University of Strathclyde
AEROSPACE **C**ENTRE of **E**XCELLENCE

A BGK-Kinetic Formulation Including Vibrational and Electronic Energy Modes within SU2

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A little bit of background

- Rethink and further advance CFD methods for the aerothermodynamics of high-performance vehicles
- Started as a research project between UoS, Lockheed Martin's Chief Scientist Office and the UK Space Agency
- Reboot under a new perspective the modelling of high-temperature effects in SU2
- Von Karman Institute for fluid dynamics and the thermochemistry library Mutation^{++}

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Aerospace Centre of Excellence @ Strathclyde

- *10 academics looking into: Future Air-space Transportation, Space Engineering Science and Computational Intelligence*
- *The CFD guys: 2 lecturers, 2 postdocs, 3 PhDs*
- *Mantra: Open-source algorithms and reproducibility*

Outline

1. The kinetic perspective
2. Calorically vs thermally perfect gas
3. Verification & Validation test cases
4. Exploitation test case
5. The road ahead

SU2
The Open-Source CFD Code

2nd Annual SU2 Developers Meeting

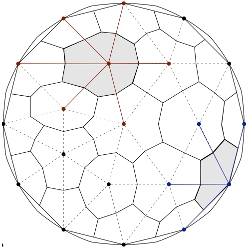
The kinetic perspective

- Attempt to obtain formulations from first principles
- Keep at minimum the adoption of heuristic relations
- Create a unified framework to address a wide range of flow physics
- Elevate the TRL of kinetic-based approaches

$$\frac{d}{dt}\int_{\mathcal{C}_i} \mathbf{w} + \sum\nolimits_{k\in\mathcal{K}_{i,\neq}} \int_{\partial\mathcal{C}_{ik}} \mathbf{j}\cdot\hat{n}_{ik} = 0$$

$$\int_{\partial\mathcal{C}_{ik}} \mathbf{j}\cdot\hat{n}_{ik} \simeq \mathbf{J}_{ik}\cdot\boldsymbol{\eta}_{ik} = R_{ik}^{-1}\mathbf{J}_{n,ik}^{R}|\boldsymbol{\eta}_{ik}|$$

with $\quad R_{ik}^{-1}\mathbf{J}_{n,ik}^{R} = \int \psi\mathbf{u}\, f(w_i, w_j)\, d\mathbf{u} d\boldsymbol{\xi}$



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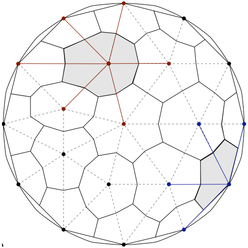


$$\frac{\partial f}{\partial t} + \mathbf{u}\cdot\nabla f = \mathcal{Q}(f_{inc.}, f_{post.}) \;\rightarrow\; \mathcal{Q}(f_{inc.}, f_{post.}) \simeq \frac{f - f_0}{\tau}$$

Calorically vs thermally perfect gas

dilute gas	T $<$ 500 K	T $\geq$ 500 K
thermally perfect (ideal) gas	$P = \rho \mathcal{R} T$	-
calorically perfect gas	$e = c_V T + e_0$	$e = \int_{T_0}^{T} c_V(T)\, dT$

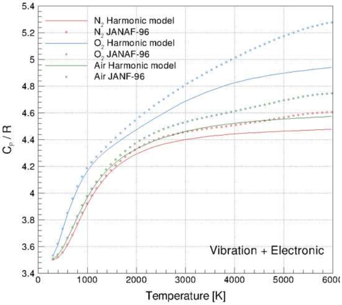
$$c_V = \frac{n}{2}\mathcal{N}k + \frac{\mathcal{N}k\left(\frac{\theta_v}{T}\right)^2 e^{\frac{\theta_v}{T}}}{\left(e^{\frac{\theta_v}{T}} - 1\right)^2} + c_V^{el.}\left(\theta_{e,i}, T, g_i\right) \quad [\mathrm{J\,/mol\,K}]$$

In the kinetic framework:

$$f_0 = f_0^{t,r}\, f_0^{vib.}\, f_0^{el.}$$

$$f_0^{vib.} = \frac{1}{Z^v}\sum_{j=1}^{\infty}\delta(\xi_v - \xi_v^j)e^{-\frac{m(\xi_v^j)^2}{2kT}}$$

$$f_0^{el.} = \frac{1}{Z^e}\mathcal{F}\left(\xi_e, T, g_i\right)$$



Scheme-to-scheme "verification"

