Multigrid for Atmospheric Data Assimilation: Analysis

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Abstract. Multigrid methods are known to provide the most efficient solvers to many well-posed boundary-value PDE problems. In the case of ill-determined problems they can supply several additional advantages. Unlike evolution problems with well-posed initial conditions which can be solved by direct marching in time, when only scattered data are known, each datum affects both earlier and later solution values, so simple marching cannot be used, and fast solvers would again require multigrid methods. Multigrid solver can provide natural regularization to the ill-posed problem, since the main ill-posedness is the long term and long range influence of fine-scale oscillations, while the multiscale large-scale interactions are mediated by coarse grids that omit those oscillations. As a model problem we treat a hyperbolic PDE: the wave equation with only approximately known coefficients. The results of a detailed Fourier analysis, comparing full-flow control with initial-value control are presented.

1 Introduction

Current assimilation methods require much more computer time and space than the direct solving of atmospheric flow equations. The main reason for this is that any measurement at any place and time should in principle affect the solution at any other place and time, which creates a huge dense matrix of influence.

Current methods are not only very slow but they are also based on highly questionable compromises such as assimilating only the data from one time interval at a time without fully correlating with other intervals and limiting control to only the initial value of the flow at some arbitrary chosen initial time instead of controlling the numerical equations at all times.

The fast multiscale algorithm could avoid such compromises and assimilate the data at a cost comparable to that of solving the direct problem because of three main reasons: (1) large-scale averages may be assimilated well enough on the coarser levels of the multiscale solver, which is not expensive; (2) deviations from any large scale average must be assimilated on some finer scale, but their correlation on that scale is local; (3) the measurements are usually less accurate than the numerical flow itself, hence their assimilation need not be done at the finest level.

In most current data assimilation approaches, the control parameters, i.e. those changed to obtain fitness of the solution to the data, are only the initial values of the solution. This makes it impossible to benefit from the details (the oscillating components) of the measurements far in time from the initial time because those details at those times are ill-determined by the initial solution, due to the fact that their phase error becomes practically random, in which case the amplitude of the entire solution which would best fit the data can be shown to tend to zero. Therefore, instead of controlling just initial values, i.e. solving *initial control problem (ICP)*, we suggest to control the *entire numerical solution*. We call this approach the *residual control problem (RCP)*. It can be effectively handled only by a *multiscale treatment*.

We present here the results of a detailed Fourier analysis, comparing full-flow control with initial-value control in a model case of 1D + time wave equation. Those results demonstrate the advantages of the RCP approach.

2 Model Problem

As a simple demonstration model we have studied a case of 1D + time wave equation:

$$u_{tt} = c\triangle u \quad in \;\; \Omega \times [0,T], \quad T \in R^+, \quad \Omega \subset R \tag{1a}$$

$$u|_{\partial\Omega} = p(t), \tag{1b}$$

$$u|_{t=0} = u_0(x), \tag{1c}$$

$$u_t|_{t=0} = g(x), \tag{1d}$$

except that part of the model, e.g. some of the functions $c(x,t)$, $u_0(x)$, $g(x)$, $p(t)$, are not known or known only partially, and instead various observations on the solution are given.

For example, let be given finitely many data $d_l \in R$, such that

$$P_l u = d_l. \tag{2}$$

The projection P_l represents a local averaging over some neigborhood, i.e.:

$$P_l u = \int p_l(x,t)u(x,t)dxdt, \qquad \int p_l(x,t)dxdt = 1,$$

when each p_l has some (small) compact support.

ICP here is to find an initial function $u_0(x)$ so that the resulting solution $u(x,t)$ of the wave equation $(1a,b,d)$ would satisfy (2) as well as possible, in the sense of minimizing the functional

$$F(u_0) = \sum_l \beta_l \Big[P_l u - d_l\Big]^2, \tag{3}$$

where $(\beta_l)^{-1}$ is an estimate of the expected square error in the measurements.

The ICP is *ill-posed* in the sense that there is no unique solution depending continuously on the data. The classical way to overcome this ill-posedness is to apply a regularization technique. The detailed description of an algorithm for solving the ICP stated above using *Tikhonov regularization* can be found in [**?**]. For the analysis of this formulation in terms of Fourier components see Sect. **??** below.

