Generation of Multiple Turbulent Flow States for the Simulations With Ensemble Averaging

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Motivation

High-fidelity turbulent flow simulations assumes:

- Eddy-resolving methods (DNS / LES / DES)
- Huge computational grids \(10^6-10^{10}-\ldots\)
- Long time integration to collect turbulent statistics \(10^4-\ldots \text{ time steps}\)
Typical DNS / LES simulation

Overall simulation: \[ T = T_T + T_A \]

*Evolution of integral velocity perturbations amplitude in a straight pipe*
Parallelization in time

Simulation with two different initial states

Simulation time per each run:

\[ T_1 = T_T + T_A / 2 \]

Overall time:

\[ T_{total} = 2T_T + T_A \]
Ensemble averaging (1)


- $m$ independent runs
- Speedup due to increase of computational resources
Typical methods for modelling incompressible turbulent flows with eddy-resolving models:

- **High-order Runge-Kutta time integration schemes (one of substeps):**

\[
\frac{u^* - u^n}{\Delta t} = - (u^n \cdot \nabla) u^n + \frac{1}{Re} \nabla^2 u^n
\]

\[
u^{n+1} = u^* - \Delta t \nabla p^{n+1}
\]

\[
\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot u^*
\]

- **Krylov subspace & Multigrid methods for solving pressure Poisson equations**
High-order Runge-Kutta time integration schemes (one of substeps):

\[
\frac{U^* - U^n}{\Delta t} = - (U^n \cdot \nabla) U^n + \frac{1}{Re} \nabla^2 U^n
\]

\[
U^{n+1} = U^* - \Delta t \nabla P^{n+1}
\]

\[
\nabla^2 P^{n+1} = \frac{1}{\Delta t} \nabla \cdot U^*
\]

«Generalized» velocity & pressure:

\[
U = \{u_1, u_2, \ldots, u_m\} \quad P = \{p_1, p_2, \ldots, p_m\}
\]

Pressure Poisson equation with multiple right-hand sides
PPE with multiple RHSs

Basic aspects for Krylov subspace & Multigrid methods:

- **Sparse matrix storage formats (e.g., CSR)**
- **Operations with vectors (linear operations, scalar products)**
  - memory bound (e.g., STREAM benchmark)
- **Sparse Matrix-Vector multiplications (SpMV)**
  - memory bound

- Generalized SpMV with multiple RHSs allows to significantly increase the performance due to increase of the computational intensity (flop per byte ratio)
Ensemble averaging (2)


- $m$ independent runs
- Speedup due to increase of computational resources


- Simultaneous modelling of $m$ states in a single run
- Speedup due to memory traffic reduction when solving pressure Poisson equation
Simulation speedup theoretical estimates (1)

\[ P_m = \frac{1 + \beta}{m + \beta} \frac{5m}{5m - 3\theta(m - 1)} \]

Three parameters:

| \( \beta = \frac{T_A}{T_T} \) | *Time intervals ratio; determined by the problem statement* |
| \( \theta \) | *SLAE solver time ratio; determined by the choice of the numerical methods used* |
| \( m \) | *Number of simultaneously modelled flow states* |
Simulation speedup as a function of a number of flow states:

\[ \theta = 0.85 \]
Generation of multiple flow states

Introducing perturbations at the transition stage ($T_B$):

\[ T_T - T_B \gtrsim T_{corr} \]
Influence on the simulation speedup

\[ T_B = 0 \]

\[ \frac{T_B}{T_T} = 0.75 \]
Computational codes

Software:

- **Linear solver for SLAEs with multiple RHSs:** BiCGStab + Algebraic Multigrid (hybrid MPI + Posix Shared Memory programming model)

- **In-house code for Direct Numerical Simulation of turbulent flows, allowing simultaneous modelling of multiple flow states**

**Test problem**

**Flow in a channel with a matrix of wall-mounted cubes:**
- **No-slip bc at the channel and cube walls**
- **Periodic bc at lateral faces**
- **Reynolds number:** \( \text{Re}_b = \frac{U_b h}{\nu} = 3854 \)
- **Integration intervals:** \( T_T = 100; \ T_A = 2000 \)

<table>
<thead>
<tr>
<th>Grid 1</th>
<th>Grid 2</th>
<th>Grid 3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Grid size</strong></td>
<td>144 x 112 x 144</td>
<td>240 x 168 x 240</td>
</tr>
<tr>
<td><strong>Cube</strong></td>
<td>52 x 38 x 52</td>
<td>100 x 74 x 100</td>
</tr>
<tr>
<td><strong>( h_x, h_z )</strong></td>
<td>0.0065( h ) – 0.054( h )</td>
<td>0.0031( h ) – 0.038( h )</td>
</tr>
<tr>
<td><strong>( h_y )</strong></td>
<td>0.0054( h ) – 0.07( h )</td>
<td>0.003( h ) – 0.044( h )</td>
</tr>
<tr>
<td><strong>Overall size</strong></td>
<td>2.32 M</td>
<td>9.68 M</td>
</tr>
</tbody>
</table>
Simulation results

Test case: Grid 1, 2.32 M cells
32 nodes, “Lomonosov-2” (448 cores)

<table>
<thead>
<tr>
<th>Flow states, m</th>
<th>$T_B / T_T$</th>
<th>CPU time, min</th>
<th>Expected speedup</th>
<th>Actual speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>1088</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>790</td>
<td>1.42</td>
<td>1.38</td>
</tr>
<tr>
<td>4</td>
<td>0.77</td>
<td>729</td>
<td>1.53</td>
<td>1.49</td>
</tr>
<tr>
<td>8</td>
<td>0.77</td>
<td>695</td>
<td>1.63</td>
<td>1.57</td>
</tr>
</tbody>
</table>
Cross-correlation for different flow states

Cross-correlation of the time series for the longitudinal velocity components of 4 flow states
Conclusion

The methodology of generation multiple uncorrelated turbulent flow states based on introducing perturbations during the transition stage has been investigated.

The performance gain theoretical estimate has been extended to cover the simulation scenario of interest.

Actual simulation speedup agrees with the proposed estimates.

The proposed methodology:
- Extends the range of applicability for the ensemble averaging approach.
- Provides additional 20% simulation speedup.
List of publications

