A Numerical Method for a Second-Gradient Theory of Incompressible Fluid Flow

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Abstract

This work concerns the development of a finite-element method for discretizing a recent second-gradient theory for the flow of incompressible fluids. The new theory gives rise to a flow equation involving higher-order gradients of the velocity field and introduces an accompanying length scale and boundary conditions. Finite-element methods based on similar equations involving fourth-order differential operators typically rely on $C^1$-continuous basis functions or a mixed approach, both of which entail certain implementational difficulties. Here, we examine the adaptation of a relatively inexpensive, nonconforming method based on $C^0$-continuous basis functions. We first develop the variational form of the method and establish consistency. The method weakly enforces continuity of the vorticity, traction, and hypertraction across interelement boundaries. Stabilization is achieved via Nitsche’s method. Further, pressure stabilization scales with the higher-order moduli, so that a classical formulation is recovered as a particular limit. The numerical method is verified for the problem of steady, plane Poiseuille flow. We then provide several numerical examples illustrating the robustness of the method and contrasting the predictions to those provided by classical Navier–Stokes theory.

Key words: finite-element, nonconforming, incompressible, fluid, second-gradient

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1 Introduction

Increasingly, continuum formulations are being explored as a means to capture phenomena at smaller and smaller length scales. An essential question con-
cerns the proper strategy for extending classical theories to capture behavior that is scale dependent. While tremendous theoretical progress has been made along these lines over the past decade, the development of robust numerical methods has lagged behind. This work concerns a new finite-element method for discretizing a theory of incompressible fluid flow that incorporates length scale effects through the introduction of higher-order gradients of the velocity field. If successful in accurately representing fluid flow at small length scales, such an approach might serve as an attractive and efficient complement to methods based on molecular dynamics or atomistics.

The origins of the second-gradient theory of fluid flow can be traced back to Gurtin [1], who developed general balance equations and associated boundary conditions for a “second-grade material” using a nonstandard form of the principle of virtual power. Gurtin’s work generalizes the early results provided by Toupin [2,3], who developed analogous conditions for an elastic body whose strain energy depends on first and second gradients of the deformation. The main contribution of Gurtin’s work is that it is independent of constitutive assumptions. As such, it is equally applicable to fluids as solids. Fried and Gurtin [4] recently adapted this framework to develop a theory of fluid flow at small length scales. Subsequently, Fried and Gurtin [5] established a connection to the Lagrangian averaged Navier–Stokes-$\alpha$ model for turbulent flow.

Aside from an extension of the Navier–Stokes equation involving higher-order gradients of the velocity field and involving an accompanying length scale, this framework provides consistent boundary conditions on free and fixed boundaries. The free boundary conditions involve the curvature of the free surface; among the conditions for a fixed boundary are generalized adherence and slip conditions, each of which involves a material length scale.

Our current interest is focused on examining further the predictions that this second-gradient theory for fluid flow provides. Accordingly, we discuss an advanced numerical method that is based on this new, higher-order continuum theory. The challenges include properly incorporating the higher-order velocity gradients and stabilizing the pressure field. The flow equation arising from the second-gradient theory involves fourth-order partial derivatives. Hence, a standard Galerkin approximation requires $C^1$-continuous basis functions such that both the velocity field and its first derivatives are continuous. Examples include functions based on Hermite polynomials. While relatively simple to construct on uniform meshes, unstructured meshes present difficulties and certain partitions are not permissible with isoparametric versions of Hermite elements; cf., e.g., Petera and Pittman [6]. Further, additional care is required to impose boundary conditions for a theory stemming from a (classically) second-order problem using elements designed for fourth-order problems. Mixed finite-element methods present a relatively expensive alternative, requiring separate approximations for primary and secondary fields; cf., e.g., Fortin and Brezzi [7].
To overcome some of the drawbacks of these traditional methods, we adapt the continuous/discontinuous Galerkin (C/DG) method proposed by Engel et al. [8]. This is essentially a nonconforming method—as the basis functions, while continuous, do not lie in the proper space for a strict Galerkin method. Continuity requirements for the derivatives are weakly satisfied by borrowing concepts from discontinuous Galerkin methods, in particular by extending the variational equation to include stabilization terms on interelement boundaries. Engel et al. [8] successfully applied the method to solve problems involving fourth-order elliptic operators arising from theories for thin beams and plates and strain gradient elasticity. Here, we develop a comparable formulation for a gradient theory for the flow of incompressible fluids.

The outline of this paper is as follows. In the next section, we introduce general balance equations and the boundary conditions developed by Fried and Gurtin [5]. Section 3 describes the weak formulation for the newly developed flow equations. In section 4, we introduce the nonconforming variational formulation and discretization with finite elements for the second-gradient theory. Numerical examples investigating the performance of the method are provided in section 5. Finally a summary and concluding remarks are given in the last section.

2 Governing Equations

We work with the generalized equations for fluid flow introduced by Fried and Gurtin [5]. The theory is based on a nonstandard form of the principle of virtual power provided by Gurtin [1]. The principle of virtual power is used as a basic tool in determining the structure of the tractions and of the local force balances. Classically, the power expended within an arbitrary control volume $R$ in the region of space occupied by the deformed body has the simple form

$$W_{\text{int}}(R) = \int_R T : \text{grad} \mathbf{v} \, dv = \int_R T_{ij} v_{i,j} \, dv \quad (1)$$

with $T$ the Cauchy stress and $T : \text{grad} \mathbf{v}$ the stress power. Fried and Gurtin [5] (see also Fried and Gurtin [4]) generalize the classical theory by including, in the internal power, a term linear in the vorticity gradient $\text{grad} \mathbf{\omega} = \text{grad} \text{curl} \mathbf{v}$. Specifically, a second-order tensor-valued hyperstress $G$ is introduced via an internal power expenditure of the form $G : \text{grad} \mathbf{\omega}$. The internal power expended within $R$ then becomes

