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An upwind local radial basis functions-finite difference (RBF-FD) method for solving compressible Euler equation with application in finite-rate Chemistry

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ABSTRACT

The main aim of the current paper is to propose an upwind local radial basis functions-finite difference (RBF-FD) method for solving compressible Euler equation. The mathematical formulation of chemically reacting, inviscid, unsteady flows with species conservation equations and finite-rate chemistry is studied. The presented technique is based on the developed idea in [58]. For checking the ability of the new procedure, the compressible Euler equation is solved. This equation has been classified in category of system of advection-diffusion equations. The solutions of advection equations have some shock, thus, special numerical methods should be applied for example discontinuous Galerkin and finite volume methods. Moreover, two problems are given that show the acceptable accuracy and efficiency of the proposed scheme.

1. INTRODUCTION

During the recent decade, the meshless methods have been employed to solve the partial differential equations (PDEs). The meshless methods don't use any mesh, element or lattice to discrete the computational domain for obtaining some numerical results. According to the basic advantages of meshless methods, these techniques may be classified as follows:

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- The global form,
- The local form.

The local meshless method is an improvement of meshless techniques where they can be split in two forms:

- Local meshless methods based on the variational (local) weak form,
- Local meshless methods based on the strong form.

In the local meshless methods based on the weak form, there are some integrals which must be computed with suitable accuracy thus these methods have more difficulty and need more CPU time. But in the local meshless methods based on the strong form there are not any integral so these techniques will be very flexible to solve models with nonlinear term.

A local meshless collocation method based on the finite difference approach is the RBFs-FD method. The RBF-FD idea has been developed in [15, 25, 26, 51, 59, 62]. Authors of [24] developed a filter approach for RBF-FD that is related to traditional hyperviscosity and which can be applied quickly in any number of dimensions. Also, some analytical explanations related to the weights of Gaussian RBF-FD formula are obtained in [3]. The main aim of [2, 4, 1] is to obtain an optimal shape parameter for RBF-FD technique. Also, some researchers studied RBF-FD method such as large-scale geoscience modeling [23], hyperbolic PDEs on the sphere [6], diffusion and reaction-diffusion equations (PDEs) on closed surfaces [55], improved meshless local Petrov-Galerkin for transient heat conduction problems [11], the interpolating moving least square-Ritz (IMLS-Ritz) analysis of laminated CNT-reinforced composite quadrilateral plates [68], etc.

One of the local meshless methods is the radial basis functions-differential quadrature (RBF-DQ) procedure. The differential quadrature method was first introduced by Richard Bellman et. al [5]. The polynomial functions have been selected as the test function [57]. For the first time, authors of [59] proposed the meshless RBFs-DQ method by using the RBFs. The RBF-DQ method is similar to the local RBF (LRBF) and RBF-FD methods. The RBFs-DQ is employed for solving several PDEs such as equations in fluid dynamic [59, 60], system of boundary value problems [13], coupled Klein-Gordon-Zakharov equations [14], doubly-curved shells made of composite materials [63], Stokes flow problem in a circular cavity [39], etc. Natural phenomena can be described by PDEs. We refer the interested reader to [65] for various applications of partial differential equations in science and engineering and also for some approaches in obtaining their solutions.

Chemically reacting flows have many applications in engineering such as hypersonic reacting flows around a blunt body, rocket nozzle combustion, pre-mixed detonation, etc. By combination of Euler and Navier-Stokes equations with species mass conservation equations and finite-rate chemical reactions a mathematical model has been obtained. Three physical processes involved in chemically reacting flows are:

- Fluid dynamics
- Thermodynamics
- Chemical reactions

As a brief explanation, we can say that the fluid dynamics process is defined by conservation of mass, momentum and energy, the thermodynamics of the reactive fluid include microscopic heat transfer between gas molecules, work done by pressure, and volume change and the Chemical reactions determine the generation and/or destruction of chemical species under the constraint of mass conservation.

Numerical solution of the Euler or Navier-Stokes equations within species conservation terms are widely used to analyze chemically reacting flows. Chemically reacting flows which may only be investigated using finite-rate chemistry extend a simple combustion to detonation of fuel-air mixtures. The Euler equation has many application such as airfoil, chemistry, explosion, deflagration, detonation, fuel-air explosives, pulse detonation engine, etc.

