Programming reaction-diffusion equation

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Abstract:

We write about programming/coding for practice of partial differential equations.

Partial differential equations express various phenomena; however, due to wide varieties of subjects, there are many approaches reach to solutions. General-purpose program products are also commercially available. We believe that making your own is also important from an educational point of view.

Although the approximation level is rough here, we adopt the forward explicit approach whose policy is easy to understand. Then, besides the diffusion and advection terms, we add biochemically interesting terms to see how the solution changes.

偏微分方程式の実習用のプログラミング・コーディングについて述べます。

偏微分方程式は拡散などの諸現象を表現する方程式です。しかし対象が多岐にわたるので、解への接近法が複数存在します。汎用的なプログラム製品も市販されています。我々は、自作するのも教育的観点からは重要と考えています。

ここでは近似レベルは粗いのですが、方針が理解しやすい前進・陽解法を採用します。そして、拡散と移流項の他に、生化学的に興味深い項を追加して、解の変化を調べます。

Keywords: Logistic map, microbe simulation

0. Introduction

A reaction-diffusion equation [1,2] is a type of partial differential equation. It is used here to examine the time(t) series change {A(x,y,z,t)} of the spatial {x,y,z} distribution of microbial populations.

Formula (1) is a fluid advection/diffusion equation, but the scalar coefficients {k,f} are constant constants in space. Equation (1) holds even when t→-t, but it cannot be solved numerically in the reverse time direction.

Microorganisms are not fluids, but since their particle size is less than 1 μm, they can be approximated as diffusing and moving in a fluid for a short period of time. Its diffusion is normally distributed turbulent diffusion. Turbulent diffusion also approaches fluid diffusion if the particle size is small. Therefore, we begin our discussion with the advection-diffusion equation.

$$\partial A(x,y,z,t)/\partial t=\{k(\partial^2/\partial x^2+\partial^2/\partial y^2+\partial^2/\partial z^2)A(x,y,z,t) + f(\partial/\partial x,\partial/\partial y,\partial/\partial z)A(x,y,z,t). \quad (1)$$

1. Expression Variant

In biochemistry, there is no use if f is a constant number in space, thus, “f”,

$$f\rightarrow\{f(x,y,z),\ (\partial/\partial x+\partial/\partial y+\partial/\partial z)f(x,y,z)=0\}, \quad (2)$$

should be. Therefore, the analytical solution of equation (1) is unknown. We will proceed with the policy of finding a numerical approximate solution.

Formula (1) is fine for A() if it is an inorganic particle such as a radioactive tracer, but if it is a bioparticle, it is necessary to handle the growth and extinction. Bioparticles consume resources to grow and disappear. Resource is a general term for nutrient salts of microorganisms. Poisons that kill microbes are also resources. It is possible that the physical properties of resources change from beneficial to toxic at a certain concentration. The advantage of writing your own program is that it naturally prompts you to consider various properties of resources.

Considering the resource as an inorganic substance, its spatio-temporal distribution {R(x,y,z,t)} is expressed by formula (1) and {k', f'(x,y,z)}. The prime of the f function means that f ≠ f', not the derivative.

The absence of the condition $(\partial/\partial x+\partial/\partial y+\partial/\partial z)f'(x,y,z)=\mathrm{div}\{f'()\}=0$ is a source such as a hot water spring in the deep sea. Because we thought about the case where there is However, if the subject is too broad, the discussion will diverge, so here we will limit the subject to the growth of microorganisms in the animal body and set source=0.

2. Spatial Meshing

Space-time is a continuous infinite set {x, y, z; t}, but it cannot be numerically processed, so it is divided into a network (mesh). If we divide the finite range [-1 μm,+1 μm; 1k time steps] by 1k (k=1000), we get (10**3)**4=10**12(8TB). It would be difficult to hold this amount of data in an array. So we make the following simplifications:

Make space two-dimensional. Do not retain data on the time axis. Set the number of divisions to 0.4k*. One type of flow field f() for resources and microorganisms. The 2D div()=0 condition calls for unidirectional flow in space.

