Time Integration for PDEs with Terms of Mixed Stiffness

• Consider a generic PDE with the following form:

\[
\frac{\partial C}{\partial t} = f(C) + g(C)
\]

• Examples:

\[
\frac{\partial C}{\partial t} = \alpha C (1 - C) + D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)
\]

• Or:

\[
\frac{\partial C}{\partial t} = \alpha_x \frac{\partial C}{\partial x} + \alpha_y \frac{\partial C}{\partial y} + D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)
\]

• Or:

\[
\frac{\partial C}{\partial t} = \frac{\partial \left( C^2 \right)}{\partial x} + D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)
\]
Split Scheme

- If we split $C$ into a stiff component $C_s$ and a non-stiff component $C_{ns}$ then we can solve the related system:

- We then use two compatible Runge-Kutta schemes to integrate the equations in lock step.

- The conditions to ensure that the explicit and implicit schemes advance at the same time in each substage have been determined and satisfied for matched implicit and explicit (imex) RK schemes which are both fourth order, six stage.

Non-Stiff Component

- Note this is an **explicit** RK scheme:

\[
\frac{\partial C_{NS}}{\partial t} = f(C)
\]

\[
f^1 = f(C^n)
\]

\[
\tilde{C}^1 = C^n
\]

\[
\tilde{C}_{NS}^1 = C_{NS}^1
\]

for \( i = 2:s \)

\[
\tilde{C}_{NS}^i = C_{NS}^n + dt \left( \sum_{j=1}^{i-1} \hat{a}_{ij} f^j \right)
\]

\[
f^i := f(\tilde{C}^i)
\]

end

\[
C_{NS}^{n+1} = C_{NS}^{n+1} + dt \left( \sum_{j=1}^{s} \hat{b}_j f^j \right)
\]
Stiff Component

• Note this is an *implicit* RK scheme:

\[ \frac{\partial C_S}{\partial t} = g(C) \]

\[ \tilde{C}^1 = C^n \]
\[ \tilde{C}_S^1 = C_s^n \]
for i=2:s
\[ \tilde{C}_S^i = C_S^n + dt \left( a_{ii} g \left( \tilde{C}^i \right) \right) + dt \left( \sum_{j=1}^{i-1} a_{ij} g^j \right) \]
\[ g^i := g \left( \tilde{C}^i \right) \]
end
\[ C_{S}^{n+1} = C_s^n + dt \left( \sum_{j=1}^{i=s} b_j g^j \right) \]
Adding The Schemes Together

\[ f^1 = f\left(C^n\right) \]
\[ \tilde{C}^1 = C^n \]
for \(i=2:s\)
\[ \tilde{C}^i = C^n + dt \left( a_{ii} g\left(\tilde{C}^i\right) \right) + dt \left( \sum_{j=1}^{i-1} a_{ij} g^j \right) + dt \left( \sum_{j=1}^{i-1} \hat{a}_{ij} f^j \right) \]
\[ g^i := g\left(\tilde{C}^i\right) \]
\[ f^i := f\left(\tilde{C}^i\right) \]
end
\[ C^{n+1} = C^n + dt \left( \sum_{j=1}^{s} b_j g^j \right) + dt \left( \sum_{j=1}^{s} \hat{b}_j f^j \right) \]
Kennedy-Carpenter 6 Stage ARK4

