Fall 2018 MATH703 Final Project Report
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Green's function solutions for 2D non-homogenous diffusion equations

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Abstract

An analytical expression for a 2D inhomogeneous transient diffusion problem and a linear advection-diffusion problem can be obtained using Green's function. Based on the homogeneous Dirichlet boundary conditions, the general expression for the Green's function including the source terms in 2D Cartesian coordinate is derived. The reduction of a 2D problem into a 1D problem using the multiplicative property of the Green's function is discussed. Examples involving a point source (using delta function) and a constant source throughout the entire field are solved using the Green's function. The results are verified by comparing with the numerical solutions. The idea of using Green's function in solving diffusion equation is applied to recognize the four different structures naturally existing in two-phase flow simulations. An illustrative example is solved to give an idea of the implementation of the Green's function solution.

Contents

1. Introduction

One of the methods used to solve an inhomogeneous, transient diffusion equation is using Green's function. In Section 2, we apply the method of using Green's function to solve a 2D transient diffusion problem in a finite domain with Dirichlet condition at the boundaries.

The multiplicative property of Green's function is one of the important properties of Green's function. With the knowledge of simple 1D Green's function solutions, we can directly construct the corresponding higher-dimensional Green's function solutions, which are sometimes not trivial to solve. We will prove this property in Section 2-1. The proof is based on a 2D Green's function.

In Section 3, we provides two numerical examples to examine the Green's function solutions. One example considers a point source term while the other one employs the constant source existing in the entire domain. The results are compared with the numerical solutions obtained using the finite difference approach with Forward-Time Central-Space (FTCS) scheme.

One of the applications using the Green's function solution for a diffusion equation is discussed in Section 4. This pertains to the numerical simulations of the two-phase flow problems. In this type of problems, an important issue is to distinguish i) liquid, ii) liquid-gas interface, iii) unresolved, and iv) gas structures. This problem can be solved by numerically solving a diffuse equation of a user-define quantity β. In this report, we will use Green's function to revisit the same problem. The procedure is detailed in Section 4.

In Section 5, the solution of 2D advection-diffusion equation, with a constant velocity, using Green's function method is discussed. The results are compared with the numerical results obtained using FTCS method.

2. Green's function for a 2D transient diffusion problem

In this section, we solve the Green's function solution for a 2D transient non-homogeneous diffusion problem. We adopt the homogeneous Dirichlet condition, that is, the quantity to be solved is zero on the boundaries.

$$\frac{\partial^2\Theta(x,y,t)}{\partial x^2}+\frac{\partial^2\Theta(x,y,t)}{\partial y^2}+\frac{1}{k}g(x,y,t>0)=\frac{1}{\alpha}\frac{\partial\Theta(x,y,t)}{\partial t}, \qquad 0<x<L_x,\ 0<y<L_y,$$

where, $\Theta =$ non-dimensional quantity $\qquad k =$ conductivity of the material

$\alpha =$ diffusivity of the material $\qquad g =$ source term

L_x and L_y are the length in the x- and y- directions

with Dirichlet Boundary Conditions (BCs): $\Theta\big|_{x=0}=\Theta\big|_{x=L_x}=\Theta\big|_{y=0}=\Theta\big|_{y=L_y}=0$

Initial Condition (IC): $\Theta\big|(x,y,t=0)=f(x,y)$

The solution, Θ, is the sum of the homogenous (Θ_h) and the Non-homogenous (Θ_p) solution,

$$\Theta=\Theta_h+\Theta_p$$

For the homogenous solution, Θ_h, it is the solution of the homogeneous part,

$$\frac{\partial^2\Theta_h(x,y,t)}{\partial x^2}+\frac{\partial^2\Theta_h(x,y,t)}{\partial y^2}=\frac{1}{\alpha}\frac{\partial\Theta_h(x,y,t)}{\partial t}, \qquad 0<x<L_x,\ 0<y<L_y$$

with BC: $\Theta_h\big|_{x=0}=\Theta_h\big|_{x=L_x}=\Theta_h\big|_{y=0}=\Theta_h\big|_{y=L_y}=0$

IC: $\Theta_h(x,y,t=0)=f(x,y)$

We solve this HG equation by using the method of separation of variable.

(i) Assume $\Theta_h(x,y,t)=\Gamma(t)X(x)Y(y)$, then the equation becomes,

$$\Gamma Y\frac{\partial^2 X}{\partial x^2}+\Gamma X\frac{\partial^2 Y}{\partial y^2}=\frac{1}{\alpha}XY\frac{\partial\Gamma}{\partial t}\Rightarrow\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=\frac{1}{\alpha\Gamma}\frac{\partial\Gamma}{\partial t}$$

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2}=-\lambda_1^2\ , \qquad \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=-\lambda_2^2\ , \qquad \frac{1}{\alpha\Gamma}\frac{\partial\Gamma}{\partial t}=-\lambda_1^2-\lambda_2^2$$

$$X(x)=C_1\sin\lambda_1 x+C_2\cos\lambda_1 x\ , \quad Y(y)=C_3\sin\lambda_2 y+C_4\cos\lambda_2 y\ , \quad \Gamma(t)=C_5e^{-\left(\lambda_1^2+\lambda_2^2\right)\alpha t}$$

(ii) The parameters C_1 and C_2 are obtained by using the BC,

$$\Theta_h\big|_{x=0}=0\Rightarrow C_2=0\ ; \quad \Theta_h\big|_{x=L_x}=0\Rightarrow C_1\sin\lambda_1 L_x=0\Rightarrow\lambda_1=\frac{m\pi}{L_x},\ m=1,2,3,...$$

(iii) Likewise for $Y(y)$:

$$\Theta_h\big|_{y=0} = 0 \Rightarrow C_4 = 0 \quad ; \quad \Theta_h\big|_{y=L_y} = 0 \Rightarrow C_3 \sin\lambda_2 L_y = 0 \Rightarrow \lambda_2 = \frac{n\pi}{L_y},\ n = 1,2,3,...$$

Hence, $\Theta_h = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} C_{mn}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha t}$, where $\lambda_m = \frac{m\pi}{L_x},\ \lambda_n = \frac{n\pi}{L_y}$

(iv) Now we solve C_{mn}.

First, we insert the IC into Θ_h, $f(x,y) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} C_{mn}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)$

Then we use the orthogonality of the eigenfunctions (which is sine function here)

$$\int_{x=0}^{L_x}\int_{y=0}^{L_y} f(x,y)\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)dxdy = C_{mn}\int_{x=0}^{L_x}\int_{y=0}^{L_y}\left(\sin^2\lambda_m x\right)\left(\sin^2\lambda_n y\right)dxdy,$$

hence, $C_{mn} = \dfrac{\int_{x=0}^{L_x}\int_{y=0}^{L_y} f(x,y)\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)dxdy}{\int_{x=0}^{L_x}\int_{y=0}^{L_y}\left(\sin^2\lambda_m x\right)\left(\sin^2\lambda_n y\right)dxdy}$,

where $\int_{x=0}^{L_x}\int_{y=0}^{L_y}\left(\sin^2\lambda_m x\right)\left(\sin^2\lambda_n y\right)dxdy = \int_{x=0}^{L_x}\left(\sin^2\lambda_m x\right)dx\int_{y=0}^{L_y}\left(\sin^2\lambda_n y\right)dy$,

where $\int_{x=0}^{L_x}\left(\sin^2\lambda_m x\right)dx = \int_{x=0}^{L_x}\frac{1}{2}\left[1-\cos 2\lambda_m x\right]dx = \frac{1}{2}\left[x - \frac{\sin 2\lambda_m x}{2\lambda_m}\right]_0^{L_x} = \frac{1}{2}\left[L_x - \frac{\sin\left(2\lambda_m L_x\right)}{2\lambda_m}\right]$,

$$\int_{y=0}^{L_y}\left(\sin^2\lambda_n y\right)dy = \frac{1}{2}\left[L_y - \frac{\sin\left(2\lambda_n L_y\right)}{2\lambda_n}\right]$$

Thus, $\int_{x=0}^{L_x}\int_{y=0}^{L_y}\left(\sin^2\lambda_m x\right)\left(\sin^2\lambda_n y\right)dxdy = \frac{1}{4}\left[L_x - \frac{\sin\left(2\lambda_m L_x\right)}{2\lambda_m}\right]\left[L_y - \frac{\sin\left(2\lambda_n L_y\right)}{2\lambda_n}\right] = \frac{1}{4}L_x L_y$

Consequently, the homogeneous solution, Θ_h, is,

$$\Theta_h = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{4\int_{x'=0}^{L_x}\int_{y'=0}^{L_y} f(x',y')\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)dx'dy'}{L_x L_y}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha t}$$

$$= \int_{x'=0}^{L_x}\int_{y'=0}^{L_y}\frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha t}\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)f(x',y')dx'dy'$$

where $\lambda_m = \frac{m\pi}{L_x}, \quad \lambda_n = \frac{n\pi}{L_y}$.

