Finite-dimensional approximations to QG dynamics

Ian Grooms

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The traditional inviscid, unforced continuously-stratified QG equations are

$$\partial_t \vartheta^+ + \mathrm{J}[\psi^+, \vartheta^+] = 0 \tag{1}$$
$$\partial_t q + \mathrm{J}[\psi, q] + \beta v = 0 \tag{2}$$
$$\partial_t \vartheta^- + \mathrm{J}[\psi^-, \vartheta^-] = 0 \tag{3}$$
$$\nabla_h^2 \psi + \partial_z \left(\frac{f_0^2}{H^2 N^2(z)} \partial_z \psi \right) = q, \quad S(z) = \frac{f_0^2}{H^2 N^2(z)} \tag{4}$$

where

$$\vartheta^{\pm} = \frac{f_0^2}{H^2 N^2} \partial_z \psi \text{ at } z = 0, 1 \tag{5}$$

Notation follows Rocha et al. (JPO 2016; RYG16). I have assumed that the dimensional z goes from 0 to H, and the above equations use a nondimensional z that goes from 0 to 1.

Energy conservation and Galerkin approximation

We want an approximate solution that has the following form

$$q_{\mathcal{N}}^G = \sum_{n=1}^{\mathcal{N}} \breve{q}_n(x, y, t) p_n^q(z), \quad \psi_{\mathcal{N}}^G = \sum_{i=1}^{\mathcal{N}} \breve{\psi}_i(x, y, t) p_n^{\psi}(z) \tag{6}$$

where $p_n^q(z)$ and $p_n^{\psi}(z)$ are a basis functions. E.g. we could use the modal expansion of RYG16, or any basis for the space of polynomials of degree $\leq n$, or finite elements, etc. The basis for q does not need to be the same as the basis for ψ. If we insert these above we get

$$\partial_t q_{\mathcal{N}}^G + \mathrm{J}[\psi_{\mathcal{N}}^G, q_{\mathcal{N}}^G] + \beta \partial_x \psi_{\mathcal{N}}^G = r_{qt} \neq 0 \tag{7}$$
$$q_{\mathcal{N}}^G - \left(\nabla_h^2 \psi_{\mathcal{N}}^G + \partial_z \left(\frac{f_0^2}{H^2 N^2(z)} \partial_z \psi_{\mathcal{N}}^G \right) \right) = r_q \neq 0 \tag{8}$$
$$\vartheta^+ + r_\vartheta^+ = (f_0/(HN))^2 \partial_z \psi_{\mathcal{N}}^G \text{ at } z = 1, \text{ and } \vartheta^- + r_\vartheta^- = (f_0/(HN))^2 \partial_z \psi_{\mathcal{N}}^G \text{ at } z = 0. \tag{9}$$

I allow some error in the boundary conditions. We don't need to allow for errors in the evolution of $\vartheta^{\pm}$ because that equation does not directly depend on the vertical structure. To put it another way, it is straightforward to enforce the following exact evolution equations:

$$\partial_t \vartheta^+ + \mathrm{J}[\psi_{\mathcal{N}}^G, \vartheta^+] = 0 \tag{10}$$
$$\partial_t \vartheta^- + \mathrm{J}[\psi_{\mathcal{N}}^G, \vartheta^-] = 0. \tag{11}$$

Note that because the Galerkin approximation $\psi_{\mathcal{N}}^G$ is not equal to the true solution ψ there will be a different kind of errors in the evolution of $\vartheta^{\pm}$, but we can still enforce the above equations to hold exactly.

We want our equations to conserve energy in the form $1/2\int|\nabla\psi_{\mathcal{N}}^G|^2+(f_0/(HN))^2(\partial_z\psi_{\mathcal{N}}^G)^2$. The standard approach to proving energy conservation is to multiply equation (7) for $\partial_t q_{\mathcal{N}}^G$ by $-\psi_{\mathcal{N}}^G$, then use equation (8) to replace $q_{\mathcal{N}}^G$, then perform multiple integrations by parts to arrive at an expression for the evolution of energy:

$$\int -\psi_{\mathcal{N}}^G\partial_t\left(\nabla_h^2\psi_{\mathcal{N}}^G+\partial_z\left(\frac{f_0^2}{H^2N^2(z)}\partial_z\psi_{\mathcal{N}}^G\right)+r_q\right)=\int\psi_{\mathcal{N}}^G(\mathrm{J}[\psi_{\mathcal{N}}^G,q_{\mathcal{N}}^G]-r_{qt})=-\int\psi_{\mathcal{N}}^G r_{qt}.$$

The hope is that we can impose appropriate conditions on r_q and r_{qt} such that the energy is conserved. E.g. a standard Galerkin condition would be to require both r_q and r_{qt} to be orthogonal to the span of the basis functions.

