Numerical integration Helfrich shape equation

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Contents

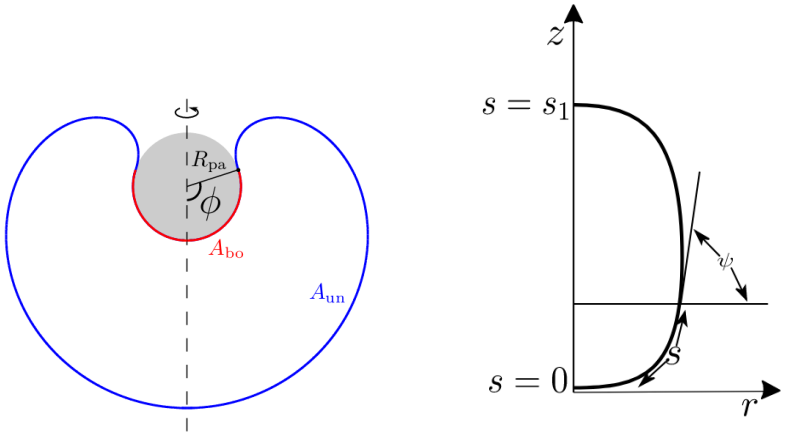
1 Introduction

In this document I will explain how to use numerical methods to solve Helfrich shape equation. The method is general but I will show how to apply it to a specific system a nano particle interacting with a membrane.
This system has been inspired by the work of [1], the code is adapted from [6] and from supplementary materials of [2].

2 Wrapping particle system

We are studying the interaction between a spherical membrane and a spherical particle. They interact with each other through an adhesive interaction. The spherical particle does not have any other properties. The membrane instead is modeled as an elastic surface following the Helfrich theory of elasticity. It has a bending modulus k and a surface tension Σ.

The system equilibrium state is the result of the interplay between two competing phenomena: the first one is the particle wrapping that decreases the free energy and the second one is the increase of energy due to the bending of the membrane surface.



(a) image taken from supplementary material of [1]

The total free energy of the system will be composed by two contribution

representing the bound and unbound segment:

$$E = E_{bo} + E_{un}$$

The bound segment of the membrane will follow the particle contour but the unbound segment does not have a trivial shape.
E_{bo} has an adhesive and a bending energy contribution: [1]

$$E_{bo} = (-2\pi|W|R_{pa}^2 + 4\pi k(1+mR_{pa})^2)(1-\cos\phi) = (-2\pi|W|R_{pa}^2 + 4\pi k)(1-\cos\phi)$$

where ϕ is the wrapping angle and we are considering a vesicle bilayer with zero spontaneous curvature, ie $m = 0$.
In order to find the shape of the unbound segment that minimizes E_{un}, for a fixed value of contact angle ϕ, and satisfies the constraints on the total membrane area $A - A_{bo}$ and enclosed volume $V + V_{bo}$ of the vesicle, we must minimize the shape functional

$$F = E_{un} + \Sigma(A - A_{bo}) - \Delta P(V + V_{bo}) = \int_{A_{un}} dA\ 2kH^2 + \Sigma(A - A_{bo})$$

where $\int_{A_{un}} dA\ 2kH^2$ is the Helfrich energy integral.

Oss: In our particle based simulations we dont have any control or constraint on the vesicle volume, we dont pay a cost to change the vesicle volume then we put the volume term equal to zero.
Assuming that the vesicle shape will be axis-symmetric around z-axis It is possible to rewrite F in terms of $s, \psi(s), x(s)$:

$$F = \int_{s_0}^{s^\star} L(s, \psi(s), x(s))\ ds$$

The mean curvature H is given by

$$H = \frac{1}{2}(C_1 + C_2)$$

From figure 2 follows that:

