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subject: Exercising the Surface Rheology Capabilities in Goma

1.0 Introduction and Summary

The Surface Rheology LDRD, a FY 2008 startup, is a combined experimental and numerical program based upon elucidating the constitutive models for the surface viscosity of langmuir films on liquid surfaces. Based partly on understanding an experimental apparatus developed and improved by Carlton Brooks [1, 2] as part of his dissertation for measure the effect on surface viscosity of films using a magnetic needle that floats on the surface, this rheometer was subsequently commercialized. A periodic force is applied to the magnetic needle, and the periodic complex response from the system is measured. The key issue to resolve is to separate out the bulk rheological response of the system from the surface rheological response; this is done via a numerical model. Carlton undertook a numerical study of the Magnetic Rod Interfacial Stress Rheometer within Matlab in his thesis [2]. One of the issues that was left unaddressed in that study was the effect of the meniscus on the response of the system, since the initial modeling approach assumed a flat interface. Thus, as one of the initial tasks in the LDRD, we have undertaken to model the curved interfaces with the rheometer within Goma [3]. We plan to combine the meniscus treatment with a surface rheology treatments within Goma, where there has been an initial implementation of the Newtonian surface viscosity term [4], to understand the effects that a real treatment of the meniscus has on measured surface viscosity properties.

In this note, we provide a description of the model development for a floating cylinder on a surface within a channel. We use Goma, as its extensive ALE free surface capabilities makes the program uniquely suited to handle this application. Of particular relevance is getting the treatment of the boundary conditions to be stable under both time dependent and steady state conditions. This actually turned out to be nonstraightforward. We anticipate that subsequent treatments of the system will then treat the oscillatory time response of the numerical model that we have set up here.

2.0 Equation System

2.1 Consitutive Modeling For Systems with Excess Surface Properties

A couple of definitions are useful. The surface gradient operator is defined as

$$\nabla_s = (\mathbf{I} - \boldsymbol{nn}) \bullet \nabla \tag{1}$$

We may think of the unity tensor in the above formulation as a combination of three dyadics

$$\boldsymbol{I} = \boldsymbol{nn} + \boldsymbol{t}_1\boldsymbol{t}_1 + \boldsymbol{t}_2\boldsymbol{t}_2 \tag{2}$$

$\boldsymbol{n}$ is the local normal to the surface. Where there is an inner surface and an exterior domain, $\boldsymbol{n}$ is defined within Goma as always pointing from the inner domain out into the outer domain (or exterior). $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ are local tangents to the surface defined in such a way that $\boldsymbol{n}$, $\boldsymbol{t}_1$, and $\boldsymbol{t}_2$ form an orthonormal basis at every point. Frequently, the symbol $\mathbf{I}_s$, the surface idemfactor tensor, is defined to represent direction which are in the plane of the surface.

$$\mathbf{I}_s = \mathbf{I} - \boldsymbol{nn} = \boldsymbol{t}_1\boldsymbol{t}_1 + \boldsymbol{t}_2\boldsymbol{t}_2 \tag{3}$$

The interfacial shear, $\mathbf{D}_s$, is a tensor defined in the plane of the surface and may be expressed as

$$\mathbf{D}_s = \frac{1}{2}[(\nabla_s \boldsymbol{v}) \cdot \mathbf{I}_s + \mathbf{I}_s \cdot (\nabla_s \boldsymbol{v})^T] \tag{4}$$

Note the dot product within Eqn. (4) combines the inner indeces of the two tensors, $(\nabla_s \boldsymbol{v})$ and $\mathbf{I}_s$ to create another tensor. This inner product is needed in order to crop the velocity changes in the normal direction which $\nabla_s \boldsymbol{v}$ actually contains. An example is useful. For cartesian coordinates, with the surface oriented in the **x** direction, $\mathbf{D}_s$ is equal to

$$\mathbf{D}_s = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \dfrac{dv_y}{dy} & \dfrac{1}{2}\left(\dfrac{dv_y}{dz} + \dfrac{dv_z}{dy}\right) \\ 0 & \dfrac{1}{2}\left(\dfrac{dv_z}{dy} + \dfrac{dv_y}{dz}\right) & \dfrac{dv_z}{dz} \end{bmatrix} \tag{5}$$

The Boussinesq Scriven model for surface rheological properties for a Newtonian approximation to the surface is given by the following formulation. $\underline{\boldsymbol{\Upsilon}}_s$ is the surface stress tensor.

$$\underline{\boldsymbol{\Upsilon}}_s = \sigma\mathbf{I}_s + \boldsymbol{\tau}_s = \sigma\mathbf{I}_s + (\kappa_s - \mu_s)(\mathbf{I}_s : \mathbf{D}_s)\mathbf{I}_s + 2\mu_s\mathbf{D}_s \tag{6}$$

The expression $\mathbf{I}_s : \mathbf{D}_s$ is actually identified as the trace of $\mathbf{D}_s$, i.e., the diagonal components oriented in the surface plane summed up.

$$\mathbf{I_s} : \mathbf{D}_s = tr(\mathbf{D}_s) = \nabla_s \cdot \boldsymbol{v} \tag{7}$$

For the example mentioned in Eqn. 5, the trace would be equal to Eqn. (8).

$$\mathbf{I_s} : \mathbf{D}_s = tr(\mathbf{D}_s) = \nabla_s \cdot \boldsymbol{v} = \frac{dv_y}{dy} + \frac{dv_z}{dz} \tag{8}$$

We note that in contrast to the full divergence of the velocity for incompressible flows, the surface divergence will easily allow for nonzero cases. A good example of dilatational flow would be a balloon expanding and contracting.

The surface excess stress tensor, also called the surface excess pressure, may be related to the bulk fields by the following expression obtained from Edward's book.

$$-(\boldsymbol{n} \cdot \|\boldsymbol{T}\|) = \boldsymbol{F}_s + \nabla_s \cdot \underline{\boldsymbol{\Upsilon}}_{\boldsymbol{s}} = \boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) \tag{9}$$

Note, the Edwards book uses the nomenclature $\|\boldsymbol{T}\| = T_{n = 0+} - T_{n = 0-}$, where the normal $\boldsymbol{n}$ dictate the direction of the interface. $\boldsymbol{T}_{in}$ is the bulk-fluid stress tensor in the $n = 0-$ direction of the interface. This is usually thought as tthe inside of the domain. $\boldsymbol{T}_{ext}$ is the stress tensor in the exterior of the domain.

2.2 Goma's Base Treatment : No Surface Excess Properties

We find it's useful to start off by describing Goma's base treatment where the surface "only" exhibits an isotropic surface tension, σ. The surface tension may be a function of the state of the two bulk fluids, 1 and 2, that are on either side of the interface $\sigma = \sigma(T, P, X_1, X_2)$. We start with the fluid momentum equation where the mesh is moving with velocity $\boldsymbol{v}_m$.

$$\rho\frac{d\boldsymbol{v}}{dt} + \rho(\boldsymbol{v} - \boldsymbol{v}_m) \cdot \nabla\boldsymbol{v} = \nabla \cdot \boldsymbol{T} + \boldsymbol{f} \tag{10}$$

where

$$\boldsymbol{T} = -p\boldsymbol{I} + 2\mu\boldsymbol{D} - \left(\frac{2}{3}\mu - \kappa\right)(\nabla \cdot \boldsymbol{v})\boldsymbol{I} \tag{11}$$

and the symmetric shear tensor, $\boldsymbol{D}$, may be represented by Eqn. (12).

$$\boldsymbol{D} = \frac{1}{2}(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T) \tag{12}$$

Residual equations for the β^{th} component of the momentum equations are then created by setting the momentum equation's error orthogonal to a set of basis functions, ϕ_i, and then integrating by parts to formulate an expression for the residual of the β th component of the momentum equation with respect to the basis function ϕ_i, $R_i^{m,\beta}$, Eqn. (13).

$$R_i^{m,\beta} = -\int_V \left(\phi_i \boldsymbol{e}_\beta \bullet \left(\rho \frac{d\boldsymbol{v}}{dt} + \rho(\boldsymbol{v} - \boldsymbol{v}_m) \cdot \nabla \boldsymbol{v} - \boldsymbol{f}\right)\right) dV - \int_V ((\nabla(\phi_i \boldsymbol{e}_\beta))^T : \boldsymbol{T}) dV + \int_\Gamma (\phi_i \boldsymbol{e}_\beta \, \boldsymbol{n} : \boldsymbol{T}) d\Gamma \tag{13}$$

Note, that we have multiplied by -1 to reach Eqn. (13). Goma's residuals formally have negative terms outside their time derivatives (in contrast to about every other code in existence). $\boldsymbol{e}_\beta$ is the unit norm directed in the β component direction, where β may represent a curvilinear coordinate system. Coming from the residual expression in Eqn. (13) the following surface term falls out, involving the stress tensor at the inside of the interface, $\boldsymbol{T}_{in}$.

$$R_i^{m,\beta} = \ldots + \int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \boldsymbol{n} : \boldsymbol{T}_{in}) d\Gamma \tag{14}$$

In Eqn. (14), $R_i^{m,\beta}$ is the momentum residual for the i^{th} basis function for the coordinate direction, β . The double dot notation in Eqn. (14) is the inner product notation, where the inner indices are contracted by an inner product before the outer indices are contracted.

