数理解析研究所講究録
1147 巻 2000 年 42-50

Infinite Precision Numerical Simulation for PDE systems and Its Applications

Hitoshi IMAI, Toshiki TAKEUCHI and Hideo SAKAGUCHI
今井　仁司，竹内　敏己，坂口　秀雄

Department of Applied Physics and Mathematics, Faculty of Engineering,
University of Tokushima, Tokushima 770-8506, Japan.

1. Introduction

Nowadays, we can easily carry out heavy numerical simulation by using cheep and powerful computers. Taking into account such changing of the computing environment, we had been looking for a new field in heavy numerical simulation.

Nonlinear problems governed by (partial) differential equations are major subjects in applied mathematics. To these problems numerical simulation often plays an important role in analysis. However, numerical errors sometimes cause troubles. The reliability of numerical results is very important, and it is usually checked by comparing numerical results in defferent precision.

From the above background we presented infinite-precision numerical simulation (IPNS) to PDE systems with smooth solutions[8, 10]. Of course, it is applicable to ODE systems. Errors in numerical simulations originate from truncation errors in discretization and rounding errors. Realization of IPNS needs arbitrary reduction of both errors. Thus, in IPNS the spectral method is used for the control of truncation errors. In particular, the spectral collocation method[1] is very useful for nonlinear problems. The order of the approximation can be controlled by the number of collocation points. Multiple precision arithmetic[11] is used for the control of rounding errors, and it is easily available by using the library on the net, e.g. http://www.lmu.edu/acad/personal/faculty/dmsmith2/FMLIB.html [15]. IPNS is also important from the theoretical view point, because it can approximate analytical solutions in arbitrary precision.

2. Boundary value problems

In this section, two simple boundary value problems are solved by IPNS.

Problem 1. Find $u(x)$ s.t.

$$u_{xx} = -\frac{\pi^2}{16}\sin\frac{(x+1)\pi}{4}, \qquad -1 < x < 1,$$

$$u(-1) = 0, \qquad u_x(1) = 0.$$

Remark 1. The exact solution to Problem 1 is

$$u(x) = \sin\frac{(x+1)\pi}{4}.$$

Numerical results are shown in Table 1[10]. Here $(N+1)$ Chebyshev-Gauss-Lobatto points are used. Extremely high accuracy is obseved.

Table 1. Maximum errors for Problem 1.(1100 digit numbers)

N	Maximum error	N	Maximum error	N	Maximum error
10	4.88×10^{-11}	90	4.32×10^{-175}	170	2.98×10^{-376}
20	6.64×10^{-27}	100	6.01×10^{-199}	180	9.38×10^{-403}
30	5.39×10^{-45}	110	3.08×10^{-223}	190	1.70×10^{-429}
40	1.54×10^{-64}	120	6.38×10^{-248}	200	1.82×10^{-456}
50	3.62×10^{-85}	130	5.76×10^{-273}	250	2.24×10^{-594}
60	1.16×10^{-106}	140	2.42×10^{-298}	300	1.20×10^{-736}
70	7.02×10^{-129}	150	4.97×10^{-324}	350	1.49×10^{-882}
80	1.03×10^{-151}	160	5.25×10^{-350}	400	1.46×10^{-1031}

Next, the following two-dimensional boundary value problem is solved.

Problem 2. Find $u(x, y)$ s.t.

$$u_{xx} + u_{yy} = -\pi^2(\sin(\pi x) + \sin(\pi y)) \quad \text{in} \quad I = (0,1) \times (0,1),$$

$$u = \sin(\pi x) + \sin(\pi y) \qquad \text{on} \quad \partial I.$$

Here, ∂I represents the boundary of I.

Remark 2. The exact solution to Problem 2 is

$$u(x, y) = \sin(\pi x) + \sin(\pi y).$$

Numerical results are shown in Table 2[10]. For the simplicity the same number of collocation points are used on both x and y. From the limitation of the memory size, IPNS is not carried out for the larger N.

Table 2. Maximum errors for Problem 2.(120 digit numbers)

N	Maximum error	N	Maximum error
5	4.24×10^{-2}	45	4.74×10^{-51}
10	3.04×10^{-6}	50	1.49×10^{-57}
15	1.37×10^{-11}	55	2.25×10^{-66}
20	1.33×10^{-16}	60	3.51×10^{-73}
25	2.47×10^{-23}	65	1.94×10^{-82}
30	5.37×10^{-29}	70	1.65×10^{-89}
35	1.26×10^{-36}	75	3.85×10^{-99}
40	9.32×10^{-43}	80	1.95×10^{-106}

3. Initial and boundary value problem

In this section, IPNS is applied to a typical initial and boundary value problem governed by the heat equation.

