# QUASI-CONVERGENCE OF AN IMPLEMENTATION OF OPTIMAL BALANCE BY BACKWARD-FORWARD NUDGING

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ABSTRACT. Optimal balance is a non-asymptotic numerical method for computing a point on an elliptic slow manifold for two-scale dynamical systems with strong gyroscopic forces. It works by solving a modified differential equation as a boundary value problem in time, where the nonlinear terms are adiabatically ramped up from zero to the fully nonlinear dynamics. A dedicated boundary value solver, however, is often not directly available. The most natural alternative is a nudging solver, where the problem is repeatedly solved forward and backward in time and the respective boundary conditions are restored whenever one of the temporal end points is visited. In this paper, we show quasi-convergence of this scheme in the sense that the termination residual of the nudging iteration is as small as the asymptotic error of the method itself, i.e., under appropriate assumptions exponentially small. This confirms that optimal balance in its nudging formulation is an effective algorithm. Further, it shows that the boundary value problem formulation of optimal balance is well posed up to at most a residual error as small as the asymptotic error of the method itself. The key step in our proof is a careful two-component Gronwall inequality.

## 1. INTRODUCTION

Optimal balance is a non-asymptotic numerical method for computing a point on an elliptic slow manifold for two-scale dynamical systems with strong gyroscopic forces. It is based on adiabatically deforming the system from the full nonlinear vector field to a linear vector field where the fast-slow splitting can be inferred from the spectrum of the associated linear operator. So long as the homotopy between linear and nonlinear vector field approximately preserves the level of fast energy, this computation yields a highly accurate approximation to a point on a nearly invariant slow manifold of the nonlinear system. The method is applicable for slow manifolds in the general sense of MacKay [13] which may not be exactly invariant as in classical singular geometric perturbation theory [5, 8]. In particular, normal hyperbolicity is not required.

While the underlying ideas are much older, optimal balance was introduced by Viúdez and Dritschel [18] in the context of semi-Lagrangian schemes for geophysical fluid flow [6, 7]. The authors observed excellent nonlinear separation of (slow) Rossby and (fast) gravity waves. Cotter [3] subsequently pointed out the connection to the theory of adiabatic invariance, investigated earlier for a finite dimensional toy model in [4]. Gottwald *et al.* [10] provide a detailed analysis of the asymptotic error of optimal balance in the same finite dimensional setting, but with a finite time horizon for the homotopy between the nonlinear and the linear system. In

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FIGURE 1. Decrease of the nudging error with the number of nudging iterations m in an application of optimal balance to the rotating shallow water equations. Shown is the spectral energy density  $E_k$ of the difference of successive nudging iterates  $q_m$  from the given basepoint potential vorticity  $q^*$  as a function of k, the modulus of the wavenumber vector. The Rossby number of this simulation is  $\varepsilon = 0.1$ . Adapted from [14].

this case, additional order conditions on the ramp function appear and prevent the use of analytic ramp functions. Nonetheless, when the ramp function is of Gevrey class 2, the balance error can be exponentially small.

The practical numerical implementation of optimal balance requires solving a boundary value problem in time. The boundary conditions are, respectively, absence of fast linear modes at the linear end of the homotopy, and the requirement that a complementary set of variables, a "basepoint coordinate" parametrizing the slow manifold, takes a specified value at the nonlinear end. When the dynamical system is low-dimensional, a standard solver for boundary value problems, sometimes even a simple shooting scheme, can be used. For large or complex models, this is not practical. However, optimal balance can be implemented via backwardforward nudging where the homotopy is repeatedly integrated backward or forward in time between the linear and the full nonlinear state. At each temporal boundary, the respective boundary condition is imposed while the complementary variables are left unchanged. This is similar, even though the precise details differ, to "backwardforward nudging" described by [1], so we borrow their terminology. The scheme as such was already used by [18] and found to work well. The key advantage of a backward-forward nudging implementation of optimal balance is that any existing numerical code can be turned into an optimal balance solver so long as the mode splitting of the linearized system is understood, which opens possibilities for accurate diagnostics even for complex operational atmosphere and ocean models.

Two theoretical questions, however, were left open until now. First, can we prove that the optimal balance boundary value problem is well posed? Second, if so, can we prove that the implementation by nudging actually converges to the solution of this boundary value problem? A detailed numerical study of optimal balance for the rotating shallow water equations in their primitive variable formulation [14, 15] found that, while the method does return well-balanced states as expected, convergence of the sequence of nudging iterates to a given basepoint takes place only up to a small residual that does not go away as the number of iterations grows large. Figure 1 shows typical diagnostic output of a simulation of a two-dimensional shallow water flow, where the basepoint variable  $q^*$  is the potential vorticity field. For selected members of the sequence of nudging iterates, indexed by m, we display the nudging residual as the difference between  $q_m$  and the prescribed basepoint  $q^*$  in terms of its spectral energy density  $E_k(q_m - q^*)$ , where the scalar total wavenumber k is defined as the modulus of the two-dimensional wavenumber vector. The best residual is reached within five iterations; subsequent iterations show no further improvement. The termination residual is very small for low spatial wavenumbers and grows somewhat larger toward high spatial wavenumbers.

In this paper, we revisit the issue mathematically in the simpler context of the finite dimensional model problem that was already used in related previous studies [4, 9, 11]. Without assuming well-posedness of the boundary value problem, we split the error into the termination residual of the iteration and the "balance error," the residual fast energy of the optimal balance formulation as analyzed in [10]. We prove that the termination residual is small and of the same order of magnitude as the balance error. This result, first, provides a rigorous foundation that optimal balance in a backward-forward nudging implementation is indeed a very effective algorithm. Second, it highlights that care must be taken to find a good termination criterion for the nudging iteration, cf. the discussion in [14, 15]. Third, it shows that we can side-step the question of well-posedness of the optimal balance boundary value problem, assumed but not proved in [10]: our result implies that the problem is well posed at worst up to a residual of the same small order of magnitude as the overall error of the method.

