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An Extension of Spectral Methods to Quasi-Periodic and Multiscale Problems

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For efficiently treating quasi-periodic and multiscale problems numerically, it is here proposed to change the number of space dimensions which is then multiplied by the number of different (incommensurable or widely separated) scales occurring in the problem. Then, all calculations are performed in this higher-dimensional space. In the higher-dimensional space the problem is a standard periodic problem where, in the presence of dissipation, only the lower-order harmonics are relevant and one can thus use all the standard spectral methods for periodic functions with a relatively small number of modes. The method is validated, using the Burgers equation, and the two-dimensional linearized Navier–Stokes equation, by comparison with standard spectral or pseudo-spectral methods (in which the dimensionality of the space is not changed but very high resolution is used). For physical problems of interest in which different widely separated scales occur, standard methods require very large computer resources; the gain in storage and CPU resources, when using the "higher dimension" method, is typically proportional to the ratio of scales.

1. INTRODUCTION

In a variety of physical problems we have to deal with fields involving more than one scale of variation in one or several space or time variables. A standard example is the one-dimensional Schrödinger equation with quasi-periodic coefficients: the potential is a combination of two periodic functions such that the ratio of the periods τ is irrational [1]. In the problem of *turbulent transport,* a velocity field with a scale a is prescribed and a passive contaminant is introduced on a scale $1/\tau$ times larger with $\tau \ll 1$ (see, e.g., [2, Sect. 9.6]). Numerical methods based on Fourier series, such as the spectral techniques [3], are not easily applied to such problems. Indeed, when using a standard spectral technique for quasi-periodic situations, we must use a rational approximation n_1/n_2 to the irrational τ, where n_1 and n_2 are integers; an accurate approximation requires then extremely high resolution. Similarly, in the multiscale case $\tau \ll 1$, a huge range of wavenumbers is required, since all scales, including intermediate ones, have to be resolved. How can we adapt the standard Fourier methods for such problems and keep the CPU and storage requirements as low as possible?

To give a first idea of our method consider a (quasi-periodic) function of one variable such that in its Fourier representation the only wavenumbers present are of the form $k = n + m\tau$, where n and m are signed integers and τ is irrational (the decomposition of k is thus unique). Such a function has the following (generalized) Fourier representation:

$$f(x) = \sum_{n,m} \hat{f}(n, m) \exp[2i\pi(n + m\tau)x]. \tag{1}$$

A two-dimensional 2π-periodic function may then be defined by

$$f_2(x, y) = \sum_{n,m} \hat{f}(n, m) \exp[2i\pi(nx + my)], \tag{2}$$

such that $f(x)$ is recovered by restriction to the line $y = \tau x$ of slope τ.

Our numerical method for dealing with PDEs involving such functions will be to change the number of space dimensions which is multiplied by the number of different (incommensurable or large) scales occurring in the problem. Then, all calculations are to be performed in this higher-dimensional space. In that space the problem becomes a periodic one which is handled by standard spectral methods.

The underlying mathematical ideas are presented in Section 2. At first sight it seems strange to be able to save computer resources and simplify calculations by "artificially" increasing the dimension of space, but this will become clear in Sections 3 and 4, where we apply our method to treat multiscale and quasi-periodic problems. The basic idea in the two cases is the same; the details however are quite different. In Subsections 3.2 and 4.2 we give examples of our method being applied to specific problems in the multiscale and quasi-periodic case, respectively.

The idea of multiplying the dimension of a problem by the number of different scales is a standard procedure both in multiscale analysis, where the "slow" variables are

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supposed to be independent of the "fast" variables (see, e.g., [4]), and in the quasi-periodic case where it is well known to scientists working in celestial mechanics (see, e.g., [5]) and in the field of linear differential equations with quasi-periodic coefficients (see, e.g., [1]). To the best of our knowledge this idea has not yet been applied for numerical purposes.

