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\textbf{ABSTRACT.} Segmenting the image into multiple regions is at the core of image processing. Many segmentation formulations of an image with multiple regions have been suggested over the years. We consider segmentation algorithm based on the multi-phase level set method in this work. Proposed method gives the best result upon other methods found in the references. Moreover it can segment images with intensity inhomogeneity and have multiple junction. We extend our method (GLIF) in [T. Dultuya, and M. Kang, Segmentation with shape prior using global and local image fitting energy, J.KSIAM Vol.18, No.3, 225–244, 2014.] using a multi-phase level set formulation to segment images with multiple regions and junction. We test our method on different images and compare the method to other existing methods.

1. INTRODUCTION

Segmentation of images with multiple regions is an important research in image segmentation field. Various works of segmentation methods have developed. Main goals of the segmentation methods are to partition an image into reasonable number of regions, to detect the objects with different intensity from background of the image and to represent the multiple junction in the image. Region based model of Mumford-Shah (MS) functional \cite{1} is fundamental approach of most segmentation methods. The nonconvexity of the (MS) functional makes it difficult to be minimized. To simplify the (MS) model, Chan and Vese (Chan-Vese)\cite{2} reformulate the (MS) functional using the level set method that introduced in \cite{3}. However, the (Chan-Vese) method is suitable for two-region image segmentation. To segment multiple regions, Vese-Chan extended their method in \cite{4}; however, multi-phase level set makes the method computationally expensive because of the re-initialization process of the level set functions. The piecewise constant (PC) and the piecewise smooth (PS) models were proposed in this extension. The (PC) model works well on the images with intensity homogeneity whereas the (PS) model can segment images with intensity inhomogeneity. Nevertheless, these methods are difficult to implement and also increases the computational cost.
Another common approach is the active contour model, which is an edge based model. Using the active contour models [10, 11, 12], the local image fitting (LIF) approach was proposed to segment images with intensity inhomogeneity in [5]. Similar approaches have been proposed in [6, 8]. They regularize the level set function using Gaussian filtering for variational level set; thus, the (LIF) eliminates the re-initialization process. The (LIF) method gives better segmentation results and is more computationally efficient than the (PS) model. We formulated another efficient approach (GLIF) in [17] for images with intensity inhomogeneity. However this model cannot segment multiple regions and cannot represent the multiple junction. We will extend the (GLIF) method using multi-phase level set formulation to partition multiple regions with junction in this work.

Organization of this paper is followed by: Section 2 introduces previous works. We review the segmentation models of images with multiple regions. Also, significant segmentation methods for images with inhomogeneity are introduced. The main contribution of this work is presented in Section 3. In Section 3, we extend our method to segment images with multiple regions using multi-phase level set method and local image fitting energy. We set a local image fitting term to cope with the intensity inhomogeneity of the image. To overcome sensitivity of initialization, a global image fitting term with multi-phase level set is considered. Numerical experiments are discussed in Section 4. At last, we conclude our work in Section 5.

2. RELATED WORKS

The first fundamental model for image segmentation was proposed by Mumford and Shah in [1]. Their main idea is to approximate an image by a simplified image as a combination of regions of constant intensities and the smoothness of the contours was disregarded. These ideas were incorporated into a variational framework; an initial image \(u_0\), find pair \((u, C)\), where \(u\) is a nearly piecewise smooth approximation of \(u_0\) and \(C\) is the set of edges. Mumford and Shah proposed to find \((u, C)\) by minimizing the following functional:

\[
F^{MS}(u, C) = \int_{\Omega-C} (u - u_0)^2 dx + \mu \int_{\Omega-C} |\nabla u|^2 dx + \nu \int_{C} d\sigma \tag{2.1}
\]

where \(\Omega\) is a bounded open set of \(\mathbb{R}^2\), \(\mu\) and \(\nu\) are nonnegative constants and \(\int_{C} d\sigma\) is the length of \(C\). Methods of solving the general (MS) model are complicated and computationally expensive, even though, (2.1) is a natural method of segmentation.

To overcome the disadvantage of (MS) functional, a region-based segmentation method with level sets was proposed by Chan and Vese [2, 13]. The level set formulation of the (Chan-Vese) model can be written as

\[
E^{Chan-Vese}(c_1, c_2, \phi) = \int_{\Omega} \left( (u_0 - c_1)^2 H(\phi) + (u_0 - c_2)^2 (1 - H(\phi)) \right) dx + \mu \int_{\Omega} |\nabla H(\phi)| dx + \nu \int_{\Omega} H(\phi) dx
\]

where \(u_0\) is a given image on the bounded open subset \(\Omega\) in \(\mathbb{R}^2\).
Vese and Chan extended their model using a multi-phase level set formulation [16] to partition multiple regions. Piecewise constant (PC) and Piecewise smooth (PS) models were proposed in [4]. The (PC) model has the advantage that it can represent multiple regions and junction.

In the (PC) model, level set functions $\phi_i : \Omega \rightarrow R, i = 1, \ldots, m$ were considered. The union of the zero-level sets of $\phi_i$ will represent the contours in the segmented image. The segments or phases in the domain $\Omega$ can be defined by the following way: Two pixels $(x_1, y_1)$ and $(x_2, y_2)$ in $\Omega$ will belong to the same phase or class if and only if $H(\Phi(x_1, y_1)) = H(\Phi(x_2, y_2))$. Here $\Phi = (\phi_1, \ldots, \phi_m)$ is the vector of level set functions and $H(\Phi) = (H(\phi_1), \ldots, H(\phi_m))$ is the vector of Heaviside functions whose components are only 1 or 0.

Up to $n = 2^m$ phases or classes can be defined in the domain of definition $\Omega$. The classes defined in this way form a disjoint decomposition and covering of $\Omega$. Therefore, each pixel $(x, y) \in \Omega$ will belong to only one class, thus there is no vacuum or overlap among the phases. The set of curves $C$ is represented by the union of the zero level sets of the functions $\phi_i$. As shown in Figure 1, we need two level set functions ($m = 2$) to represent four phases ($n = 4$) in the (PC) model. Therefore, the energy of 4 phase (PC) model for level set representation is written by:

$$E_{PC}^4(c, \Phi) = \sum_{i}^{n} \sum_{j}^{m} \int_{\Omega} (u_0 - c_{i,j})^2 H_{i,j} dx + \int_{\Omega} |\nabla H(\phi_1)| + \int_{\Omega} |\nabla H(\phi_2)|$$

where

$$H_{11} = H(\phi_1)H(\phi_2), \quad H_{12} = H(\phi_1)(1 - H(\phi_2))$$
$$H_{21} = (1 - H(\phi_1))H(\phi_2), \quad H_{22} = (1 - H(\phi_1))(1 - H(\phi_2))$$

and $c_{i,j} = \text{mean}(u_0), i = 1, 2, j = 1, 2$ in each region/phase.

Figure 2 shows the segmentation result of a noisy synthetic image with a multiple junction. Using only one level set function in Chan-Vese model (Figure 2(a)), the triple junction cannot
be represented (Figure 2(b)). If we utilize two level set functions (Figure 2(c)) in (PC) model with \( n = 4 \), the triple junction can be represented and 4 phases are extracted as shown in Figure 2(d). The (PC) model has advantage that it can represent the triple junction and more than 2 phases.

However, the authors Vese and Chan extended their model to multi-phase level set framework, it requires \( m \) level set functions and \( 2^m \) phases to detect \( 2^m \) regions. To overcome this difficulty or to reduce this storage, Lie [18] proposed Piecewise Constant Level Set Method (PCLSM). In this model, they introduced using only one level set function to detect all regions. The authors assumed that a piecewise constant level set function \( \phi = i \) in each region. The segmentation can be formulated as a minimization of the following functional:

\[
F(c, \phi) = \frac{1}{2} \int_{\Omega} |u - u_0|^2 dx + \beta \sum_{i=1}^{n} \int_{\Omega} |\nabla \psi_i| dx
\]

Where: \( u \) is formed by \( u = \sum_{i=1}^{n} c_i \psi_i \), here \( \psi_i \) are basis functions and these functions defined by using polynomial approach that is formed by

\[
\psi_i = \frac{1}{\alpha_i} \prod_{j=1, j \neq i}^{n} (\phi - j) \quad \text{and} \quad \alpha_i = \prod_{k=1, k \neq i}^{n} (i - k)
\]

and a piecewise constant level set function \( \phi \) satisfies \( \phi = i \) in \( \Omega_i \) for \( i = 1, 2, \cdots, n \).

For uniquely classifying each point or intensity in the image, they introduced a polynomial of degree \( n \) that is \( K(\phi) = \prod_{i=1}^{n} (\phi - i) \) for the constraint. Therefore they used a constraint \( K(\phi) = 0 \) and solved the following constrained minimization problem:

\[
\min_{c, \phi} F(c, \phi) \text{ subject to } K(\phi) = 0.
\]

If a given function \( \phi : \Omega \to R \) satisfies \( K(\phi) = 0 \), there exists a unique \( i \in 1, \ldots, n \) for every \( x \in \Omega \) such that \( \phi(x) = i \). Thus, each point \( x \in \Omega \) can belong to one and only one phase if \( K(\phi) = 0 \). It can be solved by the augmented Lagrangian method.

These methods work well for images with intensity homogeneity (or roughly constant in each phases) but do not work for the images with intensity inhomogeneity. So, we will discuss

Figure 2. Segmentation result of (PC) model for image with triple junction
Multiple region segmentation methods for images with intensity inhomogeneity. Most images with intensity inhomogeneity occur at medical image processing. In particular, inhomogeneities in magnetic resonance images (MRI) arise from nonuniform magnetic fields produced by ratio-frequency coils, as well as from variations in object susceptibility. Therefore, many segmentation approaches have been developed for these images.

The first approach is the (PS) model proposed by Vese and Chan [4]. The (PS) model is formulated as minimizing the following energy when \( n = 2 \) (two phase case):

\[
E_{PS}^{2}(u^+, u^-, \Phi) = \int_{\Omega} \left( (u_0 - u^+)^2 H(\phi) + (u_0 - u^-)^2 (1 - H(\phi)) \right) dx dy + \mu \int_{\Omega} |\nabla u^+|^2 H(\phi) + |\nabla u^-|^2 (1 - H(\phi)) dx dy + \nu \int_{\Omega} |\nabla H(\phi)|
\]

Here, \( u = u^+ H(\phi) + u^- (1 - H(\phi)) \) and \( \phi \) can be expressed by introducing two functions \( u^+ \) and \( u^- \) such that

\[
u(x,y) = \begin{cases} u^+(x,y), & \text{if } \phi(x,y) \geq 0 \\ u^-(x,y), & \text{if } \phi(x,y) < 0. \end{cases}
\]

This model can be extended to segment an image with intensity inhomogeneity and include two or more phases. Figure 3 shows the segmentation result of a noisy image with intensity inhomogeneity. By the second term of the functional, a noise can be removed as shown in Figure 3. Even though the (PS) model can segment an image by reducing the influence of intensity inhomogeneity, it is computationally expensive and inefficient in practice.

