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- ***AF-ADI Scheme***
  - **Approximate factorization along ξ- and η- directions**

$$\left[\mathbf{I}+\mu\Delta t\left(D_\xi^-\bar{\mathbf{A}}^+ + D_\xi^+\bar{\mathbf{A}}^-\right)\right]\left[\mathbf{I}+\mu\Delta t\left(D_\eta^-\bar{\mathbf{B}}^+ + D_\eta^+\bar{\mathbf{B}}^-\right)\right]\Delta\bar{\mathbf{U}}_{i,j}^n = -\Delta t\bar{\mathbf{R}}_{i,j}^n$$

with the factorization error $= \mu^2\Delta t^2\left(\partial\bar{A}^n/\partial\xi\right)\left(\partial\bar{B}^n/\partial\eta\right)$

  - **The resulting formulation requires block tri-diagonal matrix inversion along ξ- and η- directions.**

$$D_\xi^-\bar{\mathbf{A}}^+ = \frac{1}{\Delta\xi}\left(\bar{\mathbf{A}}_{i,j}^+ - \bar{\mathbf{A}}_{i-1,j}^+\right), D_\xi^+\bar{\mathbf{A}}^- = \frac{1}{\Delta\xi}\left(\bar{\mathbf{A}}_{i+1,j}^- - \bar{\mathbf{A}}_{i,j}^-\right)\ ;\ D_\eta^-\bar{\mathbf{B}}^+ = \frac{1}{\Delta\eta}\left(\bar{\mathbf{B}}_{i,j}^+ - \bar{\mathbf{B}}_{i,j-1}^+\right), D_\eta^+\bar{\mathbf{B}}^- = \frac{1}{\Delta\eta}\left(\bar{\mathbf{B}}_{i,j+1}^- - \bar{\mathbf{B}}_{i,j}^-\right)$$

$$\left[\mathbf{I}+\mu\frac{\Delta t}{\Delta\xi}\left(-\bar{\mathbf{A}}_{i-1,j}^+ + \left(\bar{\mathbf{A}}_{i,j}^+ - \bar{\mathbf{A}}_{i,j}^-\right) + \bar{\mathbf{A}}_{i+1,j}^-\right)\right]\underbrace{\left[\mathbf{I}+\mu\frac{\Delta t}{\Delta\eta}\left(-\bar{\mathbf{B}}_{i,j-1}^+ + \left(\bar{\mathbf{B}}_{i,j}^+ - \bar{\mathbf{B}}_{i,j}^-\right) + \bar{\mathbf{B}}_{i,j+1}^+\right)\right]\Delta\bar{\mathbf{U}}_{i,j}^n}_{\equiv\Delta\bar{\mathbf{U}}_{i,j}^*} = -\Delta t\bar{\mathbf{R}}_{i,j}^n$$

    - ξ-sweep (relaxation along the ξ-direction)

$$-\left(\mu\frac{\Delta t}{\Delta\xi}\bar{\mathbf{A}}_{i-1,j}^+\right)\Delta\bar{\mathbf{U}}_{i-1,j}^* + \left[\mathbf{I}+\mu\frac{\Delta t}{\Delta\xi}\left(\bar{\mathbf{A}}_{i,j}^+ - \bar{\mathbf{A}}_{i,j}^-\right)\right]\Delta\bar{\mathbf{U}}_{i,j}^* + \left(\mu\frac{\Delta t}{\Delta\xi}\bar{\mathbf{A}}_{i+1,j}^-\right)\Delta\bar{\mathbf{U}}_{i+1,j}^* = -\Delta t\bar{\mathbf{R}}_{i,j}^n$$

    - η-sweep (relaxation along the η-direction)

$$-\left(\mu\frac{\Delta t}{\Delta\eta}\bar{\mathbf{B}}_{i,j-1}^+\right)\Delta\bar{\mathbf{U}}_{i,j-1}^n + \left[\mathbf{I}+\mu\frac{\Delta t}{\Delta\eta}\left(\bar{\mathbf{B}}_{i,j}^+ - \bar{\mathbf{B}}_{i,j}^-\right)\right]\Delta\bar{\mathbf{U}}_{i,j}^n + \left(\mu\frac{\Delta t}{\Delta\eta}\bar{\mathbf{B}}_{i,j+1}^-\right)\Delta\bar{\mathbf{U}}_{i,j+1}^n = \Delta\mathbf{U}_{i,j}^*$$

$$\rightarrow\ \bar{\mathbf{U}}_{i,j}^{n+1} = \bar{\mathbf{U}}_{i,j}^n + \Delta\bar{\mathbf{U}}_{i,j}^n$$

