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Research Statement

Numerical simulations are rapidly taking on a more prominent role in all sciences and we rely increasingly on computers for analysis, discovery and prediction. This shift was greatly motivated by the exponential growth of the combined computational power that has continued for almost two decades. According to the Top 500 list currently there are seven petascale computers and about seventy terascale computers in North America. With these computational resources at hand, more sophisticated problems can be brought into focus and tasks can be challenged that were believed to be intractable twenty years ago.

I have been very fortunate to be in my profession because I enjoy applying mathematics to the solution of problems in engineering and science. I received my Ph.D from Novosibirsk State University (NSU) in 1999 which is in the top four research universities in Russia. In NSU I was fortunate to communicate with top mathematicians, such as Academician S.K. Godunov, Professors V.G. Romanov and S.I. Kabanikhin. My Ph.D thesis was dedicated to inverse problems of electrodynamics and optimization [11, 12]. I completed my postdoctoral training in Penn State University and in the University of Minnesota under the supervision of a great mathematician, Dr. D.N. Arnold. We developed a reformulation of the Einstein equations for applications of numerical general relativity [10]. In the following years I continued studying the Einstein equations and problems inspired by them and developed several examples of boundary conditions that do not perturb the constraint equations in numerical simulations [7, 8, 3]. My recent work is concerned with the application of analysis to the numerical solution of gas kinetic equations [9, 4]. I am interested in the development of a fast high order multidimensional deterministic solver for the Boltzmann equation [6, 5] and in the development of macroscopic models for simulation of gas flows in regimes transitional from free molecular to continuum. I am also interested in the development of a posteriori error estimates to quantify numerical and modelling errors in the solvers.

1. Deterministic solution of kinetic equations

At high altitudes and in small channels gas flows exhibit properties that are not predicted by well-established continuum models such as ones given by the Euler and the Navier-Stokes equations. Differences between the continuum predictions and the observed behaviour can include significantly different transition zones in shock waves and differences in surface effects, for example, in temperature jump, velocity slip and thermal creep. This increases uncertainty in a number of advanced technological applications such as re-entry of space vehicles, design of rocket thrusters and manufacturing and operating of microelectromecanical devices (see, e.g., Figure 1). It has been reported in [23] that experimental data is very difficult to obtain in many of these applications. Therefore, the

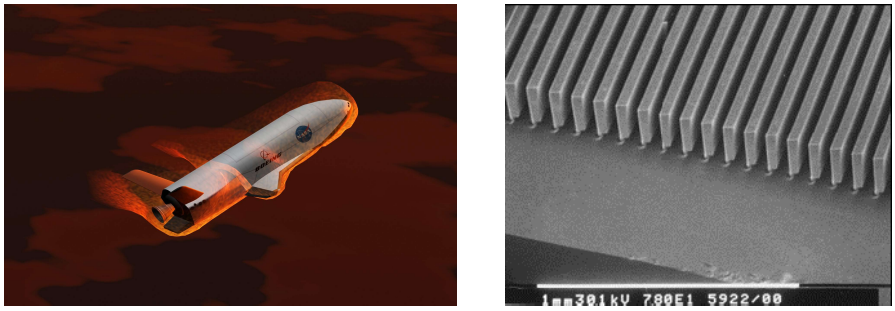

FIGURE 1. (left) Artist concept of re-entry of X-37B (image courtesy NASA). (right) Microchannels in silicon (image courtesy [19]).

development of numerical capabilities that model the physics of such flows correctly has now become very important.

The most accurate description of non-continuum flows can be done at the microscopic level using the kinetic approach. In the kinetic approach the gas is described using the molecular velocity distribution function, $f(t, \vec{x}, \vec{v})$ defined by the property that $f(t, \vec{x}, \vec{v})dx\,dv$ gives the number of molecules that at time t are located in the six dimensional volume of size $dx\,du$ around point $(\vec{x}, \vec{v})$. The distribution function is a solution of the Boltzmann equation

$$\partial_t f + \vec{u} \cdot \nabla_x f = Q(f),$$

where Q is the operator accounting for the collisions of molecules. In the simplest case of binary collisions in monoatomic gas, Q takes the form

$$Q(f) = \int_{\mathbb{R}^3} \int_0^{2\pi} \int_0^{b_*} (f(t,x,\xi')f(t,x,\xi_1') - f(t,x,\xi)f(t,x,\xi_1))|g|b\,db\,d\varepsilon\,d\xi_1\,d\xi\,, \tag{1}$$

where ξ and ξ_1 are molecular velocities before the collision, ξ' and ξ_1' are the velocities after the collision, ε and b are the azimuthal angle and the distance of the shortest approach which are parameters of the impact and b^* is the effective radius of the molecules. In more complex models, additional collision integrals and many-component distribution functions may be included to describe internal molecular degrees of freedom and chemical interaction between particles.

