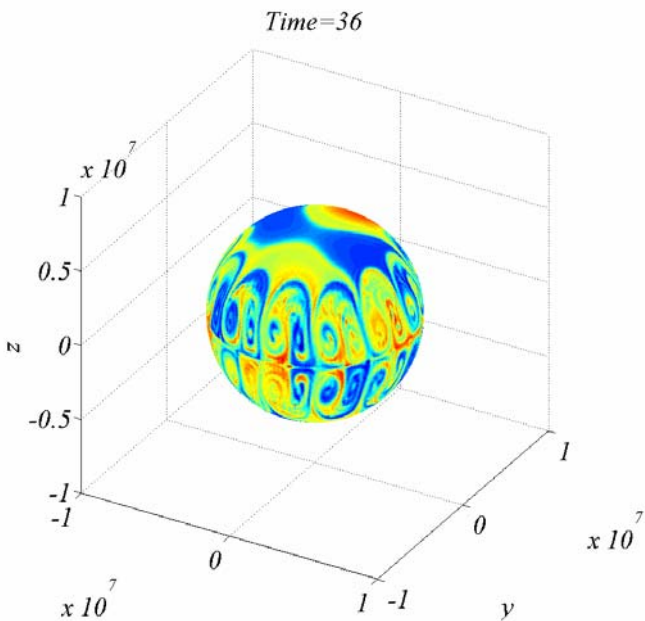Fig. 4 First chemical field after 24 hours of integration
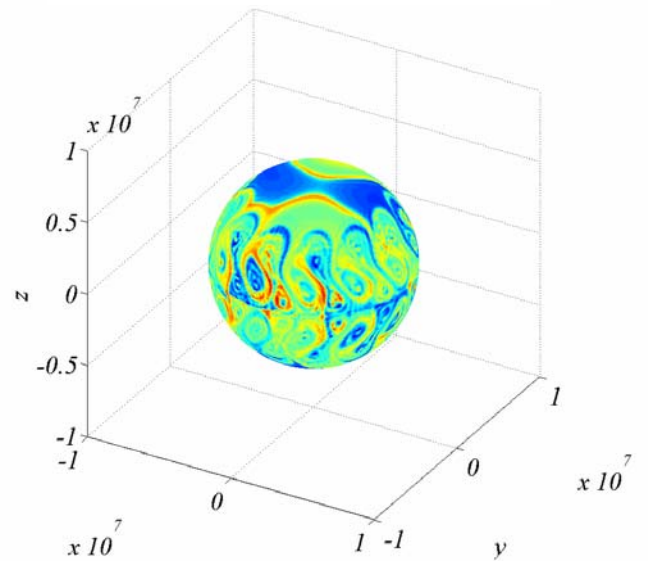

Fig. 5 First chemical field after 36 hours of integration

Fig. 6 First chemical field after 48 hours of integration