Towards the development and application of an optimal solver for continuum models of tumour growth

Fengwei YANG
Matthew HUBBARD
Peter JIMACK
Motivations

Ultimate goal is to solve complex non-linear parabolic systems by applying:

- adaptive meshing,
- second order Backward Differentiation Formula (BDF) 2 temporal scheme,
- non-linear multigrid method,
- parallel technique.
Outline

- Non-linear multigrid
- Cahn-Hilliard-Hele-Shaw (CHHS) system of equations
- Improved solver for CHHS system of equations
- Model of thin film flows
- Adaptive meshing on droplet
- Tumour model from S.M. Wise et al.
- Future plan
Non-linear multigrid

- Full Approximate Storage (FAS) scheme

  for problem on fine grid:
  - $A(u^f) = b^f$
  - $r^f = b^f - A(u^*)$

  for coarse grid correction:
  - $A(u^c) = b^c + [I_c r^f - (b^c - A(I_c u^*))]$
  - $e_{\text{correction}} = u^c - u^*$
CHHS system of equations

\[
\begin{align*}
\partial_t \phi &= \Delta \mu - \nabla \cdot (\phi u) \\
u &= -\nabla p - \gamma \phi \nabla \mu \\
\nabla \cdot u &= 0 \\
\mu &= \phi^3 - \phi - \epsilon^2 \Delta \phi
\end{align*}
\]

with Neumann boundary conditions:

\[
\begin{align*}
\partial_n \phi &= 0 \\
\partial_n \mu &= 0 \\
\partial_n p &= 0
\end{align*}
\]
on \partial \Omega

Our solver

- Cell-centred 2nd order finite difference method on rectangular grids
- PARAMESH library for mesh generation
- Fully implicit 2nd order discretization in time (BDF2)
- FAS multigrid at each time-step
- Newton-block $3 \times 3$ Red-Black (weighted) Gauss-Seidel smoother
- Full weighting restriction and multi-linear interpolation
## CHHS system of equation

<table>
<thead>
<tr>
<th>Level of grids</th>
<th>degrees of freedom</th>
<th>max No. V-cycle from our solver</th>
<th>max No. V-cycle from Wise’s solver</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>4096</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>16,384</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>4</td>
<td>65,536</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td>5</td>
<td>262,144</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>6</td>
<td>1,048,576</td>
<td>10</td>
<td>11</td>
</tr>
</tbody>
</table>

Optimal multigrid performances from our BDF2 solver and Wise’s solver with semi-implicit scheme.
Convergence tests from our BDF2 solver and Wise’s solver with semi-implicit scheme.
Droplet Spreading Flow

\[ \partial_t h = \nabla \cdot \left( \frac{h^3}{3} \nabla p \right) \]
\[ p = -\Delta h - \Pi(h) \]

with Neumann boundary conditions:
\[ \partial_n h = 0 \quad \partial_n p = 0 \quad \text{on} \quad \partial \Omega \]

\[ \text{(0,0)} \quad \text{Moving contact line} \]

Thin film \( h^* \)
Our solver

- Cell-centred 2nd order finite difference method
- PARAMESH library for mesh generation and adaptivity
- Fully implicit 2nd order discretization in time (BDF2)
- MLAT variation of FAS multigrid at each time-step
- Newton-block $2 \times 2$ Red-Black (weighted) Gauss-Seidel smoother
- Full weighting restriction and multi-linear interpolation
Droplet Spreading Flow

Changes of $h$ from Gaskell et al. (2004)

Changes of $h$ from our solver.
Droplet Spreading Flow

Optimal MG performance from Gaskell et al. (2004)

Optimal MG performance from our solver.
Adaptive meshing for initial condition of droplet.

Adaptive meshing at $t = 1 \cdot 10^{-5}$. 
Droplet Spreading Flow

Heights of droplet ($h_0(t)$)

- **adaptive meshing, CPU time = 8h 31m**
- **uniform $1024^2$, CPU time = 30h 7m**
- **uniform $512^2$, CPU time = 7h 42m**
Tumour model from Wise et al.

\begin{align*}
\frac{\partial_t \phi_T}{\partial_t \phi_D} &= M \nabla \cdot (\phi_T \nabla \mu) + S_T(\phi_T, \phi_D, n) - \nabla \cdot (u_S \phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2 \Delta \phi_T \\
\frac{\partial_t \phi_D}{\partial_t \phi_D} &= M \nabla \cdot (\phi_D \nabla \mu) + S_D(\phi_T, \phi_D, n) - \nabla \cdot (u_S \phi_D) \\
u_S &= -(\nabla p - \frac{\gamma}{\epsilon} \mu \nabla \phi_T) \\
\nabla \cdot u_S &= S_T(\phi_T, \phi_D, n) \\
0 &= \Delta n + T_C(\phi_T, n) - n(\phi_T - \phi_D)
\end{align*}

with mixed boundary conditions:

\begin{align*}
\mu = p = 0 \quad n = 1 \quad \zeta \cdot \nabla \phi_T = \zeta \cdot \nabla \phi_D = 0 \quad \text{on} \quad \partial \Omega,
\end{align*}

S. M. Wise, J. S. Lowengrub, V. Cristini,

Tumour model from Wise et al.

\[
\begin{align*}
\partial_t \phi_T &= M \nabla \cdot (\phi_T \nabla \mu) + S_T(\phi_T, \phi_D, n) - \nabla \cdot (u_S \phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2 \Delta \phi_T \\
\partial_t \phi_D &= M \nabla \cdot (\phi_D \nabla \mu) + S_D(\phi_T, \phi_D, n) - \nabla \cdot (u_S \phi_D) \\
[u_S &= -(\nabla p - \frac{\gamma}{\epsilon} \mu \nabla \phi_T)] \\
-\Delta p &= S_T(\phi_T, \phi_D, n) - \nabla \cdot (\frac{\gamma}{\epsilon} \mu \nabla \phi_T) \\
0 &= \Delta n + T_C(\phi_T, n) - n(\phi_T - \phi_D)
\end{align*}
\]

with mixed boundary conditions:

\[
\mu = p = 0 \quad n = 1 \quad \underline{\zeta} \cdot \nabla \phi_T = \underline{\zeta} \cdot \nabla \phi_D = 0 \quad \text{on} \quad \partial \Omega,
\]

S. M. Wise, J. S. Lowengrub, V. Cristini.

Optimal multigrid convergence on tumour model.
Future plan

- Validating with results from Wise et al.
- Second order convergence on tumour model
- Adaptive meshing
- Parallel implementation
- 3D