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# 論 文 集

ACMT

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# 目錄

# MS-01 Recent Developments and Applications of Meshfree Methods

## Organizer:黃琮暉 助理教授

| No. | Title | Authors |
|---|---|---|
| S01-01 | 以再生核配點架構探討雙擴散對流動力問題 | 廖羿婷, 楊子儀 |
| S01-02 | A Nodal Infinite Meshfree Approach for Unbounded Problems | Kuan-Chung Lin, Ting-Wei Chen |
| S01-03 | A Neural Particle Method for Simulating Complex Flow Geometry | 白佩鑫, 甘恆全, 王福杰, 戴義欽 |
| S01-04 | 以物質點法與分子動力學探討材料受力行為之尺寸效應 | 蘇昱臻, 賴宥蓉 |
| S01-05 | Angular Basis Functions for Solving Two-Dimensional Boundary Value Problems | Chung-Lun Kuo, Pai-Chen Guan |
| S01-06 | 結合人工智慧神經網路及等參幾何法用於船板裂縫擴展之多尺度分析 | 蕭閎文, 關百宸, 張泓棠 |
| S01-07 | 根據 TR-PIV 測量進行壓力重建計算 | 林孟鋐, 張均瑩, 楊鈞堯, 周一志, 關百宸, 林存真 |
| S01-08 | A Stabilized Reproducing Kernel Enhanced Material Point Method for Geomechanics with Fragmentation | Cameron Rodriguez*, Tsung-Hui Huang, Sung-Han Yu |
| S01-09 | An Enhanced Physics Informed Neural Networks (PINNs) for Shock Wave Modeling | Tsung-Yeh Hsieh, Yang-Ming Tsai, Tsung-Hui Huang |
| S01-10 | 以廣義有限差分法結合域外虛擬點求解二維高階偏微分方程式 | 李宗翰, 范佳銘，李柏緯，邱家麟 |
| S01-11 | 用於流體水動力計算之 IGA 半點法開發 | 石惠予, 關百宸, 王奕杰 |
| S01-12 | 用於流體動力計算之半點高階小板法開發 | 石惠予, 關百宸, 李芠蕙 |
| S01-13 | An Inverse Finite Element Method incorporated with Strain Interpolation Techniques on Structural Health Monitoring | Chu-Mou Hsiao , Min-Yi Xie , Ming-Jyun Dai |
| S01-14 | 以廣義有限差分法模擬二維方形腔內之強制熱對流問題 | 朱瓊琳, 范佳銘 |
| S01-15 | 質點法於暴洪對橋梁結構衝擊模擬中之邊界設定技術探討 | 楊文嘉 |
| S01-16 | 以基本解法配合粒子群演算法求解三維邊界值問題 | 范佳銘, 張傅俐, 朱瓊琳 |

# 以再生核配點架構探討雙擴散對流動力問題

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## 摘　要

本研究透過建立一個再生核配點架構以模擬非穩態、三相位之雙擴散對流效應的數值行為。首先參考文獻研究，推導無因次之非線性動力系統控制方程式，在強形式配點架構下於空間中進行離散，接著採用再生核函數近似各相位變數，在時間離散部分採用前向差分法，最後以二步驟牛頓法進行非線性迭代求解。在數值例題中，透過考慮不同的邊界條件、具不同幾何形狀的定義域以及改變流體參數，除了與文獻比較以驗證數值架構之正確性，進而證明所提出之再生核配點架構求解非穩態系統所具之精度與運算效率。

關鍵字：再生核配點法、雙擴散、對流、非線性、非穩態

# A Nodal Infinite Meshfree Approach for Unbounded Problems

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## Abstract

This research introduces a stable and efficient infinite meshfree approach for solving a half-space. The half-space, defined as unbounded and bounded domains by an artificial boundary, is discretized by an infinite meshfree method and a nodally-integrated reproducing kernel particle method, respectively. Using the infinite meshfree method, the size of the numerical model can be reduced to save computation time. The shape function of infinite meshfree is constructed based on a combination of a boundary singular kernel method (BSK) [1] and a dummy node approach. The BSK is used to satisfy a Kronekerle delta property on artificial edges. The dummy node approach with a Newton-Cotes integration method is used to model the infinite domain, similar to the infinite element method [2, 3]. For meshfree methods, choosing a domain integration method in the Galerkin weak form governs the stability and convergence of the solution. In this study, the nodal integration method usually needs better accuracy and stable results in meshfree methods. These issues have been addressed using naturally stabilized nodal integration [4] and variational consistency conditions [5]. The responses without a self-oscillation frequency are investigated. Finally, some conclusions are made and discussed by comparing the obtained results with the corresponding analytical solutions.

*Keywords*：meshfree methods, nodal infinite meshfree approach, unbounded problems, infinite domain, naturally stabilized, variational consistency conditions

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# A Neural Particle Method for Simulating Complex Flow Geometry

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## 摘 要

數值方法歷經長期的演進，在人工智慧的出現之後有了全新的進展。Physics-Informed Neural Networks (PINNs)[1] 不同於一般網格法需要使用繁瑣的數值技巧對計算域進行離散化，它以物理方程式作為損失函數進行神經網絡的訓練，並利用機器學習中的反向傳播算法(Backpropagation)實現自動微分(Automatic Differentiation, AD)，解算複雜的偏微分方程。大部分的 PINNs 建構在 Eulerian 的架構下，較不適用於具有移動邊界的流體行為模擬。本研究開發 NPM-LA 方法，結合 Lagrangian 架構的 PINNs (L-PINNs) [2,3] 以及粒子重置技術(Adaptive Particles)，針對邊界與內部點重置粒子分佈，改善 L-PINNs 在粒子移動時造成粒子分佈不均的現象。另外，我們善用機器學習中 inference 的特質，經由訓練完成的神經網絡，取得重置後的粒子具有物理意義的物理量。因此，NPM-LA 除了可以在計算範圍內任意增減粒子數量，也避免了數值網格加密內差所衍生的問題。透過解析解的驗證與應用案例的探討，展現 NPM-LA 動態模擬流體複雜介面的高度潛力，為未來數值模擬方法提供另一選擇。

關鍵字：Physics-Informed Neural Networks, Neural Particle Method, Interface-tracking, Adaptive particles, Complex flow geometry

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# 以物質點法與分子動力學探討材料受力行為之尺寸效應

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## 摘　要

力學模擬中關於尺寸效應之研究於近年來逐漸引起廣泛之研究興趣，主要原因為研究學者可更為深入地將材料受力行為，如微結構變化或應力波傳等，由巨觀尺度向下探討至微觀乃至於奈米尺度。探究尺寸效應之主因，系歸因於模擬方法本質上之不同。巨觀尺度之力學模擬多以連體力學為基礎進行分析，如有限元素法(Finite Element Method, FEM)或物質點法(material point method, MPM)即為兩種代表性方法，透過連續方程式描述元素或質點間之相互作用，如：內力或相對運動。反之，微觀尺度下之模擬則常見以分子動力學(Molecular Dynamics)進行模擬，此法遂利用離散函數計算原子間作用力，搭配牛頓力學進而計算個原子之運動路徑。奠基於以上關於控制方程式之差異，本研究即分別使用連續與離散方程式下之物質點法與分子動力學先進行固體材料受力行為之探討，再延伸分析氣體衝擊波問題(shock tube problem)，同時探討兩方法各自之特性與其分別所代表之尺寸效應，爾後可作為複合尺度研究之參考。

關鍵字：物質點法，分子動力學，衝擊波，剪力帶

# Angular Basis Functions for Solving Two-Dimensional Boundary Value Problems

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## Abstract

In this study, we propose a series of angular basis functions for solving the 2D boundary value problems governed by different elliptic differential operators. The proposed algorithm is a boundary type meshless method which the basis function satisfies the governing equation automatically. Instead of using radial basis function in method of fundamental solutions, we adopts angular basis function to obtain the numerical solution. Several examples are provided to demonstrate the validity and accuracy of the proposed method. Similar to other boundary type meshless method, the proposed scheme is easy to implement and performs very high accuracy.

Keywords：angular basis functions; boundary type meshless method; method of fundamental solutions; boundary value problems

# 結合人工智慧神經網路及等參幾何法用於船板裂縫擴展之多尺度分析

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## 摘　要

船體結構時常需承受複雜環境外力負荷，在同時受到微觀狀態中的缺陷及裂縫成長的影響下，應力應變關係朝高度非等向性且非線性狀態發展，進而跨尺度影響到強度評估的準確度。因此本研究結合適用於船殼幾何結構的等參幾何法(isogeometric analysis)，與運用人工智慧(artificial intelligence)中可預測微尺度裂縫成長及非等向性行為的生成對抗神經網路(generative adversarial network)，建立多尺度分析架構。大尺度分析所使用的等參幾何法，直接採用電腦繪圖使用 NURBS(non-uniform rational B-splines)函數描述幾何與取代傳統有限元素法的形函數，以確保幾何的正確性與比傳統有限元素法高的準確度與計算效率。大尺度計算的積分點上，我們根據應變不變量失效理論(strain invariant failure)，判斷積分點所代表的區域是否形成裂縫，且需進一步模擬微尺度造成的影響。為模擬微觀下的破壞行為造成的非等向性影響，本研究將積分點應變預測作為微觀尺度的邊界條件施加於代表體積單元，根據主軸應力方向生成微觀裂縫，使用圖像轉換(image to image translation)的方式，預測在不同載荷條件和方向下的應力場。為了預測在不同載荷條件和方向下的應力場，本研究通過將水平和垂直拉伸下的應力場進行線性疊加，來得到雙向拉伸下的應力場。在得到應力場後，使用最大能量釋放率準則與裂縫尖端區域的平均主軸應力來判斷微裂縫的成長距離與方向。最後將所得的微尺度平均非等向性應力應變關係傳遞回大尺度模型中，藉此達到尺度結合的目標。

關鍵字：船殼結構、多尺度分析法、等參幾何法、生成對抗神經網路、裂縫成長

# 根據 TR-PIV 測量進行壓力重建計算

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## 摘　要

在造船領域中，水動力實驗的主要目的在於獲得海洋結構物如船舶或離岸平台上的作用力，而大部分實驗僅能提供流體對物體作用的粗略測量以及總力。在所有實驗技術中，質點影像測速法（TR-PIV）可以測量局部區域內的詳細速度場，使我們可以針對目標區域進行計算。因此，本研究目標是開發一種完整的數值算法，從 TR-PIV 結果中獲得壓力資料。為了實現此目標，我們引入再生核近似法（RKA）和壓力投影法，以此重建接近結構物表面的空間壓力場。

本次的計算流程，首先使用 TR-PIV 針對接面流的計算結果做為目標數據，利用渦流識別方法使用 RKA 針對已知速度場，重新建立具有局部高階 RK 形函數的平滑速度場。而在邊界上我們考慮了幾個標準，包括渦度、速度和流線，透過這些標準作為邊界條件的施加區域。然後，在渦流區域內，採用投影方法將速度和壓力場解耦。因此，求解壓力場的控制方程式變成了泊松方程，再使用 RKA 進行離散化，以求解 PDE 並獲得高解析的壓力場。

為了驗證此作法所獲得壓力正確性，我們運用計算流體力學 CFD 求解已知流場，並將 CFD 速度場做為資料輸入程式進行壓力運算，最後比較 CFD 壓力結果與我們的數值結果，檢驗誤差。

關鍵字：渦流、再生核近似法、質點影像測速法

# A Stabilized Reproducing Kernel Enhanced Material Point Method for Geomechanics with Fragmentation

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## Abstract

Modeling geomechanics applications such as explosive mining, rock cutting, or gas-emission-induced ground explosion poses significant challenges for conventional mesh-based simulation. This is primarily because they are often unable to efficiently model fragmentation due to their susceptibility to mesh distortion. Particle methods, like the material point method (MPM), have been shown to efficiently model various types of geomechanics problems but often suffer from low accuracy and pressure instability due to immature domain integration. Because particle locations are independent from the background grid, they are suboptimal points for numerical quadrature. We present an enhanced material point framework which incorporates the reproducing kernel (RK) approximation as well as a variationally consistent integration (VCI) technique and shows increased accuracy and robustness for modeling various geomechanics applications induced by blast explosion. Appropriate stabilization for shock wave dynamics or undrained conditions would be considered and discussed. The effectiveness of the proposed framework is demonstrated through various benchmark numerical examples.

Keywords：Geomechanics, Material Point Method, Variationally Consistent Integration, Reproducing Kernel Approximation, Blast Event

# A Stabilized Reproducing Kernel Enhanced Material Point Method for Geomechanics with Fragmentation

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## Abstract

Physics-informed neural networks (PINNs) have gained prominence for their potential in advancing partial differential equations (PDEs) solvers through machine learning algorithms. Its meshfree discretization facilitates flexible spatial and temporal decomposition, sidestepping mesh intricacies and numerical timestep selection. The global deep neural network within PINNs excels in capturing intricate nonlinear solution behaviors, from discontinuities to singularities and turbulence. However, when tackling shock physics, these approaches face challenges tied to conventional collocation-based PDE discretization. We present an enhanced PINN approach for modeling shock wave problems, incorporating multiscale methods, entropy control, and total variational diminishing (TVD) regularization. Our methods are benchmarked by various Riemann problems.

Keywords：Physics Informed Neural Networks, Shock Wave, Multiscale Method, Entropy Control, TVD Regularization

# 以廣義有限差分法結合域外虛擬點求解二維高階偏微分方程式

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## 摘　要

本研究提出以廣義有限差分法(generalized finite difference method, GFDM)，結合域外虛擬點(fictitious nodes)求解二維高階偏微分方程式之邊界值問題。以電腦模擬方法分析高階偏微分方程式時，有限差分法、有限元素法、有限體積法等傳統網格法需要採用高階近似函數進行推導，推導出之高階元素或是高階控制體積可能增加數值積分之困難度或是導致無法推導出離散方程式等問題，因此過去採用傳統網格法分析高階偏微分方程式的研究較為罕見。為了能簡易且準確的模擬高階偏微分方程式，本研究提出以廣義有限差分法為基礎之電腦模擬方法求解二維高階偏微分方程式，廣義有限差分法為一局部型無網格法，可以避免複雜的網格建置等耗時工作並提高電腦模擬之計算效率。此外，廣義有限差分法採用泰勒級數展開式及移動最小二乘法推導偏微分項之表達式，其偏微分項可表示為數個鄰近點(選點數)的值和權重函數之線性累加組合，因此在求解高階偏微分方程式時，僅需將泰勒級數展開至偏微分方程式之階數，再經由移動最小二乘法便可獲得高階偏微分項的近似表達式，因此廣義有限差分法是具有彈性且簡單的空間離散方法。另外，在求解高階偏微分方程式時，計算域邊界上須同時滿足多個邊界條件，因此求解的線性代數系統為一過定系統(overdetermined system)，會造成求解上的數值不穩定問題並增加電腦模擬的誤差，本研究採用域外虛擬點的技術，在計算域邊界外設置虛擬點點位，將使得線性代數系統組成為良定系統(well-determined system)，可增加電腦模擬穩定性與準確性。本研究以四個數值案例，分別求解六階、八階、十階及十二階偏微分方程式，以驗證廣義有限差分法結合域外虛擬點的可行性及準確性，並測試不同的總點數與選點數以驗證所提出數值方法的收斂性及穩定性。

關鍵字：無網格法、廣義有限差分法、高階偏微分方程式、域外虛擬點、泰勒級數展開式。

# 用於流體水動力計算之 IGA 半點法開發

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## 摘 要

為了加速與簡化水動力分析流程，因此本研究在等參幾何法（IGA）的基礎下，引入目前尚未被使用在勢流問題中的專門用於 NURBS 函數的最佳積分方法—半點法 (half-point rule)，提出了用於水動力計算的三維 IGA 半點法。本研究提出的 IGA 半點法是一個能統一離散化，並藉由半點法去除網格劃分步驟，以及省略低階小板法建立網格的大量時間，且避免奇異積分問題的水動力計算簡化流程。IGA 半點法利用 NURBS 作為形函數描述幾何與物理場，它改善了傳統 Hess-Smith 小板法因離散化而引起幾何改變的問題，並藉由等參幾何法自由度不會被積分點限制的特性，避免了求解浮體表面速度勢時產生的奇異積分問題。另外，IGA 半點法的優勢在於引入了 Hughes 所發展的半點法，此方法藉由 NURBS 函數的連續性在跨單元上佈置積分點，它相較一般高階小板法所使用的高斯積分有更好的積分效果，可以用更少的積分點描述物體的幾何形狀與物理場分佈，且此方法完全免除劃分網格的問題與被積分網格所影響的計算精度，簡化了分析過程的複雜性。以本研究建立的 IGA 半點法計算球體附加質量並與解析解比較，結果顯示本研究的方法與解析解有良好的一致性。在積分點數 96 點的情況下，縱移以及起伏方向上的附加質量相對誤差皆為 3.7%，此誤差小於 ANSYS AQWA 在積分點數 294 個下的相對誤差 4.6 以及 4.5%，證明了此方法的可行性，並說明了 IGA 半點法在計算複雜曲面上相較傳統的小板法有更好的精度，驗證了半點法在勢流問題的適用性。

關鍵字：非均勻有理 B 樣條、等參幾何法、NURBS 小板法、高階小板法、半點法

# 用於流體動力計算之半點高階小板法開發

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## 摘 要

在水動力計算中，傳統 Hess-Smith 小板法會因離散化而導致幾何改變的問題，造就了 non-uniform rational B-spline(NURBS)函數為基底的高階小板法的出現，但該方法仍然需要構建積分網格(例如高斯積分網格)。因此本研究開發了統一離散化的半點高階小板法，直接使用 NURBS 函數及其相關的半點積分方法來計算浮體的動態行為。這種方法將不再需要表面離散化過程，並且降低了分析過程的複雜性。

關於水動力計算目前多採用 Hess-Smith 小板法(低階小板法)，此方法採用低階的點積分方式，因此對於網格的精度要求很高，需要耗費大量時間在精確網格的建立上。基於上述，本研究採用以 NURBS 為近似函數的高階小板法(無小板法) 建立水動力計算程式，高階小板法在空間幾何描述中以 NURBS 函數做為形函數，可以直接將幾何模型用在數值方法中使用，不需重建網格，而一般高階小板法還是需要建立積分網格，過程仍需要有所謂網格化的動作。為了加速分析流程與簡化計算步驟，本研究將引入由 Hughes et al.所發展的半點法積分方法(half-point rule)，是專門用在 NURBS 函數的一種積分方法，相較一般使用的高斯積分有更好的積分效果，半點法是藉由 NURBS 函數的連續性在跨單元上佈置積分點，因此完全免除劃分網格的問題與被積分網格所影響的計算精度。總結上述，本研究的目標為建立一個能統一離散化，並藉由半點法去除網格劃分步驟，省略了建立網格的大量時間的三維半點高階小板法水動力計算簡化流程。最後以本研究建立的半點高階小板法程式計算有解析解答案的球體附加質量，結果顯示本研究的方法與解析解有良好的一致性。在積分點數 96 點的情況下，縱移以及起伏方向上的附加質量相對誤差皆為 3.7%，此誤差小於 ANSYS AQWA 在積分點數 294 個下的相對誤差 4.6 以及 4.5%，證明了此方法的可行性，並且說明了半點高階小板法在計算複雜曲面上相較傳統的小板法有更好的精度。並且，本研究利用此方法計算海洋結構物常見的圓筒殼幾何模型，將合理的積分點數下所計算的水動力係數與 NURBS 小板法以及商用軟體 ANSYS AQWA 在足夠多的網格下的答案做比較，結果顯示本研究提出的方法之結果與其他兩者相當接近。總結上述的結果，證明了本研究成功建立三維半點高階小板法流程並驗證了半點法在勢流問題的適用性。

關鍵字： NURBS 小板法、高階小板法、半點法

# An Inverse Finite Element Method incorporated with Strain Interpolation Techniques on Structural Health Monitoring

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## Abstract

An inverse finite element method (iFEM) is presented to monitor structural deformations of thin-walled structures based on strain sensor data without external load and material information. In the iFEM framework, a singular stiffness matrix commonly arises with an insufficient number of strain sensors and inappropriate sensor layouts. Therefore, a numerical study in shape-sensing of thin-walled structures is implemented by using the iFEM approach incorporated with strain interpolation techniques to determine the optimal sensor layouts subjected to different types of loading conditions. It is found that the proposed approach can effectively reconstruct full-field structural deformations with minimum strain sensors. Overall, the proposed approach exhibits great potential in the structural health monitoring field.