Once having the homogeneous solution, we can easily obtain the Green's function, G, by the following relationship [1],

$$\Theta_h(x,y,t) = \int_{x'=0}^{L_x}\int_{y'=0}^{L_y} G\left(x,y,t;x',y',\tau\right)\Big|_{\tau=0} f(x',y')\,dx'dy'$$

Thus, $G(x,y,t;x',y',\tau)\big|_{\tau=0} = \frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-(\lambda_m^2+\lambda_n^2)\alpha t}(\sin\lambda_m x')(\sin\lambda_n y')$

The desired Green's function is obtained by replacing t by $t-\tau$,

$$G(x,y,t;x',y',\tau) = \frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}(\sin\lambda_m x')(\sin\lambda_n y')$$

With the Green's function, we can easily obtain the particular solution for the non-homogeneous part,

$$\frac{\partial^2\Theta_p(x,y,t)}{\partial x^2}+\frac{\partial^2\Theta_p(x,y,t)}{\partial y^2}+\frac{1}{k}g(x,y,t>0)=\frac{1}{\alpha}\frac{\partial\Theta_p(x,y,t)}{\partial t}, \qquad 0<x<L_x,\ 0<y<L_y,$$

BC: $\Theta_p\big|_{x=0} = \Theta_p\big|_{x=L_x} = \Theta_p\big|_{y=0} = \Theta_p\big|_{y=L_y} = 0$

IC: $\Theta_p\big|(x,y,t=0) = f(x,y)$

$\Theta_p(x,y,t) = \frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}G(x,y,t;x',y',\tau)g(x',y',\tau)dx'dy'$ [1],

where $G(x,y,t;x',y',\tau) = \frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}(\sin\lambda_m x')(\sin\lambda_n y')$

The final solution is, $\Theta(x,y,t) = \Theta_h(x,y,t)+\Theta_p(x,y,t)$,

$$\Theta_h(x,y,t) = \int_{x'=0}^{L_x}\int_{y'=0}^{L_y}G(x,y,t;x',y',\tau)\big|_{\tau=0}f(x',y')dx'dy'$$

where $G(x,y,t;x',y',\tau)\big|_{\tau=0} = \frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-(\lambda_m^2+\lambda_n^2)\alpha t}(\sin\lambda_m x')(\sin\lambda_n y')$.

$$\Theta_p(x,y,t) = \frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}G(x,y,t;x',y',\tau)g(x',y',\tau)dx'dy',$$

where $G(x,y,t;x',y',\tau) = \frac{4}{L_x L_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}(\sin\lambda_m x')(\sin\lambda_n y')$.

2-1. Multiplicative property of the Green's function

In the previous section, we derived the Green's function solution for a 2D transient non-homogeneous diffusion equation. Before applying this solution to the numerical examples, it is worth noting that there is an important property of the Green's function: for an multi-dimensional Green's function solution, it can be decomposed into the product of the fundamental 1D Green's function. That is, for a 2D Greens' function,

$$G(x,y,t;x',y',\tau) = G_1(x,t;x',\tau) \times G_2(y,t;y',\tau)$$

The importance of this property is that with the knowledge of the 1D Green's function which is easy to obtain, we can directly construct a higher dimensional Green's function which is sometimes not trivial to solve.

The proof of this property is given below following the work of Beck [2].

Consider the source term $g(x,y,t) = \delta(x-x')\delta(y-y')\delta(t-\tau)$.

Then a typical diffusion equation becomes,

$$\frac{\partial^2 \Theta(x,y,t)}{\partial x^2} + \frac{\partial^2 \Theta(x,y,t)}{\partial y^2} + \frac{1}{k}\delta(x-x')\delta(y-y')\delta(t-\tau) = \frac{1}{\alpha}\frac{\partial \Theta(x,y,t)}{\partial t} \quad -(e1)$$

The fundamental solution of this equation is the Green's function, $G(x,y,t;x',y',\tau)$.

Assume $G(x,y,t;x',y',\tau) = G_1(x,t;x',\tau)G_2(y,t;y',\tau) \quad -(e2)$

where $G_1(x,t;x',\tau)$ is the solution of $\frac{\partial^2 \Theta(x,t)}{\partial x^2} + \frac{1}{k}\delta(x-x')\delta(t-\tau) = \frac{1}{\alpha}\frac{\partial \Theta(x,t)}{\partial t}$,

that is, $\frac{\partial^2 G_1}{\partial x^2} - \frac{1}{\alpha}\frac{\partial G_1}{\partial t} = -\frac{1}{k}\delta(x-x')\delta(t-\tau) \quad -(e2a)$.

And, $G_2(y,t;y',\tau)$ is the solution of $\frac{\partial^2 \Theta(y,t)}{\partial y^2} + \frac{1}{k}\delta(y-y')\delta(t-\tau) = \frac{1}{\alpha}\frac{\partial \Theta(y,t)}{\partial t}$,

that is, $\frac{\partial^2 G_2}{\partial y^2} - \frac{1}{\alpha}\frac{\partial G_2}{\partial t} = -\frac{1}{k}\delta(y-y')\delta(t-\tau) \quad -(e2b)$

Since G is the fundamental solution of the equation, it shows,

$$G_2\frac{\partial^2 G_1}{\partial x^2} + G_1\frac{\partial^2 G_2}{\partial y^2} + \frac{1}{k}\delta(x-x')\delta(y-y')\delta(t-\tau) = \frac{1}{\alpha}G_2\frac{\partial G_1}{\partial t} + \frac{1}{\alpha}G_1\frac{\partial G_2}{\partial t}$$

$$G_2\left(\frac{\partial^2 G_1}{\partial x^2} - \frac{1}{\alpha}\frac{\partial G_1}{\partial t}\right) + G_1\left(\frac{\partial^2 G_2}{\partial y^2} - \frac{1}{\alpha}\frac{\partial G_2}{\partial t}\right) = -\frac{1}{k}\delta(x-x')\delta(y-y')\delta(t-\tau) \quad -(e3)$$

Because,

$$\text{LHS of } G_2 \times (e2a) + \text{LHS of } G_1 \times (e2b) = \text{LHS of } (e3),$$

we can obtain that,

$$\text{RHS of } G_2 \times (e2a) + \text{RHS of } G_1 \times (e2b) = \text{RHS of } (e3).$$

That is, $-\dfrac{1}{k}G_2\delta(x-x')\delta(t-\tau)-\dfrac{1}{k}G_1\delta(y-y')\delta(t-\tau)=-\dfrac{1}{k}\delta(x-x')\delta(y-y')\delta(t-\tau)$, if $G=G_1G_2$.

Namely, $G_2\delta(x-x')\delta(t-\tau)+G_1\delta(y-y')\delta(t-\tau)=\delta(x-x')\delta(y-y')\delta(t-\tau)$, if $G=G_1G_2$ $-(e4)$

From $(e2a)$, we know that G_1 is proportional to $\delta(x-x')H(t-\tau)$, yielding,

$$G_1 = C_1\delta(x-x')H(t-\tau)$$

From $(e2b)$, we know that G_2 is proportional to $\delta(y-y')H(t-\tau)$, yielding,

$$G_2 = C_2\delta(y-y')H(t-\tau)$$

Thus, $G_2\delta(x-x')\delta(t-\tau)+G_1\delta(y-y')\delta(t-\tau)=$

$$C_2\delta(y-y')H(t-\tau)\delta(x-x')\delta(t-\tau)+C_1\delta(x-x')H(t-\tau)\delta(y-y')\delta(t-\tau) \quad -(e5)$$

Since $\int_{t=-\infty}^{\infty}H(t-\tau)\delta(t-\tau)dt=\int_{t=-\infty}^{\infty}H(t-\tau)dH=\frac{1}{2}H^2\Big|_{-\infty}^{\infty}=\frac{1}{2}=\int_{t=-\infty}^{\infty}\frac{1}{2}\delta(t-\tau)dt$, or,

$$\int_{t=-\infty}^{\infty}H(t-\tau)\delta(t-\tau)dt=\int_{t=-\infty}^{\infty}\frac{1}{2}\delta(t-\tau)dt,$$

It shows,

$$H(t-\tau)\delta(t-\tau)=\frac{1}{2}\delta(t-\tau) \quad -(e6)$$

Insert $(e6)$ into $(e5)$,

$$\begin{aligned}
&G_2\delta(x-x')\delta(t-\tau)+G_1\delta(y-y')\delta(t-\tau)\\
&=\frac{1}{2}C_2\delta(y-y')\delta(x-x')\delta(t-\tau)+\frac{1}{2}C_1\delta(x-x')\delta(y-y')\delta(t-\tau)\\
&=\frac{1}{2}\delta(y-y')\delta(x-x')\delta(t-\tau)\left(C_1+C_2\right)\\
&=\delta(x-x')\delta(y-y')\delta(t-\tau), \text{ by setting } C_1=C_2=1
\end{aligned}$$

Since $G_2\delta(x-x')\delta(t-\tau)+G_1\delta(y-y')\delta(t-\tau)\sim\delta(x-x')\delta(y-y')\delta(t-\tau)$ which indicates that $(e4)$ is true, it proves that $\underline{G(x,y,t;x',y',\tau)=G_1(x,t;x',\tau)\times G_2(y,t;y',\tau)}$

3. Numerical examples

In this section, we will apply the Green's function solutions in Section-1 to analytically solve two different diffusion problems respectively with the source term being (i) a delta function and (ii) a constant. To narrow down the scope of analysis, the initial condition is set to be zero, so we don't need to deal with the part of the homogeneous solution.

For comparison, we also employ the numerical method to obtain the numerical solution. To reduce the difficulty of the coding, the numerical methods are rooted in the finite difference method with Forward-Time Central-Space (FCTS) scheme [3]. We don't consider Crank-Nicolson scheme which is more difficult to code, although it is more accurate and stable.

