Applications of Discontinuous Galerkin Methods to the Solution of Kinetic Equations

Alex Alekseenko

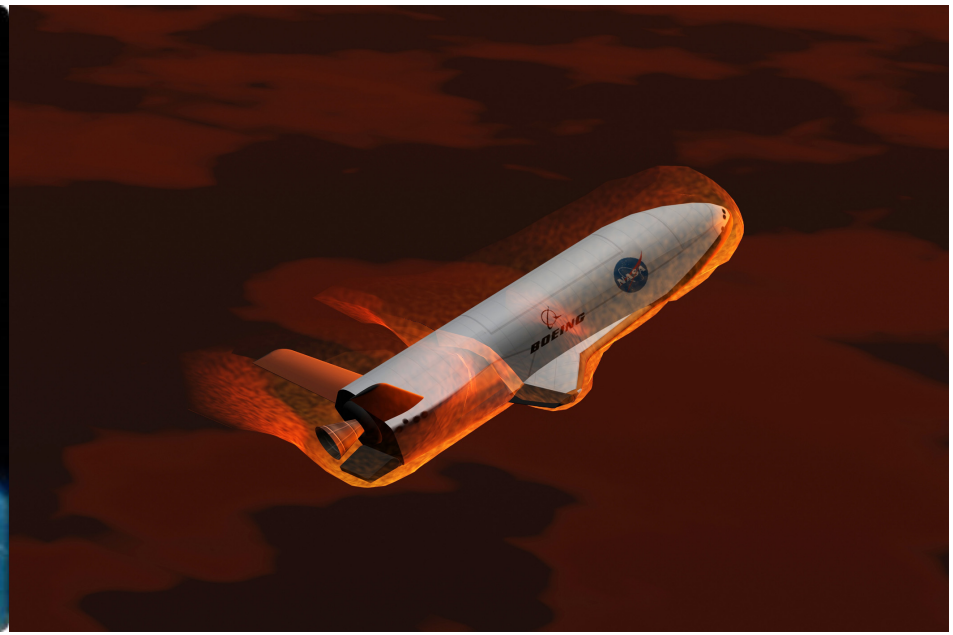
Department of Mathematics,
California State University, Northridge
on leave at AFRL at Wright-Patterson AFB

Supported by NAS RAP 2011-12, ASEE SFFP 2010

Outlook

- Applications of non-equilibrium gas flows.
- The microscopic description of gas, thermodynamic equilibrium and the Boltzmann Equation.
- The model kinetic equations.
- Discontinuous Galerkin (DG) methods
- Application of DG velocity discretization to the solution of model equations.
- Development of local time-stepping techniques for the DG discretizations.
- Development of methods for solving the Botlzmann equation based on DG methods.

Applications of Dilute Gas Flows

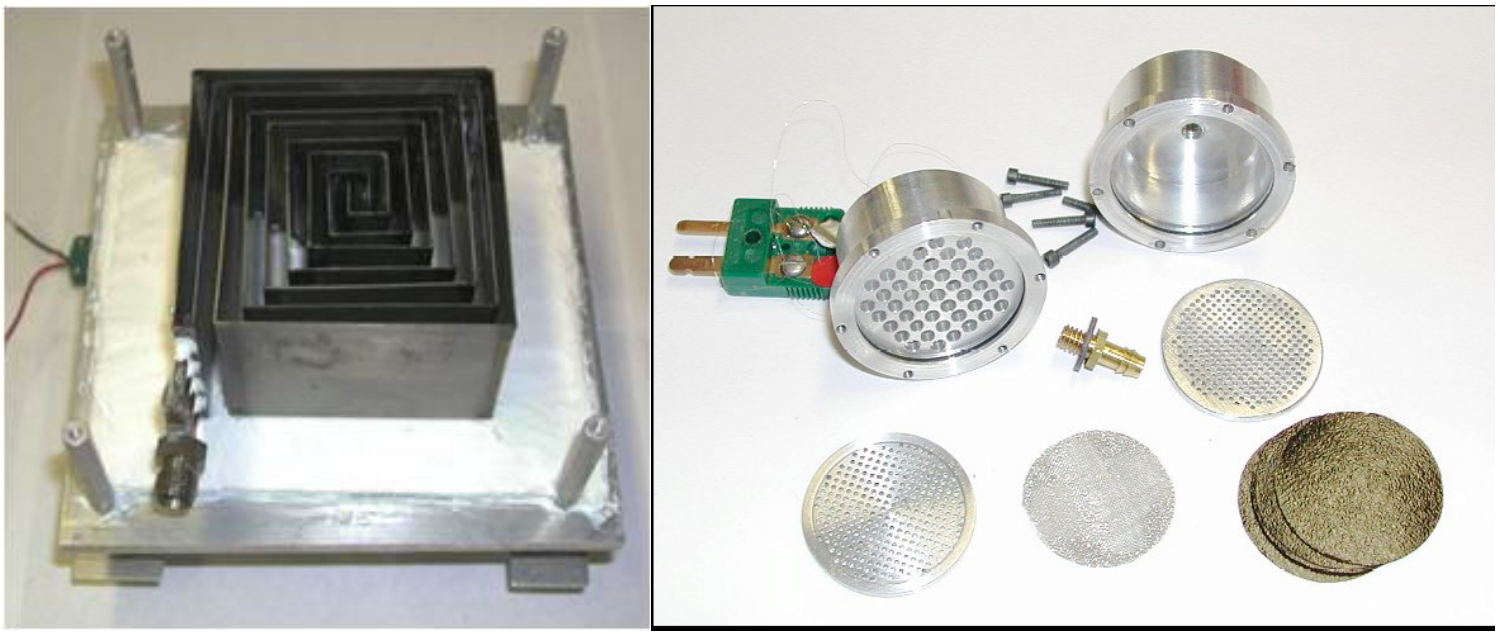


Picture credit: USAF, NASA

Applications of Dilute Gas Flows

Picture credit: NASA, JAXA

Applications of Dilute Gas Flows



Picture credit: Prof. Muntz, USC, Prof. Dunn, UCLA,

Challenges in Simulation Complex Gas Flows

Applications of high-speed high-altitude flight and flows in small channels contain regions of different flow regimes.

Regions where the flow is not in thermodynamic equilibrium (definition follows) requires kinetic description.

The solution of kinetic equations is extremely challenging, because of their high dimensionality, non-linearity, stiffness.

The Objective: Develop efficient methods for the solution of kinetic equations.

Priorities:

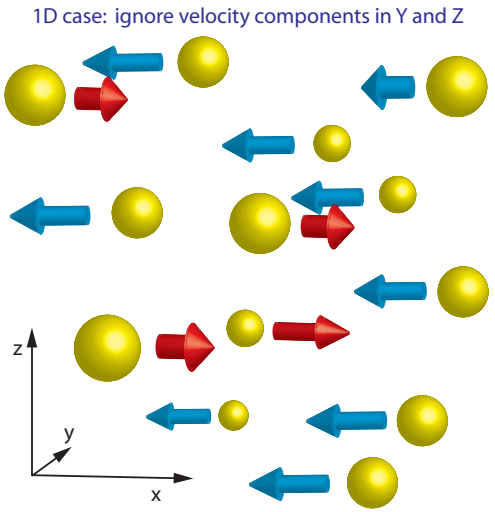
- high order, high resolution techniques.
- methods that are implicit in time.
- methods for dimensionality reduction.

