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NUMERICAL SIMULATION OF ONE-PHASE STEFAN PROBLEMS IN ARBITRARY PRECISION[1]

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1 Introduction

One-phase stefan problem is a boundary value problem involving differential equations on domains, parts of whose boundaries, the free boundaries are unknown and must be determined as part of the solution. We can find many problems in practical phenomena as stefan problems. To solve these problems are not easy because geometries of unknown domains are not simple and they are nonlinear.

On the other hand, we presented a numerical method which realizes arbitrary precision numerical simulation to PDE systems with smooth solutions. The method consists of two method, i.e. multiple precision arithmetic and the spectral collocation method. The spectral collocation method is used for the control of truncation errors and multiple precision arithmetic is used for control of rounding errors. Both errors can be reduced arbitrarily. In this paper our method is applied to one-phase stefan problems.

2 Our Method and Test Problems

2.1 Arbitrary Precision Numerical Simulation

Errors in numerical simulations originate from truncation errors in the discretization and rounding errors. The realization of arbitrary precision simulations needs arbitrary reduction

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of both errors. We presented already a simple method for numerical simulation in arbitrary precision to one- and two-dimensional free boundary problems[3, 6, 9]. Here, truncation errors in the discretization and rounding errors can be reduced arbitrarily.

The truncation errors can be reduced by raising the order of the approximation. The finite difference method , the finite element method and the boundary element method are very practical, however, they are not practical as higher order discretization formulae. On the other hand, the spectral collocation method is suitable as a higher order discretization formula. Therefore, we have adopted the spectral collocation method as a discretization method. In particular, the spectral collocation method is used here. This is because it is very useful to nonlinear problems. In the spectral collocation method, the order of the approximation can be controlled by the number of collocation points. For example, in the spectral collocation method with the Chebyshev-Gauss-Lobatto points, the N-th order approximation can be realized only by using $(N+1)$ collocation points[1].

In addition, multiple precision arithmetic[8] is used for reduction of rounding errors. A lot of FORTRAN subroutines about multiple precision arithmetic is already known. We used the library of FORTRAN subroutines on the net (http://www.lmu.edu/acad/personal/faculty /dmsmith/FMLIB.html)[2].

Our method consists of these two methods, i.e. multiple precision arithmetic and the spectral collocation method. In our method, truncation errors and rounding errors are controlled easily. This is very important in numerical simulations in applied mathematics. Of course, both errors can be reduced arbitrarily.

2.2 Test Problems

In this paper, we consider the following two test problems. These test problems are typical one-phase stefan problems.

Test Problem 1. Find u and s such that

$$\begin{aligned}
u_t(x,t) &= u_{xx}(x,t) + 2(t+2), && 0 < t, && 0 < x < s(t), \\
u(x,0) &= 1 - x^2, && && 0 < x < s(0), \\
u(0,t) &= (t+1)^2, && 0 \le t, && \\
u(s(t),t) &= 0, && 0 \le t, && \\
\frac{d}{dt}s(t) &= -\frac{u_x(s(t),t)}{2} - t, && 0 < t, && \\
s(0) &= 1.
\end{aligned}$$

Remark 1. The exact solution to Test Problem 1 is given as follows:

$$\begin{aligned} u(x,t) &= (t+1)^2 - x^2, \qquad 0 \le t, \qquad 0 \le x \le s(t), \\ s(t) &= (t+1), \qquad 0 \le t. \end{aligned}$$

Test Problem 2. Find u and s such that

$$\begin{aligned} u_t(x,t) &= \frac{4(t+1)}{\pi^2} u_{xx}(x,t) + \frac{\pi x e^{-t} \sin \frac{\pi x}{2\sqrt{t+1}}}{4(t+1)^{\frac{3}{2}}}, \\ &\qquad 0 < t, \qquad 0 < x < s(t), \\ u(x,0) &= \cos \frac{\pi}{2} x, \qquad 0 < x < s(0), \\ u(0,t) &= e^{-t}, \qquad 0 \le t, \\ u(s(t),t) &= 0, \qquad 0 \le t, \\ \frac{d}{dt} s(t) &= -\frac{e^t}{\pi} u_x(s(t),t), \qquad 0 < t, \\ s(0) &= 1. \end{aligned}$$