We simplify the above expression piece by piece. First, assuming appropriate lateral boundary conditions, we have

$$\int -\psi_{\mathcal{N}}^G\partial_t\nabla_h^2\psi_{\mathcal{N}}^G=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\nabla_h\psi_{\mathcal{N}}^G|^2.$$

Next

$$\int -\psi_{\mathcal{N}}^G\partial_z\left(\frac{f_0^2}{H^2N^2(z)}\partial_{zt}\psi_{\mathcal{N}}^G\right)=-\int_x\left[\frac{f_0^2}{H^2N^2}\psi_{\mathcal{N}}^G\partial_{zt}\psi_{\mathcal{N}}^G\right]_-^+ +\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f}{HN}\partial_z\psi_{\mathcal{N}}^G\right)^2 \tag{12}$$

$$=-\int_x\left[\psi_{\mathcal{N}}^G(\partial_t\vartheta+\partial_t r_\vartheta)\right]_-^+ +\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f_0}{HN}\partial_z\psi_{\mathcal{N}}^G\right)^2 \tag{13}$$

$$=-\int_x\left[\psi_{\mathcal{N}}^G(-\mathrm{J}[\psi_{\mathcal{N}}^G,\vartheta]+\partial_t r_\vartheta)\right]_-^+ +\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f_0}{HN}\partial_z\psi_{\mathcal{N}}^G\right)^2 \tag{14}$$

$$=-\int_x\left[\psi_{\mathcal{N}}^G\partial_t r_\vartheta\right]_-^+ +\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f_0}{HN}\partial_z\psi_{\mathcal{N}}^G\right)^2. \tag{15}$$

Putting it all together,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\nabla_h\psi_{\mathcal{N}}^G|^2+\left(\frac{f}{HN}\partial_z\psi_{\mathcal{N}}^G\right)^2=\int_x\left[\psi_{\mathcal{N}}^G\partial_t r_\vartheta\right]_-^+ +\int\psi_{\mathcal{N}}^G\partial_t r_q-\int\psi_{\mathcal{N}}^G r_{qt}.$$

The idea is that the coefficients $\breve{q}_n$ and the boundary values $\vartheta^\pm$ are known, but the coefficients $\breve{\psi}_n$ and $\partial_t\breve{q}_n$ are unknown. We can try to specify these coefficients to achieve the dual purposes of accuracy and energy conservation. Suppose we wish to impose the usual Galerkin conditions: First that r_q is orthogonal to the $\mathcal{N}$ basis functions p_n^ψ, which gives us $\mathcal{N}$ constraints on the PV inversion, then that r_{qt} is also orthogonal to the $\mathcal{N}$ basis functions p_n^ψ, which gives us another $\mathcal{N}$ constraints on the PV evolution. That will leave zero degrees of freedom to impose the boundary conditions, i.e. it won't be possible to set the error on the boundary $r_\vartheta^\pm$ to zero, and we won't be able to conserve energy. This seems to be a severe obstacle to energy conservation, since we can set the terms corresponding to r_q and r_{qt} to zero in the energy conservation equation, but we appear to be unable to control the term corresponding to $r_\vartheta^\pm$. 'Approximation B' from RYG16 is the Tulloch & Smith 2009 model; it enforces $r_\vartheta^\pm=0$ and $r_q=0$, but then doesn't have enough remaining degrees of freedom to set the terms corresponding to r_{qt} to zero.

On the other hand, RYG16 was able to achieve an energy-conserving Galerkin formulation; how was this possible? First, the 'modal' basis functions in that paper have $\partial_z p_n=0$ at the surfaces, which means that $r_\vartheta^\pm=-\vartheta^\pm$. As a result, $[\int_x\psi_{\mathcal{N}}^G\partial_t r_\vartheta]_-^+=-[\int_x\psi_{\mathcal{N}}^G\partial_t\vartheta]_-^+=0$. In 'approximation C' from RYG16 the boundary information is included in the PV inversion via delta-function sheets of PV at the boundary. This relies on the following fact, first noted by Bretherton (1966):

> The solution ψ to (4)-(5) (with inhomogeneous Neumann boundary conditions) is the same as the solution to the following PV inversion
>
> $$q-\vartheta^+\delta(z-1)+\vartheta^-\delta(z)=\nabla_h^2\psi+\partial_z\left(\frac{f_0^2}{H^2N^2}\partial_z\psi\right) \tag{16}$$
>
> with homogeneous Neumann boundary conditions $\partial_z\psi=0$.

