МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ, ЧИСЛЕННЫЕ МЕТОДЫ И КОМПЛЕКСЫ ПРОГРАММ/MATHEMATICAL MODELING, NUMERICAL METHODS AND PROGRAM COMPLEXES

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TOWARDS PCA DECOMPOSITION FOR THE WAVE-ATTRACTOR FLOWS

Research article

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Abstract

Wave attractors, being particular hydrodynamical flows forming as a result of internal or inertial waves self-focusing, are rather complicated problem from the viewpoint of both computational fluid dynamics and visualizations due to the wave instability caused by the wave amplitude augmentation. Thereby, the use of dimension reduction methods, like Principle component analysis (PCA), is of special interest and has been widely applied recently to the hydrodynamical data of such flows, especially in the numerical investigations. In this work, we discuss the particularities of PCA implementation to the wave attractor flows, methods for their acceleration, and the convergence for this class of problems.

Keywords: wave attractor, dimension reduction, PCA, numerical simulation.

О PCA-РАЗЛОЖЕНИИ В ЗАДАЧАХ С ВОЛНОВЫМ АТТРАКТОРОМ

Научная статья

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Аннотация

Волновые аттракторы, представляющие собой особые гидродинамические течения, образующиеся в результате самофокусировки внутренних или инерционных волн, являются довольно сложной задачей как с точки зрения вычислительной гидродинамики, так и визуализации из-за волновой неустойчивости, вызванной увеличением амплитуды волн. В связи с этим использование методов понижения размерности, таких как метод главных компонент (PCA), представляет особый интерес и в последнее время широко применяется к гидродинамическим данным таких потоков, особенно в численных исследованиях. В данной работе мы обсуждаем особенности применения PCA к течениям с волновыми аттракторовами, методы их ускорения и сходимость для этого класса задач.

Ключевые слова: волновой аттрактор, понижение размерности, PCA, численное моделирование.

Introduction

Internal waves play an important role in climate formation [1], [2], vertical mixing in the oceans [3], and seabed erosion [4]. Under certain circumstances [5], internal wave may self-focus, forming a coherent structure called a wave attractor [6], [7]. The latter studies showed that wave attractors tend to produce the secondary waves [8], [9], with the instability being developed of the Triadic Resonance type [10], [11], [12], [14]. For the real water reservoirs, more typical is the elongated basin form [15], [16], [17]. The investigation of wave attractor in large aspect-ratio domains [18], [19], [20] (those whose horizontal sizes are larger than vertical ones) revealed that such flows produce more (respectively, small-aspect-ratio ones) intensive instability, whose type is parametric subharmonic.

The attractor has been studied both experimentally [5], [6], [21], [23] and numerically [8], [21], [23], [25]; in recent years, the latter approach prevails [23], [26], [29], [32]. The wave nature of the attractor structure and the instability make the researcher seek advanced methods for wave attractor visualization. The more popular become mode decomposition methods like Principle Component Analysis (PCA) [33], [34]. Mainly, the most significant modes are considered for the attractor subflow, the rest are neglected as parts of instability; only [33] considers minor modes. This force to investigate the convergence of such methods and to evaluate their accuracy.

In this article, we provide a PCA-decomposition research applyingly to several wave-attractor problems. The questions of numerical application, methods, acceleration and emode number are discussed.

Research methods and principles

2.1. Numerical Setup

During this research, wave attractor flows were investigated numerically, in 2D formulation, using high-order spectral-element software *Nek5000*. The numerical approach was validated in [10], [11], [20], [21] comparing with the experiment results, the 2D approach was verified in [11], [21], [24], [32]. The work [32] provides a cross-validation between the current set-up in *Nek5000* and the simulation in *OpenFOAM* (solver *mulesQHDFoam*). However, the latter approach is mostly aimed to the large-scale structure rather than instability reproduction, while the small-scale modes are usually investigated with POD [33]; thus, the high-order *Nek5000* package known to reproduce the instability structure correctly [10] was selected.