At an interface with no surface excess properties, the following equation holds from a simpliefication of Eqn. (9) (Note, ref. [7] contains many sign errors and is not to be trusted).

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = \nabla_s \cdot (\mathbf{I}_s \sigma) = 2H\sigma \boldsymbol{n} + \nabla_s \sigma \tag{15}$$

Here, $\boldsymbol{T}_{in}$ is the stress tensor within the interior of the fluid. $\boldsymbol{T}_{ext}$ is the stress tensor on the exterior of the other fluid. $\mathbf{I}_s$ is the surface dyadic defined in Eqn. (3), and ∇_s is the surface gradient operator defined in Eqn. (1). $\boldsymbol{n}$ points out of the domain.

Frequently, the fluid in the exterior domain is a gas where the shear stress is negligible, and the value of $\boldsymbol{T}_{ext}$ reduces to $\boldsymbol{T}_{ext} = -\mathbf{I}p_{ext}$, where the minus sign is due to the definition of $\boldsymbol{T}$ (see Eqn. (11)). In this case Eqn. (15) reduces to

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in}) = -\boldsymbol{n} \cdot \mathbf{I}p_{ext} + 2H\sigma \boldsymbol{n} + \nabla_s \sigma \tag{16}$$

H is the surface mean curvature. It can be related to the surface divergence of the normal vector to the surface [7], and in fact we used this relation in deriving Eqn. (15).

$$2H = -\nabla_s \bullet \boldsymbol{n} \tag{17}$$

We may plug Eqn. (16) into Eqn. (14) to yield Eqn. (18).

$$\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \boldsymbol{n} : \boldsymbol{T}_{in}) d\Gamma = -\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n) p_{ext} d\Gamma + \int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n) 2H\sigma d\Gamma + \int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet \nabla_s \sigma) d\Gamma \tag{18}$$

It is desirable to simplify Eqn. (18) to remove explicit calculation of the surface tension gradient and the curvature. The surface divergence theorm relates surface and volume integrals of vector fields on a curved surface. Let Γ be a two dimensional surface. Let C be the one-dimensional line surrounding that surface. Let $\boldsymbol{m}$ be the normal tangent to the surface Γ along the line C that points out of the surface; $\boldsymbol{m}$ is called a binormal. Then, for an arbitray vector field, $\boldsymbol{v}$:

$$\int_{\Gamma}(\nabla_s \cdot \boldsymbol{v})d\Gamma = \int_{C}(\boldsymbol{v} \cdot \boldsymbol{m})dC - \int_{\Gamma}2H(\boldsymbol{v} \cdot n)d\Gamma \tag{19}$$

We may apply this to yield

$$\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n)2H\sigma d\Gamma = \int_{C}\phi_i\sigma(\boldsymbol{e}_\beta \cdot \boldsymbol{m})dC - \int_{\Gamma}(\nabla_s \cdot (\boldsymbol{e}_\beta\phi_i\sigma))d\Gamma \tag{20}$$

Then, we may combine to yield

$$\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n)2H\sigma d\Gamma + \int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet \nabla_s\sigma)d\Gamma = \int_{C}\phi_i\sigma(\boldsymbol{e}_\beta \cdot \boldsymbol{m})dC - \int_{\Gamma}\sigma(\nabla_s \cdot (\boldsymbol{e}_\beta\phi_i))d\Gamma \tag{21}$$

Thus, we have replaced some nasty terms with relatively easy terms that may be calculated explicitly. The final expression becomes

$$\begin{aligned}\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n)2H\sigma d\Gamma + \int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet \nabla_s\sigma)d\Gamma &= \\ \int_{C}\phi_i\sigma(\boldsymbol{e}_\beta \cdot \boldsymbol{m})dC - \int_{\Gamma}\sigma(((\mathbf{I} - \boldsymbol{nn}) \cdot \nabla) \cdot (\boldsymbol{e}_\beta\phi_i))d\Gamma &\end{aligned} \tag{22}$$

Plugging that back into Eqn. (18) yields Eqn. (23).

$$\begin{aligned}\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta\boldsymbol{n} : \boldsymbol{T}_{in})d\Gamma &= -\int_{d\Gamma} \phi_i(\boldsymbol{e}_\beta \bullet n)p_{ext}d\Gamma \\ &\quad - \int_{\Gamma}\sigma((\mathbf{I} - \boldsymbol{nn}) : \nabla(\boldsymbol{e}_\beta\phi_i))d\Gamma + \int_{C}\phi_i\sigma(\boldsymbol{e}_\beta \cdot \boldsymbol{m})dC\end{aligned} \tag{23}$$

Note we have replaced the two dot product operations in Eqn. (23) with a single double dot operation, because they are equivalent operations. The double dot operator contracts the inner indecies of the dyadic products first, before it contracts the outer indecies. Eqn. (23) is the expression that Goma has traditionally solved for when handling free surface problems. This includes the treatment of the signs. The surface integral for Eqn. (23) and its derivatives is solved for in the function `fn_dot_T()` in the file `mm_ns_bc.c`. The signs in that function agree with the signs in Eqn. (23). The point boundary condition term in Eqn. (23) is applied on the ends of free surfaces where needed. It is not needed when the contact angle is specified for the free surface.

2.2.1 Reconciliation of Signs

We may prove Eqn. (23) and especially the signs by assuming spherical symmetry, i.e., a bubble geometry. Within that geometry it’s widely known that the pressure within the bubble is greater than the pressure outside the bubble.

In spherical coordinates, and assuming symmetry in the θ and ϕ direction, the value of $\nabla(\boldsymbol{e}_r\phi_i)$ may be written as ([9] BSL, p. 837):

$$\nabla(\boldsymbol{e}_r\phi_i) = \frac{\boldsymbol{e}_\theta\boldsymbol{e}_\theta}{r} + \frac{\boldsymbol{e}_\phi\boldsymbol{e}_\phi}{r} \tag{24}$$

We may plug this value into Eqn. (23) using $\boldsymbol{n} = \boldsymbol{e}_r$ to show that

$$\int_\Gamma \sigma((\mathbf{I} - \boldsymbol{nn}) : \nabla(\boldsymbol{e}_\beta\phi_i))d\Gamma = \frac{2\sigma}{r}$$

and therefore Eqn. (23) becomes

$$-p_{in} = -p_{ext} - \frac{2\sigma}{r} \tag{25}$$

This is the expected result for a sphere. Note, for the sphere geometry, the mean curvature *H* is negative when the normal points out of the sphere. Again, this may be shown, because

$$\nabla(\boldsymbol{n}) = \nabla(\boldsymbol{e}_r) = \frac{\boldsymbol{e}_\theta\boldsymbol{e}_\theta}{r} + \frac{\boldsymbol{e}_\phi\boldsymbol{e}_\phi}{r}$$

$$H = \frac{-\nabla_s \bullet \boldsymbol{n}}{2} = -\frac{1}{2}(I - nn) : \nabla(\boldsymbol{e}_r) = \frac{1}{r}$$

Plugging the value of *H* into Eqn. (15) yields the expected relationship.

2.3 Surface Excess Properties: Linkage

Treatment for surfaces with excess properties starts with an expansion of a generalization of Eqn. (15) to include the full Boussinesq-Scriven model, Eqn. (6), for the excess surface stress tensor, $\underline{\boldsymbol{\Upsilon}}_s$. The proof starts with a derivation of the the two dimensional Cauchy’s theorum, essentially a force balance on a surface eleemtn. We then ignore the acceleration term and any other body force term which may be acting on the surface element, which is pertinent if the surface phase has an unimportant amount of surface density. The resulting equation is given in Eqn. (26).

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = \nabla_s \cdot (\underline{\boldsymbol{\Upsilon}}_s) \tag{26}$$

Note, if the acceleration of surface phase isn’t ignored the following equation would hold [2].

$$\frac{d(\rho_s \boldsymbol{v}_s)}{dt} + \nabla_s \bullet (\rho_s \boldsymbol{v}_s \boldsymbol{v}_s) \quad = \nabla_s \cdot (\underline{\Upsilon}_s) - (\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext})) \tag{27}$$

Thus,

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = \quad \nabla_s \cdot (\sigma \mathbf{I}_{\boldsymbol{s}} + (\kappa_s - \mu_s)(\mathbf{I}_{\boldsymbol{s}} : \mathbf{D}_s)\mathbf{I}_{\boldsymbol{s}} + 2\mu_s \mathbf{D}_s) \tag{28}$$

This expression needs to be linked with experimental quantities.

Changes in the surface tension are called the surface pressure,Π .

$$\Pi = \sigma_o - \sigma \tag{29}$$

o is the surface tension of a surfactant covered interface, whose concentration may vary with time and position. σ_o is the surface tension of a pure interface at isothermal and isobaric external conditions. For example, the surface tension of a pures water gas phase at 20C is 72.8 nM m^{-1}.

There are three modes for surface deformation. The first mode is dilation. The dilational modulus, E_s , may be defined as

$$E_s = \frac{d\sigma}{d \ln A} \quad . \tag{30}$$

The other two modes of in-plane deformations preserve the surface area. These two are shear and extension.