$$W_{\text{int}}(R) = \int_R (T : \text{grad} \mathbf{v} + G : \text{grad} \mathbf{\omega}) \, dv = \int_R (T_{ij} v_{i,j} + G_{ij} \omega_{i,j}) \, dv. \quad (2)$$
In conjunction with the internal power expenditure (2), Fried and Gurtin [5] introduce a corresponding external power expenditure

$$W_{\text{ext}}(R) = \int_S \left( t_S \cdot \mathbf{v} + m_S \cdot \frac{\partial \mathbf{v}}{\partial n} \right) \, da + \int_R \mathbf{b} \cdot \mathbf{v} \, dv, \quad (3)$$

in which $t_S$ and $m_S$ represent tractions on the bounding surface $S = \partial R$ of $R$, while $\mathbf{b}$ represents the net inertial and noninertial body force acting within the body. Here the term

$$m_S \cdot \frac{\partial \mathbf{v}}{\partial n},$$

which is not present in classical theories, is needed to balance the effects of the internal-power term $G : \text{grad} \omega$, which involves the second gradient of $\mathbf{v}$.

The principle of virtual power replaces $\mathbf{v}$ by $\tilde{\mathbf{v}}$ and $\omega$ by curl $\tilde{\mathbf{v}}$ and is based on the requirement that

$$W_{\text{ext}}(R, \tilde{\mathbf{v}}) = W_{\text{int}}(R, \tilde{\mathbf{v}}) \quad (4)$$

for all control volumes $R$ and any choice of the virtual velocity field $\tilde{\mathbf{v}}$. Consequences of the virtual power principle and the requirement that the internal power expenditure be frame-indifferent are that:

(i) The classical macroscopic balance $\rho \dot{\mathbf{v}} = \text{div} \mathbf{T}$ must be replaced by the balance

$$\rho \dot{\mathbf{v}} = \text{div} \mathbf{T} + \text{curl div} \mathbf{G}, \quad (5)$$

with $\mathbf{T}$ symmetric as in the classical theory.

(ii) Cauchy’s classical condition $t_S = \mathbf{T} n$ for the traction across a surface $S$ with unit normal $\mathbf{n}$ must be replaced by the conditions

$$\begin{cases}
  t_S = \mathbf{T} n + \text{div}_S (G n \times) + \mathbf{n} \times (\text{div} G - 2K G n), \\
  m_S = \mathbf{n} \times G n,
\end{cases} \quad (6)$$

in which $\text{div}_S$ is the divergence operator on $S$ and $K = -\frac{1}{2} \text{div}_S \mathbf{n}$ is the mean curvature of $S$.

When supplemented by constitutive equations for the stress and hyperstress, the balance (5) yields a flow equation. Restricting attention to incompressible fluids, we invoke the standard decomposition

$$\mathbf{T} = \mathbf{S} - p \mathbf{1}, \quad \text{tr} \mathbf{S} = 0, \quad (7)$$

of the stress into a traceless extra stress $\mathbf{S}$ and a powerless pressure $p$ and take the extra stress to be of the form

$$\mathbf{S} = 2\mu \mathbf{D}, \quad \mu > 0, \quad (8)$$
where $D = \frac{1}{2}(\text{grad} v + (\text{grad} v)^\top)$ is the stretch-rate. Further, we take the hyperstress to be of the simple linear form

$$G = \zeta \text{grad} \omega + \xi (\text{grad} \omega)^\top,$$

with $\zeta > 0$ and $-\zeta \leq \xi \leq \zeta$ to ensure non-negative dissipation.

Using (7)–(9) in (5) and assuming that the moduli $\mu$, $\zeta$, and $\xi$ are constant, we arrive at the flow equation

$$\rho \dot{v} = -\text{grad} p + \mu \Delta v - \zeta \Delta \Delta v,$$

which, in components, has the equivalent form $\rho \dot{v}_i = -p_i + \mu v_{i,jj} - \zeta v_{i,jjkk}$.

In this equation $v$ is subject to the incompressibility constraint

$$\text{div} v = 0,$$

$\dot{v}$ (often written as $Dv/Dt$) is the material time derivative of $v$, $p$ is the pressure, and $\Delta$ is the Laplace operator.

Returning to the general flow equation (10), we may identify the characteristic length scale

$$L = \sqrt{\frac{\zeta}{\mu}}.$$

Fried and Gurtin [4] refer to $L$ as the gradient length and we use that terminology here as well.

In addition to the flow equation, the theory also provides boundary conditions. In particular, the classical no-slip boundary boundary condition is replaced by the generalized adherency conditions

$$v = 0 \quad \text{and} \quad m_s = -\mu \mathbf{\omega} \times \mathbf{n},$$

in which the constitutive modulus $l \geq 0$, the adherence length, measures the strength of the fluid’s adherence to the boundary. Alternatively, the theory provides conditions at solid boundaries with slip and conditions at free surfaces, each of which involves the introduction of an additional constitutive parameter.

### 3 Variational Formulation

Because the general flow equation (5) and boundary conditions (6) follow from the application of the principle of virtual power, it is fairly straightforward

\footnote{We note that Fried and Gurtin [5] include a term proportional to the corotational rate of $D$ in the extra stress. That term is neglected here.}
to derive a variational formulation of the flow equation and the boundary conditions (13). Here rather than using an arbitrary control volume $R$, we work with the region $B$ occupied by the body at a fixed time $t$.

We consider boundary conditions in which a portion $S_{\text{free}}$ of $\partial B$ is free and the remainder $S_{\text{fxd}}$ is fixed:

\begin{align*}
\begin{aligned}
Tn + \operatorname{div}_s(Gn \times ) + n \times \operatorname{div} G &= \sigma K n \quad \text{on } S_{\text{free}}, \\
\text{and } n \times Gn &= 0 \\
v &= 0 \quad \text{and } n \times Gn = -\mu l \omega \times n \quad \text{on } S_{\text{fxd}},
\end{aligned}
\end{align*}

(14)

cf. (13). Here, $\sigma$ denotes the surface tension.

