



計算數學與科學計算 專題演講

時間：112 年 8 月 31 日 (星期四)~9 月 1 日 (星期五中午)

地點：東海大學 科技大樓五樓 ST527 演講室 [應用數學系]

第一天

開幕式 Opening : am 9:45~10:00

致詞：理學院 黃皇男院長 Huang-Nan Huang (Tunghai University)

第一場 Session 1: am 10:00~11:00

主持人：薛銘成 Ming-Cheng Shiue (National Yang Ming Chiao Tung University)

講者一 (1A)：陳鵬文 Pengwen Chen (Chung-Hsing University)

講題：Minimizing a quadratic over Stiefel manifolds

講者二 (1B)：蔣俊岳 Chun-Yueh Chiang (National Formosa University)

講題：Four extreme solutions of the conjugate discrete-time algebraic Riccati equation

第二場 Session 2: am 11:10~12:10

主持人：林敏雄 Matthew M. Lin (National Cheng Kung University)

講者一 (2A)：郭岳承 Yueh-Cheng Kuo (National University of Kaohsiung)

講題：Structure-Preserving Doubling Algorithms that Avoid Breakdowns for Nonlinear Matrix Equations

講者二 (2B)：劉青松 Ching-Sung Liu (National University of Kaohsiung)

講題：Newton-Noda iteration for nonlinear eigenvalue problems

第三場 Session 3: pm 13:30~14:30

主持人：胡馨云 Hsin-Yun Hu (Tunghai University)

講者一 (3A)：李雪甄 Hsueh-Chen Lee (Wenzao Ursuline University of Languages)

講題：Time-dependent weighted least-squares finite element methods in modeling Biot poroelasticity

講者二 (3B)：黃琮暉 Tsung-Hui (Alex) Huang (National Tsing Hua University)

講題：A Stabilized, Efficient and Bending Consistent Meshfree Formulation for Reissner-Mindlin Plate Theory

第四場 Session 4: pm 14:40~15:40

主持人：胡偉帆 Wei-Fan Hu (National Central University)

講者一 (4A)：樂美亨 Mei-Heng Yueh (National Taiwan Normal University)

講題：Recent Advances in Simplicial Surface Parameterizations

講者二 (4B)：林得勝 Te-Sheng Lin (National Yang Ming Chiao Tung University)

講題：Neural network methods for elliptic interface problems

第五場 Session 5: pm 16:00~17:45

此場次為「應用數學教育策略座談會」詳情請參閱另一份資料檔

第二天

第六場 Session 6: am 9:30~10:30

主持人：陳宏銘 Hong Ming Chen (Tunghai University)

講者一 (6A)：袁子倫 Tzu-Lun Yuan (Tunghai University)

講題：D-optimal designs for parameter estimation under semi-parametric model with multiresolution thin-plate spline bases

講者二 (6B)：王琪仁 Chi-Jen Wang (National Chung Cheng University)

講題：Structural and Dynamical Analysis of Social Networks

第七場 Session 7: am 10:50~11:50

主持人：袁子倫 Tzu-Lun Yuan (Tunghai University)

講者一 (7A)：呂秉澤 BingZe Lu (National Cheng Kung University)

講題：Error estimation of using L1-BDF2 method to solve subdiffusion equation with non-smooth data

講者二 (7B)：林佳威 Jia-Wei Lin (Tunghai University)

講題：A Two-Phase Optimal Mass Transportation Technique for 3D Brain Tumor Detection and Segmentation

閉幕式 Closing and Free Discussion: am 11:50~13:00

2023 NCTS Workshop on Computational Mathematics and Scientific Computing for Young Researchers

Minimizing a quadratic over Stiefel manifolds

Pengwen Chen (Chung-Hsing University)

Abstract:

