QUAD
The Versatile Fluid Simulator

User's Guide

Version 0.0

Hartmut Borth[1] Edilbert Kirk
Valerio Lucarini

[1]hartmut.borth@uni-hamburg.de

Contents

Part I

Model Physics

Chapter 1

Evolution equations of incompressible 2D fluids

1.1 Classical non-rotating case

The dimensional evolution equations of incompressible homogeneous 2D-fluids on the plane (see e.g. Batchelor [1967] or Canuto et al. [1988]) in vorticity velocity form

$$\zeta_t + \mathbf{u} \cdot \nabla\zeta = F + D, \tag{1.1}$$

with $\mathbf{u} = (u, v)$ the vector of velocity fields in x and y-direction, F a forcing and D a dissipation term. From homogeneity and incompressibility of the fluid we get

$$\nabla\cdot\rho\mathbf{u} = \rho\nabla \cdot \mathbf{u} = 0, \tag{1.2}$$

with ρ the fluid density. Using this property we can introduce a volume (mass) stream function measuring the volume (mass) flux across an arbitrary line from the point (x_0, y_0) to a point (x, y) via the path integral

$$\psi(x, y) - \psi(x_0, y_0) = -\int_{(x_0,y_0)}^{(x,y)} \left[\begin{pmatrix} u \\ v \end{pmatrix} \cdot \begin{pmatrix} -dy \\ dx \end{pmatrix} \right]. \tag{1.3}$$

The minus sign in front of the integral just changes the direction of positive massflux across the line and is chosen to make the classical stream function of 2D fluids compatible to the stream function (see e.g. Danilov and Gurarie [2000]) typically used for 2D rotating fluids in geosciences. In terms of the stream function ψ the integrated mass flux $\mathcal{M}$ across a line joining the points (x_0, y_0) and (x, y) is given by

$$\mathcal{M}(x_0, y_0|x, y) = -\rho H_0 \left[\psi(x, y) - \psi(x_0, y_0)\right], \tag{1.4}$$

with H_0 the depth of the fluid. At the same time the stream function ψ is connected to the velocity field (u, v) and the (relative) vorticity $\zeta = v_x - u_y$ via

$$(u, v) = (-\psi_y, \psi_x) \text{ and } \zeta = \Delta\psi. \tag{1.5}$$

Using the stream function ψ, the evolution equation (1.1 can be also written in the form

$$\zeta_t + J(\psi, \zeta) = F + D. \tag{1.6}$$

Since the velocity field is divergence free (equation 1.2) we can further derive the equivalent equation in flux form

$$\zeta_t + \nabla \cdot (\mathbf{u}\zeta) = F + D. \tag{1.7}$$

Starting from the flux form one can after repeated application of the continuity equation (1.2) finally derive an equation where the Jacobian only depends on the velocity two fields (u, v)

$$\zeta_t + \partial_x \partial_y \left(v^2 - u^2\right) + \left(\partial_x^2 - \partial_y^2\right) uv = F + D. \tag{1.8}$$

This form allows in the pseudo-spectral method (see 3.3) to reduce the number of Fourier transforms per time-step from 3 (u, v, ζ) to 2 (u, v).

1.2 Quasi-two-dimensional rotating fluids

Starting from the shallow water equation on the β-plane one can derive (see e.g. Danilov and Gurarie [2000]) an equation describing a rotating barotropic quasi-two-dimensional fluid which is a generalization of the 2D-equation (1.1). For small Rossby numbers $\mathrm{Ro} = U/Lf$, with U a typical horizontal fluid velocity at the length scale L considered and f the local coriolis paramter we get the potential vorticity (PV) q in quasi-geostrophic (QG) approximation

$$q = \left(\nabla^2 - \alpha^2\right) \psi + f, \tag{1.9}$$

where we have the modification parameter $\alpha = 1/L_{\mathrm{R}}^2$ with the Rossby-Obukhov radius of deformation $L_{\mathrm{R}} = \sqrt{gH_0}/f$ and the stream function $\psi = gh/f$. Here g is the gravitational acceleration and $h(x, y)$ the deviation of the mean fluid depth H_0 of the original shallow water layer. As in the 2-dimensional case the stream function ψ (remind the different definition) is related to the velocity fields (u, v) as defined in equation (1.5). In an unforced non-dissipative fluid the QG PV is materially conserved

$$q_t + J(\psi, q) = 0. \tag{1.10}$$

Using the linear approximation of the coriolis parameter $f = f_0 + \beta y$ and introducing again forcing and dissipation we can write the evolution equation in the form

$$q_t + J(\psi, q) + \beta \psi_x = F + D, \tag{1.11}$$

with the vorticity q given by

$$q = \left(\nabla^2 - \alpha^2\right) \psi = \zeta - \alpha^2 \psi. \tag{1.12}$$

Further one can introduce a variable mean fluid depth $H(x, y)$, which in the simple case of a linear slope in y-direction leads to a topographic β-effect (see e.g. Heijst [1994]).

In the form (1.11) and (1.12) one can simulate incompressible 2D fluids and rotating quasi-2D fluids with the same set of equations using different parameters. In this more general frame the simplest case of a non-rotating 2D incompressible fluid is characterized by a vanishing ambient vorticity gradient, i.e. $\beta = 0$, and the limit of an infinite Rossby radius $L_{\mathrm{R}} \longrightarrow \infty$ or a vanishing modification parameter $\alpha \longrightarrow 0$.

