On linear algebraic systems arising from the DGFE method for the compressible Navier-Stokes equations

Vít Dolejší

Charles University Prague
Faculty of Mathematics and Physics

Workshop Dresden-Prague
Staré Splavy, Czech Republic,
September 10-11, 2008
Our aim: efficient numerical scheme for the solution of the compressible Navier-Stokes equations,

$$\frac{\partial w}{\partial t} = \nabla \cdot G(w, \nabla w), \quad w : \Omega \times (0, T) \rightarrow \mathbb{R}^{d+2}, \quad (1)$$

space semi-discretization: $w(x, t) \approx w_h(t) \in S_{hp}, \quad t \in (0, T)$

$$\frac{\partial}{\partial t} w_h = F(t, w_h, \nabla w_h), \quad w_h : (0, T) \rightarrow S_{hp}, \quad (2)$$

system of ODEs (stiff)

ODE solver: explicit, implicit, semi-implicit
Introduction (2)

- full time-space discretization,

\[
\left( M + \tau_k C_k(w_h^{k-1}) \right) w_h^k = q_k(w_h^{k-1}),
\]

- \( w_h^k \in \mathbb{R}^{\text{DOF}}, \ k = 1, 2, \ldots, \)
- \( M \) – mass matrix,
- \( C_k \) – “discrete flux” matrix,
- \( q_k \) – RHS (boundary conditions),
- \( \tau_k \) – time step,

**Open problems:**

- linear algebra solver for (3), preconditioning ?
- stopping criterion for linear algebra solver?
- choice of \( \tau_k \)?
1 Introduction

2 Governing equations

3 Discretization

4 Linear algebra problems
Navier-Stokes equations

\[
\frac{\partial \mathbf{w}}{\partial t} + \sum_{s=1}^{d} \frac{\partial}{\partial x_s} \mathbf{f}_s(\mathbf{w}) = \sum_{s=1}^{d} \frac{\partial}{\partial x_s} \left( \sum_{k=1}^{d} \mathbf{K}_{sk}(\mathbf{w}) \frac{\partial \mathbf{w}}{\partial x_k} \right),
\]

where

- \( \mathbf{w} : \Omega \times (0, T) \rightarrow \mathbb{R}^{d+2} \),
- inviscid terms \( \mathbf{f}_s : \mathbb{R}^{d+2} \rightarrow \mathbb{R}^{d+2} \), \( s = 1, \ldots, d \),
- viscous terms \( \mathbf{K}_{sk} : \mathbb{R}^{(d+2)} \rightarrow \mathbb{R}^{(d+2) \times (d+2)} \), \( s, k = 1, \ldots, d \),
- state equation for perfect gas,
- BC + IC.
1 Introduction

2 Governing equations

3 Discretization

4 Linear algebra problems
let $\mathcal{T}_h, \; h > 0$ be a partition of $\bar{\Omega}$,

$\mathcal{T}_h = \{K\}_{K \in \mathcal{T}_h}, \; K$ are $d$-dimensional polyhedra,

let $\mathcal{F}_h = \{\Gamma\}_{\Gamma \in \mathcal{F}_h}$ be a set of all faces of $\mathcal{T}_h$,

we distinguish

- inner faces $\mathcal{F}_h^I$,
- 'Dirichlet' faces $\mathcal{F}_h^D$,
- 'Neumann' faces $\mathcal{F}_h^N$,

we put $\mathcal{F}_h^{ID} \equiv \mathcal{F}_h^I \cup \mathcal{F}_h^D$. 
Notation
Spaces of discontinuous functions

- let $p_K \geq 1$, $K \in \mathcal{T}_h$ be local polynomial degree,
- let $p = \{p_K, K \in \mathcal{T}_h\}$,
- for $p$ and $\mathcal{T}_h$ we define

$$S_{hp} = \{v; \ v \in L^2(\Omega), \ v|_K \in P_{p_K}(K) \ \forall K \in \mathcal{T}_h\}, \quad (5)$$

where $P_{p_K}(K)$ are polynomials on $K$ of degree $\leq p_K$, $K \in \mathcal{T}_h$.