*) Install the language on your PC and try to see how big an array can actually be defined. This time, I was able to define 8 4B arrays of 400 x 400 dimensions with gfortran for Windows 11, memory = 4GB (equipment for training). It can also handle future enhancements.

The discrete form of the differential operators are,

$$(\partial/\partial x)f(x,y,z)=\{f(x+1,y,z)-f(x-1,y,z)\}/dx;\ dx=f(x,y,z)-f(x-1,y,z)=..., \quad (3A)$$

$$(\partial^2/\partial x^2)f(x,y,z)=\{f(x+1,y,z)+f(x-1,y,z)-2f(x,y,z)\}/(dx)^2,..... \quad (3B)$$

2023年1月30日受付　2023年2月14日受理

(∂/∂y) is also dx=dy for simplicity. Equation (3A) is an equality, but the precision of the equation drops with the magnitude of dx(>0). must be used with caution. Common sense says dx=O(-2). O() is an argument of order, meaning O(-2) ~ 1/100. 2/100 and 0.5/100 are the same as 1/100.

3. Limitations of results and solutions

In the direction of the time axis, the A(x,y) plane is spaced at regular intervals,

IA(i,j)=integer{p*A(x,y)+q}, (4)

As, display the IA() array with office soft. "integer()" is the integerizing function. where (p,q) are constants for display such that -9 < IA() < 99. A parameter (real number) for display. Formula (1) sets the initial values of A() and f() at t=0, and calculates forward in the direction of t→∞. Therefore, the solution error accumulates. Unless the constants and flow field functions {k,f()} are also less than O(-2), you are mainly "calculating the error". You should be careful with the initial settings.

"Here, set the space to be finite." n=400, A(n,n), t=integer < 600, center point A(nh,nh), nh=n/2, dx=10/nh.

This setup considers the behavior of microorganisms within a two-dimensional plane of ± 10 [μ m].

The range that can be displayed with formula (4) is about 40 × 40 mesh, so 40 * (10/200) = 2 [μ m] square. It shows the vicinity of the center point.

When solving equation (1) in a finite space, it is necessary to set boundary conditions. Note the limitations of this approach to the solution, how far out of the plane are tails of the solution? and so on.

4. Trial

4.1 Advective/diffusion dest

Have you actually achieved your goals through numerical calculations? Let's to test. Fig.1* shows the initial distribution function of A(), and Fig.2 shows the error in the time series obtained by numerically integrating the precision of the second partial differential calculation in the difference form over the entire diffusion field. Fig.3 shows the plan view when it is diffused to "t=500". Integrating A() over the whole space is 39.3(t=0 and t=500). Even if the peak value becomes smaller due to diffusion, the total amount of A() is preserved. From these figures the programming and calculation of the diffusion term is reasonable.

*) The horizontal axis in Fig.1 is the x value. In this calculation, dx=0.1, so it is the mesh range of A(center ± 10,0,0). In Fig.2, Gaussian distribution A() is certainly diffused.

Next, Fig. 4 shows the result of adding a constant flow parallel to the x-axis in a space of y > 200 mesh. Even if we add the advection term, the integral of A() over the whole space is 39.3(t=0 and t=500). Even if the shape of A() changes due to advection, the total amount of A() is preserved. As mentioned above, this program obtained reasonable results in the advection-diffusion test.

