Direct Numerical Simulation:

As mentioned previously, direct numerical simulation (DNS) directly solves the Navier-Stokes equations, resolving all the scales of motion, with initial and boundary conditions appropriate to the flow considered. While DNS is very expensive, it provides unparalled resolution of flow details.

The numerical methods of choice in DNS are spectral and pseudo-spectral methods. Unlike finite difference, finite volume, and finite element methods, spectral methods are global methods, where the computation at any given point depends not only on neighboring points, but on information from the entire domain. Spectral methods converge exponentially, making them significantly more accurate than local methods. Pseudo-spectral methods are closely related to spectral methods but employ specialized algorithms such as the Fast Fourier Transform (FFT) to considerably reduce computational time.

To discuss the application of DNS, it helps to consider the specialized setting of homogeneous turbulence. In this setting, the solution domain is a cube of side $\mathcal{L}$, and the velocity field may be represented as a Fourier series:

$$\vec{u}(\vec{x},t) = \sum_{\vec{K}} e^{i\vec{K}\cdot\vec{x}}\, \hat{u}(\vec{K},t)$$

As discussed previously, the Fourier modes $\hat{u}(\vec{K},t)$ advance in time according to the equation:

$$\left(\frac{d}{dt} + \nu K^2\right) \hat{u}_j(\vec{K},t) = -i K_l P_{jk}(\vec{K}) \left(\hat{u}_k * \hat{u}_l\right)(\vec{K},t) \qquad (*)$$

which is precisely the Navier-Stokes momentum equation in wavenumber space. Above,

$$P_{jk}(\vec{K}) = \delta_{jk} - \frac{K_j K_k}{K^2} \qquad \text{Projection Tensor}$$

$$\left(\hat{u}_k * \hat{u}_l\right)(\vec{K},t) = \sum_{\vec{K}'} \hat{u}_k(\vec{K}',t)\, \hat{u}_l(\vec{K}-\vec{K}',t) \qquad \text{Discrete Convolution}$$

The spectral method truncates the Fourier series to a total of N^3 wavenumbers, where the even number N represents the number of modes in a single direction. The number N determines the size of the simulation, and consequently the Reynolds number that can be attained. In magnitude, the lowest non-zero wavenumber is $K_0 = 2\pi/\mathcal{L}$, and the N^3 wavenumbers represented are:

$$\vec{K} = K_0 \vec{n} = K_0 \left(\hat{e}_1 n_1 + \hat{e}_2 n_2 + \hat{e}_3 n_3\right)$$

for integer values $-\frac{1}{2}N+1 < n_i < \frac{1}{2}N$. The spectral method advances the Fourier modes in small time steps Δt according to $(*)$. Summing the triad interactions in this equation requires on the order of N^6 operations, resulting in a method of large computational cost.

To avoid the large cost associated with the nonlinear convective term, the pseudo-spectral method employs a different approach to evaluate the convection:

(i) First, the discrete Fourier transform (DFT) is used to map the velocity field from wavenumber space to physical space at a set of N^3 grid nodes.

(ii) In physical space, the nonlinear product $u_i u_j$ is evaluated at the set of N^3 grid nodes.

(iii) Finally, the DFT is used to map the nonlinear terms back to physical space, yielding the discrete convolution $\hat{u}_k * \hat{u}_\ell$, up to the scaling factor $-iK_\ell$.

The FFT may be utilized to perform the DFT in steps (i) and (iii) above, so the total cost of evaluating the nonlinear term is $O(N^3 \log N)$ for the pseudo-spectral method. This is significantly less than the cost associated with the standard spectral method. Nonetheless, the DFT introduces an aliasing error that must be removed or controlled.

Pseudo-spectral methods have enjoyed considerable success since they were first pioneered by Orszag and colleagues in the 1970s. The main numerical and computational issues in these methods are:

(i) Time-stepping
(ii) Contol of aliasing errors
(iii) Parallel implementation

These issues have been elegantly treated by the algorithm developed by Rogallo in 1981, which forms the basis for many DNS codes today. Of particular note is Rogallo's approach to control aliasing errors, which uses a low-cost combination of phase-shifts and truncation to apply the traditional 3/2 dealiasing rule promoted by Orszag. Today, there is a widely available parallel FFT package, included with FFTW, further enabling the use of pseudo-spectral methods in DNS.

The computational cost of a homogeneous turbulence simulation is largely determined by the resolution requirements. The spectral representation is equivalent to representing $\vec{u}(\vec{x},t)$ in physical space on a N^3 grid of uniform spacing:

$$\Delta x = \frac{L}{N} = \frac{\pi}{K_{max}} \qquad \text{where} \quad K_{max} = \tfrac{1}{2} N k_0 = \frac{\pi N}{L}$$

