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COMBINING A LEAST-SQUARES APPROXIMATE JACOBIAN WITH AN ANALYTICAL MODEL TO COUPLE A FLOW SOLVER WITH FREE SURFACE POSITION UPDATES

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Abstract. This paper presents a new quasi-Newton method suitable for systems that can be solved with a black-box solver for which a cheap surrogate model is available. In order to have fast convergence, the approximate Jacobian consists of two different contribution: a full rank surrogate model of the system is combined with a low rank least-squares model based on known input-output pairs of the system. It is then shown how this method can be used to solve 2D steady free surface flows with a black-box flow solver. The inviscid flow over a ramp is calculated for supercritical and subcritical conditions. For both simulations the quasi-Newton iterations converge exponentially and the results match the analytical predictions accurately.

1 INTRODUCTION

Quasi-Newton methods can be used to solve coupled problems in a partitioned way, using existing solvers for each system. A common application is fluid-structure interaction. In this paper, a new approach is presented to construct the approximate Jacobian of a (non-linear) system that can be solved with a black-box for which also a cheap surrogate model is available. To reduce the number of quasi-Newton iterations, two approximations are added: a full rank surrogate model of the system is combined with a low rank model which is constructed with known input-output pairs of the system using a least-squares technique.

The method was developed in [1] for numerically calculating 2D steady free surface flow of water and air as encountered in marine engineering. The free surface is represented with a fitting approach, i.e. the computational grid is aligned with it. As the air phase can be neglected for the envisioned flows, the free surface becomes a domain boundary whose position depends on kinematic and dynamic boundary conditions. Both the flow field and the free surface position are unknown, so that this free-boundary problem must be solved iteratively. This is done by reformulating the problem as a root-finding problem and solving it with the new quasi-Newton approach.

In Section 2 the new method to construct the approximate Jacobian is explained for a general system. The method is applied to the steady free surface problem in Section 3: first some details are given about the surrogate model for the flow solver, then the free-boundary problem is given in more detail and a solution method derived based on quasi-Newton iterations. In Section 4 the performance of the method is demonstrated by calculating the inviscid free surface flow over a ramp at different Froude numbers.

2 QUASI-NEWTON METHOD WITH LEAST-SQUARES AND SURROGATE

A general black-box system $\boldsymbol{\mathcal{S}}(\boldsymbol{x}) = \boldsymbol{y}$ is considered, with $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^{n\times 1}$ respectively the input and output of $\boldsymbol{\mathcal{S}}$. The input vector $\boldsymbol{x}$ for which $\boldsymbol{\mathcal{S}}(\boldsymbol{x}) = 0$ (i.e. the root of $\boldsymbol{\mathcal{S}}$) can be found using quasi-Newton iterations. With superscript m the iteration index, $\Delta\boldsymbol{x}^m = \boldsymbol{x}^{m+1} - \boldsymbol{x}^m$ the change in input, and $\boldsymbol{J} \in \mathbb{R}^{n\times n}$ an approximate Jacobian of $\boldsymbol{\mathcal{S}}$, a new value $\boldsymbol{x}^{m+1}$ can be calculated using the well-known formula

$$\boldsymbol{J}\Delta\boldsymbol{x}^m = -\boldsymbol{y}^m = -\boldsymbol{\mathcal{S}}(\boldsymbol{x}^m). \tag{1}$$

The iterations start with a guess $\boldsymbol{x}^0$ and continue until $\|\boldsymbol{y}^m\|$ drops below a small constant ε. It is assumed that $\boldsymbol{\mathcal{S}}$ is expensive to evaluate, so the number of quasi-Newton iterations must be as low as possible. For this purpose a Jacobian is constructed that consists of two parts which both have advantages and limitations. By combining them, a more robust and effective Jacobian is obtained.

The first approximation is a full rank surrogate model $\boldsymbol{J}_{\text{sur}}$. It can be based on e.g. analytical considerations or a low fidelity model of the system, depending on the problem at hand. It must be of full rank to ensure that Eq. 1 has a unique solution $\Delta\boldsymbol{x}^m$. The better $\boldsymbol{J}_{\text{sur}}$ approximates the behavior of $\boldsymbol{\mathcal{S}}$, the faster the quasi-Newton iterations will converge. However, if the prediction of $\boldsymbol{J}_{\text{sur}}$ is inaccurate for certain modes, these modes will slow down or even destabilize the iterations.