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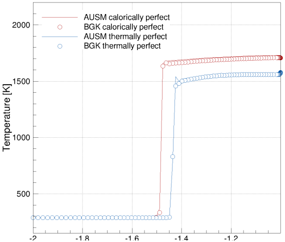
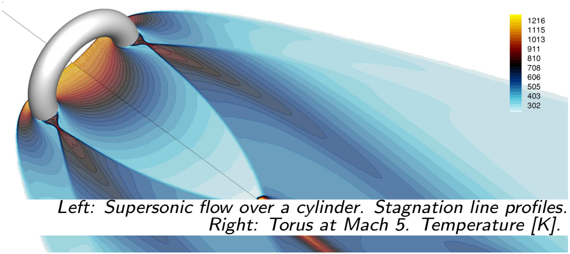
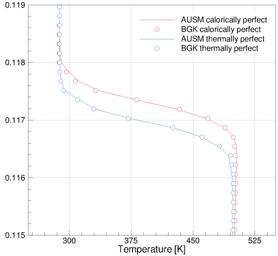
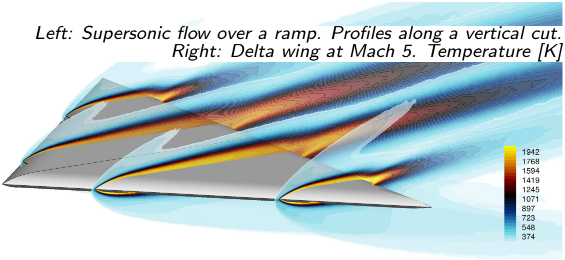




Left: Supersonic flow over a cylinder. Stagnation line profiles.
Right: Torus at Mach 5. Temperature [K].

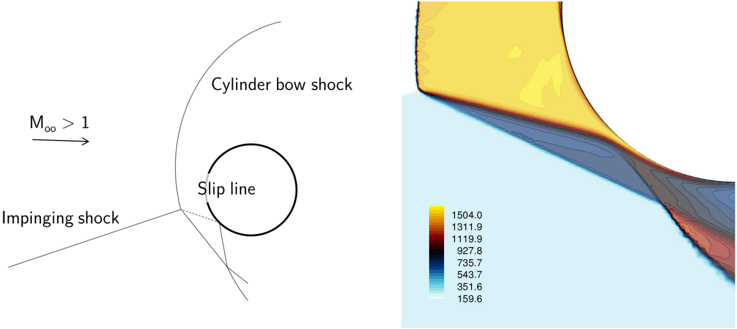


Left: Supersonic flow over a ramp. Profiles along a vertical cut.
Right: Delta wing at Mach 5. Temperature [K]



Edney type III interference over a cylinder

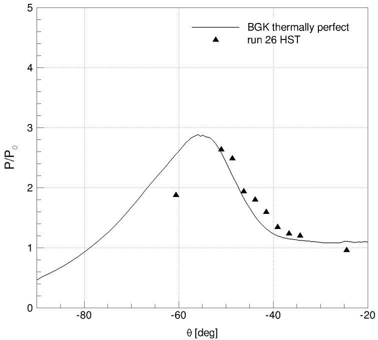
Mach	8.03	Re_R	257,498.85
T_∞ [K]	111.56	T_{wall} [K]	294.44
Elements	96,911	Nodes	69,079



Left: Schematic of type III interference pattern. Right: Temperature contours [K].

Edney type III interference over a cylinder

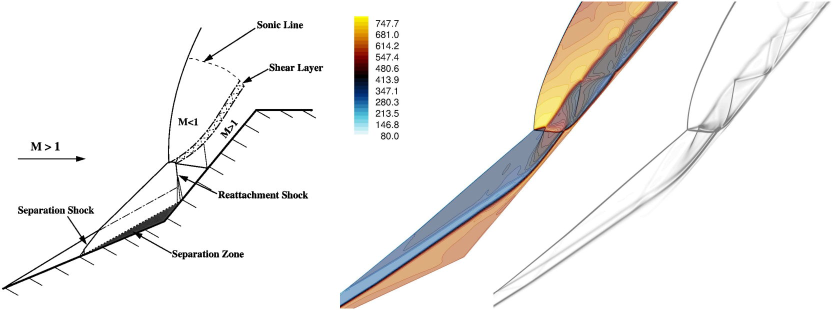
Pressure and heat flux amplification along the surface w.r.t. the undisturbed case (P_0 and q_0), i.e. with no impinging oblique shock