We refer to an arbitrary virtual field $\tilde{v}$ as kinematically admissible if

\[ \tilde{v} = 0 \text{ on } S_{\text{fxd}}. \]  

(15)

Given such a field, we consider the virtual-power balance (4) applied with $R = B$, neglecting (noninertial) body forces, and with the replacements indicated by

\[ t_s \to \sigma K n \quad \text{and} \quad m_s \to 0 \quad \text{on } S_{\text{free}}, \quad m_s \to -\mu l \omega \times n \quad \text{on } S_{\text{fxd}}. \]  

(16)

We write $\mathcal{V}$ and $\mathcal{P}$ for the spaces of admissible velocity and pressure fields, respectively. The two-field variational form reads: find $(v, p) \in \mathcal{V} \times \mathcal{P}$ such that

\[ T(v, p, \tilde{v}, \tilde{p}) = \ell(\tilde{v}) \quad \text{for all } (\tilde{v}, \tilde{p}) \in \mathcal{V} \times \mathcal{P}, \]  

(17)

where

\[ T(v, p, \tilde{v}, \tilde{p}) = \int_B (S : \operatorname{grad} \tilde{v} + G : \operatorname{grad} \operatorname{curl} \tilde{v}) \, dv + \int_{S_{\text{fxd}}} (\mu l \omega \times n) \cdot \frac{\partial \tilde{v}}{\partial n} \, da \\
- \int_B p \, \operatorname{div} \tilde{v} \, dv - \int_B \tilde{p} \, \operatorname{div} v \, dv - \int_B \rho \tilde{v} \cdot \tilde{v} \, dv, \]  

(18)

and

\[ \ell(\tilde{v}) = \int_{S_{\text{free}}} \sigma K n \cdot \tilde{v} \, da. \]  

(19)

To obtain correspondence with the particular flow equation (10), $S$ and $G$ are given by (8) and (9), respectively.
4 Discretization of the Second Gradient Theory

In this section, we introduce our numerical formulation for the second-gradient theory. Our work is based on the nonconforming method proposed by Engel et al. [8]. In this approach, the basis functions are $C^0$-continuous—so that their first and higher-order derivatives are discontinuous. Continuity of the first and higher-order derivatives is weakly enforced by adding weighted residual terms to the variational equation on element boundaries and invoking stabilization techniques. The number of unknowns per element arising for this method is considerably fewer than for alternatives based on traditional strategies such as $C^1$-continuous basis functions.

The spaces of admissible velocity and pressure fields are $V \subset H^2(B)$ and $P \subset H^0(B)$, where $H^m(B)$ denotes the classical Sobolev space of order $m$. We use a nonconforming Galerkin method to approximate the solution to (17), and we state the weak form of the variational problem in terms of finite-dimensional spaces $V^h \subset H^1(B)$ and $P^h \subset P$.

To construct the bases, we consider a regular finite-element partition $Q^h = \bigcup_{e=1}^{M} Q_e$, with $Q^h \approx B$ and $M$ the total number of elements in the mesh. We choose approximation functions which are continuous on the entire domain but discontinuous in first and higher-order derivatives across element boundaries. Further, we consider element interiors $\tilde{Q}$ defined via

$$\tilde{Q} = \bigcup_{e=1}^{M} Q_e.$$  \hspace{1cm} (20)

The union $\tilde{\Gamma}$ of interior boundaries is expressed as

$$\tilde{\Gamma} = \bigcup_{i=1}^{N_i} \Gamma_i,$$  \hspace{1cm} (21)

where $N_i$ denotes the number of element interior boundaries. In two dimensions, these refer only to those element edges that are shared by two spatially adjacent elements, and do not include edges along the physical boundary $\partial B$. Given a field $f$ on $B$, the jump $[f]$ of $f$ across the interior boundary is defined as

$$[f] = f^+ - f^-.$$  \hspace{1cm} (22)

where

$$f^\pm = \lim_{\epsilon \to 0} f(x \mp \epsilon n)$$  \hspace{1cm} (23)

and $n$ is any of the two unit normals to the interior boundary and $\epsilon > 0$. The jump operator is graphically described in Figure 1. The average $\langle f \rangle$ of $f$
across the interior boundary is defined as
\[
\langle \langle f \rangle \rangle = \frac{1}{2} (f^+ + f^-).
\] (24)

From the definitions of the jump and average operators, we have the useful identity
\[
\llbracket fg \rrbracket = \llbracket f \rrbracket \langle \langle g \rangle \rangle + \langle \langle f \rangle \rangle \llbracket g \rrbracket.
\] (25)

The method we propose to approximate the solution to flow problems arising from the second-gradient theory can then be stated as: find \((\mathbf{v}^h, p^h) \in V^h \times P^h\) such that
\[
T_{cd}(\mathbf{v}^h, p^h, \tilde{\mathbf{v}}^h, \tilde{p}^h) = \ell_{cd}(\tilde{\mathbf{v}}^h), \quad \forall (\tilde{\mathbf{v}}^h, \tilde{p}^h) \in V^h \times P^h,
\] (26)
where the bilinear form \(T_{cd}\) is defined via
\[
T_{cd}(\mathbf{v}^h, p^h, \tilde{\mathbf{v}}^h, \tilde{p}^h) = \int_{\tilde{Q}} (S^h : \text{grad}\tilde{\mathbf{v}}^h + G^h : \text{curl}\tilde{\mathbf{v}}^h) \, dv - \int_{\tilde{\Gamma}_{\text{int}}} \langle \langle \tilde{G}^h n \rangle \rangle \cdot \llbracket \text{curl}\tilde{\mathbf{v}}^h \rrbracket \, da
- \int_{\tilde{\Gamma}} \llbracket \text{curl}\tilde{\mathbf{v}}^h \rrbracket \cdot \langle \langle G^h n \rangle \rangle \, da + \tau_v \int_{\tilde{\Gamma}} \llbracket \text{curl}\tilde{\mathbf{v}}^h \rrbracket \cdot \llbracket \text{curl}\mathbf{v}^h \rrbracket \, da
- \int_{\tilde{Q}} p^h \text{div} \tilde{\mathbf{v}}^h \, dv - \int_{\tilde{Q}} \tilde{p}^h \text{div} \mathbf{v}^h \, dv - \int_{\tilde{Q}} \rho \tilde{\mathbf{v}}^h \cdot \mathbf{v}^h \, dv
\] (27)

and the linear form \(\ell_{cd}\) is defined via
\[
\ell_{cd}(\tilde{\mathbf{v}}^h) = \int_{\gamma_{\text{free}}} \sigma K n \cdot \tilde{\mathbf{v}}^h \, da - \int_{\gamma_{\text{int}}} (\mu l \omega \times n) \cdot \frac{\partial \tilde{\mathbf{v}}^h}{\partial n} \, da.
\] (28)

In (27), \(\tau_v\) denotes the velocity stabilization parameter for the interelement boundaries. The basic structure of this stabilized approach follows from Nitsche’s method [10] for enforcing constraints on interfaces.