For small problems, such as the numerical test case studied in [10], it is possible to apply a proper boundary value problem solver. The results obtained there suggest that at least in some cases, the boundary value problem is actually well-posed and the termination residual can be brought to zero. It is likely, though, that the class of problems for which quasi-convergence in the sense of this paper holds is strictly larger than the class of problems for which the boundary value problem is well posed in a strict sense.

The remainder of the paper is structured as follows. In Section 2, we introduce the model equations and sketch the standard asymptotic construction of the slow manifold. Section 3 introduces optimal balance and extends the asymptotic construction to the non-autonomous optimal balance equations. The key estimates from [10] are reviewed in Section 4 and adapted to the choice of parameters required in the context of this paper. Our new results are contained in the main Section 5: We introduce the nudging scheme and estimate the termination residual with a careful Gronwall estimate over the entire backward-forward integration cycle. The main result, quasi-convergence of the scheme, is stated as Theorem 6 or 7 for the respective case that algebraic or exponential order conditions are satisfied. The paper concludes with a discussion of scope and possible improvements to our results. A short appendix recalls a Gronwall inequality for systems of differential inequalities, one of the main ingredients in our argument.

### 2. The model

As in [4, 9, 10, 11], we consider the finite-dimensional toy model

$$\dot{q} = p \,, \tag{1a}$$

$$\varepsilon \dot{p} = Jp - \nabla V(q),$$
 (1b)

where  $q: [0,T] \to \mathbb{R}^{2d}$  is a vector of positions,  $p: [0,T] \to \mathbb{R}^{2d}$  is the vector of corresponding momenta,  $\varepsilon$  is the time-scale separation parameter considered to be small, J is the standard symplectic matrix on  $\mathbb{R}^d$  with d even, and V is a sufficiently smooth potential.

For the purpose of defining and analyzing optimal balance, this system is particularly easy because the slow subspace of the *linear* system, i.e. when V = 0, is given by p = 0. This, however, is not a true restriction but rather a convenient choice of variables. A hierarchy of slow manifold in the sense of [13] is then given by the finite power series expansion

$$p_{\text{slow}} \equiv G_n(q) = \sum_{i=0}^n g_i(q) \,\varepsilon^i \,, \tag{2}$$

where the coefficient vector fields  $g_i$  are recursively defined by

$$g_0(q) = -J\nabla V(q), g_k(q) = -J\sum_{i+j=k-1} Dg_i(q) g_j(q).$$
(3)

The series generally does not converge, but it is very easy to prove that solutions to  $\dot{q} = G_n(q)$  are shadowed by a solution of (1) for finite *n* and finite times; see, e.g., [9]. System (1) is Hamiltonian so that, provided *V* is analytic, Hamiltonian normal form theory gives exponentially close shadowing over exponentially long times [4].

# 3. Optimal balance

Optimal balance provides a numerical procedure to compute an approximation to the map (2) for a given "basepoint" q without the need to analytically compute any of the terms on the right hand side. It works by selectively turning off the nonlinear term in the equation via a "ramp function"  $\rho: [0,1] \rightarrow [0,1]$  with  $\rho(0) = 0$ and  $\rho(1) = 1$ . In addition, we assume that either  $\rho \in C^n([0,1])$  and satisfies the algebraic order condition of order  $n \in \mathbb{N}^*$ ,

$$\rho^{(i)}(0) = \rho^{(i)}(1) = 0 \quad \text{for } i = 1, \dots, n,$$
(4)

or, alternatively, that  $\rho$  is of Gevrey class 2 on [0, 1] and satisfies the *exponential* order condition

$$\rho^{(i)}(0) = \rho^{(i)}(1) = 0 \quad \text{for all } i \ge 1.$$
(5)

Recall that a function  $f \in C^{\infty}(U)$  for  $U \subset \mathbb{R}$  open is of Gevrey class s (in short,  $f \in G^{s}(U)$ ) if there exist constants C and  $\beta$  such that

$$\sup_{x \in U} \left| f^{(n)}(x) \right| \le C \, \frac{n!^s}{\beta^n} \tag{6}$$

for all  $n \in \mathbb{N}$ . Here, we need this estimate to be uniform up to the boundary of the interval [0, 1]. An example of a ramp function satisfying this condition is

$$\rho(\theta) = \frac{e^{-1/\theta}}{e^{-1/\theta} + e^{-1/(1-\theta)}} \,. \tag{7}$$

The method of optimal balance requires solving the boundary value problem in time,

$$\dot{q} = p \,, \tag{8a}$$

$$\varepsilon \dot{p} = Jp - \rho(t/T) \nabla V(q),$$
(8b)

with boundary conditions

$$p(0) = 0$$
 and  $q(T) = q^*$ . (8c)

The boundary condition at the linear end where t = 0 expresses the absence of fast motion, and the boundary condition at the nonlinear end where t = T expresses the matching with a prescribed basepoint  $q^*$ . The approximation to the slow manifold G is then given by

$$G(q^*) = p(T).$$
(9)

Optimal balance is nicely illustrated by applying it to the following classical example of an exact local slow manifold. This example is used, for instance, by MacKay [13] as a starting point for showing that generic Hamiltonian systems do not possess exactly invariant slow manifolds.

Take a slow harmonic oscillator, written in action-angle variables  $(I, \theta)$  so that the action  $I \equiv 1$  is constant and the angle  $\theta \in \mathbb{R}/2\pi$  has constant rate of change which drives, via a nonlinear coupling function  $f(\theta)$ , a fast harmonic oscillator written in complex representation, namely

$$\dot{\theta} = 1, \qquad (10a)$$

$$\varepsilon \, \dot{p} = \mathrm{i}p + f(\theta) \,. \tag{10b}$$

The form of this equation is different from (1), but can be brought into a more similar form by a change of variables the details of which do not matter for the point to be made. Expanding f as a Fourier series,

$$f(\theta) = \sum_{k \in \mathbb{Z}} f_k e^{ik\theta} , \qquad (11)$$

and inserting the ansatz  $p = G(\theta)$  into (10), we find that the slow manifold is given by

$$G(\theta) = \sum_{k \in \mathbb{Z}} f_k \frac{\varepsilon}{\mathbf{i}(k\varepsilon - 1)} e^{\mathbf{i}k\theta}$$
(12)

away from the resonances  $\varepsilon = 1/k$ . The corresponding ramped system for the optimal balance boundary value problem reads

$$\dot{\theta} = 1, \tag{13a}$$

$$\varepsilon \dot{p} = ip + \rho(t/T) f(\theta).$$
 (13b)

