Development of Generalized Low Mach Preconditioning Schemes

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Outline

- Motivation
- Approach
- Generalized Fluids Equations
- Asymptotic Theory
  - Derive appropriate preconditioning
  - Low Mach, Re, Fr and Str limits
- Discrete Formulation
  - Accuracy of Unsteady Computations
- Multiple Pseudo-Time Framework
- Summary

Motivation

- Wide range of scales
  - Inviscid: Low Mach to Hypersonic
  - Viscous: Low to high Reynolds numbers
  - Unsteady: Low to high frequencies
  - Source terms: turbulence, chemistry and phase change
- Wide range of equations of state
  - Perfect gas
  - Liquids
  - Real gases
  - Multi-component gases
  - Multiple phases

Approach

- Time-Marching or Density-Based Methods
  - Numerics related to unsteady physics & mathematics
  - Errors handled by convection and diffusion processes
- Characteristics:
  - Well suited to transonic and supersonic flows
  - Unsuited to low Mach flows because of wave stiffness
- Preconditioning
  - Pseudo-acoustic waves by altering time-derivatives
  - Inspired by Chorin's artificial compressibility (1967)
- Use Asymptotic Theory
  - Proper choice can account for all relevant limits

Fluids Equations

- Dual-Time Form:

$$\frac{\partial Q}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H$$

where

$$Q = (\rho,\ \rho u_i,\ e)^T$$

- Pseudo-time term introduced purely for numerics:
  - To derive proper discrete form
  - To act as an agency for non-linear relaxation
  - To enhance convergence of the linear solver
- Pseudo-Time Definition:
  - Ill-posed for certain equations of state (I.e., constant ρ)

Generalized Fluids Equations

- Change of Variables:

$$\frac{\partial Q}{\partial Q_p}\frac{\partial Q_p}{\partial \tau}+\frac{\partial Q}{\partial t}+\frac{\partial E_i}{\partial x_i}=\frac{\partial V_i}{\partial x_i}+H$$

where

$$Q_p=(p,\ u_i,\ T)^T$$

- Definition:

$$\frac{\partial Q}{\partial Q_p}=\begin{pmatrix}\rho_p & 0 & \rho_T\\ u_i\rho_p & \rho\delta_{ij} & u_i\rho_T\\ h_o\rho_p-(1-\rho h_p) & \rho u_j & h_o\rho_T+\rho h_T\end{pmatrix}\qquad \rho_p=\left(\frac{\partial\rho}{\partial p}\right)_T$$

Generalized Equation of State

- General State Relations

$$\rho = \rho(p,\ T) \quad h = h(p,\ T)$$

- System is well-posed for time-marching solutions
  - All variables can be updated for general fluids
  - Can be extended to multi-component gases and liquids
- But, it not necessarily well-conditioned:
  - Different time-scales control the physical processes
  - A “good” numerical scheme requires good conditioning
  - Use asymptotic theory to understand behavior and to devise appropriate preconditioning scaling

Asymptotic Analysis

- Well-established mathematical analysis tool
- Applied to CFD algorithm analysis by:
  - Guerra and Gustaffsson (1986)
  - Merkle and Choi (1987)
- Original Motivation:
  - Derive preconditioning for low Mach limit
  - Assess discrete accuracy (Guillard and Viozat, 1999)
- Contributions of the present authors (1999):
  - Analyze Euler, Navier-Stokes and unsteady scales
  - Derive appropriate preconditioning in these limits
  - Ensure discrete accuracy and convergence efficiency

Asymptotic Expansion

- Momentum Equation:

$$\left(\frac{L}{\tau_r u_r}\right)\rho\frac{\partial u}{\partial \tau}+St_r\rho\frac{\partial u}{\partial t}+\rho u\frac{\partial u}{\partial x}+\left(\frac{1}{\gamma M_r^2}\right)\varepsilon\frac{\partial p_1}{\partial x}=\frac{1}{Re_r}\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+Fr^2\rho g$$

where $p_0 = Constant$

and ε is a small parameter to be defined later.