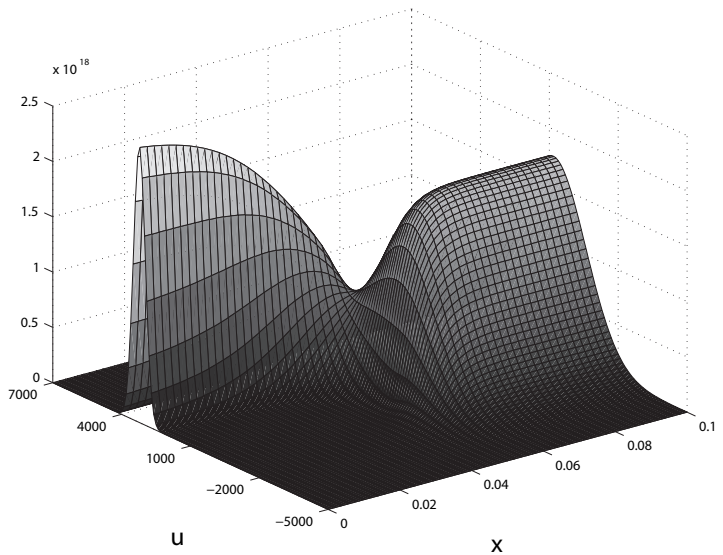
The Kinetic Description of Gas

Gas consists of particles that most of the time do not interact.

Each particle is associated with a velocity and a position.

The state of gas is described using the *molecular velocity distribution function* $f(t, \vec{x}, \vec{v})$ defined by the property that $f(t, \vec{x}, \vec{u})dxdu$ gives the number of molecules contained in a box of size $dx \times dv$ at point $(\vec{x}, \vec{u})$ of the physical space.





Macroparameters

Kinetic description is largely excessive for most of the applications. Measurable quantities of interest are usually expressed as a combination of just a few first moments of the distribution function. Here are a the first two moments:

$$n(t,\vec{x}) = \int f(t,\vec{x},\vec{v})dv \quad \text{(density)} \tag{1}$$

$$n(t,\vec{x})\vec{u}(t,\vec{x}) = \int \vec{v} f(t,\vec{x},\vec{v})dv \quad \text{(bulk velocity} \tag{2}$$

$$n(t,\vec{x})T(t,\vec{x}) = \frac{1}{3R}\int |\vec{v}-\vec{u}|^2 f(t,\vec{x},\vec{v})dv \quad \text{(temperature)} \tag{3}$$

$$n(t,\vec{x})T_{ij} = \int (v_i-u_i)(v_j-u_j) f(t,\vec{x},\vec{v})dv \quad \text{(stress tensor)} \tag{4}$$

Higher moments may be used as well in formulations.

The Thermodynamic Equilibrium

As particles collide and exchange energy, their velocities change. The gas is approaching *thermodynamic equilibrium state*. Molecular velocities of equilibrium gas are distributed according to a local Maxwellian

$$f_M(t,\vec{x},\vec{v}) = n(t,\vec{x})(2\pi RT(t,\vec{x}))^{-3/2}\exp\left(-\frac{|\vec{v}-\vec{u}(t,\vec{x})|^2}{2RT(t,\vec{x})}\right)$$

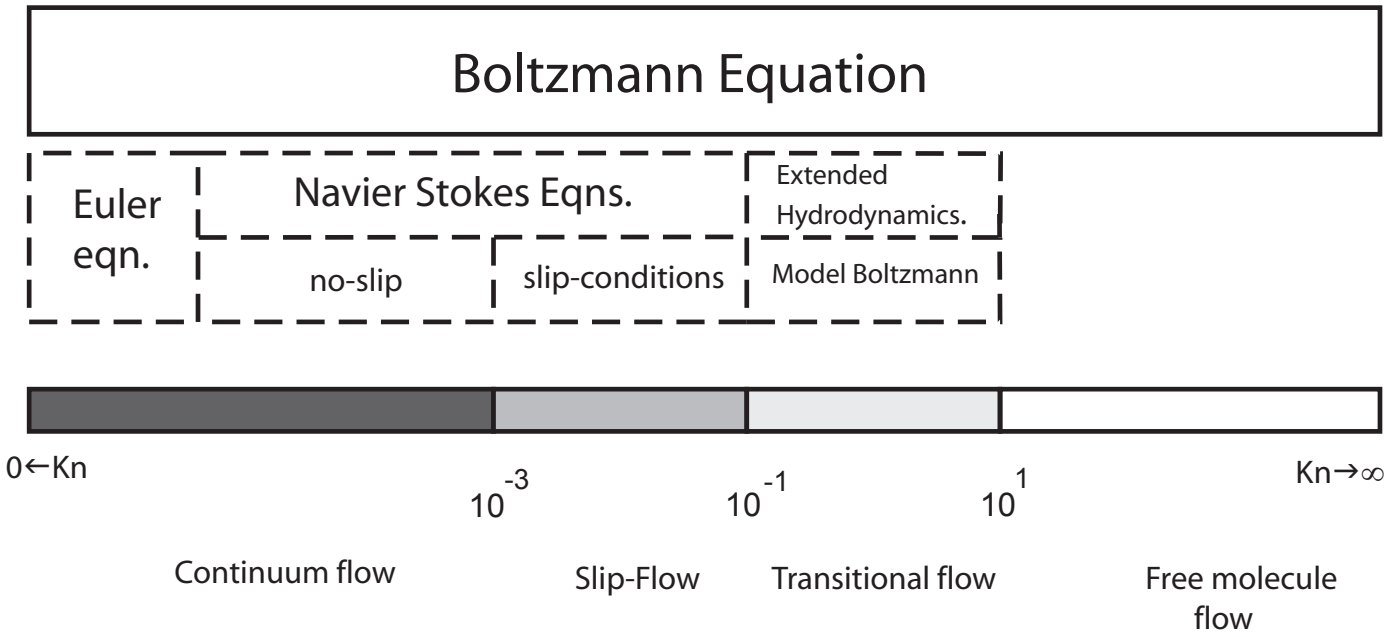
Equilibrium gas is described by just five macroparameters! We make a practical *assumption* that gas is at equilibrium if the time to reach equilibrium is small compared to the characteristic timescale of the process. In particular, we can estimate this from the gas and the process lengthscales and the gas temperature.

The Kundsen Number

Traditionally, Knudsen number is used to determine if the gas is at equilibrium.

$$\mathrm{Kn} = \frac{\lambda}{L},$$

where λ is the mean free moleculuar path and L is the characteristic lengthscale of the flow.



The Boltzmann Equation

The dynamics of gas is given the Boltzmann equation:

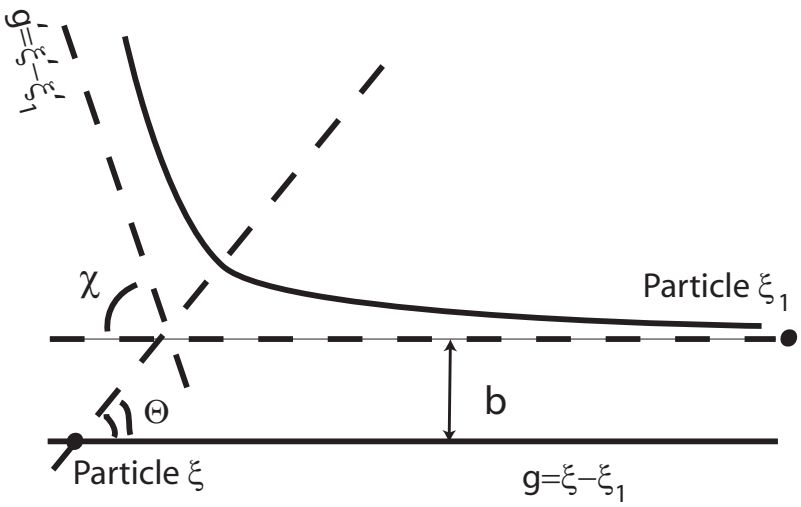
$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = Q(f, f),$$

where (no external forces, binary collisions, single species)

$$Q(f, f) = \int_{R^3} \int_0^{2\pi} \int_0^{b_0} (f' f_1' - f f_1) |g| b \, db \, d\varepsilon \, dv_1$$

Where $f = (t, \vec{x}, \vec{v})$, $f = (t, \vec{x}, \vec{v}_1)$, $f' = (t, \vec{x}, \vec{v}')$, and $\vec{v}$ and $\vec{v}_1$ are pre-collisional and $\vec{v}'$ and $\vec{v}_1'$ are post collisional velocities.

Five dimensional integration requires $O(n^5)$ operations at each point of six dimensional phase space where n is the number of D.O.F. in one dimension.



