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EXA, ZETTA, YOTTA AND BEYOND: ON THE EVOLUTION OF POISSON SOLVERS

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Abstract. In this work, we aim to shed light to the following research question: *is the complexity of numerically solving Poisson's equation increasing or decreasing for very large DNS and LES simulations of incompressible flows?* Physical and numerical arguments are combined to derive power law scalings at very high Reynolds numbers.

1 INTRODUCTION

We consider the simulation of turbulent incompressible flows of Newtonian fluids. Under these assumptions, the governing equations read

$$\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = 2\rho^{-1}\nabla\cdot(\mu\mathsf{S}(\boldsymbol{u})) - \nabla p, \qquad \nabla\cdot\boldsymbol{u} = 0, \tag{1}$$

where $\boldsymbol{u}(\boldsymbol{x},t)$ and $p(\boldsymbol{x},t)$ denote the velocity and pressure fields, and $\mathsf{S} = 1/2(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^T)$ is the rate-of-strain tensor. The density, ρ, is constant whereas the dynamic viscosity, $\mu(\boldsymbol{x},t)$, may depend on space and time. Notice that for (spatially) constant viscosity the diffusive term simplifies to $\nu\nabla^2\boldsymbol{u}$ where $\nu = \mu/\rho$ is the kinematic viscosity. Then, these equations have to be discretized both in space and time.

The basic physical properties of the Navier–Stokes (NS) equations (1) are deduced from the symmetries of the differential operators (see Ref.[1], for example). In a discrete setting, such operator symmetries must be retained to preserve the analogous (invariant) properties of the continuous equations [2, 3]: namely, the convective operator is represented by a skew-symmetric coefficient matrix, the diffusive operator by a symmetric, negative-definite matrix and the divergence is minus the transpose of the gradient operator. Therefore, even for coarse grids, the energy of the resolved scales of motion is convected in a stable manner, *i.e.* the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should be from a physical point-of-view.

On the other ands, from the pioneering turbulent channel flow simulations in the mid-'80s, DNS and LES simulations of incompressible flows have usually been carried out by means of a fractional step method (FSM) together with an explicit or semi-implicit time-integration methods for momentum, *i.e.* the convective term is virtually always integrated

with an explicit scheme whereas the diffusive term may be treated either implicitly or explicitly. This leads to the following CFL restrictions for the time-step

$$\Delta t^{conv} \sim \frac{\Delta x}{U} \qquad \Delta t^{\text{diff}} \sim \frac{\Delta x^2}{\nu}, \tag{2}$$

where Δx represents the grid spacing and U is a characteristic velocity of the large flow scales. Then, the pressure-velocity coupling is solved with a FSM leading to a Poisson equation for pressure (or some sort of pseudo-pressure),

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t}\nabla \cdot \boldsymbol{u}^p, \tag{3}$$

where $\boldsymbol{u}^p$ is a predictor velocity obtained by advancing on time the momentum equation. Once this Poisson equation is solved, the new (incompressible) velocity field is obtained, $\boldsymbol{u}^{n+1} = \boldsymbol{u}^p - \Delta t \nabla p$. Poisson equation is the most time-consuming part and the main bottleneck for extreme-scale CFD simulations. In this context, we aim to shed light to the following research question: *is the complexity of numerically solving Poisson's equation increasing or decreasing for very large DNS and LES simulations of incompressible flows?*

2 TWO COMPETING EFFECTS

The never-ending increasing capacity of modern HPC system enables running DNS simulations at higher and higher Reynolds number, Re. Estimations of how the number of grid points, N_x, and time-steps, N_t, grow with $Re = Ul/\nu$ can be easily obtained from the classical Kolmogorov theory (K41)

$$N_x^{K41} = \frac{\Delta x}{L_x} \sim \frac{\eta}{l} \sim Re^{-3/4} \qquad N_t^{K41} = \frac{\Delta t}{t_{\text{sim}}} \sim \frac{t_\eta}{t_l} \sim \frac{\eta}{l}\frac{U}{u} \sim Re^{-3/4}Re^{1/4} = Re^{-1/2}, \tag{4}$$