**Figure 3.** Segmentation result of (PS) model for noisy image

Compared to the (PS) model, a more inexpensive and accurate models were proposed in [5, 6, 7, 8, 17]. These models are based on a kernel function \( K(x) \) with a localization property that \( K(x) \) decreases and approaches zero as \( |x| \) increases. All methods choose the kernel function \( K(x) \) as a Gaussian kernel

\[
K_{\sigma}(x) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp \left( - \frac{|x|^2}{2\sigma^2} \right).
\]
with a scale parameter \( \sigma > 0 \). This scale parameter is a standard deviation of the kernel and it plays an important role. By suitable chosen, it can control the region-scalability from small neighborhoods to the entire image domain. The scale parameter should be properly chosen according to the contents of a given image. In particular, when an image is too noisy or has low contrast, a large value of \( \sigma \) should be chosen. Unfortunately, this may cause a high computational cost. Small values of \( \sigma \) can cause undesirable result as well.

We proposed global and local image fitting (GLIF) method in [17] by taking the advantage of the Chan-Vese and (LIF) models. The (GLIF) method defined the energy functional as follows:

\[
E_{GLIF}(\phi, c_1, c_2, m_1, m_2) = (1 - \alpha)E_{LIF}(\phi, m_1, m_2) + \alpha E_{GIF}(\phi, c_1, c_2)
\]

where \( \alpha \) is a positive constant such that \( 0 \leq \alpha \leq 1 \). The value of \( \alpha \) should be small when the intensity inhomogeneity in an image is severe. The local intensity fitting energy \( E_{LIF} \) is equal to the (LIF) model in [8], and the global intensity fitting (GIF) energy \( E_{GIF} \) is the term of the Chan-Vese model without regularizing term. And \( m_1 \) and \( m_2 \) are the optimal fitting functions given by following equation that is introduced in (LIF) model:

\[
\begin{align*}
m_1 &= \text{mean}(u_0 \in \{x \in \Omega | \phi(x) < 0 \} \cap W_k(x)) \\
m_2 &= \text{mean}(u_0 \in \{x \in \Omega | \phi(x) > 0 \} \cap W_k(x))
\end{align*}
\]

Here, the rectangular window function is denoted by \( W_k(x) \). They defined the local fitted image as

\[
u_{LFI} = m_1 H(\phi) + m_2(1 - H(\phi)).
\]

Then proposed local intensity fitting (LIF) energy formulation is given by

\[
E_{LIF} = \frac{1}{2} \int_{\Omega} |u_0(x) - u_{LFI}(x)|^2 dx, \quad x \in \Omega.
\]

In this model, a Gaussian filtering is applied to regularize the level set function, i.e., \( \phi = G_\gamma \ast \phi \), where \( \gamma \) is the standard deviation. Our method can segment an images with intensity inhomogeneity or multiple objects with different intensities. However, it cannot segment multiple regions. Also the proposed method cannot represent multiple junction. Therefore we will extend our method in section 3.

3. Proposed model

We extend the energy (2.2) using multi-phase level set framework. By idea of Vese-Chan model, we note the regions by \( i \), with \( 1 \leq i \leq 2^m = n \). Then the extension of our model can be written as

\[
F_n(c, m, \Phi) = \alpha \sum_{1 \leq i \leq n} \int_{\Omega} |u_0 - c_i|^2 H_i dx + (1 - \alpha) \int_{\Omega} |u_0 - \sum_{1 \leq i \leq n} m_i H_i|^2 dx
\]

Where, \( c_i = \text{mean}(u_0) \) in each region \( i \), \( m_i \) are optimal fitting functions and \( H_i \) are the Heaviside functions whose components are only 1 or 0. In this functional, the first term encourages to drive the motion of the contour far away from object boundaries and to represent multiple
juncture. And the second term enables to cope with intensity inhomogeneity. For the purpose of illustration, let us write the above energy for \( n = 4 \) phases or regions as follows.

The fitting term of the Vese-Chan model, excluding regularization terms, is given by:

\[
E^G_4 = \int_\Omega \left( |u_0 - c_1|^2 H_1 + |u_0 - c_2|^2 H_2 + |u_0 - c_3|^2 H_3 + |u_0 - c_4|^2 H_4 \right) dx
\]

\[
= \sum_{i=1}^{4} \int_\Omega |u_0 - c_i|^2 H_i dx
\]

(3.1)

where: \( H_1 = H(\phi_1)H(\phi_2), \ H_2 = H(\phi_1)(1 - H(\phi_2)), \ H_3 = (1 - H(\phi_1))H(\phi_2), \ H_4 = (1 - H(\phi_1))(1 - H(\phi_2)) \) and \( c_i = \text{mean}(u_0), \ i = 1, 2, 3, 4 \) in each region. We call this term by global image fitting (GIF) term. This term encourages to improve the convergence speed by eliminating the segmentation process’ sensitivity to initialization and to represent the multiple junction.

We extend (LIF) model on two level set functions by following:

\[
E^L_4 = \int_\Omega |u_0 - m_1 H_1 - m_2 H_2 - m_3 H_3 - m_4 H_4|^2 dx
\]

(3.2)

where

\[
m_i = \frac{K_\sigma(x) \ast (u_0(x) \cdot H_i)}{K_\sigma(x) \ast H_i}, \ i = 1, 2, 3, 4.
\]

Here, \( K_\sigma(x) \) is a Gaussian Kernel with scale parameter \( \sigma \). The scale parameter should be properly chosen depending on the contents of an image. In general, \( \sigma \) should be chosen from interval of \([1; 3]\).

The proposed energy functional consists of a local image fitting term and global image fitting term. Specifically,

\[
F_4 = (1 - \alpha)E^L_4 + \alpha E^G_4
\]

(3.3)

where \( \alpha \) is a positive constant such that \( 0 \leq \alpha \leq 1 \). The value of \( \alpha \) should be small for images with severe intensity inhomogeneity. The local image fitting term \( E^L_4 \) enables the model to cope with intensity inhomogeneity. Furthermore, it includes a local force to attract the contours and stop it at object boundaries. The global image fitting term \( E^G_4 \) allows flexible initialization of the contours. Also, it includes a global force to drive the motion of the contour far away from object boundaries.

We now discuss the numerical approximation for minimizing the \( F_4 \) functional. Constants \( c_i \) that minimize the energy in (3.3) are given by

\[
c_i = \frac{\int u_0(x) H_i(x) dx}{\int H_i(x) dx}, \ i = 1, 2, 3, 4
\]

(3.4)

By theory of calculus of variations, differentiating with respect to \( \phi_1, \phi_2 \) for fixed \( c_i \) and we obtain the following gradient descent flow

\[
\frac{\partial \phi_1}{\partial t} = -\delta(\phi_1) \left( H(\phi_2)(a_1 - a_3) + (1 - H(\phi_2))(a_2 - a_4) \right)
\]

(3.5)
\[ \frac{\partial \phi_2}{\partial t} = -\delta(\phi_2) \left( H(\phi_1)(a_1 - a_2) + (1 - H(\phi_1))(a_3 - a_4) \right) \]  

(3.6)

where \( a_i = (1 - \alpha)(u_0(x) - m_i) + \alpha(u_0(x) - c_i)^2, \ i = 1, 2, 3, 4. \)

The algorithm for solving \( F_4 \) is as follows:

**Step 1:** Initialize the level set function \( \phi_1 \) and \( \phi_2 \).

**Step 2:** Compute \( c_i \) according to (3.4).

**Step 3:** Evolve the level set function \( \phi_1 \) and \( \phi_2 \) according to (3.5), (3.6).

**Step 4:** Regularize the level set function \( \phi_j \) using a Gaussian kernel, i.e., \( \phi_j = G_\gamma * \phi_j, \ j = 1, 2 \) where \( \gamma \) is the standard deviation.

**Step 5:** Check whether the evolution is stationary. If not, return to step 3.

### 4. Experimental Results

Using gradient descent flows (3.5), (3.6) and the above algorithm, segmentation results are produced faster and require fewer iteration than the Vese-Chan and (PCLSM) models. Experimental results are illustrated in Figure 4, Figure 5 and Figure 6. Our algorithm works well on images with intensity inhomogeneity and it can segment multiple regions and can represent multiple junction (Figure 4(b,c), Figure 5(b,c) and Figure 6(b,c)). The scale parameter \( \sigma \) is equal to 3 for these images and the regularizing parameter \( \gamma \) is properly chosen 0.8. These results are better to the results of the Vese-Chan and (PCLSM) models.

In Figure 4(d), Figure 5(d) and Figure 6(d), the computed averages by (PCLSM) are illustrated. Notice that better results are produced by our method. Furthermore, computational times are relatively high using the proposed method. In Table 1, we compare the number of iterations and computational times for the (PCLSM), Vese-Chan models to our proposed method.

<table>
<thead>
<tr>
<th>Methods</th>
<th>Junction</th>
<th>Brain</th>
<th>lung</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Iterations(time(s))</td>
<td>Iterations(time(s))</td>
<td>Iterations(time(s))</td>
</tr>
<tr>
<td>Vese-Chan</td>
<td>420 (528.85)</td>
<td>200 (184.16)</td>
<td>400 (469.09)</td>
</tr>
<tr>
<td>PCLSM</td>
<td>492 (148.55)</td>
<td>679 (153.22)</td>
<td>596 (291.84)</td>
</tr>
<tr>
<td>Proposed</td>
<td>12 (25.24)</td>
<td>4 (15.23)</td>
<td>2 (6.54)</td>
</tr>
</tbody>
</table>

**Table 1. Computation time results.**
**FIGURE 4.** Segmentation result of proposed method: (a) is the given image with the initial level set; (b) is the result of proposed method; (c) is the computed average of proposed method; (d) is the computed average of the PCLSM.

**FIGURE 5.** Segmentation result of proposed method: (a) is the given image with the initial level set; (b) is the result of proposed method; (c) is the computed average of proposed method; (d) is the computed average of the PCLSM.

**FIGURE 6.** Segmentation result of proposed method: (a) is the given image with the initial level set; (b) is the result of proposed method; (c) is the computed average of proposed method; (d) is the computed average of the PCLSM.
5. Conclusion

We proposed the multi-phase level set method of image segmentation driven by global and local image fitting energy. Our method worked well for images with multiple regions and intensity inhomogeneity. Moreover, it can allowed flexible initialization of the contours. In order to cope with the intensity inhomogeneity of the image, we set a local image fitting term. To overcome initialization sensitivity and to represent multiple junction, a global image fitting term was considered. Our segmentation results were obtained faster, requiring fewer iterations than the Vese-Chan and (PCLSM) models.