$$C_1 = \frac{1}{R_1} = \frac{\sin\psi}{x(s)}$$

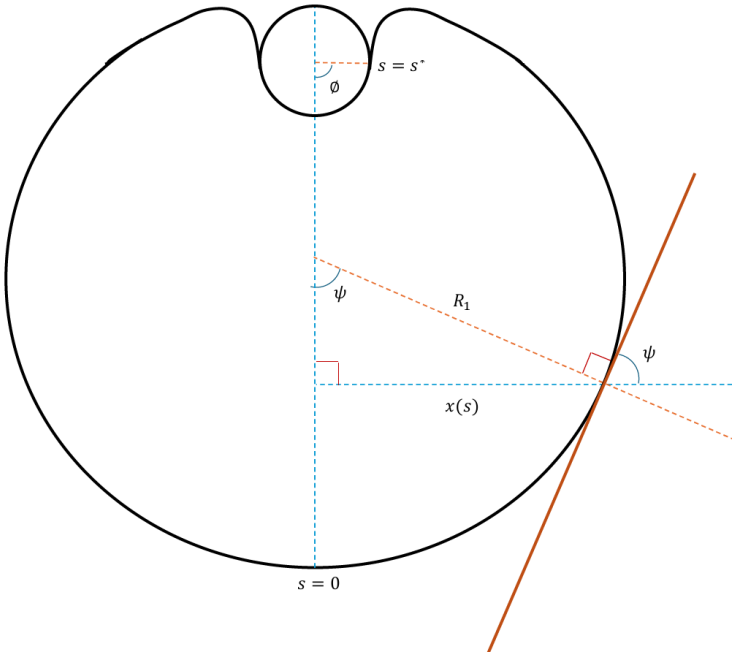


Figure 2: Visualization of the curvature

C_2 is given by the definition of curvature: the rate at which ψ changes with respect to the arc length s, which gives:

$$C_2 = \frac{d\psi}{ds}$$

C_1 defines the curvature straight into (or out of) the paper, and C_2 defines the curvature in the direction of s.
These two curvatures together give the mean curvature:

$$H^2 = \frac{1}{4}\left(\frac{d\psi}{ds} + \frac{\sin\psi}{x(s)}\right)^2$$

Now we will parameterize F in terms of $s, \psi(s), x(s)$

$$F = \int_{A_{un}} dA\ 2kH^2 + \Sigma A_{un} = \int_{s_0}^{s^\star} L(s, \psi(s), x(s))\ ds$$

For this step we need to rewrite an integral in terms of dA to an integral in terms of s. To do this we use the following formula:

$$dA = 2\pi x ds$$

applying this formula to F gives:

$$F = \int_{A_{un}} dA\ 2kH^2 + \Sigma A_{un} = \int_{s_0}^{s^\star} 2\pi x ds\ 2kH^2 + \Sigma \int_{s_0}^{s^\star} 2\pi x ds$$

Now we will add the two integrals together and fill in H:

$$F = 2\pi k \int_{s_0}^{s^\star} \frac{x}{2}\left(\dot{\psi} + \frac{\sin\psi}{x}\right)^2 + \frac{\Sigma}{k} x ds$$

To make sure the relation between x and ψ is satisfied, the Lagrange multiplier $\gamma(s)$ is added to the integral.

$$F = 2\pi k \int_{s_0}^{s^\star} \frac{x}{2}\left(\dot{\psi} + \frac{\sin\psi}{x}\right)^2 + \frac{\Sigma}{k} x + \gamma \frac{\dot{x} - \cos\psi}{2\pi k} ds$$

$$L(s, \psi, \dot{\psi}, x, \dot{x}, \gamma) = \frac{x}{2}\left(\dot{\psi} + \frac{\sin\psi}{x}\right)^2 + \frac{\Sigma}{k} x + \gamma \frac{\dot{x} - \cos\psi}{2\pi k}$$

$\gamma(s)$ is a Lagrange multiplier function that ensure the geometric relation between x and ψ is satisfied.
We aim to minimize the functional F using a variational approach, where $\delta F = 0$. Here, δF represents the variation with respect to the shape of the vesicle. Upon minimizing this functional, we obtain a system of differential equations that characterizes the shape of the vesicle.
This process is analogous to the method used in classical mechanics for minimizing the action functional with respect to a trajectory.