$$S_{hp} = S_{hp} \times \cdots \times S_{hp} \quad d+2 \text{ times} \quad (6)$$

- for $u \in S_{hp}$
  - $\langle v \rangle_\Gamma = \text{mean value of } v \text{ over face } \Gamma$
  - $[v]_\Gamma = \text{jump of } v \text{ over face } \Gamma$
Viscous terms

\[
\tilde{a}_h(w, \varphi) = \sum_{K \in T_h} \int_K \left( \sum_{k=1}^{d} K_{s,k}(w) \frac{\partial w}{\partial x_k} \right) \cdot \nabla \varphi \, dx
\]

\[
- \sum_{\Gamma \in F_h^{ID}} \int_{\Gamma} \sum_{s=1}^{\sum} \left\langle \left( \sum_{k=1}^{d} K_{s,k}(w) \frac{\partial w}{\partial x_k} \right) \right\rangle n_s \cdot [\varphi] \, dS
\]

\[
- \theta \sum_{\Gamma \in F_h^{ID}} \int_{\Gamma} \sum_{s=1}^{\sum} \left\langle \sum_{k=1}^{d} K_{k,s}(w) \frac{\partial \varphi}{\partial x_k} \right\rangle n_s \cdot [w] \, dS
\]

\[
+ \theta \sum_{\Gamma \in F_h^{D}} \int_{\Gamma} \sum_{s=1}^{\sum} \sum_{k=1}^{d} K_{k,s}(w) \frac{\partial \varphi}{\partial x_k} n_s \cdot w_B \, dS,
\]

\[\theta = 1 \text{ (SIPG)}, \ 0 \text{ (IIPG)}, \ -1 \text{ (NIPG)}.\]
Inviscid terms

\[ \tilde{b}_h(w, \varphi) = \sum_{\Gamma \in F_h} \int_{\Gamma} H \left( w|_{\Gamma}^{(p)}, w|_{\Gamma}^{(n)}, n_{\Gamma} \right) \cdot [\varphi]_{\Gamma} \, dS \]

\[ - \sum_{K \in T_h} \int_K \sum_{s=1}^d f(w) \cdot \frac{\partial \varphi}{\partial x_s} \, dx. \]

where \( H \) is a \textit{numerical flux}. 
Interior and boundary penalties

\[ J_h(w, \varphi) = \sum_{\Gamma \in F_h^{ID}} \int_{\Gamma} \sigma[w] \cdot [\varphi] \, dS - \sum_{\Gamma \in F_h^{D}} \int_{\Gamma} \sigma w_B \cdot \varphi \, dS, \]

\[ \sigma|_{\Gamma} \equiv \frac{C_W}{|\Gamma| \, Re}, \quad C_W > 0. \]
\[ \tilde{c}_h(w_h, \varphi_h) := \tilde{a}_h(w_h, \varphi_h) + \tilde{b}_h(w_h, \varphi_h) + J_h(w_h, \varphi_h) \quad (8) \]

**Space semi-discretization**

i) \( w_h \in C^1((0, T); S_{hp}) \),

ii) \[ \frac{d}{dt}(w_h(t), \varphi_h) + \tilde{c}_h(w_h(t), \varphi_h) = 0 \quad (9) \]
   \( \forall \varphi_h \in S_{hp}, \ t \in (0, T) \).

iii) \( w_h(0) \) satisfies the initial condition.
semi-discrete problem (9) represents ODEs

**explicit method** leads to a high restriction on time step (low speed flow)

**full implicit method** leads to a system of nonlinear equations in each time step

**Semi-implicit method**

- *linearize system* (9)
- *linear terms* are treated *implicitly*
- *nonlinear terms* are treated *explicitly*
Semi-implicit DGFE discretization

Formal linearization

- we define: $c_h : S_{hp} \times S_{hp} \times S_{hp} \rightarrow S_{hp}$
- $c_h$ is linear in second and third arguments,
- $c_h(w_h, w_h, \varphi_h) = \tilde{c}_h(w_h, \varphi_h) \quad \forall w_h, \varphi_h \in S_{hp}$.