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References


MATHEMATICAL UNDERSTANDING OF CONSCIOUSNESS AND UNCONSCIOUSNESS

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\textbf{ABSTRACT.} This paper approaches the subject of consciousness and unconsciousness from a mathematical point of view. It sets up a hypothesis that when unconscious state becomes conscious state, high density energy is released. We argue that the process of transformation of unconsciousness into consciousness can be expressed using the infinite recursive Heaviside step function. We claim that differentiation of the potential of unconsciousness with respect to time is the process of being conscious in a world where only time exists, since the thinking process never have any concrete space. We try to attribute our unconsciousness to a special solution of the multi-dimensional advection partial differential equation which can be represented by the finite recursive Heaviside step function. Mathematical language explains how the infinitive neural process is perceived and understood by consciousness in a definitive time.

1. INTRODUCTION

Human beings have tried to understand the world and themselves with numbers and images since the antiquity. Verbal language cannot embrace the whole scope of abstract world. Mathematics have been considered to represent different dimension of the world and mentality beyond language. The Pythagoreans believed that the principles of mathematics were the principles of all things \cite{1}. Rene Descartes claimed that scientific knowledge should be built up with the fundamentals of mathematics and geometry \cite{1}. Scientism tries to make believe that the evidence of real existence should be tested and validated only by numerical changes or visual and auditory proofs. Abstract or spiritual mental functions such as thinking, affect, and belief, which cannot be numerically positioned or physically tested, have been considered as something non-scientific and non-existent. Meanwhile, Nobel Laureate and atheist Peter

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McDawar said: That there is indeed a limit upon science is made very likely by the existence of questions that science cannot answer and that no conceivable advances of science would empower it to answer [2]. The classical physics and mathematics did not have any clue to relate brain mental function to numerical formula because mental function does not have any spatial dimension, but only having time dimension. Modern physicists solved this puzzle by confessing that the consciousness (and unconsciousness) of the person acts in the world but is not spatially extent [3]. While Freud and Jung empirically and intuitively inferred the existence of unconsciousness, contemporary modern physics made possible clarify the complex system of consciousness and unconsciousness after the collaboration of Wolfgang Pauli and Jung [4]. Despite the development of various human brain research, we still do not have a suitable set of mathematical languages to understand the consciousness [5].

We begin by introducing the recursive Heaviside step functions that the human psyche has no space to locate but exists only with time. The process of being conscious can be explained as constant process of differentiation of recursive Heaviside step function representing unconscious of human. Following Shin and Cha’s approach of which our unconsciousness to a special solution of the multi-dimensional advection-like partial differential equation, we show that humankind is totally dependent upon unconscious that is represented by the infinite recursive Heaviside step function.

2. The Advection-like Equation and Recursive Heaviside Step Function

The advection equation

\[ \frac{\partial U}{\partial t} = -c \frac{\partial U}{\partial x} \tag{2.1} \]

governs the motion of an object that moves in one \(+x\) direction by velocity \(c\), and the wave equation

\[ \frac{\partial^2 U}{\partial t^2} = c^2 \frac{\partial^2 U}{\partial x^2} \tag{2.2} \]

represents the motion in both the \(+x\) and \(-x\) directions [6]. Because the human mental state proceeds only in a forward direction in time and should not depend on any particular space coordinates, we impose the advection-like equation

\[ \frac{\partial U_n}{\partial t} = - \sum_{k=1}^{n} \frac{\partial U_n}{\partial \tau_k}, \quad (n = 1, 2, \cdots) \tag{2.3} \]

to be satisfied by \(U_n\) which denotes the \(n\)-th particular situation pertaining to an individual person. In (2.3), \(\tau_k\)‘s \((k = 1, 2, \cdots, n)\) are virtual time variables that will be elaborated.

Previously, Shin and Cha proved by induction that the recursive Heaviside step function \(U_n(t, T_n)\) is a special solution of the advection-like equation [7], under the condition that the real time \(t\) is not larger than any one of the virtual time variables \(\tau_k\)‘s. The recursive Heaviside step function \(U_n(t, T_n)\) with depth \(n\) is defined in terms of the usual Heaviside step function \(H(-t + t_0)\) by [8]

\[ U_n(t, T_n) = H \left[ -t + \tau_n U_{n-1}(t, T_{n-1}) \right] \tag{2.4} \]
Fig. 1. Heaviside step function $H(-t + \tau)$.

where

$$U_0(t, T_0) = 1, \quad H(-t + t_0) = \begin{cases} 1 & \text{when } t \leq t_0 \\ 0 & \text{when } t > t_0 \end{cases}$$

where $T_n$ in (2.4) is a set of $n$ virtual time variables $T_n = (\tau_n, \tau_{n-1}, \cdots, \tau_1)$ and $T_0$ denotes the null.

Fig. 1. shows the shape of the Heaviside step function $H(-t + \tau)$. The shape of the recursive Heaviside step function $U_n(t, T_n)$ is also same as the Heaviside step function shown above. The vertical axis means the value of the $U_n$ which represents unconsciousness and the horizontal axis represent the time, $\tau_n$ represent the present while $\tau_{n-1}, \tau_{n-2}, \cdots$ denote the past, and $\tau_{n+1}, \tau_{n+2}, \cdots$ denote the future.

3. Unconscious-to-Conscious Process

We postulate that the recursive Heaviside step function $U_n(t, T_n)$ represents individual unconsciousness about a situation from which one aspect of a person’s mental state can be formed. This postulate is conceived because $U_n(t, T_n)$ has an interesting property in which it gives a unique shape that is equal to that of the usual step function $H(-t + \tau_0)$, where $\tau_0$ is the smallest among the virtual time variables $\tau_k$ s, regardless of either the depth $n$ or the values of the other $\tau_k$ s.

We next demand that the partial derivative of the recursive Heaviside step function $U_n(t, T_n)$ with respect to the real time $t$ should be interpreted as consciousness of a person who experiences the situation represented by $U_n(t, T_n)$. Therefore, it can be said that the human brain in action is operating under a constant process of differentiation.

Figure 2 shows the typical example of recursive Heaviside step functions which represents the unconsciousness function of three persons. Jane, Paul and Bill are walking down the street together when a lost dog appeared in front of them. Jane shows no interest as she has had
no meaningful experience with a dog in the past. Paul, on the other hand, goes up to the dog and pats it on the head as he has spent a lot of time with dogs since childhood. However, Bill wants to stay away from the dog as far as he can, because he was once bitten by a dog when he was a child. Three people’s conscious reaction to a lost dog may be different according to their unconsciousness structure cumulated from past experiences. Their unconsciousness of the situation is comparable to functions $U_1$, $U_2$ for Jane, $U_3$ for Paul, and $U_4$ for Bill. Three different reactions (=consciousness) can be expressed as time derivatives $(\partial U_n(t, T_n)/\partial t)$ of human unconsciousness using the recursive Heaviside step function.

4. CONCLUSIONS

This article proves that the process of transformation of unconsciousness into consciousness can be expressed using the infinite recursive Heaviside step function and differentiation of recursive Heaviside step function with respect to current time. Differentiation of unconsciousness function $U_n(t, T_n)$ with respect to time is the process of being conscious. The human reactions depend on past times. For every moment we live and experience, the unconscious constituents are accumulated. Then the human mind has heavy and innate overlapping of unconsciousness at times $\tau_k$. For instance, if humans become unconscious ten trillion different times, there are ten trillion squared different unconscious states including instances where various states co-exist. Consciousness derives from comparison of unconsciousness from the two consecutive moments.
Lives are sum of the integral and differential of every moments and so is the consciousness, which we can never summon into our mind again, even though we have realistically experienced. Single seconds and millimeters we experience can be divided forever, which the invention of scanning tunneling microscope shows. We need to redefine unconsciousness under the umbrella of modern mathematical theorem. Efforts to postulate the existence of unconsciousness through mathematical formulas in the form of recursive Heaviside step function may help AI to imitate, assist, and potentiate human mental activities. We ardently wait further research in the converging field of mathematics, physics, and psychiatry. Development of AI requires algorithmic regeneration of human mental activities on machines. Without numerical analysis of the unconscious potential energy, we can never build up any bridge between the limitless psychological and mechanical worlds.

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REFERENCES

THE CONE PROPERTY FOR A CLASS OF PARABOLIC EQUATIONS

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ABSTRACT. In this note, we show that the cone property is satisfied for a class of dissipative equations of the form $u_t = \Delta u + f(x, u, \nabla u)$ in a domain $\Omega \subset \mathbb{R}^2$ under the so called exactness condition for the nonlinear term. From this, we see that the global attractor is represented as a Lipshitz graph over a finite dimensional eigenspace.

1. INTRODUCTION

An inertial manifold is a positively invariant finite dimensional Lipshitz manifold which attracts all solutions with an exponential rate. Thus, it contains a global attractor and the existence of an inertial manifold can explain the long time behavior of the solutions of evolutionary equations. Moreover, it allows for the reduction of the dynamics to a finite dimensional ordinary differential equation, which is called an inertial form. Inertial manifolds have been constructed for a wide class of partial differential equations. We refer to [2] and [5] for a more detailed exposition of this theory. However, the theory stands incomplete since there are important equations, including the Navier-Stokes equation, for which the inertial manifolds are not known to exist. The main reason for this is the failure of the spectral gap condition for the eigenvalues of the leading partial differential operator.

In this note, we give a new observation that leads to the existence of an inertial manifold for a class of equations of the form

$$u_t = \Delta u + f(x, u, \nabla u), \ x \in \Omega \subset \mathbb{R}^2$$

with the Dirichlet boundary condition

$$u|_{\partial \Omega} = 0.$$ 

Here, $u = u(t, x)$ is a scalar function and $\Omega$ is a rectangular domain, for which the spectral gap condition is satisfied. Until now, it is known that the gap condition holds only for special
bounded domains in $\mathbb{R}^2$ (see [5]). Furthermore, we impose a so called exactness condition on the nonlinear term:

$$f(x_1, x_2, u, p_1, p_2)_{p_1x_2} = f(x_1, x_2, u, p_1, p_2)_{p_2x_1}.$$  \hspace{1cm} (1.2)

The condition (1.2) is restrictive, but it allows $f$ to be a combination of functions $g(x, u)$, $|\nabla u|^2$ and $\nabla \phi \cdot \nabla u$ for some differentiable functions $g$ and $\phi$ in each variable. In the subsequent sections, we give the basic notations and the main results.