To simulate an attractor flow, the following equations were used:

Navier-Stokes equation in Boussinesq approximation:

$$\frac{\partial \vec{v}}{\partial t} + \left(\vec{v}, \nabla\right)\vec{v} = -\frac{1}{\rho_m}\nabla\tilde{p} + \frac{\rho_s}{\rho_m}\vec{g} + \nu\Delta\vec{v}$$

salt transport equation:

$$\frac{\partial \rho_s}{\partial t} + \left(\vec{v}, \nabla\right)\rho_s = \lambda_s \Delta \rho_s$$

The salt transport is obligatory since the startification is required for the internal wave propagation.

The last equation is the continuity one for the incompressible fluid:

$$\operatorname{div}\vec{v} = 0$$

In the incompressible flow in Bousinesq approximation energy conservation equation is not required. Here the following notations were used: $\tilde{p}$ is truncated pressure without its hydrostatical part $\tilde{p} = p - g\rho_m$, ρ_s is dissolved salt density admixture, ρ_m is the fresh water density, λ_s is salt diffusivity coefficient.

During the simulation, we used the constant uniform viscosity value $\nu = 0.01$ cm/s^2 and λ_s so that Schmidt number $Sc = \nu/\lambda_s = 700$.

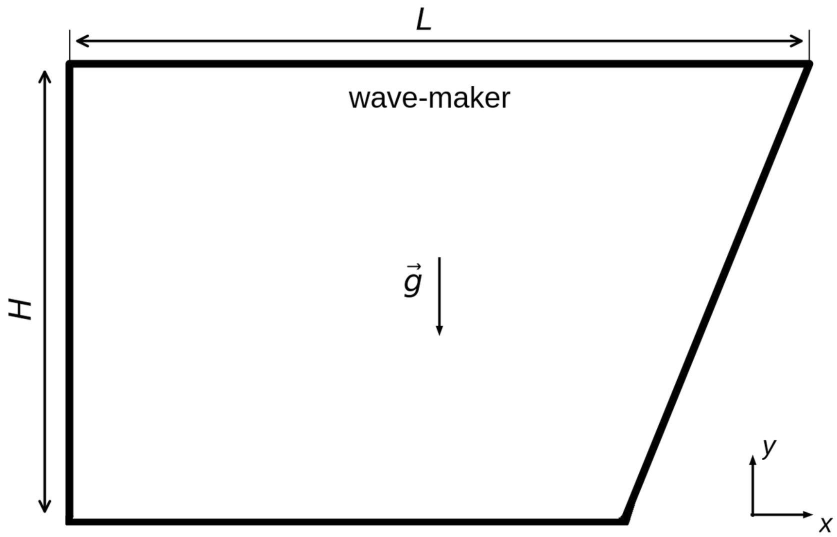

Figure 1 - Geometry sketch

The geometry in which the flow was simulated in was trapezium-shaped (Figure 1), since it is the simplest geometry in which a wave attractor can form [5]. We considered two different domain types: with low and high aspect ratio (by the aspect ratio we mean length-to-height ratio L/H), since it leads to the different instability formation [18]; in both height was $H = 40\ cm$, in small-aspect ratio domain $L = 60\ cm$, in large aspect-ratio one $L = 300\ cm$.

The simulation was run from the steady liquid (i.e., initial velocity condition was zero), initial salt density distribution was linear:

$$\rho_s(t=0) = 0.04\rho_m(1 - y/H)$$

so that buoyancy frequency was constant. The flow was exited by a moving-wall wave maker [21] situated on the top side of the area; the corresponding boundary condition was

$$\vec{v}_{wm} = \vec{e}_y \cdot a\omega_0 \sin(2\pi x/L)\sin(\omega_0 t)$$

The amplitude a was varied to provide different flow regime, the frequency ω_0 was different for different geometry types: $0.628\ s^{-1}$ for the small aspect ratio geometry and $0.149\ s^{-1}$ for the large aspect ratio one, with the forcing amplitude $a = 0.14\ cm$ was used for both geometries. The difference in the frequencies is caused by the conditions of attractor existence [7]. On the other boundaries, except the top one, vero-velocity condition was used.

For ρ_s on all the boundaries impermeability Neumann condition was set.