Euler-Lagrange equations: The solution of the minimization of functional F is given by the Euler-Lagrange equations.
In general, given a functional I:

$$I = \int_{x_a}^{x_b} L(x, f_1(x), f_2(x), \dots, \dot{f}_1(x), \dot{f}_2(x), \dots)$$

where $\dot{f}_i(x) = \frac{df_i}{dx}$ the Euler-Lagrange equations are:

$$\frac{d}{dx}\left[\frac{\partial L}{\partial \dot{f}_i}\right] - \frac{\partial L}{\partial f_i} = 0$$

The total variation δF is:

$$\delta F = \int_{s_1}^{s_2} \left[\left(\frac{d}{ds}\left[\frac{\partial L}{\partial \dot{\psi}}\right] - \frac{\partial L}{\partial \psi}\right)\delta\psi + \left(\frac{d}{ds}\left[\frac{\partial L}{\partial \dot{x}}\right] - \frac{\partial L}{\partial x}\right)\delta x\right] ds$$

The two Euler-Lagrange terms in equation must vanish separately at equilibrium, leading to the following differential equations:

$$\frac{d}{ds}\left[\frac{\partial L}{\partial \dot{\psi}}\right] - \frac{\partial L}{\partial \psi} = 0$$

Substituting will lead to

$$\ddot{\psi} = \frac{\sin\psi\cos\psi}{x^2} - \gamma\frac{\sin\psi}{2\pi k x} - \frac{\dot{x}\dot{\psi}}{x}$$

Similarly, for the second term:

$$\frac{d}{ds}\left[\frac{\partial L}{\partial \dot{x}}\right] - \frac{\partial L}{\partial x} = 0$$

Substituting here gives:

$$\dot{\gamma} = 2\pi\Sigma + k\pi\dot{\psi}^2 - \frac{k\pi\sin(\psi)^2}{x^2}$$

We can rewrite in first order terms substituing $\dot{\psi} = u$:

$$\begin{cases} \frac{d\psi}{ds} = u \\ \frac{du}{ds} = [-\frac{u}{x}\cos\psi + \frac{\cos(\psi)\sin(\psi)}{x^2} + \frac{\gamma\sin\psi}{2\pi k x}] \\ \frac{d\gamma}{ds} = [\pi k(u^2 - \frac{\sin^2\psi}{x^2}) + 2\pi\Sigma] \end{cases} \tag{1}$$

Hamiltonian function:

$$H = -L + \dot{\psi}\frac{\partial L}{\partial \dot{\psi}} + \dot{x}\frac{\partial L}{\partial \dot{x}} = \frac{1}{2}u^2 x + \gamma\frac{\cos\psi}{2k\pi} - \frac{x\Sigma}{k} - \frac{\sin\psi^2}{x}$$

H is conserved because $\frac{\partial L}{\partial s} = 0$. It also leads to the boundary condition for $\gamma(s)$ see eqs 3.7 from [7].

2.1 Physical quantity of the system

The following ones are the physical quantities or the constitutive relations involved in our system of interest:

- R_{pa} particle radius
- $|W|$ adhesive energy density for area unit
- R_{ve} radius of vesicle
- k bending rigidity

We can describe the system using two adimensional quantity:

$$r_{pa} = \frac{R_{pa}}{R_{ve}}$$

$$w = \frac{|W|R_{pa}^2}{k}$$

3 Shape ODE system

The following is the set of differential equation needed to describe the equilibrium shape of a membrane that interacts with an external particle. This system of equation is:

- ordinary because the independent variable is always $\bar{s}$.
- First order because all the derivatives are first derivative
- Non linear because of non linear terms like squares or trigonometric functions.
- it is a system because the dependent variables are coupled.

