Computational Fluid Dynamics Algorithms. Some Achievements and Challenges towards Multidisciplinary Application

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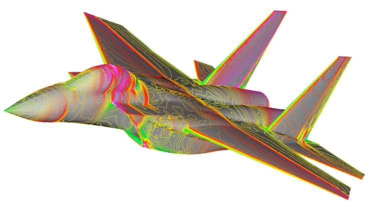
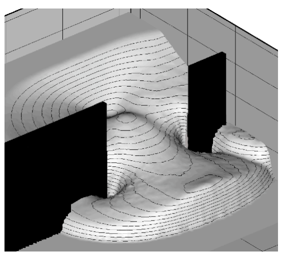
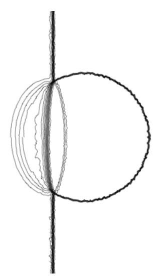
Contents

- some challenges for CFD algorithm developers

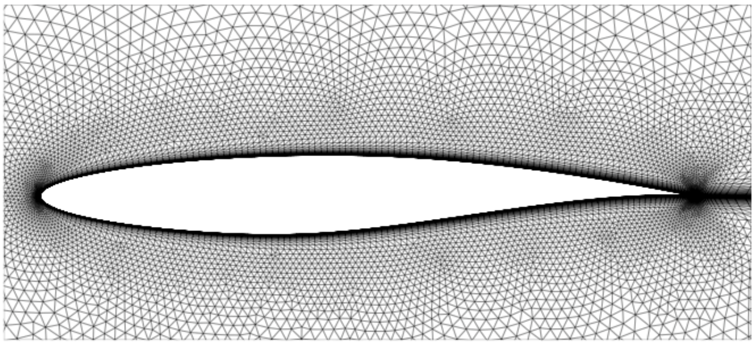
- component based CFD architecture
- a class of schemes for tetrahedral grids
- applications in hypersonic reacting flow

Modern Computational Fluid Dynamics:
Solving conservation laws dominated by
convection and nonlinear wave propagation:
flow, mass transfer, heat transfer

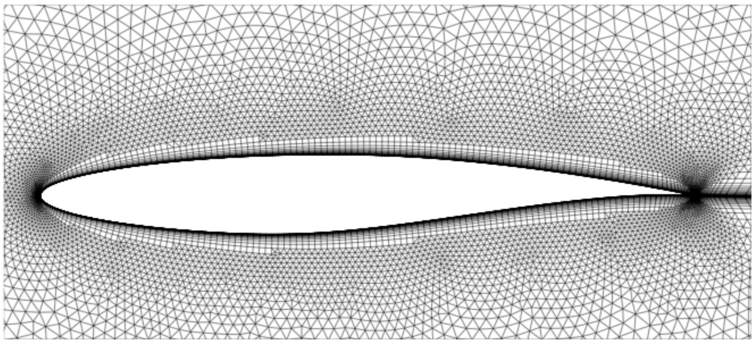
- Strong anisotropies at high Reynolds/Peclet/Schmidt nr:
  Diffusion effects in thin boundary layers and shear layers
- Strong nonlinearities: compressibility, shocks
- Complex geometries, CAD: engines, high lift systems,
  industrial processes
- Highly interdisciplinary: reacting flows, fluid-structure,
  conjugate heat transfer, aeroacoustics …

RAE 2822 case 9: $M_\infty = 0.73$, $\alpha = 2.79°$, $Re_c = 6.5 \times 10^6$



VKI THOR code:

Triangular grid, 33892 nodes



DLR Tau code:

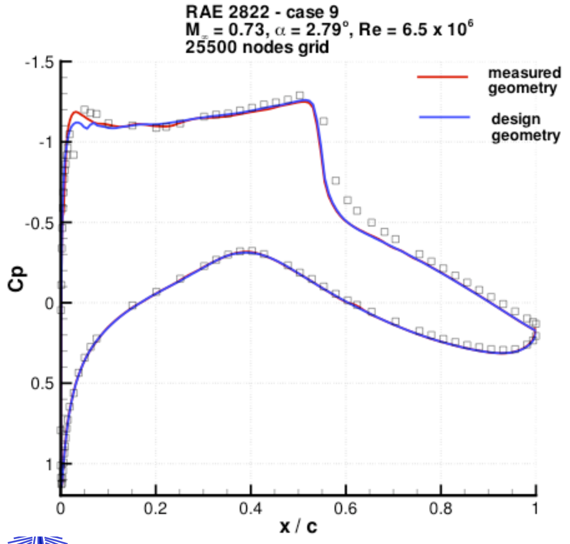
Hybrid grid, 33892 nodes

RAE 2822 case 9: $M_\infty = 0.73$, $\alpha = 2.79°$, $Re_c = 6.5 \times 10^6$

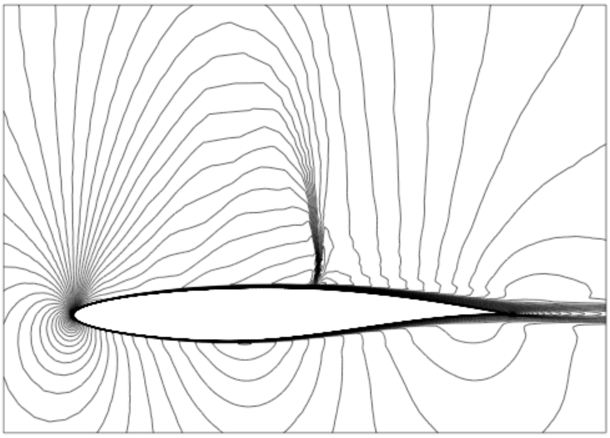
THOR MDHR scheme , S-A turbulence model

Design versus Measured Geometry

Pressure coefficient



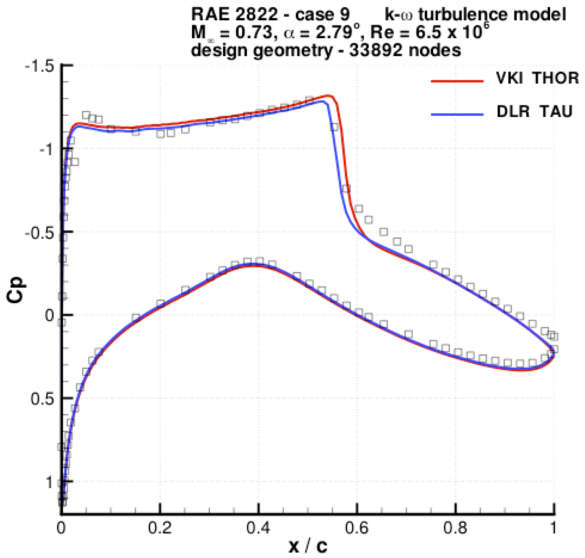
Mach number on measured geometry



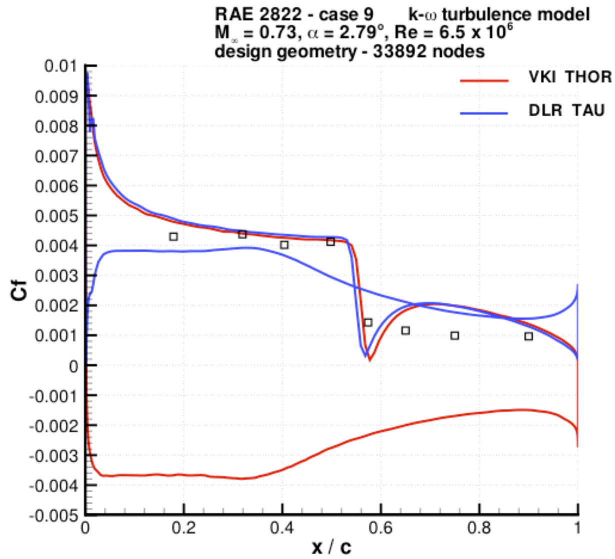
RAE 2822 case 9: $M_\infty = 0.73$, $\alpha = 2.79°$, $Re_c = 6.5 \times 10^6$

k-ω turbulence model - MDHR versus AUSM-DV

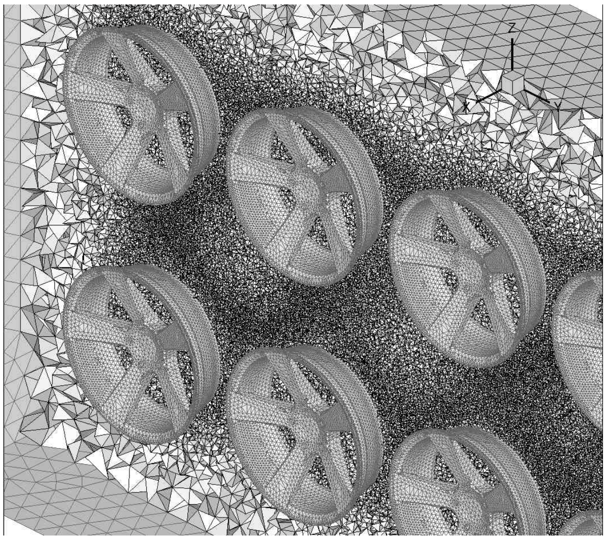
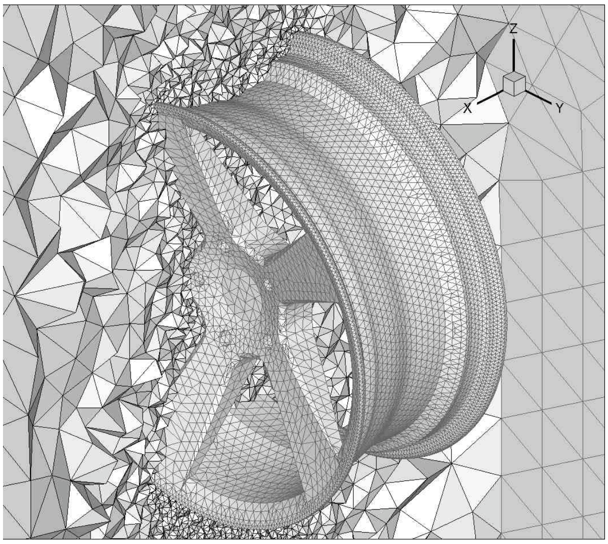
Pressure



Skin friction

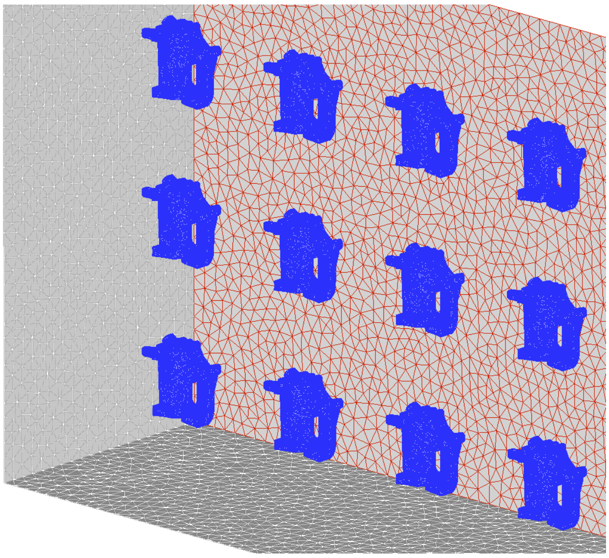
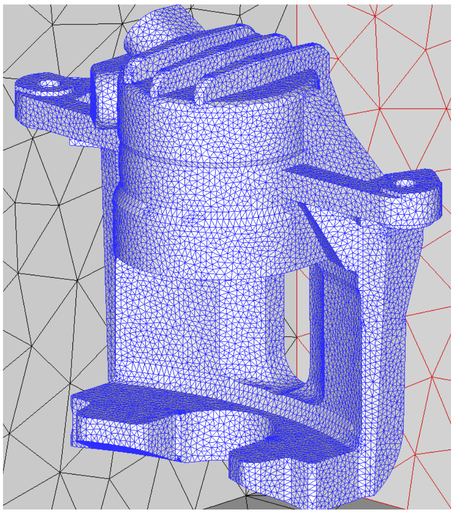


Complex geometries of industrial relevance

Chrome plating of wheels

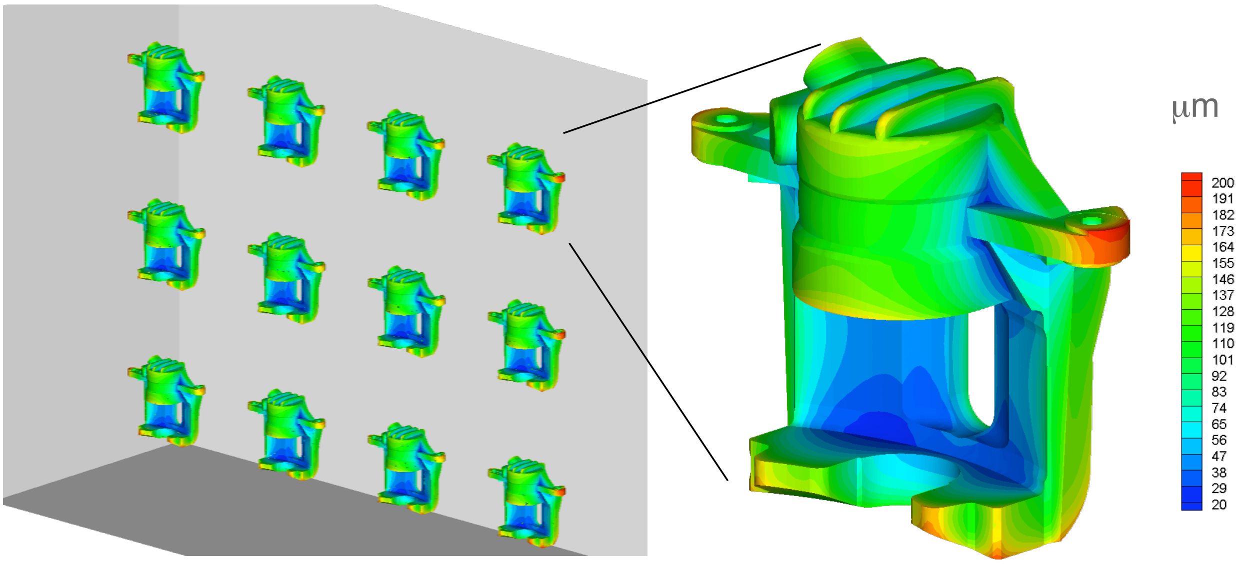
Complex geometries of industrial relevance