2.4 Goma's Treatment : Surface Excess Properties

Goma's treatment for surfaces with excess properties starts with an expansion of a generalization of Eqn. (15) to include the full Boussinesq-Scriven model, Eqn. (6), for the excess surface stress tensor, $\boldsymbol{P}_s$, after ignoring a lot of terms in the full analysis that are unimportant for

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = \quad \nabla_s \cdot (\underline{\Upsilon}_s) \tag{31}$$

Thus,

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = \quad \nabla_s \cdot (\sigma \mathbf{I}_{\boldsymbol{s}} + (\kappa_s - \mu_s)(\mathbf{I}_{\boldsymbol{s}} : \mathbf{D}_s)\mathbf{I}_{\boldsymbol{s}} + 2\mu_s \mathbf{D}_s) \tag{32}$$

Now, the first term can be manipulated with the relation

$$\nabla_s \cdot (\mathbf{I}_{\boldsymbol{s}}) \quad = 2H\boldsymbol{n}$$

to yield

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) = 2H\sigma\boldsymbol{n}+\nabla_s\sigma+\nabla_s\cdot((\kappa_s-\mu_s)(\mathbf{I}_s:\mathbf{D}_s)\mathbf{I}_s+2\mu_s\mathbf{D}_s) \tag{33}$$

The second term may be reduced via the previously derived expression

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) = 2H\sigma\boldsymbol{n}+\nabla_s\sigma+\nabla_s\cdot((\kappa_s-\mu_s)(\nabla_s\cdot\boldsymbol{v})\mathbf{I}_s+2\mu_s\mathbf{D}_s) \tag{34}$$

We should pause for a moment and reflect on Eqn. (34), as it may represent an alternative formulation to the one that will follow below. Let's rewrite Eqn. (34) in the following way

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) = 2H\sigma\boldsymbol{n}+\nabla_s\sigma+\nabla_s\cdot(\underline{\boldsymbol{\tau}}_s) \tag{35}$$

We can see that the first two terms on the rhs are consistent with the previous treatment of interfacial surface tension within Goma. The last term introduces a new tensor, $\underline{\boldsymbol{\tau}}_s$, defined as

$$\underline{\boldsymbol{\tau}}_s = ((\kappa_s-\mu_s)(\nabla_s\cdot\boldsymbol{v})\mathbf{I}_s+2\mu_s\mathbf{D}_s) \tag{36}$$

$\underline{\boldsymbol{\tau}}_s$ is a symmetric tensor with 6 unique entries. One thought would be to calculate these six intermediate entries on shell equations. Then we may use Eqn. (36) to calculate the excess contribution to the momentum balance due to the surface phase. We need to introduce intermediate variables within Eqn. (35), because Eqn. (35) involves second derivatives in the velocities, and these can not be resolved with accuracy using our current biquadratic finite element formulations. On consideration of all the issues we haver faced so far, the direct calculation of $\mathbf{D}_s$ or $\boldsymbol{\tau}_s$ via shell equation may well be the best approach, especially for non-newtonian rheology. However, that was not our initial approach in this treatment.

Well, continuing on with regrets. The second term on the rhs may be simplified assuming that κ_s and μ_s are constants (even if they aren't, the extensions to nonconstant expressions are relatively straightforward) and using the expression $\mathbf{I}_s\cdot\nabla_s=\nabla_s$:

$$\nabla_s\cdot(\mathbf{I}_s(\kappa_s-\mu_s)(\nabla_s\cdot\boldsymbol{v})) = 2H\boldsymbol{n}(\kappa_s-\mu_s)(\nabla_s\cdot\boldsymbol{v})+(\kappa_s-\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v}) \tag{37}$$

The last term may be expanded, taking care of flipping the transpose where needed, to ensure the correct idenceses are used:

$$\begin{aligned}\nabla_s\cdot(2\mu_s\mathbf{D}_s) &= \mu_s\nabla_s\cdot[(\nabla_s\boldsymbol{v})\cdot\mathbf{I}_s+\mathbf{I}_s\cdot(\nabla_s\boldsymbol{v})^T]\\ &= \mu_s[(\nabla_s\cdot\nabla_s\boldsymbol{v})\mathbf{I}_s+((\nabla_s\boldsymbol{v})^T:\nabla_s\mathbf{I}_s)]\\ &\quad+\mu_s[2H(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n}+\nabla_s\cdot(\nabla_s\boldsymbol{v})^T]\end{aligned} \tag{38}$$

Below we will make heavy use of the surface curvature dyadic, $\boldsymbol{b}$, defined as

$$\boldsymbol{b}=-\nabla_s\boldsymbol{n} \tag{39}$$

which expresses the change of the local surface normal with respect to the position (q^1, q^2) on the surface. $\boldsymbol{b}$ lies in the plane of the surface, is symmetric, and can be reduced to

$$\boldsymbol{b} = \kappa_1 \boldsymbol{e}_1 \boldsymbol{e}_1 + \kappa_1 \boldsymbol{e}_2 \boldsymbol{e}_2 \,,$$

where κ_1 and κ_2 are the principle moments of the curvature of the surface and $\boldsymbol{e}_\alpha$, which are orthogonal to one another, are the principle directions, i.e., the eigenvectors of $\boldsymbol{b}$. Also,

$$H = \frac{1}{2}(\mathbf{I}_s : \boldsymbol{b}) = \frac{1}{2}(\kappa_1 + \kappa_1) \tag{40}$$

Ok, then we use the following identities:

$$\nabla_s \mathbf{I}_s = \boldsymbol{bn} + \boldsymbol{nb}$$

So that

$$\begin{aligned} ((\nabla_s \boldsymbol{v})^T : \nabla_s \mathbf{I}_s) &= ((\nabla_s \boldsymbol{v})^T : \boldsymbol{bn}) + (\nabla_s \boldsymbol{v})^T : \boldsymbol{nb} \\ &= (\boldsymbol{b} : (\nabla_s \boldsymbol{v}))\boldsymbol{n} + \boldsymbol{b} \cdot (\nabla_s \boldsymbol{v}) \cdot \boldsymbol{n} \end{aligned} \tag{41}$$

given that $\boldsymbol{b}$ is symmetric. And we may use

$$\nabla_s \cdot (\nabla_s \boldsymbol{v})^T = \nabla_s(\nabla_s \cdot \boldsymbol{v}) - (\boldsymbol{b} \cdot (\nabla_s \boldsymbol{v}) \cdot \boldsymbol{n}) + (\boldsymbol{b} : (\nabla_s \boldsymbol{v}))\boldsymbol{n} \tag{42}$$

so that we may obtain Eqn. (43) from plugging Eqn. (41) and Eqn. (42) into Eqn. (38).

$$\begin{aligned} \nabla_s \cdot (2\mu_s \mathbf{D}_s) = \mu_s[&(\nabla_s \cdot \nabla_s \boldsymbol{v})\mathbf{I}_s + 2(\boldsymbol{b} : (\nabla_s \boldsymbol{v}))\boldsymbol{n} \\ &+ 2H(\nabla_s \boldsymbol{v}) \cdot \boldsymbol{n} + \nabla_s(\nabla_s \cdot \boldsymbol{v})\,] \end{aligned} \tag{43}$$

Collecting terms, the rhs of Eqn. (34) becomes.

$$\begin{aligned} &= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s - \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s - \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[(\nabla_s \cdot \nabla_s \boldsymbol{v})\mathbf{I}_s + 2(\boldsymbol{b} : (\nabla_s \boldsymbol{v}))\boldsymbol{n}] \\ &\quad + \mu_s[2H(\nabla_s \boldsymbol{v}) \cdot \boldsymbol{n} + \nabla_s(\nabla_s \cdot \boldsymbol{v})] \end{aligned} \tag{44}$$

$$\begin{aligned} &= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s - \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[(\nabla_s \cdot \nabla_s \boldsymbol{v})\mathbf{I}_s + 2(\boldsymbol{b} : (\nabla_s \boldsymbol{v}))\boldsymbol{n}] \\ &\quad + \mu_s[2H(\nabla_s \boldsymbol{v}) \cdot \boldsymbol{n} - \nabla_s(\nabla_s \cdot \boldsymbol{v})] \end{aligned} \tag{45}$$

$$\begin{aligned}&= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[(\nabla_s \cdot \nabla_s\boldsymbol{v})\mathbf{I_s} + 2(\boldsymbol{b} : (\nabla_s\boldsymbol{v}))\boldsymbol{n}] \\ &\quad + \mu_s[2H(\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n} - \nabla_s(\nabla_s \cdot \boldsymbol{v}) - 4H(\boldsymbol{n}(\mu_s)(\nabla_s \cdot \boldsymbol{v}))]\end{aligned} \tag{46}$$

$$\begin{aligned}&= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[(\nabla_s \cdot \nabla_s\boldsymbol{v})\mathbf{I_s} + 2H(\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n}] \\ &\quad + \mu_s[2(\boldsymbol{b} : (\nabla_s\boldsymbol{v}) - 2H(\nabla_s \cdot \boldsymbol{v}))\boldsymbol{n} - \nabla_s(\nabla_s \cdot \boldsymbol{v})]\end{aligned} \tag{47}$$

$$\begin{aligned}&= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[(\nabla_s \cdot \nabla_s\boldsymbol{v})\mathbf{I_s} + 2H(\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n}] \\ &\quad + \mu_s\left[2\left(\boldsymbol{b} : (\nabla_s\boldsymbol{v}) - 2H\left(\mathbf{I_s} . (\nabla_s\boldsymbol{v})\right)\right)\boldsymbol{n} - \nabla_s(\nabla_s \cdot \boldsymbol{v})\right]\end{aligned} \tag{48}$$