Using the optimal balance boundary conditions (8c), with  $\theta$  in place of q, we can readily write out the solution of (13b) as

$$p(T) = \int_0^T e^{i(T-t)/\varepsilon} \rho(t/T) f(\theta^* + (t-T)) dt.$$
 (14)

To see that this expression is indeed a good approximation of  $G(\theta^*)$ , we must insert the Fourier expansion for f and integrate by parts:

$$p(T) = \sum_{k \in \mathbb{Z}} f_k \int_0^T e^{\frac{\mathbf{i}(T-t)}{\varepsilon} + \mathbf{i}k(\theta^* + (t-T))} \rho(t/T) dt$$
$$= \sum_{k \in \mathbb{Z}} f_k e^{\frac{\mathbf{i}T}{\varepsilon} + \mathbf{i}k(\theta^* - T)} \int_0^T e^{(\frac{-\mathbf{i}}{\varepsilon} + \mathbf{i}k)t} \rho(t/T) dt$$
$$= \sum_{k \in \mathbb{Z}} f_k e^{\frac{\mathbf{i}T}{\varepsilon} + \mathbf{i}k(\theta^* - T)} \frac{\varepsilon}{\mathbf{i}(k\varepsilon - 1)} \left[ e^{(\frac{-\mathbf{i}}{\varepsilon} + \mathbf{i}k)T} - \int_0^T e^{(\frac{-\mathbf{i}}{\varepsilon} + \mathbf{i}k)t} \frac{\rho'(t/T)}{T} dt \right].$$
(15)

In the last equality, we have used that  $\rho(0) = 0$  so that the boundary term at t = 0 vanishes. The contribution from the first term in brackets coincides with (12). The contribution from the remainder integral is, at this point,  $O(\varepsilon)$  provided that  $\varepsilon$  is suitably bounded away from resonances. However, its order in  $\varepsilon$  can be improved by further integration by parts: So long as  $\rho^{(i)}(0) = \rho^{(i)}(T) = 0$  for  $i = 1, \ldots, n$ , the boundary terms of the (n + 1)st integration by parts vanish and the contribution from the remaining integral is  $O(\varepsilon^{n+1})$ . Thus,

$$p(T) = \sum_{k \in \mathbb{Z}} f_k \frac{\varepsilon}{i(k\varepsilon - 1)} e^{ik\theta^*} + O(\varepsilon^{n+1}).$$
(16)

To get exponential estimates, some assumption on the growth of derivatives of  $\rho$  is necessary. The corresponding analysis could proceed along the lines of [10].

We conclude that optimal balance is consistent in the case where an exact slow manifold (locally) exists, but introduces a small error even there. The interesting case, however, is when an exactly invariant slow manifold does not exist, e.g., when the action of the slow oscillator in (10) is not constant in time but varies across one or more of the resonances. Then, especially for Hamiltonian systems, exponentially accurate normal forms are the best we can expect. Optimal balance works in both cases and can be exponentially accurate, whether or not an exactly invariant slow manifold exists.

### 4. Remainder estimates

The analysis of optimal balance in [10] works by constructing an asymptotic expansion analogous to (2) for the ramped system. This expansion defines a time-dependent manifold on which the non-autonomous dynamics of (8) remains pre-dominantly slow.

The explicit form of the expansion is only used for the theoretical analysis, and reads

$$p_{\text{slow}} \equiv F_n(q,t) = \sum_{i=0}^n f_i(q,t) \,\varepsilon^i \,, \tag{17}$$

where the coefficient vector fields  $f_i$  are recursively defined by

$$f_0(q,t) = -\rho(t/T) J\nabla V(q), f_k(q,t) = -J\partial_t f_{k-1} - J \sum_{i+j=k-1} Df_i(q,t) f_j(q,t)$$
(18)

for k = 1, ..., n. An *n*-term approximation to the fast component of the motion is then given by

$$w(t) = p(t) - F_n(q, t)$$

(we suppress the dependence of w on n to keep the notation simple), and the model (8) can be rewritten in q-w variables as

$$\dot{q} = F_n + w \,, \tag{19a}$$

$$\dot{w} = \left(\frac{1}{\varepsilon}J - DF_n\right)w + R_n(q), \qquad (19b)$$

with remainder given by

$$R_n(q) = -\varepsilon^n \,\partial_t f_n(q) - \sum_{s=n}^{2n} \varepsilon^s \sum_{\substack{i+j=s\\i,j\leq n}} Df_i(q) f_j(q) \tag{19c}$$

(we suppress the explicit dependence of  $R_n$ ,  $F_n$ , and  $f_i$  on time t to keep the notation simple), and where the boundary conditions (8c) now read

$$w(0) = 0$$
 and  $q(T) = q^*$ . (19d)

In the following, we review estimates on the slow vector field and on the remainder of the asymptotic series. When the series defined in (17-19) is truncated at a fixed order n, these estimates are straightforward and stated as Lemma 1 below. When we go for exponential estimates, we need an optimal truncation of the asymptotic series. Full details can be found in [10]; Lemma 2 below states these results in the form required here, together with only a sketch of the proof.

**Lemma 1.** Let  $B(0,r) \subset \mathbb{R}^{2d}$  for some r > 0 and fix  $T_1 > 0$ . Assume that  $\rho \in C^n([0,1])$  and  $V \in C^{n+1}(B(0,r))$  for some  $n \in \mathbb{N}$ . Then there exist constants  $C_1, C_2$ , and  $C_3$  such that for any  $0 < \varepsilon < T \leq T_1$  and  $t \in [0,T]$ ,

$$||F_n(q_1, t) - F_n(q_2, t)|| \le C_1 ||q_1 - q_2||, \qquad (20a)$$

$$\|DF_n(q_1, t) - DF_n(q_2, t)\| \le C_2 \|q_1 - q_2\|,$$
(20b)

and

$$\|R_n(q,t)\| \le C_3 \left(\frac{\varepsilon}{T}\right)^n \tag{20c}$$

for any  $q_1$ ,  $q_2$ , and  $q \in B(0,r)$ . The constants may depend on  $\rho$ , V, n, and  $T_1$ , but are independent of  $\varepsilon$  and T.