The Model Equations

In the regimes when gas flows are close to equilibrium ($.1 < \mathrm{Kn} < 10$) a good approximation to the Boltzmann equation is given bv the model equations where molecular collisions are modelled by relaxation:

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = \nu(f_0 - f(t, \vec{x}, \vec{v})),$$

where f_0 is either Maxwellian (Bhatnagar-Gross-Krook, 1954) or a gaussian (ellipsoidal-statistical BGK, Holway 1966) distribution function or some other distribution function.

ν is called the collision frequency and can be large ($\nu \approx 1/\mathrm{Kn}$).

Because model equations depend only on a few macroparameters, their evaluation requires $O(n^3)$ operations at each point of three dimensional physical space

Model equations offer computational savings in evaluation of collision of about $O(n^5)$ compared to the full Boltzmann equation. However no savings in the transport part.

Discretization in the velocity space

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = \nu(f_0 - f(t, \vec{x}, \vec{v})),$$

Discrete ordinate method. Introduce $\vec{u}_j$, $j = 1, \ldots, N$ and

$$f_j(t, \bar{x}) = f(t, \bar{x}, \bar{u}_j)$$

Enforce equations at ordinates only, replace integrals with quadratures. Solve first order (nonlinear) symmetric hyperbolic system.

Choices of ordinates: Gauss-Hermite ordinates. Richter (1973), Alexeenko etal., (2008), Uniformly spaced ordinates. Mieussens (2000), Xu (2004).
Spectral-collocation method. Use basis of Hermite polynomials on Gauss-Hermite nodes. Gobbert and Cale (2007), Hauck (2010) (Virtually equivalent to discrete ordinate.)
Challenges: unclear accuracy and loss of conservation.

Convergence Analysis

Richter (1973) considered application of discrete ordinate method to steady state Couette flow. He estimated the error of discrete ordinate approximation by the errors of quadrature formulas in evaluating moments of the solution

$$\|f - f_b\|_\infty \leq \frac{q_w(\rho_{0,n} + \rho_{-1,n})}{\mathcal{T}_{0,n}(1/\lambda)}$$

where

$$\rho_{i,n} = \int_0^{2/\lambda} |T_i(s) - \mathcal{T}_{i,n}(s)|\, ds$$

where

$$T_i(s) = \int_0^\infty t^i \exp(-(t^2 + s/t))\mathrm{d}t, \quad s > 0$$

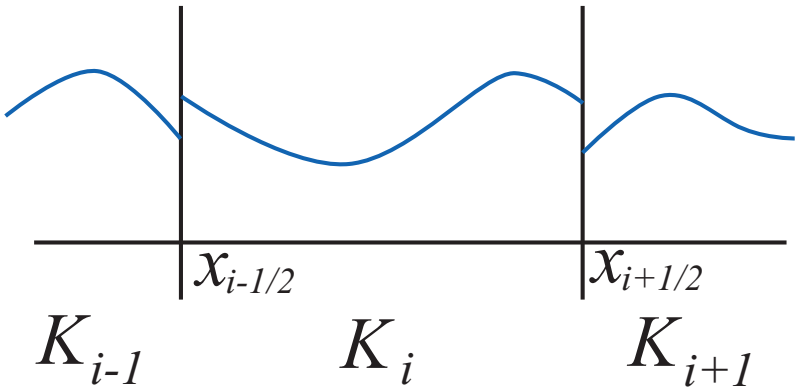
and $\mathcal{T}_{i,n}(s)$ are the corresponding quadratures

Discontinuous Galerkin Discretizations

Domain is partitioned into elements V_i, $i = 1, N$. On each V_i a finite local functional basis $\varphi_{j;i}(\vec{v})$, $j = 1, k$ is selected. Then

$$f(\vec{v})\Big|_{V_i} \approx \sum_{i=1}^{k} f_{j;i}\varphi(\vec{u})$$

Values of f on the boundaries of V_i are approximated by a *numerical flux*. Approximation of integrals of f is straightforward. Derivatives of f are approximated in a weak form using numerical flux (Cockburn, 1999).



DG Discretization in the Velocity Variable

(A., 2010) Partition the velocity space (or a bounded subset) by V_i, $i = 1, \ldots, M$. On each V_i introduce $\lambda_{l,i}(\bar{u})$ (e.g., polynomials). Seek the solution in the form

$$f(t, \bar{x}, \bar{u})|_{V_i} = \sum_l f_{l,i}(t, \bar{x}) \lambda_{l,i}(\bar{u})$$

Substitute into the BGK eqn., multiply by a basis function, integrate:

$$\mathbf{D}_i \partial_t \mathbf{f}_i(t, \vec{x}) + \partial_x \mathbf{T}_i^u \mathbf{f}_i(t, \vec{x}) + \partial_y \mathbf{T}_i^v \mathbf{f}_i(t, \vec{x}) + \partial_z \mathbf{T}_i^w \mathbf{f}_i(t, \vec{x}) = \nu \left(\int_{V_i} f_0 \lambda_{m,i} - \mathbf{D}_i \mathbf{f}_i(t, \vec{x}) \right).$$

where

$$T^u_{ml,i} = \int_{V_i} u \lambda_{l,i} \lambda_{m,i}, \quad T^v_{ml,i} = \int_{V_i} v \lambda_{l,i} \lambda_{m,i}, \quad T^w_{ml,i} = \int_{V_i} w \lambda_{l,i} \lambda_{m,i},$$

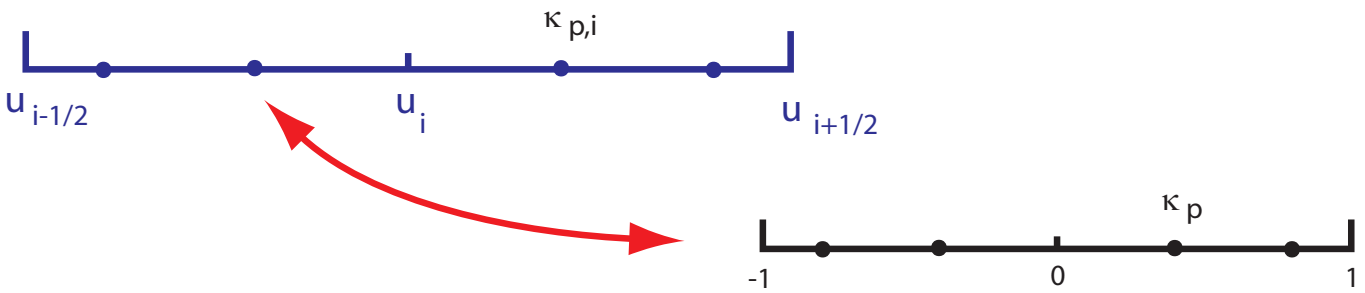
$$D_{ml,i} = \int_{V_i} \lambda_{l,i} \lambda_{m,i}.$$

Gobbert and Cale (2007) presented a global Galerkin method where $T^*_{ml,i}$ are diagonal.

Basis Functions

Efficiency of a DG method depends on sparseness of matrices $T^u_{ml,i}$, $T^v_{ml,i}$, $T^w_{ml,i}$, $D_{ml,i}$ which can be achieved by a clever match between the quadrature formulas and basis functions. Let $U_i = [u_{i-1/2}, u_{i+1/2}]$, $\Delta u_i = u_{i+1/2} - u_{i-1/2}$, $u_i = (u_{i+1/2} + u_{i-1/2})/2$. Let κ_p, $p = 1, \ldots, s$ be the nodes of Legendre's quadrature of order $2s - 1$ and

$$\kappa_{p,i} = \frac{\Delta u_i}{2}\kappa_p + u_i \quad \text{or} \quad \kappa_p = \frac{2(\kappa_{p,i} - u_i)}{\Delta u_i}$$



Basis Functions cont.