In this talk, we present one sequential subspace method (SSM) for minimizing a quadratic over Stiefel manifolds, described by orthogonal r -frames. The quadratic minimization over Stiefel manifolds has applications in generating approximate solutions for Very Large-Scale Integration(VLSI) designs and graph-based semi-supervised learning. This problem can be regarded as one generalization of a trust-region subproblem and can be used to generate an initialization in the applications. Due to non-convex structure, it has many critical points corresponding to different multiplier matrices. The desired solution can be identified with a multiplier matrix with small eigenvalues $\gamma_1, \dots, \gamma_r$. In particular, when the system matrix has k identical smallest eigenvalues d , the global solution is actually the critical point corresponding to $\gamma_i \leq d$. We prove the convergence of SSM to the global minimizer, whenever each SSM subspace contains the following SSM vectors: (i) orthogonal unit vectors associated with the current iterate, (ii) vectors corresponding to the gradient of the objective function at the current iterate, and (iii) orthogonal unit eigenvectors associated with the smallest eigenvalue of the system matrix. Fast convergence of SSM can be attained, when the gradient vector is replaced with a Newton direction, which can be computed from truncated conjugate gradient methods.

Four extreme solutions of the conjugate discrete-time algebraic Riccati equation

Chun-Yueh Chiang (National Formosa University)

Abstract:

In this talk, we consider a class of conjugate discrete-time algebraic Riccati equations(CDARE), arising originally from the linear quadratic regulation problem for discrete-time antilinear systems. Under mild and reasonable assumptions, the existence of the maximal solution to the CDARE, in which the control weighting matrix is nonsingular and its constant term is Hermitian, will be inherited to some transformed discrete-time algebraic Riccati equation (DARE). In most of the past works, it is always assumed that the Riccati-type matrix equation has a unique maximal solution X_M and another meaningful solutions are lacking in brief discussion. Our contribution fills in the existing gap in finding four extremal solutions of the CDARE. As compared to the previous works, the theoretical results presented here are merely deduced from the framework of the fixed-point iteration, using basic assumptions and elementary matrix theory. We believe the results we obtain are novel on this topic and could provide considerable insights into the study of unmixed solutions of CDARE.

Structure-Preserving Doubling Algorithms that Avoid Breakdowns for Nonlinear Matrix Equations

Yueh-Cheng Kuo (National University of Kaohsiung)

Abstract:

Structure-preserving doubling algorithms (SDAs) are efficient algorithms for solving Riccati-type matrix equations. However, breakdown may occur in SDAs. To remedy this drawback, in this paper, we first introduce Ω -symplectic forms (Ω -SFs), consisting of symplectic matrix pairs with a Hermitian parametric matrix Ω . Based on Ω -SFs, we develop modified SDAs (MSDAs), for solving the associated Riccati-type equations. MSDAs generate sequences of symplectic matrix pairs in Ω -SFs and prevent breakdown by employing a reasonably selected Hermitian matrix Ω . In practical implementation, we show that the Hermitian matrix Ω in MSDAs can be chosen as a real diagonal matrix that can reduce the computational complexity. Numerical results demonstrate a significant improvement in the accuracy of the solutions by MSDAs.

Newton-Noda iteration for nonlinear eigenvalue problems

Ching-Sung Liu (National University of Kaohsiung)

Abstract:

In this talk, we will discuss nonlinear eigenvalue problems, which encompass tensor eigenvalue problems and nonlinear Schrödinger equations. We will introduce the Newton-Noda iteration (NNI) method for finding positive eigenvectors in nonlinear problems. One notable advantage of this method is its quadratic convergence rate and the ability to preserve positivity. In other words, the vector approximating the Perron vector (or ground state vector) remains strictly positive throughout each iteration.

Time-dependent weighted least-squares finite element methods in modeling Biot poroelasticity

Hsueh-Chen Lee (Wenzao Ursuline University of Languages)

Abstract:

This study presents a time-dependent weighted least-squares (WLS) finite element method to analyze a poroelastic structure governed by Biot's consolidation model. The quasi-static model equations are transformed into a first-order system comprising four fields, and the least-squares functional is defined based on the L2 residuals of the discretized temporal equations, with weights assigned according to the time step. Various sets of weights are considered, and the coercivity and continuity properties of the functional are demonstrated. Error estimation is derived for the approximation of the primal solution variables in conforming finite element spaces. Non-physical examples are utilized in numerical experiments to illustrate the theoretical results. Furthermore, we extend this method to a benchmark problem involving brain pressure simulations, and our WLS solution agrees with the findings of published works, further validating the effectiveness of our approach. Lastly, we introduce our recent work on employing equal lower-order finite elements of the least-squares type in modeling Biot poroelasticity.