*Example-1***:** *Point source; Implemented using a 2D delta function*

The first example considers a point source term which is implemented as a 2D delta function. That is, $g(x', y') = \delta(x', y')$, which allows for some simplifications.

$$\frac{\partial^2\Theta(x,y,t)}{\partial x^2}+\frac{\partial^2\Theta(x,y,t)}{\partial y^2}+\frac{1}{k}\delta(x-x',y-y')=\frac{1}{\alpha}\frac{\partial\Theta(x,y,t)}{\partial t}, \qquad 0<x<L_x,\ 0<y<L_y,$$

BC: $\Theta\big|_{x=0}=\Theta\big|_{x=L_x}=\Theta_{y=0}=\Theta_{y=L_y}=0$; IC: $\Theta(x,y,t=0)=f(x',y')=0$

and $L_x=1,\ L_y=1,\ k=1,\ \alpha=1,\ x'=0.2,\ y'=0.2$

The analytical solution is, $\Theta(x,y,t)=\Theta_h(x,y,t)+\Theta_p(x,y,t)$,

(i) $\Theta_h(x,y,t)=\int_{x'=0}^{L_x}\int_{y'=0}^{L_y}G(x,y,t;x',y',\tau)\big|_{\tau=0}f(x',y')dx'dy'=0$

(ii)
$$\begin{aligned}\Theta_p(x,y,t)&=\frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}G(x,y,t;x',y',\tau)\delta(x-x',y-y')dx'dy'\\
&=\frac{\alpha}{k}\int_{\tau=0}^{t}G(x',y',t;\tau)d\tau\\
&=\frac{\alpha}{k}\frac{4}{L_xL_y}\int_{\tau=0}^{t}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha(t-\tau)}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)d\tau\\
&=\frac{\alpha}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\left[e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha(t-\tau)}\right]_{\tau=0}^{t}}{\left(\lambda_m^2+\lambda_n^2\right)\alpha}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)\\
&=\frac{4}{kL_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\left[1-e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha t}\right]}{\left(\lambda_m^2+\lambda_n^2\right)}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)\end{aligned}$$

Thus, $\Theta(x,y,t)=\frac{4}{kL_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\left[1-e^{-\left(\lambda_m^2+\lambda_n^2\right)\alpha t}\right]}{\left(\lambda_m^2+\lambda_n^2\right)}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)\left(\sin\lambda_m x'\right)\left(\sin\lambda_n y'\right)$,

where $\lambda_m=\frac{m\pi}{L_x}$, $\lambda_n=\frac{n\pi}{L_y}$

The numerical solution based on the FTCS scheme is determined as follows. First, we decompose the 2D delta function into the product of 1D delta function, and rewrite them as the derivative of the Heavside function,

$$\delta(x-x',y-y')=\delta_1(x-x')\delta_2(y-y')=\frac{dH_1(x-x')}{dx}\frac{dH_2(y-y')}{dy}.$$

Hence, the equation becomes,

$$\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial y^2}+\frac{1}{k}\frac{dH_1(x-x')}{dx}\frac{dH_2(y-y')}{dy}=\frac{1}{\alpha}\frac{\partial\Theta}{\partial t}$$

The discretized version using the finite difference approach with the FTCS scheme is,

$$\frac{1}{\alpha}\left(\frac{\Theta_{i,j}^{n+1}}{\Delta t}-\frac{\Theta_{i,j}^{n}}{\Delta t}\right)=\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta x^2}+\frac{\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta y^2}+\frac{1}{k}\frac{H_{1,i+1}-H_{1,i-1}}{2\Delta x}\frac{H_{2,j+1}-H_{2,j-1}}{2\Delta y}$$

$$\frac{\Theta_{i,j}^{n+1}}{\Delta t}=\frac{\Theta_{i,j}^{n}}{\Delta t}+\alpha\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta x^2}+\alpha\frac{\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta y^2}+\alpha\frac{1}{k}\frac{H_{1,i+1}-H_{1,i-1}}{2\Delta x}\frac{H_{2,j+1}-H_{2,j-1}}{2\Delta y}$$

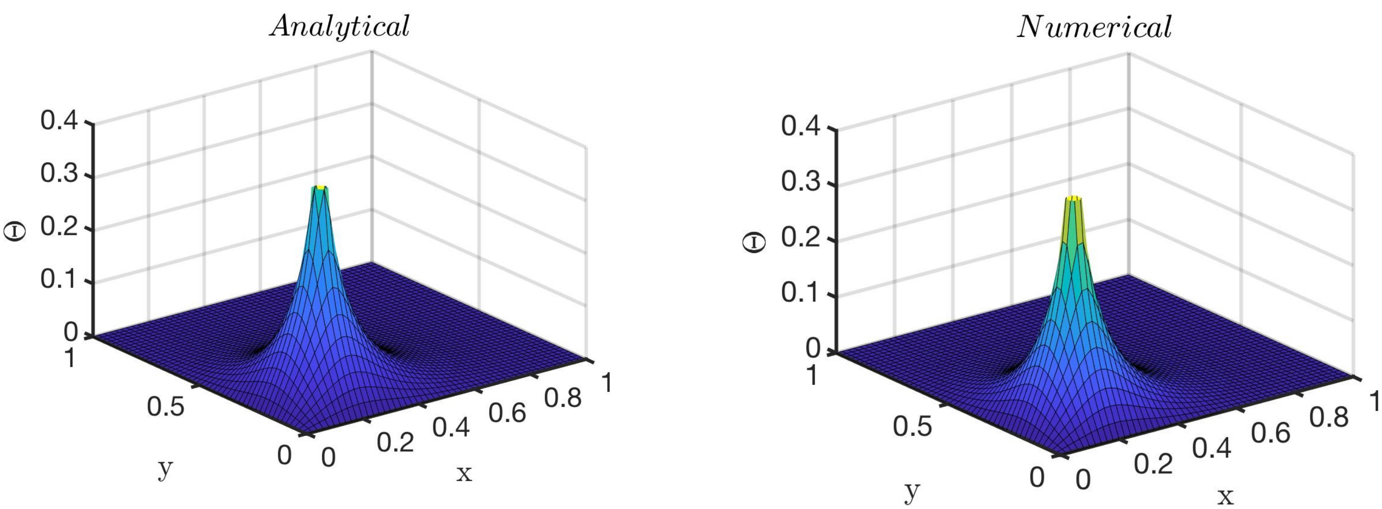
Thus, $$\Theta_{i,j}^{n+1}=\Theta_{i,j}^{n}+\left(\frac{\alpha\Delta t}{\Delta x^2}\right)\left(\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}\right)+\left(\frac{\alpha\Delta t}{\Delta y^2}\right)\left(\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}\right)+\left(\frac{\alpha\Delta t}{4k\Delta x\Delta y}\right)\left(H_{1,i+1}-H_{1,i-1}\right)\left(H_{2,j+1}-H_{2,j-1}\right)$$

The numerical solution is coded using the MATLAB programming.

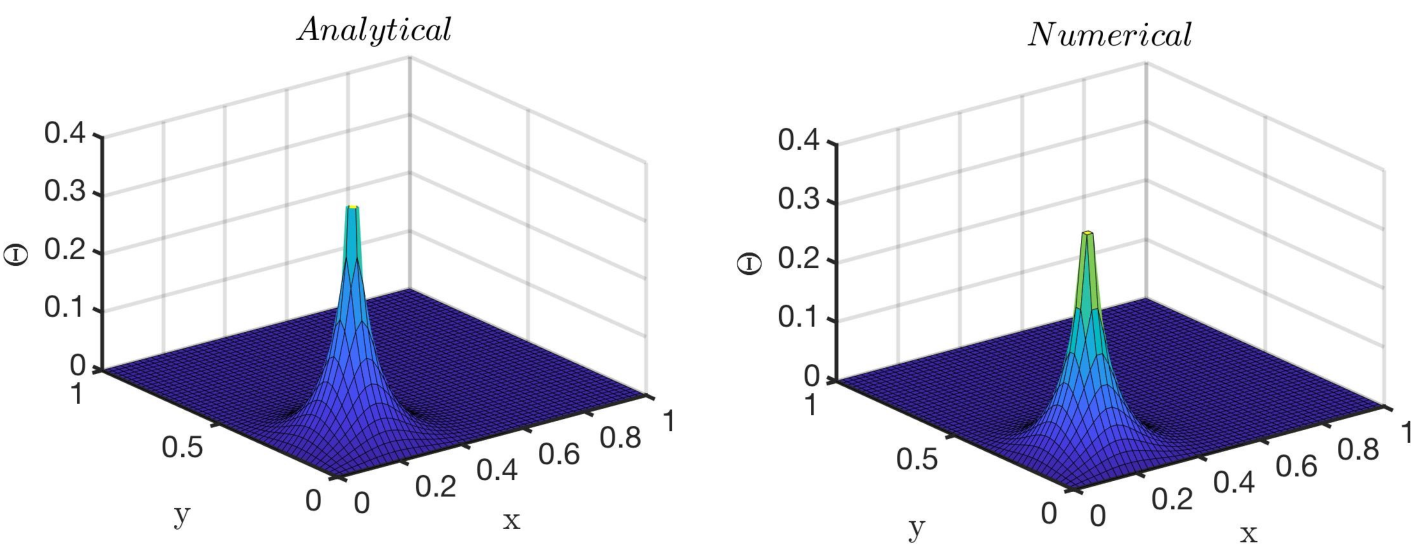
The spatial and temporal resolutions are, $\Delta x=\Delta y=0.02$, and $\Delta t=\frac{(\Delta x)^2}{4\alpha}$ to make the solutions stable.

Below are the analytical solution (left) and the numerical solution (right) at two different time instances for *Example-1*.

(i) At $t = 0.01$



(ii) At $t = 0.05$



Clearly, it shows that the analytical solution is qualitatively consistent with the numerical solution.

*Example-2***:** *Constant source throughout the domain*

The second example considers a constant source term throughout the entire computational domain. That is, $g(x', y') = C_1$.

$$\frac{\partial^2\Theta(x,y,t)}{\partial x^2}+\frac{\partial^2\Theta(x,y,t)}{\partial y^2}+\frac{C_1}{k}=\frac{1}{\alpha}\frac{\partial\Theta(x,y,t)}{\partial t},\qquad 0<x<L_x,\ 0<y<L_y,$$

BC: $\Theta\big|_{x=0}=\Theta\big|_{x=L_x}=\Theta_{y=0}=\Theta_{y=L_y}=0$; IC: $\Theta(x,y,t=0)=f(x',y')=0$

and $L_x=1,\ L_y=1,\ k=1,\ \alpha=1,\ C_1=2$

The analytical solution is, $\Theta(x,y,t)=\Theta_h(x,y,t)+\Theta_p(x,y,t)$,

(i) $\Theta_h(x,y,t)=\int_{x'=0}^{L_x}\int_{y'=0}^{L_y}G(x,y,t;x',y',\tau)\big|_{\tau=0}f(x',y')dx'dy'=0$