Define basis functions

$$\lambda_{p,i}(u) = \frac{(u-\kappa_{1,i})\cdot\ldots\cdot(u-\kappa_{p-1,i})(u-\kappa_{p+1,i})\cdot\ldots\cdot(u-\kappa_{s,i})}{(\kappa_{p,i}-\kappa_{1,i})\cdot\ldots\cdot(\kappa_{p,i}-\kappa_{p-1,i})(\kappa_{p,i}-\kappa_{p+1,i})\cdot\ldots\cdot(\kappa_{p,i}-\kappa_{s,i})}$$

(Approximate the solution by a Lagrange polynomial of degree $s-1$ on nodes $\kappa_{p,i}$.) Recall that

$$\lambda_{p,i}(\kappa_{q,i}) = \begin{cases} 1, & \text{if } p = q \\ 0, & \text{it } p \neq q \end{cases}$$

The basis functions are orthogonal (recall that the Gauss quadrature with s nodes is exact on polynomials of degree $2s-1$):

$$\int_{U_i} \lambda_{p,i}(u)\lambda_{p,i}(u)\,du = \sum_{r=1}^{s} w_r \lambda_{p,i}(\kappa_{r,i})\lambda_{q,i}(\kappa_{r,i}) = \begin{cases} w_p, & \text{if } p = q \\ 0, & \text{it } p \neq q \end{cases}$$

where w_r are the Gauss quadrature weights.

Basis Functions cont.

More importantly,

$$\int_{U_i} u\lambda_{p,i}(u)\lambda_{p,i}(u)\,du = \sum_{r=1}^{s} w_r\kappa_{r,i}\lambda_{p,i}(\kappa_{r,i})\lambda_{q,i}(\kappa_{r,i}) = \begin{cases} w_p\kappa_{r,i}, & \text{if } p = q \\ 0, & \text{it } p \neq q \end{cases}$$

In two dimensions and three dimensions, use

$$\lambda_{p,i}(u)\lambda_{q,j}(v) \qquad \text{and} \qquad \lambda_{p,i}(u)\lambda_{q,j}(v)\lambda_{r,l}(w)$$

Then the matrices

$$T^u_{ml,i} = \int_{V_i} u\lambda_{l,i}\lambda_{m,i}, \quad T^v_{ml,i} = \int_{V_i} v\lambda_{l,i}\lambda_{m,i}, \quad T^w_{ml,i} = \int_{V_i} w\lambda_{l,i}\lambda_{m,i},$$

$$D_{ml,i} = \int_{V_i} \lambda_{l,i}\lambda_{m,i}$$

are diagonal!

DG Discretization in the Spatial Variable

Partition the spatial domain by K_p, $p = 1, \ldots, N$. On each K_p introduce $\psi_{r,p}(\bar{u})$. Seek the solution in the form

$$f(t, \vec{x}, \vec{u})|_{K_j \times V_i} = \sum_{l=1}^{s} \sum_{p=1}^{\mu(l)} f_{l,i;p,j}(t) \varphi_{p,j}(\vec{x}) \lambda_{l,i}(\vec{u}),$$

where $\mu(l) = \min(\texttt{max\_degree} - l, k)$. After the standard steps, e.g. Cockburn 1999,

$$\partial_t \mathbf{f}_{ij}(t)\mathbf{C}_j - \hat{\mathbf{T}}_i^u \mathbf{f}_{ij}(t)\mathbf{C}_j^x - \hat{\mathbf{T}}_i^v \mathbf{f}_{ij}(t)\mathbf{C}_j^y - \hat{\mathbf{T}}_i^w \mathbf{f}_{ij}(t)\mathbf{C}_j^z + \mathcal{L}_{ij}^- \mathbf{f}_{ij^*}(t)\mathbf{C}_{j^*}^{\partial K} + \mathcal{L}_{ij}^+ \mathbf{f}_{ij}(t)\mathbf{C}_j^{\partial K}$$
$$= \int_{\partial K_j} \nu \Big(\sum_{m=1}^{s} (D_{lm,i})^{-1} \int_{V_i} f_0 \lambda_{m,i} - \mathbf{f}_i(t, \vec{x}) \Big) \varphi_{q,j}.$$

where j^* is the index corresponding to the adjacent element K_{j^*}

$$\mathbf{C}_j = C_{pq,j} = \int_{K_j} \varphi_{p,j}(\vec{x}) \varphi_{q,j}(\vec{x}), \quad \mathbf{C}_j^x = C_{pq,j}^x = \int_{K_j} \varphi_{p,j}(\vec{x}) \partial_x \varphi_{q,j}(\vec{x}), \quad \ldots$$

$$\mathbf{C}_{j^*}^{\partial K} = C_{pq,j^*}^{\partial K} = \int_{\partial K_j} \varphi_{p,j^*}(\vec{x}) \varphi_{q,j}(\vec{x}) d\sigma.$$

Runge Kutta Integration in Time

$$\partial_t f_j(t,x) = L(t, f_j(t,x));$$

Runge-Kutta schemes:

$$f_{n+1} = f_n + h\sum_{i=1}^{s} b_i K_i$$

$$K_i = L(t_n + hc_i, f_n + h\sum_{j=1}^{s-1} a_{ij} K_j)$$

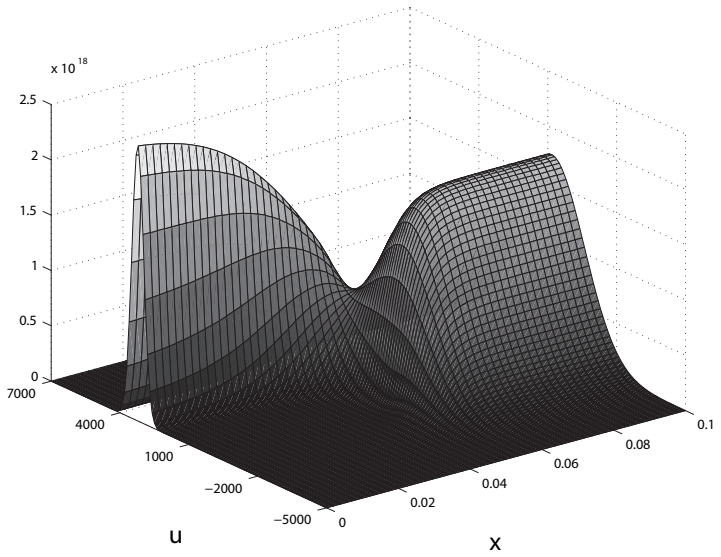
s is the degree of the method.

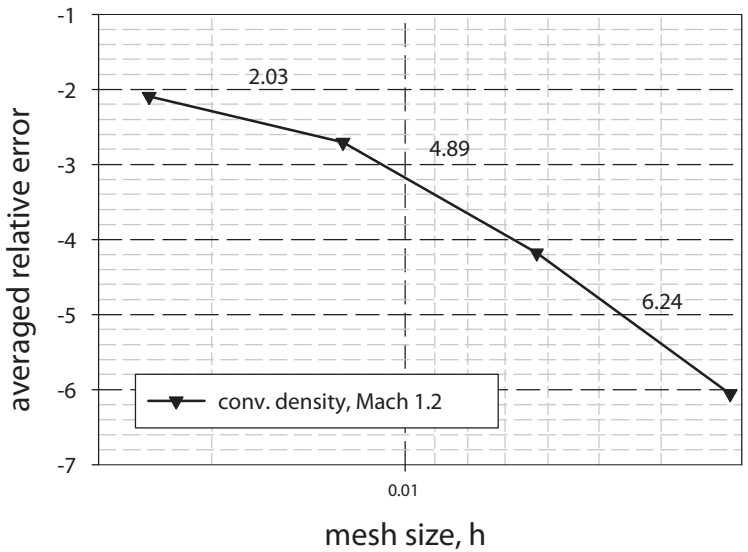
$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & & \ddots & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

The Solution to Normal Shock Wave Problem

1D Mach 10 shock wave in Argon gas. (A., 2010; A., Gimelshein and Gimelshein, 2011

The solution is obtained by fifth order Runge-Kutta method in time and a fifth order DG method in space and ninth order method in velocity.