2. FROM TWO TO ONE DIMENSIONS ... AND BACK

We shall restrict our discussion to the case where only two different scales occur; the extension to cases with more than two scales is immediate. To explain our method of extending the dimension of the problem we proceed *backwards* and explain first how, from a function depending 2π-periodically on two variables, we can obtain a function of one variable with two scales. Consider a 2π-periodic function $f_2(x, y)$ of two variables, written in terms of its Fourier series,

$$f_2(x, y) = \sum_{n,m} \hat{f}(n, m) \exp[2i\pi(nx + my)]. \tag{3}$$

The restriction (trace) of f_2 to the line $y = \tau x$ defines a one-dimensional function by the following generalized one-dimensional Fourier series,

$$f(x) = \sum_{n,m} \hat{f}_1(n + m\tau) \exp[2i\pi(n + m\tau)x], \tag{4}$$

where

$$\hat{f}_1(n + m\tau) \equiv \hat{f}(n, m). \tag{5}$$

Can this process be inverted? If τ is irrational there is a single pair of signed integers such that $n + m\tau = q$ and the corresponding q's are dense in R. Thus, from the one-dimensional quasi-periodic restriction $f(x)$ we can reconstruct the two-dimensional 2π-periodic function $f_2(x, y)$ in a unique way. This will be used in Section 4. If τ is rational the decomposition $q = n + m\tau$ is not unique unless we put some restrictions on the range of variation of n and m. For example, if $\tau = 1/K$ where K is an integer and we set $qK = k$, we know that an arbitrary integer k may be written uniquely as $k = nK + m$ provided m takes at most N consecutive values (Euclidean division). This will be used in Section 3 dealing with the multiscale case.

With the restrictions mentioned, the correspondence between the one-dimensional function $f(x)$ (the "restriction") and the two-dimensional function $f_2(x, y)$ (the "extension") is one-to-one. It is then equivalent to work, for example, with a one-dimensional quasi-periodic function or with its two-dimensional periodic extension. In practice, working with periodic functions considerably simplifies matters.

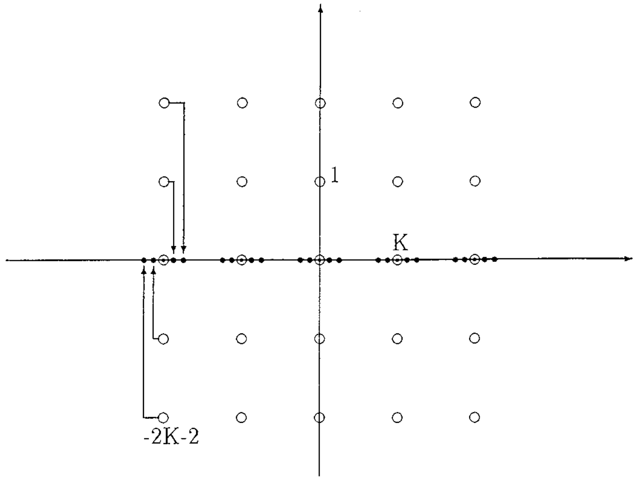

FIG. 1. Two-dimensional unfolding (shown as circles) of the one-dimensional clustering of modes for a multiscale situation ($N = M = 2$).

3. THE MULTISCALE CASE

3.1. *Theory*

We are interested in situations where two widely separated scales are present, for example, a small-scale motion on a scale $\tau \ll 1$ with a large-scale modulation on a scale of order unity. In Fourier space this corresponds to having wavenumbers of the form $k = nK + m$ with $K = \tau^{-1}$. (For the sake of simplicity K is a large even integer.)

As noted by Boyd [6] if there is a clear separation of scales the only modes with appreciable excitation are clustered around the harmonics of K, that is, they correspond to values of m such that $|m| \ll K$. The typical situation is that the maximum value of $|n|$ and $|m|$ at which the series can be truncated, denoted here N and M, respectively, depend on the accuracy required but not on the small parameter τ (although they depend on other control parameters present).

Boyd [6] observed that one can omit the mostly unexcited modes with $|m| > M$ and thereby considerably reduce storage and CPU. At first sight the decimated structure of modes, leaving only clusters around harmonics of K, is not amenable to the use of pseudo-spectral methods (including FFTs). Actually, the decimated structure, when interpreted in terms of the two-dimensional extension of Section 2, is amenable to standard two-dimensional periodic pseudo-spectral methods using $(2N + 1)(2M + 1)$ modes. This is illustrated in Fig. 1 which shows the clustering and its two-dimensional unfolding. The correspondence is shown by arrows.

By our procedure, storage has been reduced by a factor

$O(\tau)$ and CPU work is down by at least the same factor (there is an additional $\log(1/\tau)$ factor).