Numerical solution of the Boltzmann equation is extremely challenging due to the high computational costs of evaluation of the collision operator. These costs are prohibitive in realistic engineering applications plagued by massive requirements for computational grids. Therefore, new highly efficient methods for the evaluation of the collision integral need to be developed. These methods should capitalize on thorough mathematical analysis and the use of high performance computers and parallelization to a large number of processors.

Last year, in collaboration with researches at the Wright-Patterson Air Force Research Lab we developed a high order velocity discretization that has a potential to provide an efficient solution of the Boltzmann equation. Our preliminary results appeared in [6, 5]. To address the lack of accuracy in the approximation of the collision integral which is a

limitation of the existing techniques it was proposed to use nodal discontinuous Galerkin (DG) discretizations in the velocity variable [17]. It was reported in [4] that high order DG velocity discretizations exhibit good conservation of mass, momentum and energy in the solutions of model kinetic equations. Additionally, it was shown in [2] that nodal-DG basis leads to a discrete velocity equations virtually equivalent to those in discrete ordinate method, which is currently the most widely implemented technique. We therefore expect that new nodal-DG discretization can be easily combined with the existing discrete ordinate solvers.

The first step in the new method is the evaluation of the Galerkin projection of the collision operator on the DG basis function $\varphi(u)$:

$$I_\varphi = \int_{R^3} \varphi(u) \int_{R^3} \int_0^{2\pi} \int_0^{b_*} (f(t,x,\xi')f(t,x,\xi_1') - f(t,x,\xi)f(t,x,\xi_1))|g|b\,db\,d\varepsilon\,d\xi_1\,d\xi\,.$$

Kogan in [21] states that evaluation of I_φ is simpler than the evaluation of the collision operator itself, because of a number of symmetric properties that hold for it. In particular, the following representation is valid:

$$I_\varphi = \int_{R^3} \int_{R^3} \frac{1}{2} \int_0^{2\pi} \int_0^{b_*} (\varphi_p^j(\xi')+\varphi_p^j(\xi_1')-\varphi_p^j(\xi)-\varphi_p^j(\xi_1)) f(t,x,\xi)f(t,x,\xi_1)|g|b\,db\,d\varepsilon\,d\xi_1\,d\xi\,.$$

The first principles that lay the foundation for the Boltzmann equation imply that the distribution function can be removed from the integrals with respect to the impact parameters:

$$I_\varphi = \int_{R^3} \int_{R^3} f(t,x,\xi)f(t,x,\xi_1)A(\xi,\xi_1;\varphi)d\xi_1\,d\xi\,. \tag{2}$$

where

$$A(\xi,\xi_1;\varphi) = \frac{|g|}{2} \int_0^{2\pi} \int_0^{b_*} (\varphi(\xi') + \varphi(\xi_1') - \varphi(\xi) - \varphi(\xi_1))b\,db\,d\varepsilon\,.$$

We notice that operator A is symmetric in ξ and ξ_1. It is independent of time and can be pre-computed. In addition, operator A inherits symmetries of the DG discretization that can be used to dramatically reduce its storage [5]. By comparing the standard expression for the collision operator (1) with the expression for its Galerkin projection (2) we notice that the new form is much simpler. Indeed, I_φ has the form of a bilinear operator with pre-computed kernel. Due to this simple form it is straightforward to develop methods based on solution linearization and decomposition [6]. We believe that the simple form of (2) can be used to quantify the numerical errors, including the uncertainty in the DG velocity models.

