High-End Computing for Incompressible Flows

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Outline of Talk

• INTRODUCTION
  - Status
  - Major Drivers of the Current Work
• OBJECTIVE
• SOLUTION METHODS
  - Formulation / Approach
  - Summary of Solver Development
  - Current Challenges
• HEC APPLICATIONS
  - Parallel Implementation
  - Application to SSME Turbopump
• DISCUSSION
Status from Applications Point of View

- Applications to Real-World Problems
  - N-S solution of full configuration was a big goal in the 80s
  - Numerical procedures and computing hardware have been advanced enabling simulation of complex configurations

- Some Examples of Successful Applications
  - Components of liquid rocket engine
  - Hydrodynamics (Submarines, propellers, ...)
  - Ground vehicles (automobile aerodynamics, internal flows...)
  - Biofluid problems (artificial heart, lung, ...)
  - Some Earth Science problems

- Current Challenges
  - For integrated systems analysis, computing requirement is very large
    ⇒ Analysis part is still limited to low fidelity approach
  - For high-fidelity analysis, especially involving unsteady flow, long turn-around time is often a bottle neck ⇒ Acceleration of solution time is required

Major Drivers of Current Work

- To provide computational tools as an economical option for developing future space transportation systems (i.e. RLV subsystems development)

  Impact on component design ⇒ Rapid turn-around of high-fidelity analysis
  Increase durability/safety ⇒ Accurate quantification of flow
  (i.e. prediction of low-induced vibration)

Impact on system performance ⇒ More complete systems analysis using high-fidelity tools

- Target
  Turbo-pump component analysis ⇒ Entire sub-systems simulation

  Computing requirement is large:
  ⇒ The goal is to achieve 1000 times speed up over what was possible in 1992
Objectives

- Mission of Conference
  To bring together Industry and Academia & (Government)
  To nurture the next generation in computational mechanics

- Objective of the Current Talk
  To discuss some current issues in large scale computing for mission-oriented tasks

Viscous Incompressible Flow

- Formulation
  Can be viewed as a limiting case of compressible flow where the flow speed is insignificant compared to the speed of sound (Preconditioned compressible N-S eq.)
  * Artificial compressibility approach
    - Artificial Compressibility Method (Chorin, 1967; Temam, 1977)
      - ADI Scheme, FD (Central-diss) (Beam & Warming, 1978; Briley-McDonald, 1977)
      - LU-SGS, FV (Central-diss) (Yoon and Jameson, 1987...)
      - Line Relaxation, FD (Upwind) (...MacCormack, 1985)
      - GMRES, FD (Upwind)
  * Or truly incompressible
    - Pressure projection approach
      - MAC (Harlow and Welch, 1965)
      - Fractional Step Method (Chorin, 1968; Yanenko, 1971; Marchuk, 1975...)
      - SIMPLE type Pressure Iteration (Caretto et al., 1972; Patankar & Spalding, 1972...)
    - Use derived variables
      - Vorticity-Velocity (Fasel, 1976; Dennis et al., 1979; Hafez et al., 1988)
      - Stream function-vorticity
Artificial Compressibility Method

- Formulation
  \[ \frac{\partial p}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \]
  - Introduces hyperbolic behavior into pressure field.
  - Speed of pressure wave depends on the artificial compressibility parameter, \( \beta \).
  - The equations are to be marched in a time-like fashion until the divergence of velocity converges to zero.
  - Relaxes incompressibility requirement.
  - Time variable during this process does not represent physical time step.

  For time-accurate solutions
  - Iterate the equations in pseudo-time level for each time step until incompressibility condition is satisfied.
  - Efficient sub-iteration is the key for success

Artificial Compressibility Method (INS3D-UP)

- Time accuracy is achieved by subiteration
  - Discretize the time term in momentum equations using second-order three-point backward-difference formula
    \[ \frac{3q^{n+1} - 4q^n + q^{n-1}}{2\Delta t} = -(rhs)^n \]
  - Introduce a pseudo-time level and artificial compressibility,
  - Iterate the equations in pseudo-time for each time step until incompressibility condition is satisfied.
    \[ \frac{1}{\Delta \tau} (p^{n+1} - p^n) = -\beta q^{n+1} \]
    \[ \frac{1.5}{\Delta \tau} (q^{n+1} - q^n) = -(rhs)^n - \frac{3q^{n+1} - 4q^n + q^{n-1}}{2\Delta t} \]

- Code performance
  - Computing time: 50-120 ms/grid point/iteration
  - Memory usage:
    - Line-relaxation: 45 words/grid point
    - GMRES-ILU(0): 220 words/grid point
Pressure Projection Method (INS3D-FS)

- Approach in generalized coordinates
  - Finite volume discretization
  - Accurate treatment of geometric quantities
  - Dependent variables - pressure and volume fluxes
  - Implicit time integration
  - Fractional step procedure
    Solve auxiliary velocity field first,
    then enforce incompressibility condition by solving a Poisson equation for pressure.