We will now generalize 'Approximation C' from RYG16 to a general basis. Suppose only that our basis p_n^ψ has $\mathrm{d}p_n^\psi(z)/\mathrm{d}z = 0$ at the boundaries. Inserting our ansatz into the Bretherton PV inversion we find a new residual r_q

$$q_\mathcal{N}^G - \vartheta^+\delta(z-1) + \vartheta^-\delta(z) = \nabla_h^2\psi_\mathcal{N}^G + \partial_z\left(\frac{f_0^2}{H^2N^2}\partial_z\psi_\mathcal{N}^G\right) + r_q^B. \tag{17}$$

The superscript B stands for 'Bretherton' and emphasizes that this residual is different from r_q. Repeating the above analysis with the new definition of the residual r_q^B:

$$\int -\psi_\mathcal{N}^G\partial_t q_\mathcal{N}^G = \int -\psi_\mathcal{N}^G\partial_t\left(\nabla_h^2\psi_\mathcal{N}^G + \partial_z\left(\frac{f_0^2}{H^2N^2(z)}\partial_z\psi_\mathcal{N}^G\right) + \vartheta^+\delta(z-1) - \vartheta^-\delta(z) + r_q^B\right).$$

Again,

$$\int -\psi_\mathcal{N}^G\partial_t\nabla_h^2\psi_\mathcal{N}^G = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\nabla_h\psi_\mathcal{N}^G|^2.$$

As before

$$\int -\psi_\mathcal{N}^G\partial_z\left(\frac{f_0^2}{H^2N^2(z)}\partial_{zt}\psi_\mathcal{N}^G\right) = -\int_x\left[\frac{f_0^2}{H^2N^2}\psi_\mathcal{N}^G\partial_{zt}\psi_\mathcal{N}^G\right]_0^1 + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f}{HN}\partial_z\psi_\mathcal{N}^G\right)^2 = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{f_0}{HN}\partial_z\psi_\mathcal{N}^G\right)^2. \tag{18}$$

This time we used the fact that $\partial_z\psi_\mathcal{N}^G = 0$ on the boundaries. We now have a new term

$$\int -\psi_\mathcal{N}^G(\partial_t\vartheta^+\delta(z-1) - \partial_t\vartheta^-\delta(z)) = -\int_x[\psi_\mathcal{N}^G\partial_t\vartheta]_0^1 = 0.$$

The zero is because $\partial_t\vartheta^\pm = -\mathrm{J}[\psi_\mathcal{N}^G, \vartheta^\pm]$; multiplying by $\psi_\mathcal{N}^G$ and integrating yields 0. This leaves

$$\int -\psi_\mathcal{N}^G\partial_t q_\mathcal{N}^G = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\nabla_h\psi_\mathcal{N}^G|^2 + \left(\frac{f}{HN}\partial_z\psi_\mathcal{N}^G\right)^2 - \int\psi_\mathcal{N}^G\partial_t r_q^B.$$

The energy equation is now

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\nabla_h\psi_\mathcal{N}^G|^2 + \left(\frac{f}{HN}\partial_z\psi_\mathcal{N}^G\right)^2 = \int\psi_\mathcal{N}^G\partial_t r_q^B - \int\psi_\mathcal{N}^G r_{qt}.$$

To conserve energy we simply impose the usual Galerkin conditions that the residuals r_q^B and r_{qt} are orthogonal to the span of the basis functions p_n^ψ.

To be precise, if the basis for q is the same as the basis for ψ then we are imposing a traditional Galerkin condition. But there is no reason why we should enforce $\partial_z q_\mathcal{N}^G = 0$ at the boundary, so it is probably advantageous to use a more general basis for q than for ψ. In this case we are enforcing one Galerkin condition and one Petrov-Galerkin condition. A Galerkin condition requires a residual to be orthogonal to the space in which an approximate solution is sought. The residual in the PV equation r_q^B is required to be orthogonal to the span of p_n^ψ, and when solving the PV inversion we are seeking a solution $\psi_\mathcal{N}^G$ in the span of the p_n^ψ, so this is a Galerkin condition. The solution we obtain for $\psi_\mathcal{N}^G$ by imposing the Galerkin condition is optimal in the sense that it minimizes

$$-\int(\psi - \psi_\mathcal{N}^G)\left[\nabla^2(\psi - \psi_\mathcal{N}^G) + \partial_z\left(\frac{f_0^2}{H^2N^2}\partial_z(\psi - \psi_\mathcal{N}^G)\right)\right]$$

over all functions $\psi_\mathcal{N}^G$ in the subspace. RYG16 makes it look like we're minimizing the L^2 norm of the error in ψ, which is not the case.

A Petrov-Galerkin condition requires a residual to be orthogonal to a *different* subspace than the subspace in which a solution is sought. In the PV evolution equation we are seeking a solution for $\partial_t q_\mathcal{N}^G$ that is in the span of p_n^q but requiring the residual r_{qt} to be orthogonal to the span of the p_n^ψ, so this is a Petrov-Galerkin condition. In RYG16 the same basis is used for ψ and q, so it's a Galerkin condition, and in that case the approximation is optimal in the L^2 norm. I.e. the approximation $\partial_t q_\mathcal{N}^G$ is chosen to be as close as possible to $-\mathrm{J}[\psi_\mathcal{N}^G, q_\mathcal{N}^G]$ in the L^2 norm. We could do that here if we wanted to by setting $p_n^\psi = p_n^q$.