(ii) $$\Theta_p(x,y,t)=\frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}(\sin\lambda_m x')(\sin\lambda_n y')C_1\,dx'\,dy'$$

$$=\frac{\alpha C_1}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)\int_{\tau=0}^{t}e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}(\sin\lambda_m x')(\sin\lambda_n y')dx'\,dy'$$

$$=\frac{\alpha C_1}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)\int_{\tau=0}^{t}e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}\left(-\frac{1}{\lambda_n}\cos\lambda_n y'\right)_0^b\left(-\frac{1}{\lambda_m}\cos\lambda_m x'\right)_0^a d\tau$$

$$=\frac{\alpha C_1}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)\frac{1}{\alpha(\lambda_m^2+\lambda_n^2)}\left[e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}\right]_{\tau=0}^{t}\left(-\frac{1}{\lambda_n}\cos\lambda_n y'\right)_0^b\left(-\frac{1}{\lambda_m}\cos\lambda_m x'\right)_0^a$$

$$=\frac{\alpha C_1}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(\sin\lambda_m x)(\sin\lambda_n y)}{\alpha(\lambda_m^2+\lambda_n^2)}\left[1-e^{-\alpha t(\lambda_m^2+\lambda_n^2)}\right]\left(-\frac{1}{\lambda_n}\cos\lambda_n b+\frac{1}{\lambda_n}\right)\left(-\frac{1}{\lambda_m}\cos\lambda_m a+\frac{1}{\lambda_m}\right)$$

Thus, $$\Theta(x,y,t)=\frac{\alpha C_1}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(\sin\lambda_m x)(\sin\lambda_n y)}{\alpha(\lambda_m^2+\lambda_n^2)}\left[1-e^{-\alpha t(\lambda_m^2+\lambda_n^2)}\right]\left(-\frac{1}{\lambda_n}\cos\lambda_n b+\frac{1}{\lambda_n}\right)\left(-\frac{1}{\lambda_m}\cos\lambda_m a+\frac{1}{\lambda_m}\right),$$

where $\lambda_m=\frac{m\pi}{L_x},\ \lambda_n=\frac{n\pi}{L_y}$

The numerical solution using FTCS scheme is determined as follows.

The discretized version using the finite difference approach with the FTCS scheme is,

$$\frac{1}{\alpha}\left(\frac{\Theta_{i,j}^{n+1}}{\Delta t}-\frac{\Theta_{i,j}^{n}}{\Delta t}\right)=\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta x^2}+\frac{\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta y^2}+\frac{C}{k}$$

$$\frac{\Theta_{i,j}^{n+1}}{\Delta t}=\frac{\Theta_{i,j}^{n}}{\Delta t}+\alpha\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta x^2}+\alpha\frac{\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta y^2}+\frac{\alpha C}{k}$$

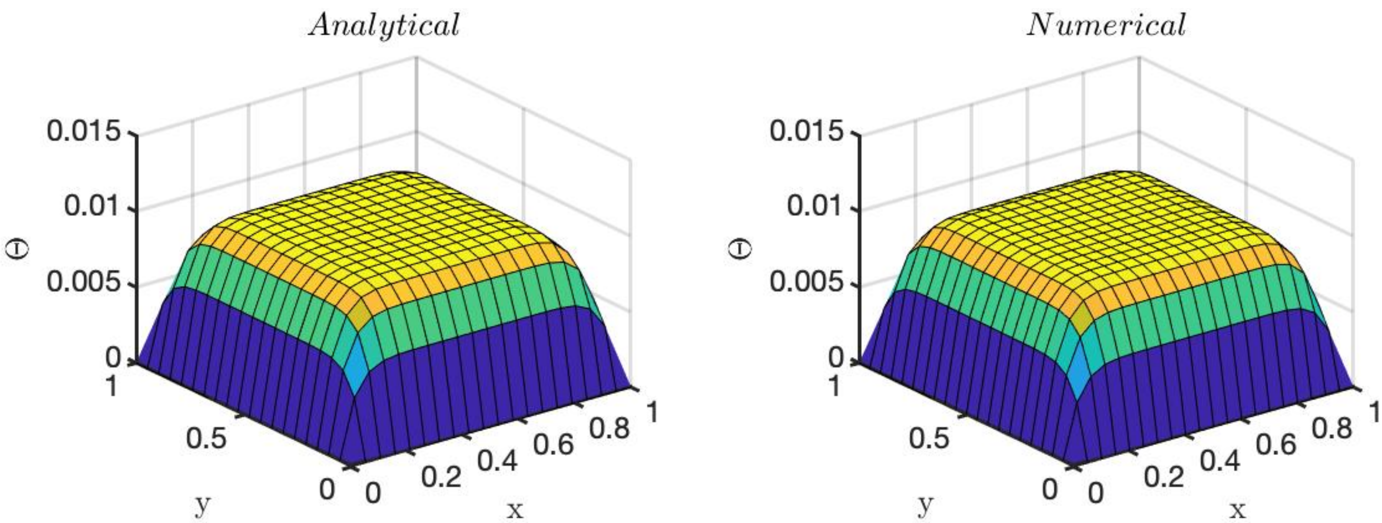
Thus, $$\Theta_{i,j}^{n+1}=\Theta_{i,j}^{n}+\left(\frac{\alpha\Delta t}{\Delta x^2}\right)\left(\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}\right)+\left(\frac{\alpha\Delta t}{\Delta y^2}\right)\left(\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}\right)+\frac{\alpha C\Delta t}{k}$$

The numerical solution is coded using the MATLAB programming.

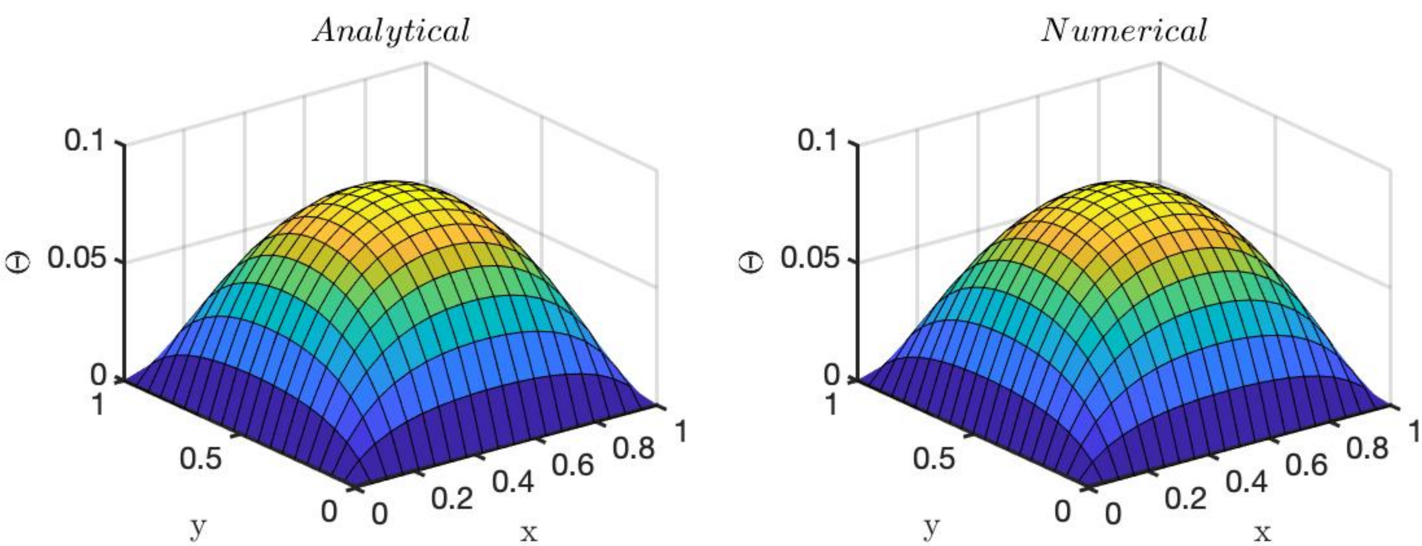
The spatial and temporal resolutions are, $\Delta x=\Delta y=0.02$, and $\Delta t=\frac{(\Delta x)^2}{4\alpha}$ to make the solutions stable.

Below are the analytical solution (left) and the numerical solution (right) at two different time instances for *Example-2*.

(i) At $t = 0.005$



(ii) At $t = 0.05$



Again, it shows that the analytical solution is qualitatively consistent with the numerical solution.

4. Applications: Structure identification in the two-phase flows

After the examination for the standard problems, we move on to the applications of the Green's function. The topic comes from one of our group research problem. Our group works on the two-phase flow simulations using the Volume of Fluid (VoF) method [4]. The principal interest of the VoF method is that the two-phase interface is advected by solving the the transport of the liquid fraction field (α). In our works, we define that $\alpha > 0.95$ if the current computational cell contains the liquid structure only. Likewise, $\alpha < 0.05$ if the cell purely contains the gas elements.

Unlike the straightforward classification of the liquid and gas cells, two different types of cells are defined for $0.05 < \alpha < 0.95$ representing the mixture of gas and liquid structures, for the purpose of accounting for the possible numerical issue. If the cell is topologically connected with the liquid element, it is defined as the interfacial cell which physically contains the gas-liquid interface. In contrast, if the cell is topologically disconnected with the liquid structures, it is called as the unresolved (liquid) structures since it stems from the problem of insufficient mesh resolution instead of physics.

Our focus is on how to identify the liquid, interfacial, unresolved, and gas structures. In our previous researches, we found out that this problem can be solved by numerically solving the discretized version of the following diffuse equation

$$\frac{d\beta}{dt} = D_1\left(\frac{\partial^2 \beta}{dx^2} + \frac{\partial^2 \beta}{dy^2}\right) + Q_1$$

- $D_1 = 0,\ Q_1 = 0$ if $\alpha < 0.05$ (gas)
- $D_1 = 1,\ Q_1 = 10^{-10}\delta\left(x - x_1, y - y_1\right)$ if $\alpha \geq 0.95$ (liquid)
- $D_1 = 1,\ Q_1 = 0$ if $0.05 \leq \alpha < 0.95$ (interface or unresolved)

where $\left(x_1, y_1\right)$ is the center cell of the liquid structures.

because of the source term in the liquid cell, the β value of the interfacial cell must be larger than that of unresolved cells due to the stronger effect of diffusion of β.