2. Notation and the main result

Let the space $H$ be a Hilbert space with an inner product $\langle \cdot, \cdot \rangle$ and a norm $\| \cdot \|$. Let $\{\lambda_j\}$ be the eigenvalues of the operator $A = -\Delta + \text{boundary condition}$ such that

$$\lambda_1 < \lambda_2 \leq \ldots \leq \lambda_N < \lambda_{N+1} \ldots,$$

and $\{\phi_j\}$ be the corresponding eigenvectors. Denote by $P$ the orthogonal projection operator from $H$ to a finite dimensional space spanned by $\{\phi_1, \phi_2, \ldots, \phi_N\}$. If $Q = I - P$, then $H$ is orthogonally decomposed as $H = PH \oplus QH$. Let $A$ be a global attractor for the solutions of the equation (1.1). Then we are interested in the question whether the projection operator $P$ restricted to $A$ is injective, i.e.,

$$P : A \rightarrow PH \text{ is injective?} \hspace{1cm} (2.1)$$

Equivalently, if $u_1(t) = p_1(t) + q_1(t)$ and $u_2(t) = p_2(t) + q_2(t)$ are two solutions with $p_1(t), p_2(t) \in PH$ and $q_1(t), q_2(t) \in QH$, then the question (2.1) can be rephrased as

$$p_1(0) = p_2(0) \Rightarrow u_1(t) = u_2(t), \text{ for all } t? \hspace{1cm} (2.2)$$

To state the main result, we recall the cone property ([4]). Let

$$u_1(t) = p_1(t) + q_1(t), \hspace{0.5cm} u_2(t) = p_2(t) + q_2(t),$$

$$\rho(t) = p_1(t) - p_2(t), \hspace{0.5cm} \sigma(t) = q_1(t) - q_2(t).$$

The cone $C_k$ is defined as a subset of $H$ by

$$C_k = \{(\rho, \sigma) \in H : \|\sigma\| \leq k\|\rho\|\} \hspace{1cm} (2.3)$$

for some $k > 0$. Then the cone property is stated as

(i) If $u_2(0) \in u_1(0) + C_k$, then $u_2(t) \in u_1(t) + C_k$ for all $t > 0$.

(ii) If $u_2(0) \notin u_1(0) + C_k$, then either $u_2(t_0) \in u_1(t_0) + C_k$ for some $t_0$ and remains there for all $t > t_0$ or $u_2(t) \notin u_1(t) + C_k$ and $\|u_1(t) - u_2(t)\| \to 0$ exponentially as $t \to \infty$.

It is well-known that the cone property is satisfied for the case of global Lipschitz nonlinearity under the gap condition (2.6) below. More precisely, we consider the equation

$$\frac{du}{dt} = -Au + F(u), \hspace{1cm} (2.4)$$

and assume the nonlinear term is global Lipschitz continuous with the constant $K$:

$$\|F(u) - F(v)\| \leq K\|u - v\|, \text{ for all } u, v \in H. \hspace{1cm} (2.5)$$
First, we prove the cone property in an equivalent but concise form.

**Proposition 1.** Let \( u_1(t) \) and \( u_2(t) \) be any two orbits in the global attractor of the equation (2.4). Under the assumption of the spectral gap condition

\[
\lambda_{N+1} - \lambda_N > \frac{(1+k)^2}{k} K, \quad (2.6)
\]

we have \( ||\sigma|| \leq k||\rho|| \) for all \( t \in \mathbb{R} \) and, therefore, the projection \( P \) is injective.

**Remark 1.** The proof is standard, however we provide a new simpler proof here.

**Proof.** Let \( u_1(t) = p_1(t) + q_1(t) \) and \( u_2(t) = p_2(t) + q_2(t) \). Then, for \( \rho(t) = p_1(t) - p_2(t) \) and \( \sigma(t) = q_1(t) - q_2(t) \), we have

\[
\begin{align*}
p_t &= -A\rho + PF(u_1) - PF(u_2), \\
\sigma_t &= -A\sigma + QF(u_1) - QF(u_2). \quad (2.7)
\end{align*}
\]

The standard estimates for \( \rho \) and \( \sigma \) give

\[
\frac{1}{2} \frac{d}{dt} ||\rho||^2 = \langle \rho_t, \rho \rangle = -||A^{1/2}\rho||^2 + <PF(u_1) - PF(u_2), \rho > \geq -\lambda_N ||\rho||^2 - K(||\rho|| + ||\sigma||)||\rho||, \quad (2.8)
\]

and

\[
\frac{1}{2} \frac{d}{dt} ||\sigma||^2 = \langle \sigma_t, \sigma \rangle = -||A^{1/2}\sigma||^2 + <QF(u_1) - QF(u_2), \sigma > \leq -\lambda_{N+1} ||\sigma||^2 + K(||\rho|| + ||\sigma||)||\sigma||. \quad (2.9)
\]

From (2.8) and (2.9), it follows that

\[
\frac{1}{2} \frac{d}{dt} (||\sigma||^2 - k^2 ||\rho||^2) \leq -\lambda_{N+1} ||\sigma||^2 + \lambda_N k^2 ||\rho||^2 + K(||\rho|| + ||\sigma||)||\sigma|| + k^2 K(||\rho|| + ||\sigma||)||\rho||. \quad (2.10)
\]

On the boundary of the cone \( ||\sigma|| = k||\rho|| \), we find that

\[
\frac{1}{2} \frac{d}{dt} (||\sigma||^2 - k^2 ||\rho||^2) \leq -(\lambda_{N+1} - \lambda_N) k^2 ||\rho||^2 + k(1 + k)^2 K ||\rho||^2 < 0, \quad (2.11)
\]

under the condition

\[
\lambda_{N+1} - \lambda_N > \frac{(1+k)^2}{k} K. \quad (2.12)
\]

This implies, once \( u_1(t) - u_2(t) \) is in \( C_k \), it will never leave it through the boundary \( ||\sigma|| = k||\rho|| \) and stays in the cone for all time.

Furthermore, if two orbits sit outside of the cone for some time \( t_0 \), then they must stay there for all \( t \leq t_0 \). That is, if \( (||\sigma||^2 - k^2 ||\rho||^2)(t_0) > 0 \) for some \( t_0 \in \mathbb{R} \), then

\[
(||\sigma||^2 - k^2 ||\rho||^2)(t) > 0
\]
for all $t \leq t_0$. From (2.9),

$$\frac{1}{2} \frac{d}{dt} \|\sigma\|^2 \leq -\lambda_{N+1}\|\sigma\|^2 + (1 + \frac{1}{k})K\|\sigma\|^2 = -a_N\|\sigma\|^2,$$

(2.13)

with

$$a_N = \lambda_{N+1} - \frac{k+1}{k}K > 0.$$

The inequality (2.13) gives

$$\frac{d}{dt}(e^{2a_N t}\|\sigma\|^2) \leq 0$$

(2.14)

or

$$e^{2a_N t_0}\|\sigma(t_0)\|^2 \leq e^{2a_N t}\|\sigma(t)\|^2, \text{ for all } t \leq t_0.$$

(2.15)

Since any orbit in the global attractor is bounded for all time, taking $t \to -\infty$, we get

$$\|\sigma\|^2 \leq k^2\|\rho\|^2,$$

(2.16)

Thus

Now, we state the main results of this note.

**Theorem 1.** Let $u_1(t)$ and $u_2(t)$ satisfy the cone property:

$$\|\sigma\| \leq k\|\rho\|, \text{ for all } t \in \mathbb{R}$$

(2.17)

with $v = u_1 - u_2 = \rho + \sigma$. Let us consider a nonlinear change of variable given by

$$V(x, t) = v(x, t)e^{-\gamma(x,t)}.$$

(2.18)

If $\gamma = \gamma(x,t)$ is any bounded smooth function for $x \in \Omega$ and $t \in \mathbb{R}$, then $V(x, t)$ also satisfies the cone property with a different constant.

**Remark 2.** The change of variable (2.18) was first used for one dimensional dissipative equations from a different point of view in [3].

**Proof.** Denote $\tilde{\rho} = PV$ and $\tilde{\sigma} = QV$. Recalling $v = Ve^{-\gamma}$, we obtain

$$\|\rho\||\tilde{\rho}| \geq \langle \rho, \tilde{\rho} \rangle \geq \langle \rho, PV \rangle \geq \langle \rho, Pve^{-\gamma} \rangle \geq \langle \rho, (\rho + \sigma)e^{-\gamma} \rangle$$

$$= \int_{\Omega} \rho^2 e^{-\gamma} dx + \int_{\Omega} \rho \sigma e^{-\gamma} dx \geq m\|\rho\|^2 - M\|\rho\||\|\sigma||,$$

(2.19)

where $m = \min e^{-|\gamma(x,t)|}$ and $M = \max e^{|\gamma(x,t)|}$.

Thus

$$\|\rho\| \leq \frac{1}{m} \|\tilde{\rho}\| + \frac{M}{m}\|\sigma\|$$

(2.20)

and then from (2.17), we have

$$\|\sigma\| \leq k\|\rho\| \leq \frac{k}{m}\|\tilde{\rho}\| + \frac{kM}{m}\|\sigma\|.$$
Without loss of generality, we may assume \( \frac{kM}{m} \leq \frac{1}{2} \) and then (2.21) becomes
\[
\frac{1}{2} \|\sigma\| \leq \frac{k}{m} \|\tilde{\rho}\|. \tag{2.22}
\]
Similarly, we have
\[
\|\sigma\| \|\tilde{\sigma}\| \geq \langle \sigma, \tilde{\sigma} \rangle = \langle QVe^{\gamma}, \tilde{\sigma} \rangle = \langle \tilde{\sigma}, (\tilde{\rho} + \tilde{\sigma})e^{\gamma} \rangle \geq m\|\tilde{\sigma}\|^2 - M\|\tilde{\rho}\|\|\tilde{\sigma}\| \tag{2.23}
\]
and
\[
\|\sigma\| \geq m\|\tilde{\sigma}\| - M\|\tilde{\rho}\|. \tag{2.24}
\]
Finally, combining (2.22) and (2.24), it yields
\[
m\|\tilde{\sigma}\| - M\|\tilde{\rho}\| \leq \|\sigma\| \leq \frac{2k}{m}\|\tilde{\rho}\|, \tag{2.25}
\]
thus, we get
\[
\|\tilde{\sigma}\| \leq \frac{mM + 2k}{m^2}\|\tilde{\rho}\|, \tag{2.26}
\]
which completes the proof. \( \Box \)