Let us observe that our procedure is actually a numerical manifestation of the multiscale technique in which the original variables are split up into "fast" and "slow." For example, the derivative performed in the Fourier space becomes the multiplication by $i(nK + m)$. In addition, with our method, there is no difficulty calculating the solution when the scale separation and/or the large-scale amplitude are finite rather than small.

3.2. *An Example: Eddy Viscosity and the Burgers Equation in One Dimension*

We used the method of extension of the dimension to calculate the eddy viscosity of the forced Burgers equation:

$$\partial_t u + u\partial_x u = \nu\partial_x^2 u + f. \tag{6}$$

The force is assumed time-independent and spatially periodic, say of period 2π. There is then a unique time-independent solution $u(x)$ with the same period, which is here called the "basic" solution. We furthermore assume $\langle f \rangle = \langle u \rangle = 0$, where angular brackets denote averages over one period.

To calculate the eddy viscosity we now add to the basic solution a small perturbation $u(x) \to u(x) + v(x, t)$, where $v(x, t)$ is assumed to have a spatial period $O(\tau^{-1})$ much larger than that of the basic solution. The perturbation satisfies

$$\partial_t v + v\partial_x u + u\partial_x v + v\partial_x v = \nu\partial_x^2 v. \tag{7}$$

If diffusive behavior is present on large scales, it will take place on a time scale $O(\tau^{-2})$. It is thus appropriate to use a multiscale formalism with the "fast" variables x, t and the "slow" variables $X = \tau x$, $T = \tau^2 t$. We are now interested in the large-scale behavior of the perturbation. For this purpose we consider $V(X, T) = \langle v(x, X, t, T)\rangle$, which is the perturbation averaged over the fast variables x, t.

Using multiscale analysis, it may be shown that V satisfies, to leading order, an unforced Burgers equation with the viscosity and the (nonlinear term) vertex renormalized by the same constant α_{eddy}, which can be obtained analytically [7],

$$\partial_t V + \alpha_{\mathrm{eddy}}(V\partial_x V - \nu\partial_x^2 V) = 0; \tag{8}$$

$$\alpha_{\mathrm{eddy}} = [\langle\exp(\psi/\nu)\rangle\langle\exp(-\psi/\nu)\rangle]^{-1}, \tag{9}$$

where ψ is the primitive of u such that $\langle\psi\rangle = 0$.

To validate our numerical multiscale method we performed numerical simulations of (7) using our method of extension of the dimension. We took a low amplitude large-scale perturbation, so as to be able to ignore the nonlinear term in (8), and scale separations of 25 and 100 ($\tau = 1/25$ and 1/100) and various values of the molecular viscosity. To obtain the numerical value of $\nu\alpha_{\mathrm{eddy}}$ we started with an initial condition v of small amplitude having all the energy in the largest scale (lowest Fourier mode $k = 1$). We then calculated $\nu\alpha_{\mathrm{eddy}}$ by watching the decay of the amplitude in the lowest mode: the logarithmic time derivative $\beta(t)$ of the amplitude of this mode converges for long times to $-\nu\alpha_{\mathrm{eddy}}$. Figure 2 shows that, after relaxation of transients, $-\beta(t)$ converges to its theoretically predicted value.

We have also repeated the calculation using a standard pseudo-spectral code which simultaneously resolves the small and large scales. The same numerical results were obtained. The storage using our method varies linearly with the separation of scales $1/\tau$ as predicted: a factor 3 for a ratio of scales of 25 and a factor 12 for a ratio of 100, as we were using 8 Fourier coefficients in the fast variables. The number of Fourier coefficients in the slow variables was 64.

Our technique can also be used to calculate the "vertex renormalisation factor," that is, the modification of the nonlinear term at large scales, which is also predicted by the theory. For this, a finite amplitude large-scale perturbation must be used. This will be presented in Ref. [8].

