A Residual-Based Compact Scheme for (Real-Gas) Flow Simulations

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Overview of the talk

- motivation of the study
- design principles for a vertex-centered RBC scheme
  & comparison with Roe's scheme
- extension to real gas
  & further comparison with Roe's scheme
- future work

Standard approach for second-order steady compressible simulations with SU2

- second-order upwind scheme with reconstruction for space accuracy coupled with a first-order upwind scheme for fast convergence to steady-state
- extended stencil for the second-order upwind scheme vs compact stencil for the first-order implicit stage
- $\oplus$ simplicity of the first-order implicit stage solution
  $\Rightarrow$ reduced cost-per-iteration
- $\ominus$ lack of stencil consistency between explicit and implicit stage
  $\Rightarrow$ reduced intrinsic efficiency of the implicit treatment (although (agglomeration multigrid is also available for convergence acceleration)

Motivation of the study

RBC scheme for second-order steady compressible simulation with SU2

- Residual Based Compact scheme = truly multi-D upwind scheme providing second-order accuracy without reconstruction on a compact stencil
- initially developed on Cartesian grids : 2nd-order accuracy achieved on a compact $3 \times 3 \times 3$ stencil (versus non-compact 5-point per direction for conventional 2nd-order upwind schemes)
- extended to unstructured grids in a cell-centered FV formulation
- present work = implementation in SU2 $\Rightarrow$ vertex-centered FV formulation

Vertex-centered formulation for RBC

Design principles : residual-based

- first-order Roe numerical flux

$$\tilde{F}_{c_{ij}} = \tilde{F}(U_i, U_j) = \left(\frac{\vec{F}_i^c + \vec{F}_j^c}{2} \right) \cdot \vec{n}_{ij} - \underbrace{\frac{1}{2} P |\Lambda| P^{-1} (U_i - U_j)}_{d_{ij}}$$

- second-order Roe numerical flux (MUSCL reconstruction)

$$\tilde{F}_{c_{ij}} = \tilde{F}(U_i, U_j; \nabla U_i, \nabla U_j)$$

  with gradient calculation $\nabla U_i, \nabla U_j$ required $\Rightarrow$ extended support

- RBC numerical flux

$$\tilde{F}_{c_{ij}} = \left(\frac{\vec{F}_i^c + \vec{F}_j^c}{2} \right) \cdot \vec{n}_{ij} - d_{ij}$$

  with the dissipative flux computed in a compact way from the residual $r = \int \nabla \cdot \vec{F}^c$ (for inviscid flows) $\rightarrow$ second-order accuracy at steady-state

Design principles : residual-based

- RBC dissipative flux

$$d_{ij} = \frac{\Delta_{ij}}{2} P|\Psi(\Lambda^{\perp}, \Lambda^{\parallel})|P^{-1} r_{ij}$$

  where the appropriate eigenvalues Ψ are computed using both the normal and tangential velocities to the face shared by i and j (in 1D $\Psi = \Lambda$; in multi-D, truly multi-D upwinding), Δ_{ij}=distance between vertices

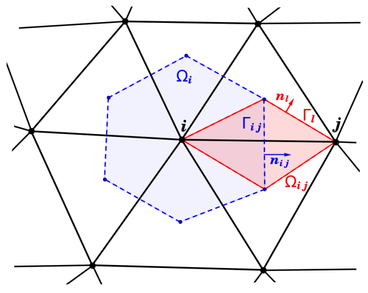
- residual r_{ij} computed on a shifted cell Ω_{ij}

$$r_{ij} = \frac{1}{|\Omega_{ij}|} \int_{\partial\Omega_{ij}} \vec{F}^c \cdot \vec{n}\, dl$$

Vertex-centered formulation for RBC

Design principles : residual-based **compact**

- residual r_{ij} computed on a shifted cell Ω_{ij} : $r_{ij} = \dfrac{1}{|\Omega_{ij}|} \sum_l \int_{\Gamma_l} \vec{F}^c \cdot \vec{n}\, dl$
- fluxes $\vec{F}^c$ to be computed at vertices + cell centers from vertex values
  $\Rightarrow$ stencil used = the one used for 1st-order upwind scheme
  but here 2nd-order dissipation (and overall accuracy) is achieved



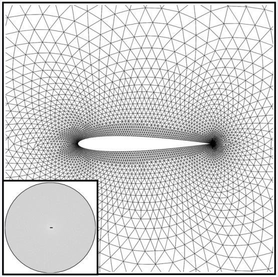
Vertex-centered formulation for RBC

Implementation (2D) in SU2

- new RBC convective flux as an alternative to Roe flux, etc
- available 1st-order implicit treatment directly re-used

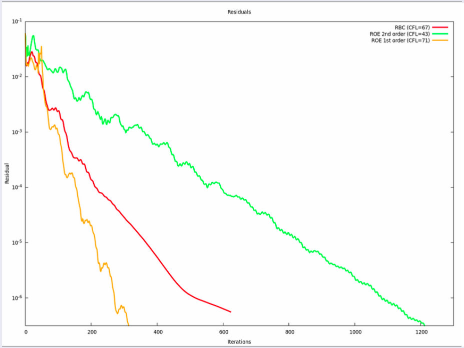
Example of application

- subsonic inviscid flow $M_\infty = 0.5$, $\alpha = 2^\circ$ over a NACA0012 airfoil
- unstructured grid (10216 triangles) provided in SU2 test-cases database