Implementation with a generic Galerkin basis

The following discussion covers how to implement this method for any Galerkin basis, i.e. it applied to the modal basis, to polynomials, to finite elements including DG, etc. For simplicity of exposition assume that the horizontal directions will be periodic and make use of the Fourier tranform so that

$$\hat{q}_n(\boldsymbol{k},t), \quad \hat{\psi}_n(\boldsymbol{k},t)$$

are the Fourier transforms of $\breve{q}_n$ and $\breve{\psi}_n$, respectively, and define vectors $\hat{\boldsymbol{q}}$ and $\hat{\boldsymbol{\psi}}$ whose n^{th} elements are $\hat{q}_n(\boldsymbol{k},t)$ and $\hat{\psi}_n(\boldsymbol{k},t)$, respectively, for $n = 1,\ldots,\mathcal{N}$. Using the Galerkin conditions, the PV inversion takes the form

$$\mathbf{B}\hat{\boldsymbol{q}} - \hat{\vartheta}^+\boldsymbol{p}^+ + \hat{\vartheta}^-\boldsymbol{p}^- = -k^2\mathbf{M}\hat{\boldsymbol{\psi}} - \mathbf{L}\hat{\boldsymbol{\psi}}$$

where

$$\left(\boldsymbol{p}^+\right)_j = p_j^\psi(1), \quad \left(\boldsymbol{p}^-\right)_j = p_j^\psi(0),$$

$$\mathbf{B}_{ij} = \int p_i^\psi(z)p_j^q(z)\mathrm{d}z, \quad \mathbf{M}_{ij} = \int p_i^\psi(z)p_j^\psi(z)\mathrm{d}z, \quad \mathbf{L}_{ij} = \int \frac{f_0^2}{H^2N^2}(\partial_z p_i^\psi(z))(\partial_z p_j^\psi(z))\mathrm{d}z$$

(in the right expression I assumed $\partial_z p_i^\psi(z) = 0$ at the boundaries and integrated by parts.) This is very similar to the standard finite-difference approach (see Grooms and Nadeau, Fluids 2017) where $\mathbf{M}$ and $\mathbf{B}$ would be the identity and $\mathbf{L}$ would be tridiagonal. In the modal basis (not polynomial) the basis functions are orthogonal so $\mathbf{M} = \mathbf{B}$ is diagonal, and they are eigenfunctions so $\mathbf{L}$ is just $\kappa_n^2\mathbf{I}$. Regardless of which basis you choose, you should evaluate the elements of $\mathbf{B}$, $\mathbf{M}$ and $\mathbf{L}$ to machine precision, either analytically if possible, or with adaptive quadrature or Gaussian quadrature with sufficient nodes. Notice that the matrix $\mathbf{L}$ is a Gram matrix based on the functions $\partial_z p_n^\psi$. If $p_1^\psi = 1$ is a basis function then the set of functions $\partial_z p_n^\psi$ is linearly dependent and $\mathbf{L}$ will be positive semi-definite. Similarly, $\mathbf{M}$ is a Gram matrix for the functions p_n^ψ, so it is symmetric positive definite.

We need a fast way to repeatedly solve the system for ψ. We need to solve for lots of different values of k^2, as well as repeatedly in time. To rapidly solve the PV inversion we can first compute the Cholesky factorization of $\mathbf{M}$ and store it: $\mathbf{M} = \mathbf{G}\mathbf{G}^T$. Then note

$$-k^2\mathbf{M} - \mathbf{L} = -\mathbf{G}(k^2\mathbf{I} + \mathbf{G}^{-1}\mathbf{L}\mathbf{G}^{-T})\mathbf{G}^T.$$

The matrix $\mathbf{G}^{-1}\mathbf{L}\mathbf{G}^{-T}$ is symmetric (and positive semi-definite) so it has an orthogonal eigenvector decomposition

$$\mathbf{G}^{-1}\mathbf{L}\mathbf{G}^{-T} = \mathbf{Q}\mathbf{D}\mathbf{Q}^T$$

where $\mathbf{D}$ is diagonal with non-negative elements and $\mathbf{Q}$ is an orthogonal matrix. This allows us to write

$$\mathbf{B}\hat{\boldsymbol{q}} + \text{ (boundary terms) } = -\mathbf{G}\mathbf{Q}(k^2\mathbf{I} + \mathbf{D})\mathbf{Q}^T\mathbf{G}^T\hat{\boldsymbol{\psi}}.$$

To obtain the solution:

- Compute $\mathbf{Q}^T\mathbf{G}^{-1}(\mathbf{B}\hat{\boldsymbol{q}} + \text{ (boundary terms) })$.
- Next multiply the previous result by $-(k^2\mathbf{I} + \mathbf{D})^{-1}$ from the left.
- Finally go back to the original basis: multiply the previous result by $\mathbf{G}^{-T}\mathbf{Q}$ from the left.