One only have to keep in mind that the stream functions different in the two cases. In the non-rotating case ψ is defined by equation (1.4). In the rotating case we get

$$h(x, y) = \frac{f}{g}\, \psi(x, y), \tag{1.13}$$

so that ψ is proportional to pressure deviations, which is not the case in the non-rotating 2D case where the relation is more complex, see e.g. Johnston and Liu [2004].

Using the property of the Jacobian $J(f, f) = 0$ for all fields $f(x, y)$ on the fluid domain equation (1.11) is equivalent to

$$q_t + J(\psi, \zeta) + \beta\psi_x = F + D, \tag{1.14}$$

where the vorticity q is still defined by equation (1.12). From this from it directly follows that that the form of the 2D Jacobian in equations (1.7) and (1.8) can be also applied in the quasi-two-dimensional rotating case.

1.3 Non-adiabatic terms

1.3.1 Laplacian viscosity and friction

Internal viscosity and external friction of the fluid are described by the dissipation term D on the left hand side of the equation (1.11). A classical way - the default reference in our model - to describe this term is to use a linear operator wich is a superposition of powers of the Laplacian. The default in the fluid simulator is

$$D\ q = -\left[\sigma\,(-1)^{p_\sigma}\,\Delta^{p_\sigma} + \lambda\,(-1)^{p_\lambda}\,\Delta^{p_\lambda}\right] q = -\left[\frac{(-1)^{p_\sigma}}{t_\sigma}\left(\frac{L_\sigma}{2\pi}\right)^{2p_\sigma}\Delta^{p_\sigma} + \frac{(-1)^{p_\lambda}}{t_\lambda}\left(\frac{L_\lambda}{2\pi}\right)^{2p_\lambda}\Delta^{p_\lambda}\right] q, \tag{1.15}$$

where L_σ and L_λ are the small and large-scale cut-off length scales. The corresponding small and large-scale "damping" time scales are given by t_σ and t_λ. The powers p_σ of small-scale viscosity are in the range of $p_\sigma \in [1, 2, 3, \ \dots\ ]$ and the powers p_λ of large-scale friction are in the range $p_\lambda \in [0, -1, -2, -3, \ \dots\ ]$. For $p_\sigma = 1$ and $p_\lambda = 0$ we speak of viscosity and linear drag (friction), for $p_\sigma > 1$ and $p_\lambda < 0$ of hyperviscosity and hypofriction (see also Danilov and Gurarie [2001]). From equation (1.15) it follows that the coefficients σ and λ can be written by

$$\sigma = \left(\frac{L_\sigma}{2\pi}\right)^{2p_\sigma}\ \frac{1}{t_\sigma} = \left(\frac{1}{k_\sigma}\right)^{2p_\sigma}\ \frac{1}{t_\sigma}\ \text{ and }\ \lambda = \left(\frac{L_\lambda}{2\pi}\right)^{2p_\lambda}\ \frac{1}{t_\lambda} = \left(\frac{1}{k_\lambda}\right)^{2p_\lambda}\ \frac{1}{t_\lambda}. \tag{1.16}$$

We have chosen the additional factor of 2π since finally the fluid domain is rescaled to multiples of 2π. Using this scaling the coefficients σ and λ are characterized respectively by the damping the time scales t_σ and t_λ as well as the cut-off wave numbers k_σ and k_λ. Above dissipation operator is a special case of dissipation operators which are polynomials with positive and negative powers of the Laplacian. In Fourier space (see subsection 3.3) the dissipation operators of this class reduce to the multiplication with polynomials in positive and negative powers of the wave numbers. More general dissipation operators can be constructed directly in Fourier space (see subsection 3.4).

1.3.2 Forcing

The forcing term F in equations (1.1) and (1.11) describes forcings due to either external processes as a wind-stress or a moving plate or non-resolved internal processes as, e.g./ baroclinic instability or diabatic heating. Both types of forcings can be described in physical or spectral space. For a constant external forcing, e.g. a wind stress or drag of a moving plate (τ^u, τ^v) given in $[N/m^2]$ and acting in x and y direction at the surface of the fluid the forcing term is given by

$$F(x, y) = \frac{1}{\rho H_0}\left(\tau_x^v - \tau_y^u\right), \tag{1.17}$$

where in the rotating quasi-2D case the height deviations h of the fluid are neglected. The forcing can also be controlled in spectral space, see subsection 3.5 below.

1.4 Geometry and boundary conditions

The evolution equations have to be completed by boundary conditions. The default geometry of the fluid domain is a square with an edge of length $L_x = L_y = L$ and the default boundary conditions are doubly periodic, i.e. $(f(x, y) = f(x + L, y + L)$ for all functions f on the fluid domain.