First order semi-implicit scheme

$$
\left( \frac{w_h^k - w_h^{k-1}}{\tau_k}, \varphi_h \right) + c_h(w_h^{k-1}, w_h^k, \varphi_h) = 0 \quad \forall \varphi_h \in S_{hp}
$$
1 Introduction

2 Governing equations

3 Discretization

4 Linear algebra problems
Basis of $S_{hp}$

Local basis

$l$ is index set, $\mathcal{T}_h = \{ K_\mu, \mu \in I \}$, $p_\mu = p_{K_\mu}, \mu \in I$,

\[ B_\mu = \left\{ \psi_{\mu,j}, \psi_{\mu,j} \in S_{hp}, \supp(\psi_{\mu,j}) \subset K_\mu, j = 1, \ldots, \text{dof}_\mu \right\}, \]

\[ \text{dof}_\mu = \begin{cases} 
2(p_\mu + 1)(p_\mu + 2) & \text{for } d = 2 \\
\frac{5}{6}(p_\mu + 1)(p_\mu + 2)(p_\mu + 3) & \text{for } d = 3 
\end{cases}, \mu \in I 
\]

<table>
<thead>
<tr>
<th>$p_\mu$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d = 2$</td>
<td>12</td>
<td>24</td>
<td>40</td>
<td>60</td>
<td>84</td>
</tr>
<tr>
<td>$d = 3$</td>
<td>20</td>
<td>50</td>
<td>100</td>
<td>175</td>
<td>280</td>
</tr>
</tbody>
</table>
**Basis of** $S_{hp}$ **(2)**

**Global basis**

$$B = \{ \psi_{\mu,j}, \psi_{\mu,j} \in B_{\mu}, j = 1, \ldots, \text{dof}_{\mu}, \mu \in I \}.$$  

**Linear algebraic representation**

$$w^k_h(x) = \sum_{\mu \in I} \sum_{j=1}^{\text{dof}_{\mu}} \xi_{k,\mu,j} \psi_{\mu,j}(x) \in S_{hp}, \quad x \in \Omega, \quad k = 0, 1, \ldots, r,$$

$$W_k = \{ \xi_{k,\mu,j} \}_{\mu \in I, j=1,\ldots,\text{dof}_{\mu}} \in \mathbf{R}^{\text{DOF}}, \quad \text{DOF} = \sum_{\mu \in I} \text{dof}_{\mu},$$

$$w^k_h(x) \leftrightarrow W_k$$
### DGFEM scheme

\[
(M + \tau_k C_k(W_{k-1})) W_k = q_k, \quad k = 1, \ldots, r, \quad (10)
\]

where
- \(W_k\) unknown vector,
- \(M\) mass matrix,
- \(C_k\) “flux” matrix representing inviscid, viscous and penalty terms,
- \(q_k\) right-hand side (BC),
- \(\tau_k\) time step.
Solution of linear algebraic problems

Linear algebraic problems

\[(M + \tau_k C_k(W_{k-1})) W_k = q_k, \quad k = 1, \ldots, r,\]

Linear algebraic solvers

- direct solvers
- iterative solvers (e.g., GMRES with preconditioning)
- multilevel solvers (e.g., $h$- or $p$-multigrids)

Restarted GMRES with preconditioning

- type of preconditioning?
- stopping criterion?
- choice of the time step?
Linear algebraic problems

\[(M + \tau_k C_k(W_{k-1}))W_k = q_k\]
Matrix structure of \((M + \tau_k C_k(W_{k-1}))W_k = q_k\)