1.1. Organization Chart for the Manuscript

In this paper we apply a local truly meshless method based on the RBF-DQ technique for solving an equation in water science in two-dimensional case. The structure of this article is as follows:

- In Section 2, we explain the LRBF-FD method.
- In Section 3, we explain the improved LRBF-FD method.
- In Section 4, we report the numerical experiments of solving the considered models for some test problems.
- Finally, a brief conclusion of the current paper has been written in Section 5.

1.2. Implementation Of Local RBFs–FD Technique

Meshfree methods are built based on scattered nodes in the problem domain [41]. One of the meshless methods is radial basis functions collocation method in global and local senses. In the current paper, we use the local radial basis functions method because this idea works for arbitrary domains and is simple for working with problems in high dimensions. Radial basis functions collocation method is known as Kansa's method [35, 36, 37].

Kansa's method was developed in 1990, in which the concept of solving PDEs by using RBFs collocation method was planned. There are different types of radial basis functions such as Multiquadratics (MQ), Gaussian (GS) and polyharmonic splines. The MQ function was originally introduced by Hardy [27] who successfully applied this method for approximating surface and bodies from field data.

Gu and his co-workers [18] developed a numerical technique based on meshless local Kriging method for solving the large deformation problems, which are geometrically nonlinear. This is the first work for the geometrically nonlinear analysis by the mentioned meshless local weak-form method. A new local point interpolation method (LPIM) is proposed in [19] to deal with fourth-order boundary-value and initial-value problems for static and dynamic analysis of beams. Authors of [20] developed an enriched radial point interpolation method (E-RPIM) for the determination of crack tip fields.

Author of [52] used a regularization method to prevent the failure of the Cholesky factorization and to improve the accuracy of symmetric positive definite (SPD) matrix factorizations when the matrices are severely ill-conditioned. The main aim of [53] is to examine how extended precision floating point arithmetic can be used to improve the accuracy of RBFs methods in an efficient manner.

Definition 2.1. [22, 66] A symmetric function $\varphi \in \mathbb{R}^d \to \mathbb{R}$ is strictly conditionally positive definite of order m, if for all sets $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d$ of distinct points, and all vectors $\lambda \in \mathbb{R}^d$ satisfying $\sum_{i=1}^{N} \lambda_i p(x_i) = 0$ for any polynomial p of degree at most $m-1$, the quadratic form

$$\lambda^T A\lambda = \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i \lambda_j \varphi(x_i - x_j),$$

is positive, whenever $\lambda \neq 0$.

We interpolate a continuous function $f : \mathbb{R}^d \to \mathbb{R}$ on a set $X = \{x_1, \ldots, x_N\}$ with choosing the radial basis function for $\varphi : \mathbb{R}^d \to \mathbb{R}$ that is radial in the sense that $\varphi(x) = \Psi(\|x\|)$, where $\|.\|$ is the usual Euclidean norm on $\mathbb{R}^d$ as we will explain in the next section. Now, we assume φ to be strictly conditionally positive definite of order m, then the interpolation function has the following form [22, 66]

$$\tau f(x) = \sum_{i=1}^{N} \lambda_i \varphi(x - x_i) + \sum_{j=1}^{l} \gamma_j p_j(x),$$

where $l = \binom{d+m-1}{m-1}$ and $\{p_1, p_2, \ldots, p_l\}$ is a basis of P_m^d. The basic problem is to find $N + l$ unknown coefficients λ_i and γ_j in which N interpolation conditions are to the following form [22, 66]

$$\tau f(x_i) = f_i, \; i = 1, \ldots, N,$$

and for l remaining conditions we use the following equations

$$\sum_{i=1}^{N} \lambda_i p_j(x_i) = 0,\ 1 \le j \le l.$$

The accuracy of many schemes for interpolating scattered data with radial basis functions and to solve partial differential equations using meshfree methods based on radial basis functions depends on a shape parameter c, of the radial basis function [41]. Also we refer the interested reader to [10, 56] for useful investigation on meshless method of radial basis functions and some related issues.