Then, we may use the following relation

$$\begin{aligned}\boldsymbol{n} \times \nabla_s[(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}] = {} & (\nabla_s \cdot \nabla_s\boldsymbol{v})\mathbf{I_s} - \nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ & + (2\boldsymbol{b} - 2H\mathbf{I_s}) \cdot (\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n}\end{aligned} \tag{49}$$

to rearrange the terms on the rhs of Eqn. (48).

$$\begin{aligned}&= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[\boldsymbol{n} \times \nabla_s[(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}] + 2H(\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n}] \\ &\quad + \mu_s\left[2\left(\boldsymbol{b} . (\nabla_s\boldsymbol{v}) - 2H\left(\mathbf{I_s} . (\nabla_s\boldsymbol{v})\right)\right)\boldsymbol{n} - ((2\boldsymbol{b} - 2H\mathbf{I_s}) \cdot (\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n})\right]\end{aligned} \tag{50}$$

Combining terms:

$$\begin{aligned}\boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) &= 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ &\quad + \mu_s[\boldsymbol{n} \times \nabla_s[(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}]] \\ &\quad + \mu_s\left[2\left((\boldsymbol{b} - 2H\mathbf{I_s}) . (\nabla_s\boldsymbol{v})\right)\boldsymbol{n} - (2(\boldsymbol{b} - 2H\mathbf{I_s}) \cdot (\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n})\right]\end{aligned} \tag{51}$$

Eqn. (51) is in agreement with Eqn. 4.2-20 on p. 110 of Edwards et al.[6]

2.4.1 Case Study: Cartesian Coordinates with flat interface with $\boldsymbol{n} = \boldsymbol{k}$.

The flat interface simplifies Eqn. (51) greatly. First, $H = 0$ and $\boldsymbol{b} = \boldsymbol{0}$, so only the second, fourth, and fifth term in Eqn. (51) is nonzero. The fourth term is

$$(\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) = (\kappa_s + \mu_s)\left(\boldsymbol{i}\frac{d}{dx}\left(\frac{dv_x}{dx} + \frac{dv_y}{dy}\right) + \boldsymbol{j}\frac{d}{dy}\left(\frac{dv_x}{dx} + \frac{dv_y}{dy}\right)\right) \tag{52}$$

The fifth term is a bit complicated. First, let's calculate $\nabla_s \times \boldsymbol{v}$. The key formula to remember for taking cross products within orthonormal coordinate systems is Eqn. (53).

$$\boldsymbol{\delta_i} \times \boldsymbol{\delta_j} = \sum_{k=1}^{3} \varepsilon_{ijk}\boldsymbol{\delta}_k \tag{53}$$

where ε_{ijk} is the permutation operator. Then, considering that $\boldsymbol{n} = \boldsymbol{k}$,

$$\begin{aligned} \nabla_s \times \boldsymbol{v} &= ((\boldsymbol{I} - \boldsymbol{nn}) \cdot \nabla) \times \boldsymbol{v} = \left(\boldsymbol{i}\frac{d}{dx} + \boldsymbol{j}\frac{d}{dy}\right) \times (\boldsymbol{i}v_x + \boldsymbol{j}v_y + \boldsymbol{k}v_z) \\ &= \boldsymbol{i}\left(\frac{dv_z}{dy}\right) + \boldsymbol{j}\left(-\frac{dv_z}{dx}\right) + \boldsymbol{k}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right) \end{aligned} \tag{54}$$

Then, taking the dot product with the surface normal again yields

$$(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n} = \frac{dv_y}{dx} - \frac{dv_x}{dy} \tag{55}$$

The surface gradient of Eqn. (55) is a vector oriented in the plane of the surface:

$$\nabla_s\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right) = \boldsymbol{i}\frac{d}{dx}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right) + \boldsymbol{j}\frac{d}{dy}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right) \tag{56}$$

so

$$\begin{aligned} \boldsymbol{n} \times \nabla_s[(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}] &= k \times \left(\boldsymbol{i}\frac{d}{dx}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right) + \boldsymbol{j}\frac{d}{dy}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right)\right) \\ &= \boldsymbol{i}\left(\frac{d}{dy}\left(\frac{dv_x}{dy} - \frac{dv_y}{dx}\right)\right) + \boldsymbol{j}\left(\frac{d}{dx}\left(\frac{dv_y}{dx} - \frac{dv_x}{dy}\right)\right) \end{aligned} \tag{57}$$

Putting this all together yields

$$
\begin{aligned}
-\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) &= \nabla_s\sigma + (\kappa_s+\mu_s)\left(\boldsymbol{i}\frac{d}{dx}\left(\frac{dv_x}{dx}+\frac{dv_y}{dy}\right)+\boldsymbol{j}\frac{d}{dy}\left(\frac{dv_x}{dx}+\frac{dv_y}{dy}\right)\right)\\
&\quad+\boldsymbol{i}\left(\frac{d}{dy}\left(\frac{dv_x}{dy}-\frac{dv_y}{dx}\right)\right)+\boldsymbol{j}\left(\frac{d}{dx}\left(\frac{dv_y}{dx}-\frac{dv_x}{dy}\right)\right)
\end{aligned}
\qquad (58)
$$

This formula agrees with Edwards, p. 112.

2.4.2 Case Study: Cylindrical Coordinates with a perfectly cylindrical interface $\boldsymbol{n} = \boldsymbol{r}$.

Let's assume that the fluid is a cylinder with $R = R(t)$ Then $\boldsymbol{n} = \boldsymbol{e_r}$ and the surface curvature tensor, $\boldsymbol{b}$, becomes:

$$
\begin{aligned}
\boldsymbol{b} &= -\nabla_s\boldsymbol{n} = -((\boldsymbol{I}_s-\boldsymbol{e}_r\boldsymbol{e}_r)\cdot\nabla)\boldsymbol{n}\\
&= -\left(\boldsymbol{e}_z\frac{d}{dz}+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\right)\boldsymbol{e}_r \quad ,\\
&= -\boldsymbol{e}_\theta\boldsymbol{e}_\theta\frac{1}{R_o}
\end{aligned}
\qquad (59)
$$

and

$$
H = \frac{1}{2}\boldsymbol{I}_s\cdot\boldsymbol{b} = -\frac{1}{2R_o} \qquad (60)
$$

so $\boldsymbol{b} - 2H\mathbf{I_s} = -\boldsymbol{e}_\theta\boldsymbol{e}_\theta\frac{1}{R_o}+\frac{1}{R_o}(\boldsymbol{e}_\theta\boldsymbol{e}_\theta+\boldsymbol{e}_z\boldsymbol{e}_z) = \frac{1}{R_o}\boldsymbol{e}_z\boldsymbol{e}_z$.

The first and second term is

$$
2H\sigma\boldsymbol{n}+\nabla_s\sigma = -\boldsymbol{e}_r\frac{\sigma}{R_0}+\boldsymbol{e}_\theta\frac{1}{R_0}\frac{d\sigma}{d\theta}+\boldsymbol{e}_z\frac{d\sigma}{dz} \qquad (61)
$$

The third term first needs a definition of the surface divergence.

$$
\begin{aligned}
\nabla_s\cdot\boldsymbol{v} &= \left(\boldsymbol{e}_z\frac{d}{dz}+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\right)\cdot(\boldsymbol{e}_r v_r+\boldsymbol{e}_\theta v_\theta+\boldsymbol{e}_z v_z)\\
&= \frac{dv_z}{dz}+\frac{1}{r}\frac{dv_\theta}{d\theta}+\frac{v_r}{r}
\end{aligned}
\qquad (62)
$$

Therefore,

$$
2H\boldsymbol{n}(\kappa_s+\mu_s)(\nabla_s\cdot\boldsymbol{v}) = \boldsymbol{e}_r\left(-\frac{(\kappa_s+\mu_s)}{R_0}\right)\left(\frac{dv_z}{dz}+\frac{1}{R_0}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_0}\right) \qquad (63)
$$

The fourth term is

$$(\kappa_s+\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v}) = (\kappa_s+\mu_s)\left(\boldsymbol{e}_z\frac{d}{dz}+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\right)\left(\frac{dv_z}{dz}+\frac{1}{r}\frac{dv_\theta}{d\theta}+\frac{v_r}{r}\right)$$

$$= (\kappa_s+\mu_s)\left(\boldsymbol{e}_z\frac{d}{dz}\left(\frac{dv_z}{dz}+\frac{1}{R_o}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_o}\right)+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\left(\frac{dv_z}{dz}+\frac{1}{R_o}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_o}\right)\right)$$

