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Determination of poroelastic properties of cartilage using constrained optimization coupled with finite element analysis

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Abstract

The feasibility of determining biphasic material properties using a finite element model of stress relaxation coupled with two types of constrained optimization to match measured data was investigated. Comparison of these two approaches, a zero-order method and a gradient-based algorithm, validated the predicted material properties. Optimizations were started from multiple different initial guesses of material properties (design variables) to establish the robustness of the optimization. Overall, the optimal values are close to those found by Cohen et al., (1998), but these small differences produced a marked improvement in the fit to the measured stress relaxation. Despite the greater deviation in the optimized values obtained from the zero-order method, both optimization procedures produced material properties that gave equally good overall fits to the measured data. Furthermore, optimized values were all within the expected range of material properties. Modeling stress relaxation using the optimized material properties showed an excellent fit to the entire time history of the measured data.

Keywords

Zero-order method; Gradient-based algorithm; Constrained optimization; Poroelasticity

1. Introduction

Articular cartilage is the bearing surface in freely movable joints. As a load bearing tissue, the mechanical properties of articular cartilage are important indicators of its ability to perform its intended functions, and methods for measuring its mechanical properties have been developed over the past 30 years. Cartilage is often modeled using biphasic or poroelastic theories, which simulate the coupled interactions between the porous solid skeleton and the mobile tissue fluid (Mow et al., 1980, Armstrong et al., 1984).

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Typically, mechanical properties are estimated by fitting a constitutive model to experimental data. Depending on the complexity of the constitutive model and experimental configuration, the relationship between the model and experiment might be expressed as an algebraic equation, the solution of a differential equation or as a computational model. For example, the isotropic and transversely isotropic properties of cartilage have been determined by fitting solutions of differential equations of biphasic material models to stress relaxation data (Mow et al., 1980, Cohen et al., 1998). In these cases material properties were determined by minimizing the squared difference between measured and predicted load intensity. Poroelastic rather than biphasic models are commonly used for computational models of cartilage since they are easily accessible in commercially available finite element (FE) codes such as ABAQUS, ANSYS, COMSOL, etc. However, Simon (1992) showed that the linear biphasic and poroelastic theories are related mathematically through a transformation of kinematic variables.

In the past twenty years, computational models have played a more prominent role in the prediction of material properties from experimental data. Computational models are particularly attractive for implementing complex tissue models such as those with fiber reinforcement, spatially varying properties, hyperelastic or viscoelastic properties (Oomens et al., 1993; Cohen et al., 1994; Wilson et al., 2004; Lei and Szeri, 2007; Liu and Ovaert, 2011; Seifzadeh et al., 2012; Fu et al., 2013; Yao et al., 2014; Reutlinger et al., 2014). Using a FE model integrated with optimization routines, material properties can be found by minimizing the squared difference between simulated and measured results such as force, stress or displacement. Diverse optimization algorithms have been used. For example, the mean values of hyperelastic properties of liver tissue were quantified using Levenberg-Marquardt optimization and verified using Monte-Carlo methods (Fu et al., 2013), and Liu and Ovaert (2011) used a differential evolution algorithm combined with a poroviscoelastic FE model to estimate viscoelastic properties of hydrogels in creep. Recently, Reutlinger et al. (2014) obtained the optimized material parameters of intervertebral disc that minimized the error between simulated displacement and experimental displacement after the bounds on hyperelastic parameters were implemented in the particle swarm optimization. In all of the examples cited above, the optimization was unconstrained. Constraints were not imposed on acceptable values of material properties or on the fit of measured to computed responses, *i.e.*, stress or displacement. In addition, the robustness of the convergence to a set of material properties was, in general, not investigated in all these investigations. Wilson et al. (2004) determined the fibril-reinforced poroviscoelastic material properties of cartilage with depth-dependent collagen orientation by fitting the reaction force and lateral displacement of the numerical results to the corresponding experimental values, but they did not provide evidence for a unique fit using different initial values of the material properties between lower and upper bounds. However, some exceptions include Lei and Szeri (2007) who showed the history of aggregate modulus converged although they did not show the convergence history of the four other material properties with different initial guesses. Seifzadeh et al. (2012) predicted the material properties of human cartilage using a fibril-reinforced poroviscoelastic model coupled with a simulated annealing algorithm (MATLAB), which searched for the robustness of optimization using several initial guesses. In each of aforementioned investigations the optimization was unconstrained.