- 478 934 face elements
- 970 267 nodes
- 5 266 106 tetrahedra

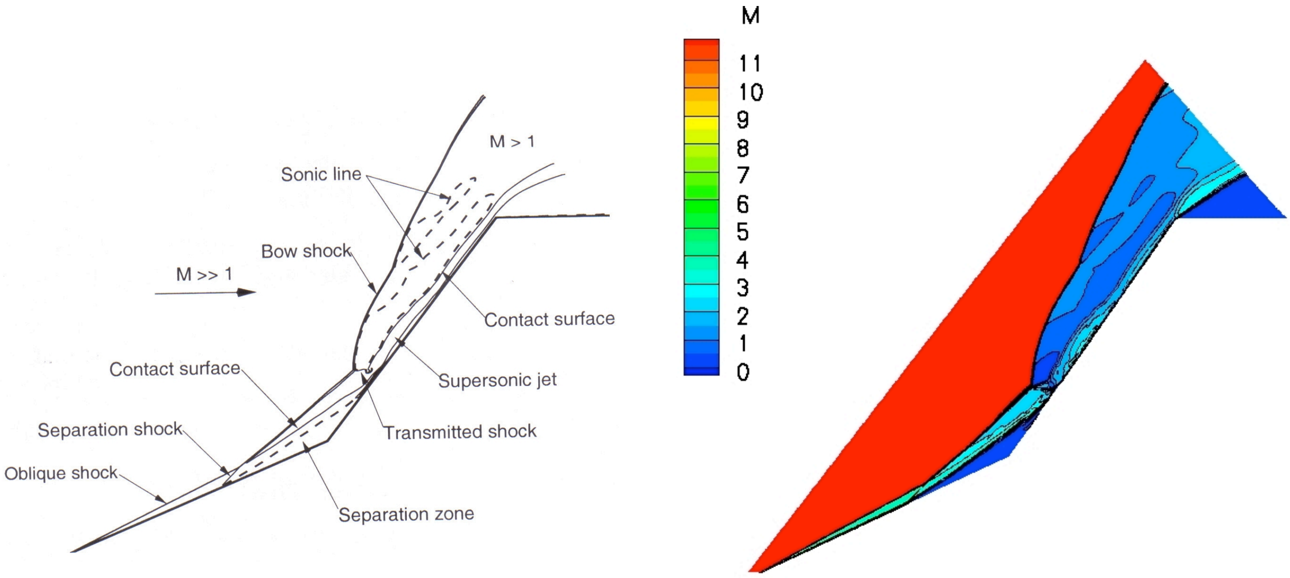
Complex geometries of industrial relevance

Layer thickness distribution



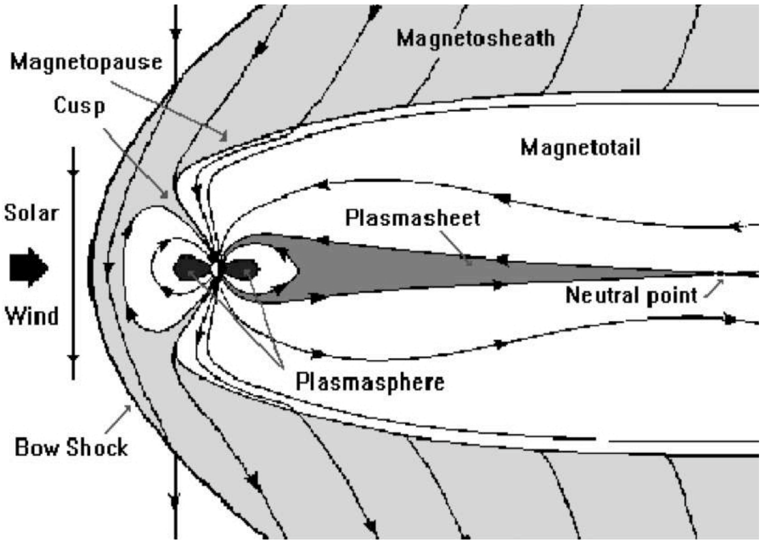
Chrome thickness layer distribution

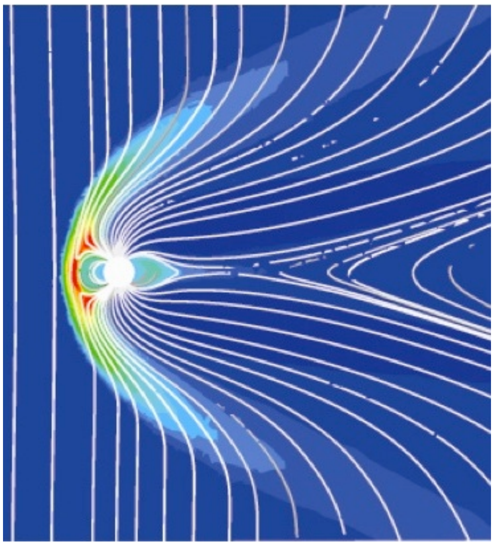
Complex physical modeling: reacting flow



Hypersonic reacting flow at Mach11, Air 5 species

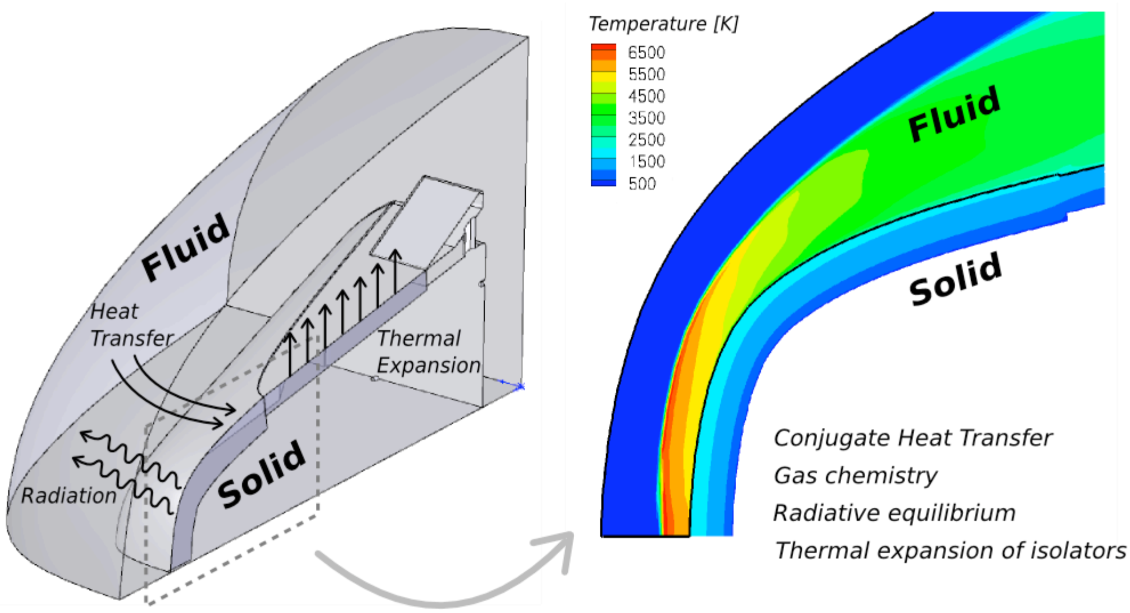
Complex physical modeling: MHD





Space weather, ideal MHD equations

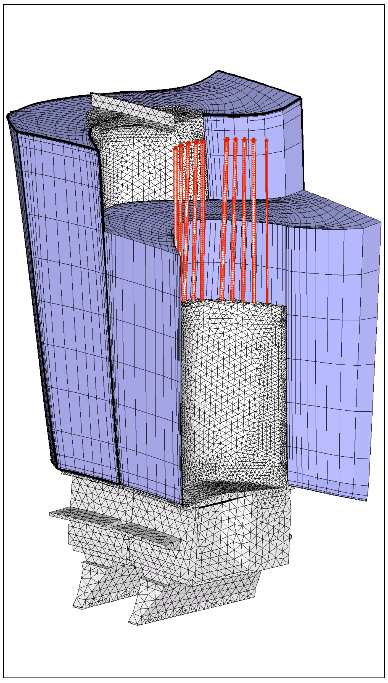
Interdisciplinary coupling: Conjugate heat transfer



Key challenges for CFD algorithms developers:

- high accuracy on non-smooth unstructured meshes:
  higher order schemes have a great future
- highly parallel: also for academic groups: multicore processors
- robustness on bad grids, implies monotone discontinuity capturing, adaptive meshes, error estimation
- grid generation for high Reynolds (Peclet –Schmidt) numbers
  cope with the anisotropies in the flow for complex CAD
- Interdisciplinary coupling, multi-physics requiring different discretizations and grids in one problem

Interdisciplinary coupling: Conjugate heat transfer

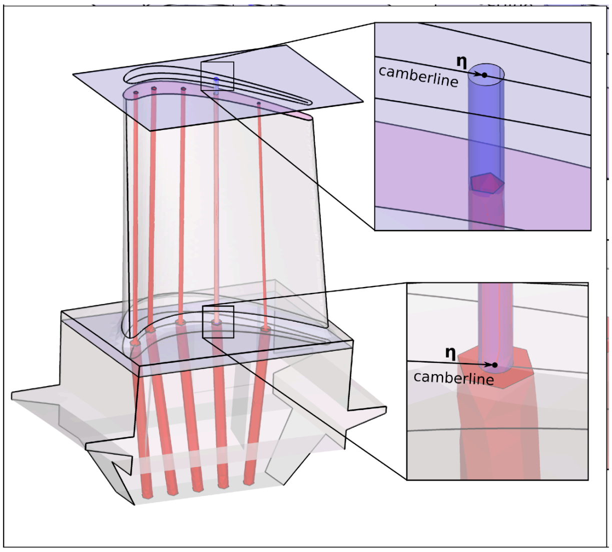


Analysis code:

Three interdisciplinary coupled domains:

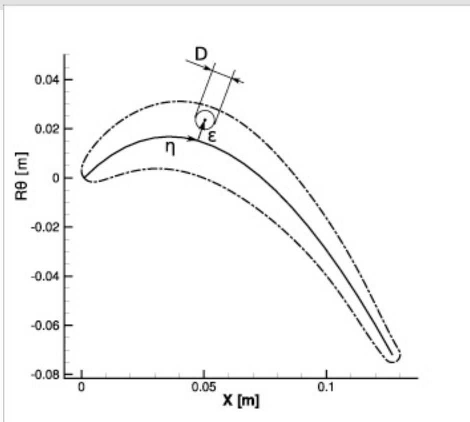
- Fluid: NS - FV
- Solid: heat conduction, thermal stresses using FEM
- Cooling channels: 1D hydraulic model with friction coefficient

Optimisation: cooling of turbine blade



Optimization case study:

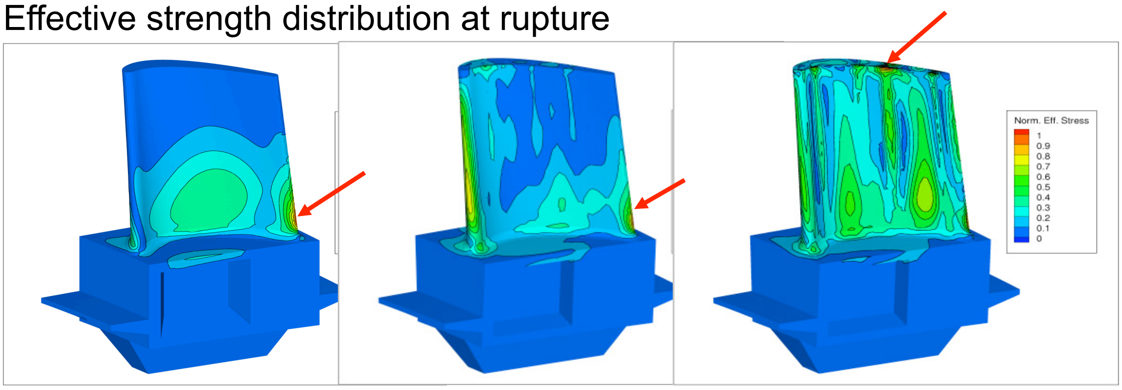
5 cooling channels,
3 parameters per channel



Optimisation of conjugate heat transfer

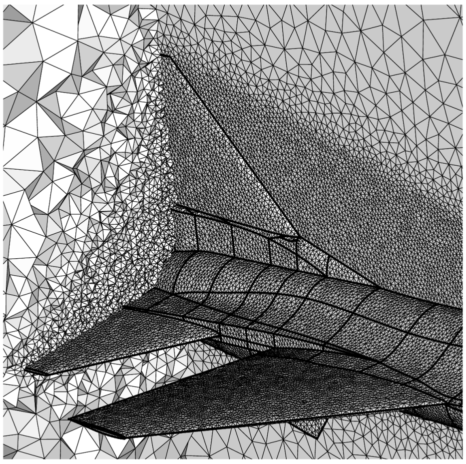
Optimise cooling for maximum life time
(not equidistribution of temperature!)

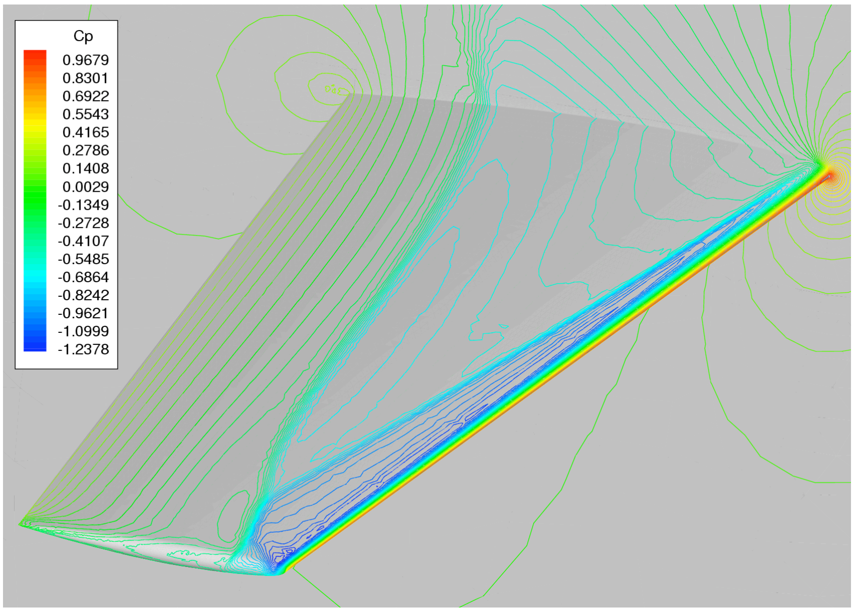
Effective strength distribution at rupture



uncooled 161 h | baseline 220 h | optimized 6872 h

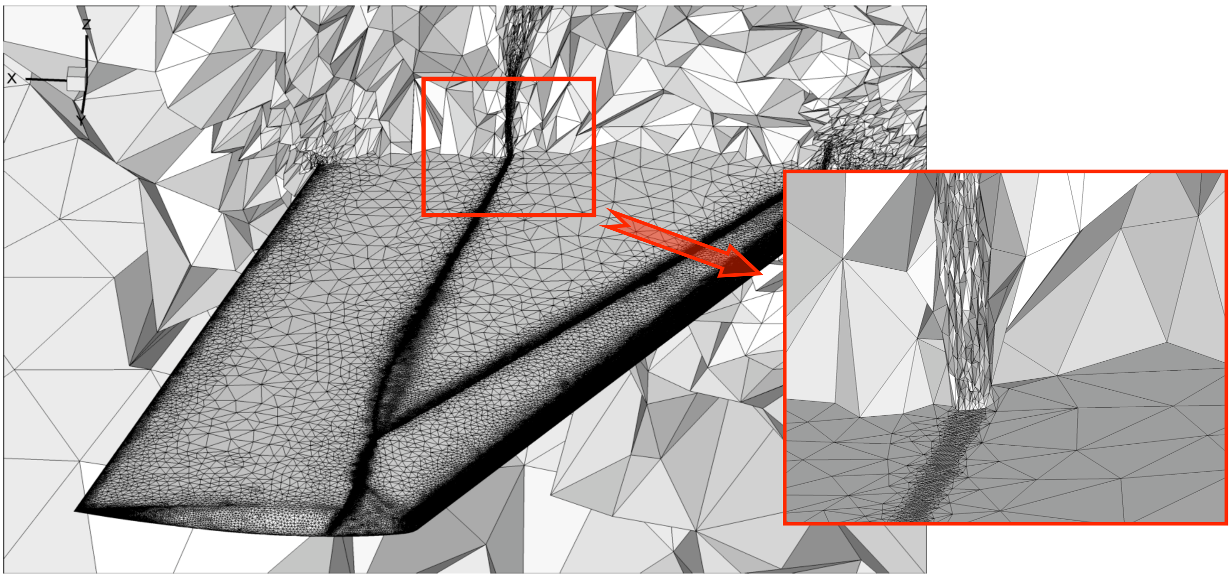
Robustness under severe mesh conditions Shocks