The 5th term is

$$\nabla_s\times\boldsymbol{v} = \left(\boldsymbol{e}_z\frac{d}{dz}+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\right)\times(\boldsymbol{e}_r v_r+\boldsymbol{e}_\theta v_\theta+\boldsymbol{e}_z v_z)$$

$$= \boldsymbol{e}_\theta\left(\frac{dv_r}{dz}\right)+\boldsymbol{e}_r\left(-\frac{dv_\theta}{dz}+\frac{1}{R_o}\frac{dv_z}{d\theta}\right)+\boldsymbol{e}_z\left(-\frac{dv_r}{d\theta}+\frac{v_\theta}{R_o}\right) \tag{64}$$

Therefore,

$$\boldsymbol{n}\cdot(\nabla_s\times\boldsymbol{v}) = \frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz} \tag{65}$$

And,

$$\nabla_s(\boldsymbol{n}\cdot(\nabla_s\times\boldsymbol{v})) = \left(\boldsymbol{e}_z\frac{d}{dz}+\boldsymbol{e}_\theta\frac{1}{r}\frac{d}{d\theta}\right)\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right)$$

$$= \boldsymbol{e}_z\frac{d}{dz}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right)+\boldsymbol{e}_\theta\frac{1}{R_o}\frac{d}{d\theta}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right) \tag{66}$$

so that

$$\boldsymbol{n}\times\nabla_s(\boldsymbol{n}\cdot(\nabla_s\times\boldsymbol{v})) = -\boldsymbol{e}_\theta\frac{d}{dz}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right)+\boldsymbol{e}_z\frac{1}{R_o}\frac{d}{d\theta}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right) \tag{67}$$

The 6th term is (68)

$$\mu_s\left[2\left((\boldsymbol{b}-2H\mathbf{I_s})\cdot(\nabla_s\boldsymbol{v})\right)\boldsymbol{n}\right] = 2\mu_s\left[\left(\frac{\boldsymbol{e}_z\boldsymbol{e}_z}{R_o}\right)\cdot(\nabla_s\boldsymbol{v})\right]\boldsymbol{e}_r$$

$$= \boldsymbol{e}_r\,2\frac{\mu_s}{R_o}\frac{dv_z}{dz} \tag{69}$$

The 7th term is (70)

$$(-\mu_s)[(2(\boldsymbol{b}-2H\mathbf{I}_{\boldsymbol{s}})\cdot(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n})] = (-\mu_s)2\left(\frac{\boldsymbol{e}_z\boldsymbol{e}_z}{R_o}\cdot(\nabla_s\boldsymbol{v})\cdot\boldsymbol{e}_r\right)$$
$$= (-\mu_s)2\left(\frac{\boldsymbol{e}_z}{R_o}\left(\frac{dv_r}{dz}\right)\right) \tag{71}$$

Combining terms

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_\theta = \frac{1}{R_0}\frac{d\sigma}{d\theta} + \frac{(\kappa_s+\mu_s)}{R_0}\frac{d}{d\theta}\left(\frac{dv_z}{dz}+\frac{1}{R_o}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_o}\right)$$
$$-\mu_s\frac{d}{dz}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right) \tag{72}$$

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_z = \frac{d\sigma}{dz} + (\kappa_s+\mu_s)\frac{d}{dz}\left(\frac{dv_z}{dz}+\frac{1}{R_o}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_o}\right)$$
$$+\mu_s\frac{1}{R_o}\frac{d}{d\theta}\left(\frac{1}{R_o}\frac{dv_z}{d\theta}-\frac{dv_\theta}{dz}\right)-2\mu_s\frac{d}{dz}\left(\frac{v_r}{R_o}\right) \tag{73}$$

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_r = -\frac{\sigma}{R_0} + \left(\frac{(\kappa_s+\mu_s)}{R_0}\right)\left(\frac{dv_z}{dz}+\frac{1}{R_0}\frac{dv_\theta}{d\theta}+\frac{v_r}{R_0}\right)+2\frac{\mu_s}{R_o}\frac{dv_z}{dz} \tag{74}$$

There are actually several differences between Eqns. (72) - (74) and the corresponding formulas in Edwards [6] p.113. Eqns. (72) - (74) include an v_r/R_o term that stems from the $\nabla\cdot\boldsymbol{v}$ formula in cylindrical coordinates. The corresponding formulas in Edwards [6] don't have the v_r/R_o term. However, I can't see why that term shouldn't exist. Also, Eqn. (73) contains an extra $-2\mu_s\frac{d}{dz}\left(\frac{v_r}{R_o}\right)$ term that stems from the 7th term in Eqn. (51) calculated in Eqn. (71). Again, it's not in Edwards, and I don't see why not. Lastly, Eqn. (74) does not contain the $-\kappa_s v_r/R_0$ term that the Edwards book has. Actually it does, but the multiplier is $\kappa_s+\mu_s$ instead of κ_s, and it's part of the $\nabla\cdot\boldsymbol{v}$ term. Resolution of these differences awaits further checking or alternative methods for derivation.

2.4.3 Case Study: Cylindrical Coordinates with a perfectly flat interface $\boldsymbol{n}=\boldsymbol{k}$.

Let's assume that the interface occurs on a plane in the axial coodinate Then, $\boldsymbol{n}=\boldsymbol{e}_z$ and the surface curvature tensor, $\boldsymbol{b}$, turns out to be identically zero. Also $H=0$.

The first and second term is

$$2H\sigma\boldsymbol{n}+\nabla_s\sigma = \boldsymbol{e}_\theta\frac{1}{r}\frac{d\sigma}{d\theta}+\boldsymbol{e}_r\frac{d\sigma}{dr} \tag{75}$$

The third term first needs a definition of the surface divergence.

$$
\begin{aligned}
\nabla_s \cdot \boldsymbol{v} &= \left(\boldsymbol{e}_r \frac{d}{dr} + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\right) \cdot (\boldsymbol{e}_r v_r + \boldsymbol{e}_\theta v_\theta + \boldsymbol{e}_z v_z) \\
&= \frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}
\end{aligned}
\tag{76}
$$

Therefore,

$$
2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) = 0 \tag{77}
$$

The fourth term is

$$
\begin{aligned}
(\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) &= (\kappa_s + \mu_s)\left(\boldsymbol{e}_r \frac{d}{dr} + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\right)\left(\frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}\right) \\
&= (\kappa_s + \mu_s)\left(\boldsymbol{e}_r \frac{d}{dr}\left(\frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}\right) + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\left(\frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}\right)\right)
\end{aligned}
$$

The 5th term is

$$
\begin{aligned}
\nabla_s \times \boldsymbol{v} &= \left(\boldsymbol{e}_r \frac{d}{dr} + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\right) \times (\boldsymbol{e}_r v_r + \boldsymbol{e}_\theta v_\theta + \boldsymbol{e}_z v_z) \\
&= \boldsymbol{e}_\theta\left(-\frac{dv_z}{dr}\right) + \boldsymbol{e}_r\left(\frac{1}{r}\frac{dv_z}{d\theta}\right) + \boldsymbol{e}_z\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right)
\end{aligned}
\tag{78}
$$

Therefore,

$$
\boldsymbol{n} \cdot (\nabla_s \times \boldsymbol{v}) = \frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r} \tag{79}
$$

And,

$$
\begin{aligned}
\nabla_s(\boldsymbol{n} \cdot (\nabla_s \times \boldsymbol{v})) &= \left(\boldsymbol{e}_r \frac{d}{dr} + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\right)\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) \\
&= \boldsymbol{e}_r \frac{d}{dr}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) + \boldsymbol{e}_\theta \frac{1}{r}\frac{d}{d\theta}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right)
\end{aligned}
\tag{80}
$$

so that

$$
\boldsymbol{n} \times \nabla_s(\boldsymbol{n} \cdot (\nabla_s \times \boldsymbol{v})) = \boldsymbol{e}_\theta \frac{d}{dr}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) - \boldsymbol{e}_r \frac{1}{r}\frac{d}{d\theta}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) \tag{81}
$$

The 6th and 7th terms are zero. Combining terms (82)

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_\theta = \frac{1}{r}\frac{d\sigma}{d\theta} + \frac{(\kappa_s+\mu_s)}{r}\frac{d}{d\theta}\left(\frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}\right) + \mu_s\frac{1}{r}\frac{d}{d\theta}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) \tag{83}$$

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_z = 0 \tag{84}$$

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext})\cdot\boldsymbol{e}_r = \frac{d\sigma}{dr} + (\kappa_s+\mu_s)\left(\boldsymbol{e}_r\frac{d}{dr}\left(\frac{dv_r}{dr} + \frac{1}{r}\frac{dv_\theta}{d\theta} + \frac{v_r}{r}\right)\right) + \mu_s\frac{d}{dr}\left(\frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r}\right) \tag{85}$$

One example of this type of flow is pure swirling flow, where $\boldsymbol{v} = \boldsymbol{e}_\theta a r$. Then, we note that

$$\boldsymbol{n}\cdot(\nabla_s\times\boldsymbol{v}) = \frac{dv_\theta}{dr} - \frac{1}{r}\frac{dv_r}{d\theta} + \frac{v_\theta}{r} = 2a \tag{86}$$

reflecting the fact that this is a pure vortex flow case/ Therefore, the derivative of this is zero and

$$\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) = \boldsymbol{0} \ . \tag{87}$$

The later formula reflects the fact that there is no shearing of the surface layer occurring for pure swirling flow. Therefore, the jump in surface traction shouldn't depend upon μ_s or κ_s .