Proof. Estimates (20a) and (20b) follow directly from the local Lipschitz property of V and its higher order derivatives. Note that the terms of  $F_k$  contain powers of  $T^{-1}$  at most up to order k. Thus, all constants in such terms can be bounded by  $C(T_1) (\varepsilon/T)^k \leq C(T_1)$ . To prove (20c), it suffices to factor out  $(\varepsilon/T)^n$  from  $R_n(q)$ , then use the available bounds on  $\rho$  and V and their derivatives together with the assumption  $\varepsilon < T < T_1$ .

To obtain exponential estimates, we assume that V is analytic and  $\rho$  is of Gevrey class 2.

**Lemma 2.** Fix r > r' > 0 and  $T_1 > 0$ . Assume that  $\rho \in G^2(0,1)$  and V is analytic on B(0,r). Then there exist positive constants  $C_1$ ,  $C_2$ ,  $C_3$ , c, and  $\gamma$ , each depending only on  $\rho$ , V, and  $T_1$ , such that if

$$n = \left\lfloor \frac{\gamma \varepsilon}{T} \right\rfloor,\tag{21}$$

then

$$||F_n(q_1) - F_n(q_2)|| \le C_1 ||q_1 - q_2||, \qquad (22a)$$

$$\|DF_n(q_1) - DF_n(q_2)\| \le C_2 \|q_1 - q_2\|, \qquad (22b)$$

and

$$|R_n(q)|| \le C_3 \,\mathrm{e}^{-c \sqrt[3]{\frac{T}{\varepsilon}}} \tag{22c}$$

for  $0 < \varepsilon < T \leq T_1$  and all  $q_1, q_2, q \in B(0, r')$ .

*Proof.* For every  $n \in \mathbb{N}$ , [10, Lemma 6] together with a Cauchy estimate asserts that

$$||F_n(q_1) - F_n(q_2)|| \le \frac{1}{r_1 - r} \sup_{q \in B(0, r_1)} ||F_n(q)|| ||q_1 - q_2||,$$
(23a)

$$\|DF_n(q_1) - DF_n(q_2)\| \le \frac{1}{(r_2 - r)(r_3 - r_2)} \sup_{q \in B(0, r_3)} \|F_n(q)\| \|q_1 - q_2\|$$
(23b)

for  $r' < r_1, r_2 < r_3 < r$ . Fixing  $r_3$ , we then need to prove that there exists  $n = n(\rho, V, T_1, \frac{\varepsilon}{T})$  such that (22c) is satisfied and  $\sup_{q \in B(0, r_3)} ||F_n(q)||$  is bounded independent of n. We briefly sketch the main ideas: The key observation is that each of the terms appearing in the expression for  $R_n$  and  $F_n$  is a product of functions which depend only on  $\rho$  and functions which depend only on V. Hence, each can be written as an inner product of a coefficient vector encoding all  $\rho$ -dependence with a coefficient vectors encoding all V-dependence as follows:

$$R_n = J \sum_{k=n}^{2n} \frac{\varepsilon^k}{T^k} \left\langle \mathcal{R}_{k+1}(\rho), \mathcal{F}_{k+1}(V) \right\rangle$$
(24a)

and

$$F_n = \sum_{k=0}^n \frac{\varepsilon^k}{T^k} \left\langle \mathcal{R}_k(\rho), \mathcal{F}_k(V) \right\rangle.$$
(24b)

A Hölder-like inequality will bound each inner product, so that we can estimate each class of coefficients separately in its respective norm. Indeed, for the  $\rho$ -dependent vectors, we use the Gevrey estimate (6),

$$|\mathcal{R}_k(\rho)| \le C \frac{(k+1)!^2}{\beta^{k+1}},\tag{25}$$

where the constants C and  $\beta$  depend only on  $\rho$  and  $T_1$ . On the other hand, using a Cauchy estimate, there exist constants  $C, \gamma > 0$  depending on V (and implicitly on B(0,r)) such that

$$\|\mathcal{F}_k(V)\|_{B(0,r_3)} \le C\left(\frac{n}{\gamma}\right)^k,\tag{26}$$

where  $\|\cdot\|_{B(0,r_3)}$  refers to the supremum norm on  $B(0,r_3)$ . Combining (25) with (26) and using the Stirling inequality in the form  $m! \leq e^{m-1} m^{m+1/2}$  for every  $m \geq 2$ , there exist constants  $C, \alpha > 0$  depending only on  $\rho$ , V, and  $T_1$  such that

$$\|R_n\|_{B(0,r_3)} \le C \sum_{k=n}^{2n} \frac{\varepsilon^k}{T^k} \frac{n^{3k}}{\alpha^k} \le C \frac{\delta^n}{1-\delta},$$
 (27)

where we have bounded the sum by the corresponding infinite geometric series under the assumption that  $\delta \equiv \frac{\varepsilon n^3}{\alpha T} < 1$ , and similarly

$$\|F_n\|_{B(0,r_3)} \le C \, \frac{1-\delta^{n+1}}{1-\delta} \,. \tag{28}$$

An optimization of the overall bound leads to the choice

$$n = \left\lfloor \left(\frac{\alpha \delta T}{\varepsilon}\right)^{\frac{1}{3}} \right\rfloor,\tag{29}$$

so that

$$||F_n||_{B(0,r_3)} \le \frac{C}{1-\delta}$$
 (30a)

and

$$\|R_n\|_{B(0,r')} \le \frac{C}{1-\delta} \,\delta^{(\alpha\delta T/\varepsilon)^{\frac{1}{3}}} \le C_3 \,\mathrm{e}^{-c\sqrt[3]{\frac{T}{\varepsilon}}} \tag{30b}$$

where, in the last inequality, we have fixed  $\delta \in (0, 1)$  such that the final constants are positive.