The nodal-DG discretization of the Boltzmann equation was implemented in Fortran. OpenMP and MPI parallelizations were used in subroutines evaluating operator $A(\xi,\xi_1;\varphi)$ and for the evaluation of (2). The MPI parallelization was successfully run on up to 320 processors. The new method was applied to the numerical solution of the problem of spatially homogeneous relaxation. In Figure 2(left) the solutions obtained by the DG-velocity method are compared to the established DCMS solutions showing excellent agreement. The conservation of mass and temperature are presented in Figure 2(right).

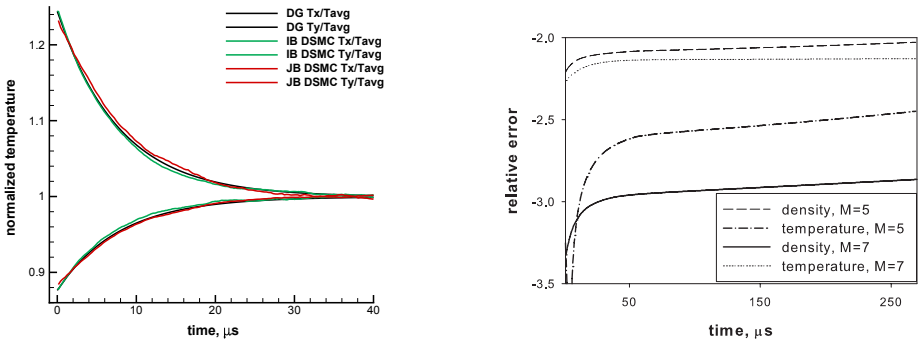

FIGURE 2. (left) Comparison of the spatially homogeneous relaxation solution to DSMC solutions (cortesy I. Boyd (IB) and J. Burt (JB). (right) Relative errors in the solution mass and temperature for different numbers of velocity cells using DG approximations by second degree polynomials.

Our next step is to extend the solver to one spatial dimension and to apply it to the solution of shock wave and heat transfer problems. A summary of future objectives is given in the concluding section.

2. DG velocity and space discretizations of model kinetic equations

In regimes of gas flows transitional from continuum to rarefied a reasonable approximation to the Boltzmann collision operator is given by a relaxation operator

$$Q(f) = \nu(f_0(t, \vec{x}, \vec{u}; f) - f(t, \vec{x}, \vec{u})),$$

where f_0 is some realizable target distribution function. The most frequently used models are the Bhatnagar-Gross-Krook (BGK), ellipsoidal-statistical (ES-BGK) and Shakhov's models. The target distributions are described by the first few integral moments of f, therefore model equations are significantly more efficient as compared to the solution of the full Boltzmann equation. One should be mindful, however, that the model equations are only appropriate for specific regimes of the gas flow. The evaluation of such regimes is an ongoing area of research, cf. [15]. However, it is a common practice to use model equation for the simulation of flows that are near continuum.

The main difficulties in simulating the model kinetic equation are high dimensionality of the solution, low order of approximations in the velocity space and the loss of conservation of mass, momentum and energy. To address these issues in collaboration with engineers in ERC, Inc., we have developed high order space and velocity DG discretizations of the BGK equation [4, 9]. Our studies have shown that high order approximations in both space and velocity are accurate, efficient and conserve mass to a high precision. We performed a unique study of convergence of solutions with respect to the velocity variable and have identified the next big obstacle for efficient simulation of gas surface interaction. We observed that in transitional zones, e.g., in the Knudsen layer the near

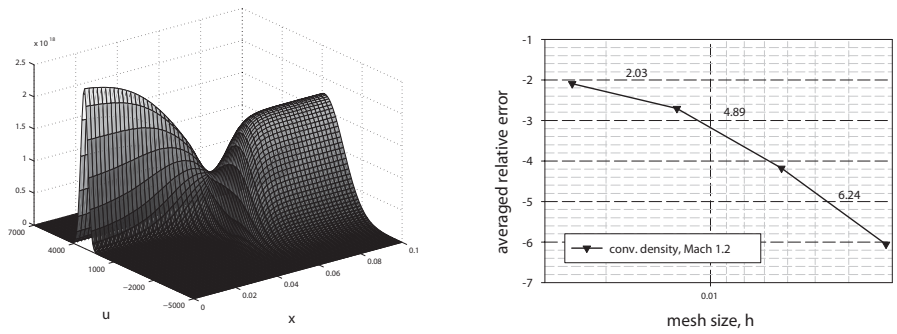

FIGURE 3. (left) 1D Mach 10 shock wave solution. (right) High order convergence of density in the shock wave problem with respect to resolution in x.