- Continuity Equation:

$$\left(\frac{L}{\tau_r u_r}\right)\left(\tilde{\rho}_p\varepsilon\frac{\partial p_1}{\partial \tau}+\tilde{\rho}_T\frac{\partial T}{\partial \tau}\right)+St_r\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}=0$$

Perturbation Parameter

- Definition:
  - Balance the pressure gradient with the dominant term in the momentum equation for various limits

- Inviscid Low Mach Limit: $\varepsilon = \gamma M_r^2$

- Viscous Low Re Limit: $\varepsilon = \gamma M_r^2 / Re$

- High Fr Limit: $\varepsilon = \gamma M_r^2 Fr^2$

- Unsteady High Str Limit: $\varepsilon = \gamma M_r^2 Str$

Dispersion Analysis

- Linearized Perturbation Equations:

$$\tilde{\Gamma}_p \frac{\partial \tilde{Q}_p}{\partial \tau} + \tilde{\Gamma}_e \frac{\partial \tilde{Q}_p}{\partial t} + \tilde{A} \frac{\partial \tilde{Q}_p}{\partial x} = \frac{\partial}{\partial x}\left(\tilde{R} \frac{\partial \tilde{Q}_p}{\partial x}\right) + \tilde{D} Q_p$$

- Solution:

$$Q_p(x,\tau) = \hat{Q}_p exp[ik(x - \omega\tau)]$$

- Dispersion Relation:

$$det\ \left[\ \tilde{\Gamma}_p(-ik\omega) + \frac{\tilde{\Gamma}_e}{\Delta t} - \tilde{D} - \tilde{A}(ik) + \tilde{R}(k^2)\ \right] = 0$$

Dispersion Analysis

- Complex Phase Speeds:

$$\omega_1 = \frac{u}{\alpha}\left[1 - \frac{i\,Str}{(k\Delta x)} - \frac{i(k\Delta x)}{PrRe}\right]$$

$$\omega_{2,3} = \frac{u}{2\alpha}\left[1 - \frac{2i\,Str}{(k\Delta x)} - i\frac{(k\Delta x)}{Re}\right] \pm S$$

where

$$S = \sqrt{\frac{u^2}{\alpha^2}\left(1 - i\frac{k\delta x}{Re}\right)^2 + \frac{4}{\varepsilon\alpha\tilde{\rho}_p}}$$

Characteristics

- Inviscid Limit:
  - Wave speeds are $\approx u, u \pm c$
  - Stiff at low Mach numbers
- Viscous Limit:
  - Wave speeds are $\approx iu/Re, u \pm c$
  - Two acoustic modes and one viscous damping mode
  - Can be stiff at low-Re
- Unsteady High Frequency Limit:
  - Wave speeds are $\approx iu\ Str, u(1 + iu\ Str) \pm c$
  - Two acoustic modes and one sink-like damping mode
  - For very high Str, three sink-like damping modes

Preconditioning

- Stiffness is due to:
  - Scaling of the first-order pressure time-derivative in continuity equation

$$\left(\frac{L}{\tau_r u_r}\right)\left(\tilde{\rho}_p \varepsilon \frac{\partial p_1}{\partial \tau} + \tilde{\rho}_T \frac{\partial T}{\partial \tau}\right) + St_r \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

- Preconditioning:
  - Rescale pressure-time derivative
  - Render pressure corrections to be order one

$$\tilde{\rho}_p \rightarrow \tilde{\rho}'_p$$

Preconditioning Scaling

- Inviscid Low Mach Limit: $$\tilde{\rho}'_p = \frac{\tilde{\rho}_p}{M^2}$$
- Viscous Low Re Limit: $$\tilde{\rho}'_p = \frac{\tilde{\rho}_p \, Re^2}{M^2}$$
- High Fr Limit: $$\tilde{\rho}'_p = \frac{\tilde{\rho}_p \, Fr^4}{M^2}$$
- Unsteady High Str Limit: $$\tilde{\rho}'_p = \frac{\tilde{\rho}_p \, Str^2}{M^2}$$