Remark 3. The proof as written above differs from the proof given in [10, Proof of Theorem 4] in two trivial respects: The analysis in [10] is done with respect to the slow time  $\tau \equiv \varepsilon t$  and considers a sequence of ramp times  $T = 1/\varepsilon$  for which  $\rho(t/T) = \rho(\tau)$ . With this choice, the ramp time T does not appear in the formulas for  $\mathcal{R}_k(\rho)$ . Here, we use fast time t, so that time-derivatives of  $\rho(t/T)$  which appear in the expressions for  $\mathcal{R}_k(\rho)$  have coefficients proportional to  $T^{-i}$ ,  $i = 0, \ldots, k$ . To account for this, we changed the definition of  $\mathcal{R}_k(\rho)$ , multiplying by  $T^k$ , so that the bound in (25) is uniform in  $T \in (0, T_1]$ . The second difference is that we estimate  $F_n$  and  $R_n$  on  $B(0, r_3)$  and B(0, r'), only requiring that V is analytic on a larger ball of radius  $r > r_3 > r'$  without an explicit requirement on their relative sizes.

# 5. The nudging scheme

To introduce the backward-forward nudging scheme, we write  $q^*$  to denote the prescribed basepoint coordinate, as before, and take an initial guess  $p_0$  for the value of the fiber coordinate  $p = G(q^*)$ . E.g.,  $p_0 = 0$  or, if explicitly available,  $p_0 = G_0(q^*)$ , cf. (2). We then construct a sequence of approximates,  $p_m$ , in the following way.

Let  $q_m^-$  and  $p_m^-$  denote the solution to the ramped system (8a,b) backward in time, endowed with the final condition

$$q_m^-(T) = q^*$$
 and  $p_m^-(T) = p_m$ . (31)

We stop the backward integration at t = 0 and initialize a *forward* solution,  $q_m^+$  and  $p_m^+$ , to (8a,b) with initial condition

$$q_m^+(0) = q_m^-(0)$$
 and  $p_m^+(0) = 0$ . (32)

#### Linear end

#### Nonlinear end

FIGURE 2. Schematic representation of the nudging cycle. The arrow annotations indicate the behavior of the implicit fast variable  $w_m$  to explain the different steps of the proof of Proposition 4.

This solution is stopped at t = T and we set

$$p_{m+1} = p_m^+(T) \,. \tag{33}$$

In the following, we prove quasi-convergence of the sequence  $\{p_m\}$  in the case of the algebraic order condition and the exponential order condition.

To analyze the scheme, it is convenient to consider the ramped system in terms of the slow-fast variables as in (19), writing  $w_m^-(t)$  and  $w_m^+(t)$  for the fast variable in the backward and forward integration steps, respectively. We emphasize that this choice relates to the theoretical analysis of the method only. Numerically,  $w_m^$ and  $w_m^+$  are not available. Similarly, we write  $w_m$  to denote the fast variable at the start of the backward-forward integration cycle. I.e.,

$$w_{m+1} = p_m^+(T) - F_n(q^*, T) \quad \text{for } m \ge 0 \tag{34}$$

and

$$v_0 = p_0 - F_n(q^*, T) \,. \tag{35}$$

 $w_0 = p_0 - F_n(q^*, T)$ . (As before, we suppress the implicit dependence of  $w_m$  on n.)

Figure 2 summarizes the nudging cycle which, in our notation, starts at the top right and goes anticlockwise. The horizontal arrows indicate the backward/forward integration steps of the ramped system along which the fast energy is adiabatically preserved. The adjustment of the phase point at the linear end is of size  $||w_m||$ by construction. At the nonlinear end, when the basepoint is restored, the adjustment in the q component, due to the structure of equation (19a), is roughly of size  $||w_m||T$ , so can be made small by choosing T sufficiently small. The precise statements and proofs are the following.

**Proposition 4.** Assume that  $\rho$  satisfies the algebraic order condition (4) of order  $n \in \mathbb{N}$  at least at time t = 0. Fix R > 0,  $T_1 > 0$ , and  $p_0, q^* \in \mathbb{R}^{2d}$  such that

$$\max\left\{\|q^*\|, \|w_0\|\right\} \le R \quad \text{for all } 0 < \varepsilon \le T_1.$$
(36)

Then there exist  $T_0 \in (0, T_1]$  and  $\theta < 1$  such that for any  $0 < \varepsilon \le T \le T_0$ , we have

$$\|w_{m+1}\| \le \theta \,\|w_m\| + c \,\frac{\varepsilon^n}{T^n} \,. \tag{37}$$

The constants  $\theta$  and c may depend on  $\rho$ , V, T<sub>0</sub>, and R, but are independent of T and m.

*Proof.* The proof consists of four steps. We initially do our analysis on a single backward-forward nudging cycle where we assume that the analog of condition (36) is satisfied at the start of the cycle, i.e.,

$$\|w_m\| \le R \,. \tag{38}$$

In the final step, we prove that this conditions is maintained when going from one nudging cycle to the next.

Step 1: Obtain a bound on the generation of fast motion during backward integration. We work under the assumption that there exists  $T_0 \leq T_1$  such that

$$\sup_{\in [0,T_0]} \max\{\|q_m^{\pm}(t)\|, \|w_m^{\pm}(t)\|\} \le 2R.$$
(39)

For the backward integration, by continuity, there is always  $T_0$  small enough such that this condition is satisfied. Using the equations for  $w_m^{\pm}$  and  $q_m^{\pm}$  and bounding the nonlinear terms via (39), we see that there exist  $C_1, C_2$ , and  $C_3$ , depending only on  $\rho$ , V, n,  $T_1$ , and R, such that

$$\pm \frac{\mathrm{d}}{\mathrm{d}t} \|q_m^{\pm}\| \le C_1 + \|w_m^{\pm}\|, \qquad (40a)$$

$$\pm \frac{\mathrm{d}}{\mathrm{d}t} \|w_m^{\pm}\| \le C_2 \|w_m^{\pm}\| + C_3 \frac{\varepsilon^n}{T^n} \,. \tag{40b}$$