where L_x and t_{sim} are the domain size and the time integration period, which are assumed to be similar to the size of the largest scales, l, and its corresponding characteristic time, $t_l \sim l/U$, *i.e.* $L_x \sim l$ and $t_{\text{sim}} \sim t_l$. For a DNS, we can also assume that $\Delta x \sim \eta$ and $\Delta t \sim t_\eta \sim \eta/u$, where $t_\eta \sim \eta/u$ and u are the characteristic time and velocity of the Kolmogorov length scales, η. Plugging this into Eqs.(2) leads to the following estimations

$$N_t^{\text{conv}} \sim \frac{\Delta t^{\text{conv}}}{t_l} \sim \frac{U}{l}\frac{l Re^{-3/4}}{U} = Re^{-3/4} \qquad N_t^{\text{diff}} \sim \frac{\Delta t^{\text{diff}}}{t_l} \sim \frac{U}{l}\frac{l^2 (Re^{-3/4})^2}{\nu} = Re^{-1/2}. \tag{5}$$

Therefore, we can conclude that

$$\frac{\Delta t}{t_l} \sim Re^{\alpha}, \tag{6}$$

where $\alpha = -1/2$ for the K41 theory (see Eq. 4) or diffusion dominated (see Eq. 5), and $\alpha = -3/4$ for convection dominated (see Eq. 5). Therefore, higher Re leads to smaller time-steps, Δt, leading to better initial guess for the Poisson equation. Namely, assuming that $\nabla \cdot \boldsymbol{u}^n = 0$ and taking p^n as initial guess, we obtain the following initial residual

$$r^0 = \nabla^2 p^n - \frac{1}{\Delta t}\nabla \cdot \boldsymbol{u}^{p,n+1} \overset{(3)}{=} \frac{1}{\Delta t}\left(\nabla \cdot \boldsymbol{u}^{p,n} - \nabla \cdot \boldsymbol{u}^{p,n+1}\right) \approx \frac{\partial \nabla \cdot \boldsymbol{u}^p}{\partial t}, \tag{7}$$

where $\nabla \cdot \boldsymbol{u}^p \approx \Delta t \nabla \cdot (\boldsymbol{u} \cdot \nabla \boldsymbol{u}) = 2\Delta t Q_G$ and $Q_G = -1/2 tr(\mathsf{G}^2)$ is the second invariant of the velocity gradient tensor, $\mathsf{G} \equiv \nabla \boldsymbol{u}$, leading to

$$r^0 \approx 2\Delta t \frac{\partial Q_{\mathsf{G}}}{\partial t}, \tag{8}$$

Therefore, smaller time-steps will benefit the convergence of Poisson solver.

On the other hand, increasing Re also leads to finer meshes (see Eq. 4) and, therefore, to more ill-conditioned systems with a wider and wider range of scales to be resolved. In the forthcoming analysis, the spectral distribution of the initial residual, $\hat{r}_k^0$, plays a crucial role. In general, we can assume a power law scaling within the internal range

$$\frac{\partial Q_{\mathsf{G}}}{\partial t} \propto k^\beta \qquad \Longrightarrow \qquad \hat{r}_k^0 \propto \Delta t k^\beta, \tag{9}$$

where k is the wavenumber. A power law scaling for Q_{G} can be derived from the $k^{-7/3}$ scaling of the shell-summed pressure spectrum [4],

$$(\hat{Q}_{\mathsf{G}})_k \propto k^2 (k^{-7/3})^{1/2} = k^{5/6}. \tag{10}$$

Then, the value of β may be estimated from the dynamics of the invariants obtained from the so-called restricted Euler equations,

$$\frac{dQ_{\mathsf{G}}}{dt} = -3R_{\mathsf{G}} \qquad \Longrightarrow \qquad \frac{\partial Q_{\mathsf{G}}}{\partial t} = -(\boldsymbol{u} \cdot \nabla) Q_{\mathsf{G}} - 3R_{\mathsf{G}} \tag{11}$$

where $R_{\mathsf{G}} = det(\mathsf{G}) = 1/3 tr(\mathsf{G}^3)$ is the third invariant of G. In summary, there are two competing effects (see Figure 1, left) when increasing Re number: time-step, Δt, decreases whereas the range of scales increases.