\[ f^1 = f(C^n) \]
\[ \tilde{C}^1 = C^n \]
\[ \tilde{C}^2 = C^n + dt \left( a_{22}g(\tilde{C}^2) \right) + dt \left( a_{21}g^1 \right) + dt \left( \hat{a}_{21}f^1 \right) \]
\[ g^2 = g(\tilde{C}^2), \quad f^2 = f(\tilde{C}^2) \]
\[ \tilde{C}^3 = C^n + dt \left( a_{33}g(\tilde{C}^3) \right) + dt \left( a_{31}g^1 + a_{32}g^2 \right) + dt \left( \hat{a}_{31}f^1 + \hat{a}_{32}f^2 \right) \]
\[ g^3 = g(\tilde{C}^3), \quad f^3 = f(\tilde{C}^3) \]
...
\[ \tilde{C}^6 = C^n + dt \left( a_{66}g(\tilde{C}^6) \right) \]
\[ \quad + dt \left( a_{61}g^1 + a_{62}g^2 + ... + a_{65}g^5 \right) \]
\[ \quad + dt \left( \hat{a}_{61}f^1 + \hat{a}_{62}f^2 + ... + \hat{a}_{65}f^5 \right) \]
\[ g^6 = g(\tilde{C}^6), \quad f^6 = f(\tilde{C}^6) \]
\[ C^{n+1} = C^n + dt \left( \sum_{j=1}^{j=6} b_j g^j \right) + dt \left( \sum_{j=1}^{j=6} \hat{b}_j f^j \right) \]
6 Stages

\[ f^1 = f(C^n) \]
\[ \tilde{C}^1 = C^n \]
\[ \tilde{C}^2 - dt\left(a_{22}g(\tilde{C}^2)\right) = C^n + dt\left(a_{21}g^1 + \hat{a}_{21}f^1\right) \]
\[ \tilde{C}^3 - dt\left(a_{33}g(\tilde{C}^3)\right) = C^n + dt\left(a_{31}g^1 + a_{32}g^2 + \hat{a}_{31}f^1 + \hat{a}_{32}f^2\right) \]
\[
\vdots
\]
\[ \tilde{C}^6 - dt\left(a_{66}g(\tilde{C}^6)\right) = C^n + dt\left(a_{61}g^1 + a_{62}g^2 + \cdots + a_{65}g^5 + \hat{a}_{61}f^1 + \hat{a}_{62}f^2 + \cdots + \hat{a}_{65}f^5\right) \]
\[ C^{n+1} = C^n + dt\left(\sum_{j=1}^{i=6} b^j g^j\right) + dt\left(\sum_{j=1}^{i=6} \hat{b}^j f^j\right) \]

We now see that there is a sequence of solves. Each stage 2-6 requires the solution of a system (as before in the ESDIRK4 scheme).
Linear $\mathbf{g}$ – discretized as $\mathbf{g}$

\[
f^1 = f\left(C^n\right)
\]
\[
\tilde{C}^1 = C^n
\]
\[
(I - dta_{22} \mathbf{g}) \tilde{C}^2 = C^n + dtg\left(a_{21} \tilde{C}^1\right) + dt\left(\hat{a}_{21} f^1\right)
\]
\[
(I - dta_{33} \mathbf{g}) \tilde{C}^3 = C^n + dtg\left(a_{31} \tilde{C}^1 + a_{32} \tilde{C}^2\right) + dt\left(\hat{a}_{31} f^1 + \hat{a}_{32} f^2\right)
\]
\[...
\]
\[
(I - dta_{66} \mathbf{g}) \tilde{C}^6 = C^n + dtg\left(a_{61} \tilde{C}^1 + a_{62} \tilde{C}^2 + a_{65} \tilde{C}^5\right) + dt\left(\hat{a}_{61} f^1 + \hat{a}_{62} f^2 + \hat{a}_{65} f^5\right)
\]
\[
C^{n+1} = C^n + dtg\left(\sum_{j=1}^{j=6} b_j \tilde{C}^j\right) + dt\left(\sum_{j=1}^{j=6} \hat{b}_j f^j\right)
\]