The high-order spectral element meshes used for the simulation are represented in Figures 2–3. The elements shapes can be arbitrary convex quadrilaterals; the orthogonality in this method is not required.

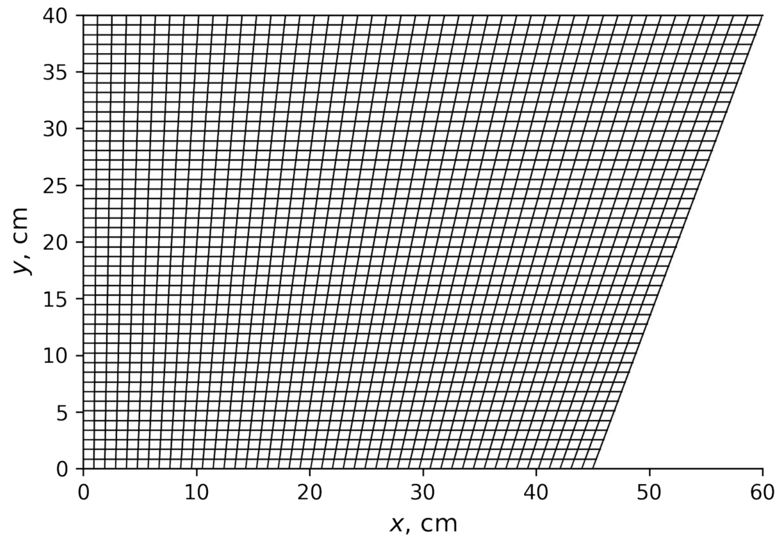

Figure 2 - Low-aspect ratio domain mesh 48x48 spectral element

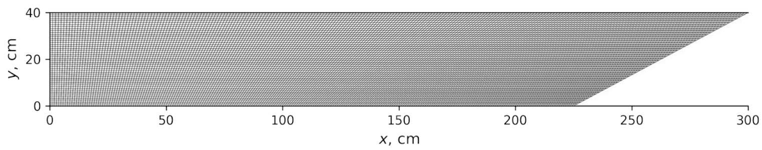

Figure 3 - Large-aspect ratio domain mesh 208x48 spectral elements

2.2. PCA

Principal component analysis represents the spatio-temporal variable $u(t, x, y)$ as follows [33], [34], [35]:

$$u(t, x, y) = \Sigma_i T_i(t) \Phi_i(x, y)$$

where spatial modes $\Phi_i(x, y)$ are normalized and mutually orthogonal in L^2 integral sense. Their corresponding temporal dependencies $T_i(t)$ are called temporal coefficients.

To calculate modes, the eigenvectors of the covariation matrix $u^T u$ are considered. It can be shown that the same vectors can be obtained as right singular vectors of the original matrix u (which is called Singular Values Decomposition (SVD)), and the coefficients can be obtained as the projection:

$$T_i(t) = \iint u(t, x, y)\, \Phi_i(x, y)\, dx\, dy$$

Such a procedure saves computational costs (time and memory).

Nevertheless, the direct SVD calculation can also be time-costly, since it calculates all the singular values and vectors (their number corresponds to the number of spatial points of the grid). For the amplification, several numerical methods are used; the most popular are ARPACK and randomized SVD. The first one creates the solution iteratively from the random initial approximation, constructing the Krylov subspace, calculating the required number of the first singular vectors; the latter one projects the original data into a random subspace with the following corrections. All the methods are available in *python3* (*scikit-learn* package).

Despite both of these methods being well-tested and reported to yield results close to the full SVD, the wave attractor flows can have a developed secondary-wave subflow that should be correctly reconstructed, and the convergence of the PCA on these problems was not investigated.

Main results

Due to the internal wave focusing, the liquid motion is localized in a specific figure, and the oscillation amplitude increases. Figure 4 represents a typical non-linear regime in the small-aspect ratio domain: the parallelogram-shaped [5] coherent structure is distorted by the secondary waves. In large-aspect ratio domain problems, this effect manifests more clearly [18], [19], [20].