Keywords：iFEM, Structural health monitoring, Strain sensor, Interpolation technique

# 以廣義有限差分法模擬二維方形腔內之強制熱對流問題

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## 摘　要

本研究採用廣義有限差分法(generalized finite difference method)搭配牛頓法(Newton method)開發電腦模擬模式，以準確且穩定地模擬具有出口與入口之二維方形腔室內之穩定強制熱對流現象。強制熱對流現象是指利用外部力驅動流體流動以實現熱交換的現象，於日常生活中常見的室內抽風扇、冷暖器的使用都涉及此現象，且隨著氣候變遷人們越加習慣待在具有冷暖氣的室內場所內，且隨著環保意識上升，通過建築物通風口增強室內流場流動帶動熱交換之綠色建築設計，皆可以說明強制熱對流現象之重要性。本研究以速度-渦度形式之奈維爾-史托克斯方程式與能量方程式描述強制熱對流問題，並首次採用廣義有限差分法為空間離散方法，搭配牛頓法作為非線性代數方程系統的求解方法，探討方形腔室在固定入口位置時，研究不同出口位置與出口大小對於二維流場和溫度場變化之影響。廣義有限差分法是一種新開發的區域型無網格法，無需建置網格和數值積分，可以大幅地提高電腦模擬效率，且具有良好的數值穩定性與自訂參數不多等優勢。廣義有限差分法利用局部化的概念，並採用泰勒級數展開式(Taylor series expansions)和移動最小二乘法(moving least squares method)來推導每個點的微分項離散式，將其與求解非線性代數方程的牛頓法結合，可以準確、穩定且有效率地模擬方形腔室內的強制熱對流現象。本研究採用多個數值案例，來驗證所開發的電腦模擬模式之可行性、一致性和有效性，並將在本研究中探討此電腦模式在未來工程問題上之應用性與延伸性。

**關鍵字：**無網格法；廣義有限差分法；牛頓法；速度-渦度方程式；強制熱對流問題。

# 質點法於暴洪對橋梁結構衝擊模擬中之邊界設定技術探討

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## 摘　要

本研究旨在探討質點法（Material Point Method）於橋樑結構受暴洪沖擊之問題中所需之流水邊界模擬技巧。此技巧延伸自土壤－結構互制問題模擬中的、基於應力邊界條件的邊界模擬技術，將在入流與出流邊界處之水流運動反應分為不可壓縮之一維流場或層流，以及應力波動反應。此基本假設意味著模擬的水體範圍必須足夠大，以確保因結構引起的紊流不致影響邊界假設的不可壓縮水流理想反應。至於因水流－結構相互作用產生的復雜應力波動則採用經典的黏滯邊界來吸收。在模擬中，傳統的質點法粒子自入流邊界處，依邊界不可壓縮流場狀態創建並發送到計算域中，並在穿過出流邊界後被消除。新提出的表面粒子則用於施加邊界應力以確保能吸收應力波的同時維持邊界應有的水流運動。本研究首先以一維應力波傳問題測試此邊界模擬技巧在質點法中的表現。其次再呈現暴洪洪峰衝擊橋樑上部結構的二維模擬結果，以顯示使用新流水邊界模擬技巧的改良效果。

關鍵字：質點法、入出流邊界、吸收邊界、暴洪、橋梁衝擊

# 以基本解法配合粒子群演算法求解三維邊界值問題

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## 摘　要

本研究採用基本解法(method of fundamental solutions, MFS)結合粒子群演算法(particle swarm optimization, PSO)來準確且高效率地求解三維線性邊界值問題。使用電腦模擬分析三維邊界值問題時，有限元素法與有限體積法等傳統網格法需要建立三維網格，並進行控制方程式離散推導或是數值積分等工作，導致電腦模擬過程非常耗時且數值結果準確性不高。為了避免建立網格與數值積分等工作，多種無網格法陸續被提出，基本解法就是其中一種具有高度發展潛力的無網格法。在基本解法分析流程中，數值解可以表示為基本解的線性累加，由於數值解表達式已經滿足控制方程式，因此計算過程中不需要內部點位參與計算，只需要一組邊界點位與一組域外源點點位。藉由邊界條件導出線性或是非線性代數方程式系統，求解過後就可以獲得源點強度，並進而獲得高準確性的電腦模擬結果。在過去的研究中發現，雖然基本解法非常簡易且具有高準確性，域外源點的空間位置可以決定數值模擬結果的準確性，因此如何決定域外源點的空間位置仍是一個值得研究的問題。在本研究中，我們採用粒子群演算法來有效且快速的搜尋域外源點的位置，粒子群演算法為一種啟發式的最佳化演算法，在每一次的搜尋中藉由群體跟個體之間的相互關係來逐漸逼近最佳的源點位置，且因粒子群演算法僅描述粒子的位置與速度，故無需大量的最佳化資訊即可進行搜尋，具有極快的收斂性。本研究採用多個三維邊界值問題，驗證結合基本解法與粒子群演算法之可行性與有效性，並將在本研究中探討所提出電腦模擬方法在未來工程問題上之可能應用。

關鍵字：基本解法；粒子群演算法；邊界值問題；無網格法；最佳化演算法

# MS-02 Microstructures and Mechanics of Materials

## Organizer: 鄒年棣 副教授兼副系主任

| No. | Title | Authors |
|---|---|---|
| S02-01 | 介觀尺度計算材料學－以離散元素法與相場法解析材料熱製程流變現象 | 蘇德徵, 柯映亘, 陳建翔, 李晨愷, 黃聰彥 |
| S02-02 | 利用圖神經網路建置辨認形狀記憶合金微結構後處理工具 | 曾翊銘, 王培德, 陳南佑, 楊安正, 鄒年棣 |
| S02-03 | Mechanical Properties of Chemically Complex Ultraelastic Alloy Using Machine Learning-enabled Potential Energy Model | Po-Yu Yang, Cheng-Lun Wu, Chun-Wei Pao |
| S02-04 | Quantum Machine Learning Frameworks for Predicting Potential Energies of Complex Material Systems | Hsu-Kai Cheng, Chun-Wei Pao, Po-Yu Yang |
| S02-05 | Computational design of organic materials in optoelectronic applications | Kun-Han Lin |
| S02-06 | Beyond the LiC6 Composition: Revisiting the Storage Capacity Limit of Graphite by Using Hybrid Machine Learning Potential Model | Po-Yu Yang, Chun-Wei Pao |
| S02-07 | Atomistic Simulation Study on the Short-range Chemical Ordering and Dislocation Behaviors in the Refractory NbTaTiV High-Entropy Alloy | I-Che Cheng, Chin-Lung Kuo |
| S02-08 | 利用機器學習方法探索材料複雜特性 | 劉禹辰 |
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| S02-10 | Phase field modeling of microstructural evolution during laser processing | Guo-Chi Li, Shih-Kai Chien, and Chuin-Shan Chen |
| S02-11 | 動力學蒙地卡羅的介觀尺度塑性模型在奈米金屬玻璃中的應用 | 羅友杰、黃仲偉、葉智仁、尾方成信、胡宣德、鄭憲清 |
| S02-12 | Very high dislocation density in advanced alloys | Hung-Wei (Homer) Yen , Binbin He, Guan-Ju Cheng, Yi-Hsuan Sun, Mingxin Huang |

# 介觀尺度計算材料學－以離散元素法與相場法解析材料熱製程流變現象

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## 摘　要

在材料科學中，介觀尺度通常用來描述介於微觀尺度（原子和晶格結構）和宏觀尺度（宏觀形狀和性能）之間的尺度範圍，一般可涵蓋從次微米級結構到毫米級結構等。介觀尺度關注材料晶粒尺寸、形狀、分布等特性，並且探討其與微觀結構組合和宏觀機械與物化行為的關聯性。介觀尺度計算材料學可大略歸類為「介觀尺度材料力學模擬」與「介觀尺度材料微結構模擬」兩大類，前者有晶體塑性有限元素法、離散元素法、離散差排動力學等以及晶格波茲曼法等，而後者則有介觀蒙地卡羅法、相場法以及細胞自動機等。

金屬冶煉和合金鑄造為現今不可或缺，但也會產生大量碳排放的材料高溫製程。因此，尋求製程參數最佳化以及新式減碳操作方案，一直受到國際冶金工業的高度重視。然而，由於材料在高溫環境下的多相流變行為和微結構演進之臨場實驗數據往往非常有限，故必須要在各種尺度下應用到可被驗證的計算材料方法以模擬金屬製程於高溫環境表現出的複雜多相流變現象。本演講將簡要說明離散元素法與相場法的計算原理，以及分享研究團隊應用這兩項介觀尺度計算材料方法為材料熱製程流變現象建模的近期應用成果。

關鍵字：介觀尺度、流變現象、離散元素法、相場法、金屬冶煉、合金鑄造

# 利用圖神經網路建置辨認形狀記憶合金微結構後處理工具

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## 摘　要

形狀記憶合金(SMAs)的微結構演變細節可以透過分子動力學(molecular dynamics, MD)計算以模擬出其動態機制與特性。然而，這類型的計算長期存在的一個問題是至今沒有一個有效率的後處理方法可以分析其分子動力學的結果。例如，Common Neighbor Analysis(CNA)僅能標示出 austentie 與 martensite 相之間的差異，卻無法區分 martensite 中不同的晶相與兄弟晶（crystal variants)。因此本研究基於 GraphSAGE 神經網絡提出一個新式的後處理工具，並利用溫度和應力誘導的 martensite transformation 的 MD 計算結果之數據集進行訓練。這個工具可以辨別出 martensite 相轉變中的高達 23 種不同的晶相，包括：orthorhombic、monoclinic 和 R 相。我們也透過未包含在訓練數據集中的特別案例(例如不可回復形狀之奈米壓痕測試)來驗證此方法之應用性與準確性。不僅如此，我們還將其應用於大尺度的 MD 模型(超過 4000 萬個原子）並與舊式演算法比較，以凸顯本方法的效率。結果顯示本方法可以迅速且準確地可視化 MD 模擬之結果。預期此工具將對於 SMA 或相關材料的原子級計算研究有相當的幫助。

關鍵字：形狀記憶合金、兄弟晶、圖神經網路、微結構

# Mechanical Properties of Chemically Complex Ultraelastic Alloy Using Machine Learning-enabled Potential Energy Model

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## Abstract

The challenge of modeling intricate alloys has ignited innovative simulations. Despite their pivotal applications, these alloys' mechanical properties remain elusive due to quantum limitations. Leveraging the power of machine learning (ML), we've harnessed the spectral neighbor analysis potential (SNAP) to delve into the ultraelastic Co25Ni25(HfTiZr)50 alloy. Our ML- enabled potential model, fine-tuned through energy and force data from density functional theory (DFT), with meticulous calibration using a Bayesian optimizer, this model adeptly predicts energies and atomic forces akin to DFT calculations. Extensive of large-scale molecular dynamics simulations, involving over 105 atoms, have been executed to unveil deformation and dislocation dynamics in nanowires and bulk structures. These simulations reveal an amorphous shear band-like domain that forms after dislocation pinning, aligning with experimental observations. Our study underscores SNAP's capability to achieve quantum-level precision in intricate alloys of five elemental constituents, providing profound insights into their deformation mechanisms.

Keywords：spectral neighbor analysis potential, density functional theory, Bayesian optimizer, LAMMPS

# Quantum Machine Learning Frameworks for Predicting Potential Energies of Complex Material Systems

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## Abstract

Construction of potential energy surface is often a crucial step for modeling and thus gaining insights into thermodynamic and kinetic behaviors of a material system with atomistic resolution. Constructing potential energy surface using first principles techniques like density functional theory (DFT), is usually computational demanding, leading to limited explored configurations as well as limitation on the allowed system sizes. The machine learning-enabled potential energy models such as the artificial neural network model have drastically reduced the computational demands, enabling evaluation of potential energy of a given material system order of magnitudes faster in time and larger in size while retaining the relative fidelity with respect to DFT. However, in most of the ML-based potential energy models, the system potential energy is assumed to be partitioned into individual atomistic contributions, which is a rather arguable approximation from DFT perspective. Hence, in this study, we propose the possibility of leveraging quantum machine learning to predict the potential energy of a material system to lift the energy partition approximation. Two quantum machine learning frameworks are constructed to predict potential energy of complex alloys, namely, the quantum convolutional neural network and the quantum deep neural network. By harnessing a novel binning approach to renormalize the atomic descriptor vectors, it is possible to train a data- and parameter-efficient quantum machine learning model that yields high prediction accuracy for systems of arbitrary sizes. The present study therefore projects a promising strategy for predicting the potential energy of a complex material system through quantum machine learning, which can become increasingly powerful with more qubits available.

Keywords：Quantum machine learning, Chemically complex alloy, DFT, Atomic fingerprints

# Computational design of organic materials in optoelectronic applications

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## Abstract

Organic materials have been widely used in various optoelectronic applications, such as organic light-emitting diodes (OLEDs) and solar cells, owing to their low cost, flexibility and low-temperature and solution processability. In addition, the versatility of synthetic organic chemistry offers possibilities for tailoring organic materials for specific applications. In this context, computational modeling allows us to truly exploit the power of organic synthesis by providing us (i) low-cost and reliable prediction of target properties and (ii) better understanding of the structure-packing-property relationship (SPPR). In this talk, I will present how computations can help in accelerating the discovery pace of organic materials in three applications: (i) hole transport materials in perovskite solar cells, (ii) thermally activated delayed fluorescence (TADF) emitters for single-layer OLEDs, and (iii) non-fullerene acceptors for organic photovoltaics.

Keywords：Computational material design; organic optoelectronic materials; multiscale simulations; charge carrier mobility

# Beyond the LiC6 Composition: Revisiting the Storage Capacity Limit of Graphite by Using Hybrid Machine Learning Potential Model

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## Abstract

Graphite is one of the most widely used negative electrode materials for lithium ion batteries (LIBs) Nowadays, the market is still looking for fast-charging, safe and performant LIBs, which drive the exploration and promotes the fundamental investigations to break through the storage capacity limit of graphite. Upon electrochemical lithium intercalation during charging, the established upper limit for reversible lithium storage capacity in graphite is acknowledged as forming LiC6 compounds and corresponds to a theoretical capacity of 372 mAh/g. Recent studies have suggested that the capacitance of graphite can potentially exceed this theoretical limit under ambient conditions. However, there remains a significant gap in our understanding of the intricate mechanisms governing overlithiation phase formation and the dynamic processes involved in lithium intercalation.

Herein, we proposed a hybrid machine learning potential model by combining the empirical potentials and the machine learning (ML) based potential energy model. This model is trained based on a series of atomistic configurations from density functional theory (DFT) calculations, covering a wide variety of stages of lithiation, including pure lithium metal, lithium plating, and overlithiated graphite intercalation compounds such as LiC2. The present study demonstrates that the hybrid machine learning approach could further extend the scope of machine learning energy models, allowing us to investigate the lithium intercalation into graphite over a wide range of intercalation capacity to unveil the underlying mechanisms of lithium plating, diffusion, and discovery of new dense graphite intercalation compounds for advanced LIBs with high charging rates and high energy densities.

Keywords: Graphite Intercalation Compound, Hybrid Machine Learning Potential Model

# Atomistic Simulation Study on the Short-range Chemical Ordering and Dislocation Behaviors in the Refractory NbTaTiV High-Entropy Alloy

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## Abstract

We employed first-principles calculations and MEAM modeling to investigate the short-range chemical ordering and dislocation behaviors in the NbTaTiV RHEA. Our first-principles calculations showed that the thermodynamic stability of this HEA can be greatly enhanced by increasing the number of Ta-V pairs while decreasing the number of V-V and Ta-Ti pairs within the alloy, indicating the tendency to form short-range chemical ordering in the NbTaTiV RHEA. Our MEAM simulations further showed that the average core energy of dislocations in the NbTaTiV RHEA is substantially lower than their constituent elements, indicating a relatively higher dislocation density with a reduced mobility in RHEA than in other BCC metals. It was also found that the average dislocation core energy in RHEA with local chemical ordering is comparable to that within the SQS structure. However, some core structures with extremely low energies were identified, which can effectively hinder the motion of dislocation to enhance the mechanical strength of the NbTaTiV RHEA.

Keywords：NbTaTiV RHEA, short-range chemical ordering, first-principles calculations, MEAM modeling

# 利用機器學習方法探索材料複雜特性

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## 摘　要

材料特性與其結構、加工、應用息息相關，如何從材料結構及其製造方法有效預測材料特性，係材料科學家、工程師關切的重要議題。計算材料科學提供不同尺度的模擬方法，嘗試預測材料在電子尺度、介觀尺度，乃至於巨觀尺度的特性表現，有效提供實驗現象的解釋，並大幅減低實驗嘗試錯誤帶來的成本。然材料特性極其複雜，並非所有特性皆具備精確解析解，因此無法透過現行計算材料科學方法進行模擬；另一方面，部分大型尺度的運算成本昂貴，相當耗時，不利於高通量運算的材料篩選。近年來，機器學習等人工智慧方法在材料領域日益熱門，以建立替代式數學模型的方法來模擬材料之複雜特性。本演講將介紹數項機器學習方法應用於材料科學探索之案例，包含中子輻射對鋼鐵材料延性脆性轉化溫度影響[1-2]、電遷移效應之有效電荷[3]、低溫共燒陶瓷之介電常數與損耗係數[4]等，探討如何透過此方法建構相應材料特性模型及其應用。

關鍵字：機器學習、材料特性

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# Layer distribution study in 2D Ruddlesden-Popper perovskites from large-scale hybrid Monte Carlo simulations enabled by machine learned energy model

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## Abstract

2D layered perovskite material exhibits increased stability in environmental conditions compared to its 3D counterpart. In addition, due to layered nature, its optoelectric properties can be easily tailored through stoichiometric ratio of perovskite and spacer components. However, the performance of 2D perovskite based photovoltaic and optoelectronic devices is lower compared to those of their 3D lead halide perovskites, in part due to the non-uniform perovskite layer distribution between intercalated hydrophobic large organic molecule spacer bilayers which has been observed in several experimental studies. In this work, we explore the relationship between the temperature and spacer layer type, namely butylammonium (BA) and phenethylammonium (PEA), and layer distribution within 2D layered perovskites. We trained quantum-accurate machine-learning enabled inter-atomic Spectral Neighbor Analysis Potential (SNAP) from carefully selected ab-initio molecular dynamics (AIMD) trajectories, which is successfully tested under canonical ensemble, enabling accurate sampling in wide phase space area. The trained energy model based on SNAP scheme was deployed within in-house developed hybrid Monte Carlo layer exchange code to study the influence of different processing temperatures on 2D perovskite material microstructure. Our large-scale atomistic simulations revealed both temperature and spacer type dependent non-uniform layer distribution. Hence, our study presented a viable scheme which could be employed to extract the microstructure details of 2D perovskites in particluar and other complex materials in general.

Keywords：2D perovskite, machine learning potential, Monte Carlo method

# Phase field modeling of microstructural evolution during laser processing

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## Abstract

Laser melting processes and solidification, commonly occurring in laser welding and metal additive manufacturing, are gaining increased attention. The laser source heats the metal to the melting point in the laser melting process, forming the melting pool. Then, the melting pool solidifies, resulting in different microstructure. By varying the processing parameters, different microstructures form. Understanding the influence of these parameters on the microstructure is essential for improving the mechanical properties of the welded structure or additive manufacturing components. This study uses a phase-field method to model the laser melting and solidification processes. We use the open-source software MOOSE (Multiphysics Object-Oriented Simulation Environment) to investigate solidification under different boundary conditions. The SPH (Smoothed-Particle Hydrodynamics) simulation provides the temperature boundary value for the phase-field model. The results show that temperature evolution strongly affects the growth of the dendritic structures and, consequently, the resulting microstructures. The influence of process parameters on microstructures and mechanical properties is also investigated.

Keywords： Laser melting, solidification, grain growth, phase-field method, MOOSE

# 動力學蒙地卡羅的介觀尺度塑性模型在奈米金屬玻璃中的應用

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## 摘　要

金屬玻璃（metallic glass, MG）展現出許多有前途的特性，如高屈服強度、低摩擦係數和高抗腐蝕、氧化和磨損能力。然而，由於剪切帶導致的局部應變和差劣的延展性，阻礙了 MGs 的作為結構材料的應用。另一方面，奈米玻璃（nanoglass, NG）由奈米尺度界面引入金屬玻璃中，組成異質性玻璃區域，可能是對抗嚴重剪應變局部化的有效策略，這設計概念已由一系列原子模擬所預測，但欠缺可與實驗相對照的數值模擬。在這項研究中，我們基於動力學蒙地卡羅（kinetic Monte Carlo, kMC）算法，提出一個新的介觀尺度模型來研究金屬玻璃和奈米玻璃的機械行為。考慮到變形過程中剪切帶的發展可以根據老化-回春-黏合-液化模型分為四個階段，我們提出一個基於 von Mises 應變的 Sigmoid 函數的可變特徵應變（variable characteristic strain, VCS）。數值模擬顯示，隨著 NG 顆粒尺寸減小到約 10 奈米，金屬玻璃材料的塑性將從非均勻變形過渡到均勻變形。這種過渡可以歸因於小顆粒尺寸阻礙了剪切帶的形成，導致應變硬化。此外，我們也引入了彈性常數的遞減功能用以表徵承載失效響應。數值模擬顯示，我們所提出的 kMC 模型對於設計納米玻璃以抵抗剪切局部化非常有效，特別是當我們可以從原子模擬中獲得適當的 VCS 時。

關鍵字：動力學蒙地卡羅、介觀尺度塑性力學、金屬玻璃

# Very high dislocation density in advanced alloys

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## Abstract

In metals, high dislocation density is demanded for strain hardening in plastic deformation. However, high dislocation density easily causes strain localization, which initiates crack formation. This paradox limits the development of high-stregnth and high-ductility materials. This presentation includes three topics. (1) A extremely high dislocation density (> $10^{16}$ $m^{-2}$) is introduced into a newly-developed steel named the D&P steel. Such a high dislocation density enables mobile dislocation avalanche, which contributes on a large local plasticity. Hence, we create a very strong (yield strength > 2 GPa) but ductile (elongation > 15%) steel with this idea. (2) The novel structural-chemical characteristics allows high dislocation density in high-entropy alloy (HEA) under deformation. We apply this principle in understanding fatigue behavior of CoCrFeMnNi HEA. It is found that dislocation aggregates is benifit for the formation of super dislocation cell. Crack propagation along the cell boundaries contributes to a low crack propagation rate (da/dN), leading to excellent resitance to fatigue failure. (3) Recently, we employ a novel approach to reaching a high capability of dislocation storage (> 5 x $10^{15}$ $m^{-2}$) in high-entropy steel (HES) in common tensile tests. This approach is realized by cooperative behavior between geometrically neccessary dislocaiton (GND) and deformation twin (DT). A strong and very ductile HES is developed via the GND-DT cooperation. In summary, a high disloation density is desired when its evolution is well understood and controlled.