This is analogous to the approach taken in finite-difference approximations of the vertical direction.

The above analysis shows that there is a diagonalizing basis. This diagonalizing basis approximates the modal basis. The elements of a column of the matrix $\mathbf{G}\mathbf{Q}$ are the coordinates of a diagonalizing basis function with respect to the basis p_n^ψ. As $\mathcal{N}$ increases we expect these diagonalizing basis functions to converge to the baroclinic modes of the full problem. This is essentially the same as what happens in the finite-difference approximation, where the eigenvectors of the matrix $\mathbf{L}$ are the ‘discrete’ baroclinic modes.

The (Petrov)-Galerkin conditions define how the PV coefficients $\breve{q}_n$ should evolve. Define the vector $\breve{\boldsymbol{q}}$ to have elements $\breve{q}_n$, and define the vector $\mathbf{NL}$ to have elements

$$\mathbf{NL}_n = \int p_n^\psi(z)\mathrm{J}[\psi_\mathcal{N}^G, q_\mathcal{N}^G]\mathrm{d}z.$$

The PV evolution then takes the form

$$\mathbf{B}\frac{\mathrm{d}}{\mathrm{d}t}\breve{\boldsymbol{q}} + \mathbf{NL}(+\beta \mathrm{i}k_x\hat{\boldsymbol{\psi}}) = 0.$$

In a fully-nonlinear implementation, one would need to repeatedly evaluate the integrals defining the elements of $\mathbf{NL}$. This could be done via quadrature. The LU factorization of the matrix $\mathbf{B}$ could be computed once, then stored.

Polynomial bases

The above considerations do not rely on any particular basis. We now specialize to polynomials. The set of polynomials of degree $\leq \mathcal{N}+1$ and with $\partial_z p = 0$ at the boundaries is a vector space of dimension $\mathcal{N}$, with an infinite number of bases, any of which could be used in the above analysis. Shen (SIAM J Sci Comput 1994; section 4) gives a basis for the space of polynomials of degree $\leq \mathcal{N}+1$ and with $\partial_z p_n^\psi = 0$ at the boundaries using a re-combination of Legendre polynomials. For this basis the matrix $\mathbf{M}$ is pentadiagonal, with the further property that an even/odd permutation will bring it into a block-tridiagonal form. This matrix has condition number about 6×10^5 for $\mathcal{N} = 1000$, which is quite good. The matrix $\mathbf{L}$ depends on the stratification $S(z) = f_0^2/N^2(z)$ and in general will be dense. (If we used a finite-element basis then $\mathbf{L}$ would be sparse.) If we use the Shen basis for p_n^ψ and the standard Legendre basis for p_n^q then the matrix $\mathbf{B}$ is upper-triangular with upper bandwidth 2, so we wouldn't even need to compute the LU factorization and solving for the time-tendency of PV would only take $\mathcal{O}(\mathcal{N})$ flops. There's no benefit to using Chebyshev since energy conservation requires us to use the standard L^2 inner product, and Chebyshev polynomials are not orthogonal in the standard L^2 inner product.

The overall cost of the PV inversion using the Shen and Legendre bases is as follows. Pre-computing the Cholesky factor of $\mathbf{M}$ is $\mathcal{O}(\mathcal{N})$ because the matrix is banded. Computing the eigenvalue decomposition of $\mathbf{G}^{-1}\mathbf{L}\mathbf{G}^{-T}$ with the basic QR algorithm should converge quickly and not cost much per iteration because the matrix is symmetric and presumably has separated eigenvalues.

- Move into the diagonalizing basis: Compute $\mathbf{Q}^T\mathbf{G}^{-1}(\mathbf{B}\hat{\boldsymbol{q}} +$ (boundary terms)). Multiplication by $\mathbf{B}$ is $\mathcal{O}(\mathcal{N})$. The cost to invert the Cholesky is $\mathcal{O}(\mathcal{N})$. The cost to multiply by $\mathbf{Q}^T$ is $\mathcal{O}(\mathcal{N}^2)$.
- Invert in the diagonalizing basis: Multiply the previous result by $-(k^2\mathbf{I}+\mathbf{D})^{-1}$ from the left. This converts from q to ψ in the diagonalizing basis. Cost is $\mathcal{O}(\mathcal{N})$.
- Finally go back to the original basis: multiply the previous result by $\mathbf{G}^{-T}\mathbf{Q}$ from the left. Cost is $\mathcal{O}(\mathcal{N}^2)$ to multiply by $\mathbf{Q}$ and $\mathcal{O}(\mathcal{N})$ to invert the Cholesky.