The RCP, on the other hand, involves minimizing the functional

$$F(\mathbf{u}) = \int_{\Omega\times[0,T]} \gamma R^2 dxdt + \int_{\partial\Omega} \gamma_1 R_1^2 dx + \int_0^T \gamma_2 R_2^2 dt + \\ + \int_0^T \gamma_3 R_3^2 dt + \sum_l \beta_l \Big[P_l u - d_l\Big]^2,$$

where γ, γ_1, γ_2, γ_3 are weight functions of x, t, u; $R = u_{tt} - \triangle u$ are the residuals of the interior equations; R_1 are residuals of the boundary conditions; R_2 and R_3 are residuals of the initial conditions. Fourier analysis for this method is reported in Sect. **??** below.

Before solving the problem numerically one should choose a suitable discretization scheme. Let h be a meshsize in x-direction and δt be a time step with $K+1$ gridpoints in the time direction, $K\delta t = T$. The discretization of the Laplacian at time $k\delta t$ is as follows:

$$\triangle^h u_j^k = \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{h^2}.$$

Consider the following second order discretizaion scheme for $(1a)$:

$$q\triangle^h u_j^{k+1} + (1-2q)\triangle^h u_j^k + q\triangle^h u_j^{k-1} = \frac{u_j^{k+1} - 2u_j^k + u_j^{k-1}}{\delta t^2}, \qquad (4)$$

where $0 \le q \le 1$ is a parameter, which has to be determined. By applying the Fourier analysis, we found that this discretization scheme is *unconditionally stable* if and only if $q \ge \frac{1}{4}$. Let us take the smallest $q = \frac{1}{4}$ which still guarantees unconditional stability, since the smaller q, the more accurate the discretization.

3 Fourier analysis

3.1 General

Assume for simplicity that

a). Ω is an infinite domain. Hence $p(t)$ in $(1b)$ is replaced just by the condition that at each time t $u(x,t)$ is a <u>*bounded*</u> function of x;

b). $g(x)$ in $(1d)$ is known to vanish.

Let $u(x,t)$ be a Fourier component of frequency ω in x-direction and amplitude $A(t)$:

$$u(x,t) = A(t)\mathrm{e}^{i\omega x}.$$

This function is discretized as follows:

$$u_j^k = A_k e^{i\Theta j}, \quad \Theta = \omega h, \quad j \in Z, \quad A_k = A(t_k), \quad k = 0,\ldots,K, \quad K\delta t = T.$$

Let us apply the discretization scheme (4) with a choosen q:

$$A_{k+1}\Big(\frac{1}{\delta t^2}+\frac{1}{h^2}\sin^2\frac{\Theta}{2}\Big)-2A_k\Big(\frac{1}{\delta t^2}-\frac{1}{h^2}\sin^2\frac{\Theta}{2}\Big)+A_{k-1}\Big(\frac{1}{\delta t^2}+\frac{1}{h^2}\sin^2\frac{\Theta}{2}\Big) = 0.$$

3.2 ICP

$$A_k = C_1\left(\frac{1-im\sin\frac{\Theta}{2}}{1+im\sin\frac{\Theta}{2}}\right)^k + C_2\left(\frac{1+im\sin\frac{\Theta}{2}}{1-im\sin\frac{\Theta}{2}}\right)^k,$$

where $m = \frac{\delta t}{h}$.

From $(1b)$ follows that $u|_{t=0} = A_0 e^{i\omega x}$. From $(1d)$ with $g(x) \equiv 0$ follows that $u_t|_{t=0} = 0 \Rightarrow \frac{A_1 - A_0}{\delta t} = 0 \Rightarrow A_1 = A_0$. Thus

$$A_k = \frac{A_0}{2}\left[\Big(1-im\sin\frac{\Theta}{2}\Big)\left(\frac{1+im\sin\frac{\Theta}{2}}{1-im\sin\frac{\Theta}{2}}\right)^k+\Big(1+im\sin\frac{\Theta}{2}\Big)\left(\frac{1-im\sin\frac{\Theta}{2}}{1+im\sin\frac{\Theta}{2}}\right)^k\right].$$