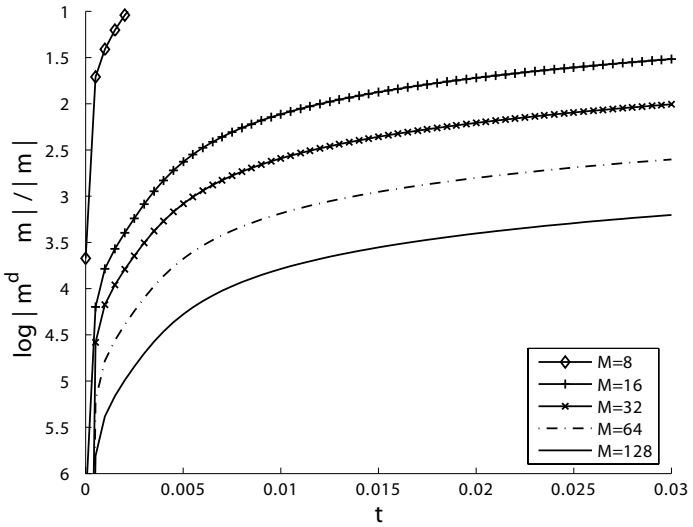




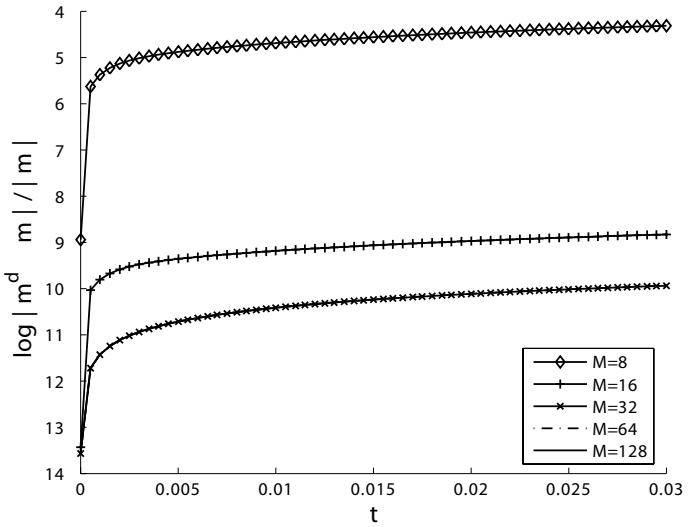
Convergence of macroparameter of density, $\int_{-\infty}^{\infty} f(t, \vec{x}, \vec{u}) du$, near the center of the wave with respect to resolution in x.

Conservation of Mass

The following plots show conservation of mass in the high order discrete velocity scheme. Notice that convergence is only second order for the 5th order scheme and high order for the 9h order scheme!



5th order in u



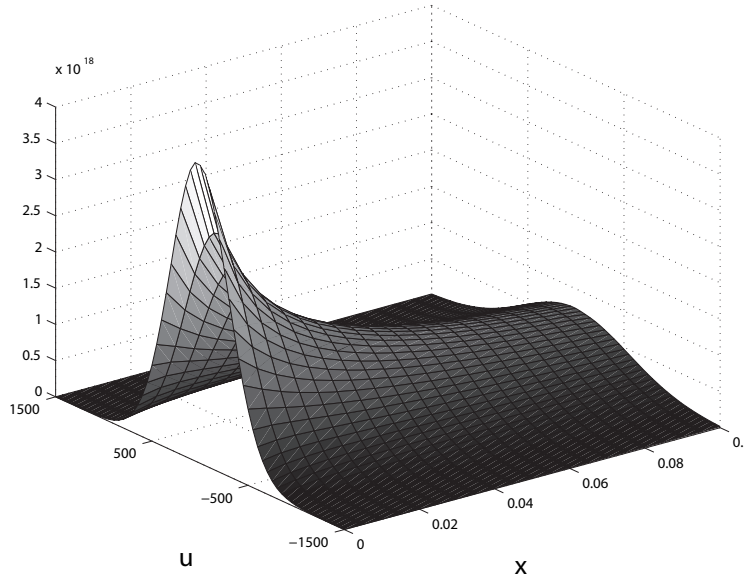
9th order in u

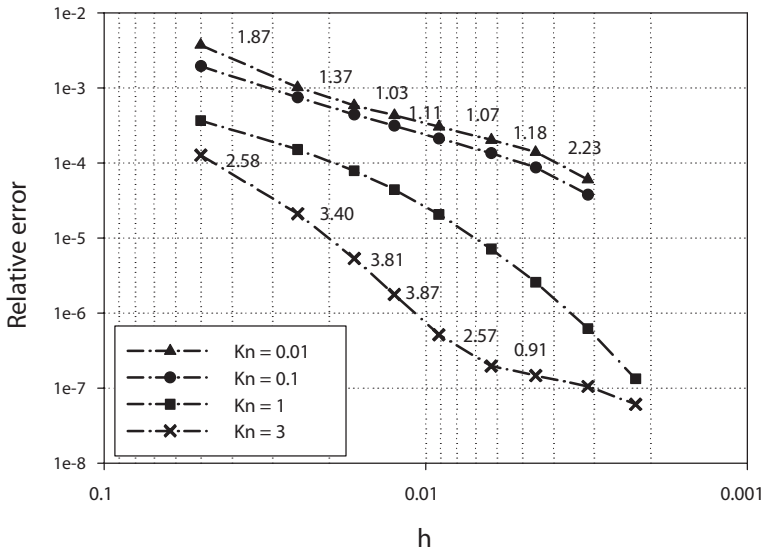
Solutions are obtained by 5th order in x scheme on 16 cells.

The Solution to Heat Transfer

1D heat transfer in Nitrogen gas.

The solution is obtained by fifth order Runge-Kutta method in time and a fifth order DG method in space and ninth order method in velocity.

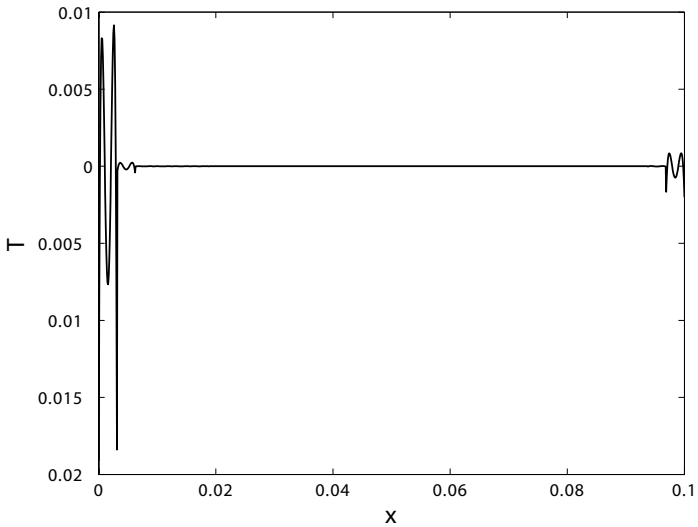




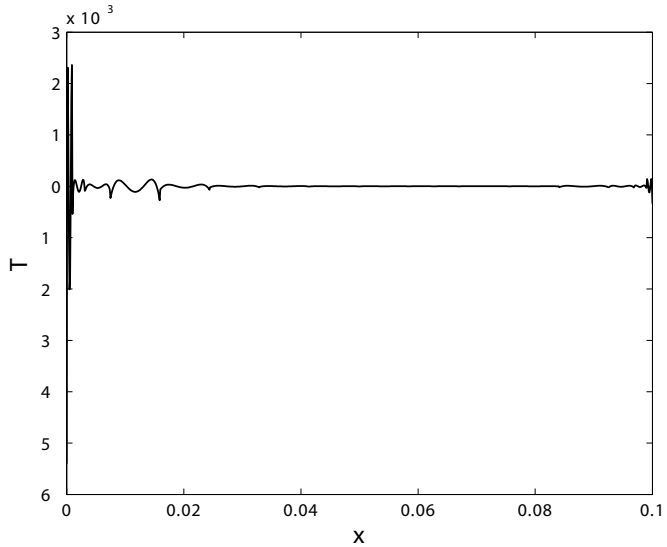
Convergence of macroparameter of density, $\int_{-\infty}^{\infty} f(t, \vec{x}, \vec{u})du$, L_2 error.

