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Development of a parallel implicit solver of fluid modeling equations for gas discharges

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ABSTRACT

A parallel fully implicit PETSc-based fluid modeling equations solver for simulating gas discharges is developed. Fluid modeling equations include: the neutral species continuity equation, the charged species continuity equation with drift-diffusion approximation for mass fluxes, the electron energy density equation, and Poisson's equation for electrostatic potential. Except for Poisson's equation, all model equations are discretized by the fully implicit backward Euler method as a time integrator, and finite differences with the Scharfetter–Gummel scheme for mass fluxes on the spatial domain. At each time step, the resulting large sparse algebraic nonlinear system is solved by the Newton–Krylov–Schwarz algorithm. A 2D-GEC RF discharge is used as a benchmark to validate our solver by comparing the numerical results with both the published experimental data and the theoretical prediction. The parallel performance of the solver is investigated.

1. Introduction

Gas discharges play an important role in modern display technologies, lighting sources, materials processing, and surface cleaning, among others. Gaining an understanding of plasma physics for these applications can often be either too difficult or too incomplete to use purely experimental techniques. With the unprecedented evolution of advanced computer technology in the past two decades, numerical fluid modeling has become an indispensable tool for understanding gas discharges. Fluid modeling, which describes the discharges based on the number density, mean velocity and mean energy of the charged and neutral species, is often used to model low-temperature plasmas by self-consistent coupling with Maxwell equations. Compared with the computationally demanding particle-in-cell method [1], one of the major advantages of the fluid modeling approach is that more complicated and realistic chemistry can be considered. However, a numerical simulation based on fluid modeling is still very time-consuming, especially for large-scale 2D or 3D computations with more chemical reactions involved [2]. To tackle these problems within a reasonable runtime while maintaining acceptable accuracy, parallelization of the fluid modeling solver is necessary. Thus, the objectives of this paper are to develop and validate a fully implicit numerical solver for gas-discharge fluid modeling equations as well as to study the related parallel performance for large scale problems.

2. Fluid modeling equations and parallel solution algorithm

In the framework of fluid modeling [3], the governing equations include: the continuity equation with drift-diffusion approximation for both electrons and ions, the continuity equation for neutral species, the energy density equation for electrons and Poisson's equation for electrostatic distribution. In our model, the flow convection effects have been omitted, and the drift and diffusion coefficients and rate constants related to electrons are functions of electron temperature. Such functional relations, obtained by a publicly available Boltzmann equation solver, BOLSIG+ [4], were prepared as a lookup table prior to the computer simulation. Except for Poisson's equation, all model equations were discretized by a fully implicit backward Euler's method on the temporal domain and finite differences with the Scharfetter–Gummel scheme for mass fluxes on the spatial domain. We applied a fully coupled Newton–Krylov–Schwarz (NKS) algorithm [5]. At each time step, the resulting large sparse algebraic nonlinear system of equations was solved by an inexact Newton method, where an additive Schwarz (AS) preconditioned Krylov-type method, e.g., BiCGStab or GMRES [6,7] was used for the solution of the Jacobian system. The parallel implementation of our fluid modeling solver was realized by a Portable, Extensible Toolkit for Scientific Computation (PETSc) [8].

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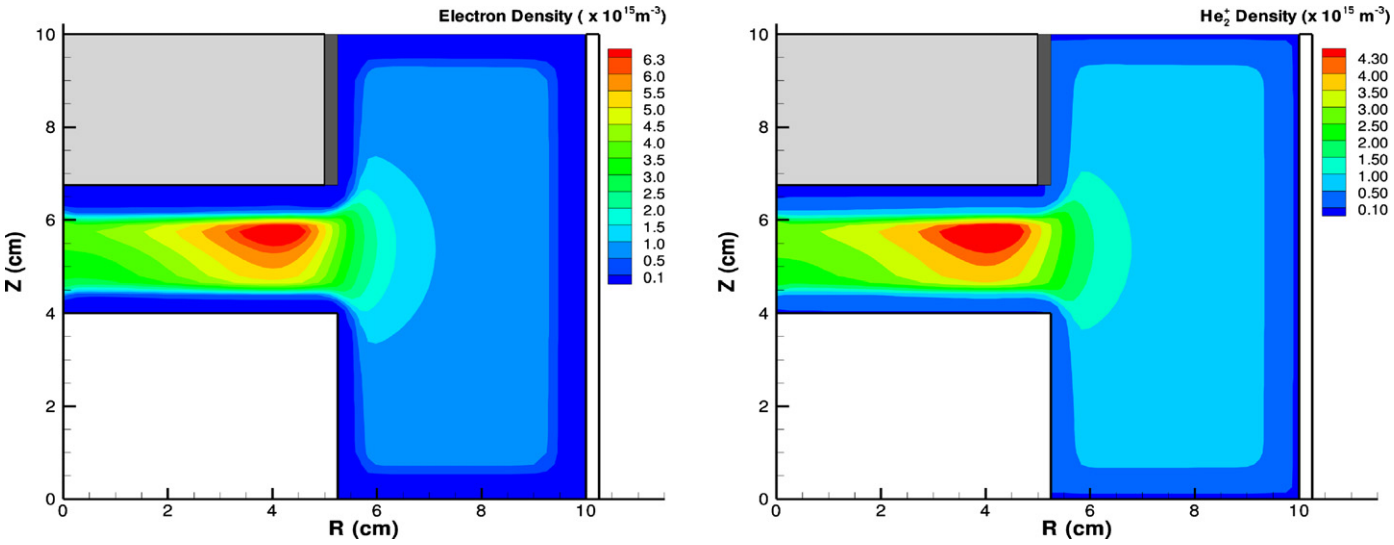