Integrating (40b) backward in time, we find

t

$$\sup_{t \in [0,T]} \|w_m^-(t)\| \le e^{C_2 T} \|w_m\| + \frac{C_3}{C_2} (e^{C_2 T} - 1) \frac{\varepsilon^n}{T^n} \le e^{C_2 T} R + \frac{C_3}{C_2} (e^{C_2 T} - 1) \frac{\varepsilon^n}{T^n}.$$
(41)

Inserting this bound into (40a) and integrating backward, we find

$$\sup_{t \in [0,T]} \|q_m^-(t)\| \le R + T \left( C_1 + e^{C_2 T} R + \frac{C_3}{C_2} \left( e^{C_2 T} - 1 \right) \frac{\varepsilon^n}{T^n} \right).$$
(42)

Thus, choosing  $T_0$  small enough, (39) is maintained also at the start of the forward integration step, with a right-hand bound of 3R/2, say. By continuity, possibly lowering the value of  $T_0$ , (39) will be maintained over the forward evolution, too. To get an explicit bound, we integrate (40b) forward. As  $\rho$  satisfies the algebraic order condition (4) of order n at t = 0, we have  $w_m^+(0) = 0$  and therefore

$$\sup_{t \in [0,T]} \|w_m^+(t)\| \le \frac{C_3}{C_2} \left( e^{C_2 T} - 1 \right) \frac{\varepsilon^n}{T^n} \,. \tag{43}$$

Finally, inserting this bound into (40a) and integrating forward, we obtain

$$\sup_{t \in [0,T]} \|q_m^+(t)\| \le R + 2T \left( C_1 + e^{C_2 T} R + \frac{C_3}{C_2} \left( e^{C_2 T} - 1 \right) \frac{\varepsilon^n}{T^n} \right).$$
(44)

Step 2: Obtain a bound on the deviation of q from the basepoint  $q^*$  after completing one full cycle. Taking the difference between the backward and the forward equation for q, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(q_m^+ - q_m^-) = F_n(q_m^+, t) - F_n(q_m^-, t) + w_m^+ - w_m^-.$$

It follows that

$$\frac{\mathrm{d}}{\mathrm{d}t} \|q_m^+ - q_m^-\| \le \|F_n(q_m^+, t) - F_n(q_m^-, t)\| + \|w_m^+ - w_m^-\|.$$
(45)

Using estimate (20a), we find that there exists  $\delta_1 = \delta_1(\rho, V, n, T_0, R)$  such that

$$\frac{\mathrm{d}}{\mathrm{d}t} \|q_m^+ - q_m^-\| \le \delta_1 \|(q_m^+ - q^-)\| + \|w_m^+ - w_m^-\|.$$
(46)

In the same manner, taking the difference between the backward and the forward equation for w, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(w_m^+ - w_m^-) = \frac{1}{\varepsilon} J(w_m^+ - w_m^-) - (DF_n(q_m^+, t)w_m^+ - DF_n(q_m^-, t)w_m^-) + R_n(q_m^+) - R_n(q_m^-).$$
(47)

Adding and subtracting  $DF_n(q_m^+,t)w_m^-$  from the right-hand side and taking the dot product with  $w_m^+ - w_m^-$ , we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \|w_m^+ - w_m^-\| \le \|DF_n(q_m^+, t)\| \|w_m^+ - w_m^-\| + \|DF_n(q_m^+, t) - DF_n(q_m^-, t)\| \|w_m^-\| + \|R_n(q_m^+)\| + \|R_n(q_m^-)\|.$$
(48)

The Lipschitz property (20b) and remainder bound (20c) then imply that there exist constants  $\delta_2$ ,  $\delta_3$ , and  $\alpha$ , only depending on  $\rho$ , V, n, R, and  $T_0$ , such that

$$\frac{\mathrm{d}}{\mathrm{d}t} \|w_m^+ - w_m^-\| \le \delta_2 \|w_m^+ - w_m^-\| + \delta_3 \|q_m^+ - q_m^-\| + \alpha \frac{\varepsilon^n}{T^n}.$$
(49)

Thus, (46) and (49) form a system of differential inequalities which can be written in matrix form as

$$\dot{z}(t) \le \delta A \, z(t) + K \,, \tag{50}$$

where  $\delta = \max{\{\delta_1, \delta_2, \delta_3\}},\$ 

$$z(t) = \begin{pmatrix} \|q_m^+(t) - q_m^-(t)\| \\ \|w_m^+(t) - w_m^-(t)\| \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \text{and } K = \begin{pmatrix} 0 \\ \alpha \left(\varepsilon/T\right)^n \end{pmatrix}, \quad (51)$$

and where we read the inequality sign component-wise. A Gronwall inequality for systems, recalled in the appendix, then shows that

$$z(t) \le z(0) + tK + \delta A \int_0^t e^{\delta(t-s)A} (z(0) + sK) ds$$
  
=  $U_1(\delta, t) z(0) + U_2(\delta, t) K$ , (52)

where the second step follows from  $A e^{\delta(t-s)A} = A e^{2\delta(t-s)}$  with

$$U_1(\delta, t) = I + \frac{1}{2} \left( e^{2\delta t} - 1 \right) A$$
 (53a)

and

$$U_2(\delta, t) = t \left( I - \frac{1}{2}A \right) + \frac{e^{2\delta t} - 1}{4\delta} A.$$
 (53b)

As  $q^+(0) = q^-(0)$ , we then obtain

$$\|q_m^+(T) - q^*\| = \|q_m^+(T) - q_m^-(T)\|$$
  
$$\leq \frac{1}{2} \left(e^{2\delta T} - 1\right) \|w_m^-(0)\| + \alpha \frac{e^{2\delta T} - 2\delta T - 1}{4\delta} \frac{\varepsilon^n}{T^n}.$$
(54)

Step 3: Translate the mismatch of the basepoint q into a bound on the fast variable w at the start of the next nudging cycle. By the triangle inequality,

$$\|w_{m+1}\| = \|p_m^+(T) - F_n(q^*, T)\|$$
  

$$\leq \|w_m^+(T)\| + \|F_n(q_m^+(T), T) - F_n(q^*, T)\|$$
  

$$\leq C \|q_m^+(T) - q^*\| + c \frac{\varepsilon^n}{T^n}$$
  

$$\leq C e^{C_2 T} (e^{2\delta T} - 1) \|w_m\| + c(T) \frac{\varepsilon^n}{T^n}.$$
(55)

Here, we used Lemma 1 together with (43) in the second inequality and estimate (54) together with estimate (41) in the third inequality. A possible explicit formula for c(T) is

$$c(T) = \alpha_1 \left( e^{2\delta T} - 2\delta T - 1 \right) + \alpha_2 \left( e^{2C_2 T} - 1 \right),$$
(56)

where  $\alpha_i = \alpha_i(\rho, V, n, T_1, R)$ . Since  $C, C_2, \delta$ , and the  $\alpha_i$  are uniform in  $m \in \mathbb{N}$  and  $T \in (0, T_0]$ , estimate (37) is satisfied by a further lowering of  $T_0$ .