<table>
<thead>
<tr>
<th>Mass Matrix (M)</th>
<th>Flux Matrix (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(M_{1,1}) 12x12</td>
<td>(C_{k,1,1}) 12x12</td>
</tr>
<tr>
<td>(M_{2,2}) 40x40</td>
<td>(C_{k,1,2}) 12x40</td>
</tr>
<tr>
<td>(M_{3,3}) 12x12</td>
<td>(C_{k,2,1}) 40x12</td>
</tr>
<tr>
<td>(M_{4,4}) 24x24</td>
<td>(C_{k,2,2}) 40x40</td>
</tr>
<tr>
<td>(M_{5,5}) 24x24</td>
<td>(C_{k,3,2}) 12x40</td>
</tr>
<tr>
<td>(M_{6,6}) 12x12</td>
<td>(C_{k,3,3}) 12x12</td>
</tr>
<tr>
<td>(M_{4,4}) 24x24</td>
<td>(C_{k,4,2}) 24x24</td>
</tr>
<tr>
<td>(M_{5,5}) 24x24</td>
<td>(C_{k,4,3}) 24x24</td>
</tr>
<tr>
<td>(M_{6,6}) 12x12</td>
<td>(C_{k,6,5}) 24x12</td>
</tr>
</tbody>
</table>

**Mass Matrix**
- \(M_{1,1}\) 12x12
- \(M_{2,2}\) 40x40
- \(M_{3,3}\) 12x12
- \(M_{4,4}\) 24x24
- \(M_{5,5}\) 24x24
- \(M_{6,6}\) 12x12

**Flux Matrix**
- \(C_{k,1,1}\) 12x12
- \(C_{k,1,2}\) 12x40
- \(C_{k,2,1}\) 40x12
- \(C_{k,2,2}\) 40x40
- \(C_{k,3,2}\) 12x40
- \(C_{k,3,3}\) 12x12
- \(C_{k,4,2}\) 24x24
- \(C_{k,4,3}\) 24x24
- \(C_{k,6,5}\) 24x12
- \(C_{k,6,6}\) 12x12
Iterative solver

Linear algebraic problems

\[(M + \tau_k C_k(W_{k-1})) W_k = q_k, \quad k = 1, \ldots, r,\]

Preconditioners
- block diagonal: fast computation & small memory
- ILU\(z\): more efficient but which \(z\)?

Block diagonal preconditioner
- preconditioner has the same block structure as \(M\),
- “small” \(\tau_k \Rightarrow\) preconditioning is very efficient,
- “large” \(\tau_k \Rightarrow\) preconditioning is inefficient
Dependence of the linear algebraic solutions on $\tau_k$

number of iterations vs. $\tau_k$

CPU-time (s) vs. $\tau_k$

DOF = 121,000, 19,147,200 nonzero matrix elements

Exponential growth?
Choice of the time step

Flow regimes

- Steady-state flow
  - “small” $\tau_k$ at the beginning of the computation,
  - “large” $\tau_k$ at the end of the computation,
- Non-steady flow
  - “small” $\tau_k$ during the whole computation.

- standard approach (e.g., [D., Kůs: IJNME, 2008]): minimize the number of time steps such that

$$\|w_h^k - w_h(t_k)\| \leq \omega_1, \quad \forall k = 1, \ldots, r$$

- It is optimal with respect to CPU-time? Open problem
Let $A_k := M + \tau_k C_k$, $A_k W_k = q_k$, $k = 1, \ldots, r$.

Let $\bar{W}_k = \{\bar{\xi}_{k,\mu,j}\}_{j=1,\ldots,\text{dof}_\mu}^{\mu \in I}$ be approximation of $W_k$.

$\bar{W}_k \leftrightarrow \bar{w}_h^k = \sum_{\mu \in I} \sum_{j=1}^{\text{dof}_\mu} \bar{\xi}_{k,\mu,j} \psi_{\mu,j} \in S_{hp}$

**Computational errors**

- **discretization error**: $e_D := w_h^k(x) - w(x, t)$,
- **algebraic error**: $e_A := \bar{w}_h^k(x) - w_h^k(x)$,
- **efficient and accurate method** $\iff \|e_A\| \approx \|e_D\|$,
- **Stop when** $\|e_A\| \leq \|e_D\|$? Open problem
let $W_k$ and $\bar{W}_k$ be the exact and approximate solutions,

error $e_k := \|\bar{W}_k - W_k\| \leq \omega$ uncomputable.