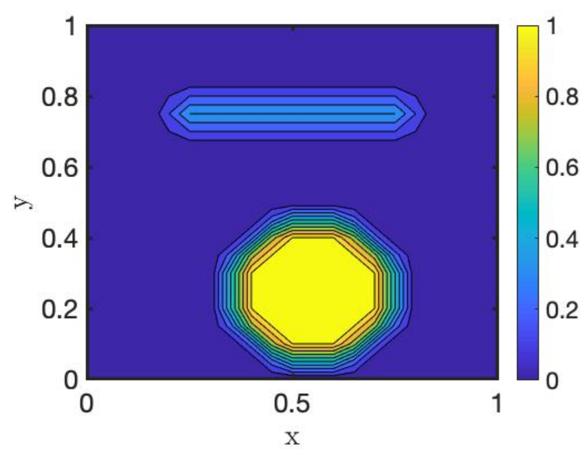
$$\beta = \frac{4 \text{ x } 10^{-10}}{kL_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\left[1 - e^{-\left(\lambda_m^2 + \lambda_n^2\right)D_1 t}\right]}{\left(\lambda_m^2 + \lambda_n^2\right)}\left(\sin\lambda_m x\right)\left(\sin\lambda_n y\right)\left(\sin\lambda_m x_1\right)\left(\sin\lambda_n y_1\right),$$

In this project, instead of solving the equation for β numerically, we solve the problem using the Green's function solution, which was given in *Example-1* (use delta function as the source term). The liquid, unresolved, interface, and gas structures are then identified by,

- liquid structure: $\beta > 3 \text{ x}10^{-12}$ and $\alpha > 0.95$
- unresolved structure: $\beta < 3 \text{ x}10^{-12}$ and $0.05 < \alpha < 0.95$
- interface: $\beta > 3 \text{ x}10^{-12}$ and $0.05 < \alpha < 0.95$
- gas structure: $\alpha < 0.05$

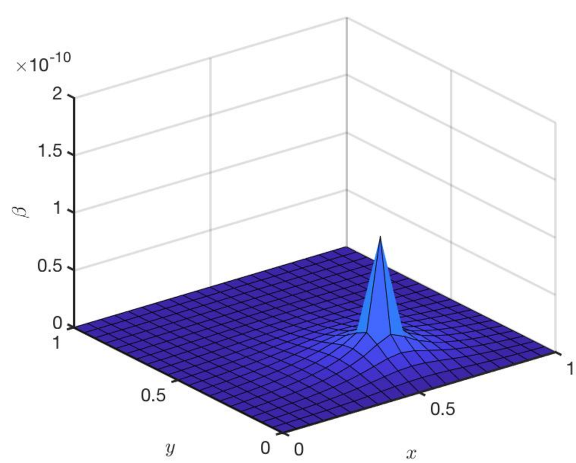
Below is the step-by step result using the MATLAB programming.

i) The initially liquid fraction fields with all the structures presented



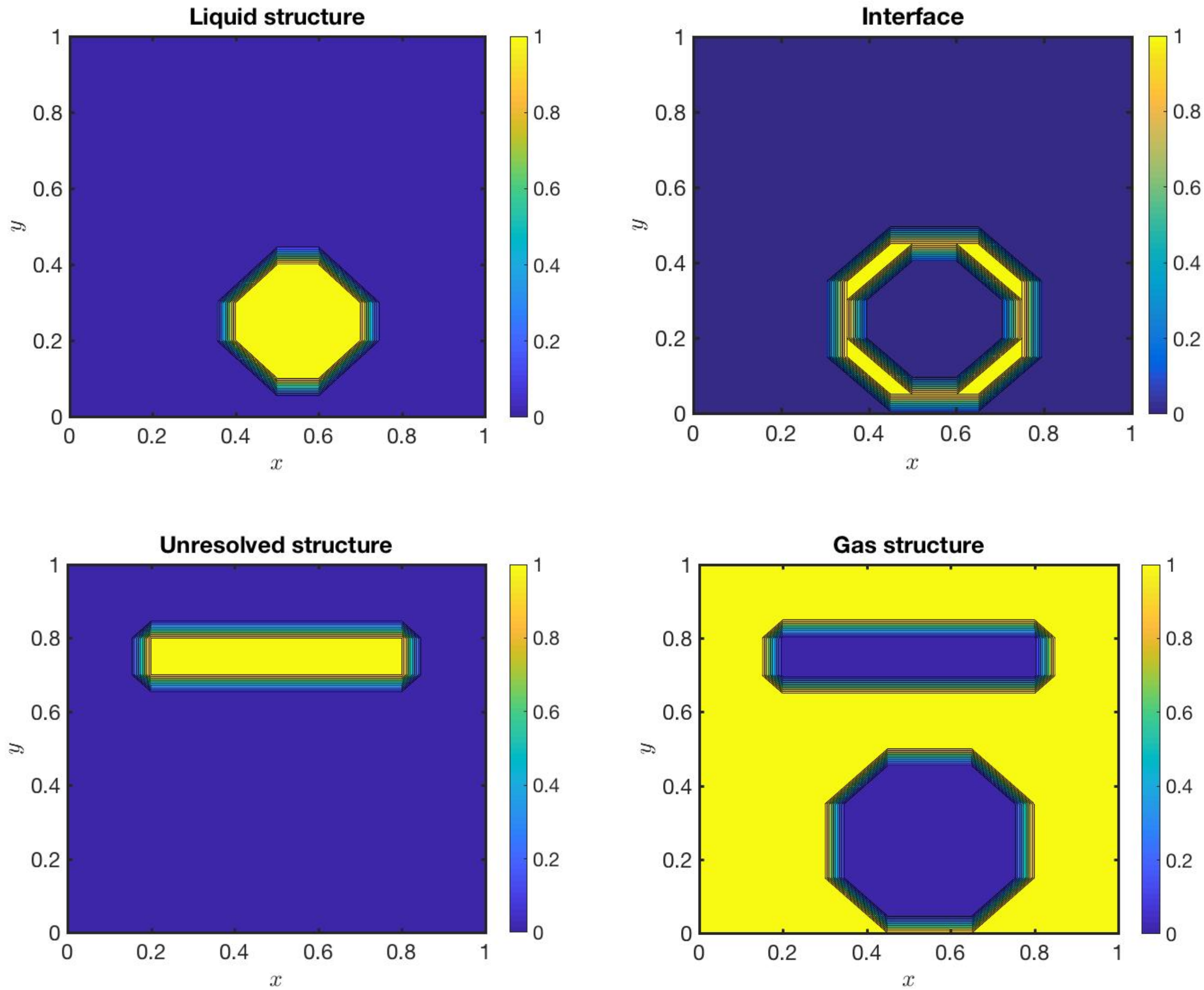
ii) The constructed β field:

The delta function as the source term is displaced in the center of the liquid structures $(x_1, y_1) = (0.55, 0.25)$



iii) The results of identification:

Liquid structure (top-left), Interface (top-right), Unresolved structure (bottom-left), and Gas structure (bottom-right).



It shows that the Greens' function solutions perform well for identifying the four different structures.

5. Green's function solution for a 2D advection-diffusion problem

Up to this point, we have finished the analysis of the Green's function for a 2D diffusion problem. As an extra topic in the last section, we will use the Green's function to solve a 2D linear advection-diffusion equation which includes the effect of advection.

$$\frac{1}{\alpha}\frac{\partial\Theta}{\partial t}+U\frac{\partial\Theta}{\partial x}+U\frac{\partial\Theta}{\partial y}=\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial y^2}+\frac{g}{k}, \qquad 0\le x\le L_x,\ 0\le y\le L_y$$

BC: $\Theta_{x=0}=\Theta_{x=L_x}=\Theta_{y=0}=\Theta_{y=L_y}=0$

IC: $\Theta(x,y,t=0)=F(x,y)$

Based on the work of Avhale and Kiwne [5], the solution is,

$$\Theta=\theta(x,y,t)\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]=\theta\exp[M(x,y,t)],$$

where $M(x,y,t)=\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t$

This can be easily confirmed when inserting this solution into the equation,

(i) $\frac{\partial\Theta}{\partial t}=\exp(M)\frac{\partial\theta}{\partial t}+\theta\exp(M)\left(-\frac{U^2\alpha}{2}\right)$; (ii) $\frac{\partial\Theta}{\partial x}=\exp(M)\frac{\partial\theta}{\partial x}+\theta\exp(M)\left(\frac{U}{2}\right)$

(iii) $\frac{\partial\Theta}{\partial y}=\exp(M)\frac{\partial\theta}{\partial y}+\theta\exp(M)\left(\frac{U}{2}\right)$;

(iv) $\frac{\partial^2\Theta}{\partial x^2}=\exp(M)\frac{\partial^2\theta}{\partial x^2}+\frac{\partial\theta}{\partial x}\exp(M)\left(\frac{U}{2}\right)+e^{\mathrm{M}}\frac{\partial\theta}{\partial x}\left(\frac{U}{2}\right)+\theta\exp(M)\left(\frac{U^2}{4}\right)$

(v) $\frac{\partial^2\Theta}{\partial y^2}=\exp(M)\frac{\partial^2\theta}{\partial y^2}+\frac{\partial\theta}{\partial y}\exp(M)\left(\frac{U}{2}\right)+\exp(M)\frac{\partial\theta}{\partial y}\left(\frac{U}{2}\right)+\theta\exp(M)\left(\frac{U^2}{4}\right)$

Insert (i) - (v) into the equation:

$$\frac{1}{\alpha}\left[\frac{\partial\theta}{\partial t}+\theta\left(-\frac{U^2\alpha}{2}\right)\right]+U\left[\begin{array}{c}\frac{\partial\theta}{\partial x}+\theta\left(\frac{U}{2}\right)\\+\frac{\partial\theta}{\partial y}+\theta\left(\frac{U}{2}\right)\end{array}\right]=\left[\begin{array}{c}\frac{\partial^2\theta}{\partial x^2}+\frac{\partial\theta}{\partial x}\left(\frac{U}{2}\right)+\frac{\partial\theta}{\partial x}\left(\frac{U}{2}\right)+\theta\left(\frac{U^2}{4}\right)+\frac{\partial^2\theta}{\partial y^2}\\+\frac{\partial\theta}{\partial y}\left(\frac{U}{2}\right)+\frac{\partial\theta}{\partial y}\left(\frac{U}{2}\right)+\theta\left(\frac{U^2}{4}\right)+\frac{g}{k\exp(M)}\end{array}\right]$$