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- For 2-D N x N mesh with single unknown at each grid point, operating count = $O(N^2)$
- μ for C-N $\leftrightarrow$ fully implicit : $\frac{1}{2\Delta\xi} \leftrightarrow \frac{1}{\Delta\xi},\ \frac{1}{2\Delta\eta} \leftrightarrow \frac{1}{\Delta\eta}$
- 3 types of errors
  - Linearization error for the implicit part
  - Factorization error to approximate the block penta-diagonal term
  - Discretization error of the residual term
- Factorization error dominant at high frequency range, and parallelization issue

- ***LU-SGS scheme***
  - **Instead of dimensional splitting, a variant of Gauss-Seidel relaxation is applied to Eq. (2) in symmetric forward & backward manner.**
    - See the works by Yoon and Jameson(1988), and others
  - **Ex) LU-SGS for 1-D case**

From $\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{0},\quad \frac{\Delta \mathbf{U}^n}{\Delta t} + (1-\mu)\frac{\partial \mathbf{F}^n}{\partial x} + \mu \frac{\partial \mathbf{F}^{n+1}}{\partial x} = \mathbf{0}$

With $\mathbf{F}^{n+1} \cong \mathbf{F}^n + \mathbf{A}^n \Delta \mathbf{U}^n,\ \mathbf{A}^n = \left(\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\right)^n \rightarrow \frac{\Delta \mathbf{U}^n}{\Delta t} + \mu\left(\frac{\partial \mathbf{A}^n}{\partial x}\right)\Delta \mathbf{U}^n = -\frac{\partial \mathbf{F}^n}{\partial x} = -\mathbf{R}\left(\mathbf{U}^n\right).$

From $\mathbf{A}^n = \mathbf{A}^+ + \mathbf{A}^-,\ \left[\mathbf{I} + \mu\Delta t\left(D^-\mathbf{A}^+ + D^+\mathbf{A}^-\right)\right]\Delta \mathbf{U}^n = -\Delta t \mathbf{R}^n$ or

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$$\Delta\mathbf{U}_i^n + \lambda\left(\mathbf{A}_i^+\Delta\mathbf{U}_i^n - \mathbf{A}_{i-1}^+\Delta\mathbf{U}_{i-1}^n\right) + \lambda\left(\mathbf{A}_{i+1}^-\Delta\mathbf{U}_{i+1}^n - \mathbf{A}_i^-\Delta\mathbf{U}_i^n\right) = -\Delta t\mathbf{R}_i^n, \quad \lambda = \mu\,\Delta t/\Delta x$$

$$\rightarrow \; -\lambda\mathbf{A}_{i-1}^+\Delta\mathbf{U}_{i-1}^n + \left[\mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)\right]\Delta\mathbf{U}_i^n + \lambda\mathbf{A}_{i+1}^-\Delta\mathbf{U}_{i+1}^n = -\Delta t\mathbf{R}_i^n \quad \text{or} \quad A\Delta\mathbf{U}^n = -\Delta t\mathbf{R}^n$$

Gauss-Seidel relaxations in a symmetric fashion as follows

- (forward sweep) $-\lambda\mathbf{A}_{i-1}^+\Delta\mathbf{U}_{i-1}^* + \left[\mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)\right]\Delta\mathbf{U}_i^* = -\Delta t\mathbf{R}_i^n$
- (backward sweep) $\left[\mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)\right]\Delta\mathbf{U}_i^n + \lambda\mathbf{A}_{i+1}^-\Delta\mathbf{U}_{i+1}^n - \lambda\mathbf{A}_{i-1}^+\Delta\mathbf{U}_{i-1}^* = -\Delta t\mathbf{R}_i^n$

By substracting forward sweep from backward sweep,

$$\left[\mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)\right]\Delta\mathbf{U}_i^n + \lambda\mathbf{A}_{i+1}^-\Delta\mathbf{U}_{i+1}^n = \left[\mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)\right]\Delta\mathbf{U}_i^* \quad \text{or} \quad U\Delta\mathbf{U}^n = D\Delta\mathbf{U}^*$$