$$\begin{cases} \frac{d\psi}{ds} = u \\ \frac{du}{ds} = [-\frac{u}{x}\cos\psi + \frac{\cos(\psi)\sin(\psi)}{x^2} + \frac{\gamma\sin\psi}{2\pi kx}] \\ \frac{d\gamma}{ds} = [\pi k(u^2 - \frac{\sin^2\psi}{x^2}) + 2\pi\Sigma] \\ \frac{dx}{ds} = \cos\psi \end{cases} \tag{2}$$

3.1 Non-dimensionalization step

$$R_{ve} = \sqrt{\frac{A}{4\pi}}$$

Given R_{ve} as length scale, k as basic energy scale and $s^\star$ as the bound arc length we can rewrite our equation in a unitless form:
The dash symbols are the unitless quantities. write in a better way, maybe in a table

$$\bar{\psi} = \psi$$

$$\bar{u} = uR_{ve}$$

$$\bar{x} = \frac{x}{R_{ve}}$$

$$\bar{\gamma} = \gamma R_{ve}$$

$$\bar{\Sigma} = \Sigma \frac{R_{ve}^2}{k}$$

$$\bar{A} = \frac{A}{4\pi R_{ve}^2}$$

$$\bar{V} = \frac{3V}{4\pi R_{ve}^3}$$

$$\bar{s} = \frac{s}{s^\star}$$

$$\bar{s^\star} = \frac{s^\star}{s^\star} = 1$$

$$\Omega = \frac{s^\star}{R_{ve}}$$

Substitute in the system we get:

$$\begin{cases} \frac{d\bar{\psi}}{d\bar{s}} = \Omega\bar{u} \\ \frac{d\bar{u}}{d\bar{s}} = \Omega[-\frac{\bar{u}}{\bar{x}}\cos\bar{\psi} + \frac{\cos(\bar{\psi})\sin(\bar{\psi})}{\bar{x}^2} + \frac{\bar{\gamma}\sin\bar{\psi}}{2\pi k\bar{x}}] \\ \frac{d\bar{\gamma}}{d\bar{s}} = \Omega[\pi k(\bar{u}^2 - \frac{\sin^2\bar{\psi}}{\bar{x}^2}) + 2\pi\bar{\Sigma}k] \\ \frac{d\bar{x}}{d\bar{s}} = \Omega\cos\bar{\psi} \end{cases} \tag{3}$$

3.2 Initial conditions and parameters

This ODE problem is not in the canonical form of initial value problem (IVP) where we know the starting conditions for every variable. The system is a boundary value problem (BVP) because we know the values of some variable at the boundaries. There are several methods to solve BVPs, we will use shooting method.
At the South Pole ($s = 0$):

$$\psi(s=0) = 0 \;\; \gamma(s=0) = 0 \;\; x(s=0) = 0$$

At the North Pole $s = s^\star$:

$$\bar{\psi}(s^\star) = \bar{\psi}^\star = \pi + \phi$$

$$\bar{x}(s^\star) = \bar{x}^\star = \frac{R_{pa}}{R_{ve}}\sin\phi = r_{pa}\sin\phi$$

$$\bar{u}(s^\star) = \bar{u}^\star = \frac{R_{ve}}{R_{pa}} = \frac{1}{r_{pa}}$$

Oss: We dont have an equation for the volume because in simulation we are not constraining it and there is no energy cost in changing vesicle internal volume.
Then, we have 3 unknown parameters:

$$\Sigma, \; s^\star, \; u_0$$

We can use some informed guesses to put some bounds on these parameters.

