Direct Numerical Simulations

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Successful modeling of physical phenomena can be formulated as coherence between experiments, theory and computations. Theory provides the conceptual framework and the basic laws. Experiment is concerned with the behavior of real systems. Computations link theory with experiments. In recent years, computational power has increased so greatly that (both theoretical and experimental) research on complex systems, described by simple laws, has relied extensively on insights obtained through direct numerical simulations (DNS).

Such is the case in turbulence research: a turbulent flow does indeed follow simple laws. These laws, for constant density and small Mach number flows, are a system of PDE's called the incompressible Navier Stokes (NS) equations:

$$\partial_t \mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -\nabla p + \nu\nabla^2\mathbf{v} \quad (1)$$

$$\nabla\cdot\mathbf{v} = 0. \quad (2)$$

In a wall-bounded domain, the NS equations must be supplemented with no-slip boundary conditions. In general, some kind of external driving is also needed in order to obtain a statistically steady state. When the Reynolds number $Re = UL/\nu$ (where U and L are typical velocity and length scales of the flow, and ν is the kinematical viscosity) is large enough, the system displays turbulent behavior: it is in a time-dependant highly nonlinear regime.

With periodic boundary conditions, the NS equations can be solved using spectral methods, with great precision and numerical efficiency (the precision of spectral methods is exponential in the resolution (rather than algebraic for e.g. finite differences methods) [1]. The basic idea is to expand the fields in (truncated) Fourier series, and to compute derivatives in Fourier space and nonlinear terms in physical space. Fast Fourier Transforms (FFT) are used to go back and forth from spectral to physical space in $O(n^D \log(n))$ operations, where D is the space dimension. These methods are quite easy to implement. As a practical illustration, we give here a toy 2D NS pseudo-spectral solver, written in Mathematica [2]. It uses the (Ψ, ω) form of the nonlinear terms, and time-stepping is carried out by the first-order Euler implicit scheme: $u_{n+1} = (1 + \nu k^2 \Delta t)^{-1}(u_n + \Delta t N(u_n))$.

The solver consists of 2 instructions to define the FFT's with proper normalization.

```
(*Viscosity, time step and resolution*)
nu=.05;dt=.05;n=16

(*FFT's*)
PhysicalToSpectral[l_]:=InverseFourier[l]/n
SpectralToPhysical[l_]:=n Fourier[l]
```

A kernel of 9 instructions.

```
(*Wavenumbers*)
Kwave=Table[I (Mod[i-1+n/2,n]-n/2),{i, n}];
KwaveSquare=Kwave^2;
Kwave[[n/2+1]]=0;

(*Derivatives*)
xDerivate[l_]:=Table[l[[i,j]] * Kwave[[i]],{i,n},{j,n
yDerivate[l_]:=Table[l[[i,j]] * Kwave[[j]],{i,n},{j,n

Laplacien[l_]:=Table[l[[i,j]] *
(KwaveSquare[[i]]+KwaveSquare[[j]]),{i,n},{j,n}]

InverseLaplacien[l_,alpha_,beta_]:=Table[l[[i,j]] /
(beta(KwaveSquare[[i]]+KwaveSquare[[j]])+alpha),{i,n}

Nonlinear[l_]:=InverseLaplacien[PhysicalToSpectral[
 SpectralToPhysical[yDerivate[l]] *
 SpectralToPhysical[xDerivate[Laplacien[l]]] -
 SpectralToPhysical[xDerivate[l]] *
 SpectralToPhysical[yDerivate[Laplacien[l]]]],
 10^-40,1.]

EulerStep[l_]:=InverseLaplacien[l+dt Nonlinear[l],1,-
```

Finally, 7 more instructions are needed to initialize the fields, run the simulation and visualize the result.

```
(*Visualizations*)
ShowMeOmega[l_]:=
ListContourPlot[Re[SpectralToPhysical[-Laplacien[l]]]

(*Initialization*)
SeedRandom[143];
Field=Table[1/(
 -KwaveSquare[[i]]-KwaveSquare[[j]]+0.001) *
 ( ( Random[]-.5)+I (Random[]-.5)/2 ),{i, n}, {j, n}]
Field[[1,1]]=0.;
Psi=PhysicalToSpectral[Re[SpectralToPhysical[Field]]]

Do[Psi=EulerStep[Psi];Psi[[1,1]]=0.,{20}];
ShowMeOmega[Psi]
```

Running this simple solver produces the visualization shown in figure 1.

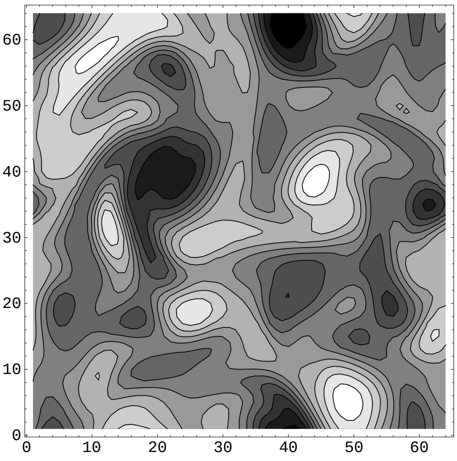

FIG. 1: A plot of the vorticity generated by the toy solver

State-of-the-art spectral solvers are very much like that above. They typically use a second-order time-stepping scheme, such as Leapfrog-Crank Nicolson: $u_{n+1} = (1 + 2\nu k^2 \Delta t)^{-1}(u_{n-1} + 2\Delta t N(u_n))$, real-to-complex-conjugate FFT's that run faster than general complex FFT's and are de-aliased [1]. As most of the computational time is spent in the FFT's, their number is reduced to a minimum. Codes are generally written in FORTRAN or C, and the FFT's are specially adapted to the machine's architecture (often written in assembly language).