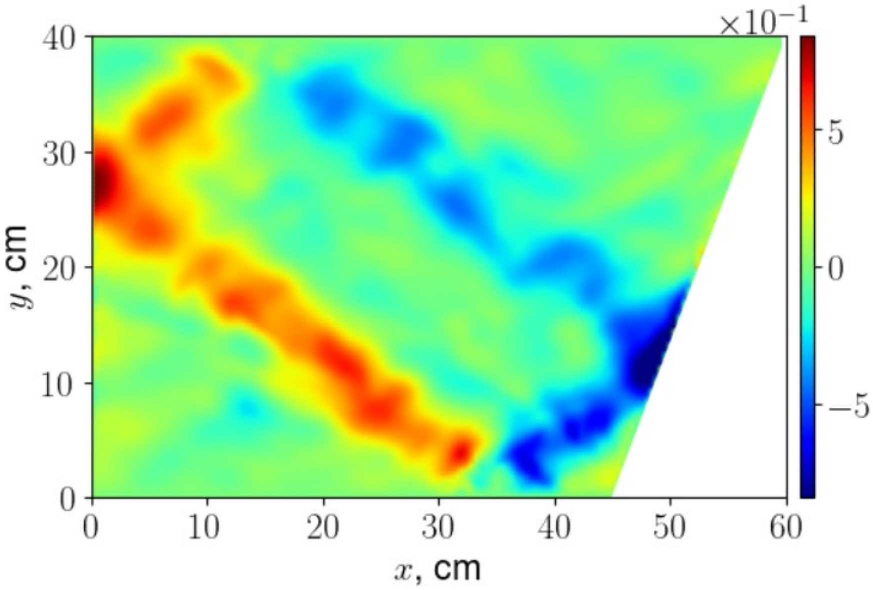

Figure 4 - Wave attractor in small-aspect ratiodo main, v_y snapshot

Note: colorbar in cm/s

The main feature of the wave attractor flow is the tendency to turn into the unstable non-linear regime even at the respectively small external forcing amplitudes a. In Figure 5–6, wave attractor in a large-aspect ratio domain; the coherent structure, formed soon after the beginning, becomes fully covered by the instability waves, and the initially monochromatic flow becomes complex (Figure 7). The black dot on Figures 5–6 is the middle of the attractor ray typically considered [5], [8], [18], [25] for the velocity evolution behaviour. In Figure 7, non-dimensional time is used on the horizontal axis ($T_0 = 2\pi/\omega_0$ — wavemaker period). Note that the wave maker amplitude, regulating the energy input in the system, was the same for both geometries.

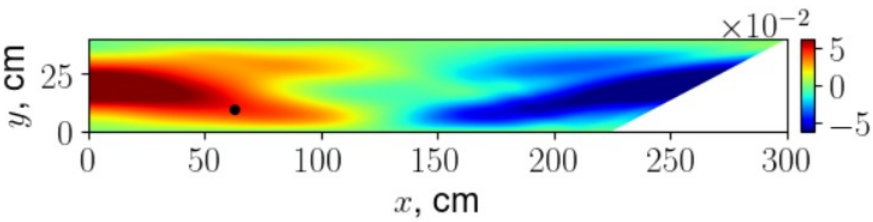

Figure 5 - Large-aspect ratio domain problem, initial attractor development befor the instability formation