Keywords：dislocation ; steel ; high-entropy alloy ;high-entropy steel ; stregnth ; ductility

# MS-03 Computational Materials and Statistical Mechanics

## Organizer: 張書瑋 副教授

| No. | Title | Authors |
|---|---|---|
| S03-01 | Ab Initio Calculations for Halide Solid Electrolytes | Chi-Hsuan Lee, Kuei-Hsien Chen, Chun-Wei Pao |
| S03-02 | 以晶體塑性有限元素法探討溶質隨機性對高熵合金力學行為影響 | 黃韋智，羅友杰，黃仲偉 |
| S03-04 | 利用分子動力學探討有機半導體光催化劑在產氫系統中的微觀作用機制 | 林婉錡，史覲瑄，游濟華 |
| S03-05 | Phosphate release pathway of dynein ATPase | Pei-Cheng Li, Yu-Bai Xiao, Shu-Wei Chang |
| S03-06 | Molecular Dynamics Studies on Bridged Structures in Ultrathin 2D MoS2 for Enhancing Toughness | Chang-Chun Chang, Chi-Hua Yu |
| S03-07 | 分子動力學模擬探討甲基丙烯酸酯改質乙二醇殼聚醣分子結構及交互作用 | 吳佳鴻，游佳欣，周佳靚 |

# Ab Initio Calculations for Halide Solid Electrolytes

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## Abstract

Lithium halides $Li_3MX_6$ (M = trivalent metal; X = Cl and Br) constitute a promising category of solid electrolytes, characterized by exceptional electrochemical stability and other desirable properties for all-solid-state batteries. This study aims to propose a material design strategy for lithium halides in high-voltage all-solid-state Li-ion batteries by comprehensively investigating crystal structures, phases, electronic properties, and ionic conductivities. First-principles calculations unveil the significant impact of varying compositional ratios between M and X on the structural properties and stabilities. The evaluation of Li-ion conductivities was conducted using *ab-initio* molecular dynamics calculations, which were enhanced by active machine learning algorithms in advance. Moreover, the replacement of $M^{3+}$ with $Zr^{4+}$ induces Li vacancies, thus amplifying Li-ion conductivities and triggering a phase transition.

*Keywords:* ab-initio molecular dynamics, ionic conductivity, structural properties.

# 以晶體塑性有限元素法探討溶質隨機性對高熵合金力學行為影響

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## 摘　要

高熵合金係由多種主元素混合而成的新型合金，因其溶質隨機分佈會造成局部的短程有序。文獻上利用分子動力學的模擬下顯示：高熵合金局部的原子排列對於合金發生塑性變形時，差排滑移的勢能造成波動，進而解釋高熵合金相較於傳統合金具有一些獨特的力學性質。然而分子動力學的模擬有時間與空間尺度上的限制，無法完全解釋大尺度的巨觀性質。本研究利用差排密度晶體塑性理論，結合溶質隨機性的特性，將統計儲存差排參數視為隨機變數，引入自定義的高熵合金有限元素模型中。透過晶體塑性有限元素可進行不同空間尺度離散的特性，建立多組不同溶質隨機尺度的模型模擬拉伸實驗，探討不同空間尺度溶質隨機性對於高熵合金的力學性質的影響。藉此將高熵合金微觀與巨觀的行為做連接，表現介觀尺度的觀察與討論溶質隨機性的範圍大小對於模型整體的影響。數值模擬的結果顯示：當溶質隨機尺度相對模型尺度的比值達到 1/16 以上，就可看出巨觀尺度下高熵合金極限強度會逐漸發散；而當兩者比值小於 1/16 十，則高熵合金極限強度會趨於收斂。。

關鍵字：高熵合金、晶體塑性有限元素法、溶質隨機性、差排密度

# 利用分子動力學探討有機半導體光催化劑在產氫系統中的微觀作用機制

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## 摘 要

本研究提出一種以第一原理計算與分子動力學為基礎的方法，模擬不同半導體光催化劑的特性，建立一套能夠觀察和分析微觀尺度下分子間之方法。近年來，光催化水分解技術因其將可再生的太陽能轉化為環保的氫氣而受到廣泛研究和關注。近期的研究顯示，透過主鏈工程策略將親水的非共軛結構單元與疏水性的共軛結構單元結合成主鏈工程型非連續共軛高分子，可以有效改善傳統共軛高分子聚合物主鏈的疏水性，並提升光催化產氫系統的效率。分子模擬在化學、材料和生物等領域中扮演重要角色，可模擬分子結構和性質等物理量。藉由分子模擬可研究微觀尺度下物質作用機制，並應用於共軛高分子材料開發和性質預測。本研究運用第一原理計算中的密度泛函理論和自然電荷分析，計算不同設計的高分子光催化劑活性位點，並觀察分子在基態和激發態下的電子分佈。透過分子動力學模擬分析軌跡文件，獲得徑向分佈函數和動態氫鍵密度數據。這些數據可用來預測氫鍵形成機率，並進一步驗證主鏈工程增加水分子和聚合物間相互作用的可能性。

總之，本研究通過結合第一原理計算和分子動力學，模擬不同高分子光催化劑的性質。透過多樣的高分子模型和不同的模擬環境，建立了能夠觀察和分析微觀尺度下分子間的作用情形。這提供了一種有效設計和優化高分子光催化劑的途徑，也為未來相關研究奠定基礎。

關鍵字：第一原理計算；分子動力學；半導盤光催化劑；共軛高分子；光催化產氫

# Phosphate release pathway of dynein ATPase

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## Abstract

Dynein is a motor protein with six AAA+ domains, it moves along microtubules in cells and plays an important role in transporting intracellular cargos. The motility is generated through an ATPconsumingcycle in the AAA+ domains. The movement of dynein is coupled to the ATP hydrolysis cycle at AAA1, and the mechanism requires AAA3 to be in a post-hydrolysis state (ADP-Pi or ADP). To further discuss the behavior of hydrolysis products release, we implement metadynamics simulation to search for the possible release pathway of Pi ($H_2PO_4^-$) at AAA1 and AAA3. The potential of mean force (PMF) obtained from the simulation is then used to calculate the lowest cost path at the two sites. By summarizing the results, we can compare the Pi release pathway and energy barrier between the two domains and deliberate the mechanism.

Keywords： dynein; motor protein; molecular dynamics simulation; metadynamics

# Molecular Dynamics Studies on Bridged Structures in Ultrathin 2D MoS2 for Enhancing Toughness

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## Abstract

2D materials possess highly functional properties due to their unique mechanical, thermal, and electrical features, positioning them as essential building blocks for future ultrathin, flexible electronics. However, they are prone to fracturing due to flaws or defects, highlighting the significance of enhancing their toughness for practical applications. In this context, we introduce architected defects to 2D materials and investigate their fracture behavior through molecular dynamics simulations. This study specifically focuses on architected defects in the form of bridges within these materials.

We create pristine $MoS_2$ samples with rectangular-shaped defects of varying widths and lengths, aiming to explore their impact on the strength and behavior of 2D $MoS_2$. All molecular dynamics (MD) simulations are conducted utilizing the Large-scale Atomic/Molecular Massively Parallel Simulator. The atomic structures and stress distributions are visualized using the OVITO software.

Our findings indicate that the length of defects in the form of parallel bridges significantly influences fracture toughness. Longer bridges exhibit the ability to notably enhance the toughness of MoS2. This strategic approach offers a means to augment the toughness of 2D materials without introducing foreign substances or altering material chemistry. As a result, it presents a universal method for enhancing their mechanical properties.

Keywords： $MoS_2$, defects, energy dissipation, bridged structure, fracture toughness, molecular dynamics

# 分子動力學模擬探討甲基丙烯酸酯改質乙二醇殼聚醣分子結構及交互作用

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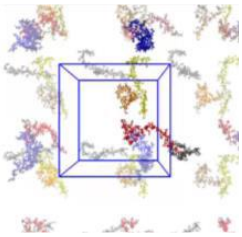
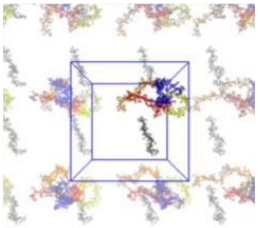
## 摘 要

在過去生物醫學領域的研究中，已發表 3D 列印技術可用於製造生物組織及器官，透過固化方法，建構複雜形狀的生物體。乙二醇殼聚醣擁有優良的生物相容性，是一種適合用於細胞生長的基礎材料，因此，以甲基丙烯酸酯改質之乙二醇殼聚醣透過光固化形成的三維結構，得以增加機械性質並應用在 3D 列印生物墨水。本研究利用分子動力學模擬方法，分析從微觀尺度下材料結構和相互作用，探討濃度、取代度改變造成之變化。根據先前文獻合成光交聯水凝膠的方法，我們修改力場，建立多個不同濃度及取代度的分子模型，包含改質、未改質、低濃度或高濃度，比較不同模型之間的氫鍵數量及分子構型變化。根據我們的觀察，甲基丙烯酸酯改質的乙二醇殼聚醣因結構關係，會大幅降低其親水性；在濃度小於 5%時，分子結構相對延展，有較高的分子間作用力；在濃度增加至 10%以上時，因為分子結構捲曲，分子間作用力則降低。希望通過微觀尺度下的分析，更瞭解材料的性質及其發展於應用的潛力。

關鍵字：分子動力學、乙二醇殼聚醣、甲基丙烯酸酯改質



5%乙二醇殼聚醣



5%甲基丙烯酸酯改質之乙二醇殼聚醣

# MS-04 Computational Metamaterials and Related Structures or Systems

## Organizer: 王雲哲 教授兼系主任

| No. | Title | Authors |
|---|---|---|
| S04-01 | 榫卯接合的地震超材料設計 | 蘇于琪，王鈺仁，周昱菁，林冠騰 |
| S04-02 | Low-frequency band-gap seismic metamaterial using dual-layer tube-type resonators | Yuan-Yo Lo, Nathan Wenzel, Tung-Yu Wu, Shiang-Jung Wang |
| S04-03 | 多模態消能機制之地震超材料研發 | 黃揚升，吳日騰 |
| S04-04 | Controlling and Generating Three-Dimensional Bioinspired Microstructures Using Transformer-Based Generative Adversarial Network | Yu-Hsuan Chiang, Bor-Yann Tseng, Chi-Hua Yu, Chuin-Shan Chen |
| S04-05 | Non-reciprocity and non-Hermiticity in the linear responses of metamaterials | Yun-Che Wang, Yasothorn Sapsathiarn |
| S04-06 | A Deep Learning Empowered Smart Representative Volume Element Method for Long Fiber Woven Composites | Mao-Ken Hsu, Chi-Hua Yu |
| S04-07 | Non-monotonicity in time-dependent Poisson’s ratio of metamaterials | Yu-Ching Lai, Yun-Che Wang |
| S04-08 | Manipulation of acoustic wave propagation through the design of metamaterials | Chien-Chun Shen, Tse-Chun Liao, Yun-Che Wang |
| S04-09 | Study of electromagnetic wave propagation in metamaterials | Chenghsuan Wei, Tse-Chun Liao, Yun-Che Wang |

# 榫卯接合的地震超材料設計

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## 摘　要

本研究以榫卯接合為基礎進行發想，提出特殊的預鑄流程以製造兩種新穎的地震超材料設計－獎盃模型與蘋果模型。兩種模型皆僅以混凝土為材料，即可達成低於 15 Hz 的帶隙。我們發現在相同的用料量下，蘋果模型的帶隙區間較獎盃模型低，然而，獎盃模型卻有較出色的衰減效果。透過暫態分析發現，兩者模型皆能在帶隙區間衰減，驗證了頻散分析的結果。最後引入 921 地震歷時，以蘋果模型為例，改變圓半徑參數，並以半徑線性變化的形式排列，驗證漸變排列的有效性。

關鍵字：地震超材料、榫卯結構、帶隙、暫態模擬、表面波

# Low-frequency band-gap seismic metamaterial using dual-layer tube-type resonators

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## Abstract

Seismic metamaterials have been widely developed in recent years as an innovative approach to earthquake-resistance technology. Artificial structures are constructed to manipulate incoming wave propagation, resulting in the formation of frequency regions known as frequency band gaps, in which the waves are blocked from reaching the safeguarded buildings. However, currently, seismic metamaterials face two major obstacles: (1) the band gap frequency generated is relatively higher than the primary frequency of earthquakes, and (2) the lack of metamaterials designed specifically for body waves. To address these drawbacks, we propose a new low-frequency (0.35Hz - 1.5Hz) seismic metamaterial unit purposefully to attenuate body waves using a dual-layer tube-type resonator. The number of unit cell rows and the manner of ordering are analyzed to determine the most favorable arrangement of metamaterial units for optimal wave reduction effect. The simulation results show that an arrangement consisting of four consecutive metamaterial units is the most economical. Moreover, the ground response analysis using actual ground motion records demonstrates that the proposed metamaterial units can reduce the spectral acceleration by half for frequency falling within the band gap, further substantiating the significant potential of the envisaged resonator.

Keywords: Seismic metamaterial, local resonance, finite element analysis, band gap

# 多模態消能機制之地震超材料研發

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## 摘　要

超材料(metamaterial)之發展最早起源於電磁波與光學領域，其利用超材料內單元晶格之特殊性質，以達到控制波傳之目的。近年來，聲學超材料蓬勃發展，而地震超材料亦為一新興研究領域。常見的地表震動主要來自於地震與施工所產生之表面波，地震所攜帶的能量能對其行經範圍的基礎建設造成巨大的破壞，而交通或施工等的震動在長時間下也會對建築疲勞與人體健康造成損害。由於此類波形具有較低的頻率，超材料的設計通常採用局部共振(local resonance)以控制單元晶格之尺寸。然而以此種機制為基礎之超材料通常具有較窄的帶隙(band gap)，難以涵蓋各種不同建物高度之自然頻率以及大型車輛與施工所產生的地表震動。本研究提出以壕溝為基礎之單元結構設計，此種單元結構能同時具有布拉格散射(Bragg scattering)與局部共振兩種消能機制，其頻散曲線(dispersion curve)中的兩個帶隙區域將分別覆蓋地震(<20Hz)與施工(40~60Hz)所產生之振動頻率範圍。此外，本研究對單元結構之材料與尺寸參數進行分析，在一些特定的參數組合下能將兩個帶隙範圍合併，使得中間段的帶隙呈現混合式的消能現象，進一步將帶隙擴大至整個低頻範圍。為確保此設計在真實環境下的可行性，本研究在數值模擬中以真實地震歷時資料來對整體效能進行評估，並將所使用的材料參數與尺寸控制在實務合理範圍內，提供現代防減震系統新的思維與策略。

關鍵字：地震超材料；表面波；週期結構；布拉格散射；局部共振

# Controlling and Generating Three-Dimensional Bioinspired Microstructures Using Transformer-Based Generative Adversarial Network

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## Abstract

Biomaterials are distinguished by their excellent material properties, largely attributable to their intricate microstructures. These properties make them particularly attractive for creating highperformance materials with diverse functionalities. This research focuses on the generation of bioinspired microstructures with predetermined characteristics. Our approach amalgamates AutoEncoder, Transformer, and Generative Adversarial Network (GAN) concepts, resulting in AETransformer-GAN. This innovative framework learns from sequential images and generates threedimensional bioinspired microstructures. Further advancements encompass a conditional model variant trained with conditional labels for refined generation control. This approach provides a highly efficient generative methodology for generating bioinspired microstructures, paving the way for designing previously unexplored hybrid microstructures with targeted properties.

*Keywords*：Bio-inspired Microstructure, Generative Adversarial Networks, Transformer

# Non-reciprocity and non-Hermiticity in the linear responses of metamaterials

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## Abstract

The homogenized properties of metamaterials can be affected by their geometrical shape, topology and constituent's material properties. As an example, the effective Young's modulus of the metamaterial can be made different in tension and compression, hence reciprocity fails in this regard. Non-reciprocal coupled-field properties have also been realized. In contrast to non-reciprocal yield stress due to the Bauschinger effects, which is caused by dislocation structures in crystalline materials, the effects of microstructure or internal energy sources are responsible for the non-reciprocity in the linear responses of metamaterials. In addition to the non-reciprocal phenomena, the metamaterials can also be made non-Hermitian due to the presence of internal energy sources. As an example, negative-stiffness induced extreme effective Young's modulus of metamaterials has been demonstrated, as well as their extreme coupled-field properties. In this talk, the non-reciprocity and non-Hermiticity in metamaterials will be discussed, and their exceptional points (EP) in homogenized properties will be emphasized. Such metamaterials may be found exceptionally useful in mitigation of vibration in seismicity, as well as noise reduction.

# A Deep Learning Empowered Smart Representative Volume Element Method for Long Fiber Woven Composites

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## Abstract

In response to the global trend of carbon reduction over the last few years, various industries have gradually begun research, design, and production of carbon fiber composite materials. The mechanical properties of woven fiber composites can be obtained by using simulation analysis software, which can reduce unnecessary waste during design and manufacturing. However, difficulties arise in the simulation analysis due to the complexity of the weaving method. With many research teams starting to implement artificial intelligence (AI) technologies in recent years, which has been widely used to overcome long-standing obstacles in many different fields. We implement a convolutional neural network (CNN), a deep learning method, to establish a model that utilizes a representative volume element for the prediction of the mechanical properties of a woven fiber composite material. The predictive model significantly streamlines the computational complexity involved in analyzing woven composite materials, resulting in a substantial reduction in processing time compared to conventional methods. Unlike traditional finite element simulations, which necessitate intricate boundary conditions and interactions on a case-by-case basis, our research simplifies these complex procedures and accommodates a wide range of scenarios. This research offers substantial advantages for industrial manufacturing, particularly in the design and mass production of woven fiber composite materials.

Keywords：finite element method, deep learning, representative volume element, carbon fiber woven composite material, mechanical properties.

# Non-monotonicity in time-dependent Poisson's ratio of metamaterials

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## Abstract

The topology and geometry of metamaterials strongly affect their effective Poisson's ratio. For isotropic, homogeneous and purely elastic metamaterials, their Poisson's ratio in the range of -1 and 0.5 is attainable. For viscoelastic materials, their Poisson's ratio is a monotonic function in time domain. In this work, the time-dependent effective Poisson's ratio of metamaterials is investigated for its non-monotonicity under the creep or stress relaxation process. The metamaterials may lose and regain their auxetic properties , i.e. negative Poisson's ratio, as time increases. Changes in microstructure inside the metamaterials during the time-dependent deformation are responsible for the non-monotonic behavior in their effective Poisson's ratio.

Keywords: metamaterials, negative Poisson's ratio, auxetic properties, viscoelasticity

# Manipulation of acoustic wave propagation through the design of metamaterials

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## Abstract

Reduction or amplification of acoustic waves in their amplitude is of practical importance in engineering applications. Through the design of the topology and geometry of metamaterials, we show the reflection and transmission of acoustic wave can be manipulated. In addition to the control of bandgaps, the incorporation of the Helmholtz resonators in the metamaterials provides additional degrees of freedom to design the metamaterials to largely increase energy absorption, hence reduce noise. Our work here demonstrates the feasibility of using metamaterials to manipulate the propagation of acoustic waves for real-world applications.

Keywords: metamaterials, acoustic wave, Helmholtz resonator, design

# Study of electromagnetic wave propagation in metamaterials

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## Abstract

In this work, the propagation of electromagnetic wave in metamaterials are investigated. The topology and geometry of the microstructure of the electromagnetic metamaterials can be designed to obtain particular effects. For electromagnetic waves in the microwave frequency range, we show, through metamaterial design, the heating capability can be largely enhanced. There is a wide range of applications for such heating capability in food or other industries. Parametric design of the electromagnetic metamaterial will be discussed.

Keywords: metamaterials, electromagnetic wave, microwave heating

# MS-05 Deep Learning in Computational Mechanics

## Organizer: 游濟華 助理教授

| No. | Title | Authors |
|---|---|---|
| S05-01 | Prediction of Li-dendrite growth with physics-informed neural network and transformer model | Yi-Chia Han, Chun-Wei Pao, Chih-Hung Chen |
| S05-02 | Toward microstructural generalization: a hybrid GNN-DMN model for multiscale materials modeling | Tung-Huan Su, Jimmy Gaspard Jean, Szu-Jui Huang, Chuin-Shan Chen |
| S05-03 | 人工智慧在高分子材料設計的應用 | 張瑋哲, 蔡宗耘, 游濟華,陳錦文, 陳俊杉 |
| S05-04 | A Deep Learning Enhanced Multiscale Modeling for Materials involving Micropores, Heterogeneities, and Micro-Cracks | Tsung-Hui Huang, Yan-Zhen Chen, Chu-Hao Wang, Tsung-Yeh Hsieh, Yu-Chun Chou, Cheng-Che Tung, Po-Yu Chen |
| S05-05 | 應用人工智能軟體探討模封材料性質變異性對於封裝體翹曲之影響 | 莊婉君, 陳伯恩 |
| S05-06 | Simulating High Re Flow Fields using Data Assisted PINN | Adhika Satyadharma, Ming-Jyh Chern, Heng-Chuan Kan |
| S05-07 | 利用圖神經網路以蛋白複合體之動態圖形結構預測蛋白功能 | 葉宏智, 陳諺霖, 簡子皓, 張書瑋 |
| S05-08 | Deep Learning Model to Predict Dendrite Structures Growth | Bor-Yann Tseng, Chen-Wei Conan Guo, Yu-Chen Chien, Jyn-Ping Wang and Chi-Hua Yu |
| S05-09 | Design Resilient Nacre-Inspired Structures Using Reinforcement Learning | 張冠輝, 蔡友晟, 曾柏諺, 游濟華 |
| S05-10 | Metamaterial Discovery for Attenuating Human-sensitive Acoustic Waves Using Deep Learning | Chun-Tat Chan, Ting-Wei Liu, Rih-Teng Wu |
| S05-11 | 應用加權 K 鄰近演算法進行波浪記錄補遺 | 吳南靖, 羅耀財, 陳俊杉 |
| S05-12 | 以機器學習方法探討中子輻射導致鋼鐵延性脆性轉換溫度效應 | 劉禹辰 |
| S03-03 | 優化 Grad-CAM 視覺化：深入解析蛋白質功能預測模型與鄰居分數重新分配 | 簡子皓, 陳諺霖,葉宏智, 張書瑋 |

# Prediction of Li-dendrite growth with physics-informed neural network and transformer model

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## Abstract

Lithium-dendrite growth at anodes has long been a well-known constraint limiting the development of lithium-ion batteries. Gaining better insights into dendrite growth mechanism is therefore a challenging yet pivotal task. Although phase-field models (PFM) serve as an effective numerical approach for modeling Li dendrite growth behaviors compatible with experiments in time and length scale, seeking for a computationally efficient scheme as a surrogate model is still imperative owing to the computationally demanding fine meshes required for PFM. Recently, deep learning (DL) has shown promising potential in learning dynamical systems. Herein, we present two DL models to capture the spatial and temporal evolution of Li dendrite growth, ion concentrations, and electrostatic potential of Li metal anode upon charging. The first model integrates the physics-informed neural networks (PINNs) with PFM. We train our PINNs model to learn PFM with imposed governing equations and boundary conditions so as to retain consistency with physics laws over training. In the second model, we develop a transformer, originated from Natural Language Processing (NLP), for the prediction of dynamic evolution of lithium dendrite growth. We use embedded dynamical systems as input sequences and predict Li deposition based on past time steps with stochastic initial conditions. The outcomes of both models yield notable consistency with those from numerical models. While additional endeavors are required to dive deeper into the application of deep learning in PFM, our findings propose an alternative platform for studying phase-field of Li-dendritic morphology.

