

PUSHING THE BOUNDARIES OF SPACE RESEARCH TO SAVE OUR FUTURE

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Numerical methods for entry flow simulations

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Outline

- Introduction
- Entry flows
- Hypersonic flows
- Numerical methods for continuum flows
- Validation
- Rarefied flows
- Numerical methods for rarefied flows
 - DSMC





"A space vehicle/object entering the atmosphere of a planet passes different flow regimes.", that is "The flow field surrounding a vehicle/object **evolves** as it descends to the surface of a planet."

• The reason for that lies in:

- the large velocity of the entering vehicle/objects (≈ 7.5 km/s for re-entry from Earth orbits and ≥ 10 km/s for planetary entries ... 30/40 and up km/s for asteroids), and
- the wide range of density and pressure with the altitude.

The large velocity of the entering vehicle/objects (\approx 7.5 km/s for reentry from Earth orbits and \geq 10 km/s for planetary entries ... 30/40 and up km/s for asteroids), means evolution from

> Hypersonic flow to Supersonic (not always ...) and finally Subsonic (not always ...)

 The wide range of density and pressure with the altitude, means evolution from

Free molecular flow

to Disturbed molecular flow (Transition regime) to Continuum flow with slip effects to **Continuum flow**



The two regimes with continuum flow, can be treated with the Navier-Stokes equations and differ only with respect to the formulation of the boundary conditions.

In the nominal case of continuum flow no-slip conditions at the wall are prescribed, whereas in the second case the **flow slips on the surface** and the temperature of the wall is different from the temperature of the gas at the wall (**temperature jump condition**).

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 The wide range of density and pressure with the altitude, means evolution from

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The two molecular regimes requires the application/solution of the Boltzmann equations describing the gas kinetic behaviour of flows. Boltzmann equations, in the context of the reentry flow problem, are usually solved by methods such as the Direct Simulation Monte-Carlo method (DSMC method)

- Definition/characterisation of hypersonic flows
- Let's start from definition/characterisation of supersonic flows:
- A flow is supersonic when the Mach number $(Ma = V_{\infty}/a)$ is >1





- Definition/characterisation of hypersonic flows
- Hypersonic aerodynamics is much different than the now conventional and experienced regime of supersonic aerodynamic.
- "Rule of thumb": hypersonic if Mach number >5
- Hypersonic flow is <u>best</u> defined as the regime where *certain physical phenomena* become progressively more important as the Mach number is increased to higher values (some phenomena may become important before reaching 5, other much after ... not crisp, but fuzzy threshold)

J. Anderson, HYPERSONIC AND HIGH TEMPERATURE GAS DYNAMICS, McGraw-Hill Book, 1989.

Definition/characterisation of hypersonic flows

Thin shock layers

The flow field between the shock wave and the body is defined as the **<u>shock</u> <u>layer</u>**, and for hypersonic speeds this shock layer can be quite thin.

Some physical complications, such as the **merging of the shock wave itself** with a thick, viscous boundary layer growing from the body surface.



FIGURE 1.13 Thin hypersonic shock tayer.

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Hypersonic Flows

Definition/characterisation of hypersonic flows

Entropy layer

Different entropy increase, then strong entropy gradients in the nose region.

This "entropy layer" flows downstream, and essentially wets the body for large distances from the nose.

The boundary layer along the surface grows inside this entropy layer, and is affected by it.



FIGURE 1.14 The entropy layer.

Definition/characterisation of hypersonic flows

Viscous interaction

Viscous dissipation: high kinetic energy is transformed (in part) into internal energy. Consider as boundary layer. The characteristics of hypersonic boundary layers are dominated by such temperature increases.

The viscosity coefficient increases with temperature, and this by itself will make the boundary layer thicker. In addition, because the pressure p is constant in the normal direction through a boundary layer, the increase in temperature T results in a decrease in density: in order to pass the required mass flow through the boundary layer at reduced density, the boundary-layer thickness must be larger.