Once the requisite decompositions have been pre-computed the inversion cost is $\mathcal{O}(\mathcal{N}^2)$. Of course, there's no particular reason why we need to go back and forth from the Shen basis to the diagonalizing basis. We could just start with the Shen basis, then compute the diagonalizing basis, then stick with the diagonalizing basis from then on. If so, the cost to invert is just $\mathcal{O}(\mathcal{N})$.

Note that the integral for $\mathbf{NL}$ is a product of three polynomials. If the basis p_n^q goes to degree $\mathcal{N}-1$ and the basis p_n^ψ goes to degree $\mathcal{N}+1$ then the product can have degree up to $3\mathcal{N}+1$. These integrals can be evaluated exactly using Gauss-Legendre quadrature with $1.5\mathcal{N}+1$ quadrature nodes. But we need to evaluate ψ at the boundaries so that we can evolve $\vartheta^\pm$ on the boundaries. We could use Gauss-Legendre-Lobatto quadrature instead; overall it would require $1.5\mathcal{N}+2$ quadrature nodes. If we used Gauss-Legendre then we would need to evaluate ψ at $1.5\mathcal{N}+1$ interior points *and* at the boundaries, and we would need to evaluate q at $1.5\mathcal{N}+1$ interior points for a total of $3\mathcal{N}+4$ polynomial evaluations. If we used Gauss-Legendre-Lobatto then we would need to evaluate ψ and q at $1.5\mathcal{N}+2$ points for a total of $3\mathcal{N}+4$ polynomial evaluations. So ultimately it's the same number of polynomial evaluations. Gauss-Legendre is easier than Lobatto.

The one drawback to using something other than Chebyshev polynomials is that it costs $\mathcal{O}(\mathcal{N}^2)$ flops to evaluate the polynomial at $\mathcal{N}$ points (vs $\mathcal{N}\ \log(\mathcal{N})$ for Chebyshev). We should, as mentioned above, just use the diagonalizing basis instead of the Shen basis. If we do that then we need to compute the matrix corresponding to the map from coordinates of a polynomial in the diagonalizing basis to values of the polynomial at the quadrature nodes. Then, to move from the coordinates in the diagonalizing basis to the values at the quadrature nodes will cost $\mathcal{O}(\mathcal{N}^2)$ and can be achieved via matrix/vector multiplication.

Overall the algorithm would be

- Start from the Shen (1994) and Legendre bases, then compute the diagonalizing basis. (The columns of the matrix $\mathbf{GQ}$ are the coefficients [in the Shen (1994) basis] of the diagonalizing basis that approximates the baroclinic modes.)
- Construct the matrix that maps from (coordinates in the diagonalizing basis) $\to$ (values on the Gauss-Legendre quadrature nodes)
- Evolve the system in time by updating q and $\vartheta^{\pm}$, then solving for ψ, etc.

In addition to the linear instability problem we should look at how rapidly the modes and deformation radii converge in the Galerkin vs FD methods and at the convergence of the interaction coefficients.

Linear instability problem

The following is an exact solution of the fully-nonlinear QG equations:

$$\bar{\psi} = -\bar{u}(z)y, \quad \bar{q} = -y\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{f_0^2}{H^2N^2(z)}\frac{\mathrm{d}\bar{u}}{\mathrm{d}z}\right), \quad \bar{\vartheta}^{\pm} = -y\frac{f_0^2}{H^2N^2(z)}\frac{\mathrm{d}\bar{u}^{\pm}}{\mathrm{d}z}.$$

We can linearize the PDE about this equilibrium solution to see whether it is stable/unstable to small perturbations. Instability of this kind of equilibrium in the QG equations is one example of something called 'baroclinic' instability. The linearized equations are

$$\partial_t\vartheta^+ + \bar{u}^+\partial_x\vartheta^+ - \frac{f_0^2}{H^2N^2}(\partial_x\psi^+)\frac{\mathrm{d}\bar{u}^+}{\mathrm{d}z} = 0 \tag{19}$$

$$\partial_t q + \bar{u}(z)\partial_x q + (\partial_x\psi)\partial_y\bar{q} + \beta(\partial_x\psi) = 0 \tag{20}$$

$$\partial_t\vartheta^- + \bar{u}^-\partial_x\vartheta^- - \frac{f_0^2}{H^2N^2}(\partial_x\psi^-)\frac{\mathrm{d}\bar{u}^-}{\mathrm{d}z} = 0 \tag{21}$$

$$\nabla^2\psi + \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{f_0^2}{H^2N^2(z)}\frac{\mathrm{d}\psi}{\mathrm{d}z}\right) = q - \vartheta^+\delta(z-1) + \vartheta^-\delta(z) \tag{22}$$

