Montestigliano Workshop | **Problem 6** Surface diffusion and reaction-diffusion equations | **Level 1 & 2** **Grady Wright**

In Problem 4 you computed differentiation matrices for the surface Laplacian on the sphere. In this problem you will look at how to use these matrices for some problems involving diffusion and reaction-diffusion on the sphere. The application of RBFs to these types of problems outlined below follows closely the method of Fuselier and Wright [6] (although that method applies to more general surfaces than the sphere).

The diffusion of a scalar valued quantity on the surface of the sphere is given by

$$\frac{\partial u}{\partial t} = \delta \Delta_{\mathcal{S}} u + f(t,u), \tag{1}$$

where $u : \mathbb{S}^2 \longrightarrow \mathbb{R}$, $\delta > 0$, $\Delta_{\mathcal{S}}$ is the surface Laplacian (or Laplace-Beltrami operator for the sphere), and f is some forcing function. Similar to the transport equation from Problem 5, we can numerically solve this equation using a method-of-lines (MOL) approach involving the differentiation matrix for the surface Laplacian from problem 4.

Following the notation of Problem 5, let $X = \{\mathbf{x}_j\}_{j=1}^N \subset \mathbb{S}^2$ and denote the vector containing samples of u at X as $\underline{u}$, and the differentiation matrix for the surface Laplacian associated with X as L_N. Then, the MOL formulation of (1) is

$$\underline{u}_t = L_N \underline{u} + f(t, \underline{u}) \tag{2}$$

Given an initial value for $\underline{u}$, this system of ODEs can be numerically solved using any number of numerical methods.[1] For example, one could use the third-order semi-implicit backward differentiation scheme (SBDF3) [1]:

$$\frac{11}{6}\underline{u}_{k+1} - 3\underline{u}_k + \frac{3}{2}\underline{u}_{k-1} - \frac{1}{3}\underline{u}_{k-2} = \Delta t \delta L_N \underline{u}_{k+1} + \Delta t \left[3f(t_k, \underline{u}_k) - 3f(t_{k-1}, \underline{u}_{k-1}) + f(t_{k-2}, \underline{u}_{k-2})\right], \tag{3}$$

for $k = 2, 3, \ldots$. Here Δt is the time-step, $\underline{u}_0$ contains the initial condition sampled at X, $\underline{u}_1$ is the solution (or an approximation) at $t = \Delta t$, and $\underline{u}_k$ is the numerical solution to (2) at $k\Delta t$. This scheme treats the diffusion term implicitly and the (possibly non-linear) forcing term f explicitly, which allows larger time-steps to be taken in the case f is not stiff. This is the numerical scheme suggested for the different problems below, but you may use a different one if you choose.

Another type of process that appears in a number of applications arising in biology, chemistry, and computer graphics is the reaction-diffusion of two species on the sphere. The prototypical form of the system of PDEs describing this process is

$$\begin{aligned} \frac{\partial u}{\partial t} &= \delta_u \Delta_{\mathcal{S}} u + f_u(t,u,v), \\ \frac{\partial v}{\partial t} &= \delta_v \Delta_{\mathcal{S}} v + f_v(t,u,v), \end{aligned} \tag{4}$$

where $u, v : \mathbb{S}^2 \longrightarrow \mathbb{R}$, $\delta_u, \delta_v \geq 0$, and f_u, f_v are (possibly non-linear) scalar functions. Using the notation above, the MOL formulation of this system is

$$\begin{aligned} \underline{u}_t &= \delta_u L_N \underline{u} + f_u(t, \underline{u}, \underline{v}), \\ \underline{v}_t &= \delta_v L_N \underline{v} + f_v(t, \underline{u}, \underline{v}), \end{aligned} \tag{5}$$

[1] Unlike the transport the problem, the differentiation matrix L_N for the surface Laplacian is guaranteed to have real, non-positive eigenvalues [7], so that no stabilization term will be necessary.

As with (2), the SBDF3 method above can be applied to discretize this system of ODEs in time.