Step 4: We finally prove that  $T_0$  can be chosen such that (38) remains satisfied in all nudging cycles provided it is satisfied initially. Estimate (55) implies, in particular, that

$$||w_{m+1}|| \le C e^{C_2 T} (e^{2\delta T} - 1) R + c(T)$$
(57)

with  $\lim_{T\to 0} c(T) = 0$ . Thus, for  $T_0$  again small enough, we ensure  $||w_{m+1}|| \leq R$ , which completes the proof.

We now turn to the analogue of Proposition 4 when V is analytic and  $\rho \in G^2(0,1)$ . Here, the truncation order n must be chosen optimally. The scheme is initialized with

$$w_0 = p_0 - F_n(q^*, T), (58)$$

which apparently depends on n. However, choosing n as in Lemma 2,  $F_n(q^*, T)$  can be bounded uniformly in  $\varepsilon < T < T_1$  for some  $T_1 > 0$ . This bound depends on  $T_1$ ,  $\rho$ , and V, in particular on the domain on which V is analytic. Thus, for a given R > 0, fix  $r_i$ , i = 1, 2, 3, such that  $2R \equiv r' < r_1, r_2 < r_3 < r \equiv 3R$  and estimates (22) are satisfied. Then, by the same steps as in the proof of Proposition 4, the following is true.

**Proposition 5.** Assume that  $\rho$  satisfies the exponential order condition (5) at least at time t = 0. Fix R > 0, S > 0,  $T_1 > 0$ , and  $p_0, q^* \in \mathbb{R}^{2d}$  such that V is analytic on B(0, 3R),

$$\|q^*\| \le R \text{ and } \|w_0\| \le S \quad \text{for all } 0 < \varepsilon < T \le T_1,$$

$$(59)$$

where n, implicit in the definition of  $w_0$ , is chosen as a function of  $\varepsilon$  and T as in Lemma 2. Then there exist  $T_0 \in (0, T_1]$  and  $\theta < 1$  such that for any  $0 < \varepsilon \leq T \leq T_0$ , we have

$$||w_{m+1}|| \le \theta ||w_m|| + d e^{-c \sqrt[3]{\frac{T}{\varepsilon}}}.$$
 (60)

The constants d and c may depend on  $\rho$ , V, T<sub>0</sub>, S, and R, but are independent of T and m.

Propositions 4 and 5 already suffice to prove quasi-convergence of the nudging sequence. However, we would like to assert that the sequence of nudging iterates not only quasi-converges to some limit, but that this limit is representative of the slow manifold of the *original* problem (1), not that of the ramped problem (8).

This requires imposing an order condition not only at t = 0 but also at t = T. Our final results can be stated in the following form.

**Theorem 6** (Algebraic quasi-convergence). Assume that  $\rho$  satisfies the algebraic order condition (4) of order  $n \in \mathbb{N}$ . Suppose  $V \in C^{n+1}(B(0,2R))$  for some R > 0 and pick  $q^*, p_0 \in \mathbb{R}^{2d}$  and  $T_1 > 0$  such that

$$\max\{\|q^*\|, \|p_0 - G_n(q^*)\|\} \le R \quad for \ all \ 0 < \varepsilon \le T_1 \,. \tag{61}$$

Choose  $T_0 \in (0, T_1]$  such that the main estimate (37) from Proposition 4 is satisfied for all  $\varepsilon < T \leq T_0$ . Then there is a constant  $C = C(\rho, V, n, T, R)$  such that the sequence of nudging iterates quasi-converges to a point  $G_n(q^*)$  on the approximate slow manifold of order n in the sense that

$$\limsup_{m \to \infty} \|p_m - G_n(q^*)\| \le C \varepsilon^n \,. \tag{62}$$

*Proof.* The order condition (4) implies that  $G_n(q^*) = F_n(q^*, T)$ . Thus, by Proposition 4,

$$\|p_{m+1} - G_n(q^*)\| = \|w_{m+1}\| \le \theta \, \|w_m\| + c \, \frac{\varepsilon^n}{T^n} = \theta \, \|p_m - G_n(q^*, T)\| + c \, \frac{\varepsilon^n}{T^n} \,. \tag{63}$$

Taking the limsup of this estimate, we find that

$$\limsup_{m \to \infty} \|p_m - G_n(q^*)\| \le \frac{c}{1-\theta} \frac{\varepsilon^n}{T^n},\tag{64}$$

which concludes the proof.

**Theorem 7** (Exponential quasi-convergence). Assume that  $\rho$  satisfies the exponential order condition (5). Fix R > 0, S > 0,  $T_1 > 0$ , and  $p_0, q^* \in \mathbb{R}^{2d}$  such that V is analytic on B(0, 3R),

$$||q^*|| \le R \text{ and } ||p_0 - G_n(q^*)|| \le S \text{ for all } 0 < \varepsilon < T \le T_1,$$
 (65)

where n is chosen as a function of  $\varepsilon$  and T as in Lemma 2. Choose  $T_0 \in (0, T_1]$ such that the main estimate (60) from Proposition 5 is satisfied. Then there are positive constants  $C = C(\rho, V, T)$  and  $D = D(\rho, V, T)$  such that

$$\limsup_{m \to \infty} \|p_m(T) - G_n(q^*)\| \le D \,\mathrm{e}^{-C\varepsilon^{-\frac{1}{3}}} \tag{66}$$

for all  $\varepsilon < T \leq T_0$ .