- Code performance
  - Computing time: 80 ms/grid point/iteration
  - Memory usage: 70 words/grid point

Pressure Projection Method

- Fractional-step
  - Solve for the auxiliary velocity field, using implicit predictor step:
    \[ \frac{1}{\Delta t}(u''_i - u'_i) = -\nabla p' + h(u'_i) \]
  - The velocity field at time level (n+1) is obtained by using a correction step:
    \[ \frac{2}{\Delta t}(u'''_i - u'_i) = -\nabla p''' + h(u''_i) - \nabla p' + h(u'_i) \]
  - The incompressibility condition is enforced by using a Poisson equation for pressure \((p' = p''' - p')\):
    \[ \nabla \cdot p' = \frac{2}{\Delta t} \nabla \cdot u' \]
Impulsively Started Flat Plate at 90°

- Time History of Stagnation Point

![Graph showing time history of stagnation point](image)

- History of INS3D Development

<table>
<thead>
<tr>
<th>Code</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>1988-1997 INS3D-UP (Robert, Kris, Kwak) INS3D-LU (Yoon, Kwak) INS3D-FS (Rosenfeld, Kris, Kwak)</td>
<td>Inducer</td>
</tr>
<tr>
<td>1998-Present Combined version (Kris, Kwak)</td>
<td>Advanced liquid sub-systems</td>
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</tbody>
</table>

**Note:** The diagrams and graphs are not described in detail in the text. The text provides a summary of the development and applications of the INS3D code, along with some visual representations of these developments.
Current Challenges

- Challenges where improvements are needed
  - Time-integration scheme, convergence
  - Moving grid system, zonal connectivity
  - Parallel coding and scalability

- As the computing resources changed to parallel and distributed platforms, computer science aspects become important such as
  - Scalability (algorithmic & implementation)
  - Portability, transparent coding etc.

- Computing resources
  - "Grid" computing will provide new computing resources for problem solving environment
  - High-fidelity flow analysis is likely to be performed using "super node" which is largely based on parallel architecture

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Supercomputing Memory and CPU Requirements
Parallel Implementation of INS3D

• INS3D-MPI
  (coarse grain)
  T. Faulkner & J. Dacles

• INS3D-MPI / Open MP
  MPI (coarse grain) + OpenMP (fine grain)
  Implemented using CAPO/CAPT tools
  H. Jin & C. Kiris

• INS3D-MLP
  C. Kiris

Parallel Implementation of INS3D

• Previous Work (SSME Impeller)
Parallel Implementation of INS3D

MPI coarse grain + OpenMP fine grain
TEST CASE: SSME Impeller

24 zones / 2.8 Million points
60 zones / 19.2 Million points

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Multi-Level Parallelism (MLP)

INS3D-MLP: MLP routines + OpenMP
Shared Memory MLP Organization for Origin 2000

MLP Process 1
Common /local/ aa, bb

MLP Process 2
Common /local/ aa, bb

Zones 1,4
OpenMP

MLP Data sharing via
Load/Stores
330 nanoseconds

Contract with
MPI at
19 microsecond

OpenMP

Zones 2,3,5

Common /global/ x,y,z
Parallel Implementation of INS3D

INS3D-MLP (NAS MLP no pin-to-node) / OpenMP

TEST CASE: SSME Impeller
60 zones / 19.2 Million points

Space Shuttle Main Engine Turbopump

Inlet Guide Vane
Impeller
Diffuser
Space Shuttle Main Engine Turbopump

Overset Grid System

Inlet Guide Vane:
15 Blades
23 Zones
6.5 M Points

Diffuser:
23 Blades
31 Zones
8.6 M Points

Shuttle Upgrade SSME-rig1

Impeller Grid:
60 Zones / 19.2 Million Grid Points
Smallest zone : 75K, Largest zone : 996K
Less than 192 orphan points.