Comparison between Roe (1st and 2nd order) and RBC (2nd order)

Subsonic inviscid flow



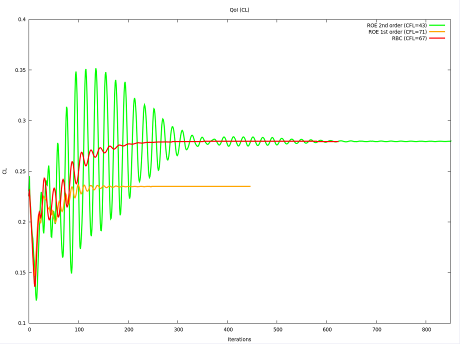


Figure: Convergence history (left : density residual, right : lift coefficient) for Roe O1, Roe O2, RBC (O2) used with their maximum allowable CFL.

- good efficiency offered by RBC (although some issue to solve with asymptotic convergence rate) for an accuracy equivalent to that of Roe O2
- cost per iteration to optimize for RBC (still $\approx +50\%$ w.r.t. Roe O2)

Extension to real-gas

Design principles

- formally unchanged numerical flux
- generalized Jacobian A_c and corresponding matrices P, P^{-1} including $\chi = \left(\frac{\partial P}{\partial \rho}\right)_e - \frac{e}{\rho}\left(\frac{\partial P}{\partial e}\right)_\rho$ and $\kappa = \frac{1}{\rho}\left(\frac{\partial P}{\partial e}\right)_\rho$
- Vinokur-Montagne Roe average for real gas
- all ingredients made available in SU2 thanks to the previous work of (Vitale *et al.*, AIAA Paper 2015)

Example of application

- transonic inviscid flow $M_\infty = 0.975$, $\alpha = 0^\circ$ over a NACA0012 airfoil
- fluid = PP10 described using Van der Waals EoS
- same first-order implicit stage

Steady solution

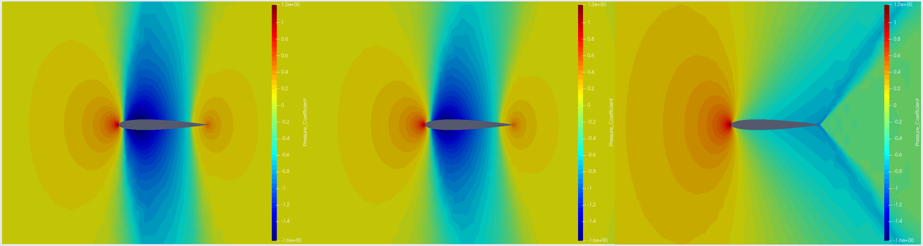


Figure: PP10 flow (VdW EoS) at $M_\infty = 0.975$. Contours of pressure coefficient : RBC (left), Roe O2 (center). RBC computation for ideal gas (right).

Comparison between RBC and Roe O2 for a real gas flow

Convergence history : PP10 flow (VdW EoS) at $M_\infty = 0.975$ over NACA0012

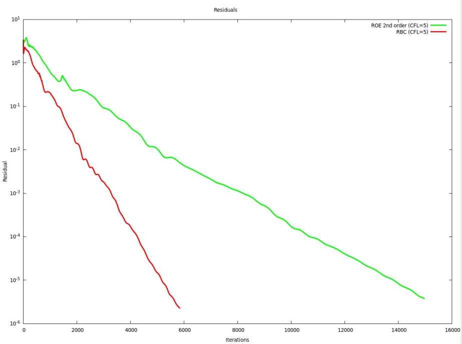


Figure: Density residual vs iterations for RBC ($CFL = 5$) and Roe O2 ($CFL = 2$). Schemes are used with their maximum allowable CFL. Cost per iteration (non-optimized) about +50% larger for RBC w.r.t. Roe O2.

- Improved efficiency offered by RBC (2D inviscid flow) for equivalent accuracy

Future work

"Straightforward" developments

- optimization of the boundary conditions (modified shifted cell)
- 3D extension for inviscid flows (perfect and real gas)

More involved developments

- proper extension to the viscous (laminar and turbulent) case
- RBC dissipative flux d_{ij} relies on the residual vanishing to achieve 2nd-order accuracy. For viscous flows,

$$r = \int \left(\nabla \cdot \vec{F}^c - \nabla \cdot \vec{F}^v \right)$$

$\Rightarrow$ the viscous flux must be computed for the balance on the shifted cell

Current work

Extension to (2D) incompressible flow

- straightforward since hyperbolic approach

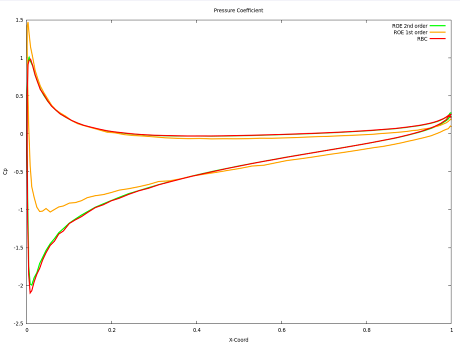


Figure: Water flow at $U_\infty = 1.775\,m/s$, $\alpha = 5°$ over a NACA0012 airfoil. Wall pressure coefficient at wall for RBC, Roe O2 and Roe O1.