- u_0 should be positive

- Ω should be equal to π in the unperturbed (no particle) case.
- Σ not too big

Boundary values of $\gamma(s)$ Hamiltonian $H(s_0) = 0$ and substituting the value for ψ and x I obtain $\gamma(s_0)\cos(\psi(s_0)) = 0$ and then $\gamma(s_0) = 0$.
Assuming that H is conserved because it is an energy, $H(s = s^\star) = 0$:

$$\gamma^\star = -2\pi R_{pa}\Sigma \tan\phi$$

4 Numerical implementation

Oss: See the code at Github repository

- assuming that the constitutive relations of the system r_{pa} and w are given and we know its values.
- you will choose a value for ϕ the wrapping angle and you will know the A_{bo} it would be cool to have the phi as optimal parameter from minimization of the total free energy instead of setting his value manually
- now you have everything to calculate the bound free energy E_{bo}
- shooting method for the unbound shape:
  - you will start with choosing random free parameters Σ, $s^\star$ and u_0
  - you will numerically integrate the ODE system knowing the initial conditions for ψ, u, γ, x
  - after the integration you calculate the residual function R as the error between the boundary conditions and the solution (obtained integrate the ODEs) at $s = s^\star$:

    $$R = (\psi(s^\star) - \bar{\psi^\star})^2 + (u(s^\star) - \bar{u}^\star)^2 + (x(s^\star) - \bar{x}^\star)^2$$

    We have three unknown free parameters so you will need three residuals to have a well defined problem.(3 residual equation, 3 unknowns). Minimize this error function corresponds to find the best parameters that match the solution with the boundary conditions. To minimize this function a variety of algorithm are possible, we will use least squares method.

- calculate the total free energy of the system
- estabilish if the total free energy is a minimum/stable state for the chosen combination of constitutive relations and contact angle ϕ.

Oss: the values obtained for the free parameters changes when you change the angle ϕ. in the same way the free parameters changed in the Felix paper when he changed m and ν.

4.1 Least squares method

This is the method we have used to minimize the residual error function. check `https://www2.imm.dtu.dk/pubdb/edoc/imm3215.pdf` for nice intro

4.2 Expansion at the South pole

At $s = 0$ $x(s)$ goes to zero and it appears as denominator and it leads to divergences causing numerical instability. An easy way to solve this is to regularize the functions at the "South pole" when $s = 0$. Regularization means Taylor expansion of all functions around $s = 0$.
First you need to expand $x(s), \psi(s), u(s), \gamma(s)$ and substitute the expansion in each equation (both sides) of the system. Then equating the coefficient of the polynomials you can get the series coefficient.

$$u(s) = u(0) + u_1 s + \frac{u_2}{2}s^2 + \frac{u_3}{6}s^3 + \frac{u_4}{24}s^4 + O(s^4)$$

$$\cos(\psi(s)) = 1 - \frac{\psi(s)^2}{2} + \frac{\psi(s)^4}{24} = 1 - \frac{1}{2}U_0^2 s^2 + \frac{U_0\psi_2}{2}s^3 + (\frac{\psi_2^2}{8} + \frac{U_0\psi_3}{6})s^4 + O(s^4);$$

Considering the simplest (and not trivial) equation from our system $\frac{dx}{ds} = \cos\psi$ and performing this substitution we'll get the coefficients for x expansion:

$$x_1 = 1,\ x_2 = 0,\ x_3 = -u_0^2,\ x_4 = 0$$

$$x(s) = s - \frac{s^3 u_0^2}{6};$$

The another equations from the system are quite challenging to deal on pen and paper and for that we have used a Mathematica script to perform the expansion.The final values for the coefficient are:

$$x_1 = 1,\ x_2 = 0,\ x_3 = -u_0^2,\ x_4 = 0$$

$$\psi_1 = u_0,\ \psi_2 = 0,\ \ \psi_4 = 0$$
$$\psi_3 = \frac{3\gamma_1 u_0 - 4\pi k u_0^3}{2\pi k} = \frac{6\pi\Sigma u_0 - 4\pi k u_0^3}{2\pi k}$$

$$\gamma_1 = 2\pi\Sigma,\ \gamma_2 = 0$$
$$\gamma_3 = \frac{4}{3}k\pi\psi_3 u_0 = 4\pi(\Sigma u_0 - \frac{2}{3}k u_0^3),\ \gamma_4 = 0$$