Keywords：Physics-informed neural networks, Transformer, Lithium deposition

# Toward microstructural generalization: a hybrid GNN-DMN model for multiscale materials modeling

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## Abstract

Designing complex materials requires comprehensive understanding of their mechanical behaviors, which gives rise to extensive research in multiscale materials modeling. Machine learning- based multiscale materials modeling seeks to speed up multiscale modeling and time-to-solution predictions of material behaviors. The deep material network (DMN) is one such model that stands out due to, on one hand, it only needs to be trained on linear elastic data and yet can be used to predict nonlinear material behaviors. On another hand, it has micromechanics building blocks with explainable parameters and hence makes DMN applicable to classes of microstructures. However, the DMN model can only be confidently used for the specific microstructure it was fitted on. Research works on this limitation however rely on rule-based interpolation strategies. In this work, we adopted a data-driven point of view to tackle this microstructural generalization issue. We cleared this roadblock by introducing graph neural network (GNN) to learn microscopic details of materials through their graph representation. This learned information is used to generate an appropriate DMN for each microstructure, and predict homogenized nonlinear material behaviors. This entire process is integrated under a single umbrella which we term as a hybrid GNN- DMN model. Examples demonstrate the validity and reliability of the approach, even when it comes to the prediction of material responses for microstructures unseen during training.

Keywords：Deep material network, Graph neural network, Graph-based mechanistic deep learning, Multiscale modeling

# 人工智慧在高分子材料設計的應用

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## 摘　要

高分子材料是世界上最廣泛使用的材料之一，其最大的特色是能透過改變單體組成種類，以及聚合的型態，得到各種不同的性質。然而由於高分子材料結構複雜的特性，以往透過實驗往往需要花費大量的時間以及金錢，才能得到具有目標性質的高分子材料。因此本研究欲以機器學習的方法，加速高分子材料開發的流程。在本研究中，主要是對於共聚高分子(co-polymer)進行性質預測以及最佳化設計。在嵌段共聚物(block copolymers)機械性能的資料集上，用深度學習建立代理模型，並透過貝葉斯優化(Bayesian Optimization)實現反向設計，能夠快速在設計空間中，找出對應目標性質的材料組成參數。針對更為複雜的無規共聚物(random copolymer)進行設計時，由於設計空間更大，即使用模擬也無法全部進行標註。因此本研究導入主動學習(active learning)，針對代理模型不確定性較大的資料進行標註，以利有效率地建立無規共聚物的代理模型。並在建立模型後，能夠透過可解釋人工智慧(Explainable AI)的方法，找出針對目標性質，各個材料組成參數的重要性。

關鍵字：高分子材料、機器學習、主動學習、最佳化

# A Deep Learning Enhanced Multiscale Modeling for Materials involving Micropores, Heterogeneities, and Micro-Cracks

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## Abstract

This presentation addresses challenges in multiscale modeling of some engineering materials, where direct numerical simulation (DNS) faces obstacles due to microscopic defects, heterogeneities, and the curse of dimensionality, leading to computationally intensive processes. To address these issues, we present a multiscale neural network enhanced finite element method (NN-FEM). This involves employing a pre-trained neural network on microstructure representative volume elements (RVEs) to construct a homogenized surrogate model tailored for macro-scale scenarios. Moreover, an energy bridging equation is formulated to establish a connection between the macroscale continuum with microstructures. The performance of the proposed NN-FEM is validated by solving a series of material examples involving micropores, heterogeneities, and micro-cracks, demonstrating superior computational efficiency and efficacy compared to the DNS results.

Keywords：Multiscale Modeling, Deep Learning, RVE, Microstructure, NN-FEM

# 應用人工智能軟體探討模封材料性質變異性對於封裝體翹曲之影響

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## 摘　要

封裝體在熱製程過程中常因各結構層間材料的機械性質不匹配而導致翹曲行為的發生，而翹曲問題往往造成機台異常與稼動率損耗。在扇出型封裝製程下，經由產線上經驗可得知封裝體在移除載台製程時將產生最大的翹曲量，因此本研究針對扇出型封裝在移除載台製程步驟時之模封材料(epoxy molding compound, EMC)的各種材料特性參數對於晶圓翹曲量影響進行探討，利用 COMSOL 物理多種耦合模擬軟體建立一扇出型封裝移除載台製程的晶圓翹曲量評估模型，搭配使用人工智能軟體進行封裝體翹曲量的不確定性分析，以期找出合適之 EMC 材料特性的評估準則。研究結果發現透過主效應分布圖得知在 EMC 中的所有機械性質中，玻璃轉化溫度(glass transition temperature, Tg)前的材料參數包含 25℃至 35℃的楊氏模數($E_L$)與熱膨脹係數(α1)對晶圓翹曲影響最大，而 EMC 在 Tg 點、Tg 點後的材料特性($E_H$、α2) 對晶圓翹曲量影響則較輕微，而經由不確定性分析結果亦可得知各材料參數的變動造成相對應封裝體翹曲量的改變量，因此藉由本研究提出之材料變異性對於封裝體翹曲量影響評估方法，可以找到關鍵材料特性參數與量化數值，達到降低封裝體翹曲量、提高生產良率的目的。

關鍵字：扇出型封裝、移除載台製程、材料性質變異性、不確定性分析

# Simulating High Re Flow Fields using Data Assisted PINN

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## Abstract

While physics informed neural network does allow the result of a neural network to obey physical laws, by just relying on the governing equation loss and boundary loss, its usage is usually limited for low Re flows. For higher Re, in order to resolve the flow field properly it requires a significant amount of collocation points, increasing its computational load. This study would focus on using several velocity measurements data in order to assist the PINN convergence, significantly lowering the collocation points requirement, thus allowing the simulation on high Re flows in a reasonable time frame. This approach is tested in 2 dimensional cavity flow at Re = 200, 1000 and 5000 with 0 to 49 paired u, v velocity data. The results shows that by using more data, the collocation points requirement to obtain the same accuracy is reduced. For Re = 200, this approach allows the simulation to be conducted 7.4 times faster and for Re = 1000, the simulation could be more than 40 times faster.

Keywords：Physics Informed Neural Network, Data Assimilation, Cavity Flow

# 利用圖神經網路以蛋白複合體之動態圖形結構預測蛋白功能

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## 摘　要

蛋白質為生命體不可或缺的一部分，不同的蛋白質功能影響著不同的生物活動，目前文獻有利用蛋白質序列，以及透過蛋白質三級結構預測蛋白質功能之方法。而圖神經網路於功能預測之研究大多侷限於處理單一肽鏈，但許多蛋白質須以蛋白複合體形式存在，才能提供生物功能。因此本研究結合蛋白質動態資訊，以及探討蛋白複合體之圖形加譯方式，藉由圖神經網路訓練出能準確預測蛋白功能之模型，並分析以三級結構與複合體預測之差異。此研究將打破以往單一肽鏈預測之限制，使蛋白能以最接近工作型態之方式進行功能預測，對未來未知蛋白之功能推測，或是設計功能性蛋白等研究有極大的幫助。

關鍵字：圖神經網路、蛋白質動力、蛋白複合體、蛋白質功能預測

# Deep Learning Model to Predict Dendrite Structures Growth

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## Abstract

The demand for highly specific and complex materials has made the development of controllable manufacturing processes crucial. Among the numerous manufacturing methods, casting is important because it is economical and highly flexible regarding the geometry of manufactured parts. Since solidification is an important stage in the casting process that influences the properties of the final product, the development of a controllable solidification process using modeling methods is necessary to create superior structural properties. However, traditional modeling methods are computationally expensive and require sophisticated mathematical schemes. Therefore, we propose a deep learning model to predict the morphology of the dendritic crystal growth solidification process, along with a reinforcement learning model to control the solidification process. By training the deep learning model with data generated using the numerical phase field method, the structure evolution of the solidification process could be successfully predicted. In addition to the structure, the input of the deep learning model also includes numerical conditions to affect the generated results. This condition is a parameter related to the degree of supercooling in the phase field simulation. Furthermore, we designed the crystal growth structures to be altered by adjusting the condition in the deep learning model by implementing reinforcement learning to control the dendritic arteries. Reinforcement learning can make the generated structure have different characteristics by giving different target conditions. This research opens new avenues for applying artificial intelligence to the optimization of casting processes, with the potential to utilize it in the processing of advanced materials and to improve the target properties of material design.

Keywords： casting, dendritic structure, generative model material, reinforcement learning, solidificatoin

# Design Resilient Nacre-Inspired Structures Using Reinforcement Learning

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## 摘　要

自然界中的生物透過億萬年的演化，進化出了千變萬化的結構、機能和適應性，形成了完美的生物系統，而生物材料是針對特定的生存環境應用而演化出來的，從骨骼到牙齒，從貝殼到蜘蛛網，自然界中的生物體具有驚人的生物力學性能和優異的功能性能。然而有些生物材料具備了這些卓越的特性，如高韌性、高強度和輕量化。仿生材料模仿了自然界中的結構和功能，以提供額外的優勢，如高強度、輕量化、自行修復和環境適應性等，從航空到建築工程，仿生材料的應用範圍廣泛，為各個領域帶來了巨大的潛力。珍珠母為當今研究最多的仿生材料之一，其珍珠層以其獨特的高韌性和輕質性能而聞名。 其獨特的結構由柔軟的珍珠質蛋白和堅硬的碳酸鈣組成，使其能夠偏轉直線擴展的裂縫，從而增加能量耗散。 然而，由於設計空間中難以處理的組合數量，珍珠質微結構的模擬具有挑戰性。 因此，我們提出了一種強化學習（RL）框架來有效地設計高韌性的珍珠質結構。 通過設計裂紋尖端的局部結構，我們將強化學習與有限元結合起來，通過替換設計空間中的軟材料和硬材料來優化結構。 從最初的晶胞開始，其中大部分珍珠層結構由軟材料組成，我們的方法通過在珍珠層結構佈置剛性和軟材料來逐漸改進珍珠層結構，以實現更高的韌性。 在進行有限元模擬和實驗測試時，優化的設計表現出對裂紋不敏感的行為和出色的抗裂性。 該設計框架可用於需要快速結構重排的合成儀器，例如生物材料和未暴露的子結構，從而提高其機械性能。

關鍵字：仿生材料；高韌性；抗裂性；珍珠質微結構；強化學習

# Metamaterial Discovery for Attenuating Human-sensitive Acoustic Waves Using Deep Learning

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## Abstract

Phononic metamaterials are engineered materials designed to exhibit specific acoustic properties, often involving the manipulation of mechanical vibration propagation in solids. It is noteworthy that the presence of a frequency band gap indicates the ability to hinder elastic waves within particular frequency ranges. Depending on the intended application, it might require to block a different range of frequencies. However, the design of metamaterials often requires a time-consuming and inefficient trial-and-error process. Recent advances in deep neural networks (DNN) have shown the capability
of solving various problems within a short amount of time, including inverse design. In this study, we propose a deep-learning-based workflow for discovering phononic plate metamaterials with a frequency band gap targeting human-sensitive acoustic noise. The forward calculations were conducted using the Finite Element (FE) method, employing the Mindlin plate formulation. Subsequently, a neural network was trained to perform inverse design. Results show that, with only 360 samples, the proposed DNN accurately achieves the target band gap with only 2% error, by optimizing five parameters that control the geometry of the unit cell. Moreover, it is observed that despite the predicted unit cell appears different from the ground-truth, the design from DNN still meets the desired target band gap, leading to the discovery of new unit cell. The comparisons between several baseline methods also demonstrate the robustness of the proposed approach.

Keywords：acoustic metamaterial; phononic crystal; noise control; deep learning; neural network; band gap; metamaterial discovery

# 應用加權 K 鄰近演算法進行波浪記錄補遺

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## 摘　要

本研究建構了一個創新的資料補遺模式，應用於台灣東北海域 4 個浮標站所組成之觀測網。該模式使用了加權 K 鄰近（WKNN）演算法。此乃常用於型態辨識之 K 鄰近（KNN）演算法的增強版。我們收集了從 2018 年 1 月 1 日至 2023 年 6 月 30 日共 48,168 筆逐時數據記錄，其中只有 18,910 筆不含缺失值。驗證結果顯示，若至少有兩個浮標站正常運作，則該模式在填補缺失波浪數據方面具有相當高的準確性。因此，我們成功地估算了 27,243 筆不完整波浪記錄中的缺失部分，使得數據完整性從 40%提高到 96%。這一改善有助於實現數據之有效維護，確保數據完整性，從而可實現即時海況監測、促進災害預防、早期警報系統與資源優化。

關鍵字：補遺模式、缺失波浪數據、加權 K 鄰近（WKNN）演算法、數據完整性

# 以機器學習方法探討中子輻射導致鋼鐵延性脆性轉換溫度效應

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## 摘　要

核子反應爐中，高能中子會提升反應爐壓力鋼板之延性脆性轉換溫度，並同時增加降伏應力（$\Delta\sigma_y$），兩者間具備線性正比關係。現有諸多物理模型可以預測不同輻射通量(flux)、輻射劑量(fluence)情形下之 $\Delta\sigma_y$，然在測試反應堆(test reactor)的加速照射實驗中，前述模型將低估高劑量情況下的脆化情形。在低通量下，隨著反應爐壓力鋼板長期運行達到 80 年或更長時間，導致高劑量的輻射情況，甚至在某些情況下劑量將達到 $10^{20}$ n/cm$^2$。儘管脆化現象在加速的高輻射通量測試反應堆中已有廣泛研究，然而，使用測試反應堆的數據將引發了輻射通量效應的問題。本研究採用機器學習方法，基於測試反應堆硬化數據進行訓練，訓練集涵蓋了各種通量、劑量、溫度及鋼種組成之複雜輸入，目標預設值為 $\Delta\sigma_y$，並以六種核心鋼板材料（CM6、LC、LD、LG、LH 和 LI）評估通量、劑量和組成之實際通量與有效通量（$\phi te/\phi t$）比值，以校準低通量-高劑量脆化之物理模型。本研究預測的 $\phi te/\phi t$ 與過去所提之物理模型估算成果相當一致，顯示機器學習方法的應用潛力[1, 2]。

關鍵字：機器學習、中子輻射、反應爐壓力鋼板、延性脆性轉換溫度

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# 優化 Grad-CAM 視覺化：深入解析蛋白質功能預測模型與鄰居分數重新分配

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## 摘　要

本研究基於過去使用的 Grad-CAM 方法，結合新的可視化技術，更深入地探究已訓練的圖神經網絡（GNN）模型對蛋白質結構的關注。我們專注於揭示模型關注的功能相關區域，並運用 Guided Grad-CAM 以及我們新提出的 Neighborhood Score Redistribution 方法進行區域可視化。這些方法旨在增進對模型解釋性的理解，進而深化對蛋白質結構的認識。通過採用 Grad-CAM 作為基礎，我們在過去已有的方法基礎上，進一步優化並結合新的技術，以提供更全面的蛋白質結構解釋。我們從功能豐富的蛋白質樣本中進行細心選擇，將這些樣本輸入 GNN 模型，並利用我們提出的方法進行熱度圖分析，我們致力於識別在不同蛋白質中重複出現的關注區域，推測其與功能相關。同時，我們的新方法 Neighborhood Score Redistribution，更進一步將 Grad-CAM 分數在不同層次分配給鄰居節點，以提升對區域關注的解釋性。透過這些綜合方法，豐富 GNN 在蛋白質研究中的應用，為生物學領域帶來新的視角，同時強化對 GNN 模型的解釋和優化能力，從而更有效地支援生命科學研究。

關鍵詞：Grad-CAM、Guided Grad-CAM、Neighborhood Score Redistribution、圖神經網絡、蛋白質結構、功能區域、可視化技術、生物信息學。

# MS-06 Advances in Artificial Intelligence and Computer Vision for Structural Health Monitoring, Autonomous Inspections and Prognostic Assessments

## Organizer: 吳日騰 助理教授

| No. | Title | Authors |
|---|---|---|
| S06-01 | 使用機器學習和統計資訊開發異常訊號的檢測和分類器 | 黃謝恭, 林天郇 |
| S06-02 | 調諧質量阻尼器之減振效能與健康狀況評估方法 | 林錦隆, 林其璋, 鄭佑典 |
| S06-03 | 高度變化的 V 型與 N 型地震防護屏障 | 蘇于琪, 王聖翔 |
| S06-04 | 結合強震預警與之半主動滾動隔震支承研發 | 莊子霆, 曾冠証, 許丁友 |
| S06-05 | Story drift and damage level estimation of buildings using relative acceleration responses with multi-target deep learning models under seismic excitation | 周肇昱, 劉倢妤, 張家銘 |
| S06-06 | 在無人工標註資料下訓練深度學習模型進行現地鋼筋影像辨識 | 黃琮煒, 陳翊翔, 林之謙, 陳俊杉 |
| S06-07 | 高擬真 RC 橋柱破壞模式預測系統之研發 | 吳亭諺, 吳日騰, 王炳雄, 林子剛, 張國鎮 |
| S06-08 | Rebar Spacing Inspection with Structure-informed Features Segmentation and Its Practical Application | Hung-Yi Chen, Shih-Jie Chuang, Tsung-Wei, Huang, Yi-Hsiang Chen, Jacob J. Lin, Chuin-Shan Chen |
| S06-09 | 結合房屋街景圖像與地震強度參數之老舊鋼筋混凝土建築反應預測 | 陳鵬宇, 李坤展 |
| S06-10 | 攝影測量技術應用於面外受力之結構磚牆的三維位移與大應變分析 | 梅可欣, 袁宇秉, 張智安, 温子漢 |
| S06-11 | 鐵皮屋頂與電力網絡在颱風下的區域脆弱性分析 | 莊于楷, 林其穎 |
| S06-12 | 考慮流固耦合交互作用之橋梁沖刷穩定性分析 | 陳柏瑋, 林子剛 |

# 使用機器學習和統計資訊開發異常訊號的檢測和分類器

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## 摘 要

結構健康監測（structural health monitoring，SHM）和結構完整性管理（structural integrity management，SIM）相關應用為了持續檢測結構狀態，海量的資料伴隨著不正常的量測數據 將不斷的被產生，不正常的量測數據會在信號處理過程中扭曲資訊，在系統識別過程中提取錯誤特徵， 在損傷檢測過程中產生錯誤結論， 最終導致在診斷（ diagnosis ）和預後（prognosis）過程中對結構狀態做出錯誤判斷。因此，開發相關技術來自動檢測與分類異常資料變得十分重要，最近利用機器學習（machine learning，ML）的方法直接處理這項任務變的越來越可行，本研究藉此提出了一種基於機器學習的分類器，此分類器由高性能的淺層神經網路（neural network，NN）建立，以期解決長期監測時可能需要線上或即時應用問題。此外，採用了校正技術來修正人工分類的錯誤，通過結合人機迴圈（ human-in-the-loop，HITL）學習來克服傳統校正技術的缺點，所提出的方法既能改進分類器又能改進資料集，預期可以作為實現全自動結構健康監測系統的基本元件。

關鍵字：結構健康監測，異常資料，機器學習，人機迴圈學習，模式識別網路

# 調諧質量阻尼器之減振效能與健康狀況評估方法

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## 摘　要

調諧質量阻尼器(Tuned Mass Dampers, TMD)已廣泛應用於工程結構之振動控制。然而，TMD 之減振效能與外力的頻率內涵(frequency content)有極大的相關性，若外力的頻涵能夠有效激發主結構的共振反應，則 TMD 的減振效能就能夠有效發揮；反之，則 TMD 的減振效能無法發揮。另一方面，若是 TMD 的頻率與主結構頻率失諧造成離頻效應(detuning effect)，即便外力的頻涵能夠有效激發主結構的共振反應，TMD 的減振效能亦無法有效發揮。職是之故，本研究旨在發展 TMD 之減振效能與健康狀況評估方法，透過外力與系統動態反應之量測，監測 TMD 與主結構之互制(interaction)情況，藉以評估在每次外力作用之下，TMD 之減振效能與其本身之健康狀態(是否離頻)。基於量測絕對加速度之方便性，本研究建議以 TMD 相對主結構加速度、與主結構相對地表加速度，作為後續評估 TMD 與主結構互制情況的依據。數值模擬與實驗結果顯示，本研究所建議之方法可有效評估 TMD 之減振效能與健康狀態。

關鍵字：調諧質量阻尼器、離頻效應、減振效能評估、健康監測

# 高度變化的 V 型與 N 型地震防護屏障

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## 摘　要

本研究以固體力學為基礎，利用晶體局部共振時，特徵長度可小於阻隔波波長的概念發展巨觀的地震超材料設計。為解決此領域在設計上製造成本昂貴的問題，我們提出容易製作的高度漸增的 V 型與 N 型地震超材料，僅使用混凝土達到低頻且寬帶隙。透過幾何參數分析，我們選擇漸增的高度來拓寬帶隙的區間。其中高度漸增的 V 型地震超材料帶隙為 7.78-14.72 Hz，而高度漸增的 N 型地震超材料帶隙為 7.40-14.80 Hz。我們亦透過全域暫態模擬，探討高度漸增的 V 型與 N 型地震超材料對 Rayleigh wave 的衰減效果。暫態結果與頻散圖結果相當一致，驗證本研究模擬的正確性。