The second approximation $\boldsymbol{J}_{\text{IQN}}$ is constructed using the IQN-ILS algorithm by Degroote et al. [2], which was developed originally for doing partitioned fluid-structure interaction with black-box solvers. $\boldsymbol{J}_{\text{IQN}}$ is a low rank approximation which is built from known input-output pairs of the system. Inputs and outputs of previous iterations are collected in the matrices

$$\boldsymbol{V}^m = \begin{bmatrix}\Delta\boldsymbol{x}^{m-1} & \cdots & \Delta\boldsymbol{x}^0\end{bmatrix}, \tag{2}$$

$$\boldsymbol{W}^m = \begin{bmatrix}\Delta\boldsymbol{y}^{m-1} & \cdots & \Delta\boldsymbol{y}^0\end{bmatrix}. \tag{3}$$

The Jacobian is then constructed with a least-squares technique:

$$\boldsymbol{J}_{\text{IQN}}^{m} = \boldsymbol{W}^{m}\boldsymbol{R}^{m^{-1}}\boldsymbol{Q}^{m^{T}} \tag{4}$$

with

$$\boldsymbol{V}^{m} = \boldsymbol{Q}^{m}\boldsymbol{R}^{m} \tag{5}$$

the economy-size QR-decomposition. With each iteration $\boldsymbol{J}_{\text{IQN}}^{m}$ grows in rank and improves. The modes which are picked up by $\boldsymbol{J}_{\text{IQN}}$ are those that hinder convergence of the quasi-Newton iterations, which are precisely those modes for which $\boldsymbol{J}_{\text{sur}}$ is inaccurate.

$\boldsymbol{J}_{\text{IQN}}^{m}$ only affects the part of $\boldsymbol{x}$ which is in range$(\boldsymbol{V}^{m})$ = range$(\boldsymbol{Q}^{m})$. As these modes can be extracted using $\boldsymbol{Q}^{m}\boldsymbol{Q}^{m^{T}}$, the combined Jacobian can be written as

$$\boldsymbol{J}^{m} = \boldsymbol{J}_{\text{IQN}}^{m} + \boldsymbol{J}_{\text{sur}}\left(\boldsymbol{I}_{n} - \boldsymbol{Q}^{m}\boldsymbol{Q}^{m^{T}}\right) \tag{6}$$

with $\boldsymbol{I}_{n}$ the identity matrix. In a nutshell: most of the work is done by the full rank surrogate model $\boldsymbol{J}_{\text{sur}}$, but the low rank least-squares based $\boldsymbol{J}_{\text{IQN}}$ is crucial to stabilize and accelerate convergence of the iterations when $\boldsymbol{J}_{\text{sur}}$ is inaccurate for some modes. The method is accordingly called *Quasi-Newton method with Least-Squares and Surrogate* and an overview of it is given in Algorithm 1.

Algorithm 1 Quasi-Newton method with Least-Squares and Surrogate.

$m = 0$
$\boldsymbol{y}^{0} = \boldsymbol{\mathcal{S}}\left(\boldsymbol{x}^{0}\right)$
while $\|\boldsymbol{y}^{m}\| > \varepsilon$ **do**
    if $m > 0$ **then**
        update $\boldsymbol{V}^{m}$, $\boldsymbol{W}^{m}$ ▷ Eqs. (2) and (3)
        QR-decomposition $\boldsymbol{V}^{m} = \boldsymbol{Q}^{m}\boldsymbol{R}^{m}$
    end if
    construct $\boldsymbol{J}^{m}$ ▷ Eq. (6)
    solve $\boldsymbol{J}^{m}\Delta\boldsymbol{x}^{m} = -\boldsymbol{y}^{m}$
    $\boldsymbol{x}^{m+1} = \boldsymbol{x}^{m} + \Delta\boldsymbol{x}^{m}$
    $m = m + 1$
    $\boldsymbol{y}^{m} = \boldsymbol{\mathcal{S}}\left(\boldsymbol{x}^{m}\right)$
end while

Note that if a surrogate model is available for the system's inverse $\boldsymbol{\mathcal{S}}^{-1}$, the quasi-Newton iteration of Eq. (1) can be rewritten as $\Delta\boldsymbol{x}^{m} = -\boldsymbol{J}^{-1^{m}}\boldsymbol{y}^{m}$, avoiding the need to solve a linear system. In addition the least-squares Jacobian $\boldsymbol{J}_{\text{IQN}}^{-1^{m}}$ does not have to be constructed explicitly, avoiding matrix-matrix products.