A Stabilized, Efficient and Bending Consistent Meshfree Formulation for Reissner-Mindlin Plate Theory

Tsung-Hui (Alex) Huang (National Tsing Hua University)

Abstract:

The Reissner-Mindlin plate and shell theory is widely used for its ability to account for shear deformations throughout the thickness of a structure, making it applicable to various engineering structures such as domes, blood vessels, and submarines. However, it suffers from the well-known issue of "shear locking" when the plate thickness approaches the Kirchhoff thin plate limit, triggering an over-stiff solution. To address this problem, a higher-order meshfree approximation utilizing the reproducing kernel (RK) approach [1] has been developed, leading to the formulation of the Kirchhoff mode reproducing condition (KMRC) and a locking-free meshfree solution [2]. Despite these advancements, the nodally integrated meshfree formulation still faces numerical challenges in three aspects: (1) instability arising from low-energy modes of nodal integration [3], (2) inaccuracy due to the violation of bending exactness in the variational equation [4], and (3) inefficiency caused by unsuitable support size [4]. This presentation introduces a computational strategy and its numerical rationale for overcoming these issues. The proposed framework is validated through the solution of various numerical examples, demonstrating its locking-free nature, better accuracy, superior robustness and increased efficiency compared to conventional approaches.

References

- [1] Chen, J. S., Hillman, M., & Chi, S. W. (2017). Meshfree methods: progress made after 20 years. *Journal of Engineering Mechanics*, 143(4), 04017001.
- [2] Wang, D., & Chen, J. S. (2004). Locking-free stabilized conforming nodal integration for meshfree Mindlin-Reissner plate formulation. *Computer Methods in Applied Mechanics and Engineering*, 193(12-14), 1065-1083.
- [3] Huang, T. H. (2022). A variational multiscale stabilized and locking-free meshfree formulation for Reissner-Mindlin plate problems. *Computational Mechanics*, 69(1), 59-93.
- [4] Huang, T. H., & Wei, Y. L. (2022). A stabilized quasi and bending consistent meshfree Galerkin formulation for Reissner-Mindlin plates. *Computational Mechanics*, 70(6), 1211-1239.

Recent Advances in Simplicial Surface Parameterizations

Mei-Heng Yueh (National Taiwan Normal University)

Abstract:

Simplicial surface parameterization aims to efficiently compute a bijective simplicial mapping between a simplicial surface and a canonical domain. The mapping induces a unified coordinate system to the surface so that geometry processing tasks on the surface are simplified to that on a planar region. In this talk, I will introduce the recent advance in computational methods and associated theoretical results for simplicial surface parameterization, including constructive and iterative approaches.

Neural network methods for elliptic interface problems

Te-Sheng Lin (National Yang Ming Chiao Tung University)

Abstract:

Neural networks have emerged as powerful tools for numerically solving partial differential equations. In this talk, we will discuss our recent work using neural network approaches to elliptic interface problems, and possible extensions to deal with models arising from interfacial phenomena. Specifically, we will introduce a structure enforcement layer in the network to enforce the inherent properties of the solutions to given problems, such as discontinuity or periodicity. The structure enforcement layer offers a new approach to solving such problems compared to traditional neural networks, which may struggle to represent discontinuous functions and may not have built-in periodicity.

***D*-optimal designs for parameter estimation under semi-parametric model with multiresolution thin-plate spline bases**

Tzu-Lun Yuan (Tunghai University)

Abstract:

Before doing data analysis and building statistical model for inferences, the experimenter will typically need to perform good designs on the settings of controllable factors. It is essential collecting useful information efficiently which may provide precise estimation of the statistical models under study and corresponding inferences. In the literature, there are many ways of making predictions based on statistical models, such as parametric models, semiparametric models, and non-parametric models. Our main interest is to investigate the design problems for certain inference problems of the multiresolution thin-plate spline basis model, developed by Tseng and Huang (2018), with uncorrelated errors. Under this semi-parametric linear model framework, we investigate the corresponding *D*-optimal designs for estimation of the unknown parameters and making prediction on the responses of the model. In this study, we will focus on the related design problems under a two-dimensional design space. Moreover, we will also apply the methodology of finding optimal designs under the multiresolution thin-plate spline basis model, to estimation and prediction problems discussed in Yuan et al. (2020a), where the behaviors of signals obtained from various differential pad placement designs of a capacitive coupling based stacked die package are investigated. For the pad placement design problems, we will select suitable semi -parametric models under different pad sizes to exhibit the patterns of the SNR values versus the frequencies, and find optimal die placement designs with given pitch distance and overlapping percentage.