Remark 2. The exact solution to Test Problem 2 is given as follows:

$$\begin{aligned} u(x,t) &= e^{-t} \cos \frac{\pi x}{2\sqrt{t+1}}, \qquad 0 \le t, \qquad 0 \le x \le s(t), \\ s(t) &= \sqrt{t+1}, \qquad 0 \le t. \end{aligned}$$

2.3 Fixed Domain Method

The spectral collocation method cannot be applied directly to one-phase stefan problems because of the restriction on the shape of the domain. Then to avoid this difficulty we use the fixed domain method which was developed in FDM[7]. A one-phase stefan problem is transformed into a fixed boundary problem using mapping functions.

We use the following variable transformation : $(x,t) \to (\xi, \tau)$ such that

$$x = x(\xi, \tau), \tag{2.1}$$

$$t = \tau \tag{2.2}$$

then

$$u_t = -\frac{\partial(u,x)}{\partial(x,t)} = -\frac{\partial(u,x)}{\partial(\xi,\tau)}\frac{\partial(\xi,\tau)}{\partial(x,t)} = -\frac{1}{J}(u_\tau x_\xi - u_\xi x_\tau), \tag{2.3}$$

$$u_x = -\frac{1}{J}u_\xi, \tag{2.4}$$
$$u_{xx} = \frac{u_{\xi\xi}}{J^2} - \frac{u_\xi x_{\xi\xi}}{J^3} \tag{2.5}$$

where

$$J = \frac{\partial(x,t)}{\partial(\xi,\tau)} = x_\xi. \tag{2.6}$$

In Test Problems 1 and 2, mapping function is given as follows;

$$x(\xi,t) = \frac{s(t)}{2}(\xi+1), \quad 0 \le t, \quad -1 \le \xi \le 1. \tag{2.7}$$

For application of the spectral collocation method in time[4, 5] the time axis is divide into intervals. In each interval the initial and boundary value problem is solved. This procedure is executed iteratively. For the application of the spectral collocation method to interval $[t_s, t_e]$ we consider the following variable transform.

$$t(\tau) = \frac{\Delta t}{2}\tau + \frac{1}{2}(t_s+t_e), \ -1 \le \tau \le 1, \ \Delta t = t_e - t_s, \tag{2.8}$$
$$\tau(t) = \frac{2}{\Delta t}(t - \frac{1}{2}(t_s+t_e)) \tag{2.9}$$

then

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau}\frac{d\tau}{dt} = \frac{2}{\Delta t}\frac{\partial}{\partial \tau}. \tag{2.10}$$

By fixed domain method in space and time, Test Problems 1 and 2 are transformed into the following Test Problems 1′ and 2′ respectively.

Test Problem 1′. Find u and $\tilde{s}$ such that

$$\begin{aligned}
\frac{2}{\Delta t}u_\tau(\xi,\tau) &= \frac{4}{\{\tilde{s}(\tau)\}^2}u_{\xi\xi}(\xi,\tau) + \frac{(\xi+1)}{\tilde{s}(\tau)}\left\{-\frac{u_\xi(1,\tau)}{\tilde{s}(\tau)} - \frac{\Delta t}{2}\tau\right. \\
&\quad \left. -\frac{1}{2}(t_s+t_e)\right\} u_\xi(\xi,\tau) + \Delta t\tau + t_s + t_e + 4, \\
&\qquad\qquad -1 < \tau \le 1, \quad -1 < \xi < 1, \\
u(\xi,-1) &= u_s(\xi), \qquad\qquad -1 < \xi < 1, \\
u(-1,\tau) &= \{\frac{\Delta t}{2}\tau + \frac{1}{2}(t_s+t_e) + 1\}^2, \qquad -1 \le \tau \le 1, \\
u(1,\tau) &= 0, \qquad -1 \le \tau \le 1, \\
\frac{2}{\Delta t}\tilde{s}'(\tau) &= -\frac{u_\xi(1,\tau)}{\tilde{s}(\tau)} - \frac{\Delta t}{2}\tau - \frac{1}{2}(t_s+t_e), \quad -1 < \tau \le 1, \\
\tilde{s}(-1) &= \tilde{s}_s.
\end{aligned}$$