Part II

Numerical Implementation

Chapter 2

Model history

Our numerical implementation goes back to a code developed by Annalisa Bracco, for more details see Bracco and McWilliams [2010]

Chapter 3

The pseudo-spectral method

The idea behind the pseudo-spectral method is first to transform the evolution equations to Fourier (spectral) space, i.e. in our example to use the eigenfunctions of the Laplacian as basis of the space of all solutions and to project the full equations onto this basis, see e.g. Canuto et al. [1988]. Second to calculate products of functions (non-linear terms) in the physical space and transform them back to Fourier space to reduce the number of multiplications necessary, which otherwise makes the spectral method computationally prohibitively expensive for problems with a large numbers of Fourier modes. This idea goes back to Kreiss and Oliger [1972]. More details on the pseudospectral method can be found, e.g. in Orszag [1972] and Fornberg [1987].

3.1 The discrete Fourier transform

Starting point for the set of basis functions are the Fourier modes $F(k_x, k_y \mid x, y)$ which are the eigenmodes of the Laplacian on the fluid domain considered (short notation $F(\mathbf{k} \mid \mathbf{x})$ with $\mathbf{k} = (k_x, k_y)$ and $\mathbf{x} = (x, y)$). We start with a doubly periodic fluid domain (default in QUAD). In this case the eigenmodes of the Laplacian are given by

$$F(\mathbf{k} \mid \mathbf{x}) = \exp\left[i\left(k_x x + k_y y\right)\right] = \exp\left[ik_x x\right]\ \exp\left[ik_y y\right], \tag{3.1}$$

and satisfy the eigenvalue equation

$$\Delta\ F(\mathbf{k} \mid \mathbf{x}) = -\left(k_x^2 + k_y^2\right)\ F(\mathbf{k} \mid \mathbf{x}), \tag{3.2}$$

with $k_x = n\ 2\pi/X$ and $k_y = m\ 2\pi/Y$ for $n, m \in [0, \pm 1, \pm 2,\ \ldots\ ]$. As can be seen form equation (3.1) the eigenmodes of the Laplacian on the two-dimensional fluid domain $F(\mathbf{k} \mid \mathbf{x}) = F(k_x \mid x)\ F(k_y \mid y)$ can be separated into a product of the eigenmodes of the 1-dimensional Laplacian. For more general domains as circular discs, annuli or the surface of spheres as well as for more general boundary conditions, i.e. for fluid domains with walls one has to choose other systems of basis functions, see e.g. Canuto et al. [1988].

Taking $L_x = X/2\pi$ and $L_y = Y/2\pi$ in x and y-direction as horizontal length scales and introducing the non-dimensional variables $\bar{x} = x/L_x$, $\bar{y} = y/L_y$, $\bar{k}_x = k_x L_x$ and $\bar{k}_y = k_y L_y$ the non-dimensional eigenvalue equation

$$\left[\frac{\partial^2}{\partial \bar{x}^2} + \frac{\partial^2}{r^2 \partial \bar{y}^2}\right]\ F(\bar{\mathbf{k}} \mid \bar{\mathbf{x}}) = -\left(\bar{k}_x^2 + \frac{\bar{k}_y^2}{r^2}\right) F(\bar{\mathbf{k}} \mid \bar{\mathbf{x}}), \tag{3.3}$$

with the aspect ratio of the fluid domain $r = L_y/L_y = Y/X$, the wave number vector $\bar{\mathbf{k}} = (\bar{k}_x, \bar{k}_y)$, where $\bar{k}_x = \bar{k}_y = 0, \pm 1, \pm 2,\ \ldots$ and the coordinate vector $\bar{\mathbf{x}} = (\bar{x}, \bar{y})$, where $\bar{x}, \bar{y} \in [0\ \ 2\pi]$. Such an approach leads to a rescaled Laplacian and is appropriate in particular for physical problems with a strong horizontal anisotropy.

Introducing a single horizontal length scale as for example $L = L_x = X/2\pi$ instead we get the non-dimensional variables $\bar{x} = x/L$, $\bar{y} = y/L$, $\bar{k}_x = k_x L = n$ and $\bar{k}_y/r = k_y L/r = m/r$. The non-dimensional eigenvalue equation now reads

$$\left[\frac{\partial^2}{\partial \bar{x}^2} + \frac{\partial^2}{\partial \bar{y}^2}\right] \; F(\bar{\mathbf{k}} \mid \bar{\mathbf{x}}) = -\left(\bar{k}_x^2 + \frac{\bar{k}_y^2}{r^2}\right) F(\bar{\mathbf{k}} \mid \bar{\mathbf{x}}), \tag{3.4}$$

with the aspect ratio of the fluid domain r defined above, the wave number vector $\bar{\mathbf{k}} = (\bar{k}_x, \bar{k}_y/r)$, where $\bar{k}_x = \bar{k}_y = 0, \pm 1, \pm 2, \ \ldots$ and the coordinate vector $\bar{\mathbf{x}} = (\bar{x}, \bar{y})$, where $\bar{x} \in [0 \ 2\pi]$ and $\bar{y} \in [0 \ r2\pi]$. In QUAD we use a single horizontal length scale keeping in mind that this choice is not optimal for problems with a strong horizontal anisotropy. In the special case of a square domain (default case in QUAD) we have $r = 1$. From now on we use, if not otherwise stated, the non-dimensional form and omit overbars.