Preconditioned Equations

- Change of Variables:

$$\Gamma_p \frac{\partial Q_p}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H$$

- Preconditioning Matrix:

$$\Gamma_p = \begin{pmatrix} \rho'_p & 0_j & \rho_T \\ u\rho'_p & \rho\delta ij & u\rho_T \\ h_o\rho'_p - (1 - \rho h_p) & \rho u_j & h_o\rho_T + \rho h_T \end{pmatrix}$$

$$\rho'_p = \rho_p \, Max[Min(\frac{1}{M^2}, \frac{Re^2}{M^2}, \frac{Fr^4}{M^2}, \frac{Str^2}{M^2}), 1]$$

Convergence Enhancement

- Dispersion Analysis
  - Complex wave speeds can again be obtained
  - Combination of particle and pseudo-acoustic modes
  - All relevant limits are seen to be well-conditioned
- System Characteristics are optimized
  - Inviscid limit: acoustic speed and particle speed
  - Viscous limit: acoustic speed and diffusion scale
  - Unsteady limit: acoustic speed and physical time scale
- Relationship to Other Preconditioners:
  - Inviscid limit similar to Turkel, van Leer, Weiss-Smith
  - Asymptotic derivation enables extension to all limits

Asymptotic Analysis of Discrete System

- Extension to Discrete Form:
  - Apply asymptotic expansions to the discrete version
  - Express scheme as central flux + artificial dissipation
- Requirements on Artificial Viscosity:
  - At most the same order as the dominant physical terms
  - All fields must have adequate dissipation
  - Use von Neumann stability analysis to verify
- Different Formulations
  - Scalar Dissipation (Jameson, Turkel)
  - Flux-Difference (Roe) or Matrix-Dissipation (Turkel)
  - AUSM- or CUSP-like (Liou, Jameson)

Different Dissipation Schemes

- Scalar Dissipation:

$$\Gamma \left. \frac{\partial Q_p}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} \right|_{cd} = \frac{\partial V_i}{\partial x_i} + H + \frac{\Delta x_i}{2} \frac{\partial}{\partial x_i} \Lambda \left(\Gamma^{-1} A \right) \frac{\partial Q}{\partial x_i}$$

- Flux-Difference or Matrix Dissipation

$$\Gamma \left. \frac{\partial Q_p}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} \right|_{cd} = \frac{\partial V_i}{\partial x_i} + H + \frac{\Delta x_i}{2} \frac{\partial}{\partial x_i} \Lambda \left| \Gamma^{-1} A \right| \frac{\partial Q}{\partial x_i}$$

- AUSM- or CUSP-like Schemes

$$\Gamma \left. \frac{\partial Q_p}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} \right|_{cd} = \frac{\partial V_i}{\partial x_i} + H + \frac{\Delta x_i}{2} \frac{\partial}{\partial x_i} \Lambda_i \frac{\partial Q}{\partial x_i}$$

where

$$\Lambda = K \left| diag(\sigma(\Gamma^{-1} A), u_i, u) \right|$$

Inviscid Limit

Scalar/Matrix Dissipation

- Without Preconditioning

$$AD = \begin{bmatrix} O(M) & O(M) & O(1) \\ O(M) & O(1/M) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- With Preconditioning

$$AD = \begin{bmatrix} O(1) & O(1) & O(1) \\ O(1) & O(1) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- Inviscid Preconditioning insures proper scaling