Here $\tilde{s}(\tau) = s(t(\tau))$ and if $t_s = 0$ then

$$u_s(\xi) = 1 - \frac{(\xi+1)^2}{4}, \qquad \tilde{s}_s = 1.$$

Test Problem 2′. Find u and $\tilde{s}$ such that

$$\begin{aligned}
\frac{2}{\Delta t}u_\tau(\xi,\tau) &= \frac{16(\frac{\Delta t}{2}\tau + \frac{1}{2}(t_s+t_e)+1)}{\{\tilde{s}(\tau)\}^2\pi^2}u_{\xi\xi}(\xi,\tau) \\
&\quad - \frac{2(\xi+1)e^{\frac{\Delta t}{2}\tau+\frac{1}{2}(t_s+t_e)}}{\{\tilde{s}(t)\}^2\pi}u_\xi(1,\tau)u_\xi(\xi,\tau) \\
&\quad + \frac{\pi\tilde{s}(t)(\xi+1)e^{-(\frac{\Delta t}{2}\tau+\frac{1}{2}(t_s+t_e))}}{8(\frac{\Delta t}{2}\tau+\frac{1}{2}(t_s+t_e)+1)^{\frac{3}{2}}}\sin\frac{\pi\tilde{s}(t)(\xi+1)}{4\sqrt{\frac{\Delta t}{2}\tau+\frac{1}{2}(t_s+t_e)+1}}, \\
&\qquad -1 < \tau \le 1, \quad -1 < \xi < 1, \\
u(\xi,-1) &= u_s(\xi), \qquad -1 < \xi < 1, \\
u(-1,\tau) &= e^{-t}, \qquad -1 \le \tau \le 1, \\
u(1,\tau) &= 0, \qquad -1 \le \tau \le 1, \\
\frac{2}{\Delta t}\tilde{s}'(\tau) &= -\frac{2e^{(\frac{\Delta t}{2}\tau+\frac{1}{2}(t_s+t_e))}}{\tilde{s}(\tau)\pi}u_\xi(1,\tau), \qquad -1 < \tau \le 1, \\
\tilde{s}(-1) &= \tilde{s}_s.
\end{aligned}$$

Here $\tilde{s}(\tau) = s(t(\tau))$ and if $t_s = 0$ then

$$u_s(\xi) = \cos\frac{\pi}{4}(\xi+1), \qquad \tilde{s}_s = 1.$$

3 Numerical Results

In this section, our method is applied to test problems.

3.1 Discretization and the Newton's Method

By applying the spectral collocation method in space and time to Test Problems 1′ and 2′, we obtain two nonlinear systems of equations, Test Problems 1″ and 2″, corresponding to Test Problems 1′ and 2′.

Test Problem 1″.

$$\frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}u_{i,l} \ - \ \frac{4}{\{s_j\}^2}\sum_{k=0}^{N_x}(D_{\xi\xi})_{i,k}u_{k,j} + \frac{z_i}{s_j}\{\frac{1}{s_j}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}$$

$$+ \ T_j\}\sum_{k=0}^{N_x}(D_\xi)_{i,k}u_{k,j} - (2T_j+4) = 0,$$

$$(i = 1, 2, \cdots, N_x - 1, \quad j = 0, 1, \cdots, N_t - 1)$$

$$\frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}s_l \ + \ \frac{1}{s_j}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j} + T_j = 0,$$