In this section, we explain the local collocation meshless method based on an arbitrary shape function. As is well-known the local interpolation procedure is as follows [23, 24]

$$\varepsilon_m f(\vec{x}) = \sum_{j \in \tau_i} \vec{\beta}_j \psi\left(\left\|\vec{x} - \vec{y}_j\right\|\right), \tag{2.1}$$

1. in which $\vec{y}$ is the set of N centers,
2. τ_i is the set of nodes that are into the stencil of i^{th} node,
3. $\vec{\beta}$ is the unknown weights that must be computed.

Also, the unknown weight can be calculated using the following interpolation conditions [23, 24]

$$\varepsilon_m f(\vec{x}_j) = f(\vec{x}_j). \tag{2.2}$$

Eq. (2.2) is equal to the following linear system of equations

$$A\vec{\beta} = f, \tag{2.3}$$

in which

$$f = \left[f(\vec{x}_1), f(\vec{x}_2), \ldots, f(\vec{x}_{|I_i|}) \right], B_{jk} = \psi\left(\left\|\vec{x}_j - \vec{x}_k\right\|_2\right),\quad j,k \in I_i.$$

A local RBFs operator (including local derivatives or etc) can be obtained as follows [23, 24]

$$\ell f(\vec{x}) = \sum_{j \in \tau_i} \vec{\beta}_j \ell \psi\left(\left\|\vec{x} - \vec{y}_j\right\|_2\right). \tag{2.4}$$

The above relation may be compacted in the following form

$$\ell f(x) = \vec{h}^T \vec{\beta}, \tag{2.5}$$

where

$$\left(h\right)_i = \psi\left(\left\|x - y_i\right\|_2\right),\quad i \in \tau_i. \tag{2.6}$$

Eqs. (2.3) and (2.5) yield

$$\ell f(\vec{x})\Big|_{\tau_i} = \left(\vec{h}^T \mathbf{B}^{-1}\right)\mathbf{f}\Big|_{\tau_i} = \left(\vec{w}_i\right)\mathbf{f}, \tag{2.7}$$

in which $\vec{w}_i$ is the stencil weights at the shape function center i [23, 24].

2. THE PROPOSED IMPROVEMENT FOR LRBFS–FD METHOD OF [58]

Shu et al [58] developed an improvement for LRBFs-DQ technique based on the upwind method. Also, it must be mentioned that the current section has been taken from [58]. The 2D unsteady compressible Euler equations are as follows

$$\frac{\partial}{\partial t}U+\frac{\partial}{\partial x}F(U)+\frac{\partial}{\partial y}G(U)=0, \tag{3.1}$$

or

$$\frac{\partial}{\partial t}U+\nabla\cdot H(U)=0, \tag{3.2}$$

in which [58]

$$\mathbf{U}=\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ e\end{pmatrix},\quad \mathbf{F}=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ u(e+p)\end{pmatrix},\quad \mathbf{G}=\begin{pmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ v(e+p)\end{pmatrix},\quad \mathbf{H}=\left[\mathbf{F}\ \mathbf{G}\right]. \tag{3.3}$$

In the above model [58]:

- U is the vector of conservative variables,
- $\left[\rho \quad \rho u \quad \rho v \quad e\right]^T$ is the primitive variables,
- $\overrightarrow{\mathbf{m}}=\left[\rho u \quad \rho v\right]^T$ is the momentum vector,
- $\mathbf{u}=\left[u \quad v\right]^T$ T is the velocity vector,
- $e=\rho\left[\varepsilon+\frac{u^2+v^2}{2}\right]$ is the total energy,
- and ε is the specific internal energy.

The pressure p is [58]

$$p=\left(\gamma-1\right)\left(e-\rho\frac{u^2}{2}\right). \tag{3.4}$$

The model (3.1) has been solved by using several numerical techniques such as adjoint-based an adaptive finite volume method [30], a novel reduced-order thrust model [40], a novel Mach-uniform numerical model [67], vortex-induced vibration for an isolated circular cylinder [69], improvement of aerodynamic characteristics [33], an adaptive finite volume method for steady case [31], a posteriori error estimator based on the variational multiscale theory [28], isogeometric finite element Navier–Stokes solver [43], compressible Navier–Stokes solvers according to the optimized upwind compact schemes [54], an adaptive WENO reconstruction [29], a discontinuous Galerkin method (DGM)