Note: colorbar in cm/s; black dot is the characteristical point

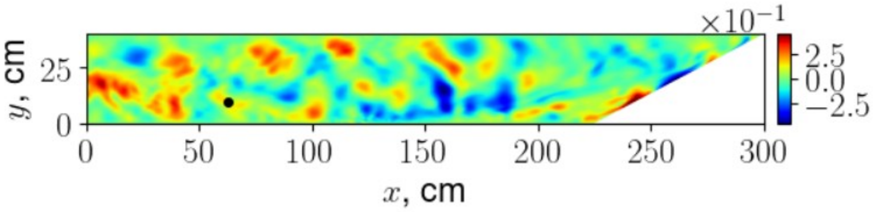

Figure 6 - Large-aspect ratio problem, v_y snapshot developed non-linear regime

Note: colorbar in cm/s, black dot is the characteristical point

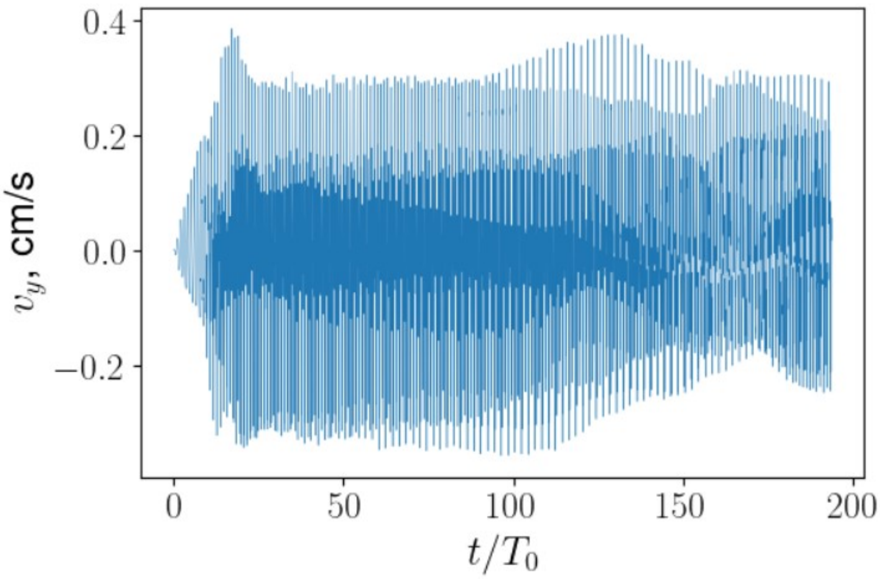

Figure 7 - Temporal behaviour of v_y in the point selected

The initial monochromacy of the wave attractor became the main idea for several of the visualization methods [33], [34] using mode decomposition. Despite the elder modes being extracted correctly and representing the attractor, nothing is said about the minor modes behavior. However, they can be used for studies of the instability of spatial structure [32], [33], and for this purpose, it is reasonable to use the methods that calculate them properly. The physical sense of the modes is the following: the first two modes correspond to the large-scale wave structure of the attractor itself [32], [34], and the rest represent the instability structure.

To check the quality of PCA decomposition, full L^2 norm residuals were calculated depending on the reconstruction modes number:

$$err = \int dt \int dx\, dy\, \left(u(t,x,y) - u^*_N(t,x,t)\right)^2,$$

where the solution reconstruction u^*_N for N modes is:

$$u^*_N(t,x,t) = \Sigma_{i=1}^{N} T_i(t)\Phi_i(x,y)$$

where N is a selected number of modes to reconstruct. The results of residual calculation by different methods are represented in Figure 8. All the methods yield approximately the same results.

