2nd-Order Implicit Methods for TRACE

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Outline

- **Introduction and Background**
  - Semi-Implicit Method
    - High-resolution methods (Wang et al, NED 2013), released in TRACE V5 P4
    - Lax-Wendroff (Wang et al, ANS2015), released in TRACE V5 P5
  - Fully implicit TRACE, released in TRACE V5 P5

- **Assessment of 2nd-Order Implicit methods for Linear Transport Problems**
  - **Time:** BDF2, Crank-Nicolson
  - **Space:** Central Difference (C-D), 2nd-order Upwind, and their combinations

- **Implementation and Assessment of 2nd-Order Implicit Methods for TRACE**
High-Resolution Methods for Semi-Implicit TRACE – a brief review
High-Resolution Methods

Linear Advection:

\[
\begin{align*}
  u_t + u_x &= 0 \\
  u(0, x) &= \begin{cases} 
  0 & 0 \leq x < 5 \\
  x - 5 & 5 \leq x < 6 \\
  1 & 6 \leq x
\end{cases}
\end{align*}
\]
BWR Single-CHAN Model

$P_{\text{out}} = 7 \text{ MPa}$

$Q = 4.5 \text{ MW}$

$P_{\text{in}} = 7.05 \text{ MPa}$
$T_{\text{in}} = 543 \text{ K}$

1$^{\text{st}}$-order in time and space

1$^{\text{st}}$-order in time
2$^{\text{nd}}$-order in space

2$^{\text{nd}}$-order in time
2$^{\text{nd}}$-order in space
Applications

- Ringhals BWR stability
- Oskarshamn-2 feedwater
  Transient Event on February 25, 1999.
  - A loss of feedwater preheaters and control system logic failure resulted in high feedwater flow and low temperature.
  - Automatic power and flow control moved the reactor into a low flow high power regime.
2\textsuperscript{nd}-Order Implicit TRACE
Implicit Discretizations for Linear Transport Equation: $u_t + u_x = 0$

- **BDF + C-D:**
  \[
  \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x} = 0
  \]

- **BDF + 2^{\text{nd}}-Order Upwind:**
  \[
  \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{3u_j^{n+1} - 4u_j^{n+1} + u_j^{n+1}}{2\Delta x} = 0
  \]

- **BDF2 + C-D:**
  \[
  \frac{3u_j^{n+2} - (4u_j^{n+1} - u_j^n)}{\Delta t} + \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x} = 0
  \]

- **BDF2 + 2^{\text{nd}}-Order Upwind:**
  \[
  \frac{3u_j^{n+2} - (4u_j^{n+1} - u_j^n)}{\Delta t} + \frac{3u_j^{n+1} - 4u_j^{n+1} + u_j^{n+1}}{2\Delta x} = 0
  \]

- **C-N + C-D:**
  \[
  \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left( \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x} + \frac{u_{j+1}^{n} - u_{j-1}^{n}}{2\Delta x} \right) = 0
  \]

- **C-N + 2^{\text{nd}}-Order Upwind:**
  \[
  \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left( \frac{3u_j^{n+1} - 4u_j^{n+1} + u_j^{n+1}}{2\Delta x} + \frac{3u_j^{n} - 4u_j^{n} + u_j^{n}}{2\Delta x} \right) = 0
  \]

- **C-N + 2^{\text{nd}}-Order Upwind/C-D:**
  \[
  \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left( \frac{3u_j^{n+1} - 4u_j^{n+1} + u_j^{n+1}}{2\Delta x} + \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x} \right) = 0
  \]
Numerical Results (1)

**BDF + C-D:** \[
\frac{U_j^{n+1} - U_j^n}{\Delta t} + \frac{U_{j+1}^{n+1} - U_{j-1}^n}{2\Delta x} = 0
\]

**BDF + 2nd-Order Upwind:** \[
\frac{U_j^{n+1} - U_j^n}{\Delta t} + \frac{3U_j^{n+1} - 4U_{j-1}^{n+1} + U_{j-2}^n}{2\Delta x} = 0
\]
Numerical Results (2)

BDF2 + C-D: \[
\begin{align*}
\frac{3U_{j}^{n+2} - (4U_{j}^{n+1} - U_{j}^{n})}{\Delta t} + \frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} &= 0
\end{align*}
\]

BDF2 + 2\textsuperscript{nd}-Order Upwind: \[
\begin{align*}
\frac{3U_{j}^{n+2} - (4U_{j}^{n+1} - U_{j}^{n})}{\Delta t} + \frac{3U_{j}^{n+1} - 4U_{j-1}^{n+1} + U_{j-2}^{n+1}}{2\Delta x} &= 0
\end{align*}
\]
"Numerical Results (3)

C-N + C-D: \[ \frac{U_{j+1}^{n+1} - U_{j}^{n}}{\Delta t} + \frac{1}{2} \left( \frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} + \frac{U_{j+1}^{n} - U_{j-1}^{n}}{2\Delta x} \right) = 0 \]