The aim of this investigation was to evaluate the feasibility of using constrained optimization to determine the material properties of a transversely isotropic porous elastic material from measured stress relaxation data. Optimization was performed using two different approaches: (a) a zero-order method, which is available in ANSYS and (b) a gradient-based solver in SmartDO, which interfaces with ANSYS via Tcl/Tk.

2. Methods

Our previously developed and validated transversely isotropic poroelastic model of unconfined compression stress relaxation (Chung and Mansour, 2013) was coupled with constrained optimization procedures. Experimental stress relaxation data for unconfined compression of growth plate were obtained from Cohen et al. (1998) who used unconstrained optimization to predict biphasic material properties ($E_t = 4.3$ MPa, $E_a = 0.64$ MPa, $\nu_t = 0.49$, $\nu_{at} = 0$ and $k = 5 \times 10^{-15} \text{ m}^4\text{N}^{-1}\text{s}^{-1}$) where the tissue was loaded at a constant strain rate of $7.6 \times 10^{-4} \text{ s}^{-1}$ to 10% strain.

Constitutive relations for a linear anisotropic poroelastic material can be constructed following the generalized Hooke's law (Detournay and Cheng, 1993; Simon, 1992; Cheng, 1997)

$$\sigma_{ij} = D_{ijkl} \varepsilon_{kl} - \alpha_{ij} p \quad (1)$$

$$p = K_m (\zeta - \alpha_{ij} \varepsilon_{ii}) \quad (2)$$

Equation (1) is the constitutive response for the porous solid, where D_{ijkl} is an elastic modulus tensor of the solid skeleton, ε_{kl} is a total elastic strain tensor, and p is the pore fluid pressure. For a transversely isotropic material D_{ijkl} has five independent material constants (Chung and Mansour, 2013), whereas for an isotropic material D_{ijkl} has two independent material constants and the Biot coefficient tensor, α_{ij} , degenerates into a scalar, i.e., $\alpha_{ij} = \alpha \delta_{ij}$ where δ_{ij} is a second-order unit tensor. Equation (2) is the constitutive response for the pore fluid, where K_m is the Biot modulus, ζ is the volumetric fluid strain, and ε_{ii} is the elastic volumetric strain which is the trace of the strain tensor.

The slow transport of fluid in porous media is governed by Darcy's law

$$q_i = -\kappa_{ij} (\nabla_j p - f_i) \quad (3)$$

where q_i is the fluid mass flow rate, κ_{ij} is a second-order permeability tensor, and f_i is the fluid body force per unit volume.

In general, a constrained optimization problem is formulated as: find a vector of design variables $\{X\} = \{x_1, x_2, \dots, x_n\}$ that minimizes the objective function $F(\{X\})$ subjected to inequality constraints on the state variables $S_i^L \leq S_i(\{X\}) \leq S_i^U$, $i = 1, 2, \dots, m$, and the lower and upper bounds on the design variables $x_k^L \leq x_k \leq x_k^U$, $k = 1, 2, \dots, n$, where n is the number of design variables, and m is the number of state variables which are the response of the design.

To implement the optimization procedures, the design variables were the transversely isotropic material properties $\{X\} = \{E_b, E_a, \nu_b, \nu_{ab}, k\}$. Lower and upper bounds on the first three design variables were set as

$$3.34\text{MPa} \leq E_t \leq 5.76\text{MPa} \quad (4)$$

$$0.36\text{MPa} \leq E_a \leq 0.59\text{MPa} \quad (5)$$

$$0.1 \leq \nu_t \leq 0.49 \quad (6)$$

as in Table 1 of Cohen et al. (1998). Bounds on permeability,

$$1.8 \times 10^{-15} \text{m}^4 \text{N}^{-1} \text{s}^{-1} \leq k \leq 5.0 \times 10^{-15} \text{m}^4 \text{N}^{-1} \text{s}^{-1} \quad (7)$$

were set from data in Villemure and Stokes (2009), as was the out of plane Poisson's ratio,

$$0.01 \leq \nu_{at} \leq 0.1 \quad (8)$$

rather than assuming it was zero as in Cohen et al. (1998). These five material properties were optimized simultaneously.