A.R. Weiting, M.S. Holden, "Experimental Study of Shock Wave Interference Heating on a Cylindrical Leading Edge", **NASA TM 100484**, *1987.*

Edney type V interference over a 25^o-50^o cone

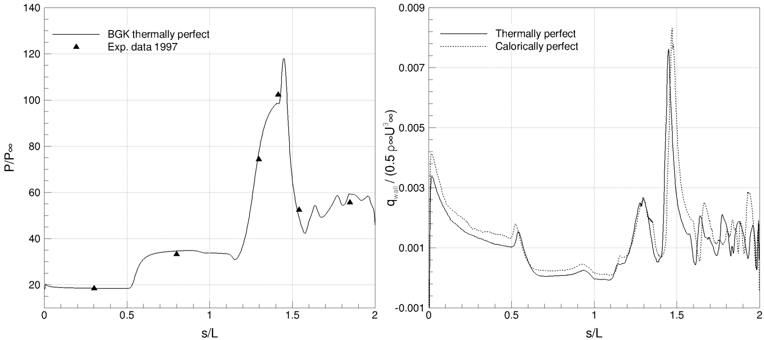
Mach	8	Re_D	2.7×10^5
T_∞ [K]	57	T_{wall} [K]	300
Elements	426,478	Nodes	428,050



Left: Schematic of type V interference pattern. Centre: Temperature contours [K]. Right: Numerical Schlieren. Contours refer to a close-up view in the corner region

Edney type V interference over a 25°-50° cone

	Calorically perfect	Thermally perfect	Δ
Integrated heat flux [W/m]	700.886	640.717	8.5%

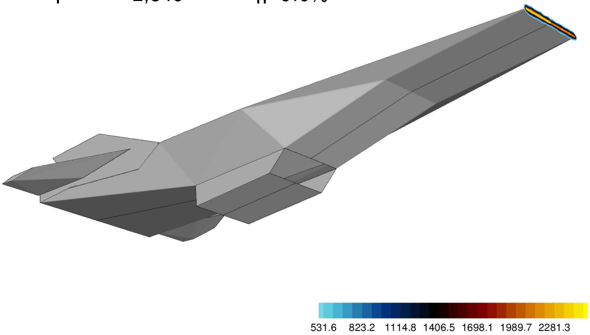


M.J. Wright, J. Olejniczak, G.V. Candler, T.D. Magruder, A.J. Smith, "Numerical and Experimental Investigation of Double-Cone Shock Interactions", **AIAA paper 97-0063**, *1997.*

Exploitation case: X43-like vehicle

Mach	7	Re_L	988,728
T_∞ [K]	239.85	h_{wall} [W/m^2]	0
Elements	10,653,216	Nodes	1,851,041

	Calorically perfect	Thermally perfect	Δ
T_0 [K]	2,590	2,340	9.6%



Temperature contours [K]. Calorically perfect (top-left), Thermally perfect (bottom-right).

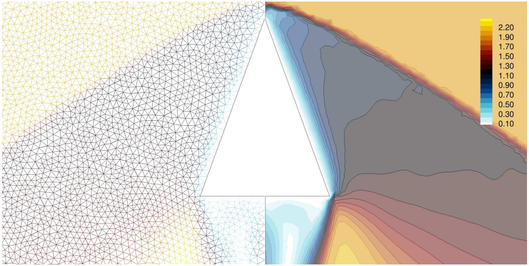
It's a long way to the top ....

1. **Multiphysics**†
   1.1 Multiple temperatures a.k.a thermal nonequilibrium
   1.2 Multi-species (frozen vs. finite-rate)
   1.3 Turbulence-Chemistry-Interaction via Eddy Dissipation Model

† *Starting with FV and progressively moving to higher-order*

2. **Adapt-by-remesh**‡
   2.1 Anisotropy
   2.2 hp-adaptivity

‡ *Integration with Gmsh*



Mach number. Anisotropic remeshing using $\mathcal{H}$(Mach) as a basis for the metric tensor.

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