3.0 Shell Variables Pertaining to the Surface Rheology Treatment

3.1 Gamma4

As a first step intermediary variables are calculated using Goma shell element capability

The 4th variable is $\Gamma_4 = (\nabla_s\times\boldsymbol{v})\cdot\boldsymbol{n}$.

The residual equation for this is

$$\int_{d\Omega} (\Gamma_4 - ((\nabla_s\times\boldsymbol{v})\cdot\boldsymbol{n}))\Phi_i d\Gamma = 0 \tag{88}$$

Using Gaussian integration the formula for ths projection equation becomes Eqn. (89).

$$R = \sum (\Gamma_4 - ((\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}))\Phi_i J_{shell} (h_1 h_2 h_3) \tag{89}$$

Let’s take a look at what this variable turns out to be, in several simple cases. Eqn. (86) demonstrates an example of a non-zero term. From the discussion in 2.4.2 and Eqn. (65), it turns out that the Γ_4 is zero in cylindrical coordinates, when there is no swirling flow, i.e., when v_θ is zero.

3.2 Surface Normal Unknowns

The surface normal may be calculated in 2D problems using the variable SH_N1 and SH_N2

$$\boldsymbol{n}^{sh} = \boldsymbol{n} = \frac{\boldsymbol{t}_1 \times \boldsymbol{t}_2}{det(\boldsymbol{J}_s)} \tag{90}$$

In 2D problems this reduces to

$$\boldsymbol{n}^{sh} = \begin{bmatrix} \text{SH\_N1} \\ \text{SH\_N2} \end{bmatrix} = \begin{bmatrix} \dfrac{t[0][1]}{det(\boldsymbol{J}_s)} \\ \dfrac{-t[0][0]}{det(\boldsymbol{J}_s)} \end{bmatrix} \tag{91}$$

The residual equations for these in 2D are

$$\int_{d\Omega} \left(\text{SH\_N1} - \frac{t[0][1]}{det(\boldsymbol{J}_s)} \right) \Phi_i d\Gamma = 0 \tag{92}$$

$$\int_{d\Omega} \left(\text{SH\_N2} + \frac{t[0][0]}{det(\boldsymbol{J}_s)} \right) \Phi_i d\Gamma = 0$$

Corresponding equations for 3D shells apply as well. The calculation of surface normals is described in the Coordinate systems memo for goma [8]. No surface diffusion was added to this equatoin. It seems to work and bunaffected by noise.

3.3 Surface Divergence of the velocity

The surface divergence of the velocity may be calculated using the following formula.

$$\Gamma_1 = \nabla_s \cdot \boldsymbol{v} = ((\mathbf{I} - \boldsymbol{nn}) \bullet \nabla) \bullet \boldsymbol{v} \tag{93}$$

Within goma this may be directly solved as

$$\Gamma_1 = ((\mathbf{I} - \boldsymbol{nn}) \bullet \nabla) \bullet \boldsymbol{v} = (\mathbf{I} - \boldsymbol{nn}):\nabla \boldsymbol{v} = \sum_{i=1}^{VIM}\sum_{j=1}^{VIM}\left(\delta_{ij}\frac{\partial v_i}{\partial x_j} - n_i n_j \frac{\partial v_i}{\partial x_j}\right) \tag{94}$$

$\nabla \boldsymbol{v}$ is the gradient of the velocity, a tensor. An explicit example of this would be the pure swirling flow with a flat interface in cylindrical coordinates, where $\boldsymbol{n} = \boldsymbol{e}_z$. In this case $\boldsymbol{v} = ar\boldsymbol{e}_\theta$. And,

$$\Gamma_1 = \nabla_s \cdot \boldsymbol{v} = \frac{\partial}{\partial r} v_r + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} = 0 \tag{95}$$

For the case of a flat interface, the variable for the surface divergence is $\Gamma_1 = \nabla_s \cdot v$ would be identically zero as v_r is equal to zero unless the domain boundaries in the radial direction are oscillating.

Another example of interest would be an expanding or contracting spherical bubble. In this case

$$\begin{aligned}\Gamma_1 = \nabla_s \cdot \boldsymbol{v} &= (\boldsymbol{e}_\theta\boldsymbol{e}_\theta + \boldsymbol{e}_\phi\boldsymbol{e}_\phi):\left(\left(\frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r}\right)\boldsymbol{e}_\theta\boldsymbol{e}_\theta + \left(\frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi} + \frac{v_r}{r} + \frac{v_\theta}{r}\cot\theta\right)\boldsymbol{e}_\phi\boldsymbol{e}_\phi\right) = 0 \\ &= \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{2v_r}{r} + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi} + \frac{v_\theta}{r}\cot\theta\end{aligned} \tag{96}$$

The residual equation for this is

$$\int_{d\Omega} (\Gamma_1 - (\nabla_s \cdot v))\Phi_i d\Gamma = 0 \tag{97}$$

Note, we have had tremendous difficulting solving Eqn. (97) in practice. The issue was that such a refined mesh was needed that the calculations ground to a halt. However, we believe it may be beneficial to rewrite Eqn. (97) to lower the order of the equation. We start with the expression, which is an expression of the surface divergence theorum.

$$\int_{d\Omega} (\nabla_s \cdot \boldsymbol{v}\Phi_i) d\Gamma = \int_{d\Omega} (\boldsymbol{m} \cdot \boldsymbol{v}\Phi_i) d\gamma - \int_{d\Omega} 2H(\boldsymbol{n} \cdot \boldsymbol{v}\Phi_i) d\Gamma \tag{98}$$

In this expression, the mean surface curvature H is equal to

$$H = -\left(\frac{1}{2}\nabla_s \bullet \boldsymbol{n}\right) = \frac{1}{2}(\kappa_{min} + \kappa_{max}) \tag{99}$$

Just for review, κ_{min} and κ_{max} are the minimum and maximum principle radii of curvature. Note for spheres the way we have defined the mean surface curvature, H is equal to $-1/r$, where the sign is correct (curvatures are negative for convex cases where $\boldsymbol{n}$ points out of the enclosed object.

We may then expand the lhs of Eqn. (98) to achieve Eqn. (100).

$$\int_{d\Omega} (\nabla_s \cdot \boldsymbol{v}\Phi_i) d\Gamma = \int_{d\Omega} \Phi_i(\nabla_s \cdot \boldsymbol{v}) d\Gamma + \int_{d\Omega} (\boldsymbol{I} - \boldsymbol{nn}):(\boldsymbol{v}(\nabla\Phi_i)) d\Gamma \qquad (100)$$

Then, we may combine the two equations to yield Eqn. (101).

$$\int_{d\Omega} \Phi_i(\nabla_s \cdot \boldsymbol{v}) d\Gamma = -\int_{d\Omega} (\boldsymbol{I} - \boldsymbol{nn}):(\boldsymbol{v}(\nabla\Phi_i)) d\Gamma + \int_{d\gamma} (\boldsymbol{m} \cdot \boldsymbol{v}\Phi_i) d\gamma - \int_{d\Omega} 2H\Phi_i(\boldsymbol{n} \cdot \boldsymbol{v}) d\Gamma \qquad (101)$$

The revised equation has some merits over the initial equation because the order of the unknown, $\boldsymbol{v}$, has been reduced by one in the expression. Therefore, we may expect that the convergence of the variable $\Gamma_1 = \nabla_s \cdot v$ will be greatly enhanced by the restatement of the equation. It also separates out important parts of the original expression. In particular, the last part of the expression, which is proportional to the mean curvature, H, is distinctly separated out, leaving terms that are exceedingly small for normal conditions that don't consist of outflow boundary conditions involving flowing surfaces, i.e., where $\boldsymbol{m} \cdot \boldsymbol{v}\Phi_i$ is nonzero.

The expression in Eqn. (100) may be written out

$$(\boldsymbol{I} - \boldsymbol{nn}):(\boldsymbol{v}(\nabla\Phi_i)) = \sum_{a=1}^{VIM} \sum_{b=1}^{VIM} \left(\delta_{ab} v_a \frac{1}{h_b} \frac{\partial \Phi_i}{\partial q_b} - n_a n_b v_a \frac{1}{h_b} \frac{\partial \Phi_i}{\partial q_b} \right) \qquad (102)$$

where h_b is the scale factor for the bth coordinate.

The edge integral, the second expression on the rhs of Eqn. (101) has not been explicitly coded up within Goma. The edge integral is zero for both symmetry boundary conditions and wall contact conditions. It is only non-zero for outflow and inflow boundary conditions with contact lines involving fluids which are flowing into or out of the domain. Our initial test cases don't include any problems of this type.

Initial numerical expeimrents using Eqn. (101) as input to the projection equation instead of the lhs of Eqn. (101) proved problematic. THe end result was that we abaondoned the effort in favor of adding surface difufsion into the projection equations and in going to more refined meshes.