From $\Delta\mathbf{U}^* = D^{-1}U\Delta\mathbf{U}^n$ and $L\Delta\mathbf{U}^* = -\Delta t\mathbf{R}^n$, we have $LD^{-1}U\Delta\mathbf{U}^n = -\Delta t\mathbf{R}^n$

$\rightarrow$ a variant of LU decomposition to invert $A\Delta\mathbf{U}^n = -\Delta t\mathbf{R}^n$

with $L = -\lambda\mathbf{A}_{i-1}^+ + \mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)$, $D = \mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right)$, $U = \mathbf{I} + \lambda\left(\mathbf{A}_i^+ - \mathbf{A}_i^-\right) + \lambda\mathbf{A}_{i+1}^-$.

- **Symmetric G-S relaxation to Eq. (2)**
  - The same procedure for 2-D case with

$$\left[\mathbf{I} + \mu\Delta t\left(D_\xi^-\bar{\mathbf{A}}^+ + D_\xi^+\bar{\mathbf{A}}^- + D_\eta^-\bar{\mathbf{B}}^+ + D_\eta^+\bar{\mathbf{B}}^-\right)\right]\Delta\bar{\mathbf{U}}^n = -\Delta t\bar{\mathbf{R}}_{i,j}^n \quad \text{or} \quad A\Delta\mathbf{U}^n = -\Delta t\mathbf{R}^n$$

- (forward sweep) $\left[\mathbf{I} + \Delta t\left\{\left(\bar{\mathbf{A}}_{i,j}^+ - \bar{\mathbf{A}}_{i,j}^-\right) + \left(\bar{\mathbf{B}}_{i,j}^+ - \bar{\mathbf{B}}_{i,j}^-\right)\right\}\right]\Delta\bar{\mathbf{U}}_{i,j}^* - \Delta t\bar{\mathbf{A}}_{i-1,j}^+\Delta\bar{\mathbf{U}}_{i-1,j}^* - \Delta t\bar{\mathbf{B}}_{i,j-1}^+\Delta\bar{\mathbf{U}}_{i,j-1}^*$

$$= -\Delta t\bar{\mathbf{R}}_{i,j}^n$$

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- (backward sweep)

$$\left[\mathbf{I}+\Delta t\left\{\left(\bar{\mathbf{A}}^{+}_{i,j}-\bar{\mathbf{A}}^{-}_{i,j}\right)+\left(\bar{\mathbf{B}}^{+}_{i,j}-\bar{\mathbf{B}}^{-}_{i,j}\right)\right\}\right]\Delta\bar{\mathbf{U}}^{n}_{i,j}+\Delta t\bar{\mathbf{A}}^{-}_{i+1,j}\Delta\bar{\mathbf{U}}^{n}_{i+1,j}+\Delta t\bar{\mathbf{B}}^{-}_{i,j+1}\Delta\bar{\mathbf{U}}^{n}_{i,j+1}$$
$$-\Delta t\bar{\mathbf{A}}^{+}_{i-1,j}\Delta\bar{\mathbf{U}}^{*}_{i-1,j}-\Delta t\bar{\mathbf{B}}^{+}_{i,j-1}\Delta\bar{\mathbf{U}}^{*}_{i,j-1}=-\Delta t\bar{\mathbf{R}}^{n}_{i,j}$$

Subtracting forward from backward sweep gives $LD^{-1}U\Delta\bar{\mathbf{U}}^{n}=-\Delta t\bar{\mathbf{R}}^{n}$.

with $L=\mathbf{I}+\Delta t\left(D^{-}_{\xi}\bar{\mathbf{A}}^{+}+D^{-}_{\eta}\bar{\mathbf{B}}^{+}-\bar{\mathbf{A}}^{-}-\bar{\mathbf{B}}^{-}\right)$, $D=\mathbf{I}+\Delta t\left(\bar{\mathbf{A}}^{+}-\bar{\mathbf{A}}^{-}+\bar{\mathbf{B}}^{+}-\bar{\mathbf{B}}^{-}\right)$,

$U=\mathbf{I}+\Delta t\left(D^{+}_{\xi}\bar{\mathbf{A}}^{-}+D^{+}_{\eta}\bar{\mathbf{B}}^{-}+\bar{\mathbf{A}}^{+}+\bar{\mathbf{B}}^{+}\right)$.