$$A_1 = 0,\ A_2 = 2\pi,\ A_3 = 0,\ A_4 = -2\pi u_0^2$$

Then if you want to reconstruct the series:

$$x(s) = x_1 s + \frac{x_2}{2}s^2 + \frac{x_3}{6}s^3 + \frac{x_4}{24}s^4 = s - \frac{u_0^2}{6}s^3$$

$$\gamma(s) = 2\pi\Sigma s + \frac{2}{9}k\pi\psi_3 u_0 s^3 = 2\pi\Sigma s + \frac{1}{9}u_0(6\pi u_0\Sigma - 4k u_0^3)s^3$$

$$\psi(s) = u_0 s + \frac{3\Sigma u_0 - 2k u_0^3}{6k}s^3$$

$$u(s) = u(0) + u_1 s + \frac{u_2 s^2}{2} + \frac{u_3 s^3}{6} + \frac{u_4 s^4}{24} = u_0 + \psi_2 s + \frac{\psi_3 s^2}{2} + \frac{\psi_4 s^3}{6} + \frac{\psi_5 s^4}{24}$$

$$= u_0 + \frac{3\Sigma u_0 - 2k u_0^3}{2k}s^2$$

This expansions still need to be non-dimensionalized.

4.3 Non-dimensionalization of the expansion

The dash symbols are the unitless quantities and we applied the same trasformations previously used.

$$\bar{x_1} = \Omega,\ \bar{x_3} = -\Omega^3 \bar{u_0}^2$$

$$\bar{\psi_1} = \Omega \bar{u_0}$$

$$\bar{\psi_3} = (3\bar{\Sigma}\bar{u_0} - 2\bar{u_0}^3)\Omega^3$$

$$\bar{u_0} = \bar{u_0}$$

$$\bar{u_1} = \frac{\Omega^2}{2}(3\bar{u_0}\bar{\Sigma} - 2\bar{u_0}^3)$$

$$\gamma_1 = 2\pi\bar{\Sigma}k\Omega$$

$$\gamma_3 = \frac{4}{3}\pi k \bar{u_0}\Omega^3(3\bar{\Sigma}\bar{u_0} - 2\bar{u_0}^3)$$

$$\bar{V_4} = \frac{9}{2}\bar{u_0}\Omega^4$$

$$\bar{A_2} = \frac{1}{2}\Omega^2,\ \bar{A_4} = -\frac{1}{2}\bar{u_0}^2\Omega^4$$

4.4 Expansion at North Pole

Simular studies [6] [2] has expanded the system also at the north pole due to the presence of divergences.
In our problem we will integrate from $s = 0$ to the contact point between particle and vesicle. If the contact point is not too close to the z-axis (rotational simmetry axis) we wont have any divergences. However it is worth checking this condition when $\phi \leq 20°$ or $\phi \geq 165°$ because the contact point became closer.

Improvement: It would be interesting to compare the numerical solution with **analytical expansion** for very small angle $\phi \to 0$. For such numerical integration is required the numerical North pole expansion in a similar way as the South pole.

4.5 More theory on Shooting method

The following two are two complex examples solved using shooting method. First for the tallest column [5] and second for optimal javelin shape [4]. Found these two papers from here `https://mathoverflow.net/questions/21257/what-is-state-of-the-art-for-the-shooting-method`

4.6 Numerical stability of the procedure

Unfortunately, we have noticed that the final value of the free parameters is affected but their initial guesses.
This is related to the fact that we have used Least squares method, a local optimization algorithm and we are not exploring all the parameters space. So we get stuck in a local minima.

TODO list

- understand concepts of stable manifold, fixed points etc
- another possibility is that our description of the system is not correct
- insted of shooting till the north pole, we can try to match the BCs in the middle of the path.