C-N + 2\textsuperscript{nd}-Order Upwind: \[ \frac{U_{j+1}^{n+1} - U_{j}^{n}}{\Delta t} + \frac{1}{2} \left( \frac{3U_{j+1}^{n+1} - 4U_{j-1}^{n+1} + U_{j-2}^{n+1}}{2\Delta x} + \frac{3U_{j}^{n} - 4U_{j-1}^{n} + U_{j-2}^{n}}{2\Delta x} \right) = 0 \]
Numerical Results (4)

**C-N + Upwind/C-D:**

\[
\frac{U_j^{n+1} - U_j^n}{\Delta t} + \frac{1}{2} \left( \frac{3U_j^{n+1} - 4U_{j-1}^{n+1} + U_{j-2}^{n+1}}{2\Delta x} + \frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} \right) = 0
\]

**C-N + Upwind/C-D with Flux Limiter**

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left\{ \frac{u_j^{n+1} + \phi^{n+1}(r_{j+1/2})}{2} \left[ \frac{u_j^{n+1} - u_{j+1}^{n+1}}{\Delta x} \right] - \frac{u_j^{n+1} + \phi^{n+1}(r_{j-1/2})}{2} \left[ \frac{u_j^{n+1} - u_{j-1}^{n+1}}{\Delta x} \right] \right\} = 0
\]

**Graphs:**
- Time steps: 100; time step size: 0.1
- Time steps: 200; time step size: 0.05
- Time steps: 400; time step size: 0.025
Observations

• All 2nd-order implicit methods studied show somewhat oscillations at discontinuities.

• The 2nd-order upwind performs better than the central difference.

• BDF is a stable method, but has large error in time integration.

• BDF2 is NOT a good method for the convection flow in terms of stability and phase error.

• C-N performs very well in combination with the upwind scheme.

• The best combination is C-N + Upwind/C-D
2\textsuperscript{nd}-Order Implicit Methods for Two-Phase Flow

The two-phase flow transport equation:

\[
\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R
\]

where \(u\) represents flow state variables, \(f(u)\) is the flux term, and \(R\) is simply considered as the source term.

\[
\frac{\partial u}{\partial t} + \left[ \frac{\partial f(u)}{\partial u} \right] \frac{\partial u}{\partial x} = R
\]

where \(\left[ \frac{\partial f(u)}{\partial u} \right] \) is the Jacobian matrix of the flux term.
TRACE Implementation

• C-N + Upwind/C-D

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left\{ \left[ \frac{\partial f(u)}{\partial u} \right]^{n+1}_j \frac{3u_j^{n+1} - 4u_{j-1}^{n+1} + u_{j-2}^{n+1}}{2\Delta x} + \left[ \frac{\partial f(u)}{\partial u} \right]^{n}_j \frac{u_{j+1/2}^{n} - u_{j-1/2}^{n}}{\Delta x} \right\} = R_j^{n+1*}
\]

• C-N + Upwind/C-D with Flux Limiters

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{2} \left\{ \left[ \frac{\partial f(u)}{\partial u} \right]^{n+1}_j \left[ u_j^{n+1} + \theta \phi^{n+1*}(r_{j+2}) \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2} \right] - \left[ u_{j-1}^{n+1} + \theta \phi^{n+1*}(r_{j-2}) \frac{u_{j-1}^{n+1} - u_{j-2}^{n+1}}{2} \right] \right\} \Delta x
\]

\[
+ \left[ \frac{\partial f(u)}{\partial u} \right]^{n}_j \left[ u_j^{n} + \vartheta \phi^{n}(r_{j+2}) \frac{u_{j+1}^{n} - u_{j}^{n}}{2} \right] - \left[ u_{j-1}^{n} + \vartheta \phi^{n}(r_{j-2}) \frac{u_{j-1}^{n} - u_{j-2}^{n}}{2} \right] \right\} \Delta x
\]

where \( \theta \) and \( \vartheta \) are the relaxation factors with values between 0 and 1 to adjust numerical diffusion for stability.

• Implemented only for the mass and energy equations.
Preliminary TRACE Results

Time Step Size Study

Nodalization Study
Thank You!
More Results
Nonlinear Flux Limiters

Theorem: Any TVD numerical method is monotonicity preserving

\[ \phi(r) = \max \left[ 0, \min \left( 1.5r, \frac{1+r}{2}, 1.5 \right) \right] \]

\[ \phi(r) = \frac{1.5(r^2 + r)}{r^2 + r + 1} \]

\[ \phi(r) = \frac{r^2 + r}{r^2 + 1} \]

\[ \phi(r) = \min \text{mod} (1, r) \]

where

\[ r_{j+1/2}^n = \begin{cases} f_j^n - f_{j-1}^n & \text{if } u_{j+1/2}^{n+1} \geq 0 \\ f_{j+1}^n - f_j^n & \text{if } u_{j+1/2}^{n+1} < 0 \end{cases} \]