[45], a compact least-squares finite volume procedure [64], a third-order finite-volume technique [17], development of a high-order finite volume method based on moving Kriging shape functions [7], transonic integro-differential and integral equations [44], a hybrid boundary element-finite volume method [32], vortex method [34], laminar and turbulent flow over different airfoils using Open FOAM [46], a numerical investigation of the effects of leading-edge protuberances on airfoil stall and post-stall performance based on the improved delayed detached eddy simulation (IDDES) method [70], a numerical study that determines how the boundary layer properties of an airfoil are modified with angle of attack [38], numerical procedure used for the Reynold's equations [42], study of the Reynold's number influences on aerodynamics of a typical supercritical airfoil [12], etc. Also, we must mention that there are many research articles on solving the Euler equations. Authors of [50] developed a Chebyshev finite difference (ChFD) method and DTM-Pade method, which is a combination of differential transform method (DTM) and Pade approximant, for solving singular boundary value problems arising in the reaction cum diffusion process.

For Eq. (3.1), we employed the LRBF-DQ technique but with a modified version that is developed in [58]. As is said in [58], the employed nodes for collocating are located at mid points i.e between the reference node and its support [58]. Using the local RBF-DQ method to discrete the spatial direction, yields [58]

$$\left.\frac{dU}{dt}\right|_i = -\sum_{k=0}^{N_I}\left[w_{i,k}^{(x)}F(U_{i,k}) + w_{i,k}^{(y)}G(U_{i,k})\right]^n. \tag{3.5}$$

According to relation (3.5) a new flux can be obtained as follows [58]

$$S_{i,k} = \alpha_{i,k}F(U_{i,k}) + \beta_{i,k}G(U_{i,k}), \tag{3.6}$$

where [58]

$$\alpha_{i,k} = \frac{w_{i,k}^{(x)}}{\sqrt{\left(w_{i,k}^{(x)}\right)^2 + \left(w_{i,k}^{(y)}\right)^2}}, \quad \beta_{i,k} = \frac{w_{i,k}^{(y)}}{\sqrt{\left(w_{i,k}^{(x)}\right)^2 + \left(w_{i,k}^{(y)}\right)^2}}. \tag{3.7}$$

By denoting

$$W_{i,k} = \sqrt{\left(w_{i,k}^{(x)}\right)^2 + \left(w_{i,k}^{(y)}\right)^2}, \tag{3.8}$$

then Eq. (3.5) can be rewritten as

$$\left.\frac{dU}{dt}\right|_i = -\sum_{k=0}^{N_1} W_{i,k}S_{i,k}. \tag{3.9}$$

However, the new flux at the mid-point can be obtained based on the Roe's scheme [58]

$$S(U_L, U_R) = \frac{1}{2}\left[S(U_L) + S(U_R)\right] - \frac{1}{2}\left|\widehat{M}\right|(U_L - U_R), \tag{3.10}$$

in which $S(U_L,U_R)$, $S(U_L)$ and $S(U_R)$ are the new flux. Also, $\widehat{M}$ denotes the constant Jacobain matrix for approximating the Jacobian matrix M. Roe [49] developed a vector Z to approximate the Jacobian matrix $\widehat{M}$. The vector U and its flux $S(U)$ can be explained in vector Z [58]

$$\mathbf{Z} = \sqrt{\rho}\begin{bmatrix}1 & u & v & H\end{bmatrix}^T. \tag{3.11}$$

The variations of U and $S(U)$ are [58]

$$(U_R - U_L) = \widehat{B}(Z_R - Z_L),\ (S_R - S_L) = \widehat{C}(Z_R - Z_L). \tag{3.12}$$

Also, the above relations can be rewritten as

$$(S_R - S_L) = \widehat{C}\widehat{B}^{-1}(U_R - U_L). \tag{3.13}$$

This results

$$\widehat{M} = \widehat{C}\widehat{B}^{-1}, \tag{3.14}$$

in which [58]

$$\begin{aligned}
\hat{\rho} &= \sqrt{\rho_L \rho_R}, \\
\hat{u} &= \frac{\sqrt{\rho_L}u_L + \sqrt{\rho_R}u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \\
\hat{v} &= \frac{\sqrt{\rho_L}v_L + \sqrt{\rho_R}v_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \\
\hat{H} &= \frac{\sqrt{\rho_L}H_L + \sqrt{\rho_R}H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}.
\end{aligned}$$