$$(j = 0, 1, \cdots, N_t - 1)$$

$$\begin{aligned} u_{i,N_t} - u_s(\xi_i) &= 0, && (i = 1, 2, \cdots, N_x - 1) \\ u_{N_x,j} - (T_j+1)^2 &= 0, && (j = 0, 1, \cdots, N_t) \\ u_{0,j} &= 0, && (j = 0, 1, \cdots, N_t) \\ s_{N_t} - \tilde{s}_s &= 0 \end{aligned}$$

where

$$\begin{aligned} (D_\tau)_{j,l} &: \text{ Chebyshev collocation first derevative in } \tau \\ (D_\xi)_{j,l}, (D_{\xi\xi})_{j,l} &: \text{ Chebyshev collocation first and second derevative in } \xi \\ u_{i,j} &= u(\xi_i, \tau_j), \\ s_j &= \tilde{s}(\tau_j), \\ z_i &= (\xi_i + 1), \\ T_j &= \frac{\Delta t}{2}\tau_j + \frac{1}{2}(t_s + t_e). \end{aligned}$$

Test Problem 2″.

$$\frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}u_{i,l} \ - \ \frac{16(T_j+1)}{\{s_j\}^2\pi^2}\sum_{k=0}^{N_x}(D_{\xi\xi})_{i,k}u_{k,j}$$

$$+ \ \frac{2z_ie^{T_j}}{\{s_j\}^2\pi}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}\sum_{k=0}^{N_x}(D_\xi)_{i,k}u_{k,j}$$

$$- \ \frac{\pi s_j z_i e^{-T_j}}{8(T_j+1)^{\frac{3}{2}}}\sin\frac{\pi s_j z_i}{4\sqrt{T_j+1}} = 0,$$

$$(i=1,2,\cdots,N_x-1, \quad j=0,1,\cdots,N_t-1)$$

$$\frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}s_l + \frac{2e^{T_j}}{s_j\pi}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}=0,$$

$$(j=0,1,\cdots,N_t-1)$$

$$\begin{aligned} u_{i,N_t}-u_s(\xi_i) &= 0, && (i=1,2,\cdots,N_x-1)\\ u_{N_x,j}-e^{-T_j} &= 0, && (j=0,1,\cdots,N_t)\\ u_{0,j} &= 0, && (j=0,1,\cdots,N_t)\\ s_{N_t}-\tilde{s}_s &= 0. && \end{aligned}$$

N_x and N_t are the order of the spectral collocation method in space and time respectively.

Here, Test Problems 1″ and 2″ are represented more general form as a nonlinear system

$$F=F_k(X)=0, \qquad i=0,1,\cdots,N_x, \qquad j=0,1,\cdots,N_t$$

$$k=1,2,\cdots,m \qquad (m=(N_x+2)(N_t+1))$$

where

$$\begin{aligned} X &= \underbrace{(s_0,s_1,\cdots,s_{N_t},u_{0,0},u_{0,1},\cdots,u_{N_x,N_t})}_{m \text{ elements}}{}^T\\ &= (X_1,X_2,\cdots,X_m)^T. \end{aligned}$$

F_k which related to Test Problem 1″ is defined as follow:

$$F_p=\begin{cases} \frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}s_l+\frac{1}{s_j}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}+T_j, & (j=0,1,\cdots,N_t-1)\\ s_j-\tilde{s}_s, & (j=N_t) \end{cases}$$

where $\qquad p=j+1, \qquad (1\le p\le N_t+1)$

$$F_q=\begin{cases} \frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}u_{i,l}-\frac{4}{\{s_j\}^2}\sum_{k=0}^{N_x}(D_{\xi\xi})_{i,k}u_{k,j} \\ \quad +\frac{z_i}{s_j}\{\frac{1}{s_j}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}+T_j\}\sum_{k=0}^{N_x}(D_\xi)_{i,k}u_{k,j} \\ \quad -(2T_j+4), \\ \qquad (i=1,2,\cdots,N_x-1, \quad j=0,1,\cdots,N_t-1)\\ u_{i,j}-u_s(\xi_i), \quad (i=1,2,\cdots,N_x-1, \quad j=N_t)\\ u_{i,j}-(T_j+1)^2, \quad (i=N_x, \quad j=0,1,\cdots,N_t)\\ u_{i,j} \qquad (i=0, \quad j=0,1,\cdots,N_t) \end{cases}$$