Residuum criterion

$$\text{res}_k := \|A_k \bar{W}_k - q_k\| \leq \omega_1,$$  
$$e_k = \|\bar{W}_k - W_k\| \leq \|A_k^{-1}\| \text{res}_k,$$
problematic for ill-conditioned $A_k$.

Preconditioned residuum criterion

$$\text{res}_k := \|P_k A_k \bar{W}_k - P_k q_k\| \leq \omega_2,$$  
problematic for block diagonal preconditioner and for large $\tau_k$. 

STOPPING CRITERION (2)
Stopping criterion (3)

Difference criterion

- **iterative process**: $\bar{\mathbf{W}}_{k-1} \rightarrow \bar{\mathbf{W}}_{k}$
  
  $\bar{\mathbf{W}}_{k-1} =: \bar{\mathbf{W}}^0 \rightarrow \bar{\mathbf{W}}^1 \rightarrow \bar{\mathbf{W}}^2 \rightarrow \ldots \rightarrow \bar{\mathbf{W}}^{sk} =: \bar{\mathbf{W}}_k$

- $\bar{\mathbf{W}}_k \rightarrow \mathbf{W}_k$ for $sk \rightarrow \infty$

- $\text{diff}_k := \|\bar{\mathbf{W}}_k^{sk} - \bar{\mathbf{W}}_k^{sk-1}\| \leq \omega_3 \quad (13)$

- may be problematic, works for steady state computations.
Comparison of stopping criteria

preconditioned residuum  difference criterion

\[ \tau_k \]

steady-state convergence  GMRES iterations

CPU time: 1285 s  437 s  DOF = 100 600.
Choice of the time step

- steady-state residuum: $\eta_k := \frac{1}{\tau_k} \| w_h^k - w_h^{k-1} \|$

Heuristic choice of the time step

$$\tau_k = \frac{1}{2\Lambda_k} \left( \frac{\eta_k}{\eta_1} \right)^{-\delta}, \quad k = 1, \ldots, r,$$

where

$$\Lambda_k = \max_{K \in \mathcal{T}_h} |K|^{-1} \max_{\Gamma \in \partial K} \max_{l=1,\ldots,d+2} \lambda_l(w_h^k|\Gamma)||\Gamma||$$

\[ \delta = 3/2 \]

- $\tau_1$ corresponds to explicit scheme with CFL=0.5,
- exponentially increasing for decreasing $\eta_k$. 

Comparison of the choice of the time step

adaptive choice of $\tau_k$ vs. heuristic

$\eta_k / \eta_0$ vs. $\tau_k$

$\# T_h = 2515$, $P_2$ approx, DOF = 60 360

<table>
<thead>
<tr>
<th>method</th>
<th>iter</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A \ 10^{-2}$</td>
<td>64</td>
<td>275</td>
</tr>
<tr>
<td>$A \ 10^{-1}$</td>
<td>54</td>
<td>266</td>
</tr>
<tr>
<td>$H \ \delta = 3/2$</td>
<td>39</td>
<td>177</td>
</tr>
<tr>
<td>$H \ \delta = 2$</td>
<td>17</td>
<td>111</td>
</tr>
</tbody>
</table>
Comparison of the choice of the time step (2)

adaptive choice of $\tau_k$ vs. heuristic

$\eta_k / \eta_0$ vs. $\tau_k$

$\# T_h = 3025$, $P_3$ approx, $\text{DOF} = 121\,000$

<table>
<thead>
<tr>
<th>method</th>
<th>iter</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A , 10^{-2}$</td>
<td>74</td>
<td>1117</td>
</tr>
<tr>
<td>$A , 10^{-1}$</td>
<td>63</td>
<td>1042</td>
</tr>
<tr>
<td>$H , \delta = 3/2$</td>
<td>59</td>
<td>863</td>
</tr>
<tr>
<td>$H , \delta = 2$</td>
<td>20</td>
<td>531</td>
</tr>
</tbody>
</table>
Subject

- preconditioner for linear algebra problem
- stopping criterion
- choice of the time step

Observation

- simple block diagonal preconditioner
- “difference” stopping criterion
- heuristic choice of the time step

Deeper analysis necessary