Using the Fourier modes $F(\mathbf{k} \mid \mathbf{x})$ we can expand all fields $g(x, y, t)$ on the fluid domain into a Fourier series

$$g(x, y, t) = \sum_{k_x=-\infty}^{\infty} \sum_{k_y=-\infty}^{\infty} \hat{g}(k_x, k_y, t) \; \exp\left[i\left(k_x x + \frac{k_y}{r} y\right)\right], \tag{3.5}$$

where $\hat{g}(k_x, k_y, t)$ are the Fourier coefficients of $g(x, y, t)$ which live on the space of wave numbers (k_x, k_y). Since $g(x, y, t)$ are real fields, the Fourier modes $\hat{g}(k_x, k_y, t)$ have the symmetry property that

$$\hat{g}(-k_x, -k_y, t) = \hat{g}^*(k_x, k_y, t), \tag{3.6}$$

where g^* is the complex conjugate of g. The Fourier coefficients $\hat{g}(k_x, k_y, t)$ are obtained by the integral

$$\hat{g}(k_x, k_y, t) = \frac{1}{r}\frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{r2\pi} \exp\left[-i\left(k_x x + \frac{k_y}{r} y\right)\right] \; g(x, y, t) \; dxdy. \tag{3.7}$$

This continous finite Fourier integral is derived from the dimensional integral

$$\hat{g}(k_x, k_y, t) = \frac{1}{XY} \int_0^X \int_0^Y \exp\left[-i\left(k_x x + k_y y\right)\right] \; g(x, y, t) \; dxdy, \tag{3.8}$$

where x,y,k_x and k_y are the dimensional variables.

To use the Fourier transform in numerical schemes to solve the evolution equation of fluids we have to approximate the continous finite Fourier integral (3.7) and the infinite Fourier series (3.5).

We start by discretizing the physical space into N grid points in x-direction and M grid points in y-direction. On the discretized grid of the physical space the continuous finite Fourier integral (3.7) reduces to the double sum

$$\hat{g}(k_x, k_y, t) = \frac{1}{NM} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \exp\left[-i\left(k_x x_n + \frac{k_y}{r} y_m\right)\right] g(x_n, y_m, t), \tag{3.9}$$

where we use the approximations $dx = \Delta x = 2\pi/N$, $dy = \Delta y = r2\pi/M$, $x_n = n \ \Delta x$ and $y_m = m \ \Delta y$ with $n \in [0, 1, \ \ldots \ , N-1]$ and $m \in [0, 1, \ \ldots \ M-1]$. The aspect ratio of the grid cell is given by $\Delta x/\Delta y = M/N \ 1/r$. For $r = M/N$ the grid cells are squares (default in QUAD $M = N$ and $r = 1$).

Next we truncate the infinite Fourier series (3.5) at wave numbers such that all modes with a higher spatial frequency (wave mumber) than the grid in physical space are omitted otherwise we would have an oversampling. The result is the finite sum

$$g(x_n, y_m, t) = \sum_{k_x=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{k_y=-\frac{M}{2}+1}^{\frac{M}{2}} \exp\left[i\left(k_x x_n + \frac{k_y}{r} y_m\right)\right] \; \hat{g}(k_x, k_y, t). \tag{3.10}$$

On the discretized grid in the physical space the modes with wave numbers $(k_x, k_y) = (-N/2, -M/2)$ and $(k_x, k_y) = (N/2, M/2)$ are identical. We omitted the mode $(k_x, k_y) = (-N/2, -M/2)$.

Using the definitions of $x_n = 2\pi\ n/N$ and $y_m = r2\pi\ m/M$ we can write equation (3.9) in discretized form as

$$\hat{g}(k_x, k_y, t) = \frac{1}{NM} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \exp\left[-i2\pi\left(\frac{k_x n}{N} + \frac{k_y m}{M}\right)\right]\ g(x_n, y_m, t) \tag{3.11}$$

and equation (3.10) as

$$g(x_n, y_m, t) = \sum_{k_x=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{k_y=-\frac{M}{2}+1}^{\frac{M}{2}} \exp\left[i2\pi\left(\frac{k_x n}{N} + \frac{k_y m}{M}\right)\right] \hat{g}(k_x, k_y, t). \tag{3.12}$$

By a shift of the wave numbers k_x and k_y corresponding to a rotation in the complex plane the double sum (3.12) can be written equivalently in the form

$$g(x_n, y_m, t) = \sum_{k_x=0}^{N-1} \sum_{k_y=0}^{M-1} \exp\left[i2\pi\left(\frac{k_x n}{N} + \frac{k_y m}{M}\right)\right] \hat{g}(k_x, k_y, t). \tag{3.13}$$

Relation (3.11) defines the discrete 2-D forward Fourier transform $\mathcal{F}_{NM}$ and relation (3.13) the discrete 2-D inverse Fourier transform $\mathcal{F}_{MN}^{-1}$ respectively. One can decompose the 2-D transformations $\mathcal{F}_{NM}$ and $\mathcal{F}_{MN}^{-1}$ into two consecutive 1-D Fourier transformations $\mathcal{F}_N$, $\mathcal{F}_M$ and $\mathcal{F}_M^{-1}$, $\mathcal{F}_N^{-1}$.