As an application of the Theorem 1, let us consider the equation (1.1) with the condition (1.2). Let \( v = u_1 - u_2 \). Then, from (1.1), we can write
\[
v_t = \Delta v + \alpha_1(x,t)v_{x_1} + \alpha_2(x,t)v_{x_2} + \beta(x,t)v, \tag{2.27}
\]
with
\[
\alpha_i(x,t) = \int_0^1 \frac{\partial f}{\partial p_i}(x,u_1 + \tau u_1 - u_2, \nabla u_1 + \tau(\nabla u_1 - \nabla u_2))d\tau, \tag{2.28}
\]
for \( i = 1, 2 \), and
\[
\beta(x,t) = \int_0^1 \frac{\partial f}{\partial z}(x,u_2 + \tau(u_1 - u_2), \nabla u_2 + \tau(\nabla u_1 - \nabla u_2))d\tau. \tag{2.29}
\]
Now the nonlinear change of variable \( V(x,t) = v(x,t)e^{-\gamma(x,t)} \) in (2.28) yields
\[
V_t = \Delta V + \sum_{i=1}^2 (2\gamma_{x_i} + \alpha_i)V_{x_i} + (\Delta \gamma + |\nabla \gamma|^2 + \sum_{i=1}^2 \alpha_i\gamma_{x_i} + \beta - \gamma_t)V. \tag{2.30}
\]
We see that the exactness condition
\[
f(x_1, x_2, u, p_1, p_2)p_{1x_1} = f(x_1, x_2, u, p_1, p_2)p_{2x_2}
\]
implies that the system
\[
\begin{align*}
2\gamma_{x_1} + \alpha_1 &= 0 \\
2\gamma_{x_2} + \alpha_2 &= 0
\end{align*} \tag{2.31}
\]
can be solved for $\gamma$. Then the new equation becomes
\[
V_t = \Delta V + \eta(x, t)V,
\] (2.32)
where
\[
\eta(x, t) = \Delta \gamma + |\nabla \gamma|^2 - 2 \sum_{i=1}^{2} \gamma_{x_i}^2 + \beta - \gamma_t
\]
and $\eta(x, t)$ and its derivatives are bounded functions. Now we apply the Proposition 1 to the equation (2.32) and obtain the cone property under the spectral gap condition (2.6). Finally, the Theorem 1 gives the cone property for the equation (1.1). This implies the global attractor is indeed Lipschitz manifold with a finite dimension.

Since the cone condition (2.26) is satisfied, we can construct an $N$-dimensional inertial manifold for (2.32) considering the negatively bounded solutions in [1].

Moreover, noting that
\[
V_{x_i} = v_{x_i} e^{-\gamma} - v e^{-\gamma} \gamma_{x_i} = v_{x_i} e^{-\gamma} - \gamma_{x_i} V
\] (2.33)
(2.30) is rewritten as
\[
V_t = \Delta V + \sum_{i=1}^{2} (2 \gamma_{x_i} + \alpha_i) v_{x_i} e^{-\gamma} + (\Delta \gamma + |\nabla \gamma|^2 - 2 \sum_{i=1}^{2} \gamma_{x_i}^2 + \beta - \gamma_t)V. \tag{2.34}
\]

If we can solve the following linear first order partial differential equation for $z = \gamma(x, y, t)$ on a rectangular domain:
\[
2v_{x_1} \gamma_{x_1} + 2v_{x_2} \gamma_{x_2} = -v_{x_1} \alpha_1 - v_{x_2} \alpha_2, \tag{2.35}
\]
then we obtain a similar equation in the form (2.32).

The coefficients in (2.35) are smooth in every variables $x_1, x_2$ and $t$. Thus, we may write (2.35) in the form
\[
a(x, y, t)u_x + b(x, y, t)u_y = c(x, y, t). \tag{2.36}
\]
We look for a bounded smooth solution $z = u(x, y, t)$ at least $C^2$ in a space variable and $C^1$ in a time variable. The standard method is solving the characteristic system (a gradient flow):
\[
\frac{dx}{ds} = a(x(s), y(s), t(s)), \ \\
\frac{dy}{ds} = b(x(s), y(s), t(s)), \ \\
\frac{dt}{ds} = 0 \tag{2.37}
\]
and integrating along the characteristic:
\[
\frac{du(s)}{ds} = c(x(s), y(s), t(s)). \tag{2.38}
\]
However, the geometry of the flow is unclear at this moment and it will be investigated in future works.

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NUMERICAL SOLUTIONS OF AN UNSTEADY 2-D INCOMPRESSIBLE FLOW WITH HEAT AND MASS TRANSFER AT LOW, MODERATE, AND HIGH REYNOLDS NUMBERS

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ABSTRACT. In this paper, we have proposed a modified Marker-And-Cell (MAC) method to investigate the problem of an unsteady 2-D incompressible flow with heat and mass transfer at low, moderate, and high Reynolds numbers with no-slip and slip boundary conditions. We have used this method to solve the governing equations along with the boundary conditions and thereby to compute the flow variables, viz. \( u \)-velocity, \( v \)-velocity, \( P \), \( T \), and \( C \). We have used the staggered grid approach of this method to discretize the governing equations of the problem. A modified MAC algorithm was proposed and used to compute the numerical solutions of the flow variables for Reynolds numbers \( Re = 10, 500, \) and \( 50000 \) in consonance with low, moderate, and high Reynolds numbers. We have also used appropriate Prandtl (\( Pr \)) and Schmidt (\( Sc \)) numbers in consonance with relevancy of the physical problem considered. We have executed this modified MAC algorithm with the aid of a computer program developed and run in C compiler. We have also computed numerical solutions of local Nusselt (\( Nu \)) and Sherwood (\( Sh \)) numbers along the horizontal line through the geometric center at low, moderate, and high Reynolds numbers for fixed \( Pr = 6.62 \) and \( Sc = 340 \) for two grid systems at time \( t = 0.0001s \). Our numerical solutions for \( u \) and \( v \) velocities along the vertical and horizontal line through the geometric center of the square cavity for \( Re = 100 \) has been compared with benchmark solutions available in the literature and it has been found that they are in good agreement. The present numerical results indicate that, as we move along the horizontal line through the geometric center of the domain, we observed that, the heat and mass transfer decreases up to the geometric center. It, then, increases symmetrically.

1. INTRODUCTION

The problem of 2-D unsteady incompressible viscous fluid flow with heat and mass transfer has been the subject of intensive numerical computations in recent years. This is due to
its significant applications in many scientific and engineering practices. Fluid flows play an important role in various equipment and processes. Unsteady 2-D incompressible viscous flow coupled with heat and mass transfer is a complex problem of great practical significance.

**NOMENCLATURE**

- $\Delta t$ time spacing
- $\Delta x$ grid spacing along $x$-axis
- $\Delta y$ grid spacing along $y$-axis
- $\frac{\partial}{\partial n}$ differentiation along the normal to the boundary
- $u, v$ dimensionless velocity components in $x, y$ coordinate directions, respectively
- $\hat{u}, \hat{v}$ pseudo-velocity components in $x, y$ coordinate directions, respectively
- $\nabla \cdot \hat{u}$ divergence of pseudo-velocity vector
- $\nabla \cdot \vec{u}$ divergence of dimensionless velocity vector
- $u^n$ $x$ component of the dimensionless velocity after $n$ iterations
- $v^n$ $y$ component of the dimensionless velocity after $n$ iterations
- $Nu$ local Nusselt number
- $Pr$ Prandtl number, $\nu/k$
- $Re$ Reynolds number, $uL/\mu$
- $i$ index used in tensor notation
- $Sh$ local Sherwood number
- $\rho$ fluid density ($kg/m^3$)
- $x, y$ coordinates
- $\bar{u}$ dimensionless velocity vector
- $C$ dimensionless concentration
- $D$ mass diffusivity ($m^2/s$)
- $Sc$ Schmidt number, $\nu/D$
- $j$ index used in tensor notation
- $k$ thermal diffusivity ($m^2/s$)

This problem has received considerable attention due to its numerous engineering practices in various disciplines, such as storage of radioactive nuclear waste materials, transfer groundwater pollution, oil recovery processes, food processing, and the dispersion of chemical contaminants in various processes in the chemical industry. More often, fluid flow with heat and mass transfer is coupled in nature. Heat transfer is concerned with the physical process underlying the transport of thermal energy due to a temperature difference or gradient. All the process equipment used in engineering practice has to pass through an unsteady state in the beginning when the process is started, and, they reach a steady state after sufficient time has elapsed. Typical examples of unsteady heat transfer occur in heat exchangers, boiler tubes, cooling of cylinder heads in I.C. engines, heat treatment of engineering components and quenching of ingots, heating of electric irons, heating and cooling of buildings, freezing of foods, etc. Mass transfer is an important topic with vast industrial applications in mechanical, chemical and aerospace engineering. Few of the applications involving mass transfer are
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absorption and desorption, solvent extraction, evaporation of petrol in internal combustion engines etc. Numerous everyday applications such as dissolving of sugar in tea, drying of wood or clothes, evaporation of water vapor into the dry air, diffusion of smoke from a chimney into the atmosphere, etc. are also examples of mass diffusion. In many cases, it is interesting to note that heat and mass transfer occur simultaneously.

Harlow and Welch [1] used the Marker-And-cell (MAC) method for numerical calculation of time-dependent viscous incompressible flow of fluid with the free surface. This method employs the primitive variables of pressure and velocity that has practical application to the modeling of fluid flows with free surfaces. Ghia et al. [3] have used the vorticity-stream function formulation for the two-dimensional incompressible Naiver-Stokes equations to study the effectiveness of the coupled strongly implicit multi-grid (CSI-MG) method in the determination of high-Re fine-mesh flow solutions. Issa et al. [5] have used a non-iterative implicit scheme of finite volume method to study compressible and incompressible recirculating flows. Elbashbeshy [6] has investigated the unsteady mass transfer from a wedge. Sattar [7] has studied free convection and mass transfer flow through a porous medium past an infinite vertical porous plate with time-dependent temperature and concentration. Sattar and Alam [8] have investigated the MHD free convective heat and mass transfer flow with hall current and constant heat flux through a porous medium. Maksym Grzywinski, Andrzej Sluzalec [10] solved the stochastic convective heat transfer equations in finite differences method. A numerical procedure based on the stochastic finite differences method was developed for the analysis of general problems in free/forced convection heat transfer. Lee [11] has studied fully developed laminar natural convection heat and mass transfer in a partially heated vertical pipe. Chiriac and Ortega [12] have numerically studied the unsteady flow and heat transfer in a transitional confined slot jet impinging on an isothermal plate. De and Dalai [14] have numerically studied natural convection around a tilted heated square cylinder kept in an enclosure has been studied in the range of $1000 \leq Ra \leq 1000000$. Detailed flow and heat transfer features for two different thermal boundary conditions are reported. Chiu et al. [15] proposed an effective explicit pressure gradient scheme implemented in the two-level non-staggered grids for incompressible Navier-Stokes equations. Xu et al. [16] have investigated the transition to a periodic flow induced by a thin fin on the side wall of a differentially heated cavity. Lambert et al. [17] studied the heat transfer enhancement in oscillatory flows of Newtonian and viscoelastic fluids. Alharbi et al. [18] presented the study of convective heat and mass transfer characteristics of an incompressible MHD visco-elastic fluid flow immersed in a porous medium over a stretching sheet with chemical reaction and thermal stratification effects. Xu et al. [20] have investigated the unsteady flow with heat transfer adjacent to the finned sidewall of a differentially heated cavity with conducting adiabatic fin. Fang et al. [21] have investigated the steady momentum and heat transfer of a viscous fluid flow over a stretching/shrinking sheet. Salman et al. [22] have investigated heat transfer enhancement of nano fluids flow in micro constant heat flux. Hasanuzzaman et al. [23] investigated the effects of Lewis number on heat and mass transfer in a triangular cavity. Schladow [24] has investigated oscillatory motion in a side-heated cavity. Lei and Patterson [25] have investigated unsteady natural convection in a triangular enclosure induced by absorption of radiation. Ren and Wan [26] have proposed a new approach
to the analysis of heat and mass transfer characteristics for laminar air flow inside vertical plate channels with falling water film evaporation.