Both of these phenomena combine to make hypersonic boundary layers grow more rapidly than at slower speeds. ("*Change of shape*")



Definition/characterisation of hypersonic flows

High temperature flows

The vibrational energy of the molecules becomes excited, and this causes the specific heats c_p and c_v to become functions of temperature. In turn, the ratio of specific heats, $\gamma = c_p/c_v$ also becomes a function of temperature.

For air. this effect becomes important above a temperature of 800 K.

As the gas temperature is further increased, chemical reactions can occur.

For an equilibrium chemically reacting gas c_p and c_v are functions of both temperature and pressure, and hence y =/(T, p).

For air at 1 atm pressure, Oxygen dissociation (O2 -> 2O) begins at about 2000 K, and the molecular oxygen is

essentially totally dissociated at 4000 K. At this temperature N2 dissociation (N2 -> 2N) begins, and is essentially totally dissociated at 9000 K. Above a temperature of 9000 K, ions arc formed (N -> N⁺ + e⁻, and O -> O⁺ + e⁻), and the gas becomes a partially ionized plasma.

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Hypersonic Flows

- Definition/characterisation of hypersonic flows
- High temperature flows

The gas temperature behind the strong shock wave can be enormous at hypersonic speeds.

- temperature in the nose region of a hypersonic vehicle can be extremely high;
- 2. The proper inclusion of chemically reacting effects is vital to the calculation of an accurate shock-layer temperature; the assumption that the ratio of specific heats γ = c_p/c_v is constant and equal to 1.4 is no longer valid.



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Hypersonic Flows

Definition/characterisation of hypersonic flows

High temperature flows

High-temperature chemically reacting flows can have an influence on <u>aerodynamic</u> <u>characteristics (lift, drag, and moments)</u> on a hypersonic vehicle/object.

For example, such effects have been found to be important to estimate the amount of body-flap deflection necessary to trim the space shuttle during high-speed re-entry.

However, by far the most dominant aspect of high temperatures in hypersonics is the resultant **high heat-transfer rates** to the surface.

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Hypersonic Flows

Definition/characterisation of hypersonic flows

High temperature flows

This aerodynamic heating takes the form of heat transfer from the hot boundary layer to the cooler surface, called **convective heating**, and denoted by q_c .

Moreover, if the shock-layer temperature is high enough, the thermal radiation emitted by the gas itself can become important, giving rise to a radiative flux to the surface called radiative heating, and denoted by q_r

- Example, for Apollo reentry, radiative heat transfer was more than 30 % of the total heating, while
- for a space probe entering the atmosphere of Jupiter, the radiative heating will be more than 95 % of the total heating.

- Although CFD can provide accurate prediction of vehicle surface pressure and temperature, it faces some challenges unique to the **high-temperature, hypersonic environment**:
 - Equations for chemical and thermal non-equilibrium must be included.
 - Definition:
 - A gas is in thermal non-equilibrium if its internal energy cannot be characterised by a single temperature, and
 - it is in chemical non-equilibrium if its chemical state does not satisfy chemical equilibrium conditions (state in which both reactants and products are present at concentrations which have no further tendency to change with time).



Chemical non-equilibrium by Damkohler number, Da, which is the ratio between the fluid motion time scale and the chemical reaction time scale:

$$Da = \frac{\tau_f}{\tau_c}$$

- When Da → ∞ the internal energy relaxation or chemical reaction time scale approaches zero and the gas is in <u>equilibrium</u>. That is its chemical state adjust immediately to changes in the flow.
- When $Da \rightarrow 0$, the reaction time scale approaches infinity, the gas is <u>frozen</u> and does not adjust to changes in the flow.

Vibration dissociation coupling

 When a gas becomes vibrationally excited, the population of the exited vibrational states increases.

Therefore, the vibrational state of a molecule affects its dissociation rate. This process is not fully understood, and simple models that can be implemented in computational methods are largely unvalidated. Even small changes in the dissociation rate can change the flow field considerably and can lead to uncertainties of integrated and local characteristics.

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Internuclear Separation

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- Finite-rate wall catalysis
- One of most important parameters that determines the convective heat transfer rate for hypersonic vehicles is the surface catalytic efficiency.