Problem 3. Find $u(x,t)$ s.t.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < t, \quad -1 < x < 1,$$

$$u(x,0) = \cos\frac{\pi x}{2}, \qquad -1 < x < 1,$$

$$u(-1,t) = 0, \qquad 0 \le t,$$

$$u(1,t) = 0, \qquad 0 \le t.$$

Remark 3. The exact solution to Problem 3 is

$$u(x,t) = \exp\left(-\frac{\pi^2 t}{4}\right)\cos\frac{\pi x}{2}, \qquad 0 \le t, \qquad -1 \le x \le 1.$$

To this problem, an iterative method is necessary for t[10]. Numerical results are shown in Table 3[10]. For the simplicity the same number of collocation points are used on both x and t.

Table 3. Maximum relative errors for Problem 3 until $t = 10$.(120 digit numbers, $\Delta t = 1$)

N	Relative error	N	Relative error	N	Relative error
5	2.148×10^{-1}	20	9.575×10^{-22}	35	1.713×10^{-44}
10	1.596×10^{-8}	25	2.502×10^{-28}	40	2.136×10^{-54}
15	9.544×10^{-14}	30	1.686×10^{-37}	45	8.011×10^{-62}

4. Inverse problems

Inverse problems are very important from the view point of engineering. Usual approaches are applications of the regularization and the least square method or AI. We tried some methods[6, 14], however we were not satisfied. Then, we applied IPNS directly to an inverse problem governed by the heat equation[9]. Here we apply IPNS directly to the following problem[3].

Problem 4. Find $u(x, y)$ s.t.

$$\begin{aligned}
\Delta u(x,y) &= 0, && \text{in } (0,1)\times(0,1),\\
u(0,y) &= 0, && 0 \le y \le 1,\\
u(1,y) &= 0, && 0 \le y \le 1,\\
u(x,0) &= 0, && 0 \le x \le 1,\\
\frac{\partial u(x,0)}{\partial y} &= \frac{1}{\pi}\sin(\pi x), && 0 \le x \le 1.
\end{aligned}$$

Remark 4. The exact solution to Problem 4 is

$$u(x,y) = \frac{1}{\pi^2}\sinh(\pi y)\sin(\pi x).$$

Numerical results are shown in Table 4. For the simplicity the same number of collocation points are used on both x and y.

Table 4. Maximum errors for Problem 4. (120 digit numbers)

N	Maximum error
10	1.25×10^{-7}
20	2.86×10^{-19}
30	1.49×10^{-30}
40	1.13×10^{-44}
50	7.22×10^{-58}
60	8.09×10^{-74}
70	5.31×10^{-89}
80	8.43×10^{-96}

5. Free boundary problems

Free boundary problems are also important from the practical view point. IPNS is applicable to free boudary problems. However, in two- or three-dimensional problems the singularity of the mapping functions becomes a big problem. Some methods for elimination of the singularity should be developed[4]. Here, IPNS is applied to a simple one-dimensional free boundary problem related to the pattern formation in diblock copolymer[12, 13].

Problem 5. Find $u^+(x,t)$, $u^-(x,t)$ and $s(t)$ which satisfy

$$
\begin{aligned}
u^+_{xx}(x,t) &= -2\frac{t+\frac{11}{4}}{t+2}, && 0<t,\ -1<x<s(t),\\
u^-_{xx}(x,t) &= 2\frac{t+\frac{3}{4}}{t+2}, && 0<t,\ s(t)<x<1,\\
u^+(s(t),t) &= 0, && 0<t,\\
u^-(s(t),t) &= 0, && 0<t,\\
u^+(x,0) &= -\frac{11}{8}\left(x+\frac{1}{2}\right)\left(x+\frac{3}{2}\right), && -1\le x\le s(0),\\
u^-(x,0) &= \frac{3}{8}\left(x+\frac{1}{2}\right)\left(x-\frac{5}{2}\right), && s(0)\le x\le 1,\\
\frac{d}{dt}s(t) &= -u^+_x(s(t),t)+u^-_x(s(t),t), && 0<t,\\
s(0) &= -\frac{1}{2},\\
u^+_x(-1,t) &= 0, && 0<t,\\
u^-_x(1,t) &= 0, && 0<t.
\end{aligned}
$$