Structural and Dynamical Analysis of Social Networks

Chi-Jen Wang(National Chung Cheng University)

Abstract:

We employ the theory of isospectral network reductions to analyze social networks. This procedure allows us to uncover the hierarchical structure of each network we considered. We apply this approach to the Southern Women Data Set, Karate Network, USAir97 Network, and Taiwan Flight Network.

Error estimation of using $L1$ -BDF2 method to solve subdiffusion equation with non-smooth data

BingZe Lu (National Cheng Kung University)

Abstract:

This presentation focuses on addressing the numerical challenges encountered when using the finite difference method in time to solve the subdiffusion equation. The subdiffusion equation is a time-fractional diffusion equation with a nonlinear source term. It is given by the following equation:

$$(1) \quad \begin{cases} \partial_t^\alpha u &= \Delta u + f(u, t) \text{ for } (x, t) \in \Omega \times \mathbb{R}^+ \\ u(x, 0) &= u_0(x) \in H_0^1(\Omega) \cap L^2(\Omega) \\ u(x, 0)|_{\partial\Omega} &= 0, \end{cases}$$

where $\alpha \in (0, 1)$ and $\partial_t^\alpha u$ is the partial Caputo derivative on time that follows the expression:

$$\partial_t^\alpha u(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \partial_t u(x, s)(t-s)^{-\alpha} ds.$$

Here, $\alpha \in (0, 1)$ represents a fractional power and $\partial_t^\alpha u$ denotes the partial Caputo derivative on time. It is defined as:

$$\partial_t^\alpha u(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \partial_t u(x, s)(t-s)^{-\alpha} ds.$$

To numerically solve this equation, we employ the finite difference method in time combined with the finite element method in the spatial domain. Specifically, we use the $L1$ method with a backward difference scheme, known as $L1$ -BDF k . In our case, we utilize the $L1$ -BDF2 scheme, which is given by:

$$\sum_{i=1}^n \left(\frac{u_{i-2} - 4u_{i-1} + 3u_i}{\Delta t} \right) \left[\frac{(t_n - t_{n-i-1})^{1-\alpha}}{\Gamma(2-\alpha)} - \frac{(t_n - t_{n-i})^{1-\alpha}}{\Gamma(2-\alpha)} \right].$$

Note that $u_{-1} = u_0$.

In this presentation, we primarily focus on analyzing the temporal errors associated with the application of the $L1$ -BDF2 scheme. Analyzing these errors is challenging due to the limited regularity of the solution, which is only C^1 . Traditional methods, such as the Taylor expansion, are not directly applicable in this scenario. Instead, we propose using the Laplace transform to analyze the error and demonstrate that the $L1$ -BDF2 scheme maintains first-order accuracy.

A Two-Phase Optimal Mass Transportation Technique for 3D Brain Tumor Detection and Segmentation

Jia-Wei Lin (Tunghai University)

Abstract:

The goal of optimal mass transportation (OMT) is to transform any irregular 3D object (i.e., a brain image) into a cube without creating significant distortion, which is utilized to preprocess irregular brain samples to facilitate the tensor form of the input format of the U-net algorithm. The BraTS 2021 database newly provides a challenging platform for the detection and segmentation of brain tumors, namely, the whole tumor (WT), the tumor core (TC) and the enhanced tumor (ET), by AI techniques. We propose a two-phase OMT algorithm with density estimates for 3D brain tumor segmentation. In the first phase, we construct a volume-mass-preserving OMT via the density determined by the FLAIR grayscale of the scanned modality for the U-net and predict the possible tumor regions. Then, in the second phase, we increase the density on the region of interest and construct a new OMT to enlarge the target region of tumors for the U-net so that the U-net has a better chance to learn how to mark the correct segmentation labels. The application of this preprocessing OMT technique is a new and trending method for CNN training and validation.