Also, according to [58], we use the following flux to obtain high-order accuracy [58]

$$S(U_L,U_R) = \frac{1}{2}\left[S(U^L) + S(U^R)\right] - \frac{1}{2}\left|A^*(U^L,U^R)\right|\left(U^L - U^R\right), \tag{3.15}$$

in which A^* is the Roe's approximate Jacobian matrix. The interested readers can find more details in [58].

3. NUMERICAL EXPERIMENTS

In this part of paper, we test the proposed new technique on two test problems. The used plate or in the other word the computational domains are rectangular that show the efficiency of the present method. We employ the **Matlab** 7 software based version of 2010 with 4 Gbyte of memory.

4.1. Test Problem 1 (Bump Geometry [7]).

As the first example, we consider a bump geometry. We employ a bump geometry that is depicted in Figure 1. Figure 2 demonstrates the graphs of approximation solution at different values of final times for Test problem 3.

4.2. Test Problem 2 (InviscidFlow [7]).

For the last problem, we apply the LRBF-DQ method for the case of an inviscid flow on a NACA 0012 airfoil with free stream Mach number $M = 0.63$ and an angle of attack $\alpha = 2^{\circ}$ [7]). Figure 3 presents transonic flow past a NACA 0012 airfoil for Test problem 2.

4. Conclusion

The advection problem may be appeared in chemistry, physics, fluid mechanics and etc. In other hand, sometimes finding their analytic solutions is so difficult. Thus, applying a useful and efficient numerical method for solving these equations is a topic of interest for researchers. Up to the best of authors' knowledge many well-known numerical procedures are not able to solve these problems. In the current investigation, we have suggested a numerical method for solving the mentioned equations. The local collocation technique is presented for solving an important equation in fluid flow equations. The method presented here is based on the upwind local RBF-DQ method. Numerical results confirm the accuracy and efficiency of the proposed scheme.

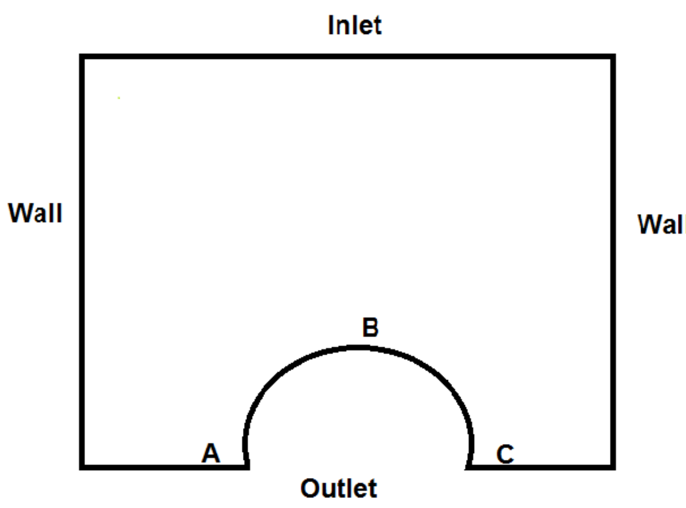


Figure 1. The computational domain for Test problem 1.