關鍵字：地震超材料、局部共振、地震工程、表面波

# 結合強震預警與之半主動滾動隔震支承研發

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## 摘　要

以往的被動式滾動隔震支承，一旦設計製作安裝至現場，則其參數已經固定不變，對於一般遠域地震波時，可有效控制受保護物體的最大加速度反應於一定範圍內，效果極為突出。但是，當受到具有速度脈衝的近斷層地震波時，則其位移反應可能超出限制而發生碰 撞，導致受保護物受損。因此本研究開發結合強震預警技術之半主動滾動隔震支承，將斜面滾動隔震支承(SRI)結合磁流變阻尼器(MR Damper)，並發展可根據初達波特徵推估最大地表速度(PGV)的卷積神經網路預測模型，建立根據 PGV 控制 MR Damper 所需電壓的控制律，當量測到初達波到達後前幾秒資訊，即可根據模型預測該地震之 PGV，並根據控制律得到該次地震下 MR Damper 所需之電壓，將電壓輸入控制系統使 SRI 之位移反應控制在門檻值之下，以在強震波來臨前調整滾動隔震支承之阻尼力，使其最大位移反應於具有速度脈衝的近斷層地震波作用下仍不至於超出界線。本研究將所提出方法加以實現，並進行振動台試驗以驗證其可行性。由試驗結果可知，所提出方法能有效限制 SRI 位移反應於門檻值下，驗證此一概念應具備其可行性。

關鍵字：卷積神經網路、斜面滾動隔震支承、半主動控制、強震預警、磁流變阻尼器

# Story drift and damage level estimation of buildings using relative acceleration responses with multi-target deep learning models under seismic excitation

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## 摘　要

損傷檢測為現今結構健康監測核心項目之一，其用於建築物受自然災害（如地震、颶風等）後之即時結構性能評估。依據當前各國結構設計規範，大多以層間變位作為結構損傷狀態指標。例如，當層間變位達 0.2 至 0.4%時，結構即存在輕微損傷。然而，過去研究文獻表明勁度在損傷前後會造成結構頻域響應的特徵變化，亦可作為損傷程度之參考依據。故本研究結合人工智慧技術，開發兩種多目標神經網路模型，僅利用樓層相對加速度即可同時預估層間變位及殘餘勁度比。其一多目標神經網路為並聯式模型，採用基於物理含義之損失函數進行最佳化。另一種為集成串接式模型，應用遷移學習預先訓練的優勢，即可微調快速重建模型。另外在兩種模型中，皆引入長短時記憶單元與傅立葉變換層以強化時、頻域特徵，大幅提升層間變位及殘餘勁度比之估計精度。本研究透過三層樓數值模型進行模型之性能探討，並以一八層樓實尺結構物進行實驗驗證，結果顯示該兩種神經網路模型於層間變位及殘餘勁度比之預測皆能達到高精度及可靠性。

關鍵字：損傷檢測、多目標神經網路、層間變位估計、殘餘勁度比估計、集成神經網路、遷移學習

# 在無人工標註資料下訓練深度學習模型進行現地鋼筋影像辨識

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## 摘　要

鋼筋混凝土一直是被廣泛使用的建築結構，為確保其結構強度符合需求，需要耗費大量時間與人力進行檢核，因此近年來使用深度學習與電腦視覺提升鋼筋檢核效率的方法獲得關注，然而目前提出的方法大多僅示範在實驗室環境中搭建的鋼筋籠，亦或是因為不足的鋼筋標註資料導致模型泛化能力不夠，只能在相似場域上有好表現。本研究提出一套使用合成資料與領域自適應的方法，在無人工標註資料下訓練深度學習模型進行現地鋼筋影像辨識。合成資料使用 BIM 模型與編寫 Revit API 的方法，在無需人力標註的情況下，生成大量且多樣的實例等級鋼筋標註資料。而合成資料與真實資料的影像在特徵空間中可能具有不同的資料分布，因此本研究開發具有領域自適應能力的 Mask R-CNN 模型，能在學習辨識鋼筋影像的同時，亦能夠消弭兩資料集間分布的不同，使得在只有合成資料有標註的情況下，也能夠在真實資料上有足夠的辨識能力。本研究在無人工標註下生成 25287 張鋼筋標註合成資料，使用此資料集訓練出的模型相較使用人工標註真實現地鋼筋資料訓練的模型相比，在測試資料集上以 AP50 作為指標，能夠獲得 27%的提升，加入領域自適應的技術後更是獲得 215%的提升。此外本研究亦從網路上收集各樣現地鋼筋影像資料供模型預測，本研究提出的模型也都有較好的預測結果，故本研究提出的方法能夠在無人工標註下提升現地鋼筋影像辨識能力， 並該方法也能作為其他缺乏人工標註資料的工程問題訓練深度學習模型的解決方案

關鍵字：現地鋼筋辨識、合成資料、建築資訊模型、領域自適應、深度學習、電腦視覺、Mask R-CNN

# 高擬真 RC 橋柱破壞模式預測系統之研發

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## 摘　要

橋梁在交通運輸中具有災害應對、資源流動等功能，為現代社會不可或缺的基礎設施，因此橋梁的結構安全性至關重要。為了量化地震後橋梁之安全及使用性能，性能設計法採用損傷指標(Damage Index)來衡量結構在最大位移及遲滯能量消散的影響，然而欲了解不同結構物在不同受力情形下之性能表現，通常需透過實際實驗獲得，龐大的成本及人力需求導致整體資料庫多有欠缺。為解決上述困難，本研究提出一條件生成對抗模型（Conditional Generative Adversarial Network），以五個不同橋柱試體之破壞影像及相對應之損傷指標、高寬比、橫向鋼筋比及縱向鋼筋體積比三種橋柱設計參數作為訓練資料，使模型能學習相關物理資訊，並能根據該物理資訊生成相對應之破壞模式。此外，本研究進一步探討兩種模型架構和三種資訊編碼策略，經實驗測試在判別網路中加入多個分支以分類及回歸輸入之條件資訊，可以有效提升模型表現，相較於一般之生成模型，Fréchet Inception Distance（FID）提升 38.88%。透過調整資訊編碼策略，可使模型於測試階段輸入未包含於訓練資料集之損傷指標，進而預測相對應之損傷影像。本研究所提出之生成模型架構能根據不同橋柱設計參數以及性能需求，生成對應之可能破壞模式，進而評估橋柱之性能表現，以供設計者評估及決策之參考。

關鍵字：橋柱破壞模式預測；深度學習；條件生成對抗模型；損傷指數；結構性能評估

# Rebar Spacing Inspection with Structure-informed Features Segmentation and Its Practical Application

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## Abstract

The process of rebar inspection holds great significance in construction, as it ensures the seismic resistance of reinforced concrete structures. However, sampling is often conducted due to concerns of the quantity, style and timeliness of rebar inspection. In light of this, our objective is to realize fast and fully-automated rebar measurement. A rebar-structure-based labeling policy is provided for training an instance segmentation Mask R-CNN model to extract two structure-informed features that sufficiently describe the rebar installation: intersections and spacings. Subsequently, a link prediction algorithm is applied to all the extracted masks, which connects all the reference points through a neighbor search in the image for Euclidean distance measurement to convert visual features into quantifiable and beneficial values in reality. Additionally, we presented a point adjustment technique that employs homography transformation with transform matrix from Apriltag to rectify points. This correction reduces the increasing error with greater distance from Apriltag. For practical application, we introduced a cross-platform application AIiS achieving rapid and convenient rebar measurement with only portable smartphones and Apriltags. In our evaluations, AIiS achieved an average detection rate of 75.97% and an average relative error of 4.59% for laboratory structured rebar slabs. Furthermore, AIiS also performed well in real construction sites and is promising for being applied for fast on-site rebar inspection.

Keywords：deep learning, rebar spacing inspection, instance segmentation, Apriltag, homography transformation, link prediction

# 結合房屋街景圖像與地震強度參數之老舊鋼筋混凝土建築反應預測

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## 摘　要

隨著世界各國朝向發展永續韌性都市，如何評估城市範圍內基礎建設的暴災風險是了解城市韌性的第一步。新近發展之機率式地震風險評估透過詳細的數值模擬來考量包含地表運動以及房屋模型的不確定性。其中結構物受震的動力反應是連結地震危害度與房屋損失的重要參數。倘若分析對象僅為一棟房屋，採用此法進行評估所需之時間與人力成本尚可接受。但針對城市範圍內大量房屋的建模與動力歷時分析所需之計算與勞力成本恐怕難以承受，尤其無法即時完成區域內的災損評估便可能導致城市防救災政策的效率下降。為此，本研究嘗試透過新近發展之人工智慧，以電腦視覺領域內廣泛使用的卷積神經網路(Convolutional Neural Network，CNN)從房屋街景圖像中擷取建築重要資訊，並搭配地表運動強度參數，如 PGA、PGV、PGD 與譜加速度等，由極限梯度提升法(XGBoosting)來預測結構物受震反應。考慮到台灣老舊混凝土建築數目龐大，本研究特別選擇非韌性鋼筋混凝土構架作為目標結構物。研究首先經由大量非線性動力歷時分析取得 1400 棟房屋之最大層間位移比，再將此結構反應用於所提之結合 CNN 與 XGBoosting 的監督式學習中，透過輸入街景圖像與地震強度參數直接預測房屋之最大層間位移比。本研究透過十折交叉驗證和網格搜索方法，來尋找最佳的超參數，包含全連結層的數量，樹的數量以及樹的最大深度。研究結果顯示，所提之架構可以有效且可靠地評估在地震作用下非韌性鋼筋混凝土構架的地震位移需求而省略進行動力歷時分析所需的成本。此種結合多源數據之機器學習方法將可有效地協助決策單位進行大規模的風險評估並訂定對應政策。

關鍵字：區域地震風險分析、卷積神經網路、極限梯度提升法、非韌性鋼筋混凝土構架

# 攝影測量技術應用於面外受力之結構磚牆的三維位移與大應變分析

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## 摘　要

如同過去各國發生的大地震,2023 年土耳其-敘利亞大地震中再一次有大量的磚牆結構倒塌或受嚴重破壞,造成嚴重傷亡和經濟損失。在該大地震中, 有不少建築結構在主震中能保持不倒,但在受多次強烈餘震作用後發生全面倒塌。因此,快速評估和監測大地震後結構的破壞程度對降低損失有關鍵性作用。本研究使用非接觸式攝影測量量測磚牆試體的變形。非接觸式攝影測量相較於接觸式量測具備低成本和高效益的特點，而且透過攝影測量可以獲得整體結構物的三維點位分布，以三維空間資訊計算結構體的應變分布。針對磚牆試體受面外力的破壞與應變分布的相關性進行討論，其中三維點位分布取得方式以兩種方法計算：(1) 佈設人工標(Target)；(2) 影像特徵點萃取(Targetless)。本研究使用格林-拉格朗日大應變計算方法分析面外受力之磚牆的變形分佈與結構行政。實驗共使用四組實驗相機，與牆面距離為 2.4m 與 4.6m 區間以及地面採樣距離(Ground Sample Distance) 0.30mm 至 0.56mm 區間。結果顯示計算得出的標點空間交會之牆面方向中誤差平均值在 0.27mm 以內、深度方向平均值在 0.60mm 至 0.64mm 之間。攝影測量得出的標點位移資料與精確度為 1mm 的雷射測距儀所量測到的成果進行比較，總結出均方根誤差(RMSE)可以在 0.7mm 以內。透過佈設間距近 10 公分且均勻分布的標點計算取得應變分布情況判斷對於磚牆在受力過程中產生之裂縫有高度相關性, 由此可作為評估磚牆結構的破壞程度與穩定性之依據。

關鍵字：格林-拉格朗日應變、大應變分析、攝影測量

# 考慮流固耦合交互作用之橋梁沖刷穩定性分析

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## 摘　要

本研究旨於探討於具沖刷現象之橋墩結構穩定性分析中，有無考慮流體-固體交互行為(fluid-solid interaction)之影響。首先利用一假想之縮尺橋墩沖刷試驗作為有限元素模擬軟體 ANSYS 之可行性評估，藉由擷取試驗之沖刷深與土壤性質等環境條件作為數值模擬邊界條件，並透過量測縮尺試體之微振資料求取數值模型目標頻率值。流固耦合模擬以其於頻率域之低誤差值顯示其在模擬沖刷橋墩之適用性。通過可行性評估後，於 ANSYS 軟體中建立西濱大橋之足尺數值模型，並根據現地鑽探資料與橋梁幾何設計進行土壤彈簧與流場之建置。透過流固耦合動態模擬與根據規範計算側向水流力加載之靜態模擬，比較我國現行橋梁設計規範於水流力定義之合理性與其不足之處。流固耦合之模擬結果顯示，以基樁之使用性與材料性質定義橋梁之安全係數，可即時透過基樁之容許相對位移與容許彎矩判定於不同沖刷條件下之橋梁安全係數。

關鍵字：數值模擬，流固耦合，橋梁沖刷

# MS-07 Recent Advances in Acoustics and Vibration

## Organizer: 陳蓉珊 副教授

| No. | Title | Authors |
|---|---|---|
| S07-01 | 內含微孔洞之降噪薄板 | 謝為宏, 陳蓉珊, 蔡宜育 |
| S07-02 | 具有中低頻段能隙之新穎複材三明治結構設計與分析 | 朱德瀚, 梁育瑞 |
| S07-03 | 以分子動力學模擬探討液滴於粗糙基底結構上受水平振動之運動機制 | 陳啟瑋, 趙士懿, 林正釧, 劉瑋文, 王安邦, 陳俊杉 |
| S07-04 | 應用輸出回饋天鉤控制律之設備物主動隔震系統 | 賴勇安, 蔡元峰 |
| S07-05 | Strain-engineering-assisted Mid IR photodetector | Chung-Chun Lu, Yu-Wei Kao, Hung-Jen Su, Chien-Kai Wang and Chien-Hao Liu |
| S07-06 | 固體材料系統由不確定簡諧激振引致響應極值之新式有限元素直接求解技術 | 柯秉良, 林昀, 林柏廷, 王建凱 |
| S07-07 | 考慮不確定性於斯托克斯流場極值反應解析之連體力學研究 | 林柏廷, 王建凱 |

# 內含微孔洞之降噪薄板

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## 摘　要

在科技快速發展的時代，噪音會影響人們身心健康，常常在交通運輸，建築施工及工業製程中產生，因此，如何有效抑制噪音是近年來重要課題，本研究提出內含微孔洞與聲學共振器之降噪薄板，著重於降低噪音，透過改變降噪板結構或微孔幾何尺寸，可調整降噪頻率以及頻寬，且利用結構設計，將空間達最大使用率。理論結果顯示同樣微孔直徑情況下，改變微孔數量，主要影響孔隙率，當孔隙率因為微孔數量增多而變大，導致 有上升，而降音頻率往高頻的趨勢。至於固定同樣微孔數量，改變微孔直徑，影響孔隙率及穿孔常數，當微孔直徑增大，孔隙率及穿孔常數也因此變大，導致 有上升，而峰值頻率往高頻的現象。如上述，可發現改變微孔直徑影響較大，因此，改變微孔直徑對模型之 影響較劇烈。若將共振腔容積做出大小不等變化，可使降噪板產生兩個峰值，而頻寬因兩個峰值相互耦合連接變寬，降噪薄板之降噪範圍藉此更廣，對此，本研究分別提出不等高及不等長結構設計。模擬使用 COMSOL Multiphysics 對阻抗管及設計之降噪板空氣通道作分析。實驗樣品使用 3D 列印方式印製，藉由聲學阻抗管量測模型獲得 ，再與理論、模擬結果比較。

關鍵字：拱形結構；荷姆霍茲共振器；微孔

# 具有中低頻段能隙之新穎複材三明治結構設計與分析

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## 摘　要

由於航空和太空應用對高強度輕量化結構的需求，複材結構的使用在近幾年來已迅速增加，而其中一種常見的複材結構稱為三明治結構，複材三明治結構通常由兩層輕薄且高勁度的面板與一層輕且相對軟的芯材所組成。另外，過去許多文獻已證實週期性結構(像是聲子晶體以及超穎材料結構)可阻擋特定頻率的波段，在工程應用上對減震以及吸音具有良好的效果。因此，本研究結合複材三明治結構以及週期性結構的概念，設計了一種細長型的新穎複材三明治結構，由兩片疊層複材板和一個具有週期性且特殊幾何形狀的芯材所組成，此結構能夠有效地阻擋彎曲波在結構中的傳遞以達到減振的效果。

本研究使用有限元素法分析單元結構的能隙行為，並探討芯材幾何結構對於能隙的影響，發現此新穎結構具有中低頻段(約 1500-2500 Hz)的彎曲波能隙。另外，為了驗證本研究提出的新穎結構具有減振能力，本研究建立全尺寸有限元素模型分析頻率響應函數(FRF)，結果顯示 FRF 的確在特定頻段區間大幅降低，並與先前所預測分析的能隙行為是一致的。最後，額外探討了此新穎複材三明治結構在單邊脫層的損傷情況下對於 FRF 的影響，分析結果得出隨著結構脫層損傷的範圍變廣，雖然結構的抗振能力下降，但抗振能力還是優於無脫層損傷之傳統複材三明治結構。

關鍵字：複材三明治結構、週期性結構、能隙現象

# 以分子動力學模擬探討液滴於粗糙基底結構上受水平振動之運動機制

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## 摘　要

在微流體控制、塗布、生醫檢測等領域，了解及控制液滴受振動所引起的運動行為和機制具有極大的價值。在本研究中，我們利用分子動力學的多體耗散性粒子動力法（ many-body dissipative particle dynamics, mDPD）來模擬液滴在粗糙基底結構上受水平振動所產生的運動行為及相關的 Cassie-Wenzel 狀態變化。多體耗散性粒子動力法考慮了液-氣體之間的相互作用， 能夠有效地描述氣-液共存系統的熱力學和流體力學特性。此外，也能夠模擬液滴與固體表面之間的接觸角和滑移現象，以及液滴內部的微觀結構和相變化過程。此研究分析液滴的運動機制，並透過液滴運動速度與實驗數據的驗證，進一步探討其運動模式與基底表面結構之間的相互作用。同時我們也探究了基板振動頻率對於液滴運動行為的影響，發現當振動模態為 Rocking mode 時會使液滴開始移動。透過粒子模擬，我們也進一步探討液滴由靜止到移動的相關機制。

關鍵字：分子動力學模擬、多體耗散性粒子動力法、液滴振動模態、液滴接觸角遲滯

# 應用輸出回饋天鉤控制律之設備物主動隔震系統

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## 摘　要

坐落於地震高風險地區的高科技廠房，由於有抗微振動的需求，廠房結構往往採用強化之抗震設計，雖然通過適當的抗震設計，廠房結構的安全已可充分確保，但結構內部的設備物仍然可能受到較大樓板加速度引起的基底擾動而遭受損失。因此，研發一可有效保護內部設備的設備物隔震系統，為高科技廠發展之一個重要的課題。傳統的天鉤控制原理，是透過模擬一天鉤阻尼器之阻尼力來抑制基底擾動，此模擬之天鉤阻尼器的一端連接到設備物，另一端則連接到空間中不受基底擾動的固定點，以主動控制方式實現。因此，傳統天鉤控制的控制效果很大程度取決於設備物絕對速度信號回饋的準確度。然而，量測設備物絕對速度信號進行控制有其難度，因此本研究改良傳統天鉤隔震之控制方法，除了量測基底的相對速度進行回饋控制以外，亦量測基底的絕對加速度並經過積分濾波後進行前饋控制，此調整不僅提高了信號測量的便利性，而且還增加了回饋信號帶來的穩定性，因此本研究所提之主動隔震系統不會輕易受到非地震外力的影響。改良的天鉤主動隔震系統不是全狀態回饋，因此可利用直接輸出回饋進行最佳化設計。從數值模擬之頻率反應函數分析結果顯示，本研究所提之天鉤主動隔震系統，可比被動隔震系統更有效降低設備物之絕對加速度，特別是對於常見地震顯著的頻率範圍。此外，地震歷時分析與振動台實驗驗證亦顯示，所提出的天鉤主動隔震系統，對於真實地震歷時具有良好的隔震效果，且對於近斷層地震或遠域地震，隔震效果沒有明顯區別，可有較高之適用性。

關鍵字：設備物隔震、天鉤控制律、主動隔震系統、直接輸出回饋、數值模擬、振動台試驗

# Strain-engineering-assisted Mid IR photodetector

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## Abstract

Strain engineering has been widely used in semiconductors and optical electronics. Various applications include the latest TSMC' 3 nm technology, 2D material-based transistors, and beam steering metasurfaces. The main concept is based on applying external strains to modify the crystal orientations for desired band diagrams and improve the output performances. In this research, we propose a strain-assisted thin film mid-infrared photodetector for optical communications in severe weather. The proposed photodetector is based on the group IV materials, GeSn, which can achieve direct bandgap via adding sufficient Sn or increasing strains. First, we will design a quarter-wavelength GeSn alloy and the operation frequency is designed at the frequency of 2.5μm, which is in the frequency range of the atmospheric window. Then, we apply external bi-axial strains to the proposed device to shift the operation frequency to the long-wavelength range by attaching the structure to a solid cylinder where the available maximum strains depend on the curvatures of the surfaces. The goal of the research is to develop a group IV photodetector with a direct bandgap in the mid and far infrared range. More details will be disclosed and discussed in the presentations.

Keywords：Strain engineering, GeSn, thin film, Mid IR detector.