Assume that the data $\{d_l\}$ are also given in terms of Fourier components, i.e. given a measurement $\overline{A_k}$ of the amplitude A_k for all $k \in I'$, I' is an index set. The functional (3) which we want to minimize now as a function of A_0 can be rewritten in the form:

$$F(A_0) = \sum_{k\in I'} \alpha_k (A_k - \overline{A_k})^2,$$

where α_k's are weight functions. α_k is proportional to an inverse of the estimated (upper bound) value of $(A_k - \overline{A_k})^2$, which can result from discretization and algebraic errors, measurements errors or modelization errors.
After solving the equation $F'(A_0) = 0$,

$$A_0 = 2\frac{\sum_{k\in I'}\alpha_k\overline{A_k}\left[\frac{(1+im\sin\frac{\Theta}{2})^k}{(1-im\sin\frac{\Theta}{2})^{k-1}}+\frac{(1-im\sin\frac{\Theta}{2})^k}{(1+im\sin\frac{\Theta}{2})^{k-1}}\right]}{\sum_{k\in I'}\alpha_k\left[\frac{(1+im\sin\frac{\Theta}{2})^k}{(1-im\sin\frac{\Theta}{2})^{k-1}}+\frac{(1-im\sin\frac{\Theta}{2})^k}{(1+im\sin\frac{\Theta}{2})^{k-1}}\right]^2}.$$

3.3 RCP

Instead of finding initial function by solving exactly $(1a-d)$ and minimizing (3), consider all A_0, A_1, ..., A_K as unknowns which have to be found by minimizing a new functional:

$$F(A_0, A_1, \ldots, A_K) = \sum_{k=1}^{K} \gamma_k R_k^2 + \overline{\gamma}\Big(\frac{A_1 - A_0}{\delta t}\Big)^2 + \sum_{k=1}^{K} \beta_k (A_k - \overline{A_k})^2,$$

where β_k's, $\overline{\gamma}$ and γ_k's are weight functions. γ_k and $\overline{\gamma}$ are of the order of the discretization error in the corresponding equations. For $k \notin I'$, $\beta_k = 0$. For $k \in I'$, β_k is proportional to an inverse of the estimated (upper bound) value of $(A_k - \overline{A_k})^2$, which results from the measurements errors. R_k is the residual of the *k-th* equation. Shortly speaking we want to reduce the residuals of (1) as much as possible while the solution fits the data best.

In order to minimize this functional the linear system of $K+1$ equations $\frac{\delta F}{\delta A_k} = 0$, $k = 0, \ldots, K$ with $K+1$ unknowns has to be solved: $\mathcal{L}\mathbf{A} = \mathbf{D}$, where $\mathbf{A} = (A_0, A_1, \ldots, A_K)$, $\mathbf{D}$ is a vector of data with components $\beta_k \overline{A}_k$ if $k \in I'$, 0 otherwise, and $\mathcal{L}$ is a $(K+1) \times (K+1)$ matrix.

Solve this linear system and find all A_0, A_1, ..., A_K at once.

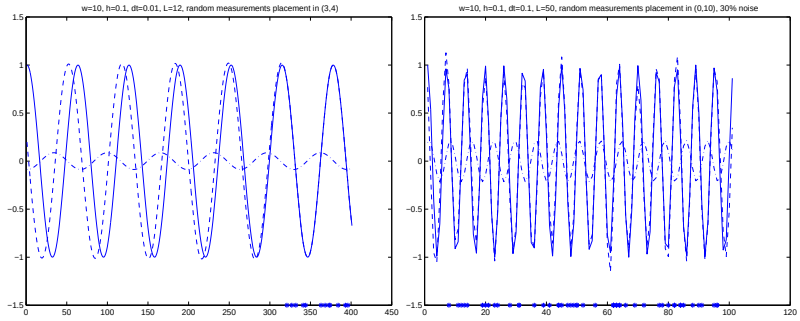
4 Numerical results: RCP vs. ICP

The exact solution of $(1a-d)$ is $u(x,t) = e^{i\omega x}\cos\omega t$. The goal is to recover the solution $\cos\omega t$ from the given data $\overline{A_k}$ for $k \in I'$ by two methods described above, the icp and rcp.

There are three main sources of errors: a). discretization and algebraic errors; b). data noise; c). modelization errors (the model doesn't describe exactly the real nature on which measurements are made). Let us consider the influence of each one on the result. The parameters on which the results depend, are:

a). frequency $\omega = \{0.1, 1, 10\}$;
b). meshsize $h = \{0.1, 0.01\}$;
c). time step $\delta t = \{0.1, 0.01\}$;
d). number of measurements $L = \{4, 12, 50, 200\}$;
e). measurements placement;
f). weight functions α_k, β_k, γ_k and $\overline{\gamma}$;
i). noise level in data;
j). modeling assumption.