For homogeneous turbulence, the box size L must be large enough to represent the energy-containing motions, and the grid spacing Δx must be small enough to resolve the dissipative scales. Consequently,

$$N \sim \frac{L}{\eta} \sim Re_L^{3/4} \sim Re_\lambda^{3/2}$$

Hence, the total number of modes increases as:

$$N^3 \sim Re_L^{9/4} \sim Re_\lambda^{9/2}$$

For the advance of the solution of homogeneous turbulence in time to be sufficiently accurate, it is necessary to have a fluid particle move only a fraction of the grid spacing Δx in a time step Δt. This motivates the Courant condition:

$$\frac{k^{1/2} \Delta t}{\Delta x} = \text{const.}$$

The duration of a simulation is typically on the order of the turbulence time-scale $\tau = k/\varepsilon$, so the number of time steps required scales like:

$$M \sim \frac{\tau}{\Delta t} \sim \frac{L}{\Delta x} \sim Re_\lambda^{9/2}$$

Now, making the strong assumptions that only $O(N^3)$ operations are required per time step, the total computational time of a simulation scales like:

$$T_G \sim N^3 M \sim Re_L^3 \sim Re_\lambda^6$$

Consequently, there is a hugely steep increase in computational cost with increasing Reynolds number. This has precluded the use of DNS for realistic flow problems. Plots of the time in days needed to perform DNS of homogeneous turbulence are included in a PDF on D2L at the link:

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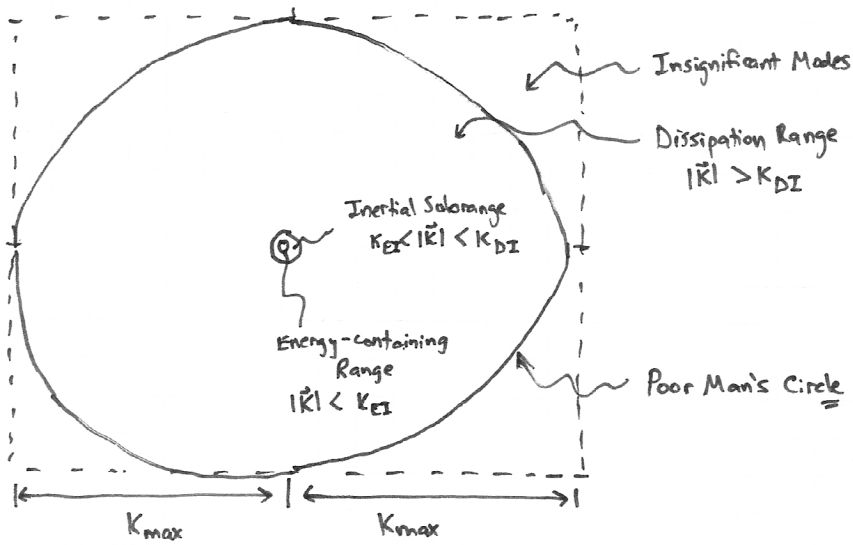
From these plots, we see that while it would take only one day to perform a DNS simulation at $Re_\lambda = 100$ on a gigaflop computer, (10^8 =) one hundred million days (or roughly 300,000 years) would be required to perform a DNS simulation at $Re_\lambda = 1000$ on a gigaflop computer. It is perhaps surprising then that a DNS simulation at $Re_\lambda = 1217$ has been performed using $N = 4096$ modes in each direction. This simulation was performed by the research group of Yokokawa in 2002 on the Earth Simulator, a testament to the enabling power of high-performance computing.

It is revealing to examine the distribution of computational effort over the various scales of turbulent motion. In wavenumber space, the modes represented lie within the cube of side $2\,K_{max}$:



In a well-resolved simulation, only modes within the sphere of radius K_{max} are significant. The dissipation range corresponds to the spherical shell of wavenumbers $|\vec{K}|$ between K_{DI} and K_{max}, where $K_{DI} = 0.1/\eta$. The inertial range corresponds to the spherical shell of wavenumbers $|\vec{K}|$ between K_{EI} and K_{DI} where K_{EI} is the wavenumber corresponding to the peaks in the energy spectrum. The energy-containing range corresponds to the sphere of wavenumbers of radius K_{EI}.

At $Re_\lambda = 70$, 99.8% of the modes have numbers $|\vec{K}|$ greater than K_{DI}, and this percentage further increases with Re_λ. Consequently, a very small percentage of modes represent motions in the energy-containing range and inertial subrange for high Re_λ.

Compared with homogeneous turbulence, the principal differences in applying DNS to inhomogeneous flows are that:

(i) Fourier representations cannot be used in directions of inhomogeneity
(ii) Physical boundary conditions (as opposed to periodic conditions) are required
(iii) Near-wall motions, characterized by the viscous length scale, introduce an additional resolution requirement

Typically, Fourier representations are employed in periodic directions and (Jacobi or Chebyshev) polynomials are employed in inhomogeneous directions. A popular alternative is the use of B-splines in inhomogeneous directions due to their high resolving power, easy implementation of boundary conditions, and ability to employ stretched grids. The largest DNS to date was of turbulent channel flow at $Re_\tau = 5200$, a simulation conducted by the research group of Robert Moser at the University of Texas at Austin on the Mira supercomputer in 2013. The simulation involved 242 billion degrees of freedom, more than 15 times larger than the previously largest channel DNS of Hoya and Jiminez, conducted in 2006. The full simulation used 300 million core hours, and each restart file in the simulation was 1.8 TB in size, with approximately eighty such files archived for long term post processing and investigation.

When it can be applied, DNS is immensely powerful. The drawback of DNS is of course its very large computational cost. The observations about the computational cost of DNS signify more than just the limitations of current computing resources. They also signify a mismatch between DNS and the objective of determining large-scale flow features in a turbulent flow. In DNS, over 99% of the effort is spent resolving the dissipation range. By contrast, the mean flow and statistics of the energy-containing range exhibit only weak Reynolds number dependencies.