The above mentioned literature survey pertinent to the present problem under consideration revealed that, to obtain high accurate numerical solutions of the flow variables, we need to depend on high accurate and high resolution method like the modified Marker-And-Cell (MAC) method, being proposed in this work. Furthermore, a modified MAC algorithm is employed for computing unknown variables $u$, $v$, $P$, $T$, and $C$ simultaneously.

What motivated us is the enormous scope of applications of unsteady incompressible flow with heat and mass transfer as discussed earlier. Literature survey also revealed that, the problem of 2-D unsteady incompressible flow with, heat and mass transfer in a rectangular domain, along with slip wall, temperature, and concentration boundary conditions has not been studied numerically. Furthermore, it has also been observed that, there is no literature to conclude availability of high accurate method that solves the governing equations of the present problem subject to the initial and boundary conditions. Moreover, in order to investigate the importance of the applications enumerated upon earlier, there is a need to determine numerical solutions of the unknown flow variables. In order to fulfil this requirement, we present numerical an investigation of the problem of unsteady 2-D incompressible flow, with heat and mass transfer in a rectangular domain, along with slip wall, temperature, and concentration boundary conditions, using the modified Marker-And-Cell (MAC) method. Though there is a well known MAC method for solving the problem of 2-D fluid flow, we present a suitably modified MAC method as well as a modified MAC algorithm to compute the accurate numerical solutions of the flow variables to the problem considered in this work.

Our main target of this work is to propose and use the modified Marker-And-Cell (MAC) method of pressure correction approach to investigate the problem of unsteady 2-D incompressible flow with heat and mass transfer. We have proposed and used this method to solve the governing equations along with no-slip and slip wall boundary conditions and thereby to compute the flow variables. We have used a modified MAC algorithm for discretizing the governing equations in order to compute the numerical solutions of the flow variables at different Reynolds numbers in consonance with low, moderate, and high. We have executed this modified MAC algorithm with the aid of a computer program developed and run in C compiler. We have also computed numerical solutions of local Nusselt ($Nu$) and Sherwood ($Sh$) numbers along the horizontal line through the geometric center at low, moderate, and high $Re$, for fixed $Pr = 6.62$ and $Sc = 340$ for two grid systems at time $t = 0.0001s$.

The summary of the layout of the current work is as follows: Section 2 describes mathematical formulation that includes physical description of the problem, governing equations, and initial and boundary conditions. Section 3 describes the modified Marker-And-Cell method, along with the discretization of the governing equations. Section 4 describes a modified Marker-And-Cell (MAC) algorithm, along with numerical computations. Section 5 discusses the numerical results. Section 6 illustrates the conclusions of this study. Section 7 provides validity of our computer code used to obtain numerical solutions with the benchmark solutions.
2. Mathematical Formulation

2.1. Physical Description. Fig. 1 illustrates the geometry of the problem considered in this study along with no-slip and slip boundary conditions. ABCD is a rectangular domain around the point \((1.0, 0.5)\) in which an unsteady 2-D incompressible viscous flow with heat and mass transfer is considered. Flow is setup in a rectangular domain with three stationary walls and a top lid that moves to the right with constant speed \((u = 1)\).

![Figure 1. Rectangular cavity](image)

We have assumed that, at all four corner points of the computational domain, velocity components \((u, v)\) vanish. It may be noted here regarding specifying the boundary conditions for pressure, the convention followed is that either the pressure at boundary is given or velocity components normal to the boundary is specified [2, pp.129].

2.2. Governing equations. The governing equations of 2-D unsteady incompressible flow with heat and mass transfer in a rectangular domain are the continuity equation, the two components of momentum equation, the energy equation, and the equation of mass transfer. These equations (2.1) to (2.5) subject to boundary conditions (2.6) and (2.7) are discretized using the modified Marker-And-Cell (MAC) method. Taking usual the Boussinesq approximations into account, the dimensionless governing equations are expressed as follows:

- **Continuity equation**
  \[
  \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (2.1)
  \]

- **x-momentum**
  \[
  \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial P}{\partial x} + \left( \frac{1}{Re} \right) \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad (2.2)
  \]

- **y-momentum**
  \[
  \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial P}{\partial y} + \left( \frac{1}{Re} \right) \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \quad (2.3)
  \]

- **Energy equation**
  \[
  \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \left( \frac{1}{Pr} \right) \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \quad (2.4)
  \]
Mass transfer equation
\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \left( \frac{1}{Sc} \right) \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right).
\] (2.5)

where \(u, v, P, T, C, Re, Pr,\) and, \(Sc\) are the velocity components in \(x\) and \(y\)-directions, the pressure, the temperature, the concentration, the Reynolds number, the Prandtl number, and the Schmidt number respectively.

The initial, no-slip and slip wall boundary conditions are given by:

\begin{align*}
\text{for } t = 0, \quad u(x, y, 0) &= 0, \quad v(x, y, 0) = 0, \quad T(x, y, 0) = 10, \quad C(x, y, 0) = 10. 
\end{align*}
(2.6)

\begin{align*}
\text{for } t > 0, \quad &\text{on boundary AB: } u = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = 0, \quad \frac{\partial C}{\partial x} = 0, \\
&\text{on boundary BC: } u = 0, \quad v = 0, \quad T = T_0 + \Delta T, \quad C = C_0 + \Delta C, \\
&\text{on boundary CD: } u = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = 0, \quad \frac{\partial C}{\partial x} = 0, \\
&\text{on boundary AD: } u = 1, \quad v = 0, \quad T = T_0 - \Delta T, \quad C = C_0 - \Delta C. 
\end{align*}
(2.7)

3. NUMERICAL METHOD AND DISCRETIZATION

3.1. Modified Marker-And-Cell (MAC) Method. Our main purpose in this work is to propose and use an accurate numerical method that solves the governing equations of the present problem subject to the initial and boundary conditions. In order to solve the equations (2.1)-(2.5) which are semi-linear coupled partial differential equations, we propose and use the modified Marker-And-Cell (MAC) method based on the MAC method of Harlow and Welch [1]. The present modified MAC method (algorithm) is a generalization of the original MAC method in the sense that the original one enable us to discretized equations (2.1)-(2.3) and hence to compute the flow variables \(u, v,\) and \(P.\) Where as, the modified MAC method (algorithm) enable us to discretized equations (2.1)-(2.5) and hence to compute the flow variables \(u, v, P, T,\) and \(C.\) Consider a modified MAC staggered grid for \(u, v,\) and a scalar node (\(P\) node), where pressure, temperature, and concentration variables are stored as shown in Fig. 2. The \(x\)-momentum equation is written at \(u\) nodes, and the \(y\)-momentum equation is written at \(v\) nodes. The energy and the mass transfer equations are written at a scalar node. Accordingly, the various derivatives in the \(x\)-momentum equation (2.2) are calculated as follows:

\begin{align*}
\left( \frac{\partial u}{\partial t} \right)^{n+1}_{i+1/2,j} &= \left( u^{n+1}_{i+1/2,j} - u^n_{i+1/2,j} \right) / \Delta t, \\
\left( \frac{\partial^2 u}{\partial x^2} \right)^{n+1}_{i+1/2,j} &= \left( u^{n+1}_{i+3/2,j} - 2u^{n+1}_{i+1/2,j} + u^{n+1}_{i-1/2,j} \right) / \Delta x^2, \\
\left( \frac{\partial^2 u}{\partial y^2} \right)^{n+1}_{i+1/2,j} &= \left( u^{n+1}_{i+1/2,j+1} - 2u^{n+1}_{i+1/2,j} + u^{n+1}_{i+1/2,j-1} \right) / \Delta y^2.
\end{align*}
(3.1)-(3.3)
\[
\left( \frac{\partial P}{\partial x} \right)_{i+1/2,j}^{n+1} = \left( P_{i+1,j}^{n+1} - P_{i,j}^{n+1} \right) / \Delta x.
\] (3.4)

Using the modified MAC method, the other terms in the \(x\)-momentum equation \((2.2)\) are written as
\[
\left( \frac{\partial u}{\partial x} \right)_{i+1/2,j}^{n} = u_{i+1/2,j}^{n} \left( u_{i+3/2,j}^{n} - u_{i+1/2,j}^{n} \right) / \Delta x,
\] (3.5)
\[
\left( \frac{\partial v}{\partial y} \right)_{i+1/2,j}^{n} = v_{i+1/2,j}^{n} \left( u_{i+1/2,j+1}^{n} - u_{i+1/2,j}^{n} \right) / \Delta y.
\] (3.6)

Here \(v_{i+1/2,j}^{n}\) is given by
\[
v_{i+1/2,j}^{n} = \left( v_{i,j+1/2}^{n} + v_{i,j-1/2}^{n} + v_{i+1,j+1/2}^{n} + v_{i+1,j-1/2}^{n} \right) / 4.
\] (3.7)

\[\text{FIGURE 2. Modified MAC staggered grid system}\]