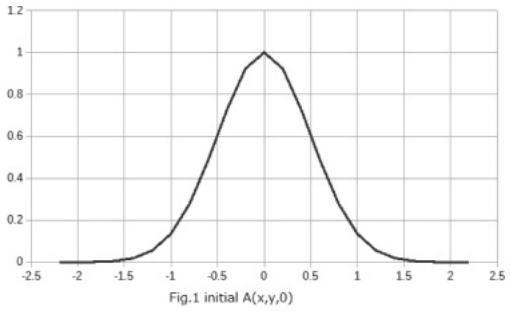

Fig.1 initial A(x,y,0)

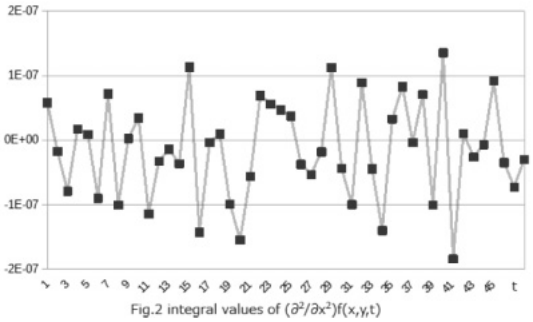

Fig.2 integral values of $(\partial^2/\partial x^2)f(x,y,t)$

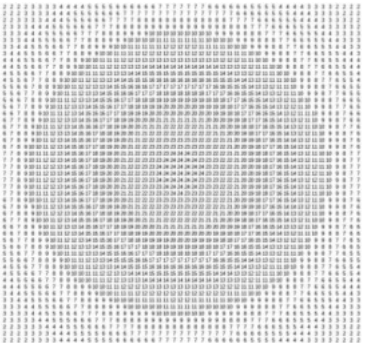
Fig.3 Distribution of A(x,y,t=500).

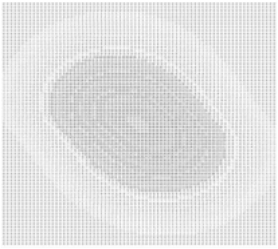
Fig.4 A(x,y,t=500) under diffuse and flow for x-direction.

4.2 Branch test

Set the branch flow as shown in Fig.5,6. Fig.7 shows changes in the value of ∫A()dxdy, and Fig.8 shows A() at t=150. Figs.5 and 6 show a flow parallel to the x-axis of "+9" from left to right and with a width of 3 meshes, which diverges in ± 45deg directions at the center point. The y-axis flow is globally 0 as a vector. It is 4 and 5 because it is a single digit display. Strictly speaking, A() of div()~O(-4) is generated instead of div()=0 (Fig.7). Fig.8 is a snap shot at t=150. The situation where the Gaussian distribution in Fig.1 is diffused and diverged is expressed. In biology, it is important where in space the distribution intensity is.

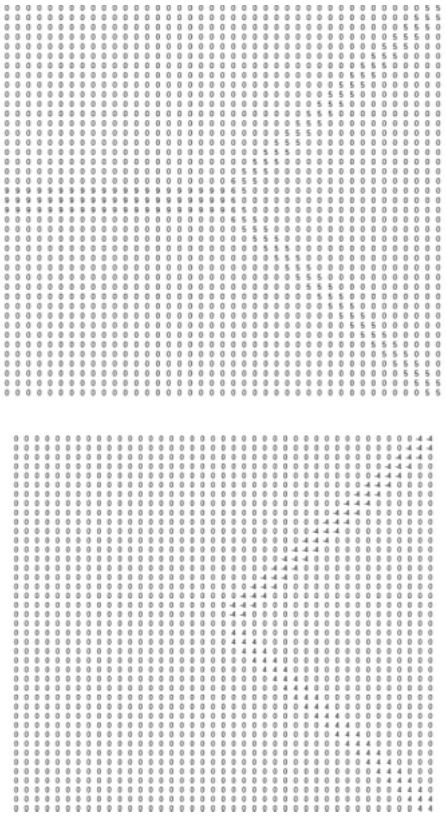

Fig.5,6 Flow of x,y-directions. It branches at the center point.