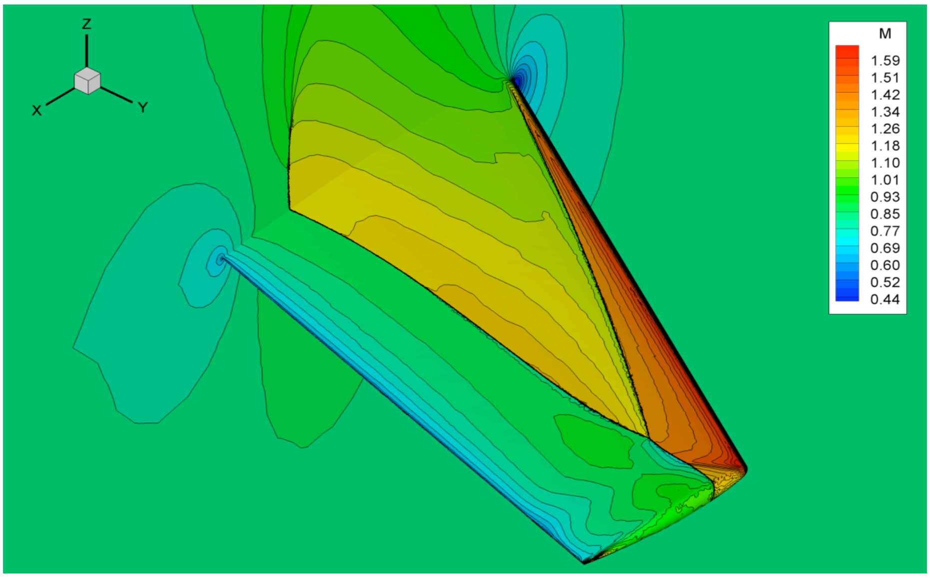
Monotone shock capturing discretizations

Anisotropic solution adaptive meshing



Grid (after 6 adaptation steps) – surface and volume grid details
(Courtesy J. Majewski, TU Warsaw)

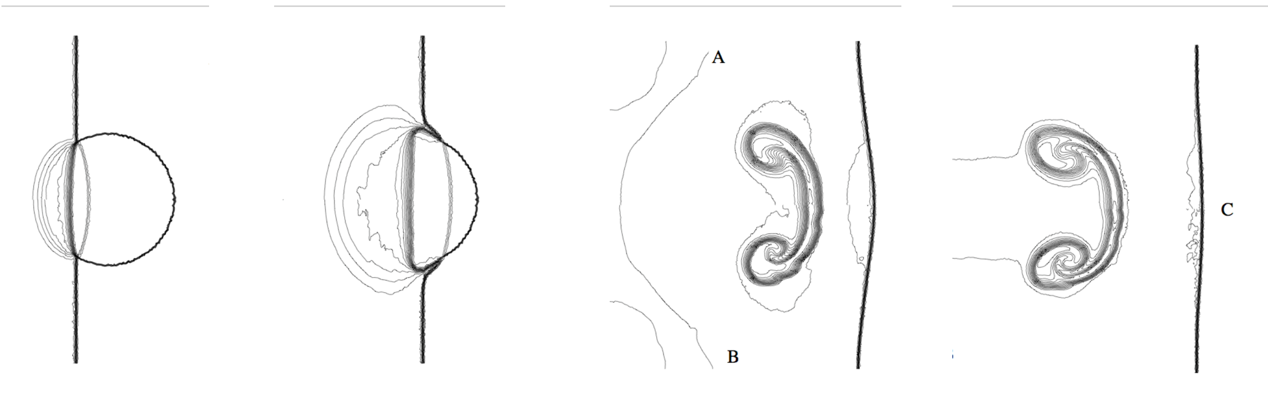
Solution adaptive meshing



ONERA M6 inviscid, transonic flow - Ma=0.8395 α=3.06º

Mach number field after 6 adaptation steps (TU Warsaw)

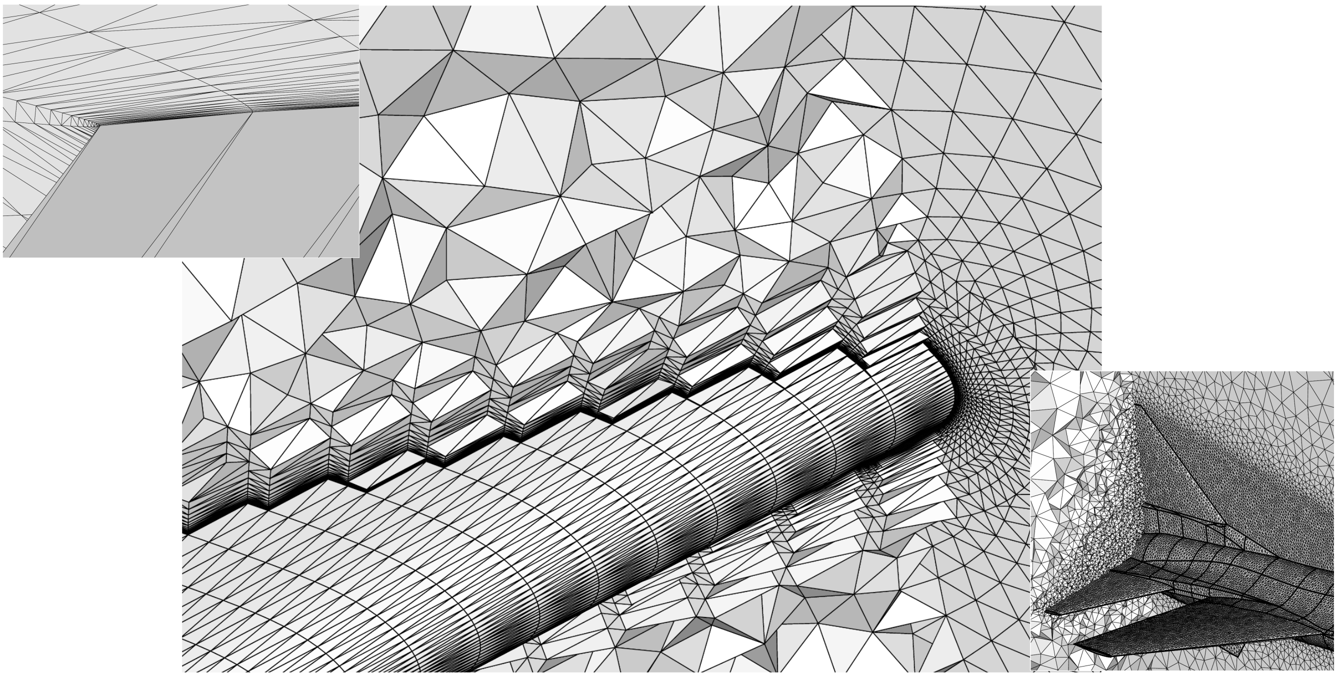
Unsteady problems:
- monotone resolution of shocks and contact layers
- accuracy in space and time



t=0.003 t=0.005 t=0.015 t=0.020

Interaction of a planar shock with a bubble

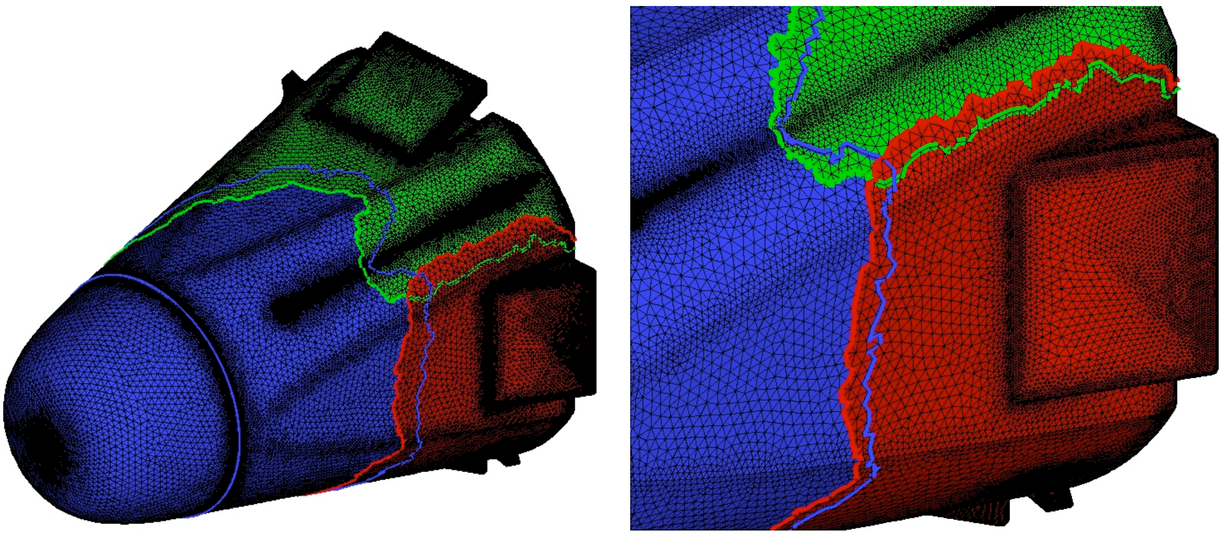
Anisotropic meshes for high Reynolds Nr flows



Wing at Reynolds 10^7 : 3 different length scales

Parallel computing based on domain decomposition

Hide communication layer from the developer



Tunable overlap region (depending on discretization)

ESA Expert vehicle

Complexity of CFD software requires new paradigm

• single discipline ⇒ multidisciplinary simulations
• coupled multiphysics
• diverse international partner institutions
• researchers from different backgrounds
• slow transfer of technology to industry

Small specialized research groups and SME's have difficulties to provide the complete chain

Two basic problems of collaboration

Technical problem

• How different numerical methods, physical models and coupling algorithms can work together?
• How to join developments from diverse researh groups to form a multi-physics simulation?

Human problem

• How preserve the efforts of the past ?
• How developers from different teams can interact?
• How to maintain intellectual property?

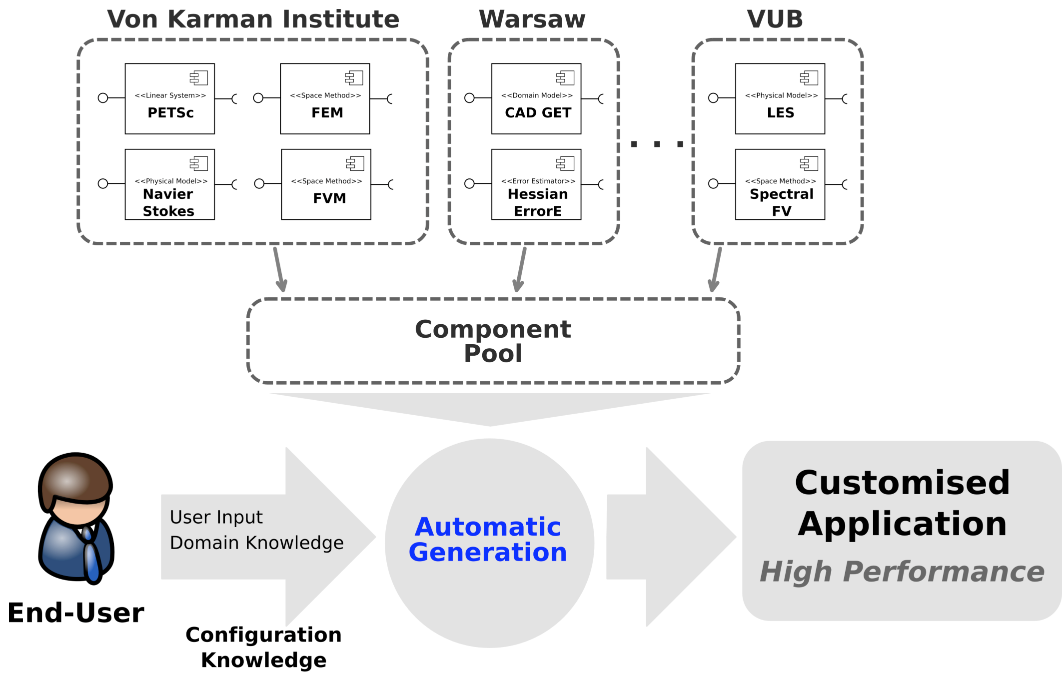
Solution: component based development

- Assemble application from basic components
  - modular components improve human cooperation
  - reusable components reduce development effort
- Modular IPR management
- Flexible interfaces between methods
- Configurable coupling algorithms
- Common standards for multi-domain data storage
- Transparent parallel communication layer

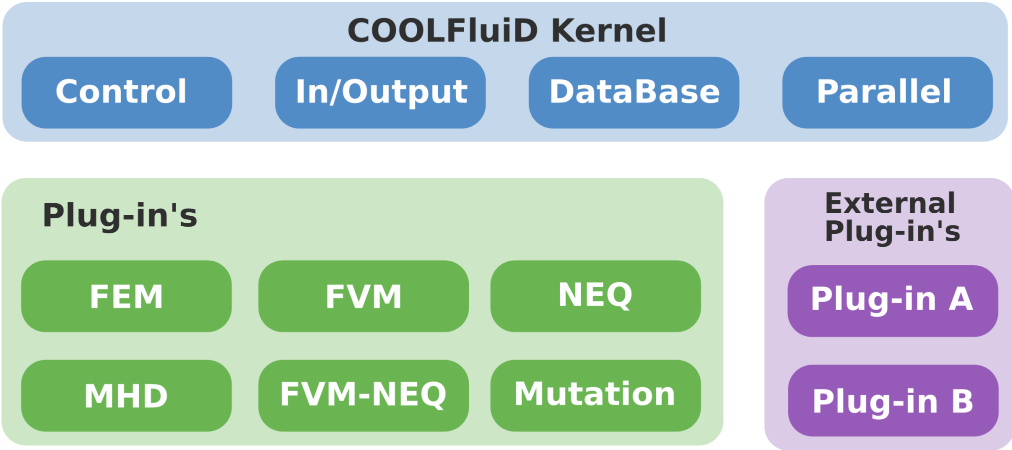
- Requires a dedicated software environment

CFD Environment

Customisable applications



Extendible framework with Plug-in policy



Component-based architecture
Complexity of software independent of number of components

Component examples: Discretization methods

- Finite Volume
- High Order Finite Element
- Residual Distribution
- Discontinuous Galerkin
- Spectral Finite Volume / Finite Difference

- Large scale computing
- Shown parallel scalability on 300+ processors

Component examples:
Physical Models

- Navier-Stokes (Incompressible to Hypersonic)
- Magnetohydrodynamics
- Structural mechanics
- Reactive species transport quations
- Heat Transfer
- Linearized Euler
- Turbulence models (RANS, LES)

- Coupling procedures amongst different models/algorithms
- Easily extendible

Component examples:
Tools

- Linear System Solvers
  Petsc, Trilinos, SAMG, Pardiso, FlexMG
- Mesh Movement and Adaptation
  Spring Analogy, Elastic Displ., Laplace Smooth,
  Rigid Move, Global remeshing
- Input / Output
  CGNS, Gambit Neutral, Gmsh, THOR, Cfmesh,
  Tecplot, VTK, Daedalus
- Time integrators / iterative solvers
  Newton Method, Runge-Kutta, Backward Euler, BDF2