- Instead of λ-based splitting $\bar{\mathbf{A}}^{\pm}=\bar{R}_{A}\Lambda^{\pm}_{A}\bar{R}^{-1}_{A}$, $\bar{\mathbf{B}}^{\pm}=\bar{R}_{B}\Lambda^{\pm}_{B}\bar{R}^{-1}_{B}$, a ρ-based splitting is introduced to avoid block matrix inversion and to maintain diagonal dominance.

$$\bar{\mathbf{A}}^{\pm}=\frac{1}{2}\left(\bar{\mathbf{A}}\pm\rho\left(\bar{\mathbf{A}}\right)\mathbf{I}\right),\ \bar{\mathbf{B}}^{\pm}=\frac{1}{2}\left(\bar{\mathbf{B}}\pm\rho\left(\bar{\mathbf{B}}\right)\mathbf{I}\right)\ \text{with}\ \rho\left(\bar{\mathbf{A}}\right)=k\left|\lambda\left(\bar{\mathbf{A}}\right)\right|_{\max}\ \text{and}\ k=1+\alpha(>0)$$

- A variant of LU decomposition to efficiently invert $A\Delta\mathbf{U}^{n}=-\Delta t\mathbf{R}^{n}$
- Complete vectorization along diagonals of *i+j=const* (or coloring scheme)
- Easily extendable to complex flows, such as chemical reacting flows
  - λ-based splitting can be used for non-calorically perfect gas.
- Parallelization issue and temporal accuracy
- LU-SGS / AF-ADI relaxation combined with MG
  - After transferring solution and residuals onto coarse grid, compute the multi-grid forcing term (***P***) and update solution $\rightarrow$ $A\Delta\mathbf{U}^{n}$ _by *LU-SGS* or *AF-ADI* $=-\Delta t(\mathbf{R}+\mathbf{P})$ _ by multi-grid

Chap. 4-7. Time-Accurate Schemes

- ***TVD R-K scheme***
  - **Higher-order R-K schemes preserving TVD stability**
    - See the works by Shu and Osher(1988), and others
    - Linearly stable R-K schemes are not sufficient to support monotonic solutions.
      - Ex: computed solutions with linearly(LS)/non-linearly(NLS) stable R-K methods

$$u_t + uu_x = 0 \text{ with } u_0(x) = \begin{cases} 1, & \text{if } x \le 0 \\ -0.5, & \text{if } x \le 0 \end{cases}$$

- One-step Euler-forward from the semi-discrete form of $u_t = L(u)$ by evaluating $F_{i+1/2}$ with a 2nd-order monotonic flux $\rightarrow$ $u^{n+1} = u^n + \Delta t L(u^n)$ with $TV(u^{n+1}) \le TV(u^n)$

- 2-stage R-K time integrations

$$\text{(LS) } u^{(0)} = u^n,\ u^{(1)} = u^{(0)} - 20\Delta t L(u^{(0)}),\ u^{(2)} = u^{(0)} + \frac{41}{40}\Delta t L(u^{(0)}) - \frac{1}{40}\Delta t L(u^{(1)}) \ \rightarrow\ u^{n+1} = u^{(2)}$$

$$\text{(NLS) } u^{(0)} = u^n,\ u^{(1)} = u^{(0)} + \Delta t L(u^{(0)}),\ u^{(2)} = \frac{1}{2}u^{(0)} + \frac{1}{2}u^{(1)} + \frac{1}{2}\Delta t L(u^{(1)}) \ \rightarrow\ u^{n+1} = u^{(2)}$$

$\rightarrow$ both are the same for linear case, but yield different solutions for non-linear case.