First consider the data without the noise, i.e. $\overline{A_k} = \cos k\omega\delta t$. If this is a high frequency component ($\omega = 10$) and data are gathered *only* far from the initial time, then the result A_0 of the icp algorithm tends to 0 as the number of measurements L increases. This happens due to the discretization and algebraic errors (phase errors). The solution of the rcp algorithm behaves



(a) (b)

Fig. 1.

(a) Data without noise. Measurements at random locations in interval (3,4). $\omega = 10$, $h = 0.1$, $\delta t = 0.01$, $L = 12$.
(b) Noised data. Noise is random number r in $(-0.5, 0.5) \times 0.3$. $\omega = 10$, $h = 0.1$, $\delta t = 0.1$, $L = 50$.
solid line: exact solution, dash dot: icp, dashed: rcp, $*$ - measurement placement.

just in the opposite way: the result is increasingly accurate as L increases (see Fig. 1a).

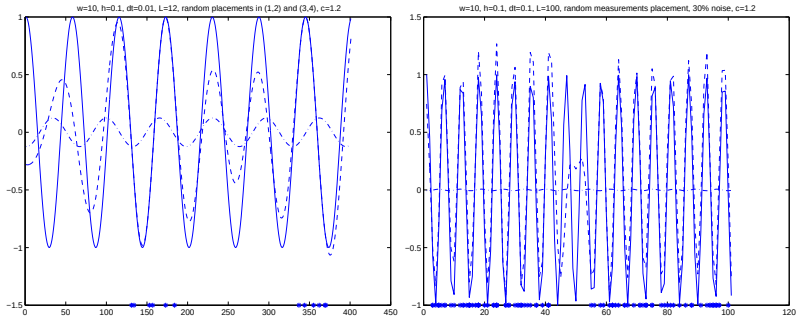
Let us calculate the phase error. Consider the equation $u_{tt} = u_{xx}$. The velocity of the analytic wave propagation in this case is $c = 1$. The discretization scheme is (4) with $q = \frac{1}{4}$. For the discrete wave $\exp^{i\gamma k \delta t} \exp^{i\omega j h}$: $\tan \frac{\gamma \delta t}{2} = \frac{\delta t}{h} \sin \frac{\omega h}{2}$. As a result, the discrete velocity is $\tilde{c} = \frac{\gamma}{\omega} \sim 1 - \frac{\omega^2 h^2}{24} - \frac{\omega^2 \delta t^2}{12}$. The error in the distance traveled by a given phase over time t is $t(c - \tilde{c}) = \frac{t\omega^2}{24}(h^2 + 2\delta t^2)$. Then the *phase error* is $\sim \frac{t\omega^3}{48\pi}(h^2 + 2\delta t^2)$.

Assume that the noise level in measurements is very small, $noise = 0.001$, we took $\beta_k = \frac{1}{0.001^2} = 1000000$. The local discretization error of the interior equation has the upper bound $err_d = \frac{h^2}{12} + \frac{2\delta t^2}{h^2} + \frac{\delta t^2}{12}$. Therefore, $\gamma_k = \frac{1}{err_d^2}$. The local discretization error of the initial condition has the upper bound $\frac{\delta t}{2}$. Therefore, $\overline{\gamma} = \frac{4}{\delta t^2}$.

Now consider another case. The measurements are placed at randomly chosen points and the data are *noised*: $\overline{A_k} = \cos k\omega\delta t + noise$, where $noise$ is 10% or 30% of a random number r between -0.5 and 0.5. Here also there are cases where the solution A_0 of icp tends to 0, while the solution of rcp gives a good approximation (see Fig. 1b).

The expected variance of a square of the random number r between -0.5 and 0.5 is $\int_{-0.5}^{0.5} r^2 dr = \frac{1}{12}$. Therefore, $\beta_k = \frac{1}{0.1^2 * \frac{1}{12}} = 1200$. Other weight functions were chosen as above.

Assume there is an error in modeling and the real equation we want to solve is $u_{tt} = c\triangle u$ with $c = 1.1$ or 1.2, while we use $c = 1$ in our numerical



(a) (b)

Fig. 2.

(a) Modeling error. Data are solutions of $u_{tt} = c\triangle u$ at random locations. $c = 1.2$. $\omega = 10$, $h = 0.1$, $\delta t = 0.01$, $L = 50$.