Many of the jump terms appearing in (27) stem from the divergence theorem as applied to volume integrals over individual elements (see the following proof.
of consistency). In particular, surface integrals involving normal flux quantities 
(such as $T_n$ or $G_n$) arise over the boundary of each element $Q_e$, where $n_e$ 
denotes the unit outward normal to $Q_e$. Since adjacent elements possess equal 
and opposite normal vectors along common interior boundaries, the choice 
of positive normal (and thus positive side) is arbitrary for any given pair. 
However, for consistency, it is important that once a positive side is identified 
on a given element interior, it is identified as such for each of the jump terms 
appearing in (27).

4.1 Consistency

The consistency of the method is derived through successive application of the 
divergence theorem to (26). Using the equality (25), we derive

$$\int_{Q_e} T^h \cdot \text{grad} \, \varepsilon^h \, dv = - \int_{Q_e} \text{div} \, T^h \cdot \varepsilon^h \, dv + \int_{S} T^h n \cdot \varepsilon^h \, da + \int_{\tilde{r}} \llbracket T^h n \cdot \varepsilon^h \rrbracket \, da$$

$$= - \int_{Q_e} \text{div} \, T^h \cdot \varepsilon^h \, dv + \int_{S} T^h n \cdot \varepsilon^h \, da$$

$$+ \int_{\tilde{r}} \left( \llbracket T^h n \rrbracket \cdot \langle \langle \varepsilon^h \rangle \rangle + \langle \langle T^h n \rangle \rangle \cdot \llbracket \varepsilon^h \rrbracket \right) \, da.$$

Similarly, the divergence theorem applied twice yields

$$\int_{Q_e} G^h \cdot \text{grad} \, \text{curl} \, \varepsilon^h \, dv = - \int_{Q_e} (\text{div} \, G^h) \cdot (\text{curl} \, \varepsilon^h) \, dv + \int_{S} G^h n \cdot \text{curl} \, \varepsilon^h \, da$$

$$+ \int_{\tilde{r}} \llbracket G^h n \cdot \text{curl} \, \varepsilon^h \rrbracket \, da$$

$$= - \int_{Q_e} (\text{curl} \, \text{div} \, G^h) \cdot \varepsilon^h \, dv + \int_{S} (G^h n \cdot \text{curl} \, \varepsilon^h + (n \times \text{div} \, G^h) \cdot \varepsilon^h) \, da$$

$$+ \int_{\tilde{r}} \left( \llbracket G^h n \cdot \text{curl} \, \varepsilon^h \rrbracket + \langle (n \times \text{div} \, G^h) \rangle \cdot \llbracket \varepsilon^h \rrbracket \right) \, da$$

$$= - \int_{Q_e} (\text{curl} \, \text{div} \, G^h) \cdot \varepsilon^h \, dv + \int_{S} (G^h n \cdot \text{curl} \, \varepsilon^h + (n \times \text{div} \, G^h) \cdot \varepsilon^h) \, da$$

$$+ \int_{\tilde{r}} \left( \llbracket G^h n \rrbracket \cdot \langle \langle \text{curl} \, \varepsilon^h \rangle \rangle + \langle \langle G^h n \rangle \rangle \cdot \llbracket \text{curl} \, \varepsilon^h \rrbracket \right) \, da$$

$$+ \int_{\tilde{r}} \left( \langle (n \times \text{div} \, G^h) \rangle \cdot \langle \langle \varepsilon^h \rangle \rangle + \langle (n \times \text{div} \, G^h) \rangle \cdot \llbracket \varepsilon^h \rrbracket \right) \, da.$$
Since $\tilde{v}^h$ is continuous on the interelement boundary $\tilde{\Gamma}$, we have $[\tilde{v}^h] = 0$, yielding

$$\int_{\tilde{Q}} T^h : \text{grad} \tilde{v}^h \, dv = - \int_{\tilde{Q}} \text{div} T^h \cdot \tilde{v}^h \, dv + \int_{S} T^h n \cdot \tilde{v}^h \, da + \int_{\tilde{\Gamma}} [T^h n] \cdot \langle \langle \tilde{v}^h \rangle \rangle \, da \quad (29)$$

and

$$\int_{\tilde{Q}} G^h : \text{grad curl} \tilde{v}^h \, dv = - \int_{\tilde{Q}} (\text{curl div} G^h) \cdot \tilde{v}^h \, dv + \int_{S} \left( [G^h n] \cdot \langle \langle \text{curl} \tilde{v}^h \rangle \rangle + [G^h n] \cdot [\text{curl} \tilde{v}^h] \right) \, da + \int_{\tilde{\Gamma}} [n \times \text{div} G^h] \cdot \langle \langle \tilde{v}^h \rangle \rangle \, da. \quad (30)$$

Here, we take advantage of the equality

$$\int_{S} G^h n \cdot \text{curl} \tilde{v}^h \, da = \int_{S} \left( \text{div}_s (G^h n \times) - 2K n \times G^h n \right) \cdot \tilde{v}^h + (n \times G^h n) \cdot \frac{\partial \tilde{v}^h}{\partial n} \right) \, da, \quad (31)$$

A detailed derivation of this equality is provided by Fried and Gurtin [5].