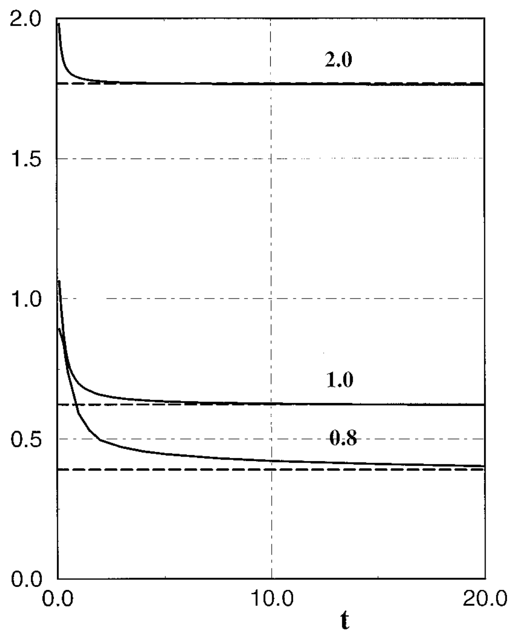

FIG. 2. Comparison of the theoretically predicted eddy viscosities $\nu\alpha_{\mathrm{eddy}}$ (dashed lines) with values obtained by our higher dimension multiscale method (scale separation, 25) by watching the relaxation of the largest mode (continuous lines) for three values of the viscosity as labelled.

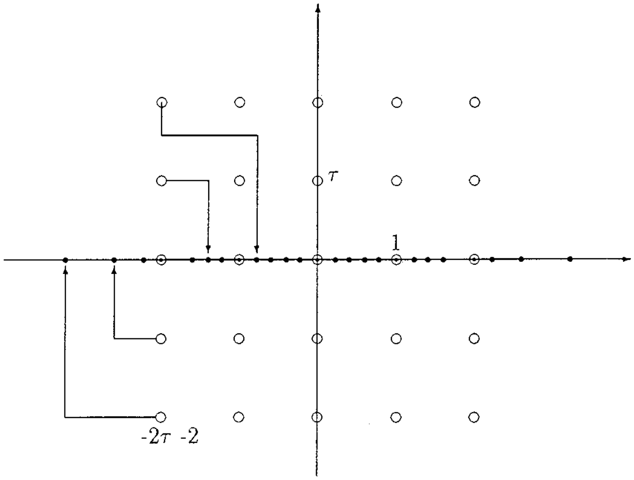

FIG. 3. Two-dimensional unfolding of Fourier space for the quasi-periodic case. The arrows show the map from (n, m) to $k = n + m\tau$ (circles to black dots).

4. THE QUASI-PERIODIC CASE

4.1. *Theory*

Quasi-periodic functions occur in a variety of different mathematical and physical problems, for example, in celestial mechanics [5], crystallography [9], and spectral theory of Schrödinger operators [1]. Such functions are interesting not only for their own sake but also because of their intermediate status between periodic and random functions.

A quasi-periodic function with only two incommensurate wavenumbers, say 1 and τ, has *by definition* the generalized Fourier representation (1), in which the coefficients $\hat{f}(n, m)$ must decrease exponentially for large values of $\sup(|n|, |m|)$ [5]. The wavenumbers $k = n + m\tau$ are dense on the real line. Hence a truncation of the form $|k| \leq k_{\max}$ still leaves infinitely many k's. A natural truncation which leaves only $O(k_{\max}^2)$ numbers of degrees of freedom is

$$\sup(|n|, |m|) \leq k_{\max}. \tag{10}$$

The Fourier geometry of quasi-periodicity is illustrated in Fig. 3 for $k_{\max} = 2$. The wavenumbers on the real line are obtained from the regular two-dimensional integer lattice by oblique projection parallel to the line of slope $-1/\tau$ so that (n, m) is mapped onto $n + m\tau$. Observe that the black dots are not clustered as in the multiscale case but appear "irregularly" distributed.

We can of course, design a *uniform* grid of wavenumbers such that the irrational numbers $n + m\tau$ within the truncation range are arbitrarily close to that grid. However, if τ is an irrational number poorly approximated by rationals (e.g., the golden mean $\tau = (\sqrt{5} - 1)/2$) extremely fine grids are needed to get good approximations. No such difficulty is present in the *natural* two-dimensional representation. With that representation the number of modes needed after numerical truncation does not depend on how irrational τ is, whereas a good one-dimensional periodic approximation requires preposterous storage and work. In other words in a one-dimensional periodic representation two modes with wavenumbers differing by a small amount Δk cannot be discriminated unless the period is at least $O(1/\Delta k)$.