Hub grid
grid for tip clearance
blade grid
background grid
Shroud grid
Parallel Implementation of INS3D

INS3D-MLP / 40 Groups
RLV 2nd Gen Turbo pump
114 Zones / 34.3M grid points

Per processor Mfloop is between 60-70.
Code optimization for cache based platforms is currently underway.
Target Mflops is to reach 120 per processor.
Increasing number of OpenMP threads is also the main objective for this effort.

SSME-rig1/ Overset Grid System

Initial Start: first time step
Velocity colored by magnitude
Impeller started at 10% of design speed

Time Step 5
Impeller rotated 2.25 degrees
Time Step 7: Impeller rotated 3-degrees at 30% of design speed

Time Step 18: Impeller rotated 8-degrees at 100% of design speed
Summary of SSME Turbopump Simulation

Problem size:
- 34.3 Million Points
- 800 physical time steps in one rotation

CPU requirement:
- One physical time-step requires less than 20 minutes wall time with 80 CPUs on Origin 2000.
- One complete rotation requires one-week wall time with 80 CPUs.

I/O:
- Currently I/O is through one processor. Timing will be improved with parallel I/O since time-accurate computations are I/O intensive.

Parallel Efficiency:
- MLP/OpenMP version requires 19-25% less computer time than MPI/OpenMP version.
- Pin-to-node for MLP version reduces computer time by 40%.

Discussion on Numerical Procedures

- Finite Difference
  - Based on Taylor series expansion ⇒ Requires smooth grid
  - Need special care for grid singularity
  - Generally easier to use fine grids near wall at high Reynolds number

- Finite Volume
  - Formulation is more physical (conservation of properties)
  - Viscous flux calculation is not as straightforward
  - Difficult to implement higher order schemes

- In actual implementation, however,
  - These differences become unclear
    - i.e. - FV in curvilinear coordinates requires lots of averaging depending on definition of variables such as staggered vs cell vertex arrangement
    - Both FD and FV implementations are very similar near grid singularities

- Major differences come from time integration scheme which also affects the computational efficiencies, especially, for unsteady flow computations
Discussion on Applications

- Rapid turn around can be accomplished through the use of
  - Algorithm: convergence acceleration such as multi-grid, and GMRES
  - Parallel implementation

- Total process time can be reduced by
  - Automatic solution process including CAD to grid procedure

- Need further development of methodology as well as physics modeling for
  - Deep understanding of flow physics such as unsteady flow characterization for
    better aeroacoustics modeling, and flow induced vibration
    \( \Rightarrow \) Is LES method mature enough for this?
  - Need to matrix IT tools to flow simulation for smart flow control and optimization

- Efficient extraction of information is still a challenge

On top of all these we still need trained CFDers to solve many unsolved real world problems, for development of flow devices and for better understanding of flow physics
Parallel Implementation of INS3D

INS3D-MPI - coarse grain
Implemented by T. Faulkner & J. Dacles

Group 1  Group 2  Group 3  Group N
Parallel Implementation of INS3D

INS3D-MPI/OpenMP
MPI (coarse grain) + OpenMP (fine grain)
Implemented by using CAPO/CAPT tools

MPI

OpenMP threads

Group 1

Group N

MPI coarse grain + OpenMP fine grain
TEST CASE: SSME Impeller
24 zones / 2.8 Million points

Number of CPUs

OpenMP Threads per MPI Group

Time (sec) per iteration

2.8M Points

- 4 MPI groups
- 12 MPI groups
- 24 MPI groups
Parallel Implementation of INS3D

MPI coarse grain + OpenMP fine grain

TEST CASE: SSME Impeller
60 zones / 19.2 Million points

Number of CPUS vs. Time (sec) per Iteration

OpenMP with two different solvers

TEST CASE: SSME Impeller
60 zones / 19.2 Million points

Number of OpenMP Threads vs. Time (sec) per Iteration
Parallel Implementation of INS3D

MPI coarse grain + OpenMP fine grain

TEST CASE: SSME Impeller
60 zones / 19.2 Million points

INS3D-MLP (NAS MLP no pin-to-node) / OpenMP

TEST CASE: SSME Impeller
60 zones / 19.2 Million points
Parallel Implementation of INS3D

INS3D-MLP/OpenMP vs. -MPI/OpenMP

TEST CASE: SSME Impeller
60 zones / 19.2 Million points

INS3D-MLP
GMRES-ILU(0) solver – 20 Groups

TEST CASE: SSME Impeller
60 zones / 19.2 Million points