5.a) *Level 1: Diffusion.* Implement a code in MATLAB following the procedure (2) for numerically solving the diffusion equation (1).

(i) Test your code for the case with no forcing ($f = 0$), $\delta = 1$, and the initial condition is given by

$$u(0, \mathbf{x}) = Y_6^0(\mathbf{x}) + \sqrt{\frac{14}{11}} Y_6^5(\mathbf{x}) + Y_{20}^5(\mathbf{x})$$

Since the initial condition is a finite combination of spherical harmonics, the exact solution is simply

$$u(t, \mathbf{x}) = e^{-t(6)(7)} \left[Y_6^0(\mathbf{x}) + \sqrt{\frac{14}{11}} Y_6^5(\mathbf{x}) \right] + e^{-t(20)(21)} Y_{20}^5(\mathbf{x}).$$

Compute the numerical solution up to $t = 0.05$ for the IMQ kernel using $N = 1849$ MD nodes, $\varepsilon = 1.75$, and a time-step of $\Delta t = 0.001$ (chosen for accuracy, not stability). Plot the numerical solution every time-step using your functions from problem 1. You should see a clear recognizable pattern emerge after a few time-steps. Compute the ℓ_2 and ℓ_∞ norm of the difference between the numerical and exact solution at the nodes X.

(ii) Experiment with different N, node sets, time-steps, and kernels to get a feel for how the method performs.

5.b) *Level 2: Turing patterns.* Since Turing's classical paper [8] that suggested how certain non-linear models of reaction and diffusion can lead to stable, heterogeneous pattern formations, there has been an explosion of research in reaction-diffusion-type models for various kinds of morphogenesis. In this problem you will implement a code for solving the Turing system (a linearized Brusselator model) on the sphere from [9]:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \delta_u \Delta_{\mathcal{S}} u + \underbrace{\alpha u(1 - \tau_1 v^2) + v(1 - \tau_2 u)}_{f_u(u,v)}, \\ \frac{\partial v}{\partial t} &= \delta_v \Delta_{\mathcal{S}} v + \underbrace{\beta v \left(1 + \frac{\alpha \tau_1}{\beta} uv\right) + u(\gamma + \tau_2 v)}_{f_v(u,v)}. \end{aligned} \tag{6}$$

Here u and v are morphogens with u the "activator" and v is the "inhibitor". If $\alpha = -\gamma$ then $(u, v) = (0, 0)$ is a unique equilibrium point of this system. By changing the diffusivity rates of u and v an instability can form that leads to different pattern formations. The cubic coupling parameter τ_1 favors the formation of stripes, while the quadratic coupling parameter τ_2 favors the formation spots [9]. The spot pattern formations are more robust than stripes and take far less time to reach "steady-state". The following are parameter values that lead to spots or stripes on the sphere [9] :

Pattern	δ_v	α	β	γ	τ_1	τ_2
Spots	$4.5 \cdot 10^{-3}$	0.899	-0.91	-0.899	0.02	0.2
Stripes	$2.1 \cdot 10^{-3}$	0.899	-0.91	-0.899	3.5	0

For the initial conditions, set the values of u and v to random values between -0.5 and 0.5 in a strip around the equator of the sphere (say for $|z| < 0.3$) and $u = v = 0$ elsewhere.

5.a) Compute the solution to (6) using parameters corresponding to spots. Try $N = 1849$ MD points, the IMQ kernel with $\varepsilon = 1.75$, and $\Delta t = 0.05$. Run the simulation until a quasi-steady-state is reached. This should be around $t = 500$. Plot the solution of the u variable on the sphere at $t = 500$ (or better yet, make a movie of the simulation!).

5.b) Repeat (i), but for the parameters corresponding to spots. As mentioned above, stripes are not as robust and take longer to develop and settle into a steady pattern. You may need to run the simulation up to about $t = 3000$. Plot the solution on the sphere at this final time. The image you get should be strikingly similar to the image on the cover of the SIAM Review Vol. 50, Issue 4. Indeed, that image was made from a simulation of the same Turing model (6) by Calhoun *et. al.* [4, 5].

