Introduction

Characteristics of computing solutions of fluid-transport equations:

- Challenging multiphysics problem if the transported entity also influences the flow, leading to two-way coupling.
- Determined by linearizing the discretized equations and solving a large sparse linear system.
- Balancing the efficiency and accuracy → direct or iterative solver.

We developed a finite volume package FVM and a solver HYMLS, both based on elements of the Trilinos EPETRA-package (see http://trilinos.sandia.gov/). HYMLS is a linear system solver for steady state incompressible Navier-Stokes equations coupled to transport equations in 2 and 3D.

Problem Setting

Our aim is to study the dynamics of fluid flow problems. In first instance we want to consider the ones related to incompressible flow.

\[
\begin{align*}
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u} &= -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f}(\phi) \\
\nabla \cdot \mathbf{u} &= 0
\end{align*}
\]

(1)

where \( \phi \) is a vector of components that are transported with the flow.

After discretization and linearized by Newton’s method, We get the structure of resulting linear systems (saddle-point system):

\[
\begin{pmatrix}
\mathbf{L} + \mathbf{N} \mathbf{Grad} \\
\text{Div}
\end{pmatrix}
\begin{pmatrix}
\mathbf{u} \\
\mathbf{p}
\end{pmatrix} =
\begin{pmatrix}
\mathbf{f}_u \\
\mathbf{f}_p
\end{pmatrix}
\]

(2)

Continuation Program FVM/HYMLS

In FVM, users create a number of routines, e.g. for the computation of the right-hand side and the Jacobian matrix. Hybrid Multilevel Linear Solver (HYMLS) is our workhorse, which is a hybrid of a direct and an iterative solver and used as preconditioner.

- Initialization
  - Partitioning + maps needed for parallelization (Epetra)
  - Set up templates for the matrix (call FVM)
  - Initialize solution
  - Continuation using LOCA (Solve linear system using HYMLS)
- Compute solution and eigenvalue

Weak Scalability in Parallel Computations

To study the weak scalability of the method on a parallel computer, we perform computations on 2D Rayleigh-Bénard convection. The computer used is an opteron cluster with infiniband connection between the nodes; every node contains 12 cores.

Time needed per unknown to make an LU factorization and to solve the equations, obtained from the table by computing \( (\text{NP} \times \text{LU fact})/4 \times (\text{NP}^2) \).

<table>
<thead>
<tr>
<th>Grid</th>
<th>NP</th>
<th>Iter</th>
<th>LU fact</th>
<th>Solve</th>
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</table>

Results for Rayleigh-Bénard Convection

RB convection has been often employed as benchmark problem for 2 and 3D NS equation solvers. Our continuation program was applied to determine the steady solutions and bifurcations of nonlinear governing equations as a function of Rayleigh number (Ra) for values of Ra up to \( 10^6 \).

Figure 2: Bifurcation diagram of flow in a cube at \( \text{Pr} = 1 \), \( \ell^2 \) norm of velocity in \( x \) direction as a function of Rayleigh number. Stable and unstable flow patterns are depicted with solid lines and dashed lines, respectively.

Figure 3: Flow patterns near the first three primary bifurcations. (a) \( x/y \) roll, (b) diagonal roll, (c) four rolls, (d) toroidal roll

Figure 4: Contours of the velocity component normal to the vertical plane \( z = 0.25 \), and velocity vector distributions for the \( x \)-roll flow pattern at \( Ra = 5730 \) and \( Ra = 20000 \), respectively.

Figure 5: Streamlines in a cubical cavity. (a) \( Ra = 10^3 \), (b) \( Ra = 10^4 \), (c) \( Ra = 10^5 \), (d) \( Ra = 10^6 \)

Results for Differentially Heated Cavity

Numerical experiments are done on a 3D cube, heated from the west wall. For low value of \( Ra \), the convection effect is less. With the increase of \( Ra \), the buoyancy force increases, resulting in a strong circulation of the fluid (clockwise rotation) and thus increasing convective heat transport.

Figure 6: Vector of velocity \( u \) and \( w \) on the plane \( y = 0 \) at \( Ra = 20000 \).

Contact

Weiyen Song, PhD
Johann Bernoulli Institute for Mathematics and Computer Science
University of Groningen
Nijenborgh 9
9747 AG Groningen
email: W.Song@rug.nl