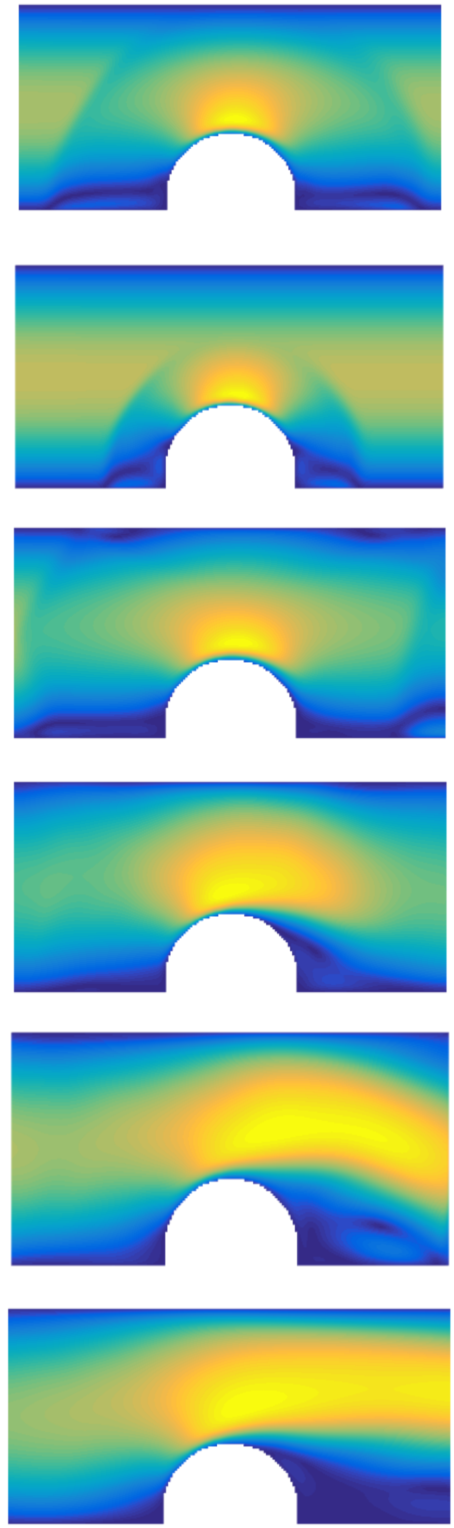
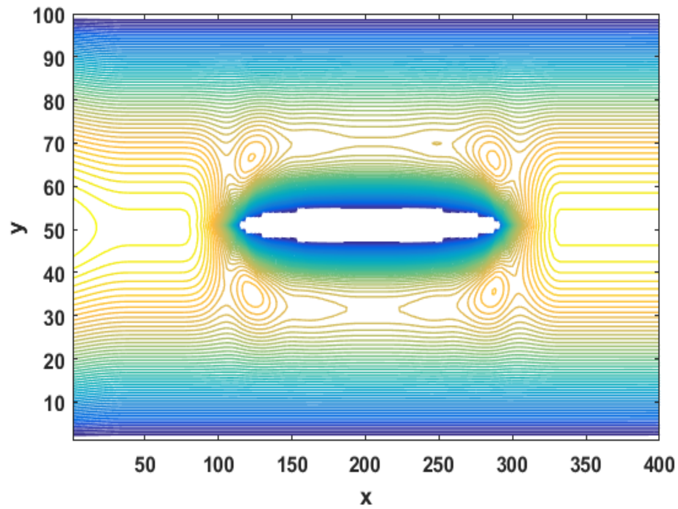