Von Karman Institute for Fluid Dynamics

A class of discretization schemes on unstructured grid:

Residual Distribution schemes

Solution methodology I: Finite Volume Method

"Physical" viewpoint: mimic physical properties

- Start from integral conservation law (FV)
  discrete conservation imposed over each cell
- Respect domain of dependence: Stabilization introduced
  through upwinding (Murmann and Cole, 1968)
- Riemann problem solution used as building block
  (Godunov, 1959)
- Impose discrete maximum principle:
  monotonicity preserving schemes, TVD, LED, …
- Higher order methods: k-exact reconstruction (Barth),
  (W)ENO (Shu), Woodward and Colella…

Solution methodology II
Finite Element / Spectral methods

"Mathematical" viewpoint

- Variational formulation
  approximaton in discrete functional spaces
- Residual method: if exact solution belongs to the discrete space, the residual must vanish
- Stabilization introduced consistently:
  Petrov Galerkin approach, least squares, SUPG, PSPG
- Inherently multidimensional
- No emphasis on maximum principles
- Higher order methods: higher order basis functions for approximation space

Try to combine the best properties of FE and FV methods:

DG methods

- From FM theory:
  FE approximation spaces, hence compact stencils
  satisfy residual property,uniformly accurate on unstructured grids
- From FV: Discontinuous representation
- From FV: Traces on element boundary compute by Riemann solvers,

Residual Distribution schemes

- From FE theory:
  FE approximation spaces, hence compact stencils
  uniformly accurate on unstructured grids
- From FV: Built-in monotonicity principles, max principle
- Avoid 1D Riemann solvers, instead: multidimensional upwinding
  = multiD dissipation (as in FEM), less grid sensitivity than FV

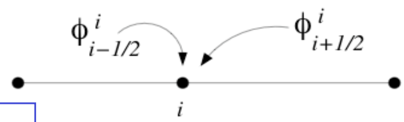
Residual Distribution in 1D (Roe 1981)
Scalar convection equation

$$\boxed{u_t + \lambda u_x = 0 \quad \text{on } \Omega \in \mathbb{R}}$$

Nodal values u_i

Equation for meshpoint i (using Euler explicit time integration):

$$\boxed{\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\beta^i_{i+1/2}\phi_{i+1/2} - \beta^i_{i-1/2}\phi_{i-1/2}}$$



Flux Difference
= Cell residual $i+1/2$:

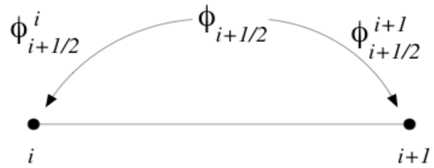
$$\boxed{\phi_{i+1/2} = \int_i^{i+1} \lambda u_x dx = \lambda(u_{i+1} - u_i)}$$

$$\boxed{\phi^i_{i+1/2} = \beta^i_{i+1/2}\phi_{i+1/2}}$$

$$\phi^i_{i+1/2} + \phi^{i+1}_{i+1/2} = \phi_{i+1/2}$$

$$\beta^i_{i+1/2} + \beta^{i+1}_{i+1/2} = 1$$

Consistency !

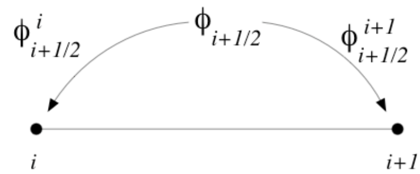


Splitting of cell residual $i+1/2$

Downwind Residual Distribution in 1D
= First Order Upwind scheme

$$\boxed{\lambda > 0 \quad \rightarrow \quad \phi^i_{i+1/2} = 0 \ , \ \phi^{i+1}_{i+1/2} = \phi_{i+1/2}}$$

$$\lambda < 0 \quad \rightarrow \quad \phi^i_{i+1/2} = \phi_{i+1/2} \ , \ \phi^{i+1}_{i+1/2} = 0$$



This defines a unique scheme with distribution coefficients

$$\boxed{\beta^i_{i+1/2} = \frac{\lambda^-}{\lambda} \quad ; \quad \beta^{i+1}_{i+1/2} = \frac{\lambda^+}{\lambda}}$$

$$\lambda^+ = \max(0,\lambda)$$

$$\lambda^- = \min(0,\lambda)$$

For problem (1) we finally end up with

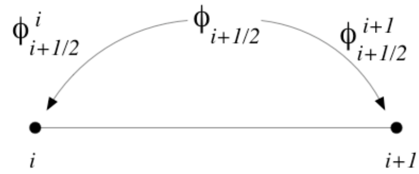
$$\boxed{\frac{u_i^{n+1} - u_i^n}{\Delta t}\Delta x = -\lambda^+ \Delta u_{i-1/2} - \lambda^- \Delta u_{i+1/2}}$$

(1^{st}order Upwind)

Downwind distribution for 1D Linear hyperbolic system Recovers Roe's Flux Difference Splitting (±1980)

Hyperbolic system: $\boxed{A = R\Lambda R^{-1}}$ Jacobian matrix

We upwind the residual on each characteristic.



This leads to the definition of a unique scheme with distribution matrices

$$\boxed{B^{i}_{i+1/2} = A^{-}\ A^{-1} \quad ; \quad B^{i+1}_{i+1/2} = A^{+}\ A^{-1}}$$

with $A^{\pm} = R\Lambda^{\pm}R^{-1}$

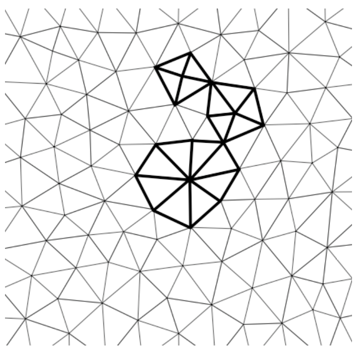
$$\boxed{\frac{U_i^{n+1} - U_i^n}{\Delta t}\Delta x = -A^{+}\Delta U_{i-1/2} - A^{-}\Delta U_{i+1/2}}$$

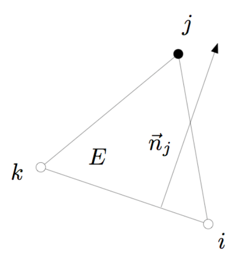
Nothing new!
(CIR)

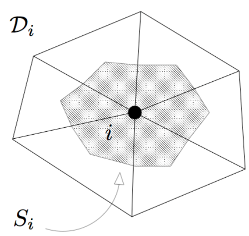
Residual Distribution in 2D

- Cell-vertex schemes on unstructured grids
- Standard *continuous* Finite Element approximation of the unknowns on P1, P2 …

$$\mathbf{u}_h(x,y,t) = \sum_{i \in \mathcal{T}_h} \psi_i(x,y)\mathbf{u}_i(t)$$







Example: linear triangles (P1)

$\mathcal{D}_i$ = support of node i

Hyperbolic system and model problems

System conservation law:

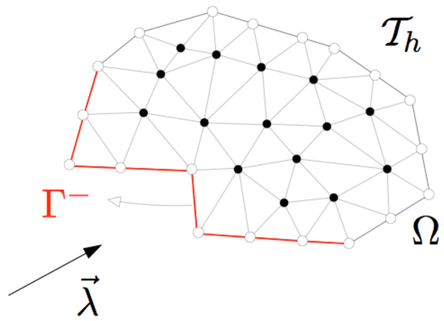
$$\boxed{\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{S}}(x,y) \qquad \text{on} \quad \Omega_T = \Omega \times [0, t_f] \subset \mathbb{R}^d \times \mathbb{R}^+}$$

Scalar convection equation:

$$\boxed{\frac{\partial u}{\partial t} + \vec{\lambda} \cdot \nabla u = \mathcal{S}(x,y)} \qquad \boxed{\boldsymbol{\mathcal{F}}(\mathbf{u}) = \mathcal{F}(u) = \vec{\lambda}\, u}$$

Steady scalar conservation law:

$$\boxed{\begin{aligned} \nabla \cdot \boldsymbol{\mathcal{F}}(u) &= 0 && \text{in} \quad \Omega \\ u &= g && \text{on} \quad \Gamma^- \\ \vec{\lambda}(u) &= \frac{\partial \mathcal{F}}{\partial u} \end{aligned}}$$



Residual Distribution method (steady problem)

❶ $\forall T \in \mathcal{T}_h$ compute : $\boxed{\phi^T = \int_T \nabla \cdot \boldsymbol{\mathcal{F}}_h(u_h)}$

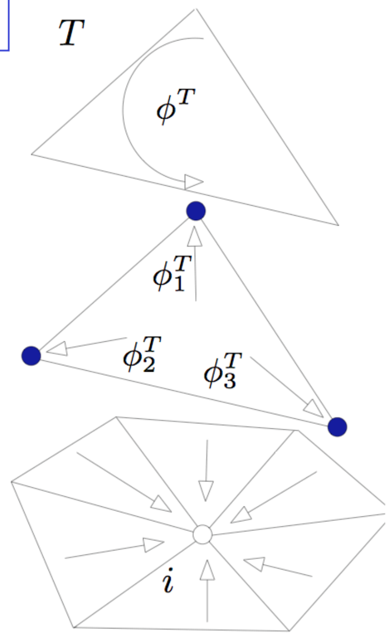
= cell Residual

❷ Distribution : $\boxed{\phi^T = \sum_{i \in T} \phi_i^T}$

Distribution coeff.s : $\phi_i^T = \beta_i^T \phi^T$

❸ Compute nodal values :
solve (evolve) = nodal update

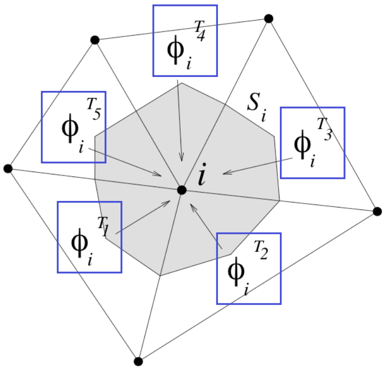
$$\boxed{u_i^{n+1} = u_i^n - \omega_i \sum_{T | i \in T} \phi_i^T}$$



Residual distribution - once more

Steady state: algebraic equation at each node:

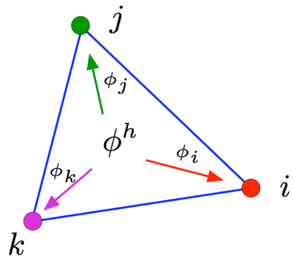
$$\sum_{T \in \mathcal{D}_i} \phi_i^T = 0 \quad \forall i \in \tau_h$$



From the viewpoint of 1 triangle:
distribute residual to its nodes.

Residual

$$\sum_{j \in E} \phi_j^E = \phi^E = \int_E \left(\vec{\lambda} \cdot \nabla u_h - \mathcal{S}_h \right) \, dx\, dy$$



Condition 1: Conservation and consistency

Main $\mathcal{HP}$: $\exists\ \boldsymbol{\mathcal{F}}_h$, continuous approximation of $\boldsymbol{\mathcal{F}}$

$$\phi^T = \sum_{j \in T} \phi_j^T = \int_T \nabla \cdot \boldsymbol{\mathcal{F}}_h = \oint_{\partial T} \boldsymbol{\mathcal{F}}_h \cdot \hat{n}$$

Flux integral computed using some quadrature rule
- Exact
- Simpson
- Gauss

Lax-Wendroff theorem (Abgrall & Barth, *SIAM J.Sci.Comp.* 24, 2002 ; Abgrall & Roe, *J.Sci.Comp.* 19, 2003)

Condition 2: Accuracy estimate

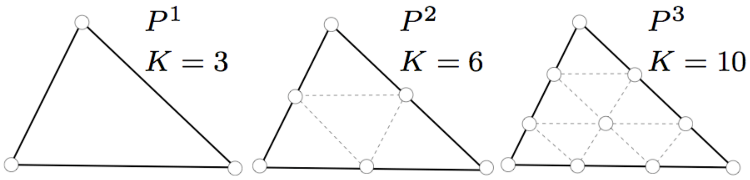
Final result

For continuous $k+1^{\text{th}}$ order space approx. (e.g. P^k Lagrange)

$$|\mathcal{E}(w_h)| \leq C'(\mathcal{T}_h, w)\|\nabla\varphi\|_\infty\, h^{k+1}$$

provided that (in 2D) $\forall i \in T$ and $\forall T \in \mathcal{T}_h$

$$\boxed{|\phi_i^T(w_h)| \leq C''(\mathcal{T}_h, w)h^{k+2} = \mathcal{O}(h^{k+2})}$$



P^k Lagrange element

Condition on the distributed
Element residual
Provides a useful
Design criterion

Design criterion: Accuracy preserving distributions

schemes for which

$$\boxed{\phi_i^T = \beta_i^T \phi^T} \qquad \sum_{j\in E} \beta_j = 1$$

with β_i^T uniformly bounded distribution coeff.s, are formally $k+1^{\text{th}}$ order accurate (for $k+1^{\text{th}}$ order spatial interpolation)

Indeed, since

$$\phi^T(w_h) = \mathcal{O}(h^{k+2})$$

One has for such schemes immediately: $\phi_i^T(w_h) = \mathcal{O}(h^{k+2})$

P1 elements: k=1 ; 2nd order, known as linearity preserving schemes
residual property in FEM
weighted residual method

Condition 3: Monotonicity (1)

$$\vec{\lambda}\cdot\nabla u = 0, \qquad \vec{\lambda} = \text{const}$$

Construct schemes for which

$$\phi_i^T = \sum_{\substack{j\in T\\ j\neq i}} c_{ij}(u_i - u_j), \quad c_{ij} \geq 0$$

LED property

Theory of positive coefficient schemes $\Rightarrow$ discrete max principle

(Spekreijse, *Math.Comp.* 49, 1987 ; Barth & Ohlberger, *Enc.Comp.Mech.*, 2004)

$$u_i^{n+1} = u_i^n - \omega_i \sum_{T|\,i\in T} \sum_{\substack{j\in T\\ j\neq i}} c_{ij}(u_i^n - u_j^n) \quad \underset{\omega_i \leq \omega_i^{\max}}{\overset{c_{ij}\geq 0}{\Longrightarrow}} \quad \min_j u_j^n \leq u_i^{n+1} \leq \max_j u_j^n$$

Godunov theorem: Linear Positive schemes are at most first order

Condition 3: Monotonicity (2)

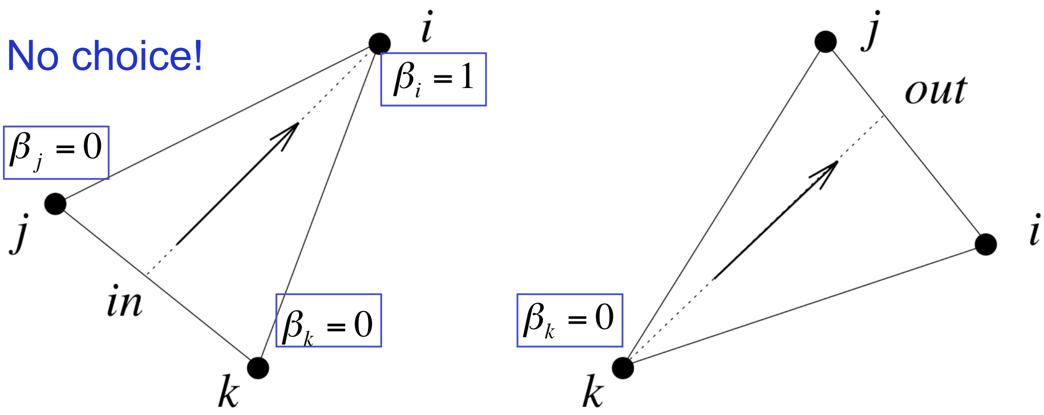
Godunov theorem:
Linear positive schemes are at most first order

Solution: nonlinear schemes higher order monotone schemes

P1: Upwind residual distribution schemes

- conclusion: require $\beta_i^T = 0$ for upwind nodes, i.e. nodes for which $k_i \le 0$

No choice!