Coefficients don't vary in the horizontal, so we take the Fourier transform

$$\partial_t\hat{\vartheta}^+ + \mathrm{i}k_x\bar{u}^+\hat{\vartheta}^+ - \mathrm{i}k_x\frac{f_0^2}{H^2N^2}\frac{\mathrm{d}\bar{u}^+}{\mathrm{d}z}\hat{\psi}^+ = 0 \tag{23}$$

$$\partial_t\hat{q} + \mathrm{i}k_x\bar{u}(z)\hat{q} + \mathrm{i}k_x(\partial_y\bar{q})\hat{\psi} + \mathrm{i}k_x\beta\hat{\psi} = 0 \tag{24}$$

$$\partial_t\hat{\vartheta}^- + \mathrm{i}k_x\bar{u}^-\hat{\vartheta}^- - \mathrm{i}k_x\frac{\mathrm{d}\bar{u}^-}{\mathrm{d}z}\frac{f_0^2}{H^2N^2}\hat{\psi}^- = 0 \tag{25}$$

$$-(k_x^2+k_y^2)\hat{\psi} + \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{f_0^2}{H^2N^2(z)}\frac{\mathrm{d}\hat{\psi}}{\mathrm{d}z}\right) = \hat{q} - \hat{\vartheta}^+\delta(z-1) + \hat{\vartheta}^-\delta(z). \tag{26}$$

We look for exponential growth so we try to find solutions with $\partial_t\hat{q} = -\mathrm{i}k_x c\hat{q}$

$$-c\hat{\vartheta}^+ + \bar{u}^+\hat{\vartheta}^+ - \frac{f_0^2}{H^2N^2}\frac{\mathrm{d}\bar{u}^+}{\mathrm{d}z}\hat{\psi}^+ = 0 \tag{27}$$

$$-c\hat{q} + \bar{u}(z)\hat{q} + (\partial_y\bar{q})\hat{\psi} + \beta\hat{\psi} = 0 \tag{28}$$

$$-c\hat{\vartheta}^- + \bar{u}^-\hat{\vartheta}^- - \frac{\mathrm{d}\bar{u}^-}{\mathrm{d}z}\frac{f_0^2}{H^2N^2}\hat{\psi}^- = 0 \tag{29}$$

$$-(k_x^2+k_y^2)\hat{\psi} + \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{f_0^2}{H^2N^2(z)}\frac{\mathrm{d}\hat{\psi}}{\mathrm{d}z}\right) = \hat{q} - \hat{\vartheta}^+\delta(z-1) + \hat{\vartheta}^-\delta(z). \tag{30}$$

For some careful choices of $\bar{u}(z)$ and $N^2(z)$ the equations can be solved analytically. For example if $\bar{u} = z$, $\beta = 0$, and $N^2(z) = N^2$ it is the 'Eady' problem. More generally you have to discretize and then solve an eigenvalue problem to find c.

To use our Galerkin formulation we need to represent the equilibrium solution using our Galerkin bases. First, set

$$\bar{u}_{\mathcal{N}}^G = \sum_{n=1}^{\mathcal{N}} \bar{u}_n p_n^\psi(z).$$

Given a $\bar{u}(z)$ we need to find $\bar{u}_n$. We can choose these coefficients to minimize the L^2 norm of the error $\bar{u}(z) - \bar{u}_{\mathcal{N}}^G(z)$, which we accomplish via a standard Galerkin condition. We need to solve the system of equations

$$\sum_{k=1}^{\mathcal{N}} \int_0^1 p_n^\psi(z) p_k^\psi(z) \bar{u}_k \mathrm{d}z = \int_0^1 p_n^\psi(z) \bar{u}(z) \mathrm{d}z, \quad n = 1, \ldots, \mathcal{N}. \tag{31}$$

This is a system of the form $\mathbf{M}\boldsymbol{u} = \boldsymbol{b}$, and we already know how to compute $\mathbf{M}$. We just need a routine to compute the integrals on the RHS, e.g. using Gauss-Legendre quadrature.

Next we need a Galerkin approximation for $\partial_y \bar{q}$. Our standard approach tells us that

$$\mathbf{B}\partial_y \bar{\boldsymbol{q}} = \mathbf{L}\partial_y \bar{\boldsymbol{\psi}} + \partial_y \bar{\vartheta}^+ \boldsymbol{p}^+ - \partial_y \bar{\vartheta}^- \boldsymbol{p}^-. \tag{32}$$

Everything on the right hand side is known, so we just need to solve for the coordinates of $\partial_y \bar{q}_{\mathcal{N}}^G$. Note that the elements of the vector $\partial_y \bar{\boldsymbol{q}}$ that we solve for in the above expression are the Galerkin coefficients of $\partial_y \bar{q}_{\mathcal{N}}^G$ in the basis p_n^q, not p_n^ψ.