The objective was to minimize

$$F(\{X\}) = 500 - 1000 \cdot f_{131s} \quad (9)$$

which brings the load intensity at 131 seconds (f_{131s}) obtained by ANSYS close to the measured value, roughly 0.245 MPa. The purpose of the offset, 500, was to ensure that the objective function remained positive throughout the optimization, and the scaling factor, 1000, raised the objective above the numerical noise (Chen, 2012). The state variables were assigned as the load intensities computed at 131, 205, 304, and 1000 seconds. Eight constraints on simulated load intensity were imposed based on measured values at 131, 205, 304 and 1000 seconds as follows:

$$0.24\text{MPa} < f_{131s} < 0.25\text{MPa} \quad (10)$$

$$0.10\text{MPa} < f_{205s} < 0.12\text{MPa} \quad (11)$$

$$0.07\text{MPa} < f_{304s} < 0.09\text{MPa} \quad (12)$$

$$0.059\text{MPa} < f_{1000s} < 0.062\text{MPa} \quad (13)$$

The computation was iterated until the conditions of convergence were satisfied. Two approaches for determining material properties were investigated, a zero-order method and a gradient-based constrained nonlinear algorithm.

For the zero-order method the mathematical statement expressed above is implemented using ANSYS. This approach only requires the dependent variables (state variables and objective function). Their derivatives with respect to the design variables are not required. The dependent variables are initially approximated within ANSYS. Then, the constrained minimization problem is converted into an unconstrained one by adding penalty functions that are based on the design and state variable constraints to the objective function. These penalty functions increase sharply when the design variables or state variables reach their limits (ANSYS, 2010). After conversion, sequential unconstrained minimization is used to search for a minimum of the approximated unconstrained objective function at each iteration. The zero-order method, which is embedded in the ANSYS design optimization module, is used to interlink the analysis database with the optimization database (Fig. 1).

The gradient-based approach used in this investigation is based on, and evolved from, the method of feasible directions (Zoutendijk 1960; Vanderplaats and Moses, 1973). Typical gradient-based algorithms require the general formulation of constrained optimization to be smooth and well-behaved, and they only search for the local optimum. Due to numerical noise caused by meshing and discretization in finite element or finite volume methods, the design point is usually trapped in the local design space. Using the conjugate feasible direction method (Chen, 2002), tunneling (Cetin et al., 1993; Levy and Montalvo, 1985) and hill climbing (Russell and Norvig, 2009; Pichitlamken and Nelson, 2003) in a gradient-based algorithm to solve the constrained optimization, it is possible for a design point to escape from local minima and achieve the global minimum. In this study, the optimization loop is an ensemble of the gradient-based algorithm in SmartDO (FEA-Opt Technology Inc., Taiwan) and the ANSYS poroelastic model that are linked (Fig. 2) using Tcl/Tk script that is given in the Supplementary data.

To test the uniqueness of the set of optimized material properties the optimization procedures were repeated with four different initial guesses (Table 1), selected to cover the feasible range for the five material properties. The final optimized values were averaged and used to simulate unconfined stress relaxation. The sum of the squared difference between simulated and measured load intensity was used to evaluate the goodness of the fit of the optimized model to the measured stress relaxation. Computations were performed on a computer with an Intel Xeon X5560 CPU at 2.79 GHz and 8 GB of RAM. These results were compared with the experimental data from Cohen et al. (1998).