1 target triangle

2 target triangle

How to split over i and j ?

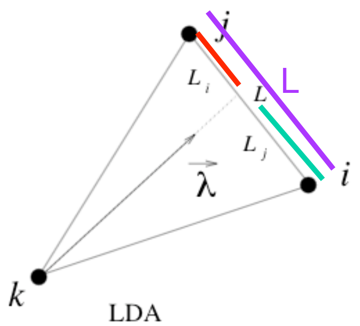
P1: A linear second order scheme: the LDA-scheme

The LDA scheme. The distribution coefficients are defined as

$$\boxed{\beta_i^{\text{LDA}} = \frac{k_i^+}{\sum_j k_j^+}.}$$

In the two target case this leads to

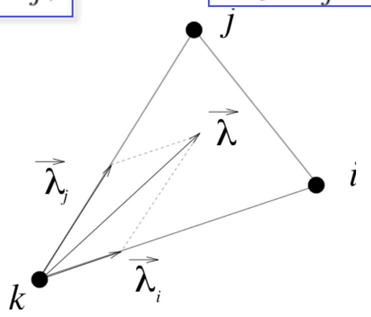
$$\boxed{\beta_i^{\text{LDA}} = -\frac{k_i}{k_k} = \frac{L_i}{L}} \quad \boxed{\beta_j^{\text{LDA}} = -\frac{k_j}{k_k} = \frac{L_j}{L}}.$$



P1: A monotone linear first order upwind scheme: the N-scheme

The N scheme. Considering the two target case, the convection vector $\vec{\lambda}$ is decomposed into components parallel to $\vec{r}_{ki} = (\vec{r}_i - \vec{r}_k)$ and $\vec{r}_{kj} = (\vec{r}_j - \vec{r}_k)$,

$\boxed{\vec{\lambda} = \vec{\lambda}_i + \vec{\lambda}_j,}$ with $\boxed{\vec{\lambda}_i \cdot \vec{n}_j = \vec{\lambda}_j \cdot \vec{n}_i = 0.}$



Hence, the residual can be decomposed into a part due to $\vec{\lambda}_i$ and a part due to $\vec{\lambda}_j$,

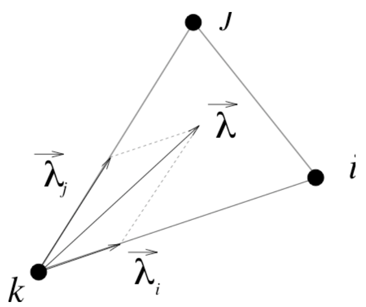
$$\boxed{\phi^T(\vec{\lambda}) = \phi^T(\vec{\lambda}_i + \vec{\lambda}_j) = \phi^T(\vec{\lambda}_i) + \phi^T(\vec{\lambda}_j).}$$

Fluctuation $\phi^T(\vec{\lambda}_i)$ is sent to i, and likewise $\phi^T(\vec{\lambda}_j)$ to node j.

the N-scheme (2)

One verifies that $\boxed{\phi^T(\vec{\lambda}_i) = k_i(u_i^n - u_k^n)}$ and $\boxed{\phi^T(\vec{\lambda}_j) = k_j(u_j^n - u_k^n)}$ which allows to check positivity under a CFL condition.

Monotone = LED under a CFL condition



However, one verifies that

$$\phi_i^T = \mathcal{O}(h^2)$$

Hence, only first order accurate!
In other words: the distribution coefficient becomes unbounded for vanishing residual

$$\beta_i^N = \frac{\phi^T(\vec{\lambda}_i)}{\phi^T(\vec{\lambda})} = \frac{\phi_i^T}{\phi}$$

Monotone Nonlinear higher order scheme

Limited nonlinear schemes (Deconinck *et al.*, *Comp.Mech.* 11, 1993 ; Sidilkover & Roe, *ICASE Report 95-10*, 1995)

1. Starting point: a positive 1st order scheme (ϕ_i^{p})
2. Devise strategy to construct a splitting (ϕ_i^*) such that

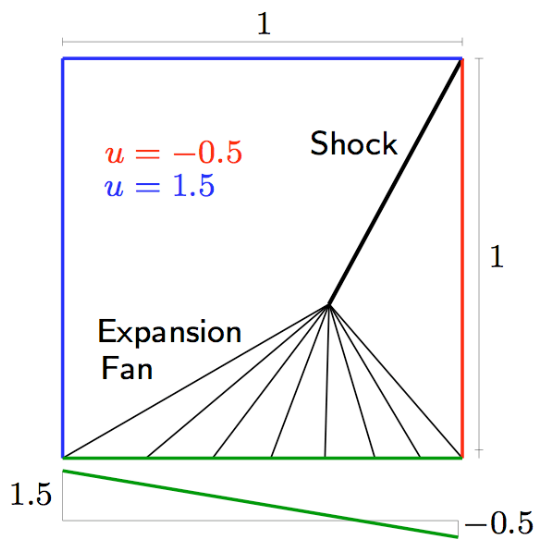
$$\phi_i^* = \alpha_i\, \phi_i^{\mathsf{p}},\ \alpha_i \geq 0 \quad \xrightarrow{c_{ij}^p \geq 0} \quad c_{ij}^* \geq 0$$

with $\alpha_i = \alpha_i(\phi^T, \{\phi_j^{\mathsf{p}}\}_{j\in T})$ limiter such that

$$\phi_i^* = \alpha_i\, \phi_i^{\mathsf{p}} = \beta_i^* \phi^T, \quad \text{with } \beta_i^* \text{ uniformly bounded}$$

Test case for monotone shock capturing

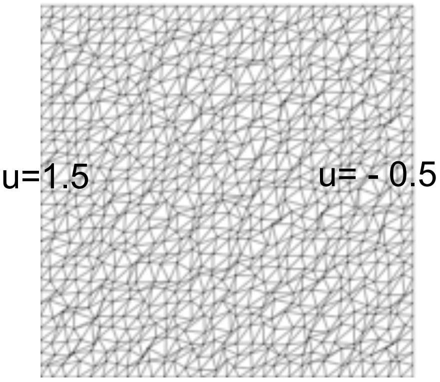
$$\nabla \cdot (\frac{u^2}{2}, u) = 0$$



Schemes on P1 triangles: Comparison for scalar conservation law

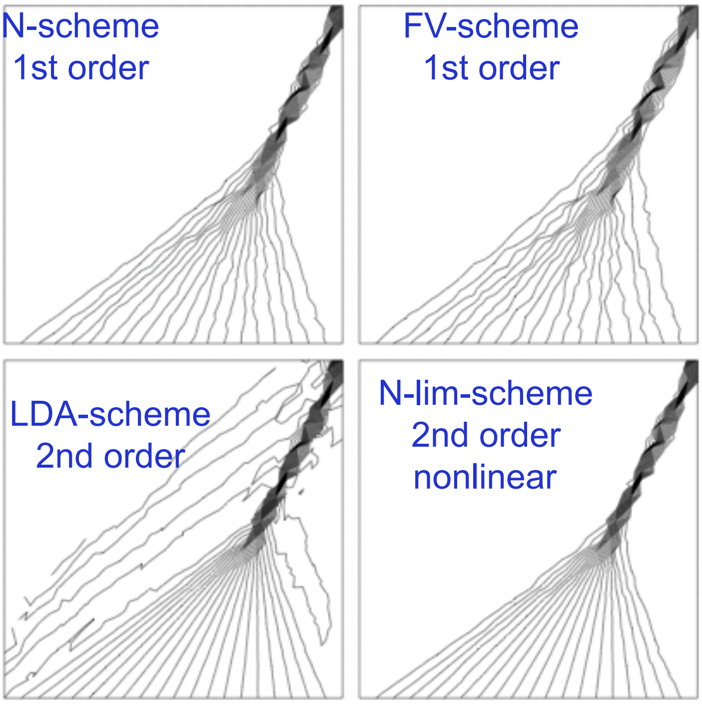
$$\nabla \cdot \mathcal{F}(u) = 0$$

$$\mathcal{F}(u) = (u^2, u)$$



u=linear between 1.5 and -0.5

Irregular mesh

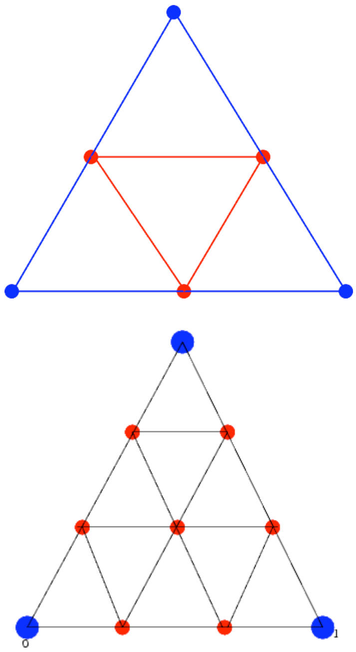


Higher order schemes on P^2 and P^3 triangles

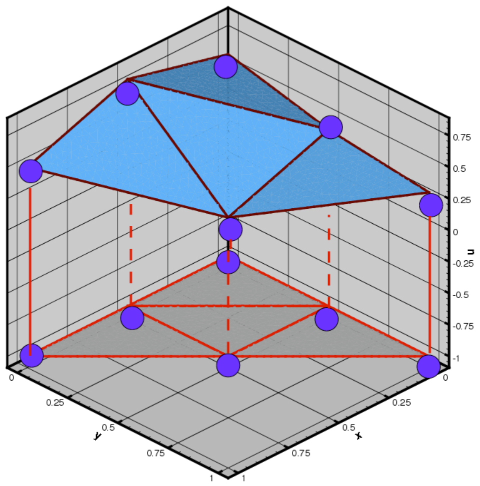
- Domain discretized by P^k element (k>1)
- Basis functions are
  quadratic for P^2
  cubic for P^3

$$\boxed{u^h(x,y) = \sum_{i \in \tau_h} \psi_i(x,y) u_i}$$

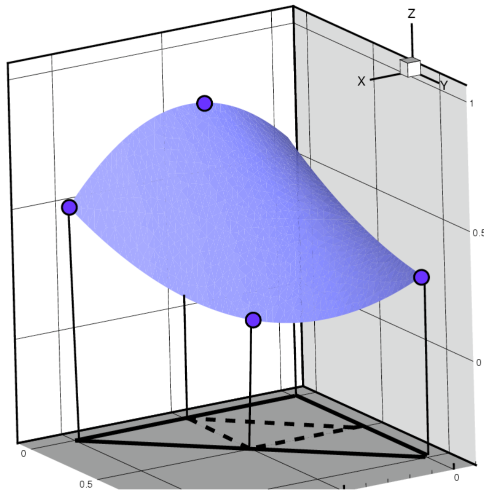
- u^h is a third (P2) or fourth (P3) order approximation of u



High order discretization



Discretization by P^1 element



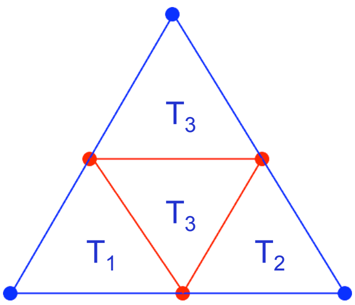
Discretization by P^2 element

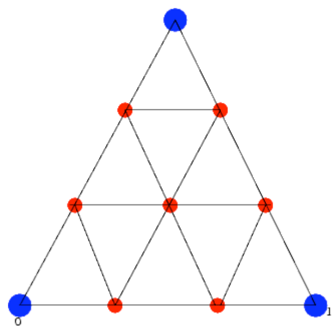
Higher order schemes on P^2 and P^3 triangles

First strategy: reuse schemes on P1 elements (1)

Construct a P1 sub-triangulation of the Pk element

$$T = \bigcup_k T_k$$





Higher order schemes on P² and P³ triangles First strategy: reuse schemes on P1 elements

- Compute Residual on sub-element E_s

$$\Phi^{E_s} = \int_{E_s} \nabla \mathcal{F}(u^h)\, d\Omega$$

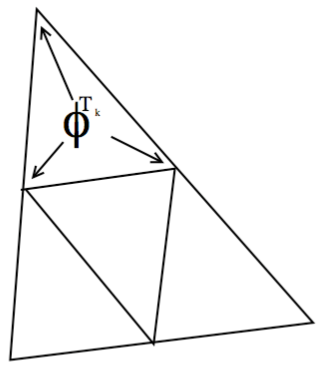
- Distribute to nodes of E_s

$$\Phi_i^{E_s} = \beta_i^{E_s} \Phi^{E_s}$$

- Solve nodal equation

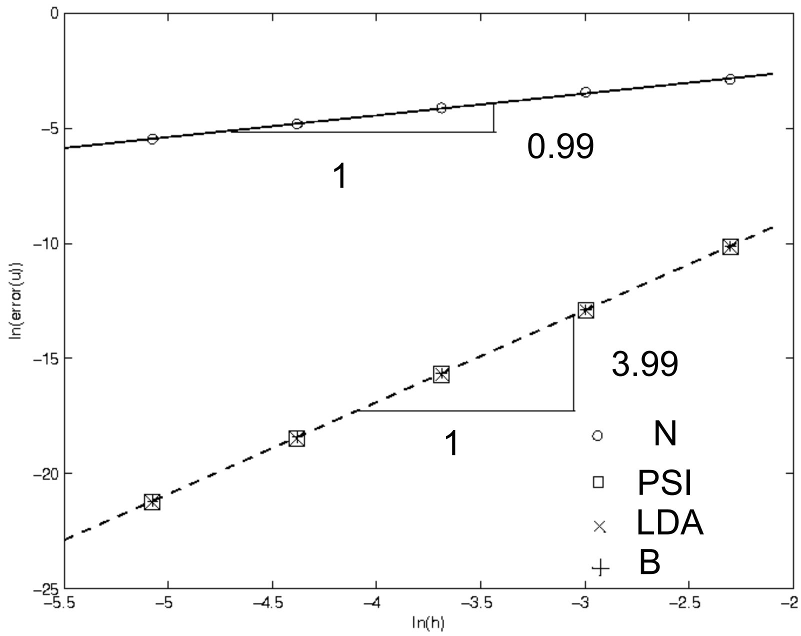
$$\sum_{E_s, i \in E_s} \Phi_i^{E_s} = 0$$

All schemes on P1 elements can be reused on the sub triangles



Spatial accuracy (steady state)

Grid convergence with P³ elements



Higher order schemes on P² and P³ triangles
Second strategy: schemes on Pk elements
Example: Pk Lax-Friedrichs scheme

$$\boxed{\boxed{\phi_i^{\mathsf{LF}} = \frac{1}{K}\phi^T} + \frac{\alpha}{K}\sum_{\substack{j\in T\\ j\neq i}}(u_i - u_j),} \quad \alpha \geq \max_{j\in T}\left|\int_T \vec{\lambda}\cdot\nabla\psi_j\right|$$