# 固體材料系統由不確定簡諧激振引致響應極值之新式有限元素直接求解技術

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## 摘　要

本研究成功開發固體材料系統由不確定簡諧激振引致響應極值之新式有限元素直接求解技術，其中基於負載響應關聯法（Load-response correlation method，簡記為 LRC 法）固體力學理論開發與有限元素法（Finite element method，簡記為 FEM）計算技術運用來準確預測出隨機簡諧外力造成固體系統之穩態振動反應極值。傳統上，對於固體系統受簡諧外力之振動響應，可透過有限元素法之時域直接積分法與頻率域簡諧模態法而得，而考量自然環境荷載，對應不同自由度隨機外力之間的關聯性時，實難不以巨量外力樣本資料之重複計算工作成果，而後統計得出系統極值振動反應。於本研究中，運用新式有限元素求解技術可直接求出系統穩態振動響應之極值，不僅大幅地降低運算所需資源與時間，還可精確地計算出不確定簡諧外力與振動響應之統計關聯特徵。

本研究使用薄板理論驗證有限元素法動力分析穩態解之正確性，再利用隨機簡諧外力引致振動模擬之極值反應統計結果，對本研究開發新式有限元素求解技術所得最大振動程度估計值進行比較，得知此新式計算方法之預測值具高度準確性。緣此，藉由本研究開發之新式分析技術，透過系統於不同工作場域隨機激振之統計特徵，可直接且一步式計算出該固體材料穩態振動響應之極值，故得以對系統振動響應極值進行敏感度分析，進而可對承受隨機簡諧外力之固體材料幾何形狀與空間分佈，得到具最佳服務性能之機械設計與相應製造方案。

關鍵字：負載響應關聯法、有限元素法、簡諧模態分析、極值響應、隨機簡諧外力

# 考慮不確定性於斯托克斯流場極值反應解析之連體力學研究

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## 摘　要

本研究提出了一種適用於不可壓縮牛頓流體的直接有限元技術，以在隨機刺激下準確地評估不確定斯托克斯流（Stokes flow）的極值響應。傳統上，有限元素法為流體材料運動特性模擬之良好計算方法，本研究根據拉普拉斯-高斯分佈的統計模型，且基於連體力學理論，推導出相應隨機刺激條件之斯托克斯流場極值解析式，並開發相關有限元素計算工具，以上新式理論與直接計算技術除能準確評估斯托克斯流峰值反應外，還可識別出與極值流場響應相對應的關鍵刺激條件。為驗證本研究致力之新式理論與計算技術能力，透過數個計算流體力學模擬計算工具所得結果比較，得知由重複模擬統計而得極端流量數據與直接解析評估之結果非常一致，從而驗證了理論方法的正確性與計算開發的準確性。

因此，藉由本論文提出考慮不確定性於斯托克斯流場極值反應解析之連體力學研究成果，可大幅減少傳統統計所需重複模擬模型之計算時間、設置成本與運算資源，進而能更有效率地對於不確定刺激條件之流場分佈，得到具最佳服務性能之精密流體機械設計方案。

關鍵字：不確定斯托克斯流、極值流場反應、不可壓縮牛頓流體、拉普拉斯-高斯分佈隨機過程、載重反應關聯法、有限元素法

# MS-08 Computational Physics and Mechanics of Biological and Bio-inspired Structural Materials

## Organizer: 劉立偉 助理教授

| No. | Title | Authors |
|---|---|---|
| S08-01 | 以晶格彈簧顆粒模型模擬多物種骨結構拉伸力學行為 | 蘇正順, 蕭羽白, 張書瑋 |
| S08-02 | 深度強化學習應用仿生微結構設計鞋中底 | 黃靖傑、陳俞文、游濟華、陳柏宇、陳俊杉 |
| S08-03 | Mechanical property of cellular materials under cyclic loading | Li-Wei Liu, Hong-Gen Chen, Zhen-En Jian |
| S08-04 | Inelastic micromechanics of nacre | Li-Wei Liu, Yuan-Jyun Shih, Jing-Yan Wang |
| S08-05 | Finite element analysis on Bauschinger effect of trabecular bone | Li-Wei Liu, Hong-Yi Wu, Po-Ho Chen |
| S08-06 | Analysis of Near-Fault Seismic Responses Using Viscoelastoplastic Structure Models | Cheng-Yuan Chen, Tsai-Ling Tsai , Li-Wei Liu, Kuang-Yen Liu |

# 以晶格彈簧顆粒模型模擬多物種骨結構拉伸力學行為

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## 摘　要

自然界中存在多樣物種，物種之間骨質結構的性質差異甚多，探討多面向的骨質特徵已成為一門研究方向。本研究旨在建立粗顆粒搭配晶格彈簧模型(LSM)，模擬經由選定的不同物種骨質透過斷層掃描後，再以圖像處理獲取的幾何形態，在最大應變為 2%下所表現的拉伸性能，如極限應力、楊氏係數等力學參數，並分析在拉伸過程的破壞行為，進而從中發現物種骨質相應的力學特性，以提供未來材料設計之參考。

關鍵字：多物種骨結構、晶格彈簧模型、拉伸行為

# 深度強化學習應用仿生微結構設計鞋中底

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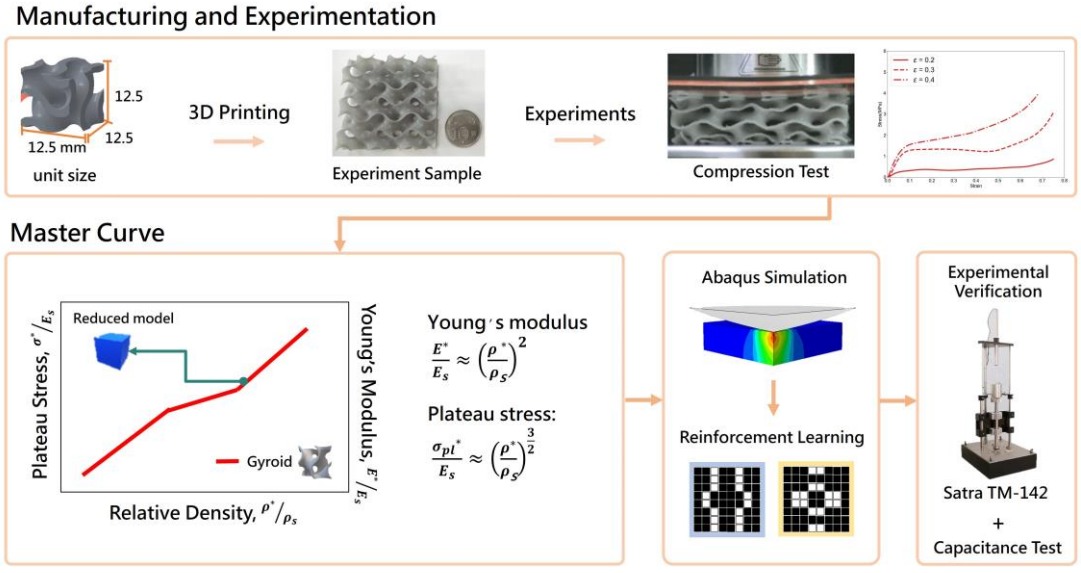
## 摘 要

科技進步驅使對多功能結構材料需求上升，全球暖化推動環保意識高漲。實現多功能性並節省材料成為工程界關切，生物材料以不同排列、幾何結構或複合材料展現卓越性質，如蝴蝶翅膀的 Gyroid 結構。然仿生結構複雜，設計成本高，人工智能解決之。經訓練的深度學習能從經驗學習，簡化複雜系統，強化學習透過環境互動，穩定有效地優化設計，將成為多功能結構材料研究的關鍵。

本研究創建了一套結構材料設計方法，以仿生材料為基礎，實現高耐衝擊性和輕量化的結合。為了解決仿生材料設計的運算耗時，本研究採用簡化模型替代複雜結構，保持結構的物理特性，解決有限元分析中的幾何複雜度。並以深度強化學習模型實現多目標設計，根據需求調整軟硬材料分佈，進行最佳化。此方法結合強化學習與有限元模擬，在迭代過程中評估設計性能，極大地降低設計成本。該方法使設計者能根據需求開展複合材料設計，靈活運用強化學習與有限元模擬，適配不同孔洞結構，解決複雜材料的設計難題，具備高度適應性和靈活性。

關鍵字：孔洞材料、仿生結構複合材料、3D 列印、深度學習、強化學習、有限元素法



# Mechanical property of cellular materials under cyclic loading

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## Abstract

Cellular materials are designed to mimic the microstructure of wood, cork, bone, and honeybees' honeycomb, exhibiting characteristics of high stiffness and lightweight. Previous research has predominantly focused on the elastic properties of cellular materials, with limited exploration into their viscoelastic behavior. This study aims to propose a viscoelastic model of a 2D cellular material, called honeycomb materials, suitable for describing the mechanical response of cellular microstructure; and validates its accuracy through experimental results and computational simulations. This model permits the exploration of the response of honeycomb materials under cyclic loading scenarios influenced by microstructure changes including different relative density (slenderness ratios) and the angle of inclined cell wall. Our results indicate that sinusoidal or cosine stress and strain inputs cause honeycomb materials to display hysteresis loops whose area reflects the energy dissipation during cyclic loading. Furthermore, among varying relative densities, the highest hysteresis loop area occurs at 5.9% of relative density for sinusoidal stress input and at 17.3% of relative density for strain input. However, under different inclined angles, the largest hysteresis loop area for both sinusoidal stress and strain inputs is observed at 60° of the inclined angle.

Keywords：Cellular materials; viscoelasticity; honeycomb materials; cyclic loading; energy dissipation.

# Inelastic micromechanics of nacre

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## Abstract

Mother-of-pearl (nacre) is a platelet-reinforced composite material highly enriched with calcium carbonate (aragonite). At the microscale, nacre is observed to be composed of protein along with numerous embedded mineral plates, resembling the arrangement of bricks (minerals) and cement (protein) in a brick wall. This unique "hard-soft mixed-layer" microstructure is believed to confer exceptional properties upon biological materials, concurrently providing high strength, toughness, and energy dissipation capacity. To gain a deeper understanding of nacre's behavior under varying loads, this study introduces a viscoelastic tension-shear chain model. Utilizing this model, the study examines nacre's responses to fixed loads, monotonic loading, and cyclic loading. Additionally, the study explores how alterations in the proportion of minerals to protein within nacre at the microscopic level impact its mechanical behavior.

Keywords： Nacre, viscoelasticity, hard-soft mixed-layer microstructure, micromechanics.

# Finite element analysis on Bauschinger effect of trabecular bone

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## Abstract

Certain bones, such as the vertebra or the femoral head, contain cellular microstructures known as "trabecular bone" which behaves anisotropic response and the asymmetric yielding in tension and compression. To investigate the mechanics of trabecular bone by using finite element simulations, we employed Voronoi honeycomb as the representation of its microstructure and adopted the generalized Hill yield function for describing its anisotropic response. To study the evolution of the yield surface within trabecular bone, we conducted mesh convergence analysis, boundary effect analysis, and size effect analysis firstly and then designed probing paths and pre-loading paths to detect yield points on the initial yield surface and subsequent yield surfaces under various pre-loading conditions. Furthermore, the resulted yield points were fitted by a convex-closed-cubic yield function which enables us to observe the evolution of yield surface. The finite element analysis revealed a consistent trend in the variation of yield surface area under axial-tension and axial-compression pre-loading paths. Additionally, there is a slight reduction observed in the yield surface area under positive and negative shear pre-loading conditions. When axial pre-loading paths were applied, they led to an increase in the aspect ratio of the yield surface. Based on observations of the yield surface evolution, we are able to identify the Bauschinger effect and the hardening behavior exhibited by the trabecular bone.

Keywords： Trabecular bone, Voronoi honeycomb, Bauschinger effect, Evolution of yield surface

# Analysis of Near-Fault Seismic Responses Using Viscoelastoplastic Structure Models

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## Abstract

This study is based on the theories of viscoelastoplasticity, and the friction mechanism of rubber bearings, deriving a simplified model. The model encompasses various friction mechanisms, different solution methods, and elastic or elastoplastic bridge piers, aiming to simulate bridges equipped with functional bearing systems. Furthermore, all models are represented using state-space equations. Through mathematical derivations, the results of time-history analyses are compared with SAP2000 or experimental data to validate the accuracy of the model. Subsequently, a parameter analysis for near-fault earthquakes is conducted to discuss the model's applicability and the effects of different friction mechanisms. After analysis, a model that most comprehensively considers the friction mechanism of rubber bearings is recommended. Additionally, the results of analyses involving models with varying friction forces indicate that, in many cases, the deformations of the bearings are significant, and the plastic deformation is smaller than that when using Coulomb friction. Furthermore, a comparison is made between the results of analyses for near-fault and far-field earthquakes to emphasize the distinctive seismic response characteristics of the model under different friction forces.

Keywords:Viscoelastoplasticity, functional bearing system, near-fault earthquakes, various friction

# MS-09 Multiphase and Multi-component Complex Flows

## Organizer: 吳清森 副教授

| No. | Title | Authors |
|---|---|---|
| S09-01 | Numerical simulation of yield stress fluids flow around an immersed object | Cheng-Chuan Lin |
| S09-02 | Well-posedness and Ill-posedness of Constitutive Relations and Continuum Simulation for Transient Compressible Granular Flows in the Inertial Regime | You-Yu Chang, Keh-Ming Shyue ,Fu-Ling Yang |
| S09-03 | 多孔介質內奈米流體之指狀對流 | 羅安成 |
| S09-04 | Growth of force chain network upon non-Bagnold Transition of Inclined Surface Granular Flows via Discrete Element Simulation | Chih-Ying Cheng, Cheng-Ting Tsai and F.L. Yang |
| S09-05 | 熱交換管內二相冰泥流擬真模擬 | 林哲鋒，楊馥菱 |
| S09-06 | Simulating an irrigation flow in root canal: Predicting the likelihood of the cavitation bubble formation | Ting-Ju Wei, Yu-Yang Chen, Cheng-Chuan Lin, Wei-Wen Liu, An-Bang Wang, Chuin-Shan Chen |
| S09-07 | Performance augmentation of a Savonius wind turbine using a cylinder deflector in front of the returning blade | Desta Goytom Tewolde, Ming-Jyh Chern |
| S09-08 | Parametric study of a flat plate for the Magnus effect VAWT performance enhancement. | Fandi D. Suprianto, Ming-Jyh Chern, Chin-Cheng Wang |
| S09-09 | 利用深度學習模型預測機翼繞流物理場 | 林冠丞，黃柏瑜，吳毓庭，游濟華 |
| S09-10 | Two-phase numerical study of particle-laden density currents using the Eulerian-Lagrangian approach | Yi-Ju Chou, Yao-Hung Tsai |
| S09-11 | 斜坡底床因波浪淺化及碎波引致土壤反應之數值模擬 | 林奕翔，林孟郁 |

# Numerical simulation of yield stress fluids flow around an immersed object

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## Abstract

In recent years, considerable research efforts in numerical simulation of yield stress fluids flow around an immersed object have been devoted because of their fundamental significance and wide applications relevant to engineering and natural sciences. In this study, the author implemented a sharp-interface-capturing volume of fluids (VOF) method into a well-developed pressure-correction solver to track the interface between two fluids. Moreover, a direct-forcing immersed boundary (IB) method was developed to consider the interaction between fluids and an immersed object. A special treatment was made to the interpolation function for the volume fraction of IB. The author simulated the typical Bingham fluid flows around a sphere under various flow conditions governed by a dimensionless Oldroyd number (Od) to validate the numerical schemes. The simulation results showed great agreement with the existing data in the literature, including the drag coefficient and the yield surface positions. The proposed simulation framework will be used to explore more complex yield stress fluid flow problems numerically, such as the granular materials flow around immersed objects, in which several issues still remain unresolved.

Keywords： Yield stress fluid, flow around an immersed subject, direct-forcing immersed boundary

# Well-posedness and Ill-posedness of Constitutive Relations and Continuum Simulation for Transient Compressible Granular Flows in the Inertial Regime

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## Abstract

Granular flows manifest in a diverse array of scenarios with significant relevance to mechanical industries, natural surroundings, and our daily routines. In the inertial and dense regimes, such flows have been successfully described by the μ(I), ϕ(I)-rheology models, which proposes that the effective friction coefficient (μ) and the solid volume fraction (ϕ) are solely functions of the dimensionless inertial number (I). While this rheological framework has been validated against both experiments and simulations in various geometries under steady-state conditions, recent research have proved that this theory is mathematically ill-posed in time-dependent problems. (Heyman *et al*., 2017)

Based on the compressible I-dependent rheology (CIDR) proposed by Barker *et al*. (2017) and the inertial compressible I-dependent rheology (iCIDR) introduced recently in Schaeffer *et al*. (2019), we implement several local μ(I), ϕ(I)-rheology models (da Cruz *et al*., 2005, Jop *et al*., 2005, Schaeffer *et al*. (2019)) to formulate our problem. We firstly prove the well-posedness of the iCIDR equation with a local μ(I) rheology model and a monotonic local ϕ(I) rheology model. Unlike the incompressible continuity and Cauchy momentum equations, in which pressure must be determined globally, all unknowns in our governing equations can be explicitly and locally specified. Hence, we employ the conventional convection-diffusion method to simulate a quasi-1D simple shear granular flow in the transient process on a collocated uniform mesh for validation.

Keywords： Granular media, Inertial compressible I-dependent rheology, μ(I), ϕ(I)-rheology models, Well-posedness, Convection-diffusion equation.

# 多孔介質內奈米流體之指狀對流

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## 摘　要

奈米流體是一種稀薄的奈米粒子懸浮液體，具有複雜的熱質傳現象。眾所皆知，其微觀的粒子泳動現象會引發異常的熱傳增強效應。探索熱傳效率增強的物理機制不僅有學術意義，更具有工業應用價值。為了達到此目的，2006 年麻省理工學院 Buongiorno 教授首先提出對流傳輸模型，方程式包含奈米粒子傳輸、質量守恆、動量守恆及能量守恆，其中各物理量間乃透過奈米粒子的泳動互相耦合，形成一套高度非線性的偏微分方程式。這套方程式與雙擴散對流的理論模型類似，數值模擬方法已經成熟，因此受到學界廣泛的認可與引用，並被推廣到很多擴充主題上，其中以多孔介質流場的研究為大宗。然而，最近一些實驗觀測與理論研究成果產生了矛盾，暗示理論模型可能存在缺陷。本研究乃藉由重新檢視舊有模型試圖進行改良，並針對多孔介質內的流場進行模擬研究。研究發現，在適當的條件下，固體邊界上可能形成一種指狀型態的高週波對流胞。這種特殊的對流現象其實已被流場穩定性分析所預示過，但一直還沒能以數值模擬來呈現。主要困難在於奈米粒子泳動的擴散時間尺度通常遠小於流體的熱擴散時間，換句話說即方程式內包含一個極大的 Lewis 數(>10 萬)使濃度梯度變得相當大，故容易導致數值發散。為了能捕捉到細緻的流場，使用傳統的數值方法就得使用高精度的網格進行計算，非常曠日廢時。本研究乃利用自行開發的數值程式(多域的頻譜方法)成功實現模擬。結果已揭露出奈米粒子傳輸的本質，對於奈米流體的熱傳增強現象之探討提供一個新的研究方向。

關鍵字：奈米流體、多孔介質流、指狀對流現象

# Growth of force chain network upon non-Bagnold Transition of Inclined Surface Granular Flows via Discrete Element Simulation

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## Abstract

Steady inclined granular flows are an important flow configuration to study the dynamic of dry granular flow. This work adopts two-dimensional discrete element simulation to study how inter-grain friction may play a role in momentum transport, other than the collision-based transport, to induce the non-Bagnold flow phenomenon reported in the literature. Special efforts were made to apply the knowledge of network science to identify the contact force chain network from particle dynamics information using the graph theory with the Louvain greedy algorithm. We studied how the number of grains born in the force chain network grows when the flow degrades from Bagnold to non-Bagnold flows. Concurrently, the stress loading ratio carried by these frictional contacts rises abruptly upon the non-Bagnold flow transition identified when the Froude number falls below 2. Both suggest that the non-local phenomenon of Bagnold velocity profile degradation occurs when sufficient grains are confined in the force chain network to assist the stress transport, replacing the collisional transport. Hence, a refined rheology model is needed to account for this friction-assisted momentum transport at a mesoscopic yet flow-dependent length scale like the currently investigated force network size.

Keywords: discrete element simulation, non-Bagnold flow transition, force network community

# 熱交換管內二相冰泥流擬真模擬

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## 摘　要

近年來,隨著再生能源發電系統占比提高,儲能成為一關鍵需解決的問題。冰泥(Ice slurry)為水與冰之混和物，被視為一良好的熱儲能材料及熱傳介質，且冰泥為固液兩相混合物，於融冰過程可吸收顯熱及潛熱；此外，冰泥具有優異的流動性，相較於固態冰，冰泥之流動性提升了其應用範圍，包含空調系統、食品、醫療、和滅火等；因此，本研究發展一數值計算DDPM (Dense Discrete Phase Method)方法探討冰泥流流場的熱傳導係數和進出口壓降。

本研究整合 Ansys Fluent 二相流計算經驗來建構擬真但有效率的數值計算，也同步建立實驗設置,利用模擬補足實驗無法觀測到的流場性質,詳究顆粒粒徑與分布對熱傳效果的影響,解決實驗中平均熱傳導係數在高冰泥濃度時的跳升。我們也將同步整合實驗與模擬的進出口壓降與 IPF 之間的關係。更期所開發的數值計算方法可應用於於未來設計擴充的應用。

關鍵字：冰泥流、DDPM、熱傳導係數、進出口壓降

# Simulating an irrigation flow in root canal: Predicting the likelihood of the cavitation bubble formation

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## Abstract

This study proposed a novel computational approach designed to predict the formation of cavitation bubbles during endodontic treatment. Cavitation effect is a pivotal cleaning mechanism within endodontics, making their prediction crucial for enhancing treatment efficacy. Our methodology employs computational fluid dynamics to simulate the endodontic file oscillating in the canal and proposes a dimensionless parameter known as the pressure gradient number (Γ). This dimensionless parameter successfully anticipates the extent of cavitation under various operational environments, such as differing drive amplitudes or the use of different endodontic instruments.

Keywords： endodontic therapy, cavitation phenomenon, computational fluid dynamics, pressure field, fluid-solid interaction

# Performance augmentation of a Savonius wind turbine using a cylinder deflector in front of the returning blade

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## Abstract

The prevalence of Savonius wind turbines and other small-scale vertical-axis wind power generation technologies is growing in urban areas. Despite having several benefits, the Savonius wind turbine has a lower power coefficient. Improvement of its performance is therefore one of the primary issues that has to be addressed. To address these issues, researchers proposed deflectors, concentrators, and directing vanes to enhance the aerodynamic performance and overall efficiency of the Savonius wind turbine. Deflectors such as flat plates and cylinders are used to redirect wind flow away from the returning blades of the turbine and reduce negative torque. As a result, the overall performance will improve. Recently, few studies on stationary and rotating cylinder deflectors have been used as an alternate design for enhancing Savonius wind turbine performance. The effects of cylinder deflector distance, diameter, and angular velocity on torque and power coefficients were investigated in these studies. However, no details were provided on the dimensions and arrangement of cylinder deflectors to the center of the returning blade. The aim of this study is to study the effect of cylinder deflector arrangements (inline and offset to center of the returning blade), cylinder diameters, and gap on the performance of the Savonius rotor at a Tip Speed Ratio of 0.8. In this study, the direct-forcing immersed-boundary approach and the Large Eddy Simulation (LES) model were utilized to simulate three-dimensional Savonius rotor models. Therefore, using a cylinder deflector significantly increased the power coefficient. The Savonius rotor performed better with the cylinder deflector aligned with the center of the returning blade than with an offset arrangement. A cylinder deflector with a radius of 0.325 meters and a horizontal gap of 0.14 achieved the highest power coefficient.