The forward Fourier transform can be decomposed as follows

$$\hat{g}(k_x, k_y, t) = \frac{1}{N} \sum_{n=0}^{N-1} \exp\left(-i2\pi \frac{k_x n}{N}\right) \left[\frac{1}{M} \sum_{m=0}^{M-1} \exp\left(-i2\pi \frac{k_y m}{M}\right) g(x_n, y_m, t)\right] \tag{3.14}$$

or using operators $\hat{g} = \mathcal{F}_{NM}\ g = \mathcal{F}_N \mathcal{F}_M g$, where the operators $\mathcal{F}_N$ and $\mathcal{F}_M$ have the matrix representation

$$\mathcal{F}_N = \frac{1}{N}\ \left(exp\left[-i2\pi \frac{k_x n}{N}\right]\right)_{k_x, n \in [0, N-1]} \quad \text{and} \quad \mathcal{F}_M = \frac{1}{M}\ \left(exp\left[-i2\pi \frac{k_y m}{M}\right]\right)_{k_y, m \in [0, M-1]} \tag{3.15}$$

For the inverse Fourier transform we get the decomposition

$$g(x_n, y_m, t) = \sum_{k_y=0}^{M-1} \exp\left(i2\pi \frac{k_y m}{M}\right) \left[\sum_{k_x=0}^{N-1} \exp\left(i2\pi \frac{k_x n}{N}\right) \hat{g}(k_x, k_y, t)\right], \tag{3.16}$$

which using operators can be written as $g = \mathcal{F}_{MN}^{-1} = \mathcal{F}_M^{-1} \mathcal{F}_N^{-1} \hat{g}$, where the operators $\mathcal{F}_N^{-1}$ and $\mathcal{F}_M^{-1}$ have the matrix representation

$$\mathcal{F}_N^{-1} = \left(exp\left[i2\pi \frac{k_x n}{N}\right]\right)_{n, k_x \in [0, N-1]} \quad \text{and} \quad \mathcal{F}_M^{-1} = \left(exp\left[i2\pi \frac{k_y m}{M}\right]\right)_{m, k_y \in [0, M-1]}. \tag{3.17}$$

Using as basic unit the exponent $\omega = \exp[-i2\pi/N]$ we can represent the one-dimensional discrete forward Fourier transform $\mathcal{F}_N$ for a vector of length N as

$$\mathcal{F}_N = \frac{1}{N} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{N-1} \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \dots & \omega^{(N-1)^2} \end{pmatrix}. \tag{3.18}$$

The inverse Fourier transform $\mathcal{F}_N^{-1}$ is given by the matrix (3.18) without the factor $1/N$, where ω is replaced by the complex conjugate $\bar{\omega} = \exp[i2\pi/N]$. The representation of the Fourier matrices for small N are the building blocks of the fast Fourier transform introduced in section (3.2). For $N = 2$, $N = 3$ and $N = 4$ we get

$$\mathcal{F}_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \mathcal{F}_3 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \bar{\omega} \\ 1 & \bar{\omega} & \omega \end{pmatrix} \quad \text{and} \quad \mathcal{F}_4 = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{pmatrix}, \tag{3.19}$$

with $\omega = -\exp(i\pi/3) = -[\cos(\pi/3) + i\ \sin(\pi/3)]$. For $N = 8$ the representation reads

$$\mathcal{F}_8 = \frac{1}{8}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & -i & -i\omega & -1 & -\omega & i & i\omega \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -i\omega & i & \omega & -1 & i\omega & -i & -i\omega \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & \omega & i & -i\omega \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & \omega & i & -i\omega & -1 & -i\omega & -i & \omega \end{pmatrix}, \tag{3.20}$$

with $\omega = \exp(-i\pi/4) = \sqrt{0.5}\,[1-i]$. Making full use of the information hidden in the structure of the Fourier matrices one can reduce the number of multiplications needed to carry out the Fourier transform from order $O(N^2)$ to order $O(N \log N)$, which makes a big difference for large N, see section 3.2.

3.2 Fast Fourier Transform

Rearranging the rows of a Fourier matrix $\mathcal{F}_N$ by collecting even and odd rows (assuming even N) we can express $\mathcal{F}_N$ in terms of $\mathcal{F}_{N/2}$. One gets

$$\mathcal{F}_N\ g_N = \begin{pmatrix} I_{N/2} & D_{N/2} \\ I_{N/2} & -D_{N/2} \end{pmatrix}\begin{pmatrix} \mathcal{F}_{N/2} & 0 \\ 0 & \mathcal{F}_{N/2} \end{pmatrix}\begin{pmatrix} g^e_{N/2} \\ g^o_{N/2} \end{pmatrix}, \tag{3.21}$$

where $g^e_{N/2}$ and $g^o_{N/2}$ are the even and odd components of the vector g_N. Moreover $\mathcal{F}_{N/2}$ is the Fourier transform of size $N/2$, $I_{N/2}$ the identity matrix of size $N/2$ and $D_{N/2}$ the diagonal matrix $D_{N/2} = diag(1, \omega_N, \ \ldots\ , \omega_N^{N/2-1})$, with $\omega_N = \exp(-i2\pi/N)$. Transforming the expression (3.21) further we can write