Scheme is LED under CFL condition

- K number of DoF per element
- ψ_j Lagrange basis fcn. relative to node j
- The LF scheme is cheap and has general formulation

Second strategy: schemes on Pk elements
Pk Limited Lax-Friedrichs scheme

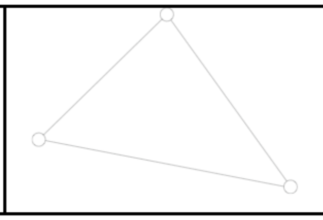
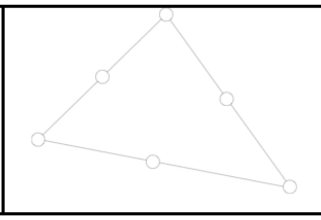
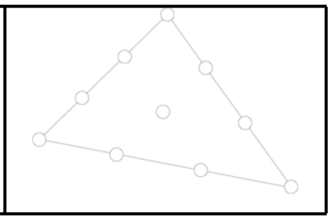
❶ $\forall T \in \mathcal{T}_h$:

(a) Compute ϕ^T (contour integral, P^k interpolation for $\mathcal{F}_h$)
(b) Compute LF distribution ϕ_i^{LF}, $\forall i \in T$
(c) Compute LF distribution coeff.s and map them
$\Rightarrow \phi_i^{\mathsf{LF}*} = \beta_i^{\mathsf{LF}*}\phi^T$, $\forall i \in T$

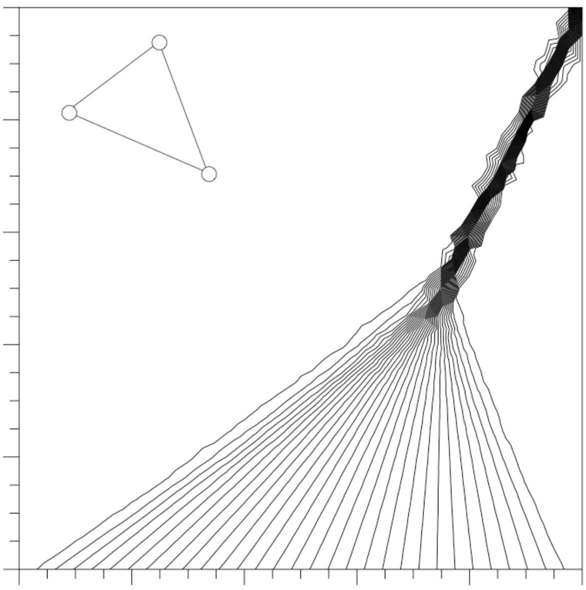
❷ Evolve nodal values : $u_i^{n+1} = u_i^n - \omega_i \sum_{T|i\in T} \phi_i^{\mathsf{LF}*}$

Apply the mapping to the LF scheme$\Rightarrow$ Limited LF scheme

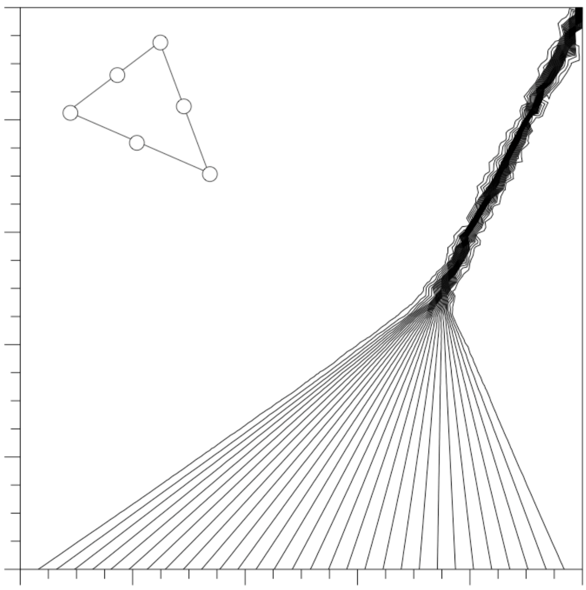
Limited LF scheme: Grid convergence

			
h	$\epsilon_{L^2}(P^1)$	$\epsilon_{L^2}(P^2)$	$\epsilon_{L^2}(P^3)$
$1/25$	0.50493E-02	0.32612E-04	0.12071E-05
$1/50$	0.14684E-02	0.48741E-05	0.90642E-07
$1/75$	0.74684E-03	0.13334E-05	0.16245E-07
$1/100$	0.41019E-03	0.66019E-06	0.53860E-08
	$\mathcal{O}^{\text{ls}}_{L^2}$ =**1.790**	$\mathcal{O}^{\text{ls}}_{L^2}$ =**2.848**	$\mathcal{O}^{\text{ls}}_{L^2}$ =**3.920**

Burgers equation - testcase with shock



LLFs scheme, P^1 interpolation



LLFs scheme, P^2 interpolation

With LSG stabilization term

Hyperbolic systems of conservation laws

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{F}}(\mathbf{u}) = \boldsymbol{\mathcal{S}}(x,y)$$

$$\boldsymbol{\mathcal{F}}(\mathbf{u}) = (\mathbf{F}(\mathbf{u}),\, \mathbf{G}(\mathbf{u}))$$

$$K(\vec{\xi},\mathbf{u}) = \frac{\partial \mathbf{F}(\mathbf{u})}{\partial \mathbf{u}}\xi_1 + \frac{\partial \mathbf{G}(\mathbf{u})}{\partial \mathbf{u}}\xi_2 = A_1\xi_1 + A_2\xi_2$$

$$\frac{\partial \mathbf{u}}{\partial t} + A_1\frac{\partial \mathbf{u}}{\partial x} + A_2\frac{\partial \mathbf{u}}{\partial y} = \boldsymbol{\mathcal{S}}(x,y)$$

$$\boldsymbol{\phi}^h = \int\limits_E \left(A_1\frac{\partial \mathbf{u}_h}{\partial x} + A_2\frac{\partial \mathbf{u}_h}{\partial y} - \boldsymbol{\mathcal{S}}_h \right) dx\, dy$$

$$\boldsymbol{\phi}^h = \sum_{j\in E} K_j \mathbf{u}_j - \frac{|E|}{3}\sum_{j\in E}\boldsymbol{\mathcal{S}}_j$$

$$K_j = \frac{1}{2}K(\vec{n}_j,\overline{\mathbf{u}})$$

$$\sum_{j\in E} K_j = 0$$

Matrix extension of scalar schemes

$$K_j^{\pm} = R_j\Lambda_j^{\pm}(R_j)^{-1} = \frac{1}{2}K^{\pm}(\vec{n}_j,\overline{\mathbf{u}})$$

Formal extension of linear schemes (N, LDA, Lax-Wendroff)

System-N scheme:

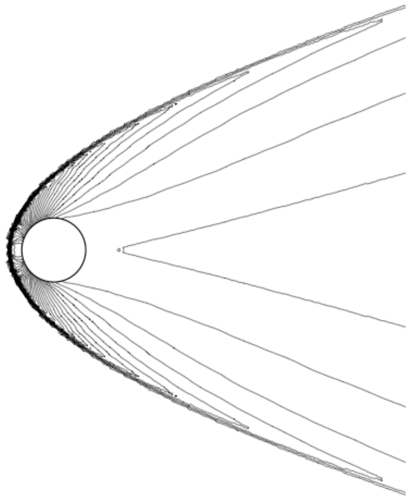
$$\boldsymbol{\Phi}_i^{T,N} = \mathbf{K}_i^{+}(\sum_j \mathbf{K}_j^{-})^{-1}\sum_j \mathbf{K}_j^{-}(\mathbf{U}_i - \mathbf{U}_j)$$

System-LDA scheme

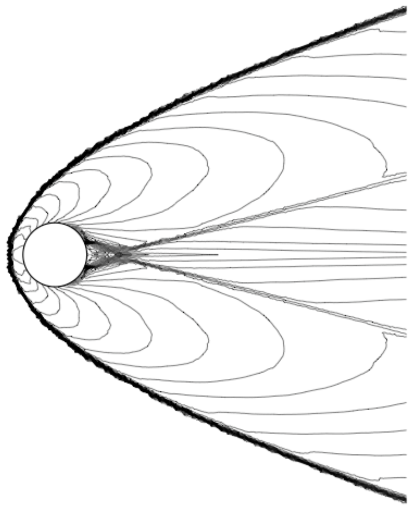
$$\beta_i^{T,LDA} = \mathbf{K}_i^{+}(\sum_j \mathbf{K}_j^{+})^{-1}$$

Example: Mach 10 flow around cylinder
Limited N-scheme on P1 elements

Pressure contours

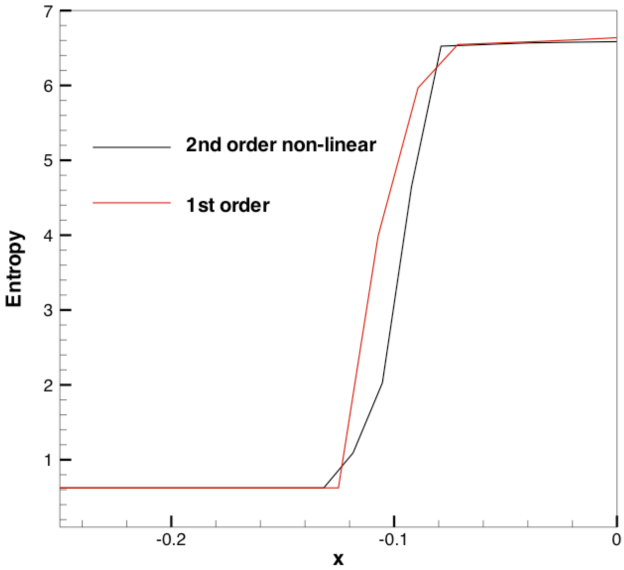


Mach number contours

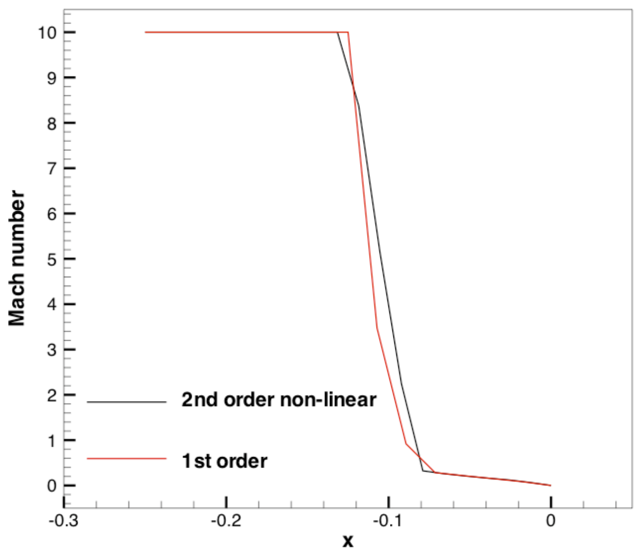


Example: Mach 10 flow around cylinder

Entropy across the shock

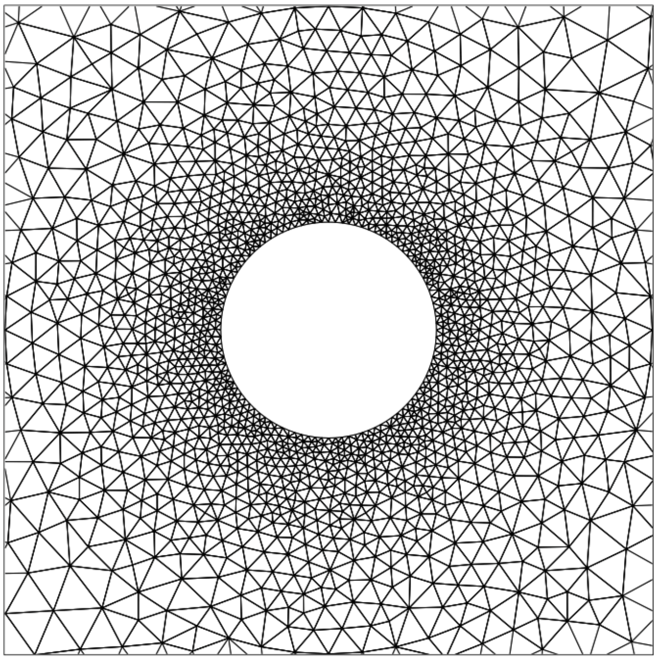


Mach across the shock

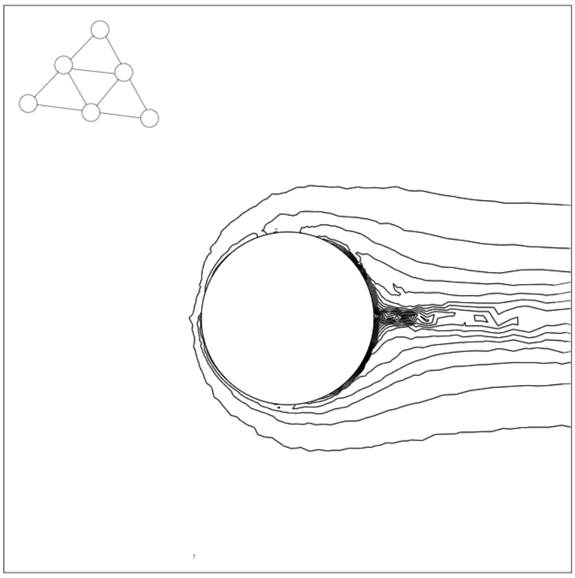


Inviscid fow round circular cylinder Mach=0.36

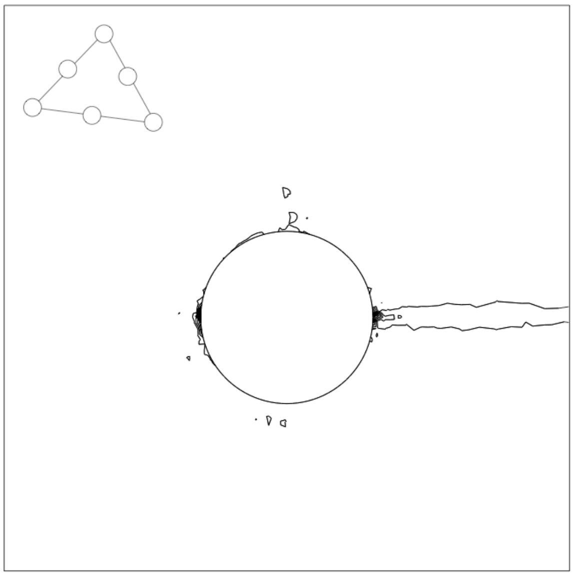
$Ma = 0.35$
flow on cylinder
Mesh :
2719 nodes
5308 elements
100 nodes
on cylinder



Inviscid fow round circular cylinder Mach=0.36
Limited LF scheme - Isolines of entropy



P1 elements



P2 elements

Same nr of DOF's

Residual distribution schemes for unsteady systems

$$\boxed{\frac{\partial u}{\partial t} + \vec{\lambda} \cdot \vec{\nabla} u = 0.}$$

First approach: Consistent Mass Matrix

$$\boxed{\sum_T \sum_j m_{ij}^T \frac{du_j}{dt} + \sum_T \beta_i^T \phi^T = 0,}$$

where in the first term on the left hand side a consistent mass matrix appears:

$$m_{ij}^T = \int\int_{|T|} w_i N_j dx =$$

Residual distribution schemes for unsteady systems Consistent Mass Matrix

$$\frac{|T|}{3} \begin{bmatrix} \frac{1}{2} + \beta_1^T - \frac{1}{3} & \frac{1}{4} + \beta_1^T - \frac{1}{3} & \frac{1}{4} + \beta_1^T - \frac{1}{3} \\ \frac{1}{4} + \beta_2^T - \frac{1}{3} & \frac{1}{2} + \beta_2^T - \frac{1}{3} & \frac{1}{4} + \beta_2^T - \frac{1}{3} \\ \frac{1}{4} + \beta_3^T - \frac{1}{3} & \frac{1}{4} + \beta_3^T - \frac{1}{3} & \frac{1}{2} + \beta_3^T - \frac{1}{3} \end{bmatrix}. \tag{5}$$

- Implicit Cranck-Nicholson time integration:

$$\boxed{\left[\frac{\mathbf{M}}{\Delta t} + \frac{\mathbf{J}}{2}\right] \Delta U^n = -R^n,}$$

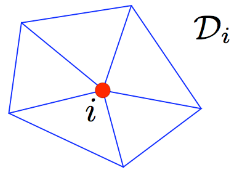
where $\mathbf{J}$ is the jacobian of the nodal residual R.