Remark 8.  $G_n$  in (66) is a truncated asymptotic series where the order of truncation grows like  $\varepsilon^{-1/3}$ . The exponent  $\frac{1}{3}$  may not be sharp, but its growth must be sublinear in  $\varepsilon^{-1}$ , in contrast with the scaling of the optimal truncation for the original fast-slow system, which goes like  $\varepsilon^{-1}$  and yields an approximation to the slow manifold to  $O(\exp(-c/\varepsilon))$ , see, e.g., [4].  $G_n$  is difficult to compute and need not be known when applying the optimal balance method in practice. Still, (66) expresses that the quasi-limit of the nudging sequence, i.e., the state returned by the optimal balance method, is exponentially well-balanced.

### 6. DISCUSSION

Our results show that, in order to guarantee quasi-convergence, one first has to choose the ramp time T sufficiently small. Quasi-convergence then holds for all  $\varepsilon \leq T$ , but to ensure small remainders, we actually need  $\varepsilon \ll T$ . This may seem restrictive, but in practice, reasonably large values of T, comparable to the natural time scales of the slow motion, work just fine [14, 15, 18].

One place where our estimates are overly conservative is the bound (39) which we apply equally to the q and w components of the transformed system. As the iterations progress, w will get successively smaller, so tracking separate bounds for q and w would improve the constants. Thus, it may be possible to start with T small and increase it as the iterations progress. This might improve the basin of quasi-convergence as well as computational efficiency. Alternatively, the basin of convergence may be extended by using damped nudging updates of the form  $p_{m+1} = p_m + \alpha (p_m^+(T) - p_m)$  with  $\alpha \in (0, 1)$ . Here, once again, our practical experience is that the algorithm is rather robust and does not usually require such measures, but there may certainly be situations where they could help.

Our method of proof only gives an upper bound on the termination residual, but does not prove that true convergence is impossible. It suggests, however, that quasi-convergence is the best we should hope for, for the following reason: Both the termination residual and the balance error arise from the same mechanism, the spurious excitation of fast degrees of freedom via the late terms of a diverging asymptotic series over an O(1)-interval of slow time. As such, we can control their amplitude, but their phases will typically depend sensitively on the initial state of a nudging cycle, and have no reason to converge. Thus, the nudging iterates land in a ball whose radius is controlled by the amplitude of the spurious fast motion, while the uncertainty of the landing point within the ball is due to the unstable fast phases. As a rule of thumb, we should expect quasi-convergence for systems that do not possess truly invariant slow manifolds.

The test problem used in this paper is a Hamiltonian system with a noncanonical symplectic matrix which structurally resembles the equations for rapidly rotating fluid flow, cf. the discussion in [4], albeit by passing the difficulties related to the functional setting and time horizon of existence of solutions for the full fluid equations. As such, it is a paradigm for a class of systems of interest in geophysical fluid dynamics. Existence of approximately invariant slow manifolds for certain Hamiltonian systems with finitely many slow degrees of freedom, without restrictions on the number of fast degrees of freedom, has been proved in [12]. The class of systems considered there differs from our model problem as the authors assume a symplectic matrix that is block-diagonal with respect to the splitting into slow and fast variables. However, the only structural feature we really use is that the fast subsystem is skew to leading order in the scale separation parameter. We therefore conjecture that optimal balance, as well as the analysis presented here, extends not only to symplectic slow manifolds as in [12], but to a much larger class of systems where, in particular, the slow subsystem is not structurally constrained. Including infinite dimensional dynamical systems will bring its own set of challenges, but progress should be possible along the lines of [12, 16, 17].

Another point of interest is the choice of time integration scheme. Solving the optimal balance boundary value problem *exactly* requires accuracy on the fast time scale, which can be very costly when the scale separation is strong. With the

nudging solver, our experience indicates that it suffices to choose a time integration scheme that is stable with a time step selected to ensure accuracy on the slow time scale, making the method more computationally feasible. A precise understanding of this phenomenon may be possible along the lines of this paper, but remains outside of the present scope.

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# Appendix

In the following, we recall a Gronwall inequality for systems which was proved in [2] and put this theorem into a form which can be used to directly obtain estimate (52).

**Theorem 9.** Fix  $n \in N^*$  and let G(t) and H(t) be real-valued, continuous, nonnegative  $n \times n$  matrices. Further, let  $z(t), a(t) \in \mathbb{R}^n$  be continuous such that

$$z(t) \le a(t) + G(t) \int_0^t H(s) \, z(s) \, \mathrm{d}s \,.$$
 (67)

Then,

$$z(t) \le a(t) + G(t) \int_0^t V(t,s) H(s) a(s) \,\mathrm{d}s \,, \tag{68}$$

where

$$V(t,\tau) = I + \int_{\tau}^{t} H(s) G(s) V(s,\tau) \,\mathrm{d}s \,.$$
(69)

The inequalities above are satisfied component-wise.

Let A denote the  $n \times n$  matrix whose components are all ones, and let  $\delta > 0$ . It is easy to check that  $\delta A$  is nonnegative. Indeed, given  $X = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$ , we have

$$X^{T}AX = \sum_{k=1}^{n} x_{k} (AX)_{k} = \sum_{k=1}^{n} x_{k} \sum_{k=1}^{n} x_{j} = \left(\sum_{k=1}^{n} x_{k}\right)^{2} \ge 0.$$
(70)

Then, writing

$$G(t) = \delta A, \quad H(t) = I, \quad \text{and } V(t,\tau) = e^{\delta(t-\tau)A}, \tag{71}$$

we easily check that  $V(t, \tau)$  satisfies (69). Theorem 9 then implies the following.

**Corollary 10.** Let  $\delta > 0$ ,  $K \in \mathbb{R}^n$ , and  $z(t) \in \mathbb{R}^n$  be differentiable such that

$$z'(t) \le \delta A \, z(t) + K \,. \tag{72}$$

Then

$$z(t) \le z(0) + tK + \delta A \int_0^t e^{\delta(t-s)A} \left( z(0) + sK \right) ds.$$
(73)

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