The feasibility of the optimal properties was further investigated by comparison with expected values for the Lamé constant, λ , and aggregate modulus, H_A . For uniaxial confined compression, the radial strain ε_{rr} and circumferential strain $\varepsilon_{\theta\theta}$ are zero. The Lamé constant λ is

$$\lambda = \frac{\sigma_{rr}}{\varepsilon_{zz}} = C_{13} = \frac{\sigma_{\theta\theta}}{\varepsilon_{zz}} \quad (14)$$

where $C_{13} = \frac{E_t V_{at}}{1 - v_t - 2v_{at}^2 E_t / E_a}$ for a transversely isotropic material (Khalsa and Eisenberg, 1997; Cohen et al., 1998). Similarly, the aggregate modulus H_A is

$$H_A = \frac{\sigma_{zz}}{\varepsilon_{zz}} = C_{33} \quad (15)$$

where $C_{33} = E_a \left[1 + \frac{2v_{at}^2 E_t / E_a}{1 - v_t - 2v_{at}^2 E_t / E_a} \right]$ for a transversely isotropic material (Khalsa and Eisenberg, 1997; Cohen et al., 1998). Values of λ and H_A were computed using the optimal solution and compared with expected values.

3. Results

The average computation time for each iteration was 9 minutes using the zero-order method and 45 minutes using the gradient-based algorithm. In general, the zero-order method converged in fewer iterations than the gradient-based method (Table 1), which greatly reduced the overall computation time for this approach.

Each of the four sets of initial guesses for the five material properties converged to optimized values (Figs. 3–7). However, properties did not always converge to the same set of values (Table 1). In all cases, the standard deviations of the predicted material properties using the zero-order method were greater than those using gradient-based algorithm (Table 2). Three of the five coefficients (E_b , E_a and v_t) converged to the same value using the gradient-based approach. The out-of-plane Poisson's ratio v_{at} had the greatest variation, relative to the mean, when determined using the zero-order approach. However, using the gradient-based approach the standard deviation was an order of magnitude smaller than the mean. For permeability, the deviations were one and two orders on magnitude smaller than the mean for the zero-order and gradient-based approaches. These results suggest the gradient-based method yields more precise estimates of material properties. The variability in predicted coefficients between two approaches was low, except for the out-of-plane Poisson's ratio. For this coefficient, the gradient-based approach predicted a value that was approximately 63% lower than that predicted by the zero-order approach. However, simulated stress relaxation (Figure 9) suggests that the differences between coefficients predicted by the zero-order and gradient-based approaches have little effect on the simulated stress relaxation.

Using the final optimized properties, the Lamé constant λ was found to be 0.519 ± 0.381 MPa using the zero-order method and 0.303 ± 0.104 MPa using the gradient-based algorithm, while the aggregate modulus H_A was calculated as 0.647 ± 0.063 MPa using the zero-order method and 0.6070 ± 0.012 MPa using the gradient-based algorithm.

Simulated stress relaxation, using the average value of each of the five optimized material properties, resulted in an excellent overall fit of the peak, equilibrium and transition regions to the measured data in Cohen et al. (1998) (Fig. 9). The sum of squared differences between the measured and simulated load intensity were 0.0044, 0.0042 and 0.0042 for least-squares optimization (Cohen et al., 1998), zero-order method and gradient-based algorithm, respectively.

4. Discussion

By coupling procedures for constrained optimization with a finite element model, this study shows that it is possible to determine optimized material properties that can provide an excellent fit of the model to measurements throughout the entire history of stress relaxation. We choose to model stress relaxation since previous work (Armstrong et al., 1984; Brown and Singerman, 1986) showed that fitting the peak and equilibrium values was not possible whereas creep has been well fit. The approach used here differs from previous work that used unconstrained optimization to minimize the squared difference between measured and computed values of force, stress or displacement (Cohen et al., 1994; Wilson et al., 2004; Lei and Szeri, 2007; Liu and Ovaert, 2011; Seifzadeh et al., 2012; Fu et al., 2013; Yao et al., 2014; Reutlinger et al., 2014). In this investigation, the objective was to minimize the modeled stress relative to the measured value at the end of the applied ramp displacement, subject to constraints on the stress at selected times during stress relaxation and on acceptable values of material properties. To the best of our knowledge, this is the first investigation that used constrained nonlinear optimization to determine the material properties of soft tissues.