We now see that there is a sequence of solves. Each stage 2-6 requires the solution of a system (as before in the ESDIRK4 scheme).
Incorporating the Mass Matrix $\mathbf{M}$ for Symmetry
(specific to our DG formulations)

\[ f^{1} = f\left( C^{n} \right) \]
\[ \tilde{C}^{1} = C^{n} \]
\[ (\mathbf{M} - dta_{22}\mathbf{g})\tilde{C}^{2} = \mathbf{M}C^{n} + dtg\left( a_{21}\tilde{C}^{1} \right) + dt\left( \hat{a}_{21}.f^{1} \right) \]
\[ (\mathbf{M} - dta_{33}\mathbf{g})\tilde{C}^{3} = \mathbf{M}C^{n} + dtg\left( a_{31}\tilde{C}^{1} + a_{32}\tilde{C}^{2} \right) + dt\left( \hat{a}_{31}.f^{1} + \hat{a}_{32}.f^{2} \right) \]
... 
\[ (\mathbf{M} - dta_{66}\mathbf{g})\tilde{C}^{6} = \mathbf{M}C^{n} + dtg\left( a_{61}\tilde{C}^{1} + a_{62}\tilde{C}^{2} + ... + a_{65}\tilde{C}^{5} \right) + dt\left( \hat{a}_{61}.f^{1} + \hat{a}_{62}.f^{2} + ... + \hat{a}_{65}.f^{5} \right) \]

\[ \mathbf{M}C^{n+1} = \mathbf{M}C^{n} + dtg\left( \sum_{j=1}^{6} b_{j}\tilde{C}^{j} \right) + dt\left( \sum_{j=1}^{6} \hat{b}_{j}.f^{j} \right) \]

\[ C^{n+1} = \mathbf{M}^{-1}\left( \mathbf{M}C^{n+1} \right) \]

Where for example $\mathbf{g}$ is the diffusion operator

\[ \mathbf{g} = DM\left( D_{x}^{D}D_{x}^{N} + D_{y}^{D}D_{y}^{N} \right) \]
Kennedy-Carpenter Additive RK Schemes

\[ f^1 = f \left( C^n \right) \]
\[ \tilde{C}^1 = C^n \]
\[ \left( M - dt \gamma g \right) \tilde{C}^2 = MC^n + dtg \left( a_{21} \tilde{C}^1 \right) + dt \left( \hat{a}_{21} f^1 \right) \]
\[ \left( M - dt \gamma g \right) \tilde{C}^3 = MC^n + dtg \left( a_{31} \tilde{C}^1 + a_{32} \tilde{C}^2 \right) + dt \left( \hat{a}_{31} f^1 + \hat{a}_{32} f^2 \right) \]

... 

\[ \left( M - dt \gamma g \right) \tilde{C}^6 = MC^n + dtg \left( a_{61} \tilde{C}^1 + a_{62} \tilde{C}^2 ... + a_{65} \tilde{C}^5 \right) + dt \left( \hat{a}_{61} f^1 + \hat{a}_{62} f^2 ... + \hat{a}_{65} f^5 \right) \]

\[ MC^{n+1} = MC^n + dtg \left( \sum_{j=1}^{6} b_j \tilde{C}^j \right) + dt \left( \sum_{j=1}^{6} \hat{b}_j f^j \right) \]

\[ C^{n+1} = M^{-1} \left( MC^{n+1} \right) \]

- K-C set up the imex schemes so that the Butcher block diagonal entries
- \( a_{22} = a_{33} = a_{44} = a_{55} = a_{66} = \gamma \)
- Thus the same matrix needs to be inverted at stages 2-5
Mixed Implicit Explicit Runge Kutta Scheme (IMEX RK)

• Many papers. Example:

  -- or --

Fourth Order, 6 Stage

Notes:
1) \( \text{bhat} = b \)
2) See p 176 of Kennedy/Carpenter
K-C ARK4 IMEX Scheme

- 87-91 sum up stiff terms
- 93-96 sum up non-stiff terms
- 98-102 invert system
- 104 evaluate $f(C_{\tilde{j}})$
- 107-119 piece together $C^{n+1}$
- Dr Day will discuss the use of umPERM stages.
Project Lab Time

• Start working on your projects.