3 APPLICATION TO STEADY FREE SURFACE FLOW

Before the free-boundary problem is solved with the new quasi-Newton technique, a free surface perturbation analysis is discussed in Section 3.1. Not only does this analysis provide the basis for constructing the flow solver's surrogate model, it also shows that additional conditions are needed to obtain a unique free surface solution for subcritical flows. In Section 3.2 the 2D steady free surface problem is discussed in more detail, then it is expressed as a free-boundary problem and finally a solution algorithm based on quasi-Newton iterations is outlined.

3.1 Surrogate model from perturbation analysis

In [3] the 2D inviscid free surface flow over a flat bottom is investigated in detail. This flow is characterized by its Froude number $\mathrm{Fr} = U/\sqrt{gh}$ which is based on the average flow velocity U and flow depth h. The steady flow solution of this case is a horizontal free surface and a uniform velocity U. It is shown in [3] that when the free surface height $\eta(x)$ is perturbed with a sine wave, the free surface pressure $p(x)$ changes proportionally. This analysis leads to a relation between free surface height perturbations $H(k)$ and pressure perturbations $P(k)$ in the wavenumber domain:

$$P(k) = L(k)H(k) \tag{7}$$

with

$$L(k) = \rho g \left(\mathrm{Fr}^2 \frac{kh}{\tanh kh} - 1 \right). \tag{8}$$

Here ρ is the density, g the gravitational acceleration and $k = 2\pi/\lambda$ the wavenumber. This relation between perturbations can be used to approximate the Jacobian of a general 2D free surface flow. An expression for $\boldsymbol{J}_{\mathrm{sur}}$ for uniform free surface grids is derived in [1] using the discrete Fourier transform. For stretched free surface grids $\boldsymbol{J}_{\mathrm{sur}}$ can be calculated using the convolution theorem as explained in [4].

The behavior of free surface flow changes at $\mathrm{Fr} = 1$. For supercritical flow ($\mathrm{Fr} > 1$), the wave speed of surface gravity waves is smaller than the flow speed U for all wavenumbers so that disturbances can only travel downstream. For subcritical flow ($\mathrm{Fr} < 1$) this is not the case: waves below a certain wavenumber travel faster than the flow, so disturbances can travel upstream. This change in behavior corresponds to a zero in $L(k)$, Eq. (8): the wave with this wavenumber travels at the same speed as the flow and thus appears stationary. This so-called *steady gravity wave* is a solution of the flow and therefore gives no change in pressure ($L = 0$). This is problematic: it means that for subcritical flow, this wave can be present with arbitrary phase and amplitude without influencing the free surface pressure. As a consequence, two additional conditions will need to be added to find a unique solution for the free-boundary problem.

3.2 Solving the free-boundary problem with quasi-Newton

The 2D immiscible steady flow of water and air as encountered in marine engineering is considered as application. The free surface is represented with a fitting approach, which means that the computational grid is aligned with it. Due to the large density difference with water, the air phase can be neglected for these flows. The free surface then becomes a domain boundary whose position depends on kinematic and dynamic boundary conditions. For steady flow, the kinematic boundary condition (KBC) requires that the flow is tangential to the free surface. The dynamic boundary condition (DBC) requires continuity of the stresses at the free surface. This condition can be split into tangential and normal components which can be simplified. To fulfill the tangential DBC the shear stresses at the free surface must be zero. For the normal DBC the pressure must be constant along the free surface.

The flow field and free surface position cannot be determined simultaneously by a standard CFD solver, so the free-boundary problem needs to be solved iteratively: in one step the flow field is solved with a given free surface position, in the other step a new free surface position is calculated. The distribution of the free surface boundary conditions over these two steps varies between different methods found in literature [5, 6, 7].