For simplicity, we will implement a fully explicit version of the time-splitting (fractional time-step) method, for both the viscous and the diffusion terms. When this method is applied to the \(x\)-momentum equation on the staggered grid from time level \(t^n\) to \(\hat{t}\) yields the following equation at the intermediate step:
\[
\frac{u_{i+1/2,j}^{n+1} - u_{i+1/2,j}^{n}}{\Delta t} = \frac{u_{i+1/2,j}^{n+1} - u_{i+3/2,j}^{n}}{\Delta x} + \frac{v_{i+1/2,j}^{n} \left( u_{i+1/2,j+1}^{n} - u_{i+1/2,j}^{n} \right)}{\Delta y} + \frac{2u_{i+1/2,j}^{n} - 2u_{i+1/2,j}^{n} - u_{i-1/2,j}^{n} + u_{i+1/2,j}^{n} - u_{i+1/2,j}^{n+1} - u_{i+1/2,j}^{n+1}}{Re \Delta x^2} + \frac{2u_{i+1/2,j+1}^{n} - 2u_{i+1/2,j}^{n} + u_{i+1/2,j}^{n} - u_{i+1/2,j}^{n+1} - u_{i+1/2,j}^{n+1}}{Re \Delta y^2}.
\] (3.8)
Similarly for the \( y \)-momentum equation we obtain the following equation:

\[
\frac{\Delta t}{Re} \sum_{i,j} \left( \begin{array}{c}
\hat{v}_{i,j+1/2} - v^{n}_{i,j+1/2} \\
\hat{v}_{i+1,j+1/2} - v^{n}_{i+1,j+1/2} + \frac{v^{n}_{i,j+1/2} - v^{n}_{i,j+3/2}}{2}
\end{array} \right) + \frac{v^{n}_{i+1,j+1/2} - 2v^{n}_{i,j+1/2} + v^{n}_{i-1,j+1/2}}{Re \Delta x^2} + \frac{v^{n}_{i,j+3/2} - 2v^{n}_{i,j+1/2} + v^{n}_{i,j-1/2}}{Re \Delta y^2},
\]

(3.9)

Practical stability requirement obtained from the Von Neumann analysis for the Euler explicit solvers are given by Peyret and Taylor [4, 148], given in equations (3.10) and (3.11). It may be noted here that these relations establish stability requirement of the discretized equations associated with the original MAC method. Where as the present physical problem contains additional flow variables associated with heat and mass transfer equations ((2.4) and (2.5)). For which the discretized equations are in (3.19) and (3.20). However there is a need to define stability requirement which are proposed by us in equations (3.12) and (3.13). In fact, these two relations contain \( Pr \) and \( Sc \), associated in heat and mass transfer equations.

(3.10)
\[
\left( |u| + |v| \right)^2 \Delta t Re \leq 4,
\]

(3.11)
\[
\frac{\Delta t}{Re} \left[ \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right] \leq 5,
\]

(3.12)
\[
\Delta t_{\text{max}} \left[ \frac{\left( \frac{u_{i+1,j}}{\Delta x} + \frac{v_{i,j}}{\Delta y} \right)}{Re} + \frac{2}{Pr} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \right] \leq 1,
\]

(3.13)
\[
\Delta t_{\text{max}} \left[ \frac{\left( \frac{u_{i,j+1}}{\Delta x} + \frac{v_{i,j}}{\Delta y} \right)}{Re} + \frac{2}{Sc} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \right] \leq 1.
\]

Now advancing from \( t^n \) to \( \hat{t} \) and then \( \hat{t} \) to \( t^{n+1} \) one obtains the elliptical pressure equation:

\[
\frac{\nabla \cdot \hat{u}}{\Delta t} = \nabla^2 P^{n+1}.
\]

(3.14)

The corresponding homogeneous Neumann boundary condition for pressure is given by:

\[
\frac{\partial P^{n+1}}{\partial n} = 0.
\]

(3.15)

Now using central difference scheme:

\[
\frac{P^{n+1}_{i+1,j} - 2P^{n+1}_{i,j} + P^{n+1}_{i-1,j}}{\Delta x^2} + \frac{P^{n+1}_{i,j+1} - 2P^{n+1}_{i,j} + P^{n+1}_{i,j-1}}{\Delta y^2} = \frac{1}{\Delta t} \left[ \frac{\hat{u}_{i+1/2,j} - \hat{u}_{i-1/2,j}}{\Delta x} + \frac{\hat{v}_{i,j+1/2} - \hat{v}_{i,j-1/2}}{\Delta y} \right].
\]

(3.16)

We obtain the velocity field at the advanced time level \( (n + 1) \), for each velocity component, this equation gives

\[
u^{n+1}_{i+1/2,j} = \hat{u}_{i+1/2,j} - \frac{\Delta t}{\Delta x} \left( P^{n+1}_{i+1,j} - P^{n+1}_{i,j} \right),
\]

(3.17)
energy equation is written as follows:
\[ v_{i,j+1/2}^{n+1} = \hat{v}_{i,j+1/2} - \frac{\Delta t}{\Delta y} (P_{i,j+1}^{n+1} - P_{i,j}^{n+1}). \] (3.18)

The modified MAC staggered grid quotients of different derivatives which appeared in the energy equation is written as follows:
\[
\left( \frac{\partial T}{\partial t} \right)^{n+1}_{i,j} = \left( T^{n+1}_{i,j} - T^n_{i,j} \right) / \Delta t,
\left( \frac{\partial T}{\partial x} \right)^{n}_{i+1,j} = \left( T^n_{i+1,j} - T^n_{i,j} \right) / \Delta x,
\left( \frac{\partial T}{\partial y} \right)^{n}_{i,j+1} = \left( T^n_{i,j+1} - T^n_{i,j} \right) / \Delta y,
\left( \frac{\partial^2 T}{\partial x^2} \right)^{n}_{i+1,j} = \left( T^n_{i+1,j} - 2T^n_{i,j} + T^n_{i-1,j} \right) / \Delta x^2,
\left( \frac{\partial^2 T}{\partial y^2} \right)^{n}_{i,j+1} = \left( T^n_{i,j+1} - 2T^n_{i,j} + T^n_{i,j-1} \right) / \Delta y^2.
\]

The discretized form of the energy equation (2.4) is given by:
\[
\frac{T^{n+1}_{i,j} - T^n_{i,j}}{\Delta t} = u^n_{i,j} \frac{T^n_{i,j} - T^n_{i+1,j}}{\Delta x} + u^n_{i,j} \frac{T^n_{i,j} - T^n_{i,j+1}}{\Delta y} + \frac{T^n_{i+1,j} - 2T^n_{i,j} + T^n_{i,j-1}}{Pr \Delta x^2} + \frac{T^n_{i,j+1} - 2T^n_{i,j} + T^n_{i,j-1}}{Pr \Delta y^2}.
\] (3.19)

The modified MAC staggered grid quotients of different derivatives which appeared in the mass transfer equation is written as follows:
\[
\left( \frac{\partial C}{\partial t} \right)^{n+1}_{i,j} = \left( C^{n+1}_{i,j} - C^n_{i,j} \right) / \Delta t,
\left( \frac{\partial C}{\partial x} \right)^{n}_{i+1,j} = \left( C^n_{i+1,j} - C^n_{i,j} \right) / \Delta x,
\left( \frac{\partial C}{\partial y} \right)^{n}_{i,j+1} = \left( C^n_{i,j+1} - C^n_{i,j} \right) / \Delta y,
\left( \frac{\partial^2 C}{\partial x^2} \right)^{n}_{i+1,j} = \left( C^n_{i+1,j} - 2C^n_{i,j} + C^n_{i-1,j} \right) / \Delta x^2,
\left( \frac{\partial^2 C}{\partial y^2} \right)^{n}_{i,j+1} = \left( C^n_{i,j+1} - 2C^n_{i,j} + C^n_{i,j-1} \right) / \Delta y^2.
\]

The discretized form of the mass transfer equation (2.5) is given by:
\[
\frac{C^{n+1}_{i,j} - C^n_{i,j}}{\Delta t} = u^n_{i,j} \frac{C^n_{i,j} - C^n_{i+1,j}}{\Delta x} + u^n_{i,j} \frac{C^n_{i,j} - C^n_{i,j+1}}{\Delta y} + \frac{C^n_{i+1,j} - 2C^n_{i,j} + C^n_{i,j-1}}{Sc \Delta x^2} + \frac{C^n_{i,j+1} - 2C^n_{i,j} + C^n_{i,j-1}}{Sc \Delta y^2}.
\] (3.20)

We note that \( u^n_{i,j} \) is not defined on \( u \) node and \( v^n_{i,j} \) is not defined on \( v \) node. Therefore in order to obtain these quantity, we use averaging as given below:
\[
u^n_{i,j} = \frac{1}{2} \left( v^n_{i+1/2,j} + v^n_{i-1/2,j} \right) \quad \text{and} \quad v^n_{i,j} = \frac{1}{2} \left( v^n_{i,j+1/2} + v^n_{i,j-1/2} \right).
\] (3.21)
4. Numerical Computations

We have used a modified MAC algorithm to the discretized governing equations in order to compute the numerical solutions of the flow variables at different Reynolds numbers in consonance with low, moderate, and high. This modified MAC algorithm has an advantage over the original MAC algorithm in discretizing and computing the solutions of any number of governing equations and the flow variables augmented to the basic physical problem of a 2-D simple fluid flow. We have executed this modified MAC algorithm with the aid of a computer program developed and run in C compiler. The input data for the relevant parameters in the governing equations like Reynolds number ($Re$), Prandtl Number ($Pr$), and Schmidt number ($Sc$) has been properly chosen compatible with the present problem considered.

4.1. Modified MAC Algorithm. We summarize the sequence of computational steps involved in the modified MAC algorithm as follow:

4.1.1. Prediction Step.
- Using (3.8) and (3.9), calculate $\hat{u}$ and $\hat{v}$ at their respective grid point locations.
- Apply the initial and boundary conditions given in equations (2.6) and (2.7) respectively.
- These equations will be solved algebraically because time advancement is fully explicit.
- Linear stability conditions (3.10), (3.11), (3.12), and (3.13) must be obeyed.
- Divergence of the velocity field must be calculated at every time step, using the velocity field at the advanced time level, $(n + 1)$,

$$
\nabla \cdot \hat{\mathbf{u}} = \frac{u^{n+1}_{i+1/2,j} - u^{n+1}_{i-1/2,j}}{\Delta x} + \frac{v^{n+1}_{i,j+1/2} - v^{n+1}_{i,j-1/2}}{\Delta y}.
$$

Figure 3. The rectangular staggered computational grid
4.1.2. Pressure Calculation.
- Calculate pressure from Pressure-Poisson equation (3.14).
- Boundary condition applied to the pressure equation at all boundaries is the homogeneous Neumann boundary condition given by (3.15). This equation is solved at the pressure $(ij)$. Note that the Euler explicit time-advancement calculates the actual thermodynamic pressure (scaled by the constant density) and not a pseudo-pressure.

4.1.3. Velocity Correction.
- Obtain the velocity field at the advanced time level $(n+1)$, for each velocity component, this equation gives
  \[
  u_{i+1/2,j}^{n+1} = \hat{u}_{i+1/2,j} - \Delta t \frac{\Delta x}{2} (P_{i+1,j}^{n+1} - P_{i,j}^{n+1}),
  \]
  \[
  u_{i,j+1/2}^{n+1} = \hat{v}_{i,j+1/2} - \Delta t \frac{\Delta y}{2} (P_{i,j+1}^{n+1} - P_{i,j}^{n+1}).
  \]

4.1.4. Temperature Calculation.
- Calculate the numerical solutions for temperature profiles by using equations (3.19) and (3.21).