Fig. 1. Simulated cycle averaged plasma properties of helium GEC.

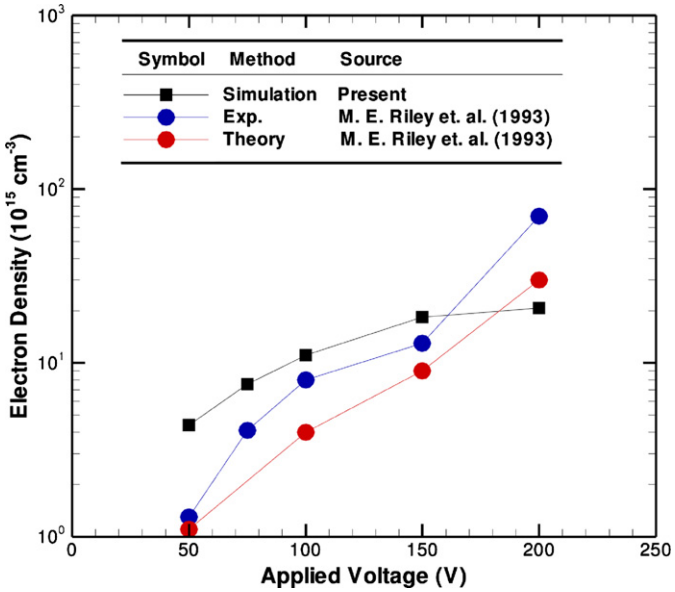

Fig. 2. Comparison of computed electron densities as a function of the zero-to-peak applied RF voltage with the experimental data and the theoretical prediction.

3. Results and discussion

A GEC discharge simulation was conducted as a benchmark problem. Both the power and grounded electrodes were 2 inches in radius, the electrode gap was 1 inch in length, the applied peak-to-peak voltage was 150 V, the frequency was 13.56 MHz, and the background pressure for pure helium was 500 mTorr. The gas temperature was assumed to be 400 K. A 52×61 non-uniform grid and a total of 200 time steps per RF cycle were employed. One overlapping layer for AS and LU decomposition as a subdomain solver was used. Convergence criteria for the Newton and Krylov subspace methods were 5×10^{-5} and 10^{-4}, respectively.

The cycle-averaged electron and molecular ion densities are shown in Fig. 1. The results indicate that the maximum value occurred near the outer edge between two electrode gaps where the electric field was large. In addition, molecular ions were the dominant ion species, rather than atomic ions. Similar trends were found in the previous study [9].

Fig. 2 shows a comparison of the simulated peak electron densities with the theoretical prediction and the experimental data [10] for various applied voltages. Note that only the 1-D electron Boltzmann equation was used for the theoretical prediction, which was questionable for the present 2-D case. Thus, the data were included for reference only. In general, the simulation data followed the trend of the measurements reasonably well, except for the lowest (50 V) and the highest (200 V) cases. Note that the electron densities were measured by a microwave interferometer probing through the center along the radial direction at the midpoint between the electrodes by integrating the data along the line-of-sight path. The data were only correct if the densities were uniform throughout the microwave path, which was obviously not true for the current test cases. Nevertheless, the simulated data were in reasonable agreement with the measurements.

Fig. 3 shows the speedup analysis and runtime per time step with respect to the number of processors. The simulation conditions used for the parallel performance studies were similar to