In this paper the conditions are distributed in such a way that the free-boundary problem becomes a root-finding problem. The black-box system of this problem is the flow solver $\boldsymbol{\mathcal{F}}$ which uses a free-slip wall at the free surface boundary—this way the KBC and tangential DBC are satisfied in the flow solver step. The input and output of $\boldsymbol{\mathcal{F}}$ are respectively the free surface height $\boldsymbol{\eta} \in \mathbb{R}^{n\times 1}$ and the free surface pressure $\boldsymbol{p} \in \mathbb{R}^{n\times 1}$, so that $\boldsymbol{p} = \boldsymbol{\mathcal{F}}(\boldsymbol{\eta})$. The normal DBC requires that $\boldsymbol{p} = p_{\text{cst}}\mathbf{1}$ with $\mathbf{1}$ the all-ones vector. This cannot yet be formulated as a root-finding problem as p_{cst} is unknown. It follows from the perturbation analysis in Section 3.1 that changing the value of p_{cst} corresponds to a change of the average free surface height. Instead of specifying p_{cst} it is more convenient to impose e.g. the free surface inlet height $\boldsymbol{\eta}(0) = h$ to fix the average free surface height. p_{cst} is removed from the normal DBC by subtracting the average value (or constant mode) from the pressure. The flow solver $\boldsymbol{\mathcal{F}}$ and pressure $\boldsymbol{p}$ after removing the average value are denoted as $\boldsymbol{\mathcal{F}}_{\emptyset}$ and $\boldsymbol{p}_{\emptyset}$, so that the normal DBC becomes

$$\boldsymbol{\mathcal{F}}_{\emptyset}(\boldsymbol{\eta}) = \boldsymbol{p}_{\emptyset} = 0. \tag{9}$$

This is a root-finding problem for a black-box system $\boldsymbol{\mathcal{F}}_{\emptyset}$ with input $\boldsymbol{\eta}$ and output $\boldsymbol{p}_{\emptyset}$, which can be solved with quasi-Newton iterations. The inlet height condition must be added to the system for a unique solution. With $\boldsymbol{J}^m$ the approximate Jacobian of $\boldsymbol{\mathcal{F}}_{\emptyset}$, the iterative scheme becomes:

$$\begin{cases} \boldsymbol{J}^m \, \Delta\boldsymbol{\eta}^m = -\boldsymbol{p}_{\emptyset}^m \\ \Delta\boldsymbol{\eta}^m(0) = h - \boldsymbol{\eta}^m(0) \end{cases} \tag{10}$$

This system has $n+1$ equations for n unknowns and must therefore be solved with least-squares. The system is still well-determined though, because the rank of $\boldsymbol{J}$ is $n-1$ due to subtraction of the average value from $\boldsymbol{p}$.

In Section 3.1 it is explained that for subcritical flow two additional conditions need to be added to ensure that the free surface solution is unique. A physically relevant option is to require that the free surface is flat upstream. This is enforced by the conditions

$$\boldsymbol{\eta}(i) = h \qquad \text{with} \qquad i = i_1, i_2 \tag{11}$$

where $\boldsymbol{x}(i_1)$ and $\boldsymbol{x}(i_2)$ are points close to the domain inlet $\boldsymbol{x}(0)$. Adding these conditions, the system that has to be solved in the quasi-Newton iterations becomes:

$$\begin{cases} \boldsymbol{J}^m \, \Delta\boldsymbol{\eta}^m = -\boldsymbol{p}_\emptyset^m \\ \Delta\boldsymbol{\eta}^m(i) = h - \boldsymbol{\eta}^m(i) \qquad \text{with} \qquad i = 0, i_1, i_2 \end{cases} \tag{12}$$

The *Free Surface Quasi-Newton method with Least-Squares and Surrogate* (FreQ-LeSS) is summarized in Algorithm 2.

Algorithm 2 Free Surface Quasi-Newton method with Least-Squares and Surrogate.

