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NP-Hard Problems in Computational Large Deformation Mechanics and Canonical Dual Finite Element Method

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Nonconvex phenomena arise naturally in large classes of engineering applications. It is known that in the modelling of phase transitions, large deformed structures, and super-conducting materials, the total free energy functional is usually nonconvex due to certain internal variables. Traditional FEM for solving non-linear solid mechanics usually leads to nonconvex optimization problems. Due to the lack of global optimality criteria, traditional numerical approaches for solving nonconvex minimization problems in global optimization are fundamentally difficult or even impossible. Therefore, most of nonconvex minimization problems are considered as **NP-hard** (i.e., Non deterministic method for solving the problem within Polynomial times) [1,2]. Unfortunately, this well-known fact in computer science and global optimization is not fully recognized in computational mechanics. It turns out that many local search finite element methods and commercial software have been used extensively for solving nonconvex large deformation problems.

Canonical duality theory [1,2,3] is a methodological and potentially powerful theory which can be used not only for modelling complex phenomena within a unified framework, but also for solving a large class of nonconvex/nonsmooth/discrete problems in non-linear mechanics and global optimization. This theory was developed from Gao and Strang's original work for solving the following general nonconvex variational problem [4].

$$\min \quad \Pi(u) = \int W(\nabla u)\, d\Omega - \int f\, u\, d\Omega - \int t u\, d\Gamma$$

where $W(F)$ is a nonconvex (or even nonsmooth) stored energy. The key idea of the canonical dual transformation is to choose a geometrically nonlinear (objective) operator $E = \Lambda(u)$ and a convex energy $V(E)$ such that $W(\nabla u) = V(\Lambda(u))$. By the convexity of $V(E)$, the complementary energy $V^*(T)$ can be uniquely determined by Legendre transformation $V^*(T) = E{:}T - V(E)$. Therefore, the nonconvex functional $\Pi(u)$ can be written as

$$\Xi(u,T) = \int [\, \Lambda(u){:}T - V^*(T)]\, d\Omega - \int f\, u\, d\Omega - \int t u\, d\Gamma$$

Based on this total complementary functional, a pure complementary energy $\Pi^c(T)$ was first obtained in 1999 [5]. It was discovered by Gao and Strang in [4] that if $\Lambda(u)$ is a pure quadratic operator (such as the Cauchy-Green strain), then $G(u,T) = \int \Lambda(u){:}T\, d\Omega$ is the so-called *complementary gap function* and its positive sign provides a global optimality condition for the nonconvex variational problem. In 1996 it was realized that the negative gap function can be used to identify the biggest local min and local max. Therefore, a triality theory was proposed first in post-buckling analysis of a large deformed beam model [5], and then generalized to global optimization problems. It was shown by Gao an Ogden that in phase transitions of solids, global optimal solutions could be nonsmooth and can't be obtained by any Newton type method [6]. By the total complementary energy $\Xi(u,T)$, a mixed finite element method has been developed for solving large deformed elasto-plastic mechanics problems [7]. Recently, after an open problem has been solved, the canonical duality-triality theory has been established [8].

Theorem 1 *Suppose that ($\underline{u}$,$\underline{T}$) is a critical point of $\Xi(u,T)$, then $\underline{u}$ is a critical point of $\Pi(u)$. If $G(u, \underline{T}) \geq 0$ $\forall u \neq 0$, then $\underline{u}$ is a global minimizer of $\Pi(u)$ and*

$$\Pi(\underline{u}) = \min \Pi(u) = \min_u \max_T \Xi(u,T) = \max_T \min_u \Xi(u,T)$$

If $G(u, \underline{T}) < 0$ $\forall u \neq 0$, then $\underline{u}$ is a biggest local maximize if and only if

$$\Pi(\underline{u}) = \max \Pi(u) = \max_u \max_T \Xi(u,T) = \max_T \max_u \Xi(u,T)$$

If $G(u, \underline{T}) < 0$ $\forall u \neq 0$ and dim u = dim T, *then $\underline{u}$ is a biggest local minimize if and only if*

$$\Pi(\underline{u}) = \min \Pi(u) = \min_u \max_T \Xi(u,T) = \min_T \max_u \Xi(u,T)$$

Based on this triality theorem, a powerful canonical dual finite element method has been developed with successful appellations in phase transitions of solids and post-buckling analysis of a large deformed beam [9,10]. In this talk, we will show that many nonconvex problems in engineering mechanics are actually not NP-hard and can be solved completely by the canonical dual finite element method. The local minimal solution is very sensitive to the size of meshes. This talk should bring some fundamentally new insights into computational nonlinear mechanics.

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