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A stabilized finite element formulation for liquid shells and its application to lipid bilayers

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A B S T R A C T

This paper presents a new finite element (FE) formulation for liquid shells that is based on an explicit, 3D surface discretization using C^1-continuous finite elements constructed from NURBS interpolation. Both displacement-based and mixed displacement/pressure FE formulations are proposed. The latter is needed for area-incompressible material behavior, where penalty-type regularizations can lead to misleading results. In order to obtain quasi-static solutions for liquid shells devoid of shear stiffness, several numerical stabilization schemes are proposed based on adding stiffness, adding viscosity or using projection. Several numerical examples are considered in order to illustrate the accuracy and the capabilities of the proposed formulation, and to compare the different stabilization schemes. The presented formulation is capable of simulating non-trivial surface shapes associated with tube formation and protein-induced budding of lipid bilayers. In the latter case, the presented formulation yields non-axisymmetric solutions, which have not been observed in previous simulations. It is shown that those non-axisymmetric shapes are preferred over axisymmetric ones.

1. Introduction

Biological membranes form the boundaries of cells and cell-internal organelles such as the endoplasmic reticulum, the Golgi complex, mitochondria and endosomes. Mechanically they are liquid shells that exhibit fluid-like behavior in-plane and solid-like behavior out-of-plane. They mainly consist of self-assembled lipid bilayers and proteins. At the macroscopic level, these membranes exist in different shapes such as invaginations, buds and cylindrical tubes [69,58,41,56]. These shapes arise as a result of the lateral loading due to cytoskeletal filaments and protein-driven spontaneous curvature. Cell membranes undergo many morphological and topological shape transitions to enable important biological processes such as endocytosis [9,35,43], cell motility [30] and vesicle formation [21,8]. The shape transitions occur as a result of lateral loading on the membranes from cytoskeletal filaments, such as actin, from osmotic pressure gradients across the membrane, or from