$m = 0$
$\boldsymbol{p}_\emptyset^0 = \boldsymbol{\mathcal{F}}_\emptyset\left(\boldsymbol{\eta}^0\right)$
while $\left\|\boldsymbol{p}_\emptyset^m\right\| > \varepsilon$ **do**
    if $m > 0$ **then**
        update $\boldsymbol{V}^m$, $\boldsymbol{W}^m$ ▷ Eqs. (2) and (3)
        QR-decomposition $\boldsymbol{V}^m = \boldsymbol{Q}^m\boldsymbol{R}^m$
    end if
    construct $\boldsymbol{J}^m$ ▷ Eq. (6)
    solve system for $\Delta\boldsymbol{\eta}^m$ ▷ Fr > 1: Eq. (10) | Fr < 1: Eq. (12)
    $\boldsymbol{\eta}^{m+1} = \boldsymbol{\eta}^m + \Delta\boldsymbol{\eta}^m$
    $m = m + 1$
    $\boldsymbol{p}_\emptyset^m = \boldsymbol{\mathcal{F}}_\emptyset\left(\boldsymbol{\eta}^m\right)$
end while

4 INVISCID FREE SURFACE FLOW OVER A RAMP

The free surface method is demonstrated by calculating the inviscid free surface flow over a ramp as shown in Fig. 1, using the same geometry and flow parameters as Muzaferija and Perić [5]. The total mechanical energy E (in J/kg) is conserved between inlet and outlet of the domain. Assuming a uniform flow velocity in each section, it can be shown that

$$E_i = \frac{U_i^2}{2} + gh_i + gy_{\mathrm{b},i} = \mathrm{cst} \tag{13}$$

with U_i the flow velocity, h_i the depth of the flow and $y_{\mathrm{b},i}$ the vertical position of the bottom. Combining Eq. (13) with the continuity equation gives analytical expressions

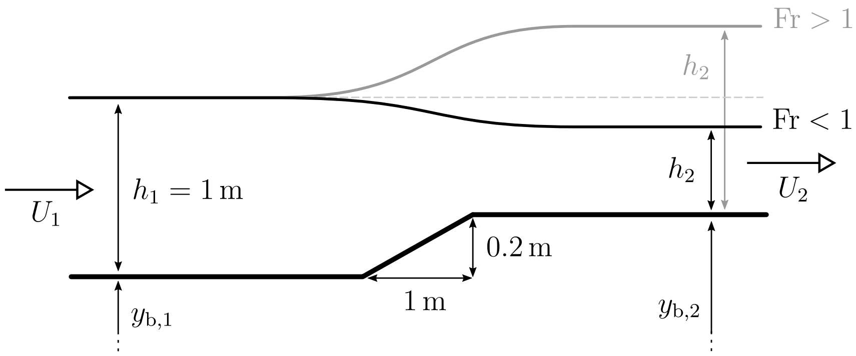

Figure 1: Definition of free surface flow over a ramp [5].

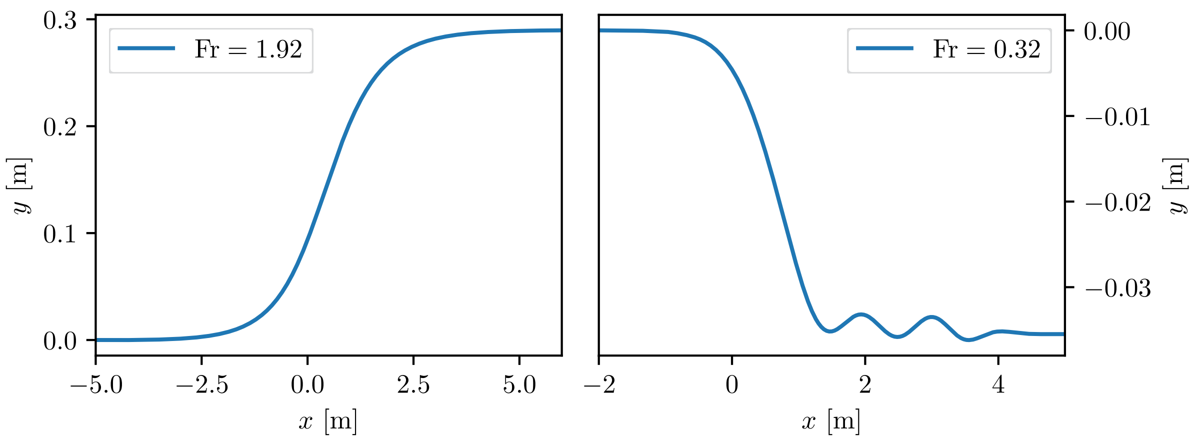

Figure 2: Free surface for supercritical and subcritical flow calculations. The values are plotted with respect to the inlet height. The ramp is located between $x = 0\,\mathrm{m}$ and $x = 1\,\mathrm{m}$.

for the outlet water depth h_2 and outlet velocity U_2 for known inlet conditions and ramp geometry.