Heat Transfer Problem

1D Heat Transfer Problem for argon: Initial density $d_i = 10^{-4}$. Temperature is $T_l = 300$K on the right wall and $T_r = 1000$K. Diffusion boundary conditions.
There are spurious oscillation near walls in the bulk velocity. These however, can be treated to some extend by using non-uniform spatial grids.



Av. vel., uniform grid in x



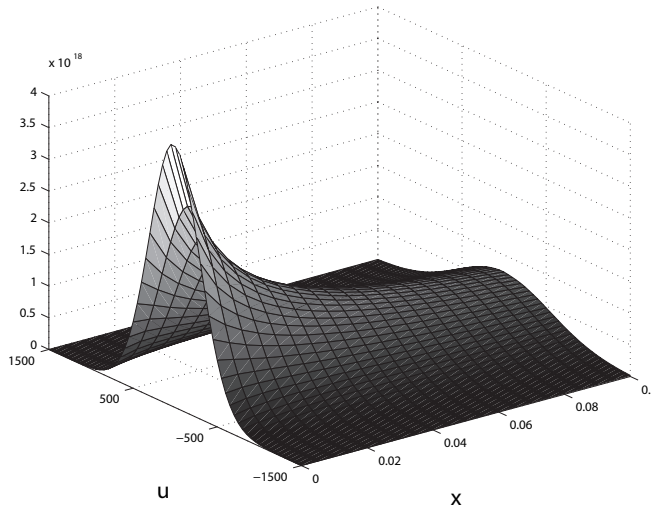
Av. vel., 1/8-1/4-1/2 grid

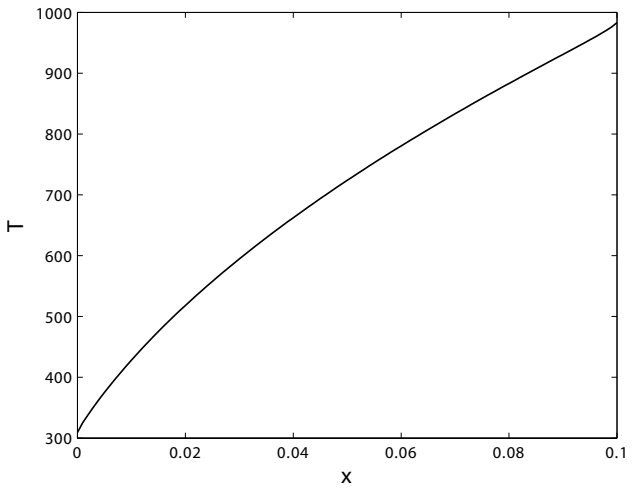
Solutions are obtained by 5th order in x on 32 cells and 9th order in u on 32 cells

Numerical Effects of Gas Surface Interaction

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{u}) + \vec{u} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{u}) = \nu(t, \vec{x})(f_0(t, \vec{x}, \vec{u}) - f(t, \vec{x}, \vec{u}))$$

In fact, the solution to the heat transfer has a tiny discontinuity in the direction of velocity variable at the wall because of the use of diffuse boundary conditions. This is indicated by the temperature jump.

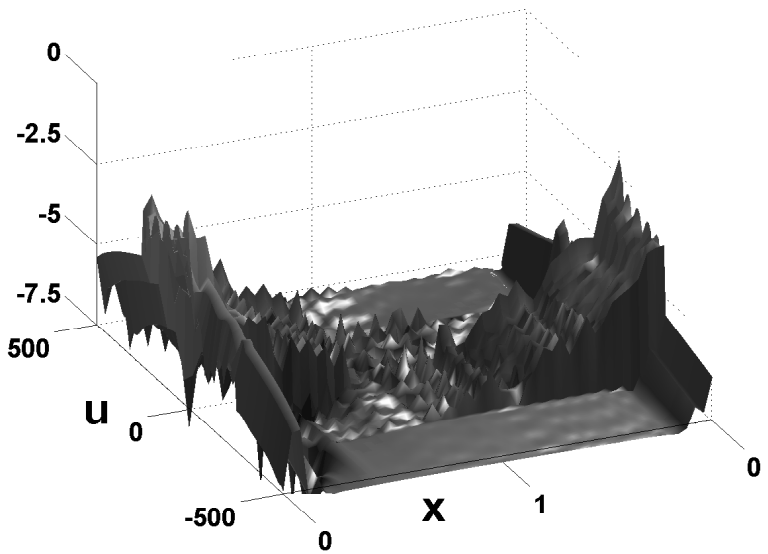


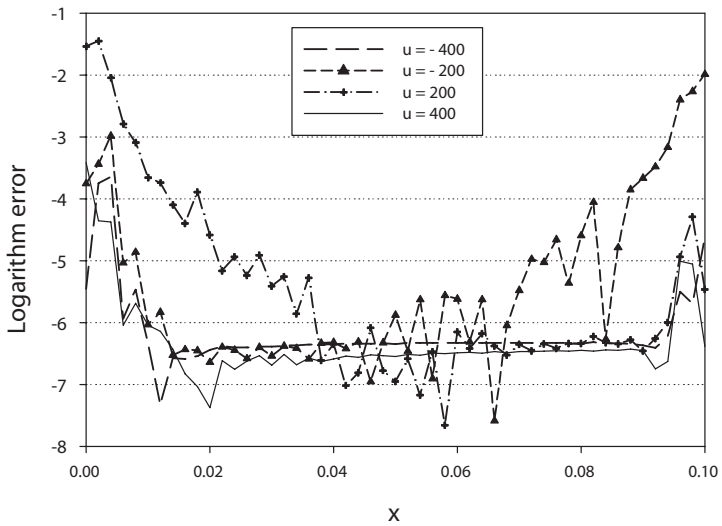


This discontinuity makes the collision term dominant near the wall and the model equation becomes stiff.

Error Pollution due to the Equation Stiffness

A comparison of solutions with different spatial resolution allows to see the sources of error.





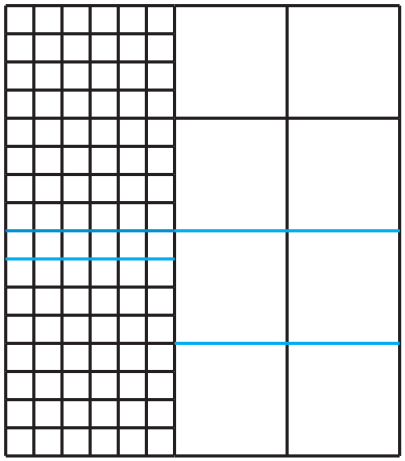
Idea 1: use mesh refinement in u near zero in combination with a mesh refinement in x. Idea 2: Use implicit time integration.

Multiple Spatial Grids and Local Timestepping

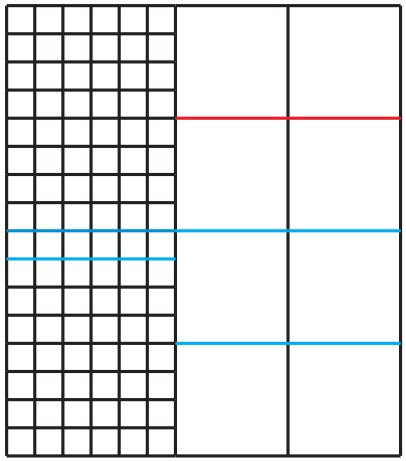
Joint work with Patrick Medina: Use local mesh refinement to overcome stiffness. However, small cells will put a restriction on the time step when explicit time integration is used.
Local time stepping (LTS): use different time step size on different grids. Grotte and Diaz, 2009, Grotte, 2010, Grotte and Teodorova, 2011.
The new Local Time Stepping DG discretization:

- hierarchical collection of meshes in x;
- use DG discretization in the spatial variable;
- use local time integration is by multiple time stepping (Adams-Bashforth, Adams-Moulton); use uniform RK time-stepping to calculate the values required in the multistep integration.
- use interpolation to advance finer meshes, make sure that course meshes advance in time first;