where $\quad q = (N_t+1)(i+1)+(j+1), \qquad N_t+2 \le q \le (N_x+2)(N_t+1).$

Similarly, F_k which related to Test Problem 2″ is defined as follow:

$$F_p = \begin{cases} \frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}s_l + \frac{2e^{T_j}}{s_j\pi}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}, & (j=0,1,\cdots,N_t-1) \\ s_j - \tilde{s}_s & (j=N_t) \end{cases}$$

where $\quad p = j+1, \qquad (1 \le p \le N_t+1)$

$$F_q = \begin{cases} \frac{2}{\Delta t}\sum_{l=0}^{N_t}(D_\tau)_{j,l}u_{i,l} - \frac{16(T_j+1)}{\{s_j\}^2\pi^2}\sum_{k=0}^{N_x}(D_{\xi\xi})_{i,k}u_{k,j} \\ \quad +\frac{2z_ie^{T_j}}{\{s_j\}^2\pi}\sum_{k=0}^{N_x}(D_\xi)_{0,k}u_{k,j}\sum_{k=0}^{N_x}(D_\xi)_{i,k}u_{k,j} \\ \quad -\frac{\pi s_j z_i e^{-T_j}}{8(T_j+1)^{\frac{3}{2}}}\sin\frac{\pi s_j z_i}{4\sqrt{T_j+1}}, \\ (i=1,2,\cdots,N_x-1, \quad j=0,1,\cdots,N_t-1) \\ u_{i,j}-u_s(\xi_i), \quad (i=1,2,\cdots,N_x-1, \quad j=N_t) \\ u_{i,j}-e^{-T_j}, \quad (i=N_x, \quad j=0,1,\cdots,N_t) \\ u_{i,j} \quad (i=0, \quad j=0,1,\cdots,N_t) \end{cases}$$

where $\quad q = (N_t+1)(i+1)+(j+1), \qquad N_t+2 \le q \le (N_x+2)(N_t+1).$

Futhermore, we obtain the iteration scheme by the Newton's method

$$X^{(n+1)} = X^{(n)} - A^{-1}F(X^{(n)}) \qquad n=0,1,2,\cdots$$

where

$$A = \frac{\partial(F)}{\partial(X)}, \qquad A^{-1} \text{ inverse of } A.$$

We can also write the iteration scheme

$$AX^{(n+1)} = AX^{(n)} - F(X^{(n)}) \qquad n=0,1,2,\cdots$$

then we use the Gauss elimination method to solve simultaneous linear equations.

3.2 Numerical Results

For test problems, the spectral collocation method with the Chebyshev-Gauss-Lobatto points and 60 digit numbers have been used. For evaluation of the numerical results, the maximum error is used. The maximum error is difined such that

$$\max_k \mid X_k^{(exact)} - X_k^{(numer)} \mid, \quad (k=1,2,\cdots,m)$$

where

$$X_k^{(exact)} \ : \ \text{the computed value of exact solution at collocation point } k$$

$$X_k^{(numer)} \ : \ \text{the computed value of numerical solution at collocation point } k$$

$$m = (N_x + 2)(N_t + 1) \ : \ \text{total collocation points}$$

Table 1. Maximum errors for Test Problem 1.

$N_x = N_t$	Max. Error	$N_x = N_t$	Max. Error
3	6.088×10^{-58}	10	8.946×10^{-59}
4	3.016×10^{-58}	15	1.728×10^{-59}
6	3.698×10^{-58}	20	1.397×10^{-59}
8	7.357×10^{-59}	25	5.597×10^{-60}

For Test Problem 1, we use $\Delta t = 1$. Numerical calculation is executed only for the first interval $[0, \Delta t]$. Here, we use the same order approximation in space and time for simplicity. The results are superior in precision. This is because the exact solution to Test Problem 1 is polynomial in space and time.