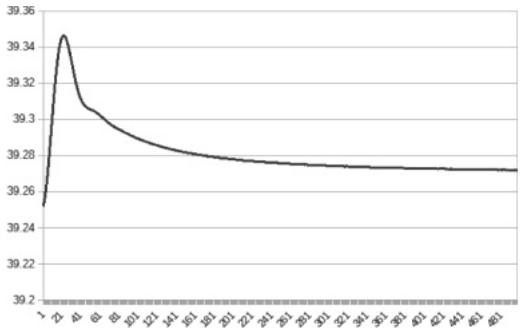

Fig.7 Changes of integrals of A(). When numerically solving a differential equation with a finite-difference approximation using meshes, errors are transiently visible when the high-valued points spread over a narrow range.

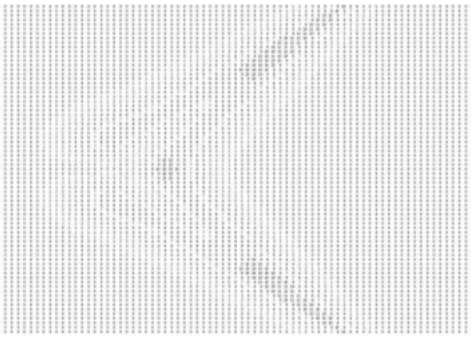

Fig.8 Distribution of A(x,y,150).

5. Add Logistic Map Term

"A() = constant" so far. If we think of A() as the microorganism distribution, it increases or decreases depending on time t and resource distribution R(x, y, t). Resources also advect-diffusion. We need a different advection-diffusion equation than A(). The solution of the two equations is

Y(x,y,t)={A(x,y,t+1),R(x,y,t+1)};

Y(x,y,t+1)=kY(x,y, t){1-Y(x,y,t)}, (5)

A logistic map (discrete logistic equation) is known, on which the description on the Japanese version [3] of Wikipedia is helpful for understanding the property.

There, it is stated that it is a formula for the number of individuals when "organisms live in the environment and there is no movement of individuals between the environment and the outside".

This map generates chaos depending on the value of the coefficient k. Here, we recognize the biological significance of this mapping and use it as a recurrence formula that expresses the number of living organisms.

Until now, dx = 1/20, but from now on, dx = 1/5, which is 4 times the 8 x 8 [μm] plane. Adopt a wide range of space even if the accuracy is reduced.

Equation (5) is

A(x,y,t+1)=A(x,y,t)R(x,y,t), (6A)

w=R(x,y,t)-mA(x,y,t);

if(w>0)R(x,y,t+1)=w, else A(x,y,t+1)=0, (6B)

and transform. If k=1 in the original formula, it quickly converges to A()=0.

Formula (6) expresses the situation where m resources are consumed and A() increases or decreases in proportion to the population of A(). If the resources in a mesh become 0, the population of that mesh dies. R() does not change. Therefore, when $t \to \infty$, the number of individuals becomes 0.

Calculate the divergent advection and diffusion of microorganisms under the condition of uniform resource distribution in all spaces and no advection-diffusion of resources.

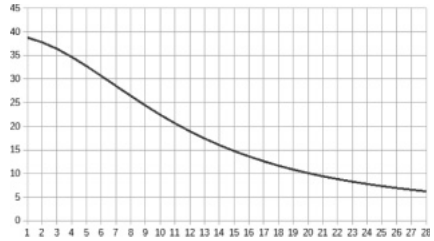

Fig.9 Total mass change in A(..,t) up to t<29. Consuming the resource in a plane, total mass changes from 39.3 to 6.23. Using parameters: m=+1/39.3, R(x,y,t=0)=1, diffused parameter k=1/1000 in the plane, flow parameters are in Fig.5,6.

Fig.10 Snap shots of A(x,y,t=29,59,89), in which the mass of A() are 6.23, 2.31, 1.41, respectively.
The change depends on a parameter “m=1/39.3” used in Fig.9.
Distribution of microorganisms that advect and diffuse while consuming resources along the flow that diverges at an angle of 45 degrees from the central point.