Two cases are simulated: a supercritical and a subcritical flow. For both cases the ramp is $0.2\,\mathrm{m}$ high, $h_1 = 1\,\mathrm{m}$, density $\rho = 1\,\mathrm{kg/m^3}$ and gravity $g = 9.81\,\mathrm{m/s^2}$. The supercritical flow has $U_1 = 1\,\mathrm{m/s}$ (Fr = 1.92), the subcritical flow $U_1 = 6\,\mathrm{m/s}$ (Fr = 0.32). In the flow solver the bottom and free surface are modeled as free-slip walls. At the outlet a hydrostatic pressure is imposed, at the inlet a uniform velocity U_1. For both simulations, the initial free surface is horizontal and corresponds to the inlet height. Structured quadrilateral grids are used, with 100 cells in the y-direction and 50 cells per meter in the x-direction. As the free surface grid is uniform, $\boldsymbol{J}_{\mathrm{sur}}$ is constructed based on Eq. (8) and the discrete Fourier transform, as described in [1].

The free surface for both cases is shown in Fig 2. The supercritical free surface is a smooth curve, while the subcritical free surface has the characteristic wave train downstream of the obstacle. To avoid wave reflections at the outlet, a wave damping zone is

Table 1: Analytical result for outlet depth h_2 and error in numerical result.

Fr	h_2 (analytical)	h_2 (numerical)
1.92	1.089730 m	−0.008 %
0.32	0.763544 m	+0.127 %

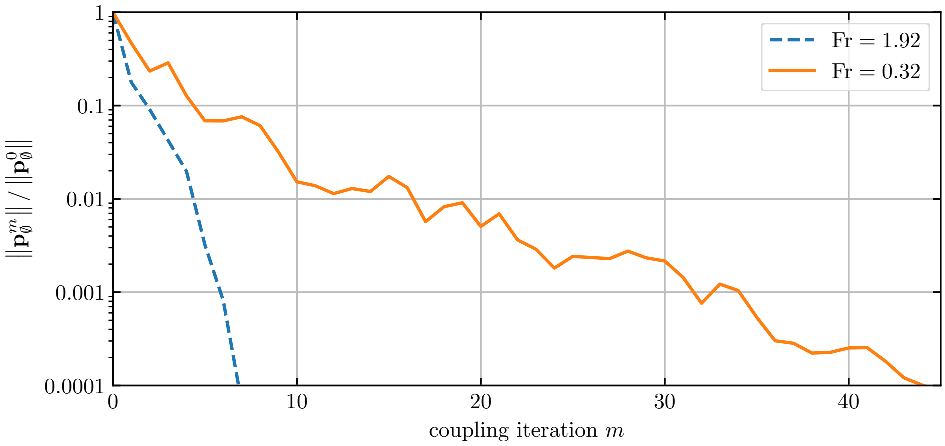

Figure 3: Normalized pressure residuals of the quasi-Newton iterations.

implemented near the outlet using momentum source terms [8]. In Table 1 the outlet depth of the flow h_2 is given: the analytical result based on Eq. (13) is compared to the result of the simulations, giving excellent results. The subcritical result is a bit less accurate, most likely because of the wave train and the damping zone.

Fig. 3 shows the residuals for both cases: they converge exponentially and in a low number of iterations. The subcritical case takes longer: this is due to the presence of the steady gravity wave, which makes the steady free surface problem –and the root-finding problem– much harder to solve.

5 CONCLUSIONS

This paper presents a new quasi-Newton method suitable for systems that can be solved with a black-box solver for which a cheap surrogate model is available. In order to have fast convergence, the approximate Jacobian consists of two different contribution: a full rank surrogate model of the system is combined with a low rank least-squares model based on known input-output pairs of the system. It is then shown how this method can be used to solve 2D steady free surface flows with a black-box flow solver. The inviscid flow over a ramp is calculated for supercritical and subcritical conditions. For both simulations the quasi-Newton iterations converge exponentially and the results match the analytical predictions accurately.

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