3 ON THE SOLVER CONVERGENCE

Using the Parseval's theorem, we can relate the L2-norm of the residual with the integral of $\hat{r}_k$ for all the wavenumbers

$$||r||^2 = \int_\Omega r^2 dV = \int_1^{k_{\max}} \hat{r}_k^2 dk, \tag{12}$$

where $k_{\max} \approx 1/\eta \sim Re^{3/4}$. Then, the residual after n iterations can be computed as

$$||r^n||^2 = \int_1^{k_{\max}} \left(\hat{\omega}_k^n \hat{r}_k^0\right)^2 dk \overset{(6),(9)}{\approx} \int_1^{Re^{3/4}} \hat{\omega}_k^{2n} Re^{2\alpha} k^{2\beta} dk, \tag{13}$$

where $\hat{\omega}_k = \hat{r}_k^{n+1}/\hat{r}_k^n$ is the convergence ratio of the solver. For instance, for a Jacobi solver, $\hat{\omega}_k = \cos(\frac{\pi}{2}\rho)$ where $\rho \equiv k/k_{\max}$. In this case, using a quadratic approximation of the $\cos(x) \approx 1 - 4x^2/\pi^2$ leads to

$$||r^n||^2 \approx \frac{Re^{2(\alpha+3/4(\beta+1/2))}}{2(2n+1)}. \tag{14}$$

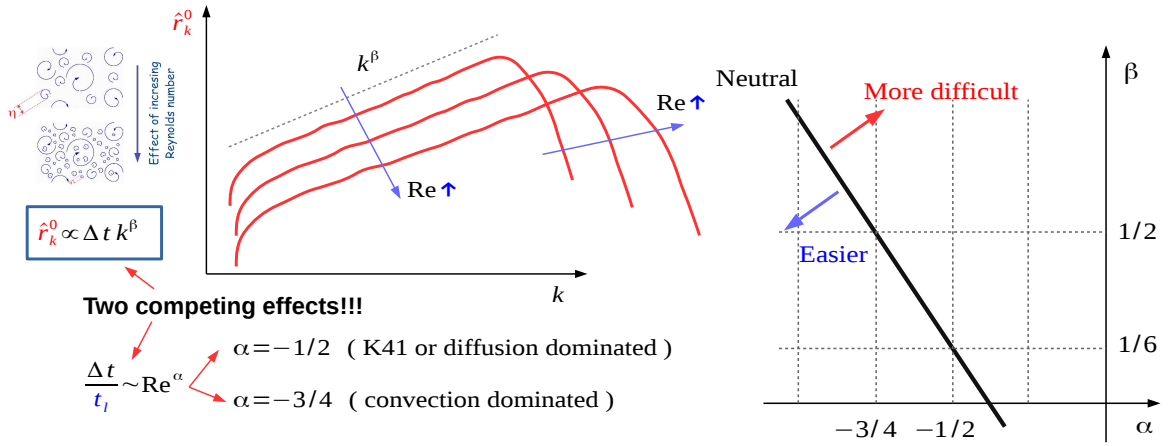

Figure 1: Left: illustrative explanation of the two competing effects on the solution of Poisson's equation when increasing Re number: time-step, Δt, decreases whereas the range of scales increases. Right: $\{\alpha, \beta\}$ phase space. Solid black line corresponds to $\propto Re^0$ in Eqs.(14) and (15), *i.e.* neutral effect of Re-number in the total number of iterations.

This analysis can be extended for a multigrid (MG) solver with $l_{\max} \approx \frac{3}{4}\log_2 Re$ levels and Jacobi as smoother

$$||r^n||^2 \approx \frac{Re^{2(\alpha+3/4(\beta+1/2))}}{2(2n+1)} \left\{ \left(\sum_{l=0}^{l_{\max}} \frac{(3/4)^{2n+1}}{2^{2l}} \right) + \frac{1}{2^{2l_{\max}+1}} \right\}. \tag{15}$$

Notice that compared with Eq.(14), the convergence is strongly accelerated by the term in brackets, which in the limit tends to $(3/4)^{2n}$. Nevertheless, the power law scaling with Re is the same; therefore, the regions defined in the $\{\alpha, \beta\}$ phase space remain unchanged (see Figure 1, right). DNS of homogeneous isotropic turbulence are being carried out to find out the exact value of β in Eq.(9). Results will be presented during the conference.

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