If Parameter “m” is positive, microorganisms will decrease, and if negative, they will proliferate. There is no m<0 in reality, and when m=-0.01/39.3<0 in the simulation, A() changes from 39.3→42.1→48.3.

Returning to the original Logistic mapping formula, when the resource is 0, A() = 0 & R() = A(). Consider the case where resources are circulating in the form of microorganisms.

We set,

w=A(x,y,t)R(x,y,t), (7A)

A(x,y,t+1)=k*w*(1-w), (7B)

w2=R(x,y,t)-A(x,y,t),

if(w2>0)R(x,y,t+1)=w2, else A(x,y,t+1)=0,

R(x,y,t+1)=A(x,y,t), (7C)

Moving the k value in equation (7B) from 1.01 to 1.06 gives Figure 11.

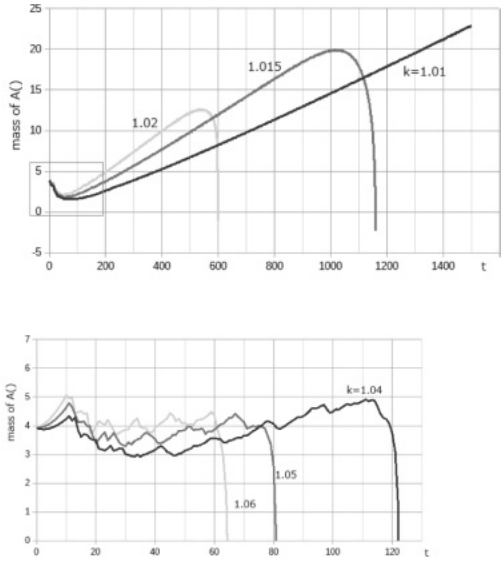

Fig.11 Change of A(x,y,t) under k=1.04~1.06. Increasing the k value in Eq. (7B) results that is faster proliferation, but resource shortages lead to early extinction. It did not become extinct until t=1.5k under reasonable diffusion rate (k=1.01).

Conclusion:

We introduce a programming example of the reaction-diffusion equation. We add the logistic map term as a reaction of microorganisms, modify it, and simulate the growth and extinction process of microbial assemble. A logistic map is characterized by a single scalar parameter. In this simulation, we set uniform resources for whole space and simplified microbial growth process (close to the original map), but due to the action of advection-diffusion terms, the growth and destruction became complicated. Reaction-diffusion equation is an equation with a potential that expresses microbial growth and destruction in user designed resource-space.

References

[1] T.Aoyama, “A simulation of Virus Diffusion”, Informatio, vol.19. pp.117-128, 2022.7; https://edo.repo.nii.ac.jp/index.php?action=pages_view_main&active_action=repository_view_main_item_snippet&index_id=84&pn=1&count=20&order=7&lang=japanese&page_id=13&block_id=21; Jan. 30, 2023. confirmed the article.

[2] There are few examples in which the reaction-diffusion equation has been applied biologically, and there was the following paper.
We undrstand following messages, “A reaction-diffusion model describing the spatial distribution and temporal development of tumor tissue, normal tissue, and excess H+ ion concentration is presented.”
Robert A. Gatenby; Edward T. Gawlinski,
"A Reaction-Diffusion Model of Cancer Invasion"
Cancer Res (1996.12.1) 56 (24): pp.5745–5753.

[3] https://ja.wikipedia.org/wiki/; we confirm the article at Jan. 20, 2023.

捕捉:

Biochemical implications of this calculation:
With minor viral illnesses such as the common cold, your throat will be sore first, and as the cold progresses, your nose may become stuffy. The stuffy nose will eventually improve, and before you know it, you'll be completely healed.
Describe the progression of these symptoms.

この計算の生化学的意味:
風邪などの軽度のウイルス性疾患では、まず喉が痛くなり、風邪が進行すると鼻が詰まることがあります。
鼻づまりはやがて改善し、いつの間にか完治する。これらの症状の進行(炎症部の動き)について説明しています。