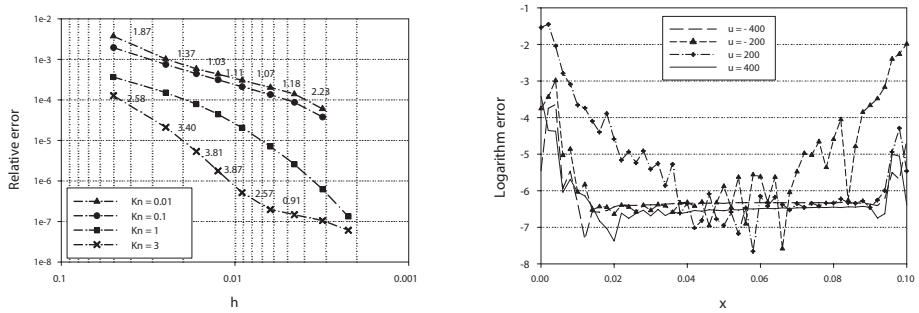

FIGURE 4. (left) Slow convergence of density with respect to x in the heat transfer problem. (right) Relative error in the velocity distribution function shown for different velocities. Slow velocities have the maximum error pollution

walls interacting with gas, the model equations become stiff. The stiffness is due to the physical effect of temperature jump and velocity slip in the rarefied gas. As the result, high order DG approximations converge only with low order, see Figure 4 [4, 9]. Presently, we use two approaches to overcome the stiffness of the equations. The first approach is the development of high order fully implicit time integrators for model equations. In 2010 I developed an ultra weak variational formulation (UWVF) for model equations. Currently, the new formulation is being implemented in Fortran. The second approach is to use local mesh refinement and local time stepping to allow the use of the explicit time integrators. The development of local time-stepping schemes for DG space and velocity discretizations of model equation is the topic of study for my student, Mr. Patrick Medina who had just received his Masters degree from CSUN. We are in the final stage of the investigation and plan to submit a paper this winter.

3. Constraint-preserving boundary conditions for artificial domain boundaries

Artificial domain boundaries are frequently introduced in wave propagation problems to avoid computations in infinite space or in regions where solution behaves in a very simple manner. As a rule, the solution is not known and can not be measured on the artificial boundary. Instead, properties of the equations and empirical knowledge about the problem are used to construct boundary conditions that will produce a reasonable approximation to the original problem. Artificial boundaries may arise in domain decomposition and multiscale applications. The most familiar examples of artificial boundaries arise in acoustics and electromagnetism. The method of Schwartz iteration and the so-called non-reflecting or transparent boundary conditions are examples of methods of handling artificial boundaries in these applications.

Handing artificial boundaries may be even more involved if the problem has differential constraints. Examples of systems with constraints are the Maxwell equations, the incompressible Navier-Stokes equations, and the Einstein equations of gravitation. Such systems are overdetermined in the sense that they contain more equations than the unknowns. Special techniques need to be designed for these systems to enforce the differential constraints. Often, the conditions imposed on the artificial boundaries become a major source of the violation of the discrete constraint equations. This issue in particular became a serious obstacle in numerical general relativity, cf. [18], where the loss of stability of the numerical solution was attributed to the violations of the constraint equations. The need to keep the constraint quantity from growing stipulated the search for the so-called constraint preserving conditions, or conditions that guarantee that the norm of the constraint quantities does not increase with time.

Many approaches has been proposed to this problem, most notable of which perhaps were [20, 22, 13, 14]. However, no general theory for the design of well posed initial boundary value problems for evolution systems with differential constraints was developed. Motivated by the lack of such theory I proposed to look at the well-posedness of equations that are related to the constrained evolution system in question via addition of a combination of constraint to the principal part that evolve the constraint equations statically. In [7] this approach was successfully applied to the model problem of vector wave equation subject to divergence free constraint. By analysing the subsidiary system that propagates the divergence constraint statically, new sets of constraint-preserving boundary conditions (CPBCs) were constructed and analysed.