Recombination Rate Parameter

- Non-equilibrium thermal radiation
- The modelling of thermal radiation from the flow field remains a <u>major</u> <u>challenge</u>.
- For high energy flows where radiative heating is important, there may be a significant increase in the heat transfer rate due to nonequilibrium.
- This process is very difficult to model because there are many complicated rate-dependent processes competing for the thermal energy produced by the shock wave.

- Equations for viscous, turbulent and **chemical** non-equilibrium flow:
 - Navier–Stokes equations (including mass and energy conservation)
 - equations for a turbulence model, and
 - the species continuity equations.

- For **thermal** non-equilibrium:
 - the energy conservation of vibrationally excited molecules, and
 - the energy equation for electron modes

(Laminar, perfect gas, and the equilibrium gas case are each included, and can simply be extracted)

(the equations that represent chemical and thermal non-equilibrium flows contain source terms that may add stiffness to the numerical scheme used for the solution of the governing equations)

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- Discretisation of the domain and the equations (usually by Finite Volume approach)
- Set of boundary conditions





Figure 1. Standard Cartesian Volume Mesh



Figure 3. Final Mesh after 2nd Stage of Refinement

Hypersonic blunt body problem

- First practical solution by Moretti and Abbett in **1966**
- Time-marching finite-difference technique of Euler equations
- The unsteady Euler equations are hyperbolic with respect to time, no matter whether the flow is locally subsonic or supersonic.





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• What happened in last 20/25 years:

- The chemistry models reaction rates, vibration-dissociation coupling models, etc. – are still largely the same.
- Still have serious problems associated with predicting <u>the stagnation</u> point heating, particularly for very blunt capsule-like geometries.
- The computational method had to be adapted and the code completely rewritten for the parallel cache based computer architecture of current machines (clusters, GPU).
- Improvements in numerical methods are at least as important as improvements in computer hardware in increasing the degree of difficulty of present-day simulations.

• What happened in last 20/25 years:

- Grid generation remains a major problem, often consuming considerably more time than actually running a simulation (100 million element grids)
- Data management and flow <u>visualization</u> are very time consuming and can be difficult (many interesting problems are unsteady, resulting in increased run times and severe solution analysis problems).
- Not as much progress in the validation of simulations as in increasing the complexity of the calculations.









Schemes, such as upwind, for improved shock capturing.

- The advancements in <u>multigrid algorithms</u> that have significantly accelerated the convergence to steady state over a single-grid algorithm. This technology is still <u>not fully developed for the treatment</u> <u>of chemical source terms</u> but the prospects exist for considerable further enhancements to the convergence rate.
- <u>Local preconditioning</u>: algorithmic enhancement to address problems associated with convergence and truncation errors in very low velocity flows, such as the stagnation region of a blunt body.



Validation - Test facilities

- "Wind" Tunnels
 - Shock tunnels
 - Expansion tunnels
- Simulated conditions
- 3<Mach<30



- The simulation of all flight conditions in a wind tunnel is not possible. Flight Reynolds numbers and flight Mach numbers associated with high enthalpy flows are critical to simulate.
- Operation time
- << 1 sec (≈20 ms for shock tunnels,
 ≈0.2 ms for expansion tunnels)





DLR

Validation - Test facilities

Hypersonic Plasma Tunnels

Borrelli & Martucci, ISBN 978-953-307-623-2, 2011



• (CIRA) SCIROCCO Plasma Wind Tunnel (PWT)

built in 2001 in collaboration with the European Space Agency (ESA) as a special wind tunnel capable of simulating the thermal conditions of space vehicles re-entering from low Earth or interplanetary orbits (from the Moon or Mars), thereby improving flight safety in this very sensitive phase. The facility is typically focused on the development and qualification of thermal protection systems for aerospace use. Electric arc heaters are used to generate high air temperatures **up to 10,000** ° **C**. The dimensions of the test chamber, the **70MW electric arc**, the size of the jet and the level of automation make SCIROCCO the largest and most advanced plasma tunnel in the world.



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Validation - In flight tests

- In flight-measurement constitutes the only way to obtain data for prediction tools validation and calibration under real conditions
- BUT flight measurements:
 - are expensive



- require considerable time for preparation, and
- (complete) repeatability is not always possible.