The consistency of the method then follows upon substituting the results (29), (30), and (31), into (27), viz.

$$0 = T_{cd}(v^h, p^h, \tilde{v}^h, \tilde{p}^h) - \ell_{cd}(\tilde{v}^h)$$

$$= \int_{\tilde{Q}} (\text{curl div} G^h + \text{div} T^h - \rho \tilde{v}^h) \cdot \tilde{v}^h \, dv - \int_{\tilde{\Gamma}} \langle \langle \tilde{G}^h n \rangle \rangle \cdot [\text{curl} \tilde{v}^h] \, da$$

$$+ \int_{\tilde{\Gamma}} [T^h n + n \times \text{div} G^h + \text{div}_s (G^h n \times) - 2K n \times G^h n] \cdot \langle \langle \tilde{v}^h \rangle \rangle \, da$$

$$+ \int_{\tilde{\Gamma}} [n \times G^h n] \cdot \left\langle \left\langle \frac{\partial \tilde{v}^h}{\partial n} \right\rangle \right\rangle \, da$$

$$+ \int_{S_{\text{free}}} (T^h n + n \times \text{div} G^h + \text{div}_s (G^h n \times) - 2K n \times G^h n - \sigma K n) \cdot \tilde{v}^h \, da$$

$$+ \int_{S_{\text{free}}} (n \times G^h n) \cdot \frac{\partial \tilde{v}^h}{\partial n} \, da + \int_{S_{\text{free}}} (n \times G^h n - \mu \omega \times n) \cdot \frac{\partial \tilde{v}^h}{\partial n} \, da$$

$$+ \tau_v \int_{\tilde{\Gamma}} [\text{curl} \tilde{v}^h] \cdot [\text{curl} \tilde{v}^h] \, da.$$  

(32)
From (32) we deduce the second gradient equations

\[
\text{div} T^h + \text{curl} \text{div} G^h = \rho \dot{v}^h \quad \text{in } \tilde{Q}, \tag{33}
\]

\[
\begin{aligned}
T^h n + n \times \text{div} G^h + \text{div}_s (G^h n \times) - 2K n \times G^h n &= \sigma K n \\
\text{and } n \times G^h n &= 0 \\
n \times G^h n &= -\mu \omega \times n \quad \text{on } S_{\text{fix}},
\end{aligned}
\tag{34}
\]

and the jump conditions

\[
\begin{aligned}
\left[ \text{curl} v^h \right] &= 0, \\
\left[ T^h n + n \times \text{div} G^h + \text{div}_s (G^h n \times) - 2K n \times G^h n \right] &= 0, \\
\left[ n \times G^h n \right] &= 0,
\end{aligned}
\tag{35}
\]

While (33) enforces the flow equation on the element interiors, (34) enforces the boundary conditions on free and fixed surfaces of the flow domain, (35)_1 ensures the continuity of the first derivatives across the interelement boundaries, and (35)_2,3 ensure the continuity of the tractions across the interelement boundaries. On replacing \(v\) and \(p\) in (26) by \(v^h\) and \(p^h\), we obtain the Galerkin orthogonality condition

\[
T_{cd}(e_v, e_p, \tilde{v}^h, \tilde{p}^h) = 0 \quad \forall (\tilde{v}^h, \tilde{p}^h) \in V^h \times P^h, \tag{36}
\]

where \(e_v = v^h - v\) and \(e_p = p^h - p\) are the errors for the velocity and pressure fields, respectively.

### 4.2 Element Choice and Additional Pressure Stabilization

We restrict attention to problems for which the inertial terms appearing in (27) can be neglected. Extensions to time-dependent flows and the nonlinearities associated with the material derivative of the velocity field for the second gradient theory are left for a future work.

We will base our formulation on one that is stable for the classical theory, namely: four-node isoparametric quadrilateral elements with piecewise-quadratic basis functions for the velocity field and linear (discontinuous) basis functions for the pressure field. Three-dimensional generalizations of these elements are readily available and widely used in practice.
To begin, we introduce the space

$$P^j(Q_e) = \{v : v \text{ is a polynomial of degree } \leq j \text{ on } Q_e\}$$

(37)
of complete polynomials over element $Q_e$. Using $N$ to denote the number of nodes in the mesh, we then write

$$\{\phi_I\} = \{\phi_I \in C^0(Q^h) : \phi_I|Q_e \in P^2(Q_e)\}, \quad I = 1 \ldots N,$$

(38)

for the set of quadratic Lagrangian isoparametric functions. The approximation to the velocity field is then given by

$$v^h(x) = \sum_{I=1}^{N} \phi_I(\xi(x))v_I,$$

(39)

where $v_I$ is the nodal value at node $I$ and $\xi$ the coordinates in a reference element.

For the pressure field, we introduce the set

$$\{M_I\} = \{M_I \in H^0(Q^h) : M_I|Q_e \in P^1(Q_e)\}, \quad I = 1 \ldots M,$$

(40)
of linear element-based (discontinuous) shape functions. The approximation to the pressure field $p$ can then be written as

$$p^h(x) = \sum_{I} M_I(x)p_I.$$

(41)

The approximations (39) and (41) over quadrilateral elements are stable for the classical problem of Stokes flow; cf., e.g., Hughes [9]. We therefore expect stability to also hold for sufficiently small gradient lengths $L$. However, for larger gradient lengths, we should not expect these elements to be stable. Accordingly, we investigate the use of additional pressure stabilization. In particular, we follow the approach of Hughes and Franca [11] and add terms of the form

$$- \sum_{e \in F} \tau_p \int_e \|p^h\|^{2} \|\tilde{p}^h\| \, da,$$

(42)

to the nonconforming approximation (27), where $\tau_p$ is the pressure stability parameter. Importantly, the addition of this term does not affect the consistency proof presented earlier; indeed, this term simply enforces continuity of the pressure field between elements.