After simplification, it shows the advection-diffusion equation is converted into a diffusion equation,

$$\frac{1}{\alpha}\frac{\partial\theta}{\partial t}=\frac{\partial^2\theta}{\partial x^2}+\frac{\partial^2\theta}{\partial y^2}+\frac{g}{k\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]},\qquad 0\le x\le L_x,\ 0\le y\le L_y$$

BC: $\theta_{x=0}=\theta_{x=L_x}=\theta_{y=0}=\theta_{y=L_y}=0$

IC: $\Theta(x,y,t=0)=F(x,y)=\theta(x,y,t=0)\exp\left[\frac{U}{2}(x+y)\right]$, i.e., $\theta(x,y,t=0)=f(x,y)=F(x,y)e^{\frac{-U(x+y)}{2}}$

Now we can easily solve this diffusion equation by by Green's function. From the previous derivation,

$$\theta=\theta_h+\theta_p$$

(i) $\theta_h=\int_{x'=0}^{L_x}\int_{y'=0}^{L_y}G(x,y,t;x',y',\tau)\big|_{\tau=0}\left\{F(x',y')\exp\left[\frac{-U(x'+y')}{2}\right]\right\}dx'dy'$

$$G(x,y,t;x',y',\tau)\big|_{\tau=0}=\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-(\lambda_m^2+\lambda_n^2)\alpha t}(\sin\lambda_m x')(\sin\lambda_n y')$$

(ii) $\theta_p(x,y,t)=\frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}G(x,y,t;x',y',\tau)\frac{g(x',y',\tau)}{\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]}dx'\,dy'$

$$G(x,y,t;x',y',\tau)=\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)e^{-\alpha(\lambda_m^2+\lambda_n^2)(t-\tau)}(\sin\lambda_m x')(\sin\lambda_n y')$$

where $\lambda_m=\frac{m\pi}{L_x},\quad \lambda_n=\frac{n\pi}{L_y}$.

Then we obtain the actual solution, Θ, which is,

$$\Theta=\theta_h\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]+\theta_p\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right],\quad 0\le x\le L_x,\ 0\le y\le L_y$$

5-1. *Example-3: Point source; Implemented using a 2D delta function*

We present an example pertaining to the 2D advection-diffusion equation. The point source term is again implemented as a 2D delta function, i.e., $g(x', y') = \delta(x', y')$,

$$\frac{1}{\alpha}\frac{\partial\Theta}{\partial t}+U\frac{\partial\Theta}{\partial x}+U\frac{\partial\Theta}{\partial y}=\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial y^2}+\frac{\delta(x-x_s,y-y_s)}{k},\qquad 0\le x\le L_x,\ 0\le y\le L_y$$

BC: $\Theta_{x=0}=\Theta_{x=L_x}=\Theta_{y=0}=\Theta_{y=L_y}=0$

IC: $\Theta(x,y,t=0)=F(x,y)=0$

and $L_x=1,\ L_y=1,\ k=1,\ \alpha=1,\ U=1,\ x'=0.2,\ y'=0.2$

The analytical solution is, $\boxed{\Theta=\theta_h\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]+\theta_p\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]}$

(i) $\theta_h=\int_{x'=0}^{L_x}\int_{y'=0}^{L_y}G(x,y,t;x',y',\tau)\big|_{\tau=0}\left[F(x',y')e^{\frac{-U(x'+y')}{2}}\right]dx'dy'=0$

(ii) $\theta_p(x,y,t)=\frac{\alpha}{k}\int_{\tau=0}^{t}d\tau\int_{x'=0}^{a}\int_{y'=0}^{b}G(x,y,t;x',y',\tau)\frac{\delta(x-x_s,y-y_s)}{\exp\left[\frac{U}{2}(x+y)-\frac{U^2\alpha}{2}t\right]}dx'\,dy'$

$$=\frac{\alpha}{k}\int_{\tau=0}^{t}\frac{\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)\exp\left[-\alpha\left(\lambda_m^2+\lambda_n^2\right)(t-\tau)\right](\sin\lambda_m x_s)(\sin\lambda_n y_s)}{\exp\left[\frac{U}{2}(x_s+y_s)-\frac{U^2\alpha}{2}t\right]}d\tau$$

$$=\frac{\alpha}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(\sin\lambda_m x)(\sin\lambda_n y)(\sin\lambda_m x_s)(\sin\lambda_n y_s)\int_{\tau=0}^{t}\frac{\exp\left[-\alpha t\lambda_m^2-\alpha t\lambda_n^2+\alpha\tau\lambda_m^2+\alpha\tau\lambda_m^2\right]}{\exp\left[\frac{U}{2}(x_s+y_s)-\frac{U^2\alpha}{2}t\right]}d\tau$$

$$=\frac{\alpha}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(\sin\lambda_m x)(\sin\lambda_n y)(\sin\lambda_m x_s)(\sin\lambda_n y_s)}{\alpha\lambda_m^2+\alpha\lambda_m^2}\left\{\exp\left[\begin{array}{l}\tau\left(\alpha\lambda_m^2+\alpha\lambda_m^2\right)-\alpha t\lambda_m^2-\alpha t\lambda_n^2\\-\frac{U}{2}(x_s+y_s)+\frac{U^2\alpha}{2}t\end{array}\right]\right\}_{\tau=0}^{t}$$

$$=\frac{\alpha}{k}\frac{4}{L_xL_y}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(\sin\lambda_m x)(\sin\lambda_n y)(\sin\lambda_m x_s)(\sin\lambda_n y_s)}{\alpha\lambda_m^2+\alpha\lambda_m^2}\left\{\begin{array}{l}\exp\left[-\frac{U}{2}(x_s+y_s)+\frac{U^2\alpha}{2}t\right]\\-\exp\left[-\alpha t\lambda_m^2-\alpha t\lambda_n^2-\frac{U}{2}(x_s+y_s)+\frac{U^2\alpha}{2}t\right]\end{array}\right\}$$

The numerical solution based on the FTCS scheme is determined as follows. First, we rewrite the delta function as the product of the derivative of the Heavside function,

$$\frac{1}{\alpha}\frac{\partial\Theta}{\partial t}+U\frac{\partial\Theta}{\partial x}+U\frac{\partial\Theta}{\partial y}=\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial y^2}+\frac{1}{k}\frac{dH_1(x-x')}{dx}\frac{dH_2(y-y')}{dy}$$

The discretized version using the finite difference approach with FTCS scheme is,

$$\frac{1}{\alpha}\left(\frac{\Theta_{i,j}^{n+1}}{\Delta t}-\frac{\Theta_{i,j}^{n}}{\Delta t}\right)+U\left(\frac{\Theta_{i+1,j}^{n}-\Theta_{i-1,j}^{n}}{2\Delta x}+\frac{\Theta_{i,j+1}^{n}-\Theta_{i,j-1}^{n}}{2\Delta y}\right)=$$
$$\frac{\Theta_{i+1,j}^{n}-2\Theta_{i,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta x^2}+\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta y^2}+\frac{1}{k}\frac{H_{1,i+1}-H_{1,i-1}}{2\Delta x}\frac{H_{2,j+1}-H_{2,j-1}}{2\Delta y}$$

$$\Theta_{i,j}^{n+1}-\Theta_{i,j}^{n}+\alpha U\Delta t\left(\frac{\Theta_{i+1,j}^{n}-\Theta_{i-1,j}^{n}}{2\Delta x}+\frac{\Theta_{i,j+1}^{n}-\Theta_{i,j-1}^{n}}{2\Delta y}\right)=$$
$$\alpha\Delta t\frac{\Theta_{i+1,j}^{n}-2\Theta_{i,j}^{n}+\Theta_{i-1,j}^{n}}{\Delta x^2}+\alpha\Delta t\frac{\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}}{\Delta y^2}+\frac{\alpha}{k}\Delta t\frac{H_{1,i+1}-H_{1,i-1}}{2\Delta x}\frac{H_{2,j+1}-H_{2,j-1}}{2\Delta y}$$

Thus,

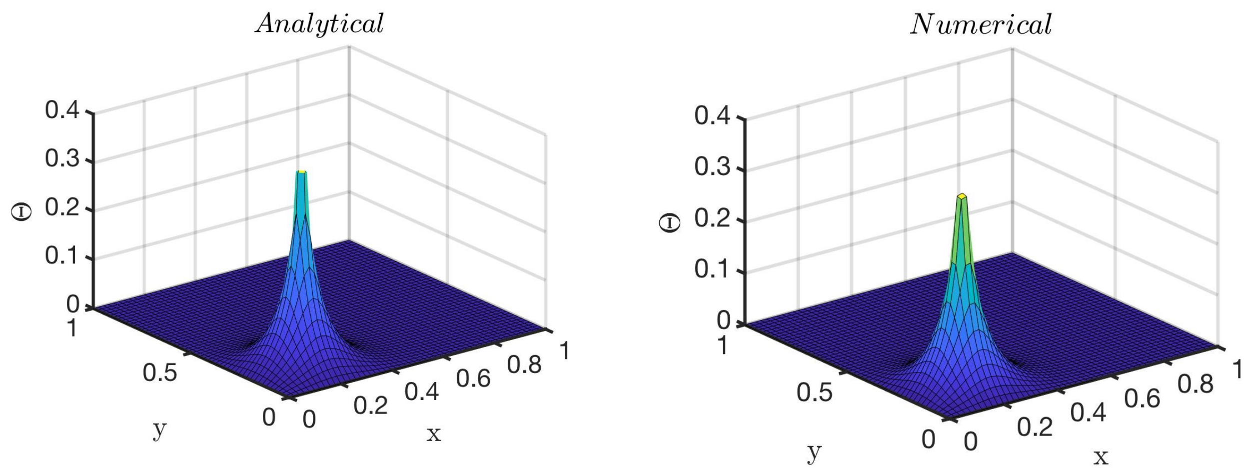
$$\boxed{\begin{aligned}\Theta_{i,j}^{n+1}&=\Theta_{i,j}^{n}-\frac{\alpha U\Delta t}{2}\left(\frac{\Theta_{i+1,j}^{n}-\Theta_{i-1,j}^{n}}{\Delta x}+\frac{\Theta_{i,j+1}^{n}-\Theta_{i,j-1}^{n}}{\Delta y}\right)+\left(\frac{\alpha\Delta t}{\Delta x^2}\right)\left(\Theta_{i,j+1}^{n}-2\Theta_{i,j}^{n}+\Theta_{i,j-1}^{n}\right)\\&\quad+\left(\frac{\alpha\Delta t}{\Delta y^2}\right)\left(\Theta_{i+1,j}^{n}-2\Theta_{i+1,j}^{n}+\Theta_{i-1,j}^{n}\right)+\left(\frac{\alpha\Delta t}{4k\Delta x\Delta y}\right)\left(H_{1,i+1}-H_{1,i-1}\right)\left(H_{2,j+1}-H_{2,j-1}\right)\end{aligned}}$$

The numerical solution is coded using the MATLAB programming.