Results from DNS of 2D turbulence have included the transition from an early-time k^{-4} inertial range to a latter time k^{-3} range, for flows developing from large-scale initial data [3]. An important finding has been the identification of the spontaneous emergence of long-lived coherent vortices when the DNS is run for a long time [4]. Long-time behavior of 2D turbulence is an active field of research, using DNS with a resolution of up to 1024^2 [5].

The biggest general periodic computations to date in 3D turbulence have a resolution of up to 512^3 (performed on a CM5 massively parallel machine) [6, 7]; 256^3 computations are common on Cray supercomputers [8]. The Taylor-Green vortex, a periodic flow with symmetries that can be used to save time and memory, has been simulated with resolutions up to 864^3 on a Cray2 [9, 10].

When studying 3D turbulence, the basic limitation of DNS is their lack of resolution. From Kolmogorov scaling one knows that the dissipation scale is $\ell_d \sim \ell_I R_I^{-3/4}$, where ℓ_I is the injection length scale and R_I is the Reynolds number. To accommodate this range of scales the DNS's resolution must scale as $n \sim R_I^{3/4}$, which implies computer memory scaling as $R_I^{9/4}$ and a total operation count scaling as $R_I^3 \log(R_I)$ [11]. State-of-the-art 3D DNS, in the early 90's, typically have an R_I of a few thousand (and a Taylor-scale Reynolds number R_λ of a few hundred). Given these limitations, why have DNS been so popular in the recent past? A first remark is that, with R_λ a few hundred, one starts to see Kolmogorov scaling (over, say, a decade). So one can argue that the DNS has something to do with turbulence. It can be used to validate turbulence models [12]. Another point is the possibility of getting information about any computable quantity. Indeed, suppose we want to see a cumulative distribution plot (the integral of the p.d.f.) of e.g. the x-derivative of the vorticity field computed in our toy Mathematica 2D DNS. The following 2 instructions:

```
ShowMeDistribution[l_]:=ListPlot[
 Transpose[{Sort[Re[Flatten[l]]],
 Table[N[(i-1)/n^2],{i,n^2}]}]]
ShowMeDistribution[
 SpectralToPhysical[xDerivate[Laplacien[Psi]]]]
```

will produce the plot shown in figure 2. This is indeed the very power of DNS: any quantities of interest, can be computed, plotted and studied.

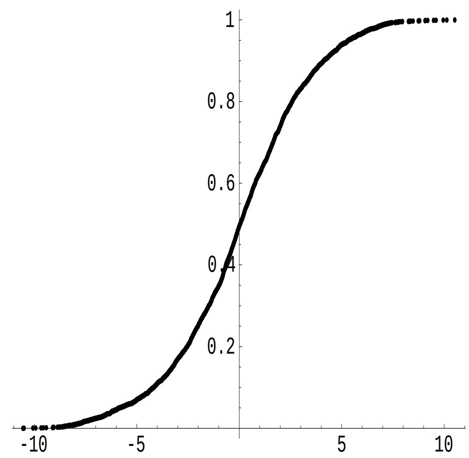

FIG. 2: Cumulative distribution of the vorticity gradient (x-component) corresponding to the situation displayed in Figure 1.

Evidence for the presence of vortex blobs, sheets, and filaments, in 3D DNS of turbulence, were first obtained in the early 80's [13]. At about the same time, the first Kolmogorov $k^{-5/3}$ inertial range was reported in a DNS [14]. It is impossible to give here an exhaustive list of all the important contributions that followed in the numerous papers published from the mid 80's to the early 90's. Perhaps two main results should be mentioned at this point, as they have both motivated new experiments that go beyond statistical analysis of one-point velocimetry data.

The first result is the DNS data on strain statistics and vorticity alignment with the eigenvector corresponding to its middle eigenvalue [15]. This result has been confirmed in sophisticated hot-wire measurements [16], that shed new light on the geometrical distribution of turbulent small scales.

The second result is the utilization of DNS to gain insight about the coherent structures present in 3D turbulent flows and their physical signatures [9, 17]. These DNS have confirmed the presence of vortex filaments and sheets, and demonstrated the dominant effect of vortex filaments on the pressure field. Pressure field visualizations and histograms, obtained in the DNS have paved the way for new experiments that have directly visualized vortex filaments in actual turbulent flows [18].

These new experiments have, in turn, focused the attention of the turbulence community on the study of small-scale geometry, filamentation and vortex breakdown, as a basic dynamical mechanism in 3D turbulence.

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[2] The Mathematica source code, together with some extra functions needed to de-aliase, compute spectra, etc..., can be obtained by sending e-mail to: *brachet@physique.ens.fr*

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