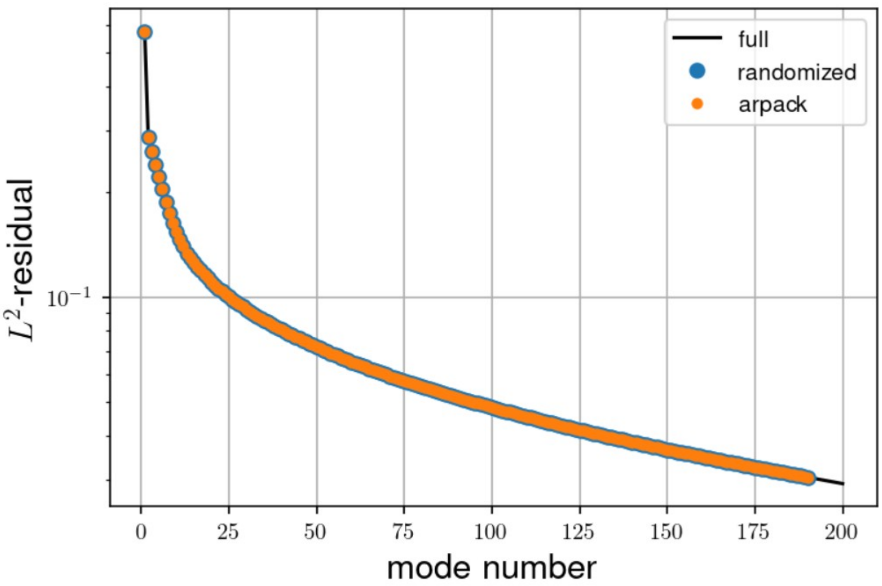

Figure 8 - Residuals in small-aspect ratio problem decomposition

Since that, all the methods can be used for the detailed reconstruction of the solution. The advantages of the non-full methods are their time-loss gain. In Figure 9, the computational times for the methods considered depending on the mode numbers are represented. The randomized SVD is only a little faster than the APRACK method, and both are 30–100 times faster than full SVD. The computational time only slightly depends on the mode number; full SVD is mode number-independent since all the modes are calculated and then the minor ones are neglected.

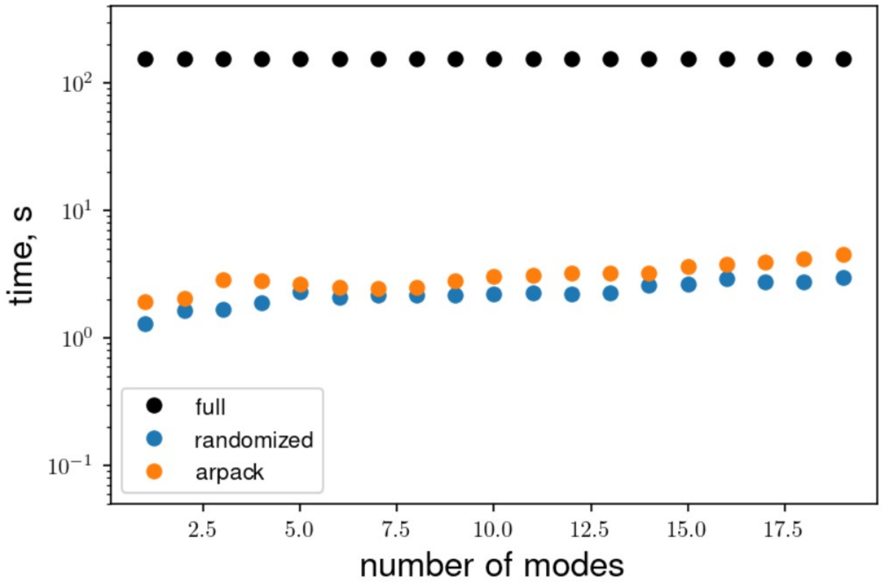

Figure 9 - Execution times for different SVD calculation methods

The large-aspect ratio flow has a more developed instability (Figure 6), which results in slower residual attenuation compared to small-aspect ratio flows, as shown in Figure 10. This means that far more mode numbers should be considered to reach the same reconstructuon error level.