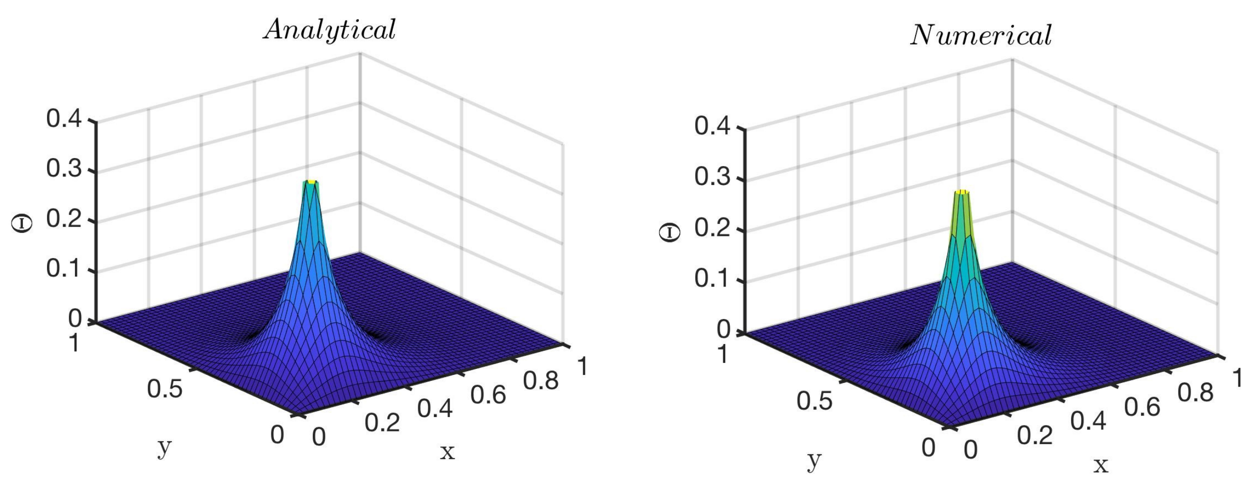
The spatial and temporal resolutions are, $\Delta x=\Delta y=0.02$, and $\Delta t=\dfrac{(\Delta x)^2}{4\alpha}$ to make the solutions stable.

Below are the analytical solution (left) and the numerical solution (right) at two different time instances for *Example-3*.

(i) At $t = 0.01$



(ii) At $t = 0.05$



As expected, the analytical solution is qualitatively consistent with the numerical solution.

Conclusions and future works

We use the Green's function to solve the 2D transient inhomogeneous problem respectively described by i) diffusion equations and ii) advection-diffusion equations. Green's function is derived for a finite domain and with homogeneous Dirichlet boundary conditions. The results for a point source and a constant source term, are obtained using the Green's function method. These results are compared with the numerical results obtained using Forward-Time and Central-Space (FTCS) method. The FTCS method is used for numerical analysis instead of Crank-Nicolson method, due to the ease of implementation of FTCS method. Comparing the results using Green's function and numerical method show a decent qualitative agreement. However, the numerical method converges to a true solution only when the conditions of the stability and convergence are satisfied, which depend on the space and time discretization and the discretization method used. The multiplicative property of a 2D Green's function is derived and it's application in reducing a 2D problem to a 1D problem is discussed.

Apart from the standard problems, the Green's function is also applied in identifying the liquid, interface, unresolved, and gas structures in a two-phase fluid simulations using the VoF method. This problem is modeled by a diffusion equation of diffusing a scalar field, and is then solved adopting the Green's function method. The results also show a successful application.

The present work involves Green's function solution for 2D diffusion and advection-diffusion equations for a point source and constant source term. The analysis could be extended for a source term which is a function of space and time. Also, the analysis could be extended for a 3D problem. A representative example is solved for identification of liquid, unresolved, interface and gas structures in a two phase flow simulations. This analysis could be used in two-phase simulations involving practical applications, for instance, the simulation of the liquid spray problems.

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Appendix: MATLAB code

1. Example-1

```
% ─────────────────────────────────────────────────────────────
clc; clear; close all;

% delta function is placed in (x,y)=(0.2, 0.2)
alpha=1;        k=1;            % diffusivity
dx=0.02;        dy=dx;          % dx, dy
Lx=1;           Ly=1;           % length of x, y
x=0:dx:Lx;      y=0:dy:Ly;      % x-, y-coordinate
Nx=length(x);   Ny=length(y);   % size of x-, y-coordinate

% time step
Nt=100;
dt=(dx^2/alpha)/4; % stable criterion
tf=Nt*dt

% group parameter
cox=alpha*dt/dx^2;            coy=alpha*dt/dy^2;
cog=alpha*dt/4/k/dx/dy;

% define mesh; use X' and Y' to convert into common convention
[X,Y]=meshgrid(x,y);     X=X';   Y=Y';

% initial condition
numer_sol=zeros(Nx,Ny);
for i = 1 : Nx
    for j = 1 : Ny
        numer_sol(i,j)=0;
    end
end

% Heavside function in x-dirction, H(x)=H(x-0.2)
H1=zeros(Nx,1);
for i = 1 : Nx
       if i>=(0.2/dx+1)
           H1(i)=1;
       else
           H1(i)=0;
       end
end

% Heavside function in y-dirction, H(y)=H(y-0.2)
H2=zeros(Ny,1);
for j = 1 : Ny        % loop for x-coordinate marching
```

```
        if j >= (0.2/dx+1)
            H2(j)=1;
        else
            H2(j)=0;
        end
end


% ------  analytical solution using Green's function -----------
%
xp=x(0.2/dx+1);     yp=y(0.2/dx+1);
% (x,y)-coordinate of delta function

t=tf;               % time
xx=xp;     yy=yp;
% (x,y)-coordinate; here we observe (x,y)=(0.2, 0.2)

mlim=100;    nlim=100;
% m=[0,inf], n=[0,inf]; I use 100 to approximate inf
term_3=zeros(mlim,nlim);    sum_temp=zeros(mlim,1);
analy_sol=zeros(Nx,Ny);
for i = 1 : round(Nx)
    for j = 1 : round(Ny)
    for m = 1 : mlim    % summation over m; m=[0,inf]
    lam_m=m*pi/Lx;
    for n = 1 : nlim   % summation over n=[0,inf]
        lam_n=n*pi/Ly;
        term_1=sin(lam_m*xp)*sin(lam_n*yp)/(lam_m^2+lam_n^2)...
                *(1-exp(-(lam_m^2+lam_n^2)*alpha*t));
        term_2=sin(lam_m*X(i,1))*sin(lam_n*Y(1,j));
        term_3(m,n)=term_2*term_1;
    end
    sum_temp(m)=sum(term_3(m,:));
    end
    analy_sol(i,j)=sum(sum_temp)*4/k/Lx/Ly;
    end
end
figure;         surf(X,Y,analy_sol);
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Analytical$','Interpreter','latex');
set(gca,'XTick',0:0.2:1.0);
zlim([0 0.4]); set(gca,'ZTick',0:0.1:0.4);
%
% ----- end of analytical solution ------
```

```
% ------  numerical solution -----------
%
% initialize temporary data to store f(i,j) at next time step
temp=zeros(Nx,Ny);
temp(:,1)=0;        temp(:,end)=0;
% boundary condition at y=0 and y=1
temp(1,:)=0;        temp(end,:)=0;
% boundary condition at x=0 and x=1

for k = 1 : Nt   % loop for time marching
    % use FTCS to update f(i,j) at next time step
    for i = 2 : Nx-1        % loop for x-coordinate marching
        for j = 2 : Ny-1    % loop for y-coordinate marching
          temp(i,j)=numer_sol(i,j+coy*(numer_sol(i,j+1)-...
               2*numer_sol(i,j)+numer_sol(i,j-1))+...
               cox*(numer_sol(i+1,j)-2*numer_sol(i,j)+...
               numer_sol(i-1,j))+...
               cog*(H1(i+1)-H1(i-1))*(H2(j+1)-H1(j-1));
        end
    end
numer_sol=temp;   % update f(i,j) for next time-step calculation
end

figure;         surf(X,Y,numer_sol);
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Numerical$','Interpreter','latex');
set(gca,'XTick',0:0.2:1.0);
zlim([0 0.4]); set(gca,'ZTick',0:0.1:0.4);
% ----- end of numerical solution ------
```