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List of important symbols

$\mathbf{1}$	identity tensor in $\mathbb{R}^3$
$\boldsymbol{a}_\alpha$	co-variant tangent vectors of surface $\mathcal{S}$ at point $\boldsymbol{x}$; $\alpha=1,2$
$\boldsymbol{A}_\alpha$	co-variant tangent vectors of surface $\mathcal{S}_0$ at point $\boldsymbol{X}$; $\alpha=1,2$
$\boldsymbol{a}^\alpha$	contra-variant tangent vectors of surface $\mathcal{S}$ at point $\boldsymbol{x}$; $\alpha=1,2$
$\boldsymbol{A}^\alpha$	contra-variant tangent vectors of surface $\mathcal{S}_0$ at point $\boldsymbol{X}$; $\alpha=1,2$
$\boldsymbol{a}_{\alpha,\beta}$	parametric derivative of $\boldsymbol{a}_\alpha$ w.r.t. ξ^β
$\boldsymbol{a}_{\alpha;\beta}$	co-variant derivative of $\boldsymbol{a}_\alpha$ w.r.t. ξ^β
$a_{\alpha\beta}$	co-variant metric tensor components of surface $\mathcal{S}$ at point $\boldsymbol{x}$
$A_{\alpha\beta}$	co-variant metric tensor components of surface $\mathcal{S}_0$ at point $\boldsymbol{X}$
a	class of stabilization methods based on artificial shear viscosity
A	class of stabilization methods based on artificial shear stiffness
$b_{\alpha\beta}$	co-variant curvature tensor components of surface $\mathcal{S}$ at point $\boldsymbol{x}$
$B_{\alpha\beta}$	co-variant curvature tensor components of surface $\mathcal{S}_0$ at point $\boldsymbol{X}$
$\boldsymbol{B}$	left surface Cauchy–Green tensor
$c^{\alpha\beta\gamma\delta}$	contra-variant components of the material tangent
$\boldsymbol{C}$	right surface Cauchy–Green tensor
γ	surface tension of $\mathcal{S}$
$\Gamma^\gamma_{\alpha\beta}$	Christoffel symbols of the second kind
$\mathrm{d}a$	differential surface element on $\mathcal{S}$
$\mathrm{d}A$	differential surface element on $\mathcal{S}_0$
$\delta\ldots$	variation of ...
e	index numbering the finite elements; $e=1,\ldots,n_{\mathrm{el}}$
ϵ	penalty parameter
$\mathbf{f}^e$	finite element force vector of element Ω^e
g	expression for the area-incompressibility constraint
G	expression for the weak form
G^e	contribution to G from finite element Ω^e
$\mathbf{g}^e$	finite element 'force vector' of element Ω^e due to constraint g
H	mean curvature of $\mathcal{S}$ at $\boldsymbol{x}$
H_0	spontaneous curvature prescribed at $\boldsymbol{x}$
I	index numbering the finite element nodes
$I_1,\ I_2$	first and second invariants of the surface Cauchy–Green tensors
$\boldsymbol{i}$	surface identity tensor on $\mathcal{S}$
$\boldsymbol{I}$	surface identity tensor on $\mathcal{S}_0$
J	surface area change
k	bending modulus
k^*	Gaussian modulus
K	initial in-plane membrane bulk modulus
K_{eff}	effective in-plane membrane bulk modulus
$\mathbf{k}^e$	finite element tangent matrix associated with $\mathbf{f}^e$ and $\mathbf{g}^e$
κ	Gaussian curvature of surface $\mathcal{S}$ at $\boldsymbol{x}$
$\kappa_1,\ \kappa_2$	principal curvatures of surface $\mathcal{S}$ at $\boldsymbol{x}$
L_I	pressure shape function of finite element node I
$\lambda_1,\ \lambda_2$	principal surface stretches of $\mathcal{S}$ at $\boldsymbol{x}$
m_e	number of pressure nodes of finite element Ω^e
$m_\nu,\ m_\tau$	bending moment components acting at $\boldsymbol{x}\in\partial\mathcal{S}$
$\bar{m}_\nu,\ \bar{m}_\tau$	prescribed bending moment components
$M^{\alpha\beta}$	contra-variant bending moment components
μ	initial in-plane membrane shear stiffness
μ_{eff}	effective in-plane membrane shear stiffness
n_{no}	total number of finite element nodes used to discretize $\mathcal{S}$
n_{el}	total number of finite elements used to discretize $\mathcal{S}$
n_{mo}	total number of finite element nodes used to discretize pressure q
n_e	number of displacement nodes of finite element Ω^e
$N^{\alpha\beta}$	total, contra-variant, in-plane membrane stress components
N_I	displacement shape function of finite element node I
$\boldsymbol{n}$	surface normal of $\mathcal{S}$ at $\boldsymbol{x}$
$\boldsymbol{N}$	surface normal of $\mathcal{S}_0$ at $\boldsymbol{X}$
$\mathbf{N}$	array of the shape functions for element Ω^e
ν	in-plane membrane shear viscosity
$\boldsymbol{\nu}$	normal vector on $\partial\mathcal{S}$
ξ^α	convective surface coordinates; $\alpha=1,2$
P	class of stabilization methods based on normal projection; projection matrix
q	Lagrange multiplier associated with area-incompressibility
$\mathbf{q}$	array of all Lagrange multipliers q_I in the system; $I=1,\ldots,n_{\mathrm{mo}}$
$\mathbf{q}_e$	array of all Lagrange multipliers q_I for finite element Ω^e; $I=1,\ldots,m_e$
S^α	contra-variant, out-of-plane shear stress components
$\mathcal{S}$	current configuration of the surface
$\mathcal{S}_0$	initial configuration of the surface
$\boldsymbol{\sigma}$	Cauchy stress tensor of the shell
$\sigma^{\alpha\beta}$	stretch related, contra-variant, in-plane membrane stress components
$\boldsymbol{t}$	effective traction acting on the boundary $\partial\mathcal{S}$ normal to $\boldsymbol{\nu}$
$\bar{\boldsymbol{t}}$	prescribed boundary tractions on Neumann boundary $\partial_t\mathcal{S}$
$\boldsymbol{T}$	traction acting on the boundary $\partial\mathcal{S}$ normal to $\boldsymbol{\nu}$
$\boldsymbol{T}^\alpha$	traction acting on the boundary $\partial\mathcal{S}$ normal to $\boldsymbol{a}^\alpha$
$\mathcal{V},\ \mathcal{Q}$	admissible function spaces