$$\mathcal{F}_N\ g_N = \begin{pmatrix} I_{N/2} & I_{N/2} \\ I_{N/2} & -I_{N/2} \end{pmatrix}\begin{pmatrix} I_{N/2} & 0 \\ 0 & D_{N/2} \end{pmatrix}\begin{pmatrix} \mathcal{F}_{N/2} & 0 \\ 0 & \mathcal{F}_{N/2} \end{pmatrix}\ P_N^2\ g_N \tag{3.22}$$

where P_N^2 is a permutation matrix reordering the vector components into 2 blocks (even and odd). Since the Fourier operators $\mathcal{F}_N$ are symmetric we can write

$$\mathcal{F}_N\ g_N = \left[\mathcal{F}_2 \otimes I_{N/2}\right]\ diag(I_{N/2}, D_{N/2})\ \left[I_2 \otimes \mathcal{F}_{N/2}\right]\ P_N^2\ g_N, \tag{3.23}$$

Taking $N = 8$ as example.

3.3 Evolution equations in Fourier space

The basic advantage of the Fourier representation is that differential operators as ∂_x, ∂_y, $\partial_x\partial_y$, ∇, Δ are transformed to simple multiplication operators ik_x, ik_y/r, $-k_xk_y/r$,$(ik_x, ik_y/r)$, $-(k_x^2+k_y^2/r^2)$ in spectral space with $i=\sqrt{-1}$. Differential equations in physical space are thus reduced to algebraic equations in spectral space.

In the Fourier space it is now straight forward to determine the stream function $\hat{\psi}(k_x,k_y,t)$ and the corresponding velocity fields $\hat{u}(k_x,k_y,t)$ and $\hat{v}(k_x,k_y,t)$ once the vorticity field $\hat{q}(k_x,k_y,t)$ is known. The vorticity equation (1.12) of the quasi-2D rotating case reduces to

$$-\left(k_x^2+\frac{k_y^2}{r^2}+\alpha^2\right)\hat{\psi}(k_x,k_y,t)=\hat{q}(k_x,k_y,t), \tag{3.24}$$

which in the case for $\alpha\neq 0$ can always be solved for the stream function

$$\hat{\psi}(k_x,k_y,t)=-\frac{1}{k_x^2+k_y^2/r^2+\alpha^2}\;\hat{q}(k_x,k_y,t). \tag{3.25}$$

In the case $\alpha=0$ equation (3.25) is still valid except for the zero mode. Here we set $\hat{\psi}(0,0,t)=0$, which is consistent with the definition (1.13) of the stream function and the double periodic boundary conditions. Further the velocity field is simply given by

$$\hat{u}(k_x,k_y,t)=-i\frac{k_y}{r}\;\hat{\psi}(k_x,k_y,t)=i\;\frac{k_y/r}{k_x^2+k_y^2/r^2+\alpha^2}\;\hat{q}(k_x,k_y,t) \tag{3.26}$$

and

$$\hat{v}(k_x,k_y,t)=ik_x\;\hat{\psi}(k_x,k_y,t)=-i\;\frac{k_x}{k_x^2+k_y^2/r^2+\alpha^2}\;\hat{q}(k_x,k_y,t). \tag{3.27}$$

The evolution equations (we use the general quasi-2D rotating case) reduce in Fourier space for every wave number pair $\mathbf{k}=(k_x,k_y)$ to an ordinary differential equations

$$\hat{q}_t(\mathbf{k},t)=i\frac{k_x\beta}{k_x^2+k_y^2/r^2+\alpha^2}\;\hat{q}(\mathbf{k},t)-\hat{J}(\mathbf{k},t)+\hat{F}(\mathbf{k},t)+\hat{D}(\mathbf{k},t). \tag{3.28}$$

In the case of vanishing Jacobian, Forcing and Dissipation we get a linear equation which can be solved exactly for every wave number pair $\mathbf{k}=(k_x,k_y)$ and has the solution

$$\hat{q}(\mathbf{k},t_0+\Delta t)=\exp\left[i\;\frac{k_x\beta}{k_x^2+k_y^2/r^2+\alpha^2}\;\Delta t\right]\;\hat{q}(\mathbf{k},t_0), \tag{3.29}$$

with $\hat{q}(\mathbf{k},t_0)$ the initial condition at time t_0 and the time interval $\Delta t=t-t_0$. The system can still be solved exactly if one includes a linear dissipation term $\hat{D}$. For more details see subsection 3.4. The Jacobian $\hat{J}$, forcing $\hat{F}$ and dissipation $\hat{D}$ are treated in a separate subsection each, since there are different ways to represent and define them.

3.4 Dissipation schemes

By default viscosity (internal dissipation) and friction (dissipation at the boundaries of the fluids) is parameterized by positive and negative powers of the Laplacian respectively given by equation (1.15). In spectral space the dissipation operator reads

$$D\;\hat{q}(\mathbf{k})=-\left[\sigma\left(k_x^2+k_y^2\right)^{p_\sigma}+\lambda\left(k_x^2+k_y^2\right)^{p_\lambda}\right]\hat{q}(\mathbf{k}). \tag{3.30}$$

Using the definitions σ and λ of (1.16) we can write the dissipation operator (3.30) in the form

$$D\;\hat{q}(\mathbf{k})=-\left[\frac{1}{t_\sigma}\left(\frac{1}{k_\sigma}\right)^{2p_\sigma}\left(k_x^2+k_y^2\right)^{p_\sigma}+\frac{1}{t_\lambda}\left(\frac{1}{k_\lambda}\right)^{2p_\lambda}\left(k_x^2+k_y^2\right)^{p_\lambda}\right]\hat{q}(\mathbf{k}). \tag{3.31}$$

Mind that $p_\lambda\leq 0$.