Figure 2. Graphs of approximation solution with different values of final times to test Problem 1.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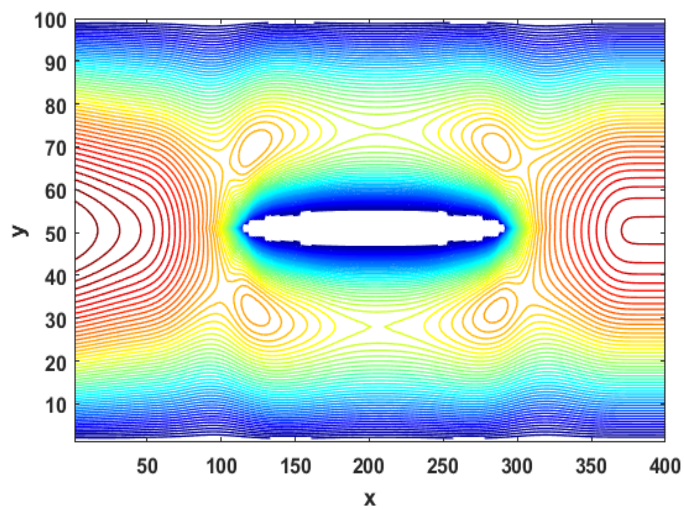
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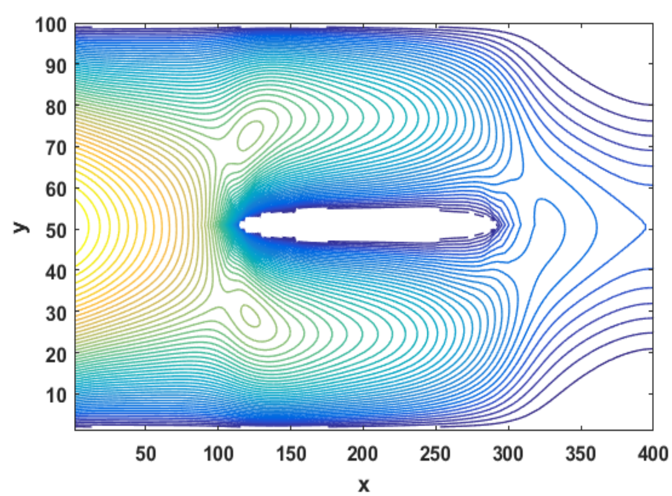
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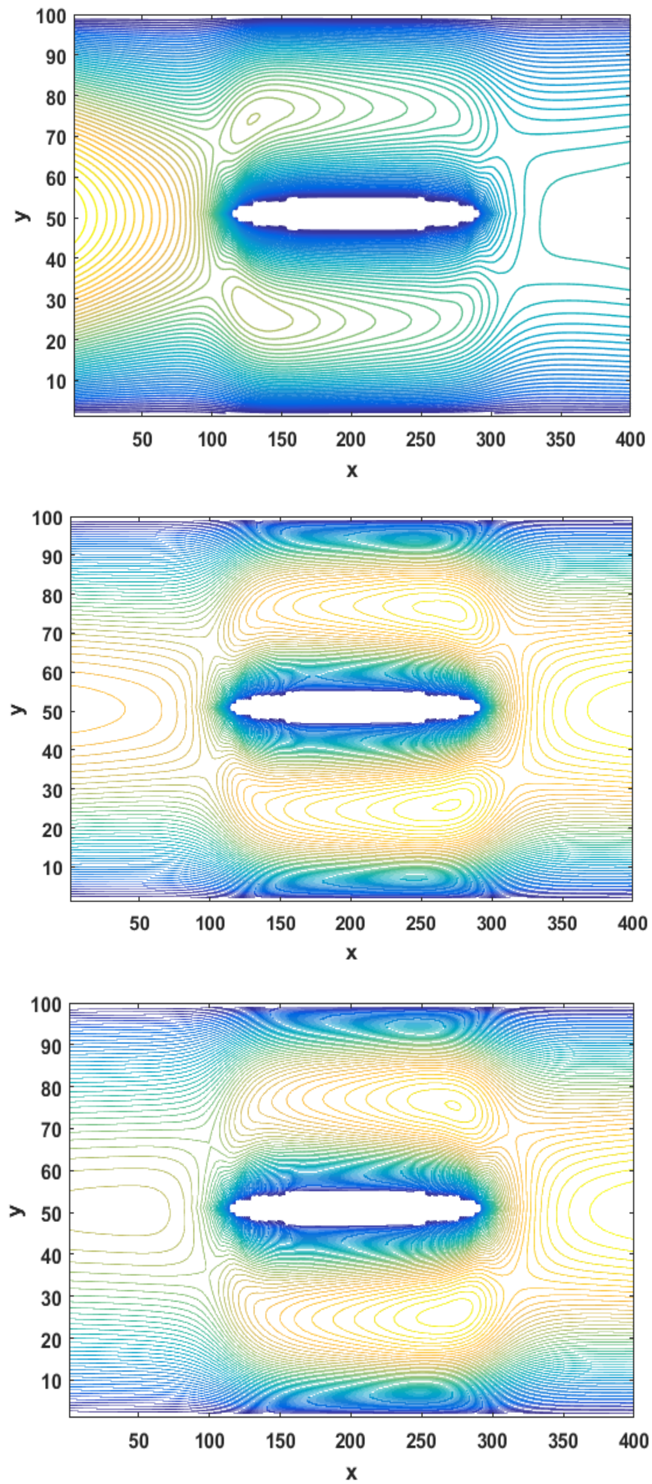

Figure 3. Graphs of approximation solution with different values of final times to test Problem 2.

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