When actually trying to numerically solve PDEs with quasi-periodic coefficients, certain difficulties, not present in the periodic case, can be expected, irrespective of the use of a standard pseudo-spectral method or the higher dimension method. The main difficulty has to do with denominators: large values of n and m ensure smallness of the coefficients but the dissipation, usually proportional to $k^2 = (n + m\tau)^2$, need not be large. Hence interactions involving high (n, m) modes with small $|k|$ can lead to unpleasant resonances. When a parameter controlling the dissipation, say the viscosity, is decreased the amount of resolution required may therefore increase dramatically.

4.2. *An Example: Eddy Viscosity and Two-Dimensional Quasi-Periodic Flow*

We are here interested in the response of a prescribed two-dimensional incompressible "basic" flow $\mathbf{u}(\mathbf{r})$ to a weak uniform shear. It is well known that, provided that the basic flow is parity invariant (possesses a center of symmetry), the leading-order response is a flux of momentum Φ_{ij} linearly proportional to the applied shear $\partial_i v_j$. In general the relation involves a fourth order tensor ν_{ijlm}, called the eddy viscosity:

$$\Phi_{ij} = -\nu_{ijkl}\, \partial_k v_l. \tag{11}$$

The general theory of the eddy viscosity can be found in [11], where it is shown that the eddy viscosity is expressible in terms of the solution of the Navier–Stokes equation linearized around the basic flow u:

$$\partial_t v_i + \partial_j(u_i v_j + u_j v_i) = -\partial_i P + \nu \partial_{jj}^2 v_i, \qquad \partial_j v_j = 0. \tag{12}$$

Numerical implementation for *periodic* two-dimensional basic flow may be found in [10]. Solving the linearized Navier–Stokes equation with *quasi-periodic* flow has, to the best of our knowledge, never been attempted. This is however of considerable interest because it is known that, in two dimensions, rotational symmetry of order n with $n > 5$ implies isotropy of all fourth order tensors, and hence of the eddy viscosity. Within the framework of periodic flow the only possible instance is six-fold symmetry, which corresponds to a triangular lattice. Indeed, there exists no regular periodic tiling of the two-dimensional

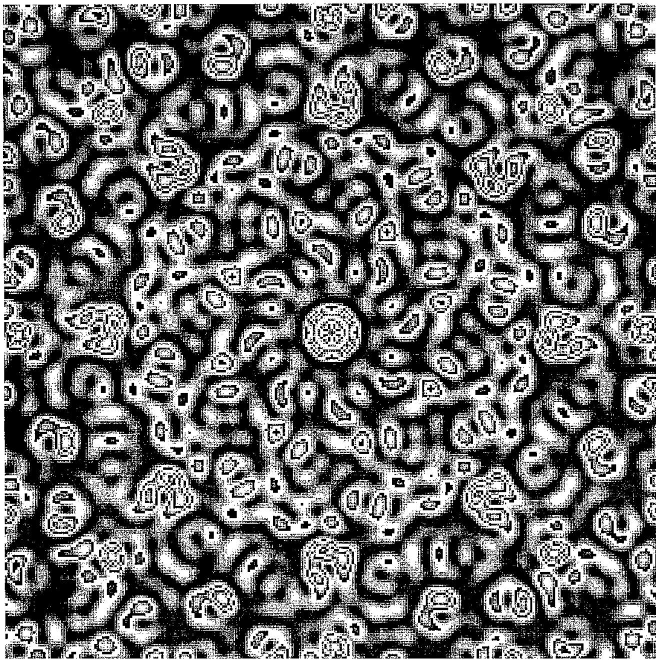

FIG. 4. Streamfunction of the eight-fold symmetrical quasi-periodic flow, the eddy viscosity of which is determined by our method.

plane with more than six-fold symmetry. All other rotational symmetries can be implemented only with quasi-periodic tilings.

Eight-fold rotational symmetry is particularly easy to implement since it requires only two incommensurable length scales, say 1 and $\sqrt{2}$. A simple way to construct a flow with such symmetry is to excite a finite set of wavevectors of the form

$$\mathbf{k} = (n_1 + n_2\sqrt{2}, n_3 + n_4\sqrt{2}), \tag{13}$$

where n_1, n_2, n_3, and n_4 are integers, and then to perform rotations by $2\pi j/8$ for $j = 1, \ldots, 8$. Figure 4 shows an example of the streamfunction of such a flow which has $8 \times 4 = 32$ different wavevectors excited. The eight-fold symmetry is very conspicuous.