The reliability of the optimized properties was checked by changing the initial guesses and testing the uniqueness of the solution. Initial values were chosen based on estimates in the literature rather than over an arbitrarily wide range as suggested in Julkunen et al. (2013). Despite the range of initial values, computations show that the five optimized material properties and the reduction in the objective function are insensitive to the initial guess values. Overall, the deviation in the optimized values was less for the gradient-based algorithm than for the zero-order method. As compared to the zero-order method, the gradient-based algorithm converged to a lower value of the objective function (Fig. 8) but it needs longer calculation times. Although all of the optimized material properties determined by either method are in the range of reported data for growth plate (Villemure and Stokes, 2009), this does not guarantee that a global minimum has been found. It is possible that another set of parameters, within or outside of the range tested, could be found which would give an equally good fit to the experimental stress relaxation data.

Additionally, values of the Lamé constant, λ , and aggregate modulus, H_A , are also feasible when compared with those from previous studies (Cohen et al., 1998; Bursa et al., 1999). The value for the Lamé constant estimated from the optimal results, 0.519 ± 0.381 MPa (zero-order method) or 0.303 ± 0.104 MPa (gradient-based algorithm) appears feasible based on the range in Bursa et al. (1999), 0.37 ± 0.26 MPa to 0.40 ± 0.28 MPa. However, a direct comparison is not possible since they evaluated patellar articular cartilage instead of growth plate. Our optimal estimate of H_A , 0.647 ± 0.063 MPa (zero-order method) or 0.607 ± 0.012 MPa (gradient-based algorithm) is similar to that predicted for growth plate, 0.64 MPa (Cohen et al., 1998). Although reasonable, these values for λ and H_A were not verified in comparison with measured values for growth plate. Furthermore, we have not investigated the influence of the predicted material properties on radial deformation (DiSilvestro and Suh, 2001).

The present FE constrained optimization improved the best curve-fit of Cohen et al. (1998) by fitting the peak, equilibrium and transition regions of the stress relaxation. It also appears that the constrained optimization gives a better fit than was achieved in other investigations that used different optimization algorithms. For example, multiple stress relaxation steps at small strain (Li et al., 2005) resulted in a good fit only for the lowest strain, 0.6%. Similarly, the approach used by Julkunen et al. (2013) fit peak and equilibrium stress in some but not all strain steps (2% per step for 10 steps). Since each of these investigations used fibril-reinforced models, a direct comparison of optimization approaches cannot be made.

A good fit to stress relaxation was accomplished without imposing $v_{at}=0$ as in Cohen et al. (1998), or with negative values of v_{at} as in our previous investigation (Chung and Mansour, 2013). This optimization, and a previous investigation of articular cartilage suggest that $v_{at} \neq 0$ (Bursa et al., 1999). Despite the greater deviation in the optimized values obtained from the zero-order method, both optimization procedures produced constants that gave equally good fits to the measured data. This is consistent with our previous results that showed that the material properties do not contribute equally to the simulated load intensity (Chung and Mansour, 2013). Although the difference in v_{at} between the two optimization approaches was relatively large, we have shown that v_{at} has relatively little effect on the relaxed stress.

Clearly, there is a complex relationship between material properties and mechanical response, even in simple loading such as stress relaxation. If this approach were to be applied to stress relaxation with multiple strain steps (Li et al., 2005; Julkunen et al., 2013), the functional form of the objective function would not change. However, the value of the load intensity would be changed for each step based on the measured peak for the corresponding step. Although we have found material properties that give an excellent fit to stress relaxation, this does not imply that these properties or the transversely isotropic model would be applicable to more complex loading scenarios, or whole joint models with healthy or pathological cartilage. In this investigation the maximum strain was 10%, which is within the linear range for cartilage. However, the applicability of constrained optimization in the nonlinear range has yet to be demonstrated.

In summary, this approach is robust and effective for identification of material properties from experimental results using FEA with constrained optimization. Although the transversely isotropic poroelastic model is used throughout this study, it should be possible to apply this technique to other constitutive models such as a fibril-reinforced poroviscoelastic model, and the procedure can, in principle, be applied to other tissues e.g. articular cartilage in other tests such as confined compression, creep and indentation.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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Fig. 1.

The flow of the design optimization using the zero-order method (subproblem approximation method) established within the ANSYS parametric design language. The approximated unconstrained objective function was minimized until the convergence tolerance of 0.001 is reached.

Fig. 2.