To verify the robustness of the new constraint preserving boundary conditions, I have developed the Runge-Kutta Discontinuous Galerkin (RKDG) methods for the wave equation in the first order in time and second order in space form. This is the first RKDG discretization of the second order vector-equations, however discretizations of second order scalar equations are studied in [1, 16]. The boundary conditions derived in [7] were implemented in two dimensions and their performance compared to some more traditional choices. The new boundary conditions produced a stable numerical solution. Also, in the case when zero incoming modes conditions were used at the artificial boundary, the new

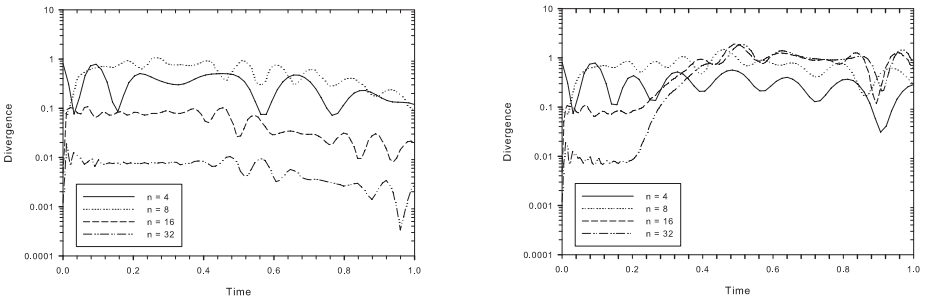

FIGURE 5. L^2 norm of the divergence for CPBCs (left) and the standard conditions (right). Spurious reflections do not converge with spatial resolution for standard boundary conditions.

conditions resulted in the smallest reflection in the constraint quantity (see Figure 5). Additionally, the stability restrictions on the time step were evaluated. The findings were consistent with the results for the scalar wave equation in [1]. More details on this study can be found in [8]

4. Research plans

The development of numerical methods for applied problems is an exciting profession. My short term plans include collaboration with engineers at Air Force Research Lab on the solution of kinetic equations of gas dynamics. The following objectives are set forward:

- Development of extremely efficient deterministic solvers for the Boltzmann equation. It is planned to extend the DG solver to one spatial dimension. This will involve a large scale MPI implementation. The approach will be generalized to mixtures of gases and gases with external degrees of freedom. The new efficient DG basis based on the multi-wavelets will be proposed and implemented.
- The numerical errors in the evaluation of Boltzmann collision operator will be studied. I am particularly interested in the development of a posteriori error estimates for approximating the collision operator. These estimates will play a key role in adaptive velocity discretizations that will be developed.
- Macroscopic models inspired by the moments methods and DG methods will be developed. Modelling error will be estimated for gas flows in near-continuum regime using both theoretical estimates and the reference solutions of Boltzmann equation
- High order methods for the solution of model kinetic equations will be developed using both explicit and implicit integration in time. Effect of the stiffness of the model equations in transitional zones will be investigated.
- Macroscopic models inspired by the moments methods and DG methods will be developed. Modelling error will be estimated for gas flows in near-continuum

regime using both theoretical estimates and the reference solutions of Boltzmann equation

Overall, the goal of this investigation is the development of highly efficient and very robust techniques for simulating gas flows

In the long term, I plan to consider the return to the problem of constraint-preserving boundary conditions and apply the technique developed in [22] to the BSSN formulation of general relativity. The high-order non-reflective boundary conditions for the wave equations will be implemented and their performance compared to other boundary conditions. In addition, I plan to work on an inverse problem in pharmokinetics. I am currently co-advising a Ph.D. student, Mr. Daulet Bakytov, in Kazakhstan on the numerical solution of inverse problem of pharmokinetics. I hope to develop a new approach to this problem in collaboration Mr. Bakytov and my Ph.D. adviser, Dr. S. Kabanikhin. I am also interested in the solution of problems with multiple temporal scales such as found in the problem of transmitting signals in neural cells.

In conclusion, I am genuinely fascinated by the developments in biology, chemistry, physics and engineering and the new challenges they bring to mathematics. Computational mathematics will continue to be the main frontier of collaboration between mathematics and other disciplines. The possibility of such collaboration and its impact makes my profession truly enjoyable!

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