Keywords： Savonius wind turbine, cylinder deflector, power coefficient, direct-forcing immersed-boundary, Large Eddy Simulation.

# Parametric study of a flat plate for the Magnus effect VAWT performance enhancement

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## Abstract

The Magnus effect VAWT harness the principle of the Magnus effect in conjunction with a vertical axis orientation. This mechanism relies on the Magnus force produced by rotating cylinders to propel the rotor and to generate power. The proposed method involved installing a flat plate near each rotating cylinder to generate a higher Magnus force. As the configuration of the plate affects both the flow pattern and the Magnus force exerted on the blade, the current study intends to identify an optimal blade configuration consisting of a rotating cylinder and a flat plate.

Direct-forcing immersed boundary (DFIB) numerical model was used to simulate the flow past a rotating cylinder with a flat plate at different configurations, and the Box-Behnken Design for the response surface methodology (RSM) was applied to find an optimized flat plate arrangement that would produce the highest Magnus force.Three design parameters were examined, specifically the plate's length (L/D), the gap between the plate and the cylinder (g/D), and the plate's orientation angle (β). The Reynolds number was 5,000, and the cylinder's spin ratio was 2. The findings suggested that the flat plate can enhance the Magnus force on a blade by approximately 25% at (L/D = 1, g/D = 0.1, β = 40°), and that the torque coefficient produced by the rotor is higher when compared to a blade without a flat plate.

Keywords： Magnus effect; Response surface methodology (RSM); Direct-forcing immersed boundary (DFIB) method.

# 利用深度學習模型預測機翼繞流物理場

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## 摘　要

翼型（Airfoil）是一種幾何形狀結構，具有製造升力的氣動特性，廣泛應用於飛機機翼、風力渦輪機葉片、直升機螺旋槳、發動機葉片等。儘管市面上有許多設計良好的翼型，但仍有許多產品無法在現有翼型中尋找到適合自身氣動性能或氣流特性的翼型。因此，我們希望利用人工智慧的深度學習模型結合計算流體力學來進行翼型設計與開發，以降低時間和金錢成本，為需要探討翼型繞流場的領域提供資源支持。

本研究採用兩種深度學習模型來加速計算流體力學，以翼型繞流為例進行實際應用。流體力學模擬使用 S-A 湍流模型，分析 NACA 翼型繞流的物理場和空氣動力係數，並透過 102 種不同翼型和 0-12 度攻角來建立深度學習所需的資料集。兩種深度學習方法分別為條件式生成對抗網絡模型（cGAN）和雙重輸入之卷積神經網絡模型（CNN）。條件式生成對抗網絡模型能夠透過幾何和流體力學條件輸入來預測翼型繞流壓力場。雙重輸入卷積神經網絡模型結合翼型繞流壓力場輸入和流體力學條件輸入，透過 cGAN 預測的壓力場圖像和流體力學條件數值來預測升力係數。這兩種深度學習方法的串接能夠快速預測翼型繞流的流體力學性質，為翼型開發領域提供了一種準確且高效的開發方法。同時，也促進了翼型自動優化與設計的研究發展。

關鍵字：翼型繞流，人工智慧，深度學習，計算流體力學，有限體積法

# Two-phase numerical study of particle-laden density currents using the Eulerian-Lagrangian approach

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## Abstract

Density currents are fundamental phenomenon in fluid dynamics. In the context of environmental flows in estuaries and lakes, the density difference can arise from the presence of suspended fine sediments, known as turbidity currents. While some numerical models have represented turbidity currents by introducing a Stokes settling velocity to the concentration field, a more accurate portrayal requires the consideration of particle-turbulence interactions, best captured through extensive particle tracking. In this study, we investigate particle dynamics in detail within turbidity currents using a Eulerian-Lagrangian model tailored for solid-liquid flows. Our focus is on understanding the long-term resuspension induced by vortices, a behavior driven by the non-diffusive nature of particles. This leads to distinctive deposition patterns depending on different particle sizes. Additionally, we explore the propagation speed and distance of the front under varying physical conditions, such as particle settling velocity and Grashof number. We also highlight the difference between the present two-phase treatment and the traditional passive scalar assumption.

Keywords： Turbidity current, Eulerian-Lagrangian model, deposition

# 斜坡底床因波浪淺化及碎波引致土壤反應之數值模擬

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## 摘　要

台灣四面環海，在進行海岸工程規劃時，波浪造成的底床土壤反應是需要考慮的重點。當波浪從外海傳遞至近岸時，波浪會因深度改變而產生折射、淺化與碎波等現象，而淺化與碎波效應對於底床有著顯著的影響。目前關於波浪淺化與碎波造成底床土壤反應的研究仍相當有限。為了探討此現象，本研究應用開源流體力學計算軟體 OpenFOAM 建立數值模式，包含了波浪模組 waves2Foam 與土壤模組 upFoam，模擬規則週期波通過海岸斜坡底床之淺化與碎波現象，以及造成之底床多孔彈性土壤的孔隙水壓與應力變化。波浪模擬中應用了 stress-ω 紊流模式，以避免傳統的紊流模式在碎波時常出現的紊流強度高估的現象。經與實驗結果（水波部分）及解析解（土壤部分）之比較，可確定本模式之準確性。研究中探討了 spilling wave 與 plunging wave 兩種碎波型態、土壤含水飽和率以及滲透係數對於底床土壤之影響。從結果可以發現，在淺化階段波高隨著水深變淺而逐漸升高，引致之土壤超額孔隙水壓也逐漸增大。在碎波後波高會大幅降低，土壤之超額孔隙水壓也隨之降低；但因水下逆流現象，超額孔隙水壓的週期振盪會朝正值偏移。若比較兩種碎波型態之影響範圍，plunging wave 會比 spilling wave 將孔隙水壓傳遞至更深處土壤底部。從孔隙水壓的分佈來看，滲透係數值越大則孔隙水壓傳遞越深，且發現隨著滲透係數的減少會有較明顯的相位延遲現象發生，而土壤飽和率 $S_r$ 值越大則有越大的孔隙水壓分佈。

關鍵字：斜坡底床、波浪淺化、碎波、多孔彈性土壤、OpenFOAM

# MS-10 Machine Learning and Deep Learning in Harbor and River Engineering Applications

## Organizer: 蘇元風 助理教授

| No. | Title | Authors |
|---|---|---|
| S10-01 | 利用機器學習方法提升暴雨事件時洪水預測之準確度 | 蔡可安, 蔡文柄 |
| S10-02 | 以深度學習方法預測濁水溪流域地下水位 | 何紹維, 蔡文柄 |
| S10-03 | 機器學習結合雲端遙測平台 Sentinel-1 及 Sentinel-2 影像進行土地利用分類 | 鄭群儒, 蘇元風 |
| S10-04 | 不同油污偵測感應器於海域油污監測與擴散之分析 | 甘翊萱,高奕翔, 蕭宇倫, 林育銓, 韓仁毓 |

# 利用機器學習方法提升暴雨事件時洪水預測之準確度

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## 摘 要

氣候變遷導致極端水文事件發生頻率提高，莫拉克颱風在 2009 年對台灣造成約 700 人死亡及失蹤、一百多億的災損，根據觀測資料顯示每小時降雨強度來到 100 毫米，此類型的降雨模式在近幾年愈發頻繁的發生，不穩定的降雨模式為洪水預報帶來嚴苛的挑戰。本研究嘗試利用機器學習的方法來解決傳統模型在面對極端水文事件的不足，結合卷積神經網路(Convolutional Neural Network ,CNN)及長短期記憶模型(Long Short-Term Memory ,LSTM) 的特性進行洪水預測，利用卷積神經網路善於自動提取數據中的特徵以及長短期記憶模型可以在較長的時間序列中進行學習且不會遺漏關鍵訊息的特性。將數據放入卷積神經網路進行訓練後得到的輸出作為長短期記憶模型的輸入，讓最後的輸出可以同時擷取兩個模型的優點。此外，利用機器學習的技術可以使本研究的模型與傳統的水文模型相比，在更短的時間內得到更準確的模型，進而更快地提供即時的淹水資訊以利應變可能產生的災情，通過本研究的模型，在面對暴雨的情況下，事先預測都市區域容易產生淹水災害的區域，提供可以作為預防性撤離的參考資料，減少洪水帶來的損害。

關鍵字：機器學習、卷積神經網路、長短期記憶模型、都市淹水

# 以深度學習方法預測濁水溪流域地下水位

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## 摘　要

因河道坡陡流急和降雨時空間分配不均，台灣極大部分的雨水未能經過有效利用就流入海中，又因面積狹小使得建立水庫儲水方式效果有限，使得台灣在擁有豐沛降水量的前提下卻也非常容易遇到缺水的問題，因此地下水一直以來都是台灣非常重要的水資源。然而影響地下水位的變量多且複雜，建立傳統模型的過程往往需要高度的知識量與人力，本研究將利用機器學習方法純資料驅動的特性，使模型自動去尋找輸入資料間的關係，嘗試去預測未來的地下水位。

研究區域為台灣中部濁水溪沖積扇平原一帶，收集了研究區域內數個地下水位站的日資料作為目標變量，同時收集了其他資料例如降雨量、溫度、測站經緯度或地下水井高程等作為輸入變量，對以上數據進行整理並正規化後輸入模型，嘗試利用長短期記憶模型（LSTM）來預測未來數天之地下水位，並以均方根誤差（root-mean-square error, RMSE）、納許效率係數（Nash-Sutcliffe efficiency coefficient, NSE）等評估指標確認模型可信度。

關鍵字：地下水位、機器學習、深度學習、LSTM

# 機器學習結合雲端遙測平台 Sentinel-1 及 Sentinel-2 影像進行土地利用分類

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## 摘　要

近年來，地表變動的監測與分析在自然災害防治及環境管理上扮演著重要角色，針對崩塌地判釋，過去方法大多依賴於現場調查及航照分析，然而這些方法耗時且人力成本高昂。隨著遙測技術這些年來不斷更新，利用高解析度光學衛星影像成為現在的主要趨勢，但光學影像易受天氣條件限制，導致某些時刻無法正確判釋。近年來有一個新興的大數據平台叫做 Google Earth Engine(簡稱 GEE)，此雲端遙測平台內可進行各種光學衛星影像、數值高程模型(DEM)資料等等的下載、分析、可視化，本研究的目標就是結合該平台內的光學與雷達影像進行崩塌地判釋，期望能提高判釋效率及準確性。

本研究利用 GEE 平台內的 Sentinel-1 SAR 和 Sentinel-2 MSI 影像，結合機器學習技術，包括：支援向量機(Support vector machine,SVM)與隨機森林(Random Forests, RF)來進行土地利用分類。我們將研究區劃分為五個類別：草地與農地、森林、水體、裸露地、建築，並利用紅光、近紅外光及 NDVI 等波段與參數作為機器學習模型的輸入資料。儘管光學影像在正常情況下就已經有不錯的表現，但在雲層干擾下，其判釋效果仍會受到限制。因此，我們引入了雷達影像，以克服光學影像的局限性。透過此研究，期望能夠更準確的判釋出崩塌裸露地區域，從而能夠為自然災害防治及環境管理上提供更有力的支持。

關鍵字：Google Earth Engine、機器學習、衛星影像、土地利用分類

# 不同油污偵測感應器於海域油污監測與擴散之分析

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## 摘 要

臺灣四面環海且地處東南亞海運主要航道，由於地理位置特殊，使得社會、人文、經濟和自然資源皆與海洋環境息息相關，加之國際貿易興盛及工業發展需求，促使各類船舶經常航行於臺灣四周海域。而高雄港為我國第一大商港，每年皆有約一億公噸以上的貨運吞吐量，雖帶來可觀的貿易效益但也無形增加海洋汙染之風險，任何船舶的意外甚至是蓄意所造成之溢油事件，都可能造成港區內遭受重大油污染或是化學品污染災害。據統計 110 年高雄港內發生了 46 件油汙染事件，其中僅有 2 件確定行為人，其餘 95%的事件為不明油汙染事件。因此，瞭解並即時監測港區周邊海域是否有油污等污染物並能確定事件發生之證據尤為重要。本計畫先透過室內模擬對熱紅外線與雷射螢光感測兩種油汙偵測儀器進行感測能力的分析與比較，並到高雄港進行實地驗證。研究成果顯示兩種儀器各自有適合的任務目標，熱紅外適合大範圍偵測；雷射螢光感測適合判斷是否真有油汙發生。建議相關管理單位採複合使用，以協助清潔船監測並辨識海面上肉眼難以察覺之油污污染物之分布，達成海洋污染災害的防治及淨化。

關鍵字：油污、船用柴油、雷射螢光感測、熱紅外線影像

# MS-11 Machine Learning on Earthquake Engineering and Disaster Prevention

## Organizer: 張蔚慈 副研究員

| No. | Title | Authors |
|---|---|---|
| S11-01 | A Novel Window Detection Model for UAV-based Disaster Response System | Hong-Bo Huang , Rih-Teng Wu |
| S11-02 | 結合隨機森林與主動式學習之鋼筋混凝土柱塑鉸參數預測 | 陳鵬宇，李坤展 |
| S11-03 | 以圖強化學習最佳化非線性歷時分析下之結構斷面設計 | 周遠同，黎光曜，張慰慈，黃尹男，陳俊杉 |
| S11-04 | Ground Motion Selection for Nonlinear Response-History Analysis of Buildings | I-Hsiang Chang, Wei-Tze Chang, Yin-Nan Huang, Chuin-Shan Chen, Wen-Yu Chien, Hsun-Jen Liu |
| S11-05 | 影像量測與深度學習於結構裂縫偵測之實作 | 莊英甫，楊元森 |
| S11-06 | 整合機器學習與電腦繪圖技術應用於風機扇葉振動影像分析方法 | 詹偉詳，楊元森 |
| S11-07 | Identification of Infrasonic Signals of Tatun Volcano Group with Unsupervised Machine Learning | Wei-Tze Chang, Yin-Cherng Lin, Ya-Chuan Lai, Min-Hung Shih, Chun-Yun Chou, Lin, Cheng-Horng Lin, Jen-Yu Han, and Chuin-Shan Chen |
| S11-08 | 含深度學習之非線性數值子結構及時複合實驗技術開發與驗證 | 陳沛清，徐上祈，范萬軒 |
| S11-09 | Advanced LiDAR-based SLAM and Autonomous UAV Exploration for Post-Disaster Assessment in Severely Impacted Buildings | Chun-Sheng Lee, Chuin-Shan Chen, Wei-Tze Chang |
| S11-10 | 結合電腦視覺與深度學習於建物耐震性能初步評估 | 王迎芃，邱聰智，張家銘，林子為[2]，宋隆洧 |

# A Novel Window Detection Model for UAV-based Disaster Response System

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## Abstract

In recent years, Unmanned Aerial Vehicles (UAVs) have led to increasingly diverse applications in various fields. Object detection within complex disaster scenarios has emerged as a significant research topic for the realization of efficient disaster prevention and rescue operations by UAVs in unknown environments. Particularly, windows often serve as an alternative point of access to indoor spaces, and the enhancement of window detection are therefore critical for rescue efficiency. However, the number of disaster-related building imagery that can be utilized for model training is highly limited. To address these issues, we propose a novel model named Fopen-YOLO (i.e., Find opening-YOLO). We train the model on non-disaster building imagery sourced from Google Street View images to ensure generalization capability for unpredictable scenarios, thereby facilitating the identification of windows in disaster-affected buildings. Compared to the baseline YOLO-v5 model, our model architecture integrates Coordinate Attention Mechanisms (CA) and Bidirectional Feature Pyramid Networks (BiFPN) to place greater emphasis on the spatial contextual information surrounding windows. Additionally, lightweight module Ghost Convolution (GhostConv) and the adaptive activation function Mate-Activate or Not (Mate-ACON) are employed to minimize model parameters and enhance generalization, respectively. Results have demonstrated that the proposed Fopen-YOLO outperforms the baseline deep learning models across various datasets, including a 4.3% increasing in accuracy for Google Street View images, a 26.6% improvement for UAV-captured images, and a 21.2% boost in performance for window detection in disaster scenarios.

Keywords: UAVs, Object detection, Deep learning, YOLO-v5, Disaster prevention and rescue

# 結合隨機森林與主動式學習之鋼筋混凝土柱塑鉸參數預測

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## 摘　要

鋼筋混凝土 (RC) 建築是台灣常見之的建築材料，其優勢為成本低且易於施工。過往的地震災害中可發現，RC 柱受側向力產生之變形關係對建築物的抗震性能有著顯著的影響。因此，如何精確評估柱中塑性鉸的背骨曲線參數和遲滯迴圈的劣化參數對於評估 RC 建築的抗震性能、潛在的損傷程度和損失極為重要。既有分析技術在模擬 RC 塑鉸時，是採用經由實驗數據迴歸所得的經驗公式來描述其背骨曲線。使用上，往往需要多次校準數值模型，過程既耗時又費力。倘若針對單一 RC 建物進行詳細的耐震評估，此一方法尚可接受。但若分析對象為城市範圍內大量之 RC 房屋，其計算成本過高，恐無法即時得知災損情況。為解決此一問題，本研究提出一基於隨機森林的數據驅動機器學習方法，用於預測在 OpenSees 中常用的 Modified Ibarra-Krawinkler 材料模型中的 7 個非線性參數，這些參數描述了背骨曲線中的降伏轉角、極限轉角以及遲滯迴圈中的強度與勁度劣化速率。為了開發機器學習模型，本研究彙整了 475 個 RC 柱試體之側推曲線與遲滯迴圈，這些試體具有廣泛的材料參數、幾何特性與配筋細節，並且有撓曲、撓剪與剪力破壞的試體。值得注意的是，本研究納入了過往從未考慮過的高強度 RC 試體來訓練隨機森林模型。為了克服費時的標籤過程，本研究融入了主動式學習的架構，可由少數經詳細校正後的試體模型來協助標籤其他未經校正之模型塑鉸參數，結果顯示其性能優於現有方法。此研究成果將有助於針對城市內大量 RC 建築物進行地震災害的風險評估，來協助政府訂定災防相關政策。

關鍵字：隨機森林、主動式學習、鋼筋混凝土柱、塑性鉸、遲滯迴圈

# 以圖強化學習最佳化非線性歷時分析下之結構斷面設計

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## 摘　要

結構斷面設計為一迭代的設計過程，一常見之實務目標為產生符合法規強度要求並同時降低材料成本之最佳斷面組合。然而，在此迭代設計過程中存在兩項主要挑戰：首先非線性歷時分析所需的高時間成本使得設計過程通常使用快速的靜力分析。雖然靜力分析成本較低，但卻無法準確考慮結構在設計及最大考量地震下之動力及塑性反應。其次，由於斷面設計具有巨大的設計空間，窮舉每種可能的設計並非可行之最佳化方法。因此，本研究旨在利用 AI 技術，結合線性靜力分析及非線性歷時分析作為結構強度之檢核方法，以開發一深度學習模型，對不同幾何形狀之鋼結構進行斷面設計之最佳化。本研究將鋼結構表示成圖 (graph) 資料結構，並使用包含圖神經網路 (graph neural network) 及強化學習 (reinforcement learning) 之深度學習模型進行訓練。此模型會生成兩組設計：第一組為在僅考慮靜力分析法規作為檢核條件時，AI 所得到的最佳的斷面設計組合；第二組則同時考慮了靜力分析及非線性歷時分析法規下之斷面設計組合。通過大量對結構斷面之設計空間進行取樣，此深度學習方法可以比 90% 以上採樣得到之設計更好、使用更少的材料用量。此外，測試集之結果顯示，多考量了非線性歷時分析的設計，確實讓結構在最大考量地震等級下有更好的層間位移比表現。

關鍵字：圖神經網路、強化學習、斷面最佳化設計、耐震設計、非線性歷時分析

# Ground Motion Selection for Nonlinear Response-History Analysis of Buildings

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## Abstract

Selection and scaling of input ground motions is crucial for the response-history analysis of a building. For this issue, the National Center for Research on Earthquake Engineering (NCREE) under the National Applied Research Laboratories (NARLabs) established the “Taiwan Recorded Ground Motion Database for Structural Response-History Analysis” and then developed it into the “platform of Input Motion Selection for Taiwan” (INMOST) which can identify a small set of ground-motion records whose elastic response spectra closely match the code-defined design response spectrum for any specific location in Taiwan. This study performed a series of nonlinear response-history analyses for sample code-compliance RC special moment frames using a significant number of ground motions. This comparison aims to understand the impact of selecting ground motion solely based on elastic response spectra, as well as to explore the advantages and potential of a ground-motion selection procedure that takes into account the nonlinear responses of a building.