Flow chart of finite element analysis integrated with the gradient-based optimization algorithm for the determination of material properties from experimentally measured data. Convergence of the minimization of the objective function was simultaneously satisfied with two criteria: the absolute convergence, $|F(X^{q+1}) - F(X^q)| < 0.001$, and the relative convergence, $|[F(X^{q+1}) - F(X^q)] / F(X^q)| < 0.0001$.

Fig. 3.
History of the first design variable E_t evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 4.

History of the second design variable E_a evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 5. History of the third design variable v_t evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 6.

History of the forth design variable v_{at} evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 7. History of the fifth design variable k evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 8.

History of the objective function evolved from (a) zero-order method and (b) gradient-based algorithm during optimization.

Fig. 9.

Experimental unconfined compression stress-relaxation data, analytical solution with the least-squares optimization (Cohen *et al.*, 1998) and corresponding finite element simulations with the zero-order and gradient-based optimizations for the transversely isotropic model.

Table 1

Initial guesses of material properties (E_b , E_a , ν_b , ν_{ab} , k) are set relatively far from one another in the space between their lower and upper bounds to solve for the corresponding optimized material parameters. Best fit values found by Cohen et al. (1998) are also given. The percent differences between the best fit values found by Cohen et al. (1998) and the mean values found in this investigation are given in the last two rows of the table. The Young's modulus and permeability are expressed in units of MPa and $\text{m}^4\text{N}^{-1}\text{s}^{-1}$, respectively. Case a refers to the zero-order method, and Case b refers to the gradient-based algorithm.

Initial guesses of parameters		Iterations	Optimized parameters (E_b , E_a , ν_b , ν_{ab} , k)
Case 1a	(3.5, 0.35, 0.15, 0.02, 1.8×10^{-15})	57	(5.7534, 0.5895, 0.4580, 0.0102, 4.4813×10^{-15})
Case 1b	(3.5, 0.35, 0.15, 0.02, 1.8×10^{-15})	36	(5.7600, 0.5900, 0.4900, 0.0207, 4.2129×10^{-15})
Case 2a	(4.0, 0.40, 0.20, 0.04, 2.0×10^{-15})	18	(5.7530, 0.5895, 0.4680, 0.0300, 4.2580×10^{-15})
Case 2b	(4.0, 0.40, 0.20, 0.04, 2.0×10^{-15})	26	(5.7600, 0.5900, 0.4900, 0.0382, 4.1159×10^{-15})
Case 3a	(4.5, 0.48, 0.30, 0.06, 3.0×10^{-15})	21	(5.7546, 0.5895, 0.4892, 0.0517, 4.0383×10^{-15})
Case 3b	(4.5, 0.48, 0.30, 0.06, 3.0×10^{-15})	25	(5.7600, 0.5900, 0.4900, 0.0224, 4.2042×10^{-15})
Case 4a	(5.0, 0.56, 0.40, 0.08, 4.0×10^{-15})	16	(5.7535, 0.5861, 0.4890, 0.0726, 3.8890×10^{-15})
Case 4b	(5.0, 0.56, 0.40, 0.08, 4.0×10^{-15})	27	(5.7600, 0.5900, 0.4900, 0.0223, 4.2047×10^{-15})
Best fit values from Cohen et al. (1998)			(4.3000, 0.6400, 0.4900, 0.0000, 5.0000×10^{-15})
Predicted error of Cohen et al. (1998) from Case a			(33.80%, 8.016%, 2.837%, N/A, 16.67%)
Predicted error of Cohen et al. (1998) from Case b			(33.95%, 7.813%, 0.000%, N/A, 16.31%)

Table 2

Material properties (mean and standard deviation) were obtained from the zero-order method (Case a) and gradient-based algorithm (Case b).

	E_t (MPa)	E_a (MPa)	ν_t	ν_a	k ($\times 10^{-15} \text{ m}^4 \text{ N}^{-1} \text{ s}^{-1}$)
Case a	5.7536 ± 0.0007	0.5887 ± 0.0017	0.4761 ± 0.0156	0.0411 ± 0.0269	4.1666 ± 0.2588
Case b	5.7600 ± 0.0000	0.5900 ± 0.0000	0.4900 ± 0.0000	0.0259 ± 0.0082	4.1844 ± 0.0458