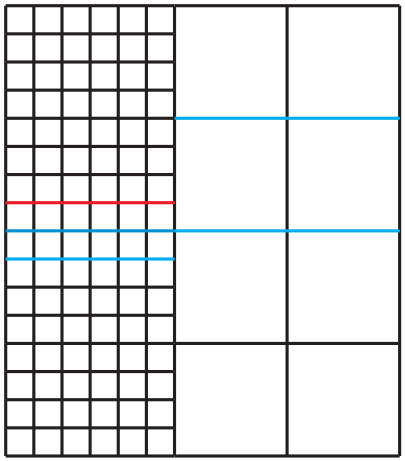
Local Time Stepping



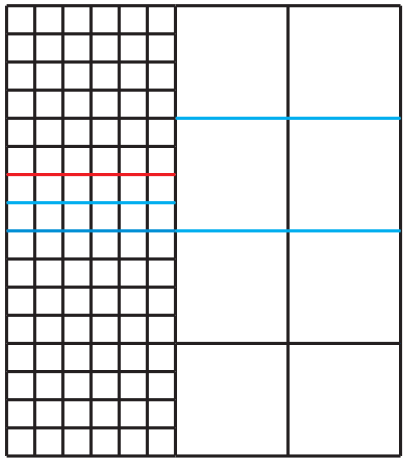
Step 0.



Step 1.



Step 3.

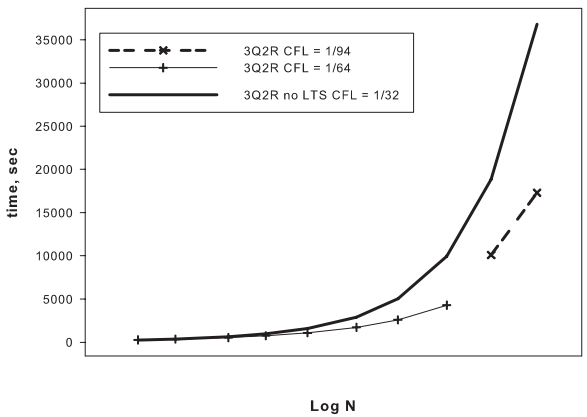


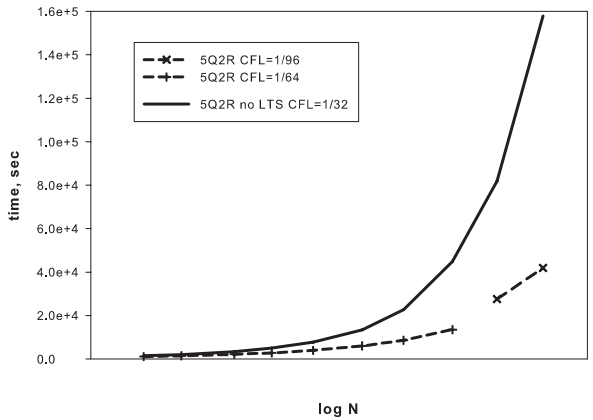
Step 4.

1D traces on the course mesh are interpolated by Hermite interpolating polynomials or splines.

Time and Convergence Improvement

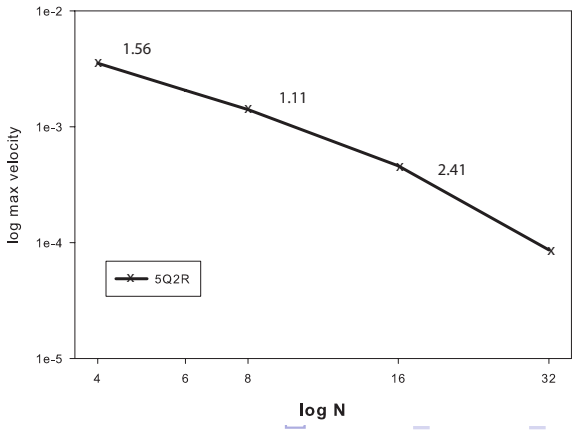
LTS has much smaller CFL stability constant ($\Delta t/\Delta x < CFL$) as compared to the uniform time stepping (UTS) method. However, the LTS techniques give overall savings of 2-3 times.





Comparison of computational time for LTS and UTS.

On a locally refined mesh spurious velocity oscillations decrease faster than a on uniform meshes



Motivation for UWVF

Implicit time integrators are known to be significantly faster for steady-state problems and have better stability properties when applied to stiff problems.

Ultra Weak Variational Formulations (UWVF) are generalizations of DG methods. Cessenat and Depress, 1998; Darrigrand and Monk, 2006, Huttunen, Monk, Collino, and Kaipio, 2004.

UWVF inherit many nice properties from DG formulations: they can handle complicated geometries, h-p refinement. They add flexibility in designing the solution and test spaces.

In UWVF, the equations are reduced to the equations on the skeleton of the mesh which in general is coupled to a system of local equations. This results in a reduced number of unknowns (but not in non-linear or case). The method is somewhat demanding on storage for test functions in hon-homogeneous or nonlinear case.

A Toy UWVF Example

Consider an application of UWVF to an ODE:

$$\partial_t f(t) = \nu(f_0(t) - f(t)), \quad t \in [0, T]$$
$$f(0) = g$$

where ν is constant and $f_0(t)$ is given. Partition the time interval in $T_k = [t_{k-1/2}, t_{k+1/2}]$. Introduce $f_k = f|_{T_k}$. DG discretization follows by multiplying the equation by a test function ρ_k integration over T_k. Integrating by parts, we obtain:

$$\int_{T_k} f_k \partial_t \rho_k dt + f_k(t_{k+1/2})\rho_k(t_{k+1/2}) - f_k(t_{k-1/2})\rho(t_{k-1/2}) = \int_{T_k} \nu(f_0 - f_k)\rho_k dt$$

We replace $f_k(t_{k-1/2})$ with $f_{k-1}(t_{k-1/2})$ to allow communication between intervals (upwind flux):

$$\int_{T_k} f_k \partial_t \rho_k dt + f_k(t_{k+1/2})\rho_k(t_{k+1/2}) - f_{k-1}(t_{k-1/2})\rho(t_{k-1/2}) = \int_{T_k} \nu(f_0 - f_k)\rho_k dt$$

A Toy UWVF: Test Functions

Consider the DG formulation with upwind flux.

$$\int_{T_k} f_k \partial_t \rho_k dt + f_k(t_{k+1/2})\rho_k(t_{k+1/2}) - f_{k-1}(t_{k-1/2})\rho(t_{k-1/2}) = \int_{T_k} \nu(f_0 - f_k)\rho_k dt$$

To derive UVWF, assume that ρ_k solve

$$\begin{aligned} \partial_t \rho(t) &= \nu \rho_k(t), \quad t \in T_k \\ \rho_k(t_{k+1/2}) &= 1. \end{aligned}$$

The DG scheme reduces to a system on the "skeleton of the mesh" with respect to the boundary data $\xi_k = f_k(t_{k+1/2})$:

$$f_k(t_{k+1/2})\rho_k(t_{k+1/2}) - f_{k-1}(t_{k-1/2})\rho(t_{k-1/2}) = \int_{T_k} \nu f_0 \rho_k dt$$

Finally, we restore $f_k(t)$ by solving

$$\begin{aligned} \partial_t f_k(t) &= \nu(f_0(t) - f_k(t)), \quad t \in T_k \\ f_k(t_{k-1/2}) &= xi_{k-1}. \end{aligned}$$

UWVF for the BGK Equation

We consider 4D rectangular partition $\Pi_{kj} = [t_{k-1/2}, t_{k+1/2}] \times R_j$ of $[0, T] \times \Omega$, where $R_j = [x_{j-1/2}, x_{j+1/2}] \times [y_{j-1/2}, y_{j+1/2}]$ $\times [z_{j-1/2}, z_{j+1/2}]$. Introduce test functions $\rho(t, x)$ on Π_{kj}.