Second approach
Space-time residual distribution schemes

$$\boxed{u_t + \vec{\lambda}\cdot\nabla u = 0 \quad \text{on} \quad \Omega \times [t_0, t_{fin}] \subset \mathbb{R}^2 \times \mathbb{R}^+}$$

Given the nodal values at time $t^n < t_{fin}$, the nodal values at time $t^{n+1} > t^n$ are the solution of the algebraic system

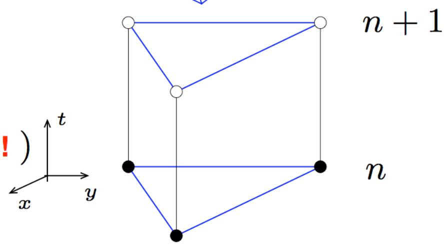
$$\boxed{\sum_{T\in\mathcal{D}_i} \phi_i = 0 \quad \forall i \in \tau_h} \qquad (3)$$



System (3) is obtained as follows (Abgrall and Mezine, *JCP* 2003).

1. $\forall T \in \tau_h$: computation of *space-time* cell residual

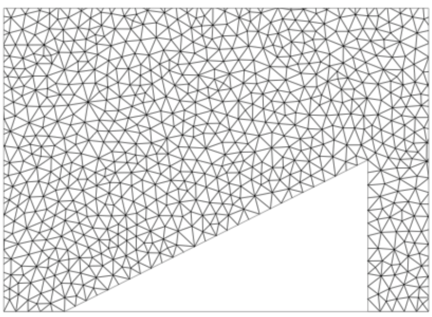
$$\boxed{\phi^h = \int_{t^n}^{t^{n+1}} \int_T \left(u_t^h + \vec{\lambda}\cdot\nabla u^h\right)\, d\Omega dt} \quad (\textbf{Implicit schemes !})$$



2. $\forall i \in T$: residual distribution $\rightarrow \phi_i$.

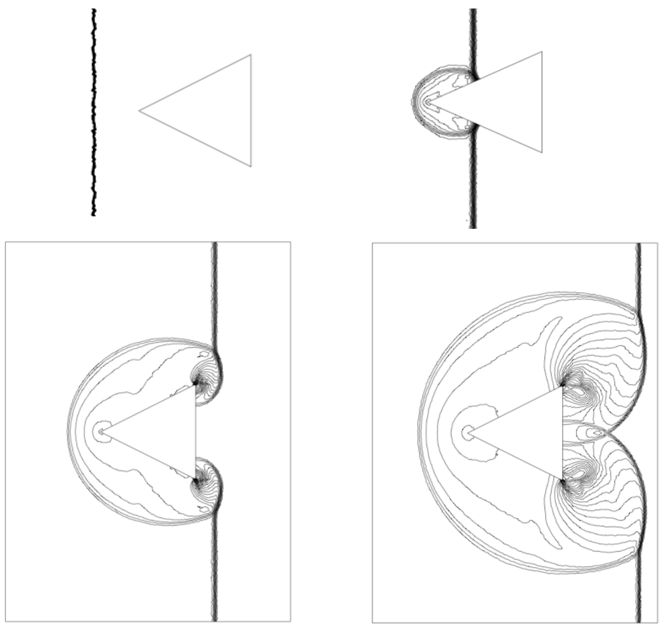
   Distribution coefficients: $\boxed{\beta_i = \dfrac{\phi_i}{\phi^h}}$

Example unsteady Euler : Mach 1.6 shock hitting a finite wedge

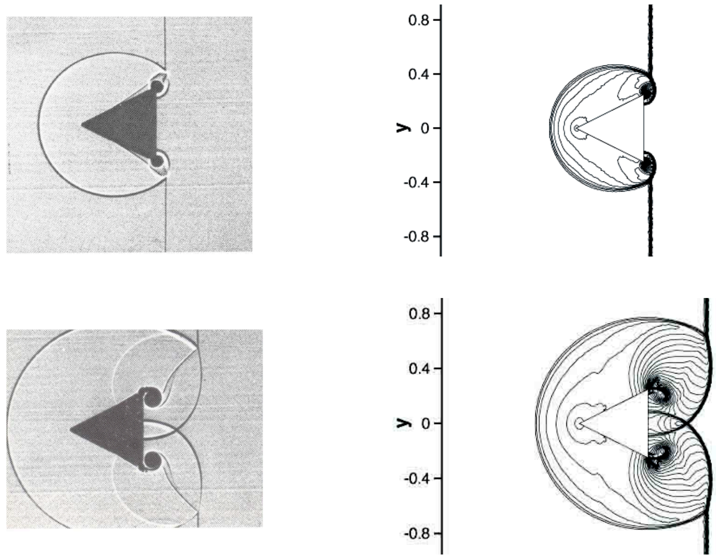


Course mesh: h= 1/50

Solutions on real mesh:
h=1/100
at
t=0, 0.25, 0.5, 0.6875



Mach 1.6 shock hitting a finite wedge
Comparison with schlieren



t=0.5

t=0.6875

Left: Schlieren picture Right: time dependent simulation

Density contours for planar Mach 1.6 shock over wedge

Viscous terms:

Steady Convection-diffusion equation
and
Steady Navier-Stokes equations

Basic idea for discretization of viscous terms:

$$\vec{\lambda}.\nabla u^h(x,y) - \nabla.(\nu \nabla u^h(x,y)) = 0$$

- Use the Petrov-Galerkin interpretation equivalent to RDS

$$\omega_i = N_i + (3\beta_i^T - 1)S^T$$

- For P1 elements this leads to a standard Galerkin Finite Element discretization for the diffusion operator (elliptic part)

Application

Hypersonic reacting flows

Thermal and Chemical non-equilibrium

Conservation equations for Thermal and chemical non-equilibrium

$$\frac{\partial \mathbf{U}}{\partial \mathbf{P}}\frac{\partial \mathbf{P}}{\partial t} + \frac{\partial \mathbf{F}_i^c}{\partial x_i} = \frac{\partial \mathbf{F}_i^d}{\partial x_i} + \mathbf{S} \qquad \mathbf{U} = (\rho_s, \rho\mathbf{u}, \rho E, \rho_m e_m^v)^T \qquad \mathbf{P} = (\rho_s, \mathbf{u}, T, T_m^v)^T$$

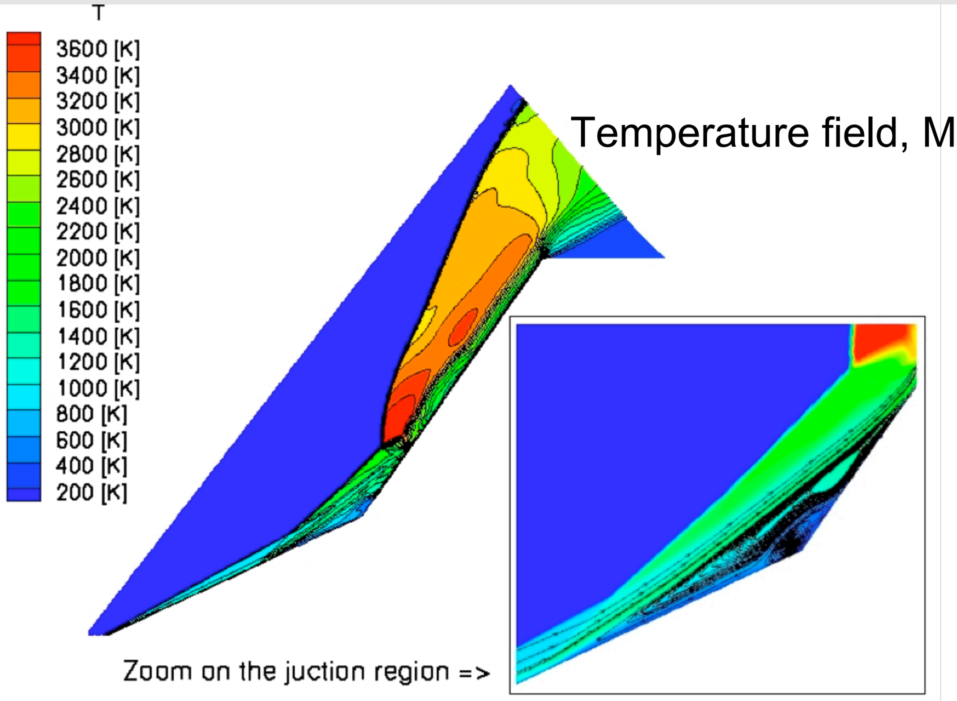
$$\mathbf{F}_i^c = \begin{pmatrix} \rho_s \mathbf{u} \\ \rho\mathbf{u}\mathbf{u} + p\hat{I} \\ \rho\mathbf{u}H \\ \rho_m \mathbf{u} e_m^v \end{pmatrix}, \quad \mathbf{F}_i^d = \begin{pmatrix} -\rho_s \mathbf{u}_s^d \\ \bar{\bar{\tau}} \\ (\bar{\bar{\tau}}\cdot\mathbf{u})^T - \mathbf{q} - \sum_s \rho_s h_s \mathbf{u}_s^d \\ -\rho_m h_m^v \mathbf{u}_m^d - \mathbf{q}_m^v \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} \dot{\omega}_s \\ \mathbf{0} \\ \mathbf{0} \\ \Omega^{vt} + \Omega^{CV} + \Omega^{VV} \end{pmatrix}$$

$y_s = \rho_s/\rho$ is the mass fraction of species s

Air 5 (O_2, N_2, N, O, NO) or Air 11 species

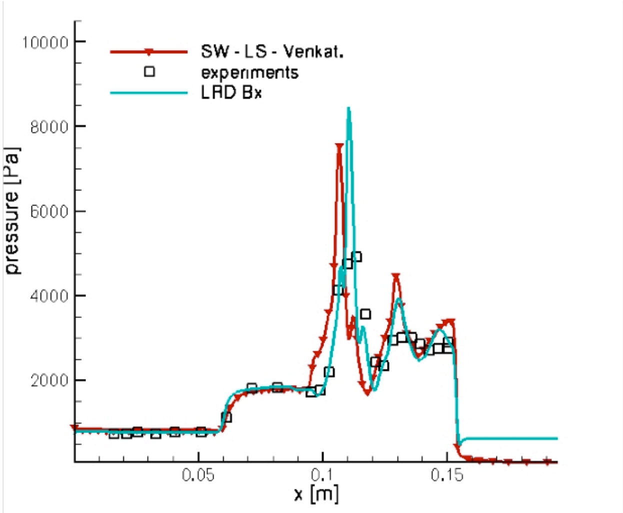
Three temperature model: roto-translational (T) + vibrational modes for O_2 and N_2

Hypersonic flow over double cone – non reacting (run 35)

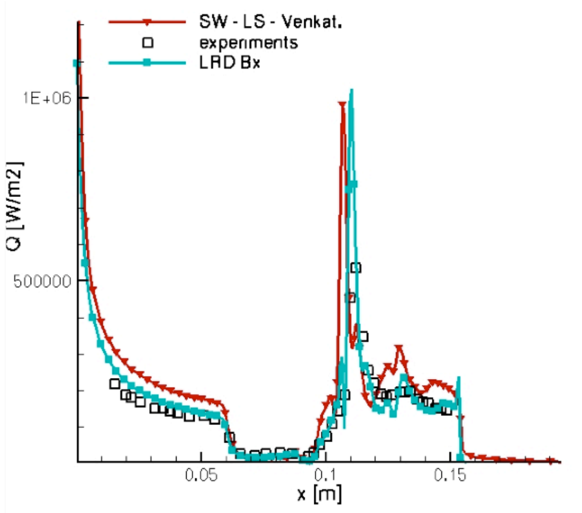


Temperature field, Mach nr = 8

Hypersonic flow over double cone – non reacting (run 35)



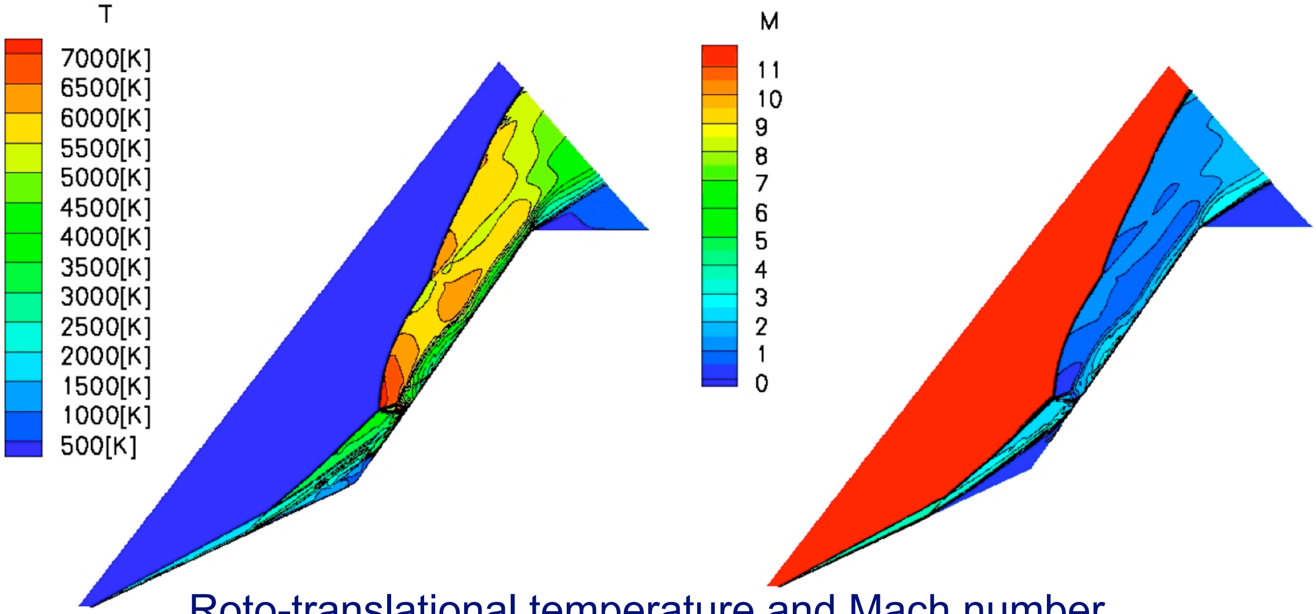
(a) Surface pressure



(b) Surface heat flux

Comparison between Finite Volume, Residual Distribution method and experiments

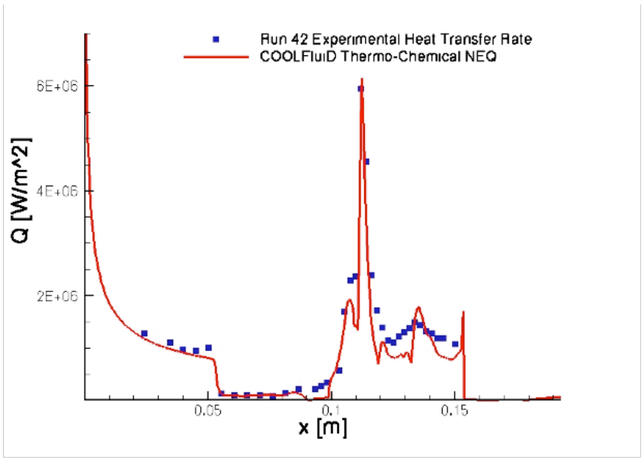
Mach 11 hypersonic flow over double cone Thermo-Chemical non-equilibrium (run 42)