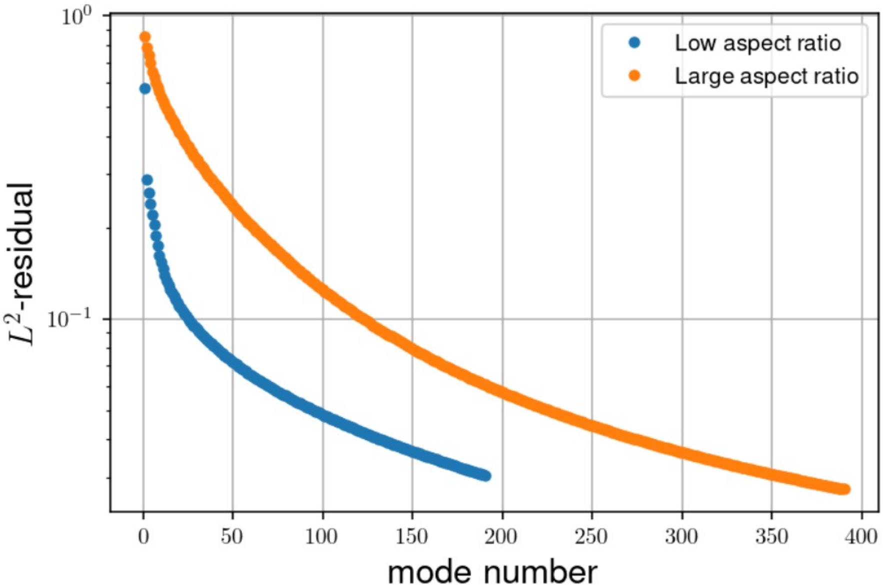

Figure 10 - Comparison of reconstruction residuals for different aspect ratio

Despite this, all the methods yield the same result, the same as for the small-aspect ratio problem (Figure 11), which allows to extrapolate the ability of the indirect SVD computation method using a wide class of wave attractor problems.

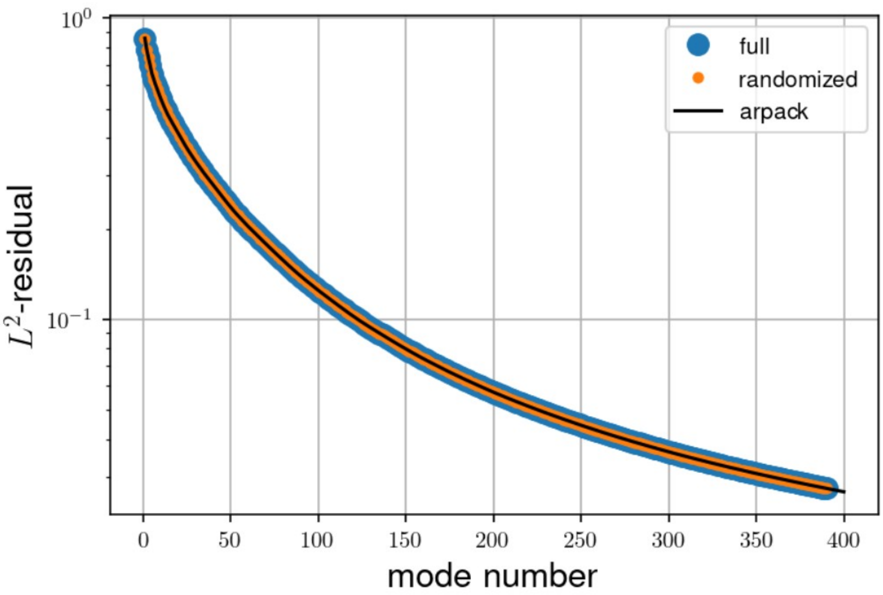

Figure 11 - Large-aspect problem residuals

Despite the advantages of the acceleration, the PCA method does not turn out to be very fine itself. As can be comprehended from Figure 10, for a 3% residual, it requires 200 modes for the small-aspect ratio case and 400 modes for the large-aspect ratio one. The convergence is stable but slow, which limits the investigation of the instability by PCA modes with moderate-instability cases only.

Conclusion

The PCA decomposition was considered for the wave attractor problems. Both full SVD and reduced methods yield the same accuracy of by-mode reconstruction, which allows to use the latter one without significant losses. It was found that their use can accelerate the computation up to 100 times, with the fastest being the *randomized SVD* approach.

The large-aspect ratio problems demonstrate less residual decrease with the used mode number and thus require more modes for the same accuracy in comparison with the small-aspect ratio problems. This makes the indirect SVD methods application even more preferable.

Withal, PCA method converges slowly and requires about several hundred modes for a precise enough reconstruction, which limits the investigation of secondary waves, forming the instability, with this method.

Конфликт интересов

Не указан.

Рецензия

Все статьи проходят рецензирование. Но рецензент или автор статьи предпочли не публиковать рецензию к этой статье в открытом доступе. Рецензия может быть предоставлена компетентным органам по запросу.

Conflict of Interest

None declared.

Review

All articles are peer-reviewed. But the reviewer or the author of the article chose not to publish a review of this article in the public domain. The review can be provided to the competent authorities upon request.

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