- TVD-stable, multi-stage R-K schemes by optimizing standard R-K coefficients
  - One-step TVD scheme: $u^{n+1} = u^n + \Delta t L(u^n) \equiv EL(u^n)$ with $TV(u^{n+1}) \le TV(u^n)$
  - Multi-stage TVD R-K schemes: from general m-stage R-K method as

$$u^{(0)} = u^n,\quad u^{(k)} = \sum_{j=0}^{k-1}\left(\alpha_{jk}u^{(j)} + \beta_{jk}\Delta t L(u^{(j)})\right) \text{ with } \sum_{j=0}^{k-1}\alpha_{jk} = 1,\ 1 \le k \le m,\quad u^{n+1} = u^{(m)}$$

Chap. 4-7. Time-Accurate Schemes

If α_{jk} and β_{jk} are all positive, $u^{(k)}$ can be regarded as a convex combination of EL operators as

$$u^{(k)} = \sum_{j=0}^{k-1} \alpha_{jk} \left(u^{(j)} + \Delta t_j L(u^{(j)}) \right) = \sum_{j=0}^{k-1} \alpha_{jk} EL(u^{(j)}) \text{ with } \Delta t_j = \frac{\beta_{jk}}{\alpha_{jk}} \Delta t. \text{ Thus, } TV(u^k) \le TV(u^{k-1})$$

For m-stage R-K methods, search optimal positive α_{jk}, β_{jk} yielding a maximal CFL time-step.

- 2-stage/2nd-order TVD R-K schemes

$$u^{(1)} = u^{(0)} + \Delta t L(u^{(0)}), \quad u^{(2)} = \frac{1}{2} u^{(0)} + \frac{1}{2} u^{(1)} + \frac{1}{2} \Delta t L(u^{(1)})$$

- 3-stage/3rd-order TVD R-K schemes

$$u^{(1)} = u^{(0)} + \Delta t L(u^{(0)}), \quad u^{(2)} = \frac{3}{4} u^{(0)} + \frac{1}{4} u^{(1)} + \frac{1}{4} \Delta t L(u^{(1)}), \quad u^{(3)} = \frac{1}{3} u^{(0)} + \frac{2}{3} u^{(2)} + \frac{2}{3} \Delta t L(u^{(2)})$$

- m-stage/m th-order TVD R-K schemes?
  - 5-stage/4th-order SSPRK scheme
  - Non-linearly stable R-K schemes with maximal CFL number and minimal complexity

- ***Dual Time Stepping with 2^nd^-order Backward Differencing Formula***
  - **2nd-order A-stable BDF**

$$\frac{d\mathbf{U}}{dt} = -\mathbf{R}(\mathbf{U}) \rightarrow \frac{3}{2\Delta t}\mathbf{U}^{n+1} - \frac{2}{\Delta t}\mathbf{U}^{n} + \frac{1}{2\Delta t}\mathbf{U}^{n-1} + \mathbf{R}\left(\mathbf{U}^{n+1}\right) = \mathbf{0}$$

- (Dahlquist's stability barrier theorem) For $y_t = f\left(y, t\right)$, general linear multi-step methods of $\sum_{i=0}^{k} \alpha_i y_{n+i} = \sum_{i=0}^{k} h\beta_i f_{n+i}$ can acheive 'A-stability' with the maxim order of '2'.

Chap. 4-7. Time-Accurate Schemes

- **Instead of linearizing the implicit residual term, solve the full non-linear BDF by introducing a pseudo-time derivative.**
  - Define extended residual, $\mathbf{R}^*(\tilde{\mathbf{U}})$, in terms of $\tilde{\mathbf{U}}$

$$\mathbf{R}^*(\tilde{\mathbf{U}}) \equiv \frac{3\tilde{\mathbf{U}} - 4\mathbf{U}^n + \mathbf{U}^{n-1}}{2\Delta t} + \mathbf{R}(\tilde{\mathbf{U}}) = \mathbf{0}$$

$$\xrightarrow[\text{to update solution, } \tilde{\mathbf{U}}\text{, by sub-iterations in terms of } \tau]{\text{introduce a pseudo-time derivative term}} \frac{d\tilde{\mathbf{U}}}{d\tau} + \mathbf{R}^*(\tilde{\mathbf{U}}) = \mathbf{0} \qquad \text{Eq.(3)}$$

  - two-time scale: physical-time(t) for time accuracy and pesudo-time(τ) for convergence

- **Solution of the original BDF can be recovered by converging Eq. (3).**
  - Explicit scheme
    - Modified R-K schemes, such as (4,2) and (5,3) schemes, with local time stepping
    - Implicit residual smoothing and multi-grid
  - Implicit schemes, such as LU-SGS or AF-ADI with multi-grid

- **With a fast convergence of inner iterations, an efficient 2nd-order time-accurate scheme allowing a larger Δt can be obtained.**