Viscous Limit

Scalar/Matrix Dissipation

- With Inviscid Preconditioning

$$AD = \begin{bmatrix} O(1/\mathrm{Re}) & O(1) & O(1) \\ O(\mathrm{Re}) & O(1) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- With Preconditioning

$$AD = \begin{bmatrix} O(1) & O(\mathrm{Re}) & O(1) \\ O(1) & O(1/\mathrm{Re}) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- Viscous preconditioning insures proper scaling

Unsteady Limit

Scalar/Matrix Dissipation

- With Preconditioning

$$AD = \begin{bmatrix} O(Str) & O(1) & O(1) \\ O(1/Str) & O(1) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- With Preconditioning

$$AD = \begin{bmatrix} O(1) & O(1/Str) & O(1) \\ O(1) & O(Str) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- Unsteady preconditioning does not scale correctly

Unsteady Limit

AUSM-/CUSP-like Form

- Formulation:

$$\Gamma \frac{\partial Q_p}{\partial \tau} + \frac{\partial Q}{\partial t} + \left.\frac{\partial E_i}{\partial x_i}\right|_{cd} = \frac{\partial V_i}{\partial x_i} + H + \frac{\Delta x_i}{2} \frac{\partial}{\partial x_i} \Lambda_i \frac{\partial Q}{\partial x_i}$$

$$\Lambda = K \left| diag(\sigma(\Gamma^{-1} A), u_i, u) \right|$$

- With Unsteady Preconditioning

$$AD = \begin{bmatrix} O(1) & 0 & O(1) \\ O(1) & O(1) & 0 \\ 0 & 0 & O(1) \end{bmatrix}$$

- Now, the dissipation terms are scaled correctly

Robustness Issues

- Preconditioning has robustness difficulties:
  - Presence of stagnation regions
  - Influence of large pressure changes
- Stagnation Regions
  - Global cut-off (Turkel and others)
  - We employ a “local” maximum definition
- Large-Scale Pressure Changes at Low Mach
  - Linearly stable only for errors in the dynamic pressure
  - Non-linear instability caused by “fast” waves
  - Due to changes in the thermodynamic/acoustic pressure

Remedy

- Note:
  - Preconditioning necessary for efficiency and accuracy
  - Robustness demands are different
- Standard Approaches
  - Use physical system until “fast” waves are eliminated
  - Use “unsteady” form until “fast” waves are eliminated
  - Need to devise a clean framework for “switching”
- Multiple Pseudo Time Framework:
  - Use preconditioning for discretization
  - Do not use for non-linear time-marching
  - Use preconditioning for linear solver iterations

Multiple-Time Formulation

$$\Gamma_1 \frac{\partial Q_p}{\partial \tau_1} + \Gamma_2 \frac{\partial Q_p}{\partial \tau_2} + \Gamma_3 \frac{\partial Q_p}{\partial \tau_3} + \frac{\partial Q}{\partial t} + \frac{\partial E_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H$$

- Outermost Time: Accuracy
  - Choose preconditioning for accurate flux formulation
- Intermediate Time: Robustness
  - For non-linear time-marching to maintain robustness
  - Use physical time-derivatives
- Innermost Time: Efficiency
  - Choose preconditioning to optimize linear convergence

Properties

- Artificial Dissipation Time-Step
  - Set to infinity
- Non-linear Time-Step
  - Start at small values and ramp up to infinity
  - Not limited by linear solver stability restrictions
- Linear Solver
  - Start at infinity and reduce to optimal value for scheme
  - Inner iterations can be done at each non-linear step
  - Similar to unsteady computations
  - LU decomposition of matrix inverse may be stored

Summary

- Derived a preconditioning approach:
  - Suitable for all Mach, Re, Str, Fr, etc.
  - Enables accurate discrete formulation at all limits
  - Enables efficient linear solver convergence
  - Preferable not to introduce at non-linear iteration level
- Asymptotic Analysis
  - Derivation of preconditioning
  - Assessment of accuracy
- Time-Marching:
  - Provides a link between numerics and physics