3.3.1 Adding a surface diffusion term

We still have problems with this term. Therefore, let's add in a surface diffusion term. Consider a concentration of a surface species c that undergoes reaction and diffusion. We may write a continuity equation for c.

$$\frac{dc}{dt} + k_f - k_r c = D(\nabla_s \cdot \nabla_s c) \tag{103}$$

By analogy with Eqn. (103), we may write a diffusion addition for Γ_1 keeping track of signs. We will ignore the time dependence, assuming steady state behavior of *c*.

$$-\int_{d\Omega} ((\nabla_s \cdot v) - \Gamma_1)\Phi_i d\Gamma + \int_{d\Omega} D(\nabla_s \cdot \nabla_s \Gamma_1)\Phi_i d\Gamma = 0 \tag{104}$$

We may do the normal integration by parts using the surface divergence theorum. We note that the $\boldsymbol{n} \cdot \nabla_s \Gamma_1 = 0$ term simplifies the resulting expression.

$$-\int_{d\Omega} ((\nabla_s \cdot v) - \Gamma_1)\Phi_i d\Gamma - \int_{d\Omega} D(\nabla_s \Phi_i \cdot \nabla_s \Gamma_1) d\Gamma + \int_{d\gamma} \Phi_i(\boldsymbol{m} \cdot D\nabla_s \Gamma_1) d\gamma = \quad 0\ \mathrm{T} \tag{105}$$

The middle term may additionally be simplified to yield

$$\begin{aligned} -\int_{d\Omega} ((\nabla_s \cdot v) - \Gamma_1)\Phi_i d\Gamma - \int_{d\Omega} D(\nabla\Phi_i \cdot \nabla\Gamma_1 - (\boldsymbol{n} \cdot \nabla\Phi_i)(\boldsymbol{n} \cdot \nabla\Gamma_1)) d\Gamma \\ + \int_{d\gamma} \Phi_i(\boldsymbol{m} \cdot D\nabla_s \Gamma_1) d\gamma = 0 \end{aligned} \tag{106}$$

We don’t believe the edge term needs to be implemented at this time for the projection equations for any of the projection equations employed. Eqn. (106) has been implemented with Goma. It appears to be very successful at eliminating problems with the inclusion of noise within the porjection equations.

3.4 Surface Calculation of the Curvature

The local curvature of the surface is calculated as a shell variable, Γ_2 of the velocity may be calculated using the following formula.

$$\Gamma_2 = -\frac{1}{2}\nabla_s \cdot \boldsymbol{n} = -\frac{1}{2}((\mathbf{I} - \boldsymbol{n}\boldsymbol{n}) \bullet \nabla) \bullet \boldsymbol{n} \tag{107}$$

Within goma this is solved as

$$\Gamma_2 = ((\mathbf{I}-\boldsymbol{nn})\bullet\nabla)\bullet\boldsymbol{v} = \sum_{i=1}^{VIM}\sum_{j=1}^{VIM}\left(\delta_{ij}\frac{\partial n_i}{\partial x_j} - n_i n_j\frac{\partial n_i}{\partial x_j}\right) \tag{108}$$

An explicit example of this would be a pure sphere. In that case $\boldsymbol{n} = \boldsymbol{e}_r$, and

$$\Gamma_2 = -\frac{1}{2}\nabla_s\cdot\boldsymbol{n} = -\frac{1}{2}\left((\mathbf{I}-\boldsymbol{nn})\bullet\left(\frac{\boldsymbol{e}_\theta\boldsymbol{e}_\theta}{r}+\frac{\boldsymbol{e}_\phi\boldsymbol{e}_\phi}{r}\right)\right) = -\frac{1}{r} \tag{109}$$

A surface diffusion term was added to the equation system as well. This was put in because the curvature variable was observed to have oscillations in its value when the shear viscosity was set to nominal values. These oscillations eventually caused the simulations to break down. The equation that's solved is Eqn. (110).

$$-\int_{d\Omega}\left(\left(-\frac{1}{2}\nabla_s\cdot\boldsymbol{n}\right)-\Gamma_2\right)\Phi_i\,d\Gamma - \int_{d\Omega}D(\nabla\Phi_i\cdot\nabla\Gamma_2-(\boldsymbol{n}\cdot\nabla\Phi_i)(\boldsymbol{n}\cdot\nabla\Gamma_2))d\Gamma + \int_{d\gamma}\Phi_i(\boldsymbol{m}\cdot D\nabla_s\Gamma_2)d\gamma = 0 \tag{110}$$

In order to solve issues that arose at r = 0 under cylindrical coordinates we implemented the following boundary condition, which is implemented on the edge of a shell using a collocation strategy.

$$\int_{d\gamma}(\boldsymbol{m}\cdot\nabla\Gamma_2)d\gamma = 0 \tag{111}$$

The card is called GAMMA2_DERIV_SYMM. An example of its implementation is given below.

BC = GAMMA2_DERIV_SYMM NS 101 5 0.0

Collocation boundary conditions are usually applied on the nodes along a side set. However, Goma has been changed for this and the corresponding GAMMA1 boundary condition to apply collocation conditions at a node set consisting of a single point. ***m*** is the binormal vector introduced in Eqn. (19). It is the normal tangent to the surface along the line that points out of the surface. Eqn. (111) is applied at the r = 0 point, and replaces the equation at that point, in order to ensure symmetry is enforced. When the shear surface viscosity is nonzero, this additional constraint is apparently necessary.

3.5 Surface Calculation of $\nabla_s \boldsymbol{v} \cdot \boldsymbol{n}$

This term is nonzero because the surface normal operates on the right index and not on the left index of $\nabla_s \boldsymbol{v}$.

$$\boldsymbol{\Gamma_3} = \nabla_s \boldsymbol{v} \cdot \boldsymbol{n} = ((\mathbf{I} - \boldsymbol{nn}) \bullet \nabla \boldsymbol{v}) \bullet \boldsymbol{n} \tag{112}$$

$\boldsymbol{\Gamma_3}$ is a vector quantity. Each of its scalar components, β, is evaluated from the following equation, Eqn. (113).

$$-\int_{d\Omega} ([(\nabla_s \boldsymbol{v} \cdot \boldsymbol{n}) \cdot \boldsymbol{e}_\beta] - \Gamma_3^\beta)\Phi_i \, d\Gamma - \int_{d\Omega} D(\nabla\Phi_i \cdot \nabla\Gamma_3^\beta - (\boldsymbol{n} \cdot \nabla\Phi_i)(\boldsymbol{n} \cdot \nabla\Gamma_3^\beta))\, d\Gamma + \int_{d\gamma} \Phi_i (\boldsymbol{m} \cdot D\nabla_s \Gamma_3^\beta)\, d\gamma = 0 \tag{113}$$

3.6 Surface Terms

Putting it all together, from the finite element formulation, the difference in the normal stresses applied on either side of an interface arises naturally. We have shown that this difference can be expressed by Eqn. (114).

$$\begin{aligned} \boldsymbol{n} \cdot (\boldsymbol{T}_{in} - \boldsymbol{T}_{ext}) = {} & 2H\sigma\boldsymbol{n} + \nabla_s\sigma + 2H\boldsymbol{n}(\kappa_s + \mu_s)(\nabla_s \cdot \boldsymbol{v}) + (\kappa_s + \mu_s)\nabla_s(\nabla_s \cdot \boldsymbol{v}) \\ & + \mu_s[\boldsymbol{n} \times \nabla_s[(\nabla_s \times \boldsymbol{v}) \cdot \boldsymbol{n}]] \\ & + \mu_s\left[2\left((\boldsymbol{b} - 2H\mathbf{I_s}) . (\nabla_s\boldsymbol{v})\right)\boldsymbol{n} - (2(\boldsymbol{b} - 2H\mathbf{I_s}) \cdot (\nabla_s\boldsymbol{v}) \cdot \boldsymbol{n})\right] \end{aligned} \tag{114}$$

Let's review what there is already. There are two boundary conditions that apply. One is the CAPILLARY boundary condition. The other is the CAPILLARY_SHEAR_VISC boundary condition.

They are both integrated boundary conditions applied on surfaces. The CAPILLARY boundary condition imposes the following equation on single sided interfaces.

$$\boldsymbol{n} \cdot (\boldsymbol{T}_{in}) = (2)H\sigma\boldsymbol{n} - \boldsymbol{n}P_{ex} + \nabla_s\sigma \tag{115}$$

The CAPILLARY card may also be used for internal surfaces between fluid regions. The formulation turns out to be almost the same. The CAPILLARY card picks one side of the interface (or the user can pick the side alternatively) to be the primary side and implements the same boundary condition with $P_{ex} = 0$. This turns out to implement Eqn. (15) exactly, creating the jump in the pressure across the interface exactly if discontinuous P1 presure interpolations are chosen.