Remark 5. The exact solutions to Problem 5 are

$$
\begin{aligned}
u^+(x,t) &= -\frac{t+\frac{11}{4}}{t+2}(x-s(t))(x+2+s(t)), && 0\le t,\ -1\le x\le s(t),\\
u^-(x,t) &= \frac{t+\frac{3}{4}}{t+2}(x-s(t))(x-2+s(t)), && 0\le t,\ s(t)\le x\le 1,\\
s(t) &= -\frac{1}{t+2}, && 0\le t.
\end{aligned}
$$

The spectral collocation method cannot be applied directly to free boundary problems due to the unknown shape of the domain. To avoid this difficulty, we use the fixed domain method using mapping functions[5, 16].

Numerical results are shown in Table 5. N_x and N_t represent the number of collocation points in x and t, respectively. N_x is fixed to be 2. This is because the exact solutions are polynomial of degree 2 in space. Of course, for more general problems N_x should be changed as N_t.

Table 5. Maximum errors for Problem 5. ($\Delta t = 0.1$, 500 digit numbers)

N_t	Max. Error	N_t	Max. Error
20	7.362×10^{-40}	140	1.570×10^{-269}
40	3.800×10^{-78}	160	8.325×10^{-308}
60	1.998×10^{-116}	180	4.416×10^{-346}
80	1.056×10^{-154}	200	2.343×10^{-384}
100	5.588×10^{-193}	220	1.243×10^{-422}
120	2.961×10^{-231}	240	6.598×10^{-461}

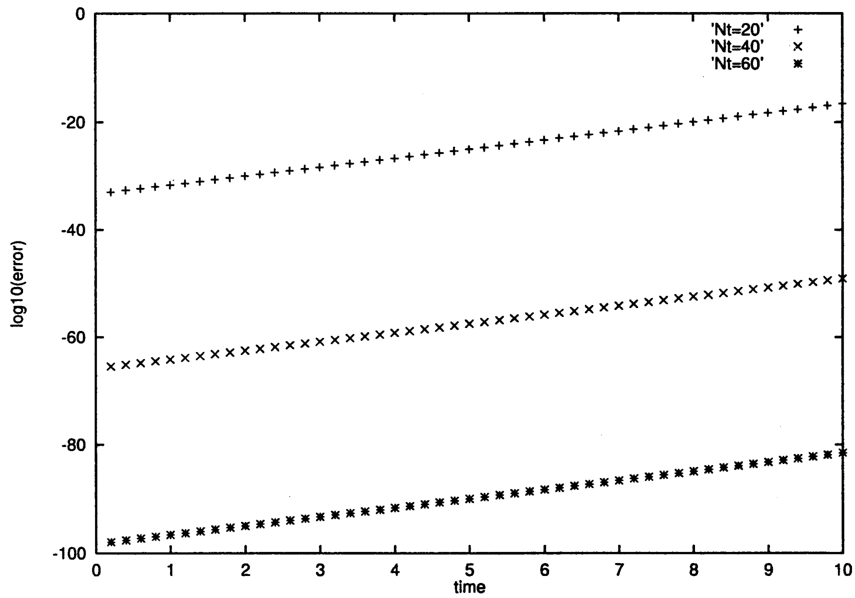

Fig. 1. Behavior of maximum error for Problem 5. ($\Delta t = 0.2$, 150 digit numbers).

Table 5 shows errors in the first interval $[0, \Delta t]$. The growth of errors is observed in Fig. 1. This interesting phenomenon originates in the mathematical property of the problems.

6. Parallel computing by PVM

IPNS requires huge computer resources. Then, we developed parallel computing by PVM (Parallel Virtual Machine)[2]. The utilization of PVM has two merits that we can use the larger memory area than that of the single computer and we can reduce computational time by pararell computing.

In IPNS the Gauss elimination method for solving a linear system in multple precision needs much CPU time. Then, we developed its parallel computing program by PVM and applied it to the Cauchy problem in the section 4. The PVM cluster used here is shown in Fig. 2.