To approximate the weight functions $\tilde{v}^h$ and $\tilde{p}^h$, we use expansions analogous to (39) and (41). Upon substituting these expressions into (27) (neglecting inertial terms) and invoking the arbitrariness of the weight functions, we obtain
the linear algebraic system of equations

\[
\begin{bmatrix}
K_c + K_g & G_c \\
G_c^\top & S
\end{bmatrix}
\begin{bmatrix}
d_v \\
d_p
\end{bmatrix}
= \begin{bmatrix}
f_v \\
f_p
\end{bmatrix},
\]

(43)

which can be solved to yield \(d_v\) and \(d_p\).

5 Numerical Examples

5.1 Benchmark Problem: Plane Poiseuille Flow

Fig. 2. Schematic of the channel for the problem of plane Poiseuille flow. The coordinates in the directions downstream and out of the plane are \(x\) and \(z\).

We consider the problem of steady, laminar flow through an infinite, rectangular channel formed by two parallel surfaces separated by a gap \(h\) (Figure 2). Writing

\[
u = \mathbf{v} \cdot \mathbf{e}_x, \quad v = \mathbf{v} \cdot \mathbf{e}_y, \quad (44)
\]

for the horizontal and vertical components of the velocity field, we consider problems with solutions of the form

\[
u = u(y), \quad v = 0, \quad (45)
\]

as shown in Figure 2. An analytical solution to this problem for the flow equation (10) with generalized adherency conditions (13) was developed by Fried and Gurtin [4] for a theory different from that considered here. Nevertheless, the solution to the problem of plane Poiseuille flow is identical for both theories.

The pressure field is only known up to an arbitrary additive constant with gradient

\[\text{grad} \, p = -\beta \mathbf{e}_x, \quad \text{with} \quad \beta = \text{constant}; \quad (46)\]

without loss of generality, we assume that \(\beta > 0\). The solution for the velocity field can be decomposed into classical and generalized contributions as

\[u(y) = u_c(y) + u_g(y), \quad (47)\]
where

\[ u_c(y) = \frac{\beta h^2 y}{2\mu} \left( 1 - \frac{y}{h} \right) \]  

(48)

is the classical solution of the analogous problem for a Navier–Stokes fluid and

\[ u_g(y) = -\frac{\beta h^2}{2\mu} \frac{b_l L}{h \sinh \frac{h}{L}} \left( \sinh \frac{h}{L} - \sinh \frac{y}{L} - \sinh \frac{h - y}{L} \right) \]  

(49)

arises from higher-order terms characterized by the gradient length \( L \). In view of the signs of \( L, l, \) and \( h \), the constant

\[ b_l = \frac{\frac{2L}{T} + \frac{l}{T}}{1 + \frac{l}{T} \tanh \frac{\frac{h}{2L}}{h}} \]  

(50)

is a nonnegative dimensionless measure of the effective adhesion length. The specialized conditions of weak and strong adherence arise respectively from the limits setting \( l \to 0 \) and \( l \to \infty \).

Although the solution (49) is essentially one-dimensional in nature, we use it to establish a two-dimensional boundary value problem to verify the finite-element formulation described in Section 4. The approach we follow is to prescribe boundary conditions consistent with (49) on an arbitrary, finite “computational domain” \( Q^h \). We then quantify the error in the numerical approximation to the velocity \( \mathbf{v} \) and pressure \( p \) fields on the interior of the domain using suitable error norms. This procedure requires a-priori knowledge of the solution and is only used for verifying the numerical formulation. More general boundary conditions will be discussed subsequently.

![Boundary conditions](image)

Fig. 3. Computational domain and boundary conditions for the channel flow studies.

We take advantage of the symmetry of the solution (49) about the midplane of the channel and consider a numerical domain with dimensions \([0, h/2] \times [h/2, h]\)
as shown in Figure 3. On the midplane of the channel, the velocity field is constrained to be symmetric and a zero hypertraction is enforced. The top surface of the channel is considered fixed and we prescribe the generalized adherence conditions (13). It bears emphasis that while the vertical component of the velocity field is fixed to vanish on all of the boundaries of the computational domain, it is not constrained on the interior of the domain.

What remains is to designate boundary conditions on the vertical computational surfaces. Here, we choose to prescribe the velocity field only at the left (inlet) boundary according to the exact solution (49). Zero hypertractions are prescribed at the inlet and outlet.

To check convergence in the velocity field, we use the $L_2$-norm of the error $e_v = v^h - v$. Since the pressure field is known only up to a constant, the appropriate norm to check convergence is the $L_2$-norm of the error $e_p = \text{grad} p^h - \text{grad} p$ in the gradient of the pressure field. In the following, we report error norms that are normalized by those of the solution.

We begin by examining the limiting case of $l \to 0$, corresponding to weak adherence conditions on the channel walls. We set the gradient length $L$ equal to $h/4$. Figure 4 provides convergence results obtained using a sequence of uniform meshes with equidistant nodal spacing $dy = dx$ in each of the coordinate directions. We observe a rate of convergence in the $L_2$-error norm of the velocity field that lies between quadratic and cubic. For a discretization of a classical Navier–Stokes problem using the isoparametric quadratic shape functions, a cubic rate is optimal; cf. Hughes [12]. Figure 5 juxtaposes the solution (49) and the finite-element approximation $v^h$ obtained using a $4 \times 4$ uniform mesh. The latter is shown above the midplane $y/h = 0.5$ and the numerical approximation is seen to be indistinguishable from the solution.

For the pressure field, we obtain nearly a quadratic rate of convergence in the $L_2$ norm of $e_p$. We are not aware of any studies detailing the accuracy of the pressure approximation for the mixed formulation described herein. However, this rate is above that expected based on the best approximation error for a linear field.

The accuracy and rate of convergence in the velocity and pressure fields was found to be sensitive to the particular choice of the stability terms $\tau_v$ and $\tau_p$. Without any stabilization, for example, we observed much lower accuracy in both fields. The results shown were obtained using $\tau_p$ and $\tau_v$ proportional to $\zeta/h_e$ where $h_e$ denotes the width of the element edges. Such a scaling with mesh spacing is likely the minimum requirement to maintain convergence, and is consistent with error estimates provided in Engel et al. [8]. We anticipate that much better results could be obtained using stabilization parameters that are more closely related to the solution. This is an area for future work.
Fig. 4. Convergence results for the benchmark problem for weak adherence boundary conditions.