With the addition of surface viscosity, extra terms are needed at the interface. These are represented by terms in Eqn. (114) that are not in Eqn. (15). These are listed in Eqn. (116).

$$\begin{aligned}\boldsymbol{n}\cdot(\boldsymbol{S}_{extra}) &= 2H\boldsymbol{n}(\kappa_s+\mu_s)(\nabla_s\cdot\boldsymbol{v}) + (\kappa_s+\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v})\\ &\quad + \mu_s[\boldsymbol{n}\times\nabla_s[(\nabla_s\times\boldsymbol{v})\cdot\boldsymbol{n}]]\\ &\quad + \mu_s\left[2\left((\boldsymbol{b}-2H\mathbf{I}_{\boldsymbol{s}}) . (\nabla_s\boldsymbol{v})\right)\boldsymbol{n} - (2(\boldsymbol{b}-2H\mathbf{I}_{\boldsymbol{s}})\cdot(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n})\right]\end{aligned} \tag{116}$$

The CAPILLARY_SHEAR_VISC boundary condition calculates these extra terms and implements them on top of the CAPILLARY card. These are integrated weakly in the galerkin format just as the CAPILLARY card terms..

$$\int_\Gamma \left(\phi_i\boldsymbol{e}_\beta\boldsymbol{n}\cdot\boldsymbol{S}_{extra}\right)d\Gamma \tag{117}$$

Let's break down each term in Eqn. (116) and figure out how we are to solve it.

$$\int_\Gamma \phi_i(\boldsymbol{e}_\beta\cdot\boldsymbol{n})2H(\kappa_s+\mu_s)(\nabla_s\cdot\boldsymbol{v})d\Gamma \tag{118}$$

The CAPILLARY_SHEAR_VISC card uses the routine apply_surface_viscosity(). Within the routine the following implementation described by Eqns. (119) to (123) is carried out.

$$2H\boldsymbol{n}(\kappa_s+\mu_s)(\nabla_s\cdot\boldsymbol{v}) = 2\Gamma_2\boldsymbol{n}(\kappa_s+\mu_s)(\Gamma_1) \tag{119}$$

$$(\kappa_s+\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v}) = (\kappa_s+\mu_s)\nabla_s(\Gamma_1) \tag{120}$$

$$\mu_s[\boldsymbol{n}\times\nabla_s[(\nabla_s\times\boldsymbol{v})\cdot\boldsymbol{n}]] = \mu_s[\boldsymbol{n}\times\nabla_s\Gamma_4] = \mu_s[\boldsymbol{n}\times\nabla\Gamma_4] \tag{121}$$

$$\mu_s\left[2\left((\boldsymbol{b}-2H\mathbf{I}_{\boldsymbol{s}}) . (\nabla_s\boldsymbol{v})\right)\boldsymbol{n}\right] = \mu_s[2((\boldsymbol{b}-2\Gamma_2\mathbf{I}_{\boldsymbol{s}}) : (\nabla_s\boldsymbol{v}))\boldsymbol{n}] \tag{122}$$

$$\mu_s[-(2(\boldsymbol{b}-2H\mathbf{I}_{\boldsymbol{s}})\cdot(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n})] = \mu_s[-(2(\boldsymbol{b}-2\Gamma_2\mathbf{I}_{\boldsymbol{s}})\cdot\boldsymbol{\Gamma}_{\mathbf{3}})] \tag{123}$$

In Eqns. (122) to (123), the surface diadic is calculated from

$$\mathbf{I}_{\boldsymbol{s}} = \mathbf{I} - \boldsymbol{nn} \tag{124}$$

In Eqns. (119) to (123), all of the terms only involve single derivatives. Note, we have used Γ_2 in Eqn. (122) to Eqn. (123). It simplifies the arithmetic. However, we wonder whether that is the source of inconsistency. The term $\boldsymbol{b} - 2\Gamma_2\mathbf{I}_{\boldsymbol{s}}$ should be equal to zero identically for planes, cylinders, and spheres. Therefore it might seem that the same interpolation scheme should be used for all element of that vector. However, the significance of this has yet to be checked.

An example example input deck section for the surface equations is provided below

```
 MAT = surface 5
  Coordinate System = CYLINDRICAL
  Element Mapping   = isoparametric
  Mesh Motion = ARBITRARY
  Number of bulk species = 0

        Number of EQ = 7
        EQ = n_dot_curl_v Q2    gamma4 Q2             1.
        EQ = shell_normal1 Q2   SH_N1  Q2             1.
        EQ = shell_normal2 Q2   SH_N2  Q2             1.
        EQ = SHELL_SURF_CURV Q1 gamma2  Q1            1.
        EQ = SHELL_SURF_DIV_V Q1 gamma1  Q1            1.
        EQ = GRAD_V_DOT_N1 Q2 gamma3_1  Q2            1.
        EQ = GRAD_V_DOT_N2 Q2 gamma3_2  Q2            1
```

The CAPILLARY_SHEAR boundary condition is applied via the following cards.

```
#
#      CAPILLARY
#        Set the surface tension at the interface
#
BC = CAPILLARY SS 1 72. 0.0 0.0
BC = CAPILLARY_SHEAR_VISC SS 1 1.0 1.0 1.2 4.8
```

The first two doubles (after the identification of the side set on which the boundary condition is applied, i.e., SS 1) are the surface shear viscosity and the surface dilatational viscosity. The last two doubles on the card are optional parameters indicating the initial time and final time for a ramp of the surface viscosity values. If those numbers are on the card, a linear time ramp in the values of τ_s and κ_s from an initial value of zero for both of those parameters is carried out between the two times. For example in the case above the surface viscosity terms are ramped up form 1.2 to 4.8 seconds. This time ramp has been found to be useful in starting out the time dependent calculations. In those calculations there is frequently an oscillatory quasi-equilibration period at the start of the calculations, and it is easier to achieve the quasi-equilibrium without the addition of the surface viscosity terms.

3.7 Other Boundary conditions

For the cylindrical geometry cases where we are solving fluid mechanics at r = 0, we have implemented a boundary condition imposing a zero radial gradient at r = 0 for the axial velocity. An example of the card usage is

```
#        Set the axial velocity’s radial derivative
#
BC = DVZDR_ZERO SS 4
```

This boundary condition is applied as a collocated boundary condition, therefore throwing out the surface integral at r = 0 which is problematic in any case. Note, in all cases setting the radial velocity to zero is employed.

3.8 Results of the Capillary Bubble Problem.

It became clear at the end of the program that there were unresolved issues in the formulation that prevented the oscillating bubble problem from being solved correctly. In particular it was found using a heuristic approach that a sign on one of the surface rheology terms had to be flipped in order for the equations to be solved successfully.

$$\begin{aligned}\boldsymbol{n}\cdot(\boldsymbol{T}_{in}-\boldsymbol{T}_{ext}) &= 2H\sigma\boldsymbol{n}+\nabla_s\sigma+2H\boldsymbol{n}(\kappa_s+\mu_s)(\nabla_s\cdot\boldsymbol{v})+(\kappa_s+\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v})\\ &\quad+\mu_s[\boldsymbol{n}\times\nabla_s[(\nabla_s\times\boldsymbol{v})\cdot\boldsymbol{n}]]\\ &\quad+\mu_s\left[2\left((\boldsymbol{b}-2H\mathbf{I}_s)\cdot(\nabla_s\boldsymbol{v})\right)\boldsymbol{n}-(2(\boldsymbol{b}-2H\mathbf{I}_s)\cdot(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n})\right]\end{aligned} \tag{125}$$

The sign of the term that had to be flipped was the last term on the first line, $(\kappa_s+\mu_s)\nabla_s(\nabla_s\cdot\boldsymbol{v})$. Without flipping this term, the solution appeared to gain energy even under quiescent conditions. Recirculations would appear in the bubble problem that revolved in both directions depending upon the starting conditions. When the sign was flipped to a negative value, this degree of freedom disappeared. This behavior is characteristic of a non-null null-space for the jacobian for the positive sign and the violation of the first law of thermodynamics.

Just to reiterate, there is no theoretical basis for the flipping the sign. The fact that it was necessary indicates that there is an error within Goma of some sort.

While I was able to solve dilatational viscosity problems with this kluge of an arbitrary value of κ_s, I was not able to do the same for the shear surface viscosity problems. The culprit was the first term on the last line of Eqn. (125). Even flipping the sign didn't help that term. The calculations reached a point where it appeared that the problem became ill-conditioned and the step changes in the solution variables did not decrease along with the residual values. Again, this is characteristic of a Jacobian that is near singular, with a non-null null vector. The null vector seemed to include mostly surface terms involving the vector $(\nabla_s\boldsymbol{v})\cdot\boldsymbol{n}$, which appeared to be constant and the value of $(\nabla_s\cdot\boldsymbol{v})$, whose value was constant throughout the bubble surface. This null vector also included a contribution from ΔP the pressure drop accross the bubble surface.

3.9 Recommendation

It's recommended that an approach based on returning to a raw formulation of the surface stresses be used. The starting condition for this formulation would be Eqn. (32). In this formulation the shell variables to be used would be the individual components of $\boldsymbol{D}_s$, of which there are 6 (because it's symmetric). We are guessing here that using the raw surface strain components $\boldsymbol{D}_s$ should less problematic just as using the raw bulk strain tensor is less problematic for bulk viscosity formulations.

An additional advantage for this formulation is that non-newtonian formulations for the surface shear and dilational viscosities could be employed in a rigorous and straightfoward manner, once the method is verified using newtonian viscosities.

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