We have applied our higher dimension method to solving the linearized Navier–Stokes equation (12) and evaluating the eddy viscosity which here reduces to a number, because of the isotropy implied by the eight-fold symmetry. Since the basic flow has two dimensions and there are two incommensurable scales, our method leads to solving a four-dimensional periodic PDE. The circles in Fig. 5 give the variation of the eddy viscosity with the molecular viscosity for the flow shown in Fig. 4. Our calculations used 16^4 modes and we checked that high order harmonics are well damped within the range of molecular viscosities shown.

In order to compare our higher dimension calculation with a standard calculation using a two-dimensional pseudo-spectral method, we should approximate the irrational $\sqrt{2}$ by a rational number p/q. In order to be able to represent essentially the same harmonics as in the higher dimensional case with 16^4 modes we need at least $(16p)^2$ modes. We thus used the approximation $\sqrt{2} \approx 7/5$ and 256^2 modes. In a rational approximation the eight-fold symmetry reduces actually to an exact four-fold symmetry, but one very close to the original eight-fold symmetry. Still, four-fold symmetry allows the presence of one spurious anisotropic tensor in the eddy viscosity. In Fig. 5 the diamonds give the isotropic part of the eddy viscosity which is, for the range of molecular viscosity used here, within one percent of the result from the (numerically more accurate) higher dimensional method. There is also, as predicted, a spurious anisotropic contribution, shown as squares, which reaches values up to 6 percent of the isotropic part.

For values of the molecular viscosities less than 0.2 (not shown) the numerics deteriorate very quickly unless much higher resolution is used. This is caused by resonances of the sort discussed in Section 4.

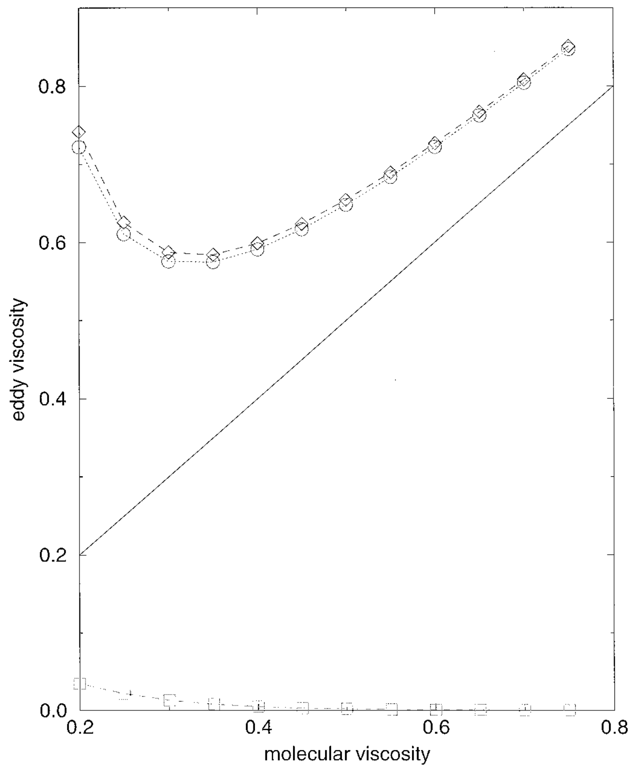

FIG. 5. Eddy viscosity of the quasi-periodic flow shown in Fig. 4. The circles correspond to our higher dimensional method using 16^4 modes. The diamonds are obtained using a standard two-dimensional pseudo-spectral method applied to a periodic approximation with 256^2 modes; this also gives a *spurious* anisotropic contribution to the eddy viscosity, shown as squares.

Two concluding remarks are in order. We observe that quasi-periodicity can achieve a very large range of scales (wavenumbers) without recourse to excessively many modes. For example, in two dimensions for the irrational value of $\sqrt{2}$ used above, if we use $(17 \times 12)^2 = 204^2$ modes, it may be checked that the ratio between the largest and smallest wavenumber is about 10^4. This is about 30 times larger than would be achieved with a periodic flow having a comparable number of modes. It is therefore suggested that quasi-periodic flow simulated with our technique could be used, e.g., to simulate turbulence with a substantial inertial range. Such a strategy may turn out to be more effective than using periodic flow with symmetry [12].

Finally, we observe, that the increasing of the dimension, which has for many years been the mathematician's natural vision of quasi-periodic functions, has been demonstrated here to be also the most effective way to deal with such a function numerically.

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