Fig. 5. Contour plot of velocity field normalized by $\beta h^2/2\mu$ for weak adherence boundary conditions. The finite-element approximation is shown above the channel center $y/h = 0.5$ and the solution (49) is shown below this line.

Figure 6 compares numerical and exact solutions for the case of generalized adherence conditions ($l > 0$) on the channel wall, using various ratios $l/L$ of adherence length to gradient length. The numerical results were obtained at the outflow ($x/h = 0.5$) boundary of the computational domain. All of the numerical results shown in Figure 6 are for a uniform mesh of $4 \times 4$ elements. The results indicate an excellent match between the numerical and exact velocity fields, particularly given the coarseness of the mesh. Figure 7 shows the
contours of the normalized pressure gradient obtained for the particular choice of $l/L = 0.1$. As expected, the pressure gradient is almost constant and the maximum error is less than 3%.

![Graph of velocity profiles](image1)

Fig. 6. Exact and numerical velocity profiles at the outlet boundary of the computational domain for various ratios $l/L$ of adherence length to gradient length. All numerical results were obtained on a $4 \times 4$ uniform mesh.

![Contour plot of pressure gradient](image2)

Fig. 7. Contour plot of the normalized pressure gradient $\mathbf{e}_x \cdot \nabla p / \beta$ for channel flow with generalized adherence boundary conditions ($l/L = 1.0$).

A convergence study with generalized adherence boundary conditions on the
channel walls yields results that are qualitatively similar to those arising for weak adherence boundary conditions. Figure 8 compares the relative error norms for the two cases. The generalized adherence results were obtained using \( t/L = 0.1 \). We report that the rates of convergence are nearly unaffected with generalized adherence boundary conditions, and a slight increase in accuracy was observed with increasing mesh refinement.

![Graph](image.png)

Fig. 8. Convergence results for the benchmark problem for weak and generalized adherence boundary conditions.

As a final verification test, we report results using skewed meshes. Figure 9 shows velocity contours for the case of generalized adherence boundary conditions with the skewed mesh geometry superimposed over the finite-element approximation to \( \mathbf{v} \). The numerical results once again compare favorably to the solution.

We note that this benchmark problem also permits us to examine other choices for boundary conditions and their effect on the numerical solution. Heywood et al. [13] proposed a simple method to prescribe a pressure drop between artificial inlet and outlet boundaries such as the left and right boundaries in Figure 3. Writing \(-P\) for the desired pressure drop between the artificial inlet and outlet boundaries, the approach amounts to replacing the prescribed velocity boundary condition at the inlet with a traction

\[
\mathbf{t} = -Pe_x.
\]  

Using such an approach, we obtain nearly identical results to those obtained using the boundary conditions described in Figure 2. This approach will be used in Section 5.3 to study flow through a channel with a step.
5.2 Flow Past a Cylinder

The second benchmark problem that we consider involves steady, laminar flow past a right circular cylinder. We consider a domain of height $h$ and width $w$ containing a circular obstacle of diameter $d$ (Figure 10). The boundary conditions for the hypertraction $\mathbf{m}_g$ and the horizontal and vertical components $u$ and $v$ of the velocity field are indicated in the Figure. On the cylinder surface, no slip conditions are considered along with generalized adherence boundary conditions ($l > 0$). A uniform velocity in the $x$-direction at the inlet boundary is applied. The computational domain is taken as $h/w = 1$, and $h/d = 4$. We find that the mesh shown in Figure 11 of 288 quadratic elements provides sufficiently converged results for all of the problems presented below.

Figure 12 compares numerical approximations for the horizontal component of the velocity field for the classical Navier–Stokes theory and the gradient theory. The results correspond to generalized adherence boundary conditions ($l > 0$) on the cylinder surface, with $L/d = 1.0$ and $l/L = 10.0$. The two solutions are seen to be qualitatively quite similar, with perhaps the greatest difference occurring in the vicinity of the cylinder. This is not surprising given the generalized adherence condition there.

Figure 13 displays contour plots of the vertical component of the velocity field for the classical Navier–Stokes theory and the gradient theory. Only minor qualitative and quantitative differences between the two flows can be observed,
Fig. 10. Problem description for flow past a cylinder with velocity and hypertraction boundary conditions.

Fig. 11. Mesh for studies of flow past a cylinder.

but the adherence near the cylinder boundary is clearly identifiable. Figure 14 shows the pressure distributions for the classical (left) and gradient (right) flows. As expected, these results show a pressure drop as the flows pass the cylinder. Moreover, we find that the pressure field upstream of the cylinder for the gradient theory is greater than that predicted by the classical theory.

Figure 15 compares the horizontal velocity components for the classical theory with those of weak- and generalized-adherence boundary conditions under the gradient theory. The numerical results correspond to the flow profiles along a vertical line along the middle ($x/h = 0.5$) of the computational domain. All of the numerical results shown in the Figure were obtained using a mesh of 288 elements. The results indicate that the velocity profiles at small length...
Fig. 12. Contour plots of the normalized horizontal velocity component for the classical theory (left) and the gradient theory (right) with generalized adherence boundary conditions. Results for the gradient theory correspond to \( L/d = 1.0 \) and \( l/L = 10.0 \).

Fig. 13. Contour plots of the normalized vertical velocity component for the classical solution (left) and the gradient (right) solution with generalized adherence boundary conditions. Results for the gradient theory correspond to \( L/d = 1.0 \) and \( l/L = 10.0 \).

Fig. 14. Contour plots of pressure field for the classical solution (left) and the gradient (right) solution with generalized adherence boundary conditions.
scales are smaller than those of classical theory. Moreover, the slope around the cylinder decreases with increasing gradient and adherence lengths ($L$ and $l$).