4.1.5. Concentration Calculation.
- Calculate the numerical solutions for concentration profiles by using equations (3.20) and (3.21).

5. Results and Discussion

We used the modified Marker-And-Cell (MAC) method to carry out the numerical computations of the unknown flow variables $u, v, p, T,$ and $C$ for the present problem. We have executed the modified MAC algorithm mentioned above with the aid of a computer program developed and run in C compiler. To verify our computer code, the numerical results obtained by the present method were compared with the benchmark results reported in [3]. It is seen that the results obtained in the present work are in good agreement with those reported in [3] at low Reynolds number $Re = 100$. This indicates the validity of the numerical code that we developed.

Based on the numerical solutions for $u$-velocity, Fig. 4 illustrates the variation of $u$-velocity along the vertical line through the geometric center of the rectangular domain at low, moderate, and high Reynolds numbers $Re = 10, 500,$ and $50000$. We can see that, for a given $Re = 10$ and $Re = 500$, $u$-velocity first decreases from the bottom boundary of the rectangular domain.
It, then, increases to the upper boundary. But, for \( Re = 50000 \), \( u \)-velocity increases from the bottom boundary to the upper boundary of the rectangular domain. We also observe that, the absolute value of \( u \)-velocity decreases with increase in Reynolds number.

![Figure 4](image)

**Figure 4.** \( u \)-velocity along the vertical line through the geometric center of the domain at low, moderate, and high \( Re \) for a fixed \( Pr = 6.62 \) and \( Sc = 340 \) for grid \( 32 \times 32 \) at time \( t = 0.0001 \) s.

Based on the numerical solutions for \( v \)-velocity, Fig. 5 illustrates the variation of \( v \)-velocity along the horizontal line through the geometric center of the rectangular domain. It is clear that for a given \( Re \), \( v \)-velocity decreases from the left boundary to the right boundary. Further, the absolute value of \( v \)-velocity decreases with increase in Reynolds number.

![Figure 5](image)

**Figure 5.** \( v \)-velocity along the horizontal line through the geometric center of the domain at low, moderate, and high \( Re \) for a fixed \( Pr = 6.62 \) and \( Sc = 340 \) for grid \( 32 \times 32 \) at time \( t = 0.0001 \) s.

Based on the numerical solutions for pressure, Fig. 6 illustrates the variation of pressure in the rectangular domain. We observed that, for \( Re = 10 \), the pressure is oscillatory in nature.

![Figure 6](image)
However, for \( Re = 500 \) and \( Re = 50000 \), we observed the pressure decrease from the left boundary to the right boundary. Further, the absolute value of pressure increases with increase in Reynolds number.

![Figure 6](image)

**Figure 6.** Pressure variation at low, moderate, and high \( Re \) for a fixed \( Pr = 6.62 \) and \( Sc = 340 \) for grid \( 32 \times 32 \) at time \( t = 0.0001 \) s.

Based on the numerical solutions for temperature, Fig. 7 illustrates the variation of temperature at different Reynolds numbers (\( Re = 10, 500, \) and \( 50000 \)), along the vertical line through the geometric center of the rectangular domain. It is clear that for a given \( Re \), temperature increases from the bottom boundary to the upper boundary.

![Figure 7](image)

**Figure 7.** Temperature variation at low, moderate, and high \( Re \) for a fixed \( Pr = 6.62 \) and \( Sc = 340 \) for grid \( 32 \times 32 \) at time \( t = 0.0001 \) s.

Based on the numerical solutions of concentration, Fig. 8 illustrates the variation of concentration at different Reynolds numbers (\( Re = 10, 500, \) and \( 50000 \)), along the vertical line through the geometric center of the rectangular domain. It is clear that for a given \( Re \), concentration increases from the bottom boundary to the upper boundary.

![Figure 8](image)
Figure 8. Concentration variation at low, moderate, and high Re for a fixed Pr = 6.62 and Sc = 340 for grid 32 × 32 at time t = 0.0001 s.

Grid dependence tests have been conducted on two grid systems (16 × 16 and 32 × 32). In order to evaluate the effect of the two grid systems on the natural convection flow in the rectangular domain, three representative quantities are evaluated numerically: the volumetric flow rate (Q), average Nusselt number (\( \bar{Nu} \)), and average Sherwood number (\( \bar{Sh} \)) across the horizontal centerline of the rectangular domain, which are defined as (also see [24, 25])

\[
Q = \frac{1}{2} \int_{-\frac{L}{2}}^{\frac{L}{2}} |v| dx, \tag{5.1}
\]

\[
\bar{Nu} = \frac{1}{L} \int_{-\frac{H}{2}}^{\frac{H}{2}} \left( \frac{vT - \frac{\partial T}{\partial y}}{2\Delta T} \right) dx, \tag{5.2}
\]

\[
\bar{Sh} = \frac{1}{L} \int_{-\frac{H}{2}}^{\frac{H}{2}} \left( \frac{vC - \frac{\partial C}{\partial y}}{2\Delta C} \right) dx, \tag{5.3}
\]

where local Nusselt number (\( Nu \)), and local Sherwood number (\( Sh \)) is defined as follows:

\[
Nu = vT - \frac{\partial T}{\partial y}, \tag{5.4}
\]

\[
Sh = vC - \frac{\partial C}{\partial y}. \tag{5.5}
\]

In the present problem length, \( L \) of the rectangular domain varies from 0 to 2, height, \( H \) varies from 0 to 1, \( \Delta T = 0.5 \), and \( \Delta C = 0.5 \). Then the volumetric flow rate (\( Q \)), average Nusselt
number ($\overline{Nu}$), and average Sherwood number ($\overline{Sh}$) across the horizontal centerline of the rectangular domain, take the form

\[ Q = \int_{0}^{2} |v| \, dx, \quad \text{(5.6)} \]

\[ \overline{Nu} = \int_{0}^{2} vT - \frac{\partial T}{\partial y} \, dx, \quad \text{(5.7)} \]

\[ \overline{Sh} = \int_{0}^{2} vC - \frac{\partial C}{\partial y} \, dx. \quad \text{(5.8)} \]

In order to investigate heat transfer from the bottom to the top wall of the rectangular domain, we have computed the numerical solutions of local Nusselt number for two different grid systems along the horizontal line through the geometric center of the domain at different Reynolds numbers. Fig. 9 illustrates comparison of computed local Nusselt number ($Nu$) from the hot bottom wall to the cold top wall at time $t = 0.0001s$.

![Figure 9](image)

**Figure 9.** Variation of local Nusselt number ($Nu$) profiles along the horizontal line through the geometric center at low, moderate, and high $Re$ for a fixed $Pr = 6.62$ and $Sc = 340$, (a) for grid $16 \times 16$ and (b) for grid $32 \times 32$, at time $t = 0.0001s$.

From this figure, we observe that, as we move along the horizontal line through the geometric center of the domain, heat transfer decreases up to the geometric center. It then, increases symmetrically.

In order to investigate mass transfer from the bottom to the top wall of the rectangular domain, we have computed the numerical solutions of local Sherwood number for two different grid systems along the horizontal line through the geometric center of the domain at different Reynolds numbers.

Fig. 10 illustrates comparison of computed local Sherwood number ($Sh$) from the hot bottom wall to the cold top wall at time $t = 0.0001s$. From this figure, we observe that, as we
move along the horizontal line through geometric center of the domain, mass transfer decreases upto the geometric center. It, then, increases symmetrically.

6. CONCLUSIONS

In this study, we have proposed a modified Marker-And-Cell (MAC) method to investigate the problem of an unsteady 2-D incompressible flow with heat and mass transfer at low, moderate, and high Reynolds numbers with no-slip and slip boundary conditions. We have used this method to solve the governing equations along with the boundary conditions and thereby to compute the flow variables, viz. $u$-velocity, $v$-velocity, $P$, $T$, and $C$. We have used the staggered grid approach of this method to discretize the governing equations of the problem. A modified MAC algorithm was proposed and used to compute the numerical solutions of the flow variables for Reynolds numbers $Re = 10$, $500$, and $50000$ in consonance with low, moderate, and high Reynolds numbers.

Numerical solutions for $u$-velocity illustrates the variation of $u$-velocity along the vertical line through the geometric center of the rectangular domain at low, moderate, and high Reynolds numbers $Re = 10$, $500$, and $50000$. We have observed that, for a given $Re = 10$ and $Re = 500$, $u$-velocity first decreases from the bottom boundary of the rectangular domain. It, then, increases to the upper boundary. But, for $Re = 50000$, $u$-velocity increases from the bottom boundary to the upper boundary of the rectangular domain. We also observed that the absolute value of $u$-velocity decreases with increase in Reynolds number. The numerical solutions for $v$-velocity illustrates the variation of $v$-velocity along the horizontal line through the geometric center of the rectangular domain. We have observed that, for a given $Re$, $v$-velocity decreases from the left boundary to the right boundary. Further, we also observed that the absolute value of $v$-velocity decreases with increase in Reynolds number.
Numerical solutions for pressure illustrate the variation of pressure in the rectangular domain. We have observed that, for $Re = 10$, the pressure is oscillatory in nature. However, for $Re = 500$ and $Re = 50000$, we observed the pressure decrease from the left boundary to the right boundary. Further, we have also observed that the absolute value of pressure increases with increase in Reynolds number. The numerical solutions for temperature illustrate the variation of temperature at different Reynolds numbers ($Re = 10$, $500$, and $50000$), along the vertical line through the geometric center of the rectangular domain. We have observed that, for a given $Re$, temperature increases from the bottom boundary to the upper boundary. The numerical solutions of concentration illustrate the variation of concentration at different Reynolds numbers ($Re = 10$, $500$, and $50000$), along the vertical line through the geometric center of the rectangular domain. We have observed that, for a given $Re$, concentration increases from the bottom boundary to the upper boundary.

Based on the computed local Nusselt number ($Nu$) from the hot bottom wall to the cold top wall at time $t = 0.0001s$, we have observed that, as we move along the horizontal line through the geometric center of the domain, heat transfer decreases up to the geometric center. It, then, increases symmetrically. Based on the computed local Sherwood number ($Sh$) from the hot bottom wall to the cold top wall at time $t = 0.0001s$. We have observed that, as we move along the horizontal line through geometric center of the domain, mass transfer decreases up to the geometric center. It, then, increases symmetrically.

7. Code Validation

To check the validity of our present computer code used to obtain the numerical results of $u$-velocity and $v$-velocity, we have compared our present results with those benchmark results are given by Ghia et al. [3] and it has been found that they are in good agreement.

![Figure 11](image_url)  
**Figure 11.** Comparison of the numerical results of $u$-velocity along the vertical line through the geometric center of the square cavity for $Re = 100$. 

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