2. *Example-2*

```
% ———————————————————————————————————————————————————————————————
clc; clear; close all;

x1=linspace(0,1,20)';
y1=linspace(0,1,20)';
[X1,Y1]=meshgrid(x1,y1);

Lx=1; Ly=1; % domain lengths in 2D
a=1; b=1;   % boundaries
alpha=1;    % diffusivity
tf=0.05;    % final time at which the temperature is evaluated
k=1;        % conductivity
g=2;        % source term
N=1000;     % number of terms considered in the series

% ------  analytical solution -----------
Tp=zeros(length(x1),length(y1));
for i=1:length(x1)
    for j=1:length(y1)
        Tp(i,j)=0;
        for m=1:N
            lm=m*pi/Lx;
            for n=1:N
                ln=n*pi/Ly;
                Tp(i,j)=Tp(i,j)+ ((4/(Lx*Ly))*g*...
                    ((1-exp(-alpha*(lm^2+ln^2)*tf))...
                    /(alpha*(lm^2+ln^2)))...
                    *sin(lm*x1(i,1))*((cos(lm*a)-1)/lm)...
                    *sin(ln*y1(j,1))*((cos(ln*b)-1)/ln));
            end
        end
    end
end

%% Final solution
T=Th+(alpha/k)*Tp;

%% plot
surf(X1,Y1,T)
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Analytical$','Interpreter','latex');
set(gca,'XTick',0:0.2:1.0);
```

```
% ------  numerical solution -----------
dx=0.05;            dy=dx;      % dx, dy
x=0:dx:Lx;      y=0:dy:Ly;      % x-, y-coordinate
Nx=length(x);   Ny=length(y);   % size of x-, y-coordinate


% time step
Nt=80;
dt=(dx^2/alpha)/4; % stable criterion
tf=Nt*dt

% group parameter
cox=alpha*dt/dx^2;
coy=alpha*dt/dy^2;
cog=alpha*dt/k;

% define mesh; use X' and Y' to convert into common convention
[X,Y]=meshgrid(x,y);     X=X';   Y=Y';

% initial condition
numer_sol=zeros(Nx,Ny);
for i = 1 : Nx
    for j = 1 : Ny
        numer_sol(i,j)=0;
    end
end

%
% initialize temporary data to store f(i,j) at next time step
temp=zeros(Nx,Ny);
temp(:,1)=0;        temp(:,end)=0;
% boundary condition at y=0 and y=1
temp(1,:)=0;        temp(end,:)=0;
% boundary condition at x=0 and x=1

for k = 1 : Nt   % loop for time marching
    % use FTCS to update f(i,j) at next time step
    for i = 2 : Nx-1         % loop for x-coordinate marching
        for j = 2 : Ny-1     % loop for y-coordinate marching
         temp(i,j)=numer_sol(i,j)+coy*(numer_sol(i,j+1)...
                   -2*numer_sol(i,j)+numer_sol(i,j-1))+...
                   cox*(numer_sol(i+1,j)-2*numer_sol(i,j)...
                   +numer_sol(i-1,j))+cog*g;
        end
    end
```

```
    numer_sol=temp;
    %  update f(i,j) for next time-step calculation
end
figure;         surf(X,Y,numer_sol);
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Numerical$','Interpreter','latex');
set(gca,'XTick',0:0.2:1.0);
% ----- end of numerical solution ------
```

```
% ____________________________________________________________
N=1000;      % Number of terms in series
g=1e-10;     % Source term
tf=0.05;     % final time
Lx=1; Ly=1; % domain length
a=1;  b=1;  D=1;  k=1;  % Diffusivity and conductivity
X1=0.55;     Y1=0.25;  % Coordinates where delta function is used


Beta = zeros(21,21);
for i=1:21
    for j=1:21
        Beta(i,j)=0;
        for m=1:N
            lm=m*pi/Lx;
            for n=1:N
                ln=n*pi/Ly;
                Beta(i,j)=Beta(i,j)+((4/(Lx*Ly))*g*((1-...
                    exp(-D*(lm^2+ln^2)*tf))/(D*(lm^2+ln^2)))...
                    *sin(lm*X(i,j))*sin(lm*X1)...
                    *sin(ln*Y(i,j))*sin(ln*Y1));
            end
        end
    end
end
figure(2); surf(X,Y,Beta);
xlabel('$x$','Interpreter','latex');
ylabel('$y$','Interpreter','latex');
zlabel('$\beta$','Interpreter','latex');


%% Liquid structure
Liq=zeros(21,21);
for i=1:21
    for j=1:21
        if (Beta(i,j)>3e-12 && A(i,j)>0.95) % Condition
            Liq(i,j)=1;
        end
    end
end
figure(3); contourf(X,Y,Liq);
xlabel('$x$','Interpreter','latex');
ylabel('$y$','Interpreter','latex');
```

```
%% Interface
Int=zeros(21,21);
for i=1:21
    for j=1:21
        if (Beta(i,j)>3e-12 && A(i,j)<0.95 && A(i,j)>0.05)
        % Condition
            Int(i,j)=1;
        end
    end
end
figure(4); contourf(X,Y,Int);
xlabel('$x$','Interpreter','latex');
ylabel('$y$','Interpreter','latex');


%% Unresolved structure
Unresolved_Struct=zeros(21,21);
for i=1:21
    for j=1:21
        if (Beta(i,j)<3e-12 && A(i,j)<0.95 && A(i,j)>0.05)
        % Condition
            Unresolved_Struct(i,j)=1;
        end
    end
end
figure(5); contourf(X,Y,Unresolved_Struct);
xlabel('$x$','Interpreter','latex');
ylabel('$y$','Interpreter','latex');


%% Gas structure
Gas=zeros(21,21);
for i=1:21
    for j=1:21
        if (A(i,j)<0.05)    % Condition
            Gas(i,j)=1;
        end
    end
end
figure(6); contourf(X,Y,Gas);
xlabel('$x$','Interpreter','latex');
ylabel('$y$','Interpreter','latex');
```

4. *Example-3*

```
% ----------------------------------------------------------------------
clc; clear; close all;

% delta function is placed in (x,y)=(0.2, 0.2)

alpha=1;     k=1;     U=1;  % diffusivity and addiction velocity
dx=0.02;        dy=dx;             % dx, dy
Lx=1;           Ly=1;              % length of x, y
x=0:dx:Lx;      y=0:dy:Ly;         % x-, y-coordinate
Nx=length(x);   Ny=length(y);      % size of x-, y-coordinate

% time step
Nt=100;
dt=(dx^2/alpha)/4; % stable criterion
tf=Nt*dt

% group parameter
cou=alpha*U*dt/2;   cox=alpha*dt/dx^2;
coy=alpha*dt/dy^2;  cog=alpha*dt/4/k/dx/dy;

% define mesh; use X' and Y' to convert into common convention
[X,Y]=meshgrid(x,y);     X=X';   Y=Y';

% initial condition
numer_sol=zeros(Nx,Ny);
for i = 1 : Nx
    for j = 1 : Ny
        numer_sol(i,j)=0;
    end
end

% Heavside function in x-dirction, H(x)=H(x-0.2)
H1=zeros(Nx,1);
for i = 1 : Nx
       if i>=(0.2/dx+1)
           H1(i)=1;
       else
           H1(i)=0;
       end
end

% Heavside function in y-dirction, H(y)=H(y-0.2)
H2=zeros(Ny,1);
for j = 1 : Ny         % loop for x-coordinate marching
```

```
        if j >= (0.2/dx+1)
            H2(j)=1;
        else
            H2(j)=0;
        end
end



% ------  analytical solution using Green's function -----------
%
xp=x(0.2/dx+1);     yp=y(0.2/dx+1);
% (x,y)-coordinate of delta function

t=tf;                % time
xx=xp;      yy=yp;
% (x,y)-coordinate; here we observe (x,y)=(0.2, 0.2)

mlim=100;          nlim=100;
% m=[0,inf], n=[0,inf]; I use 100 to approximate inf
term_5=zeros(mlim,nlim);    sum_temp=zeros(mlim,1);
analy_sol=zeros(Nx,Ny);
for i = 1 : round(Nx)
    for j = 1 : round(Ny)
    for m = 1 : mlim    % summation over m; m=[0,inf]
    lam_m=m*pi/Lx;
    for n = 1 : nlim   % summation over n=[0,inf]
        lam_n=n*pi/Ly;
        term_1=sin(lam_m*xp)*sin(lam_n*yp)/(lam_m^2+lam_n^2);
        term_2=sin(lam_m*X(i,1))*sin(lam_n*Y(1,j));
        term_3=exp(-U/2*(X(i,1)+Y(1,j))+U*U*alpha/2*t);
        term_4=exp(-alpha*t*lam_m^2-alpha*t*lam_n^2-...
               U/2*(X(i,1)+Y(1,j))+U*U*alpha/2*t);
        term_5(m,n)=term_1*term_2*(term_3-term_4);
    end
    sum_temp(m)=sum(term_5(m,:));
    end
    analy_sol(i,j)=sum(sum_temp)*4/k/Lx/Ly*...
                   exp(U/2*(X(i,1)+Y(1,j))-U*U*alpha/2*t);
    end
end
figure;         surf(X,Y,analy_sol);
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Analytical$','Interpreter','latex');
```

```matlab
set(gca,'XTick',0:0.2:1.0);
zlim([0 0.4]); set(gca,'ZTick',0:0.1:0.4);
%
% ----- end of analytical solution ------




% ------  numerical solution -----------
%
% initialize temporary data to store f(i,j) at next time step
temp=zeros(Nx,Ny);
temp(:,1)=0;         temp(:,end)=0;
% boundary condition at y=0 and y=1
temp(1,:)=0;         temp(end,:)=0;
% boundary condition at x=0 and x=1

for k = 1 : Nt   % loop for time marching
 % use FTCS to update f(i,j) at next time step
  for i = 2 : Nx-1        % loop for x-coordinate marching
   for j = 2 : Ny-1    % loop for y-coordinate marching
    temp(i,j)=numer_sol(i,j)...
    -cou*((numer_sol(i+1,j)-numer_sol(i-1,j))/dx+...
    (numer_sol(i,j+1)-numer_sol(i,j-1))/dy)...
    +cox*(numer_sol(i+1,j)-2*numer_sol(i,j)+numer_sol(i-1,j))...
    +coy*(numer_sol(i,j+1)-2*numer_sol(i,j)+numer_sol(i,j-1))...
    +cog*(H1(i+1)-H1(i-1))*(H2(j+1)-H1(j-1));
   end
  end
  numer_sol=temp;
% update f(i,j) for next time-step calculation
end

figure;         surf(X,Y,numer_sol);
xlabel('x','Interpreter','latex');
ylabel('y','Interpreter','latex');
zlabel('$\Theta$','Interpreter','latex');
title('$Numerical$','Interpreter','latex');
set(gca,'XTick',0:0.2:1.0);
zlim([0 0.4]); set(gca,'ZTick',0:0.1:0.4);
% ----- end of numerical solution ------
```