(b) Three kinds of errors. Data at random locations, random r in $(-0.5, 0.5)$. $\omega = 10$, $h = 0.1$, $\delta t = 0.1$, $L = 100$, $noise = 0.3r$, $c = 1.2$.

solid line: exact solution, dash dot line: icp, dashed: rcp, $*$ - measurement placement.

solver. Then again there are cases where the solution A_0 of icp tends to 0, while the solution of rcp gives a good approximation (see Fig. 2a).

When all three kinds of errors exist, the result of the icp algorithm is practically zero-function, while rcp algorithm is still successful in approximation the real solution at least in the neighborhood of the measurements (see Fig. 2b).

5 Summary

In this paper we presented just one aspect of how multiscale computational methods can contribute to data assimilation problems (and similarly to other inverse problems).

Also multiscale formulations provide ill-posed problems with additional tools, including: one-shot solution of non-linearities; local refinement techniques; space+time parallel processing; unlimited correlation ranges and efficient representation of direct and inverse covariance matrices; multiscale organization of the observational data and in particular coarse-scale representation of oscillatory data; etc. (see Sect. 4.3 of [**?**]).

Multigrid solvers can provide natural regularization to many ill-posed problems, since the main ill-posedness in those problems is the long term and long range influence of fine-scale oscillations, while the multiscale large-scale interactions are mediated by coarse grids that omit those oscillations.

The general data assimilation RCP is an optimization problem which leads to a system of hyperbolic equations with corresponding boundary, initial and

terminal conditions. Usually time-dependent hyperbolic problems are solved by forward marching in time, but the measurements introduce backward time couplings as well. Hence, a simple marching in time could not be applied here.

Traditional multigrid solvers are not effective for this problem either, because some "characteristic" high-frequency components are non-local (their size is determined by conditions many meshsizes away) exactly on all those grids which are fine enough to approximate such components. On the other hand, on coarser grids such components cannot be approximated, because the grid does not resolve their oscillations or resolves them with large phase errors.

Our next goal is to develop a more sophisticated efficient multigrid method for solving this kind of problems which embeds forward and backward time marching in a partly distributive relaxation process.

References

1. Brandt, A. (1981): Multi-grid Solvers for Non-Elliptic and Singular-Perturbation Steady-State Problems, Weizmann Institute of Science.
2. Brandt, A. (1984): Multigrid Techniques: 1984 Guide, with Applications to Fluid Dynamics, 191 pages, ISBN-3-88457-081-1, GMD-Studie Nr. 85, Available from GMD-AIW, Postfach 1316, D-53731, St. Augustin 1, Germany.
3. Brandt, A. (2002): Multiscale Scientific Computation: Review 2001. In: Barth, T.J., Chan, T., Haimes, R. (eds) Lecture notes in comp. science and eng. Springer. **20**, 3–95.
4. Brandt, A. (1994): Rigorous Quantitative Analysis of Multigrid: I. Constant Coefficients Two Level Cycle with L_2 norm. SIAM J. Numer. Anal., **31**, 1695–1730.
5. Brandt, A., Livshits, I. (1997): Way-ray multigrid method for standing wave equations. Electr. Trans. Numer. Anal., **6**, 162–181.
6. Brandt, A., Diskin, B. (1999): Multigrid solvers for the non-aligned sonic flow: constant coefficient case, Report WI/GC-8, 1997, Comp. and Fluids, **28**, 511–549.
7. Calderon, A. (1980): On an inverse boundary value problem, Seminar on Numerical Analysis and its Applications. In: Meyer, W., Raupp, M. (eds) Brazilian Mathematical Society, Rio de Janeiro, 1–7.
8. Czajkowski, M. (1996): Iterative solution of an initial control problem for the wave equation, Universität Düsseldorf, Germany.
9. Gandlin, R. (1999): Solvers for some Inverse Problems. Proposal for Ph.D. Thesis, Weizmann Institute of Science.
10. Gandlin, R. (2000): Multigrid solvers for some Inverse Problems. Intermediate report, Weizmann Institute of Science.
11. Morozov, V.A., (1984): Methods for Solving Incorrectly Posed Problems, Springer-Verlag.
12. Sylvester, J., Uhlmann, G. (1987): A global uniqueness theorem for an inverse boundary value problem, Annals of Math., **125**, 153–169.