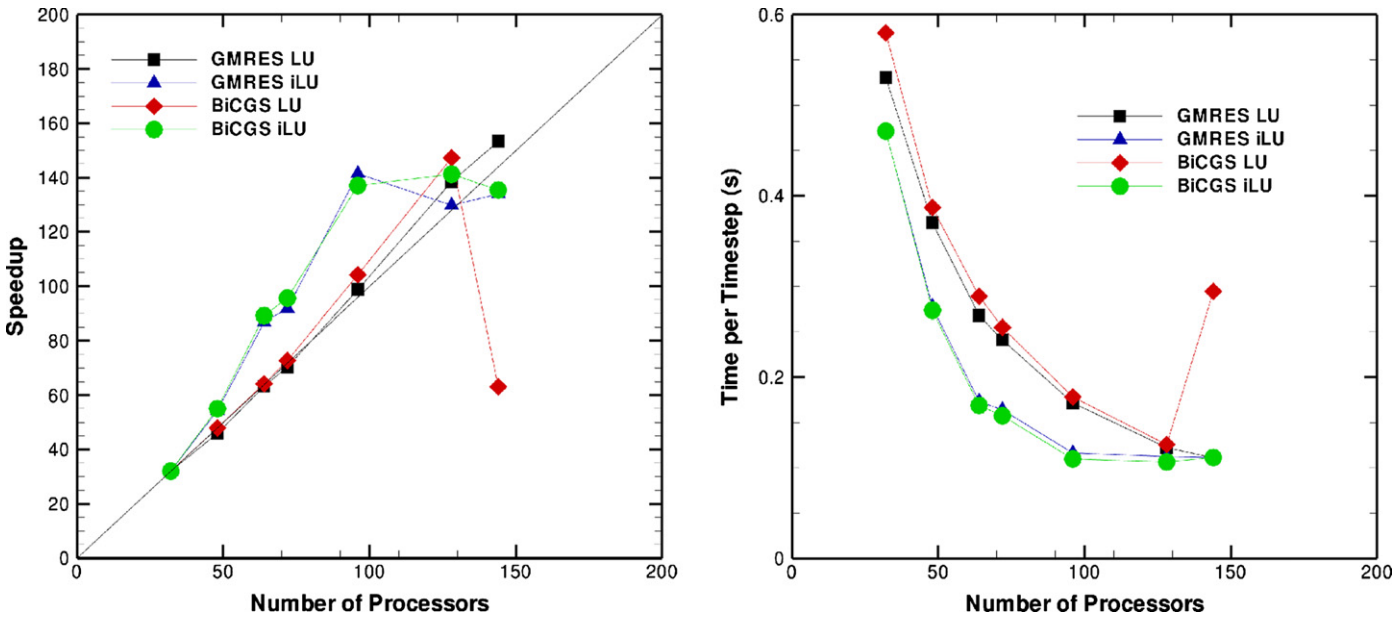

Fig. 3. Speedup analysis (left) and the runtime per time step (right) with respect to the number of processors.

those for the parallel code validation, except that we now considered a 122×123 uniform grid and $V_{pp} = 200$ V. We investigated the parallel performance of the solver by using two types of the Krylov subspace method, GMRES and BiCGStab in conjunction with standard AS pre-conditioners, where the subdomain problems were solved by either the LU decomposition or the ILU(0) (incomplete LU decomposition with zero level fill in). All of the calculations were done on a V'ger cluster system (Xeon 3 GHz, dual core, dual CPU) at the Center for Computational Geophysics, National Central University, Taiwan. The results show that the combination of ILU(0) as a subdomain solver, with either GMRES or BiCGStab, performed the best in terms of runtime, and a nearly linear speedup was found up to 144 processors.

4. Concluding remarks

A fully parallel fluid modeling code for gas discharges was developed on top of PETSc, and the parallel solution algorithm was based on the fully coupled and fully scalable NKS algorithm. The validations showed reasonable agreement with measurements for a GEC. Very good parallel performance was also found for the developed code.

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References

[1] C.K. Birdsall, A.B. Langdon, Plasma Physics via Computer Simulations, Institute of Physics Publishing, Philadelphia, USA, 1991.
[2] H.C. Kim, F. Isa, S.S. Yang, M. Radmilovic-Radjenovic, J.K. Lee, J. Phys. D: Appl. Phys. 38 (2005) 283.
[3] F.F. Chen, Introduction to Plasma Physics and Controlled Fusion, Vol. 1: Plasma Physics, 2nd ed., Plenum Press, New York, USA, 1984.
[4] G.J.M. Hagelaar, L.C. Pitchford, Plasma Source Sci. Technol. 14 (4) (2005) 722.
[5] X.-C. Cai, W.D. Gropp, D.E. Keyes, R.G. Melvin, D.P. Young, SIAM J. Sci. Comput. 19 (1996) 246.
[6] H.A. van der Vorst, SIAM J. Sci. Stat. Comput. 13 (1992) 631.
[7] Y. Saad, H.S. Martin, SIAM J. Sci. Stat. Comput. 7 (1986) 856.
[8] S. Balay, K. Buschelman, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, B.F. Smith, H. Zhang, PETSc Web page, http://www.mcs.anl.gov/petsc, 2009.
[9] T. Martens, A. Bogaerts, W. Brok, J. Van Dijk, Anal. Bioanal. Chem 388 (2007) 1583.
[10] M.E. Riley, K.E. Greenberg, G.A. Hebner, P. Drallos, J. Appl. Phys. 75 (1994) 2789.