5.c) *Level 2: Spiral waves.* Spiral waves can be observed in many excitable chemical, biological, and physical media. Important examples include Belousov-Zhabotinsky (BZ) chemical reactions and electrical activity in the membranes of organisms. While numerical methods have been developed for these models in planar domains (see [2, 3] and the corresponding software EZ-Spiral), there has been growing interest in studying these models on non-planar surfaces, such as the sphere, since most physically relevant problems occur on curved surfaces. In this problem you will implement a code for solving, on the surface of the sphere, the following simplified model for spiral waves developed by Barkely [2] that captures the dynamics of many excitable media:

$$\begin{aligned} \frac{\partial u}{\partial t} =& \delta_u \Delta_{\mathcal{S}} u + \underbrace{\frac{1}{\alpha} u\,(1-u)\left(u - \frac{v+b}{a}\right)}_{f_u(u,v)}, \\ \frac{\partial v}{\partial t} =& \delta_v \Delta_{\mathcal{S}} v + \underbrace{u - v}_{f_v(u,v)}\ , \end{aligned} \tag{7}$$

where u and v can be viewed as some chemical concentrations or as membrane potential and current. The parameters a, b, and α govern the reaction kinetics and δ_u and δ_v are the diffusivities of the u and v species respectively. The parameter α is chosen as $\alpha << 1$ so that the u field takes on the values $u = 0$ or $u = 1$ almost everywhere, with a thin interface (or reaction zone) separating these two regions.

Solve the system (7) using the initial conditions

$$\begin{aligned} u(0, \mathbf{x}) &= \frac{1}{2}\left[1 + \tanh(2x + y)\right], \\ v(0, \mathbf{x}) &= \frac{1}{2}\left[1 - \tanh(3z)\right], \end{aligned}$$

where $\mathbf{x} = (x, y, z)$ is a point on the unit sphere. and the following values for the parameters: $a = 0.75$, $b = 0.02$, $\alpha = 0.02$, $\delta_v = 0$, and $\delta_u = 1.5(2\pi/50)^2$ (these choices are motivated by the values found in [3] for a simulation on 2-D planar domain). Try $N = 1849$ MD points, the IMQ kernel with $\varepsilon = 1.75$, and $\Delta t = 0.02$. Plot the solution every 10 time-steps to see visualize the wave that develops.

References

[1] U. M. Ascher, S. J. Ruuth, and B. T. R. Wetton, *Implicit-explicit methods for time-dependent partial differential equations*, SIAM J. Numer. Anal., 32 (1995), pp. 797–823.

[2] D. Barkley, *A model for fast computer simulation of waves in excitable media*, Physica D, 49 (1991), pp. 61–70.

[3] D. Barkley, *Barkley model*, Scholarpedia, 3 (2008), p. 1877.

[4] D. Calhoun and C. Helzel, *A finite volume method for solving parabolic equations on logically cartesian curved surface meshes*, SIAM Journal on Scientific Computing, 31 (2010), pp. 4066–4099.

[5] D. A. Calhoun, C. Helzel, and R. J. LeVeque, *Logically rectangular grids and finite volume methods for pdes in circular and spherical domains*, SIAM review, (2008), pp. 723–752.

[6] E. J. Fuselier and G. B. Wright, *A high-order kernel method for diffusion and reaction-diffusion equations on surfaces*, Journal of Scientific Computing, (2013), pp. 1–31.

[7] R. B. Platte and T. A. Driscoll, *Eigenvalue stability of radial basis function discretizations for time-dependent problems*, Comp. Math. Appl., 51 (2006), pp. 1251–1268.

[8] A. Turing, *The chemical basis of morphogenesis*, Philos. Trans. R. Soc. B, 237 (1952), pp. 37–52.

[9] C. Varea, J. Aragon, and R. Barrio, *Turing patterns on a sphere*, Phys. Rev. E, 60 (1999), pp. 4588–4592.