5 Future works

- Northpole expansion
- Compare the Energy with the unperturbed spherical vesicle $E = 8\pi k$ (maybe 4 ?)
- generalize the method to another system, look at extracting a membrane tube [3]

A Jacobian Matrix

This ODE system now is written in the standard form:

$$\frac{d}{d\bar{s}}\mathbf{Y} = \mathbf{f}(\mathbf{Y})$$

where

$$\mathbf{Y} = (\bar{\psi}, \bar{u}, \bar{\gamma}, \bar{x}, \bar{A}, \bar{V})$$

and

$$\mathbf{f} : \mathbb{R}^6 \to \mathbb{R}^6$$

The Jacobian is needed for the algorithm used by Felix but in principle with Runge-Kutta methods is not neeeded because it is calculated by finite difference method.

Oss: Now the following quantities are not dashed but they are already in their adimensional form, so consider for example $\psi(s)$ as $\bar{\psi}(\bar{s})$.
However:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{Y}} \\ \frac{\partial f_2}{\partial \mathbf{Y}} \\ \vdots \\ \frac{\partial f_n}{\partial \mathbf{Y}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial \bar{\psi}} & \frac{\partial f_1}{\partial \bar{u}} & \frac{\partial f_1}{\partial \bar{\gamma}} & \cdots & \cdots \\ \frac{\partial f_2}{\partial \bar{\psi}} & \frac{\partial f_2}{\partial \bar{u}} & \frac{\partial f_2}{\partial \bar{\gamma}} & & \\ \vdots & \vdots & & & \\ \frac{\partial f_n}{\partial \bar{\psi}} & \frac{\partial f_n}{\partial \bar{u}} & \frac{\partial f_n}{\partial \bar{\gamma}} & \cdots & \cdots \end{bmatrix}$$

$$\mathbf{J} = \begin{bmatrix} 0 & a_{12} & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 \\ a_{31} & a_{32} & 0 & a_{34} & 0 & 0 \\ a_{41} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{54} & 0 & 0 \\ a_{61} & 0 & 0 & a_{64} & 0 & 0 \end{bmatrix}$$

$$a_{12} = \frac{df_\psi}{du} = \Omega$$

$$a_{21} = \frac{df_u}{d\psi} = \Omega(\frac{u}{x}\sin\psi + \frac{1}{x^2}\cos^2\psi - \frac{1}{x^2}\sin^2\psi\frac{\gamma}{2\pi kx}\cos\psi)$$

$$a_{22} = \frac{df_u}{du} = -\frac{\Omega}{x}\cos\psi$$

$$a_{23} = \frac{df_u}{d\gamma} = \Omega\frac{\sin\psi}{2\pi kx}$$

$$a_{24} = \frac{df_u}{dx} = \Omega(\frac{u}{x^2}\cos\psi - 2\frac{\cos\psi\sin\psi}{x^3} - \frac{\gamma\sin\psi}{2\pi kx^2})$$

$$a_{31} = \frac{df_\gamma}{d\psi} = \Omega(-\pi k\frac{\cos\psi}{x^2})$$

$$a_{32} = \frac{df_\gamma}{du} = \Omega\pi k2u$$

$$a_{34} = \frac{df_\gamma}{dx} = 2\Omega\pi k\sin\psi\frac{1}{x^3}$$

$$a_{41} = \frac{df_x}{d\psi} = -\Omega\sin\psi$$

$$a_{54} = \frac{df_A}{dx} = \Omega$$

$$a_{61} = \frac{df_V}{d\psi} = \Omega\frac{3}{4}x^2\cos\psi$$

$$a_{64} = \frac{df_V}{dx} = \frac{3}{2}\Omega x\sin\psi$$

B Non-dimensionalization of E_{bo} and E_{un}

$$\bar{E_{bo}} = (-2\pi\bar{W}r_{pa}^2 + 4\pi)(1-\cos\phi)$$

$$\bar{E_{un}} =$$

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