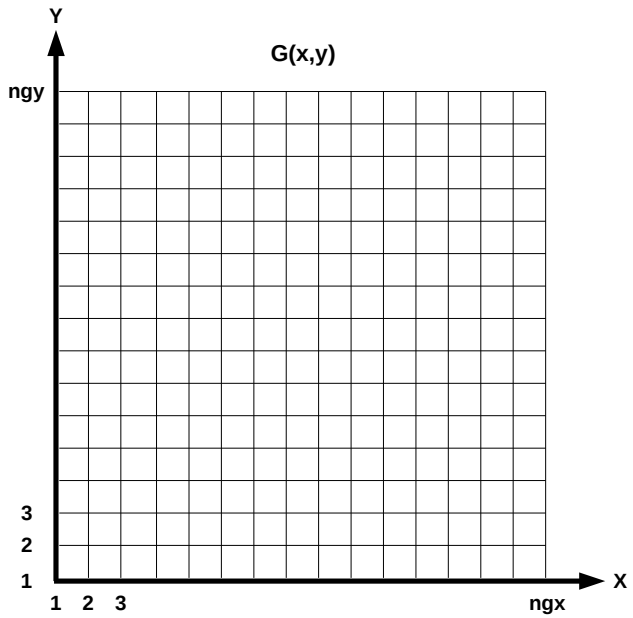

Figure 3.1: In physical space functions $g(x, y)$ are represented on a regular grid with ngx grid points in x-direction and ngy grid points in y-direction. At present in QUAD only the default $ngx = ngy$ is implemented.

3.5 Forcing schemes

3.6 Time-stepping schemes

3.7 The grid representation in QUAD

In physical space all fields $g(x, y)$ are real and are represented on a regular grid. Figure 3.7 shows the grid for for a horizontal resolugion of $ngx = ngy = 16$. Grid point read in or written out by QUAD are given in this format. In spectral space we have complex fields which in QUAD are either represented as complex $c(k_x, k_y)$ or as real $f(k_x, k_y)$ fields. Plate (a) in figure 3.7 shows the wave number grid for the internal complex representation $c(k_x, k_y)$ of spectral fields. Due to the symmetry propreties 3.6 it is sufficient to represent the fields only on half of the space wave number space, i.e. for the wave numbers

$$(k_x,\ k_y) \in \{\ k_x \in [\ 0, 1,\ \ldots\ nkx\ ]\ \text{ and }\ k_y \in [\ 0,\ \ldots\ , nky, -nky,\ \ldots\ , -1\ ]\}. \tag{3.32}$$

As described above we use the 2/3-truncation, so that the bounds nkx and nky are given by

$$nkx = ngx/3\ \text{ and }\ nky = ngy/3, \tag{3.33}$$

where non-integer part of the division is omitted. In our example from above $nkx = nky = 5$. As one can see the wave-numbers in y-direction are not centered around zero. Plate (b) of figure 3.7 shows the internal real representation $f(k_x, k_y)$ of spectral fields. In y-direction the spectral grid remains the same as in the case of the complex representation. In x-direction the number of coordinate points is doubled, even coordinates starting from 0 hold the real part $\mathcal{R}(c(k_x, k_y))$ and the odd coordinates starting from 1 hold the imaginary part $\mathcal{I}(c(k_x, k_y))$ of the complex fields $c(k_x, k_y)$. This is the format QUAD reads in or writes out spectral fields. While prescribing complex fields $c(k_x, k_y)$ in spectral space to QUAD it is important to keep in mind

