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Methods for Computational Fluid Dynamics Aiming Quantum Computing

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This work investigates linearization techniques for the Navier-Stokes equations (NSE) using the Taylor-Green Vortex (TGV) benchmark, with applications to Quantum Computing (QC). Pre-processing NSE for QC will open avenues for faster fluid simulations in the future [4].

Quantum algorithms require linear formulations, as quantum operations follow the superposition principle through unitary transformations [2]. This fundament is shown in Dirac notation:

$$U\left(a|\psi_1\rangle + b|\psi_2\rangle\right) = aU|\psi_1\rangle + bU|\psi_2\rangle, \tag{1}$$

where U is a unitary operator ($U^\dagger U = I$), $|\psi_i\rangle$ represent quantum state vectors, and $a, b \in \mathbb{C}$ are complex probability amplitudes. The nonlinear convective term $(\mathbf{u}\cdot\nabla)\mathbf{u}$ in NSE violates this linearity requirement, necessitating specialized approximation techniques. The TGV problem provides an ideal test case for its exact analytical solution and periodic boundary conditions [1, 7].

The TGV test case is governed by the incompressible NSE [7]:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu\nabla^2\mathbf{u}, \quad \nabla\cdot\mathbf{u} = 0, \tag{2}$$

where $\mathbf{u}$ is the velocity field, p is the pressure, ν is the kinematic viscosity, and t is time.

The analytical solution for TGV is [7]:

$$\mathbf{u}_{\text{analytical}} = \begin{pmatrix} A\cos(ax)\sin(by)\sin(cz)e^{-\nu(a^2+b^2+c^2)t} \\ B\sin(ax)\cos(by)\sin(cz)e^{-\nu(a^2+b^2+c^2)t} \\ C\sin(ax)\sin(by)\cos(cz)e^{-\nu(a^2+b^2+c^2)t} \end{pmatrix}, \tag{3}$$

where A, B, C, a, b, and c are constants, and x, y, and z are Cartesian coordinates.

The studied methods are:

1. **Local Temporal Linearization:** Approximates the nonlinear term using a Taylor series expansion around equilibrium $\mathbf{u}_0$ [6]:

$$(\mathbf{u}\cdot\nabla)\mathbf{u} \approx (\mathbf{u}_0\cdot\nabla)\mathbf{u}_0 + \alpha\left[(\mathbf{u}_0\cdot\nabla)\delta\mathbf{u} + (\delta\mathbf{u}\cdot\nabla)\mathbf{u}_0\right], \tag{4}$$

where $\delta\mathbf{u} = \mathbf{u} - \mathbf{u}_0$ is a small perturbation, and α is a coefficient that calibrates the velocity field at each time step.

2. **SVD Matricial Tensorial Linearization:** Uses Singular Value Decomposition (SVD) to approximate velocity fields in low-rank format, reducing complexity while preserving flow features. The 3D fields are reshaped into 2D matrices, decomposed via SVD, and rebuilt using dominant singular components:

$$\mathbf{u}_{\text{approx}} = \mathbf{U}_{:,1:r}\cdot\mathbf{S}_{1:r,1:r}\cdot\mathbf{V}^T_{1:r,:}, \tag{5}$$

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where $\mathbf{U}$, $\mathbf{S}$, and $\mathbf{V}$ are singular vectors and values, and r is the rank. The linearized fields are updated as:

$$\mathbf{u}_{\text{linearized}} = \mathbf{u}_{\text{approx}} - \alpha \mathbf{u}_{\text{approx}} \Delta t, \tag{6}$$

where α is a linearization coefficient and Δt is the time step. This approach aligns with low-rank solvers for Navier-Stokes equations [3].

3. Logarithmic Linearization: This method linearizes nonlinear velocity terms by applying a logarithmic transformation to $|\mathbf{u}|$, ensuring positivity with a small constant $\epsilon = 10^{-10}$. Linearization is performed in log-space and mapped back via the exponential function, preserving velocity direction [5]:

$$\mathbf{u}_{\log} = \log(|\mathbf{u}| + \epsilon), \quad \mathbf{u}_{\text{linearized}} = \exp\left(\mathbf{u}_{\log} - \alpha \mathbf{u}_{\log} \Delta t\right) \cdot \frac{\mathbf{u}}{|\mathbf{u}|}, \tag{7}$$

where α is a linearization coefficient and Δt the time step.

Numerical experiments used a 64^3 grid, 2π domain, $\nu = 0.01$ m^2/s, $\Delta t = 0.001$ s, third-order Runge-Kutta time integration [1], and finite-differences for spatial derivatives.
The methods yielded comparable accuracy to standard NSE:

- **Navier-Stokes**: MSE = 0.049062, Absolute Error = 0.161511
- **Local Temporal**: MSE = 0.049062, Absolute Error = 0.161511
- **SVD**: MSE = 0.049001, Absolute Error = 0.161220
- **Logarithmic**: MSE = 0.049049, Absolute Error = 0.161493

The SVD method showed superior performance, demonstrating potential for quantum computing applications where linear formulations are essential.

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