Fig. 15. Comparison of the normalized horizontal velocity component profiles in the middle ($x/w = 0.5$) of the computational domain for the classical theory and weak- and generalized-adherence boundary conditions on the cylinder surface with the gradient theory.

5.3 Step Flow

We consider a steady, laminar flow through a channel with a sudden area expansion as shown in Figure 16. We prescribe a pressure drop $-P$ between the inlet and outlet boundaries as shown in the Figure. The vertical component of the velocity field is also fixed to zero at the inlet and outlet boundaries. On the top and bottom surfaces, no-slip boundary conditions are enforced, and weak adherence ($l = 0$) conditions are considered for the gradient theory. The dimensions of the computational domain are taken such that $w_1/w_2 = 3$, $h_1/h_2 = 5/2$, and $h_1/w_1 = 5/6$.

Figure 17 and 18 provide contour plots of the numerical solution of the horizontal and vertical velocity components for classical (left) and gradient (right) flows. The numerical results were obtained using a uniform mesh of 176 elements. As expected, the results reveal a qualitative difference between classical and gradient theories. Figure 19 provides the pressure comparison at the same contour level between classical and gradient theories. The results clearly show the same net pressure drop between inlet and outlet boundaries. A profile of the horizontal velocity field at the outlet of the computational domain is shown...
Fig. 16. Geometry and boundary conditions for the step flow problem. The coordinates in the directions downstream and out of the plane are $x$ and $z$.

in Figure 20. The gradient theory clearly predicts smaller flow rates compared to the classical for the same pressure drop across the step. The results for the gradient theory shown in Figures 17–20 were all obtained using $L/h_2 = 0.25$.

![Contour plot](image)

**Fig. 17.** Contour plot of normalized horizontal velocity component predicted using the classical theory (left) and the gradient theory (right) with weak adherence boundary conditions.

We next examine the variation in flow rates with aspect ratio $h_1/h_2$ for a fixed pressure drop. We calculate the flow rates $Q$ for a sequence of steps ranging from $h_1 = h_2$ (the straight channel) to $h_1 = 2.5h_2$. We use the flow rate $Q_1$ obtained for the straight channel in each case (classical and gradient) to normalize the subsequent results. Figure 21 shows the normalized flow rates as a function of step ratio $h_1/h_2$ for a sequence of increasing ratios $L/h_2$ of gradient to physical lengths. The results predict that the flow rate of the classical theory is always greater than that of the gradient theory. Moreover,
Fig. 18. Contour plot of vertical velocity component for the classical solution (left) and the gradient (right) solution with weak adherence boundary conditions.

Fig. 19. Contour plot of normalized pressure fields for the classical (left) and gradient (right) theories for the step flow problem.

flow rates are seen to decrease relative to the straight channel rate as the gradient length is increased relative to the physical length. We note that the introduction of the corner to the problem results in a marked decrease in flow rates (before a more gradual increase with increasing step size) for large $L/h_2$. This may be attributable to the increased role that corner singularities may play with regard to dissipation for the gradient theory.
Fig. 20. Normalized horizontal velocity profiles at the outlet of the computational domain for the classical theory and the gradient theory for the step flow problem.

Fig. 21. Normalized flow rates as a function of step ratio $h_1/h_2$ for a sequence of increasing ratios $L/h_2$ of gradient to physical lengths.

### 6 Summary and Conclusions

In this paper, we described a finite-element method for a second-gradient theory of fluid flow. The second gradient theory incorporates gradients of the vorticity field that are power-conjugate to a hyperstress in a nonstandard principle of virtual power. The theory gives rise to a flow equation that is fourth-order in the velocity field, and incorporates associated higher-order boundary conditions. Rather than employing $C^1$-continuous basis functions or a fully mixed
approach, we base our method on a recent formulation for fourth-order elliptic problems that employs $C^0$-continuous basis functions. Continuity of higher-order velocity derivatives is then enforced between elements using a variation of Nitsche’s [10] method, involving jump quantities across interelement boundaries. Using this formulation, we based our approach on second-order elements that are stable for the classical Navier-Stokes theory for incompressible fluid flow. Additional terms were added to properly stabilize the discontinuous pressure field.

Using our finite-element method, we then examined several numerical examples. First, the method was verified using an analytical solution to a Poiseuille flow problem derived by Fried and Gurtin [4]. An excellent match between numerical and analytical results was obtained, as were near-optimal rates of convergence in appropriate error norms for the velocity and pressure fields. The numerical method was also shown capable of capturing effects for a range of boundary conditions stemming from the second-gradient theory, from weak to strong adherence. Results were obtained using stabilization parameters that scale with the second-gradient moduli and the inverse of the mesh spacing. Additional problems of flow past a cylinder and step flow were then examined, and numerical predictions based on the second-gradient theory were compared to those of the classical theory. Consistent with the additional sources of dissipation associated with the hyperstress and the generalized adherence boundary conditions, the second-gradient theory predicts lower flow rates and shows a marked difference near boundaries due to the effect of the adherence boundary conditions.

This work is based on a theory of fluid flow that involves the gradient of the vorticity field [5]. It shares several common features with an earlier theory based on the full second-gradient of the velocity field [4]. The earlier theory involves an additional hyperpressure field not present in the vorticity-based theory considered here. A numerical formulation based on the earlier theory would thus require a three-field approach that would be more difficult to ensure stability. Since both theories yield identical flow equations, however, we do not anticipate significant qualitative differences in the flow profiles.

Future work will focus on extending our approach to time-dependent flows beyond the steady Stokes flows considered herein. This work should serve as an excellent starting point for a formulation based on the generalization of the LANS-$\alpha$ theory for turbulent flow obtained by Fried and Gurtin [5], for example. Importantly, we intend to examine methods that can better tie the stabilization parameters to the solution in a particular problem. Along these lines, Mourad et al. [14] have recently developed a method to relate the stabilization parameters in Nitsche’s [10] method to the relationship between coarse and fine scales in a solution. In principle, such a strategy could be applied to the present work, provided that a suitable approximation for the
fine-scale can be identified.

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