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Rarefied flows

• The degree of rarefaction is defined by the Knudsen number

 $K_n = \frac{\lambda}{L}$

- λ is the molecular mean free path (average value of the path length between two collisions with other molecules)
- *L* is the characteristic length scale of the considered system



C. White, Benchmarking, Development and Applications of an Open Source DSMC Solver, PhD thesis, 2013.

DSMC method

 In the transition and free-molecular regimes non-equilibrium effects dominate and a solution to the Boltzmann equation must be sought

$$\frac{\partial\left(nf\right)}{\partial t} + \mathbf{c}\frac{\partial\left(nf\right)}{\partial \mathbf{r}} + \mathbf{F}\frac{\partial\left(nf\right)}{\partial \mathbf{c}} = J\left(f, f^*\right)$$



$$J(f, f^*) = \int_{-\infty}^{\infty} \int_{0}^{4\pi} n^2 \left(f^* f_1^* - f f_1 \right) c_r \xi d\Omega dc_1$$

 It is difficult to obtain exact analytical solutions to the Boltzmann equation due to the non-linear nature of the collision integral.

C. White, Benchmarking, Development and Applications of an Open Source DSMC Solver, PhD thesis, 2013.

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DSMC method

- Then: numerical methods to find solutions to the Boltzmann equation.
- Direct simulation methods enable the difficulties associated with the particulate nature of the gas (the collision integral of the Boltzmann equation) in analytical solutions to be used as an advantage.
- Simulation particles represent real molecules, and their positions, velocities and energies are stored and updated with time as the simulation proceeds. By far, the most successful numerical method for solving rarefied gas flows in the transition regime has been the direct simulation Monte Carlo method (DSMC)*.

*G. A. Bird. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford Science Publications, Oxford University Press Inc, New York, 1994.

C. White, Benchmarking, Development and Applications of an Open Source DSMC Solver, PhD thesis, 2013.

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DSMC method

- DSMC is a stochastic particle-based method based on the kinetic theory of diluted gases.
- **Kinetic theory** is a statistical theory of the dynamics of systems formed from a great number of individual molecules. It describes the macroscopic behaviour of a system in terms of the microscopic molecule movements and interactions, utilising probability theory. These molecule interactions are always considered as binary collisions in kinetic theory; since the gas is dilute it is very unlikely that three or more molecules will be involved in a single collision event.



C. White, Benchmarking, Development and Applications of an Open Source DSMC Solver, PhD thesis, 2013.

Background to dsmcFoam:

- OpenFOAM (Open Field Operation and Manipulation) CFD Toolbox
- Freely available and open source (GNU GPL)
- Flexible set of efficient C++ modules for solving complex fluid flows
- JWFL/CFASTT Groups at Strathclyde use OpenFOAM
- MD code developed in group
- Create new DSMC code using existing algorithms for MD initialisation and particle tracking in unstructured, arbitrary polyhedral meshes
- dsmcFoam tested successfully [1]

[1] Scanlon, et al (2010), Computers and Fluids, 39, 2078-2089.

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Why OpenFOAM ?

- C++ code flexibility, hierarchical structure, inheritance features
- Solvers, utilities and libraries fully extensible
- Modular nature allows facile new model incorporation
- Advanced error checking at compile and run times
- Robust solver and utility executables
- Can easily handle complex 3D geometries
- Unlimited parallel processing capability
- Open source + free

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dsmcFoamStrath Capabilities

- Arbitrary geometry
- Multi-species
- Vibrational energy
- Chemical reactions
- New boundary condition framework
- Low- and high-speed DSMC solutions possible
- New field measurement property framework
- Everything is easily extendible

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Skylon hypersonic concept vehicle – demonstration of powerful meshing capacity in OpenFOAM



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Comparisons of dsmcFoam predictions with the MONACO DSMC code for chemically reacting air flow over a cylinder at Ma = 25 and 82 km altitude. dsmcFoam uses the Quantum-Kinetic approach for chemistry modelling.

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Summary

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"Numerical methods for entry flow simulations" END





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