Next we need equations for the evolution of $\hat{\vartheta}^\pm$ and $\hat{q}_n$. The discrete evolution equations for $\hat{\vartheta}^\pm$ are simple because $\partial_z \bar{u}_{\mathcal{N}}^G = 0$ at the boundaries, even if $\partial_z \bar{u} \neq 0$:

$$(-c + \bar{u}_{\mathcal{N}}^G(z=1))\hat{\vartheta}^+ = 0, \quad (-c + \bar{u}_{\mathcal{N}}^G(z=0))\hat{\vartheta}^- = 0. \tag{33}$$

It will be convenient to eliminate $\hat{\psi}_n$ formally as follows

$$\hat{\boldsymbol{\psi}} = -\left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \mathbf{B}\hat{\boldsymbol{q}} + \hat{\vartheta}^+ \boldsymbol{\psi}^+ - \hat{\vartheta}^- \boldsymbol{\psi}^-.$$

The vectors $\boldsymbol{\psi}^\pm$ are

$$\boldsymbol{\psi}^+ = \left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \boldsymbol{p}^+, \quad \boldsymbol{\psi}^- = \left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \boldsymbol{p}^-.$$

Once we have this, we can write the discrete PV evolution equation as follows

$$-c\mathbf{B}\hat{\boldsymbol{q}} + \left[\bar{\mathbf{U}} - (\bar{\mathbf{Q}}_y + \beta\mathbf{M})\left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \mathbf{B}\right]\hat{\boldsymbol{q}} + (\bar{\mathbf{Q}}_y + \beta\mathbf{M})(\hat{\vartheta}^+ \boldsymbol{\psi}^+ - \hat{\vartheta}^- \boldsymbol{\psi}^-) = 0 \tag{34}$$

$$\left(\bar{\mathbf{U}}\right)_{jk} = \int_0^1 p_j^\psi(z) p_k^q(z) \bar{u}_{\mathcal{N}}^G(z) \mathrm{d}z, \quad \left(\bar{\mathbf{Q}}_y\right)_{jk} = \int_0^1 (\partial_y \bar{q}_{\mathcal{N}}^G) p_j^\psi(z) p_k^\psi(z) \mathrm{d}z$$

We can now write a generalized eigenvalue problem for c as follows

$$\left[\begin{array}{c|c|c} \bar{u}_{\mathcal{N}}^G(z=1) & 0 & 0 \\ \hline (\bar{\mathbf{Q}}_y + \beta\mathbf{M})\boldsymbol{\psi}^+ & \bar{\mathbf{U}} - (\bar{\mathbf{Q}}_y + \beta\mathbf{M})\left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \mathbf{B} & -(\bar{\mathbf{Q}}_y + \beta\mathbf{M})\boldsymbol{\psi}^- \\ \hline 0 & 0 & \bar{u}_{\mathcal{N}}^G(z=0) \end{array}\right] \begin{pmatrix} \hat{\vartheta}^+ \\ \hat{q} \\ \hat{\vartheta}^- \end{pmatrix} =$$

$$c \left[\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline 0 & \mathbf{B} & 0 \\ \hline 0 & 0 & 1 \end{array}\right] \begin{pmatrix} \hat{\vartheta}^+ \\ \hat{q} \\ \hat{\vartheta}^- \end{pmatrix} \tag{35}$$

The top and bottom rows require either $c = \bar{u}_{\mathcal{N}}^G(z=1) = \bar{u}_{\mathcal{N}}^G(z=0)$ or $\hat{\vartheta}^\pm = 0$. The only realistic option is the latter, so the eigenvalue problem simplifies to

$$\left[\bar{\mathbf{U}} - (\bar{\mathbf{Q}}_y + \beta\mathbf{M})\left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1} \mathbf{B}\right]\hat{\boldsymbol{q}} = c\mathbf{B}\hat{\boldsymbol{q}}. \tag{36}$$

The linear instability analysis will in general proceed as follows

- Choose $\bar{u}$ and $N^2(z)$. (and f_0 and H and β and $\mathcal{N}$)
- Use (31) and (32) to construct the Galerkin approximations $\bar{u}^G_{\mathcal{N}}$ and $\partial_y \bar{q}^G_{\mathcal{N}}$.
- Construct all the matrices $\mathbf{B}$, $\mathbf{M}$, $\mathbf{L}$, $\bar{\mathbf{U}}$, $\bar{\mathbf{Q}}_y$
- Construct the matrices in (36) and pass the whole thing to a generalized eigenvalue solver, searcing for the eigenvalue with largest imaginary part. If the imaginary part of the eigenvalue is positive then there is exponential growth with rate k_x times the imaginary part of c. If you don't want to use a generalized eigenvalue solver, you could just find eigenvalues of the matrix

$$\mathbf{B}^{-1}\left[\bar{\mathbf{U}} - (\bar{\mathbf{Q}}_y + \beta\mathbf{M})\left((k_x^2 + k_y^2)\mathbf{M} + \mathbf{L}\right)^{-1}\mathbf{B}\right].$$

Note that despite what I said in the previous sections about using the diagonalizing basis, this entire section still uses the Shen/Legendre bases. In particular, the eigenvector will be coefficients of $q^G_{\mathcal{N}}$ in the Legendre basis.