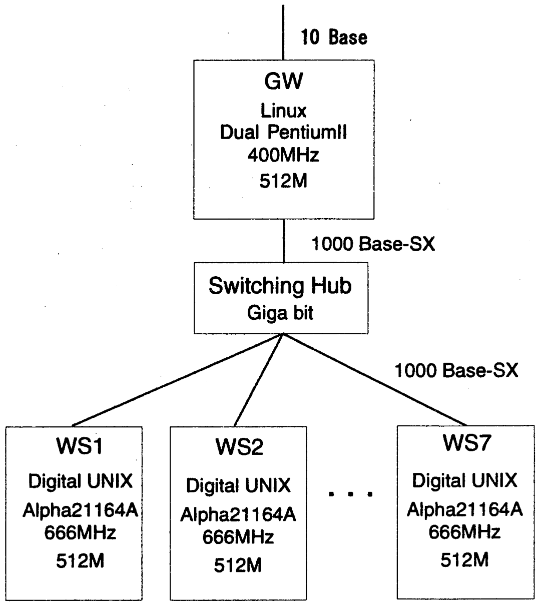

Fig. 2. PVM cluster.

The following tables show results of numerical experiments.

Table 6. Computational time(sec). (120 digit numbers)

$N_x = N_y$	Non-PVM 1CPU	2-slaves	4-slaves	6-slaves
20	161	91	52	40
30	2005	1027	542	381
40	11640	5904	3053	2093
50		22946	11694	7987
60			36005	24344
70				61388

Table 7. Ratio of p-slaves to Non-PVM&1CPU.

$N_x = N_y$	2-slaves	4-slaves	6-slaves
20	1.77	3.10	4.03
30	1.95	3.70	5.26
40	1.97	3.81	5.56

These results show IPNS is suitable for parallel computing. This is because computational time of the message passing is much less than that of multiple precision arithmetic.

7. Conclusion

In the paper some applications of infinite-precision numerical simulation(IPNS) to PDE systems and its parallel computing are shown. Extremely high accuracy is observed. This means numerical results by IPNS are very helpful for theoretical analysis. Its application to higher dimensional problems is our future work.

Acknowledgements

This work is partially supported by Grants-in-Aids for Scientific Research (Nos. 09440080, 10354001), Japan Ministry of Education, Science, Sports and Culture.

References

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

[2] A. Geist, et al., PVM, The MIT Press, 1994.

[3] H. Han and H.-J. Reinharat, Some stability estimates for Cauchy problems for elliptic equations, J. Inv. Ill-Posed Problems **5**(5)(1997), 1-18.

[4] H. Imai and H. Kawarada, One-Component Asymmetric Plasmas in a Symmetric Vessel, Japan Journal of Applied Mathematics, **5**(2)(1988), 173-186.

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

[6] H. Imai, Application of the Fuzzy Theory and Spectral Collocation Methods to an Ill-Posed Shape Design Problem With a Free Boundary, in "Inverse Problems in Mechanics," Eds. S. Saigal and L.G. Olson, **186**, pp.103-107, The American Society of Mechanical Engineers, 1994.

[7] H. Imai, et al., Numerical Computations of Free Boundary Problems in Quadruple Precision Arithmetic Using an Explicit Method, GAKUTO International Series, Mathematical Sciences and Applications **11**(1998), 193-207.

[8] H. Imai, et al., On Numerical Simulation of Partial Differential Equations in Arbitrary Precision, RIMS Kokyuroku, Kyoto University **1040**(1998), 92-99.(in Japanese)

[9] H. Imai et al., A direct approach to an inverse problem, GAKUTO International Series, Mathematical Sciences and Applications **12**(1999), 223-232.

[10] H. Imai, T. Takeuchi and M. Kushida, On Numerical Simulation of Partial Differential Equations in Infinite Precision, Advances in Mathematical Sciences and Applications **9**(2)(1999), 1007-1019.

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

[12] Y. Nishiura and I. Ohnishi, Some mathematical aspects of the micro-phase separation in diblock copolymers, Physica D **84**(1995), 31-39.

[13] I. Ohnishi and H. Imai, Modified Hele-Shaw moving boundary problem related to some phase transition phenomena, Bulletin of the University of Electro-Communications **11**(1)(1998), 17-28.

[14] A. Sasamoto, H. Imai and H. Kawarada, A Practical Method for an Ill-Conditioned Optimal Shape Design of a Vessel in Which Plasma Is Confined, in "Inverse Problems in Engineering Sciences", Eds. M. Yamaguti et al., pp.120-125, Springer-Verlag, 1991.

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

[16] Tarmizi, T. Takeuchi, H. Imai and M. Kushida, Numerical simulation of one-dimensional free boundary problems in infinite precision, Advances in Mathematical Sciences and Applications **10**(2)(2000). (in press)