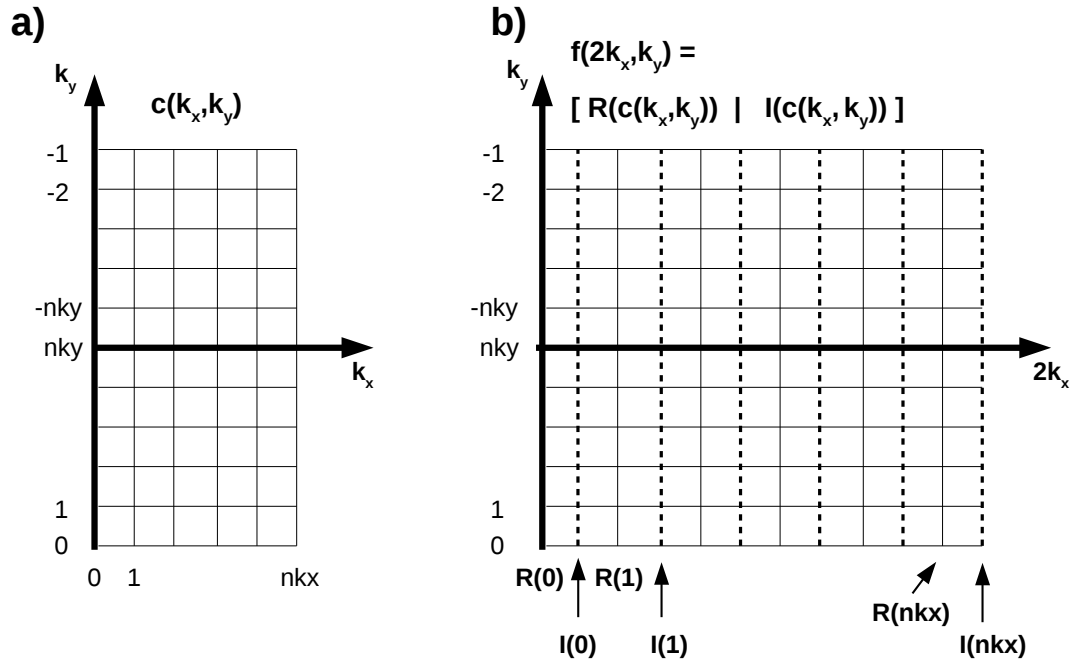

Figure 3.2: Functions in spectral space are represented either as complex fields c or as real fields f containing in the first spectral coordinate k_x the real and imaginary parts of c in an alternating series.

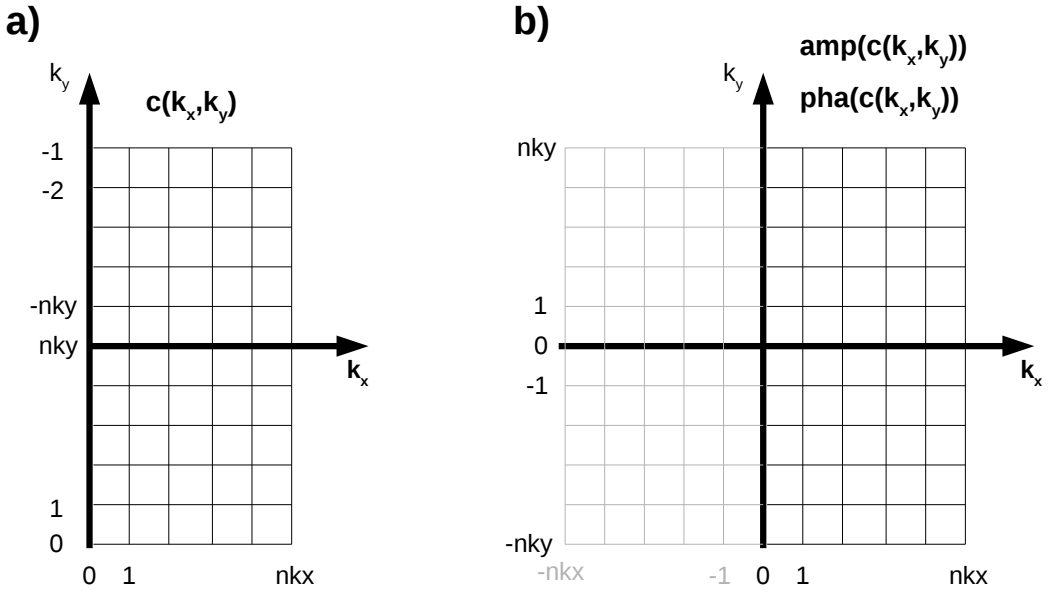

Figure 3.3: Internally spectral fields are given for the non-centered wave numbers given by equation (**??**), for the visualization in the GUI the amplitudes and phases of the complex spectral fields are represented on thee centered wave-number grid given by equation (3.34)

that on the k_y-axis ($k_x = 0$) values are not completely arbitrary, otherwise unphysical complex fields in phyiscal space are created. First $c(0,0)$ has to be zero, it represents the average of the field in physical space. In the case of vorticity cq we get $cq(0,0) = 0$. For the remaining values $(0, k_y)$ the symmetry properties 3.6 have to be satisfied, i.e. on the k_y-axis spectral fields must satisfy the condition $c(0, k_y) = c^*(0, -k_y)$. In the Graphical User Interface (GUI) spectral fields are visualized on a centerd wave-number grid

$$(k_x,\ k_y) \in \{\ k_x \in [\ -nkx,\ \ldots\ , nkx\ ] \ \text{ and } \ k_y \in [\ -nky,\ \ldots\ , nky\ ]\ \}. \tag{3.34}$$

Visualized are the amplitudes amp and phases pha of the complex fields

$$amp(c) = \sqrt{\mathcal{R}^2(c) + \mathcal{I}^2(c)} \ \text{ and } \ pha(c) = \tan^{-1}(\frac{\mathcal{I}(c)}{\mathcal{R}(c)}). \tag{3.35}$$

Chapter 4

Reference test cases and performance

Part III

Using the Model

Chapter 5

Implementing the model

Chapter 6

Running the model

Chapter 7

Analysing the model output

Chapter 8

Modifying the model

Part IV

Appendix

Appendix A

Namelists and parameters

Basic Control Namelist quad_nl

nx	64	grid points in x-direction
ny	64	grid points in y-direction (nx = ny)
nstop	10000	integration time steps
nout	50	time steps between 2D outputs

Appendix B

Moduls and basic model variables

Appendix C

Structure of code and flow scheme

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