Table 2. Maximum errors for Test Problem 2.

$N_x = N_t$	$t = 1$		
	$\Delta t = 1$	$\Delta t = 0.2$	$\Delta t = 0.05$
4	6.979×10^{-04}	1.716×10^{-04}	7.927×10^{-05}
6	2.041×10^{-06}	7.281×10^{-07}	3.568×10^{-07}
8	3.007×10^{-08}	1.850×10^{-09}	6.166×10^{-10}
10	6.336×10^{-10}	3.047×10^{-12}	8.708×10^{-13}
15	5.225×10^{-14}	6.789×10^{-20}	1.913×10^{-20}
20	5.086×10^{-18}	3.722×10^{-28}	1.038×10^{-28}
25	5.435×10^{-22}	7.444×10^{-37}	1.408×10^{-37}
30	6.164×10^{-26}	7.043×10^{-44}	8.110×10^{-47}

For Test Problem 2, we use $\Delta t = 1,\ 0.2,\ 0.05$. Numerical calculation is executed for the interval $[0, 1]$. Here, we use the same order approximation in space and time for simplicity. Table 2 show that the results for small Δt are mostly better than the results for large Δt in precision. Here, we can not adopt large $N_x = N_t$ due to the restriction on the computing resources.

4 Conclusion

We considered a method for numerical simulation in arbitrary precision. It consists of the spectral collocation method and multiple precision arithmetic. One-phase stefan problems whose exact solution are known are solved by this method. The numerical results are satisfactory in accuracy. Numerical simulation of one-phase stefan problems in arbitrary precision is possible by using the spectral collocation method and multiple precision arithmetic.

References

[1] Canuto, C. et al., *Spectral Methods in Fluid Dynamics,* Springer, NewYork, 1988.

[2] David, M. Smith. "A FORTRAN Package For Floating-Point Multiple-Precision Arithmetic". *Transactions on Mathematical Software.* 17, pp.273-283(1991).

[3] Imai, H., Takeuchi, T. and Kushida, M., On Numerical Simulation of Partial Differential Equations in Infinite Precision, *Advances in Mathematical Sciences and Applications*, Vol.9, in press.

[4] Imai, H., Shinohara, Y. and Miyakoda, T., Application of Spectral Collocation Methods in Space and Time to Free Boundary Problems, *"Hellenic European Research on Mathematic and Informatics '94 (E.A. Lipitakis, ed.)," Hellenic Mathematical Society*, Vol.2, pp.781-786(1994).

[5] Imai, H., Shinohara, Y. and Miyakoda, T., On Spectral Collocation Methods in Space and Time for Free Boundary Problems, *" Computational Mechanics '95(eds. S.N.Atluri, G.Yagawa and T.A.Cruse)"*, Springer, **1**, pp.798-803(1995).

[6] Imai, H., Takeuchi, T., Sakaguchi, H., Shinohara, Y. and Tarmizi., On Numerical Simulation of Partial Differential Equations in Arbitrary Precision, *RIMS Kokyuroku*, Kyoto Univ., *1040*, pp.92-99(1998), in Japanese

[7] Katano, Y., Kawamura, T. and Takami, H., Numerical Study of Drop Formation from a Capillary Jet Using a General Coordinate System, *"Theoretical and Applied Mechanics," Univ. Tokyo Press* pp.3-14(1986).

[8] Knuth, D. E., *The Art of Computer Programming*, Addison-Wesley, 1981.

[9] Takeuchi, T., Imai, H., Tarmizi., Shinohara, Y., Sakaguchi, H. and Miyakoda, T., On Numerical Simulation of Partial Differential Equations in Arbitrary Precision, *Science International(Lahore)* **10**(5), in press