Integrate the discrete velocity model over Π_{kj} by parts and transfer all derivatives onto ρ. Use numerical flux $\Phi(f)$ (say, upwind):

$$-\int_{\Pi_{kj}} f_p \partial_t \rho - \int_{\Pi_{kj}} f_p (\vec{\chi}_p \cdot \nabla)\rho + \int_{R_j} f_p(t_{k+1/2})\rho(t_{k+1/2}) - f_p^{ext}(t_{k+1/2})\rho(t_{k-1/2})$$
$$+ \int_{t_{k-1/2}}^{t_{k+1/2}} \int_{\partial R_j} \vec{\chi}_p \cdot \vec{n} \Phi(f_p)\rho = \int_{\Pi_{kj}} \nu(f_0(\vec{\chi}_p) - f_p)\rho$$

Require that ρ solves

$$\partial_t \rho + (\vec{\chi}_p \cdot \nabla)\rho = c(\vec{x})\rho$$
$$\rho|_{\vec{\chi}_p \cdot n > 0} = \varphi(t, x), \qquad \rho|_{t = t_{k+1/2}} = 0.$$

UWVF for the BGK Equation (cont.)

Equation on the faces of the mesh:

$$\int_{R_j} f_{kjp}(t_{k+1/2})\rho_{kj}(t_{k+1/2}) + \int_{t_{k-1/2}}^{t_{k+1/2}} \int_{\partial R_j} \vec{\chi}_p \cdot \vec{n}\Phi(f_{kjp}, \xi_{kjp})\rho_{kj}$$
$$= \int_{\Pi_{kj}} (\nu f_0(\vec{\chi}_p) - (\nu - c) f_{kj,p})\rho_{kj}$$

The local solutions f_{kjp} satisfy

$$\partial_t f_{kjp} + (\vec{\chi}_p \cdot \nabla) f_{kjp} = \nu(f_0(\vec{\chi}_p) - f_{kjp})$$
$$f_{kjp}|_{\vec{\chi}_p \cdot n > 0} = \xi_{kjp}, \qquad f_{kjp}|_{t=t_{k-1/2}} = f_{k-1,jp}(t_{k-1/2}).$$

The new unknowns are traces ξ_{kjp} and local solutions f_{kjp}.

Summary of the Algorithm

$$\int_{R_j} f_{kjp}(t_{k+1/2})\rho_{kj}(t_{k+1/2}) + \int_{t_{k-1/2}}^{t_{k+1/2}} \int_{\partial R_j} \vec{\chi}_p \cdot \vec{n}\Phi(f_{kjp}, \xi_{kjp})\rho_{kj} = \int_{\Pi_{kj}} (\dots f_{kj,p})\rho_{kj}$$

$$\partial_t f_{kjp} + (\vec{\chi}_p \cdot \nabla) f_{kjp} = \nu(f_0(\vec{\chi}_p) - f_{kjp})$$

$$f_{kjp}|_{\vec{\chi}_p \cdot n > 0} = \xi_{kjp}, \qquad f_{kjp}|_{t=t_{k-1/2}} = f_{k-1,jp}(t_{k-1/2}).$$

- choose Lagrange basis function on Guass-Lobatto nodes.
- the test functions ρ_{kj} are calculated for each basis function on the faces of the mesh.
- the equations of the faces and the local equations are solved by a split iteration.
  - set the initial approximation for $f_{kjp} = f_{k-1,jp}$ and some consistent ξ_{kjp}.
  - solve the local problems for an update f_{kjp}. Local problems are non-linear. Use Broyden update.
  - solve equation on faces explicitly for an update of traces ξ_{kjp}.

The Deterministic Solution of the Boltzmann Equation

The model equations are efficient, however, sometimes they fail to approximate the true physics. In this case, one has to solve the Botlzmann equation.

Presently, the direct statistical method Monte-Carlo simulations are the prevailing methods.

Because of the statistical noise, DSMC methods are difficult to couple to continuum solvers, e.g., Navier-Stokes solvers. Also, they are prohibitively slow for slow flows and transient flows.

Deterministic methods can be used in these cases, however their solution is still expensive. Examples: Tcheremissine 2006, Bobylev and Rjasanow 1999, Aristov 2001.

Existing deterministic techniques do not allow for high Mach number simulations and generally are limited to steady problems in one and two dimensions.

With Dr. Josyula, AFRL, we proposed a deterministic approach based on the DG velocity discretization that generalizes the approach of Tcheremissine

The DG Velocity Dicretization

Consider the Boltzmann equation:

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = Q(f, f),$$

where $Q(f, f)$ is the collision operator:

$$Q(f, f) = \int_{R^3} \int_0^{2\pi} \int_0^{b_0} (f' f_1' - f f_1) |g| b \, db \, d\varepsilon \, dv_1$$

Recall, that in DG formalism, we partition the velocity space by V_i, $i = 1, \ldots, M$ and seek the solution in the form

$$f(t, \bar{x}, \bar{u})|_{V_i} = \sum_l f_{l,i}(t, \bar{x}) \varphi_{l,i}(\bar{u})$$

We use the DG discrete velocity formulation with the Lagrange basis. The discrete transport part has the form of a diagonal symmetric hyperbolic system (many recipes are available). The challenging part is the evaluation of the collision integral.

The DG Discrete Velocity Collision Operator

Consider the projection of the collision operator to a DG basis function

$$I_\varphi = \int_{R^3} \varphi(\vec{\xi}) \int_{R^3} \int_0^{2\pi} \int_0^{b_*} (f(\vec{\xi}')f(\vec{\xi}_1') - f(\vec{\xi})f(\vec{\xi}_1))|g| b \, db \, d\varepsilon \, d\xi_1 \, d\xi$$

The following identity is valid, (e.g., Kogan 1995)

$$\begin{aligned} I_\varphi &= \int_{R^3} \int_{R^3} f(\vec{\xi})f(\vec{\xi}_1) \frac{|g|}{2} \int_0^{2\pi} \int_0^{b_*} (\varphi(\vec{\xi}') + \varphi(\vec{\xi}_1') - \varphi(\vec{\xi}) - \varphi(\vec{\xi}_1)) b \, db \, d\varepsilon \, d\xi_1 \, d \\ &= \int_{R^3} \int_{R^3} f(t, \vec{x}, \vec{\xi}) f(t, \vec{x}, \vec{\xi}_1) A(\vec{\xi}, \vec{\xi}_1; \varphi) d\xi_1 \, d\xi \end{aligned}$$

where

$$A(\vec{\xi}, \vec{\xi}_1; \varphi) = \frac{|g|}{2} \int_0^{2\pi} \int_0^{b_*} (\varphi(\vec{\xi}') + \varphi(\vec{\xi}_1') - \varphi(\vec{\xi}) - \varphi(\vec{\xi}_1)) b \, db \, d\varepsilon \,. \quad (5)$$

The operator A depends only on the velocity discretization and the collision model and is pre-computed. No interpolation of f is required.

Some Properties of the New Method.

Advantages:

- No interpolation of f;
- Operator A is pre-computed;
- The velocity discretization is high-order;
- The integration over R^6 is very sparse and is rather $O(n^3)$
- An elegant mathematical formulation. Symmetry, periodicity of A.
- Easy application of implicit techniques, UVWF.

Challenges:

- Large CPU and storage costs to evaluate A, need to use big computers;
- Still high costs to evaluate the collision integral, need to study accuracy to increase efficiency;

DG Methods for Kinetic Equations. Summary

The DG Velocity Collision Integral: Need to experiment with different basises, study the accuracy and to increase efficiency. Develop implicit methods for the Boltzmann equation. Development of a posteriory error analysis. Develop model error analysis for model equations.

Graduate students: Implementaion of UWVF, use of software packages (DIAL II, ClawPack). Experiment with different Galerkin basis. Development of efficient evaluation of A.

Undergraduate students: Interdisciplinary research team to research energy harvesting using thermal transpiration. Simulation of rarefied gas flows.

Future goal: Development of model reduction techniques. Quantification of uncertainty in solution due to the uncertainty in model and in data. Development of ultra-fast template-based solutions. Development of large scale code.

Thank you!