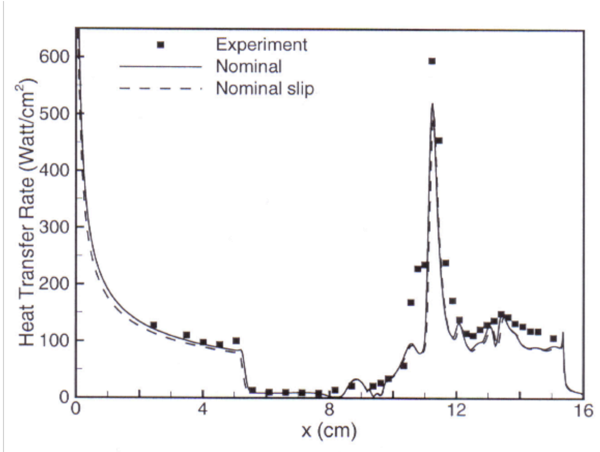
Roto-translational temperature and Mach number, RDS (256 x 512 mesh)

Von Karman Institute for Fluid Dynamics

Mach 11 hypersonic flow over double cone
Thermo-Chemical non-equilibrium (run 42)



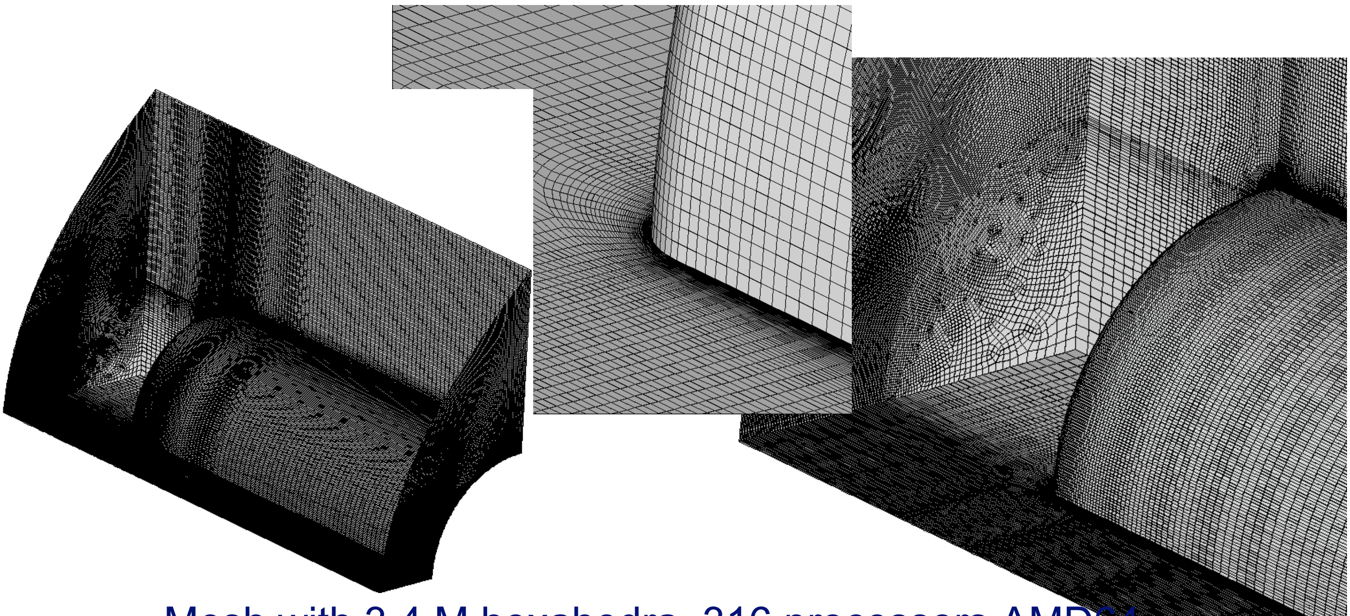
(a) Surface heat flux given by BCx scheme



(b) Surface heat flux given by [106]

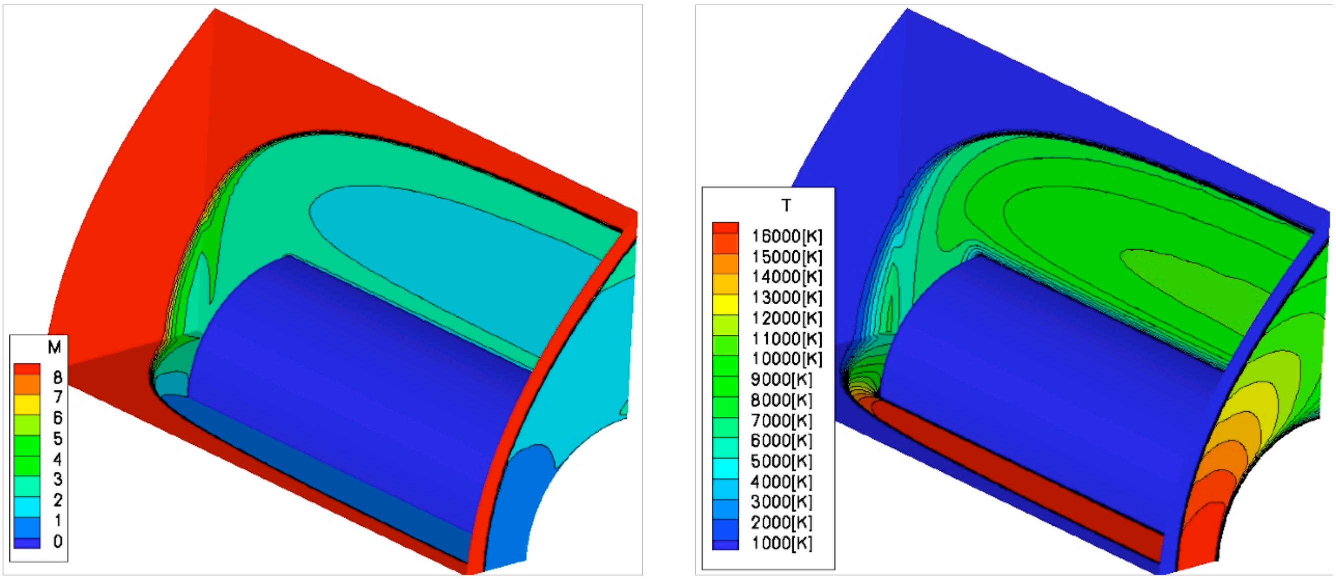
Comparison between Finite Volume and RDS (256 x 512 mesh)

Mach 18 hypersonic flow around Cylinder (DLR)
5-species air, Thermo-Chemical non-equilibrium



Mesh with 3.4 M hexahedra, 316 processors AMD64
Finite Volume scheme, AUSM+

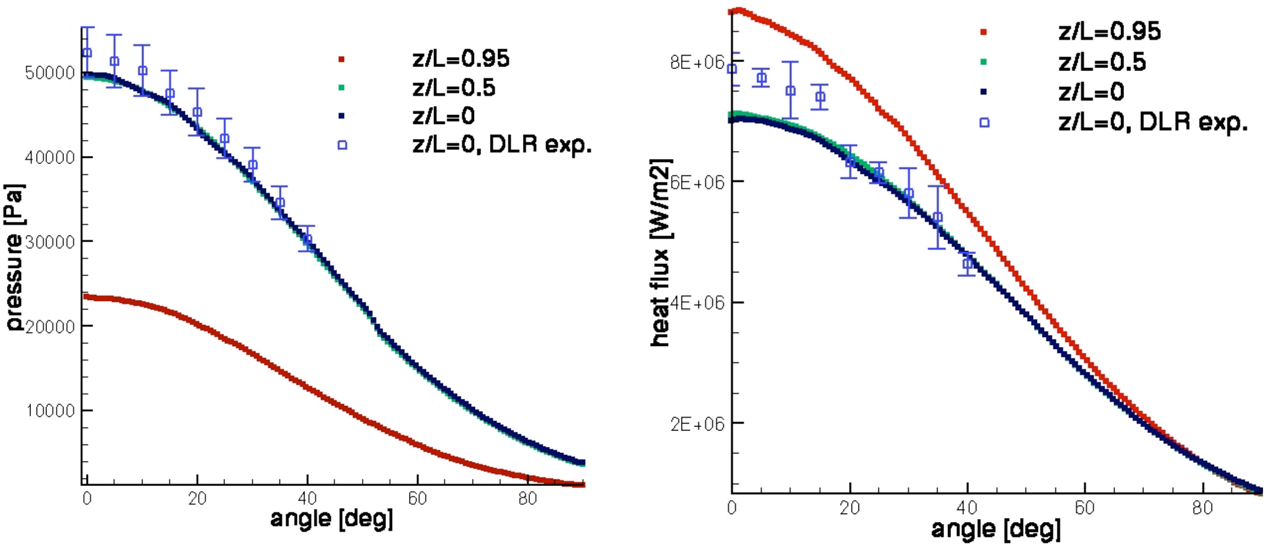
Mach 8 hypersonic flow around Cylinder (DLR)
5-species air, Thermo-Chemical non-equilibrium



(a) Mach number (b) Roto-translational temperature

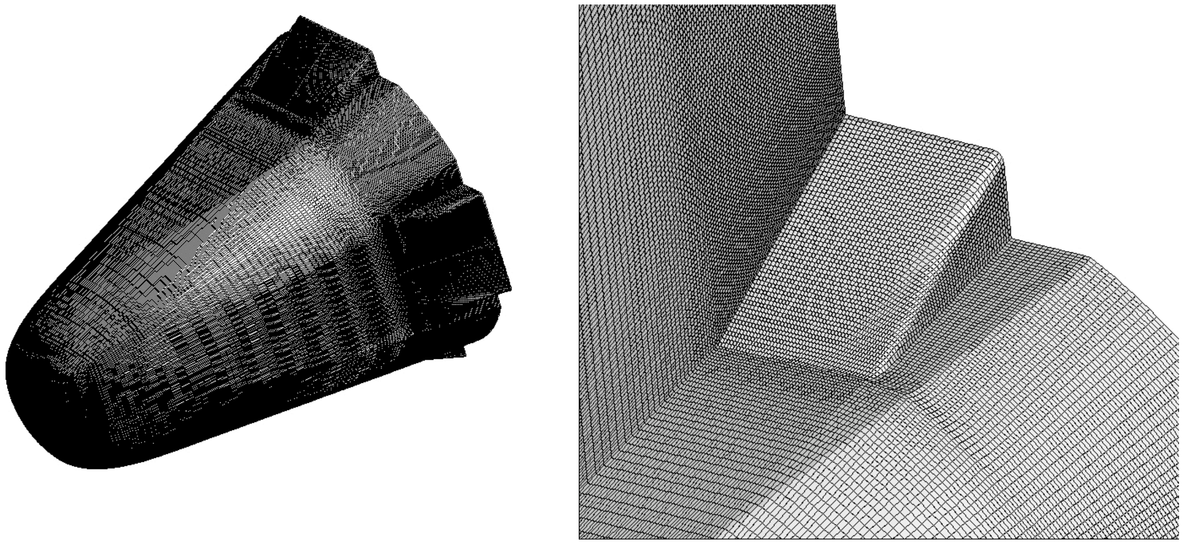
Finite Volume scheme, AUSM+

Mach 8 hypersonic flow around Cylinder (DLR)
5-species air, Thermo-Chemical non-equilibrium



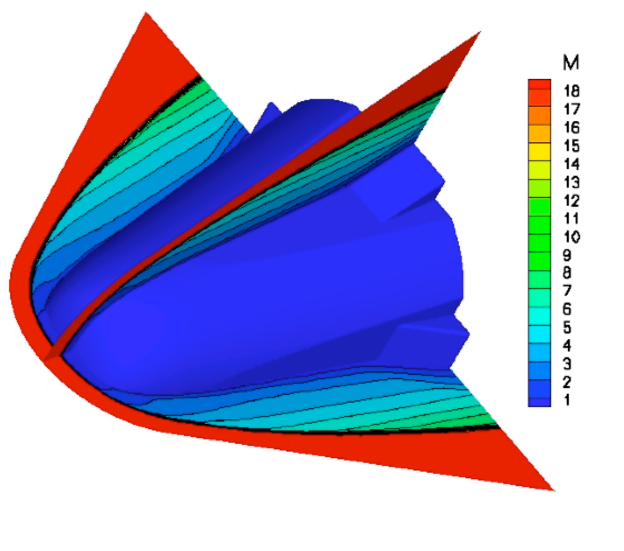
Pressure and heat flux at different spanwise locations

Mach 18 hypersonic flow around EXPERT vehicle 5-species air, Thermo-Chemical non-equilibrium

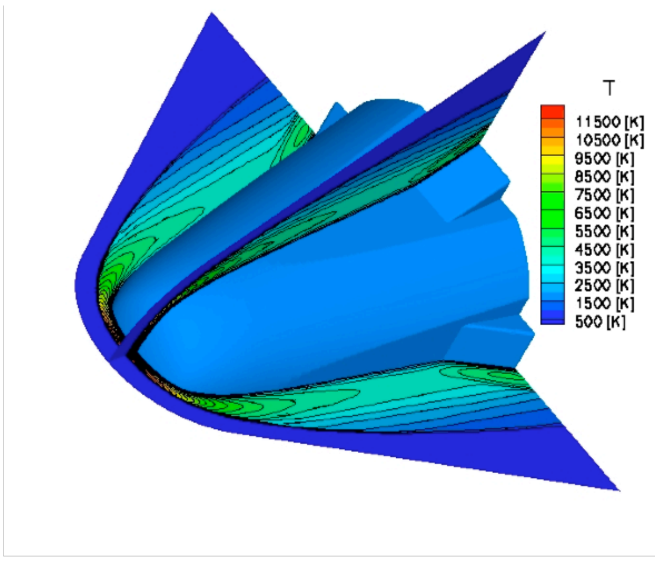


Mesh with 3.3 M hexahedra, 316 processors AMD64
Finite Volume scheme

Mach 18 hypersonic flow around EXPERT vehicle Thermo-Chemical non-equilibrium



(a) Mach number



(b) Roto-translational temperature

Conclusions and challenges

- CFD is going mainstream, large scale computations become standard
- Complex physics: reacting flows, combustion, electromagnetic …
- Complex industrial CAD geometries
- Interdisciplinary coupling extremely important

- Biggest challenge: how to cope with this, especially at academic level:
  (component based collaborative development platform)
- Other challenges: Higher order methods: work only started (DG, RDS)
- Challenge of hybrid anisotropic unstructured meshes