Keywords: dynamic analysis, ground-motion selection and scaling, Input Motion Selection for Taiwan (INMOST)

# 影像量測與深度學習於結構裂縫偵測之實作

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## 摘　要

表面裂縫對於牆體結構的健康監測和安全性評估是一個非常重要的指標。目前常採用人工目視的方式進行表面裂縫檢測，工作時間成本高，檢視人員的工作環境也可能具有危險性。近年來由於機器學習技術的發展與普及性快速地進步，利用機器學習的手段來進行混凝土表面裂縫偵測與分析，有機會可改善這些問題。目前相關的研究發表數量相當多，但這些成果大多僅適用於特定屬性的訓練資料，而其特性與廣泛使用性則較少被探討。

本研究透過設計並實作縮尺牆體結構實驗，後續利用深度學習進行影像裂縫分析，並以各方法應用於裂縫量測之結果與位移場差分法做比較，藉此探討結構健康監測各應用面的發展性。藉由對各項量測結果之分析比較與歸納，對未來開發結構健康監測系統，建立影像量測品質及流程架構之依據，並探討各影像量測技術之適用場合、效率、精度及可能產生誤差之原因。

關鍵字：影像量測、結構實驗、裂縫量測、結構監測、深度學習

# 整合機器學習與電腦繪圖技術應用於風機扇葉振動影像分析方法

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## 摘　要

風機扇葉的監測因扇葉之位移不易量測且風機所在位置較為嚴苛，其監測任務對於研究人員來說是一項非常困難的挑戰。影像式量測與監測技術具有遠距量測、低硬體成本，與易於維護等優勢，對於風機葉片振動量測與監測具有相當的潛力。影像式監測系統的開發在過去幾年研究人員的共同努力之下，現已能取得良好的量測精度，然而傳統基於模板匹配法之影像追蹤法須於待測物表面進行特徵塗佈與粘貼靶標以利演算法進行追蹤，實務上要在結構物上進行標記作業可能較難以被接受。

本研究利用有限元素分析軟體 OpenSees 模擬真實離岸風機的運動行為，並結合電腦繪圖軟體 Blender 模擬現實環境條件，例如霧、海浪、天空和陽光等建立大量擬真動態影像。以機器學習之圖像分割技術分割出風機扇葉之影像，利用本研究開發之演算法追蹤分割圖像中風機扇葉尖端位置進行位移量測獲取結構頻率，以探討該流程於離岸風機扇葉結構監測之可行性。本研究結果顯示結合機器學習方法進行風機扇葉面外位移量測與力學分析之結果有相當高的契合度，利用機器學習圖像分割方法不須事先於待測風機表面進行標記即可進行量測工作，可大幅提升實務應用的接受度。

關鍵字：影像量測、虛擬環境、風機扇葉振動分析、Blender、OpenSees、機器學習

# Identification of Infrasonic Signals of Tatun Volcano Group with Unsupervised Machine Learning

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## Abstract

Infrasonic signals of large fumarole fields imply important information related to volcanic activities, which directly reflects the changes in the state of the magma or hydrothermal system underground. Variations in the number, type, location, and magnitude of fumarole activities may indicate volcanic anomalies. However, infrasonic signals can be caused by other events, such as earthquakes, gusts, extreme weather, and even human activities, which are not easy to process and identify. This research studied infrasonic records from the Tatun Volcano Group (TVG) in Taiwan. The signals were transformed into the frequency domain via the Fast Fourier Transform (FFT) to understand its characters. The Power Spectral Density (PSD) was retrieved as the critical feature for unsupervised machine learning, and the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) clustering algorithm was applied to identify the special events of the volcano. The research results will then be developed into an automatic platform of TVG for achieving real-time monitoring and simplifying considerable data for geoscience experts.

Keywords: infrasonic signal, identification, volcanic, frequency, unsupervised machine learning

# 含深度學習之非線性數值子結構及時複合實驗技術開發與驗證

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## 摘　要

近年，即時複合實驗在地震工程等領域蓬勃發展，結合數值子結構和實驗子結構節省傳統實驗架設之成本。然而，處理複雜結構時，數值子結構運算成本龐大，且需確保數值和實驗子結構互動一致，避免時間延遲導致實驗不穩。為應對此，本研究引入基於長短期記憶（Long Short-Term Memory,LSTM）神經網絡的深度學習模型作為數值子結構代理。模型輸入輸出符合實驗架構，標竿為三層樓單跨黏滯阻尼非線鋼結構。在阻尼力強健性訓練上，透過五種線性阻尼器地震歷時分析，確保 LSTM 模型可處理非線性阻尼力並穩定在取樣頻率 40Hz 進行實驗。為克服時間延遲，研究不僅運用相位補償，還在訓練過程中讓 LSTM 學習處理延遲輸入，維持準確預測。結果證實，這種訓練機制有效解決時間延遲，展現深度學習模型於即時複合實驗之潛力。最終，本研究在不增設硬體下，簡化 LSTM 模型，並調整區域採樣步驟，成功實現取樣頻率 100Hz 和 200Hz 之即時複合實驗。此工作為複雜結構的即時實驗提供了可行方法。

關鍵字：即時複合實驗、深度學習、LSTM、時間延遲、非線性結構反應預測

# Advanced LiDAR-based SLAM and Autonomous UAV Exploration for Post-Disaster Assessment in Severely Impacted Buildings

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## Abstract

Engaging in a rescue operation is a pivotal endeavor within post-disaster assessments, requiring the efficient localization of individuals in need within collapsed structures. Therefore, comprehending the interiors of buildings after disasters becomes imperative. To achieve this, a well-suited solution emerges in the form of an autonomous UAV (Unmanned Aerial Vehicle) system with LiDAR-based (Light Detection And Ranging) SLAM (Simultaneous Localization And Mapping) technology. Our UAV system has high maneuverability, autonomous navigation, and object recognition capabilities, deftly overcoming environmental challenges like low-light and non-GPS signal scenarios. Our UAV system features three subsystems. The algorithm system processes data from onboard sensors such as LiDAR, IMU, and camera utilizing the online Cartographer SLAM algorithm for real-time localization and the YOLOv7 model for object detection. This perceptual data empowers the UAV to make corresponding decisions regarding path planning. The client system, facilitated by ROS (Robot Operating System), integrates UAV functionalities, ensuring sensor harmony. Simultaneously, the cloud platform generates a high-definition (HD) map by amalgamating LiDAR and IMU data. Moreover, it integrates outcomes from the image-based segmentation model onto the HD map, ensuring a more faithful representation of the actual environment. Through this integrated framework, our system empowers rescue missions by providing real-time insights into collapsed structures, enhancing the safety and effectiveness of rescue teams.

Keywords： UAV, Cartographer SLAM, YOLOv7, ROS, object detection

# 結合電腦視覺與深度學習於建物耐震性能初步評估

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## 摘　要

耐震初步評估為一可快速診斷建物耐震性能方法。於過去研發之耐震初步評估方法中，需透過人工讀取工程藍圖中重要資訊，如相關構件之截面積，但該步驟相當耗費時間與人力成本。因此，本研究研發一套基於電腦視覺與深度學習方法之影像辨識方法，由工程藍圖中提取建物重要構件之截面積，結合過去研發之耐震初步評估方法，降低人工判讀圖資之時間與減少人為失誤之可能性。本研究提出的方法中，首先本法會透過影像辨識的方式，找出結構圖或建築圖中之結構柱並相互套疊，自動化框選出建築圖中之牆體，再透過人工智慧深度學習，分出不同類型的牆體，之後由本研究應用影像處理技術，提出牆長度及厚度計算方法，可擷取牆截面積的關鍵參數，最後藉由柱、牆之類型與截面積，可套入過去研發之耐震初步評估計算方法，即可得出耐震初步評估分數。目前已對 181 棟建物進行此方法之評估，正確預測的準確率達 90.6%，符合工程應用的信心程度可達 96.1%。

關鍵字：鋼筋混凝土加強磚造建物、耐震能力初步評估、影像處理、電腦視覺、深度學習

# MS-12 Recent Advances in Numerical Modeling in Geomechanics and Geotechnical Engineering

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| S12-02 | Seismic Performance of Building on Liquefiable Sites improved with Structural Wall | Yu-Wei Hwang, Shu-Ci Yang |
| S12-03 | 填充材與潛盾隧道中大口徑輸水管線受震之互制行為探討 | 楊世凡, 葉馥瑄, 葛宇甯, 張凱評, 周采青, 張宏華, 汪嘉誠 |

# 以物質點法探討光華崩塌地滑動深度與運動行為

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## 摘　要

為有效掌握邊坡災害的風險，以及進行邊坡整治工程的規劃，現場的環境資訊與長期的監測資料成為上述工作推動的重要參考依據。然而，受限於山區險峻之地形條件，以及氣候劇烈變動之不利因素，地表下的資訊，例如地下水、地質、構造、地中變形等，難以取得充分的資料。此結果導致邊坡崩塌機制的評估困難，並導致後續整治工程的規劃完成度不足，以及治理成效不理預期等問題。本研究擬透過以物質點法為基礎發展之數值模式來克服上述問題，相較於過去以有限元素法為基礎發展之模式，僅能預測到崩塌發生階段的變形行為，本研究所提模式得以接續預測後續崩塌流體到堆積停止之行為，透過此模式將有利於探討不同深度滑動同時發生之邊坡破壞現象。本研究選定桃園市復興區光華崩塌地為案例，並以現場側傾管、地表位移和多期數值地形等資料作為模式之驗證參數。透過三維模擬結果顯示，光華崩塌地除上邊坡崩積層不穩定之外，破碎岩層中 40~50 m 處亦存在一深層滑動面，邊坡破壞先從上邊坡崩積層處發生，然後再從破碎岩層中的深層發生破壞，並致使光華邊坡的整體滑動。模式模擬的光華崩塌運動行為與現場監測資料具有一致性，且當滑動塊體崩移至趾部山溝，受束口效應提供抑制阻擋效果亦能於模擬結果中呈現，說明本研究所提之模式得以合理預測光華崩塌地的複雜運動行為。模式的預測結果得以回饋地表下現場難以取得之資訊，例如地下水、地中變形等，相關資訊之提供，將有助於未來邊坡災害風險的掌握和邊坡整治工程的規劃。

關鍵字：物質點法、大規模變形、滑動面分析、破壞後行為

# Seismic Performance of Building on Liquefiable Sites improved with Structural Wall

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## Abstract

The stiff structural wall or Diaphragm wall have been commonly used as liquefaction countermeasures for existing building(s) on potentially liquefiable ground. However, the state-of-practice for such mitigation designs is typically for free-field conditions, without considering seismic soil-structure interaction (SSI) and soil-structural wall interaction (SSWI). In particular, the mechanism of SSWI for liquefaction mitigation is still not well understood. Three-dimensional (3D), fully-coupled, nonlinear finite element analyses are used to evaluate how structural wall design and ground motion characteristics affect the seismic performance of inelastic, shallow-founded structures on liquefiable sites. An enclosed structural wall system was placed around the perimeter of a hypothetical, isolated, shallow-founded structure with a small distance. The numerical simulations showed that structural wall notably affects the seismic performance of isolated building in terms of settlement, tilt, and acceleration through (1) restriction to shear strains/deformations and (2) restraint of inward and outward excess pore water pressure migration. On the other hand, increasing shaking intensity reduced the efficiency of structural wall on foundation settlement reduction, while evolutionary ground intensity measures were better correlated with the liquefaction-induced foundation settlement, regardless of mitigation or not. The insight from this study aims to develop future design recommendations on the role of structural wall on mitigation of liquefaction.

Keywords： liquefaction, soil-structure interaction, finite element analysis, structural walls

# 填充材與潛盾隧道中大口徑輸水管線受震之互制行為探討

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## 摘　要

近年來，大口徑供水管道之埋設除了以明挖覆蓋之方式，另有以潛盾隧道工法進行供水管道之埋設。在過去的地下管線研究中，多探討土壤與地下管線直接接觸的互制行為；然而，潛盾工法中的管線非直接與土壤接觸，管線與隧道間係灌注膠結填充材使得隧道與管線成一複合體，然填充材之強度與灌注量與管線間互制行為研究甚少，故需進一步探究。因此，本研究以有限元素法軟體 ABAQUS 進行三維數值模擬，探討隧道環片與 U 型鑄鐵管間之填充材以「三種抗壓強度（10、40 與 140 kgf/cm$^2$）」、「兩種澆灌量（滿灌與半滿灌）」等設定條件下，地下管線受外力加載條件下伸長量、轉角的變化。本研究於 ABAQUS 建立三維模型，並以擬靜態方式進行分析外，另以大地工程界常用之有限元素程式 PLAXIS2D 建立二維平面應變模型，並輸入真實地震波進行動態分析，交互驗證與比對二維及三維模型分析結果中填充材之應力分布。數值模擬分析結果顯示，滿灌填充量案例中，延性鑄鐵管較半滿灌填充量中的延性鑄鐵管發生較大之轉角與伸長量，而填充材之材料強度對於管線之轉角與伸長量幾無影響，僅於管線發生最大伸長量發生處具較明顯差異；此外，填充材的應力分布於二維動態分析及三維擬靜態分析中趨勢相近，故填充材與管線間受震行為影響可透過三維數值模擬搭配擬靜態之受力方式進行，有別於二維平面應變分析，三維分析可獲得管線的轉角與伸長量。

關鍵字：地下管線、潛盾隧道、填充材、有限元素法、擬靜態分析、動態分析

# MS-13 Applications of Boundary Element Method/Boundary Integral Equation Method

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| No. | Title | Authors |
|---|---|---|
| S13-01 | Adomian Decomposition Method for First Order Linear PDE Systems with Unprescribed Data | Tzon-Tzer Lu |
| S13-02 | Indentation over a poroelastic layered system | Zhiqing Zhang, Ernian Pan, Jiangcun Zhou, Chih-Ping Lin, Shuangbiao Liu, Qian Wang |
| S13-03 | 以力學解釋宇宙萬象 | 林聰悟 |
| S13-04 | Symbolic derivations for complete factorized series expansions of the dyadic Green's functions for equations of equilibrium in homogeneous solid full-space governed by isotropic linear continuum theory of elastic mixture | Yang-Jye Lee, Tsung-Jen Teng |
| S13-05 | New Locations of Source Nodes for Method of Fundamental Solutions Solving Laplace's Equation; Pseudo Radial-Lines | Hung-Tsai Huang, Li-Ping Zhang, Zi-Cai Li, Ming-Gong Lee |
| S13-06 | Meshfree boundary integral equation method for solving the steady state heat conduction in exchanger tubes containing slits | Jia-Wei Lee, Hung-Wen Yang and Jeng-Tzong Chen |
| S13-07 | 向量式有限元理之論發展與工程應用回顧 | 王仁佐，王仲宇 |
| S13-08 | An Efficient Solver for Fractional Diffusion Equations | Chung-Lin Tseng, Wei-Cheng Wang |

# Adomian Decomposition Method for First Order Linear PDE Systems with Unprescribed Data

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## Abstract

In this paper, we like to explore the full power of Adomian decomposition method (ADM), especially its symbolic capability. We will demonstrate this method, together with splitting technique, to compute the explicit closed-form solutions of first order linear systems of partial differential equations with unprescribed initial conditions, and even with parameters. These features are those normal numerical methods fail to do. Our examples include many prototype hyperbolic and elliptic systems possessing analytical solutions, e.g. the linearised equations of gas dynamics. We conclude that ADM is far more powerful than existing numerical methods.

Keywords： Adomian decomposition method, splitting technique, closed-form solution, power series, unprescribed data, PDE system.

# Indentation over a poroelastic layered system

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## Abstract

We derive a general solution of indentation over a multilayered half-space consisting of transversely isotropic and poroelastic materials. The rigid disk-shaped indenter is subjected to a vertical force of Heaviside time-variation. The solution is expressed in terms of the recently introduced powerful Fourier-Bessel series (FBS) system of vector functions combined with the unconditionally stable dual-variable and position method for dealing with layering. Since the problem is a mixed boundary-value one, the Green's functions due to a vertical ring-load are first derived which are then utilized in the integral least-square formulation to derive the solution. In terms of the FBS vector system, the expansion coefficients, which are further called Love numbers, are discrete, and therefore can be pre-calculated and used repeatedly for different field points on the surface. As such, the solution based on the new FBS system is more efficient and accurate than the previous integral-transform methods. This new and discrete vector system is particularly attractive for dealing with mixed boundary-value problems where time-variation is involved. Numerical examples are carried out to validate the accuracy of the proposed solution, and to demonstrate the effect of material layering, geometry, and hydraulic boundary conditions on the contact performance of the material system.

Keywords: FBS system of vector functions; dual-variable and position method; layered poroelasticity; transverse isotropy; Love number; consolidation

# 以力學解釋宇宙萬象

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## 摘　要

近代物理於一百多年前以 Michelson-Morley 實驗否定以太的存在並放棄牛頓力學。事實上日本學者於 25 年前已經實驗証明微中子有質量且充滿於太空中。微中子即為三百多年前以來所認定的光電磁波與萬有引力的介子"以太"。只是以太一直被誤以為不具質量而且絕對靜止。一旦以太有質量，就會跟隨地球轉，M-M 實驗就量不到預想的相對運動，因此以該實驗否定以太的存在是錯誤的。有質量的以太粒子相互碰撞就會有反彈力而造成壓力。所有的現象自然都可用力學來分析：如用有質量的以太造成的壓力變化解釋萬有引力，用有質量且會旋轉的以太即可傳遞光電磁波。而不必用所謂的隔空使力來解釋萬有引力或磁力，真空可以傳播光電磁波等無理的論調。一百多年前 Maxwell-Boltzmann 所提出的 M-B 速度分布最近我們也用力學方法得到証明，因此亦適用於空氣與以太混合的情形。故可利用力學方法得到合理而準確的以太質量。這也間接証明以太確實是光電磁波的傳播介子。再者熱容比本來是由實驗得來的統計熱力學的係數，亦可用力學的能量關係求得。所以統計熱力學就可以從純力學的觀點來分析。另外從粒子的碰撞分析可以看出粒子的碰撞確實存在隨機性但仍然可以用力學做分析。所以力學不僅能做巨觀的確定性分析，亦可做微觀的個別粒子的運動行為分析。由這些分析可以了解分子的特性。

關鍵字：以太，微中子，以太質量，波速，壓力，熱容比，體積模數，移動動能，轉動動能，應變能。

# Symbolic derivations for complete factorized series expansions of the dyadic Green's functions for equations of equilibrium in homogeneous solid full-space governed by isotropic linear continuum theory of elastic mixture

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## Abstract

In this talk, we are going to present a complete factorized series expansions of the dyadic Green's functions for the equations of static equilibrium in solid full-space governed by isotropic linear continuum theory of elastic mixtures (abbreviated as "EM theory" in the sequel).

By "factorized series expansion", we mean that each term of this series expansion is expressed as the product of a vector function of the position vector of the field point and a vector function of the position vector of the source point.

All vector functions in this series expansion can be proven to be included in two infinite sequences of fundamental solutions of source free static equilibrium in solid full-space governed by EM theory.

The first sequence consists of fundamental solutions which are regular in the sense that these functions are regular when the dependent position vector is in region with finite distance from the origin, which should be included inside this region. Moreover, these regular fundamental solutions may be proven to be complete in representing solutions of internal BVPs in finite solid region governed by EM theory.

The second sequence consists of fundamental solutions which are singular in the sense that these functions are singular when the dependent position vector is in region with finite distance from the origin. Moreover, these singular fundamental solutions may be proven to be complete in representing solutions of external BVPs in a semi-finite solid region governed by EM theory. By "external BVPs", we mean that the target region is a semi-infinite region external to a finite region including the origin.

By "symbolic derivation", we mean that we are going to present all closed-form expressions for all results derived in this study.

Keywords： dyadic Green's function, fundamental solution, continuum theory of elastic mixture

# New Locations of Source Nodes for Method of Fundamental Solutions Solving Laplace's Equation; Pseudo Radial-Lines

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## Abstract

Consider Laplace's equation in a bounded simply-connected domain $S$, and solve it by the method of fundamental solutions (MFS). The source nodes must be located outside the domain boundary $\Gamma = (\partial S)$ $\Gamma\ (= \partial S)$. How to select better source nodes $(R_i$ is essential to the MFS in both theory and computation. In this paper, we study new locations of source nodes along pseudo radial-lines outside $\Gamma$. Denote the source nodes by $(R_i, \phi_i^*)$ in polar coordinates, where $R_i > \rho_{\max} = \max \rho|_\Gamma$ $R_i > \rho_{\max} = \max_\Gamma \rho$ but angle $\phi_i^*$ is fixed. We propose new algorithms using two pseudo radial-lines. Two different angles $\phi_1^*$ and $\phi_2^*$ are fixed, and the source nodes as $(R_i, \phi_1^*)$ and $(R_i, \phi_2^*)$ are chosen, where $R_i \in [R_0, R_{\max}]$ $R_i \in [R_0, R_{\max}]$. Adaptive error estimates are derived by using the numerical coefficients obtained. We study two kinds of locations of source nodes, Case I: uniform $R_i \in [R_0, R_{\max}]$ $R_i \in [R_0, R_{\max}]$ and Case II: uniform $x_i = \rho_{\max} / R_i \in [a, b]$ $x_i = \dfrac{\rho_{\max}}{R_i} \in [a, b]$, where $a = \rho_{\max} / R_{\max}$ $a = \dfrac{\rho_{\max}}{R_{\max}}$ and $b = \rho_{\max} / R_0$ $b = \dfrac{\rho_{\max}}{R_0}$. Locations of source nodes are defined by four parameters (i.e., $R_0$ $R_0$, $R_{\max}$ $R_{\max}$, $\phi_1^*$ and $\phi_2^*$) in Cases I and II. Numerical experiments are carried out for Cases I and II, and better parameters are found. Two radial-lines of Case II are antenna-like and radar-line-like. Based on the sensitivity index, Case II offers better numerical performance. The algorithms of two radial-lines converge fast; both Cases I and II are satisfactory for scientific/engineering problems. In summary, the algorithms for new two pseudo radial-lines in Cases I and II have been established to enrich the MFS family, and the new algorithms and techniques seeking better source nodes in this paper are further developments of the MFS.

Keywords：Method of fundamental solutions, pseudo radial-lines, adaptive errors, error analysis, stability analysis, Laplace's equations, selection of source nodes, sensitivity index.

# Meshfree boundary integral equation method for solving the steady state heat conduction in exchanger tubes containing slits

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## Abstract

This paper proposes the meshfree boundary integral equation method (BIEM) to determine the conduction shape factor heat of exchanger tubes containing slits. The main difference between the present method and the conventional boundary element method is that the adaptive exact solution and Gaussian quadrature are simultaneously employed to technically calculate the singular integral. When dealing with the problem containing a slit or so-called degenerate boundary, a rank-deficient problem of influence matrix due to a degenerate boundary may occur. To overcome it, we introduce the dual BIEM with the hypersingular boundary integral equation to obtain independent equations for a collocation point on the slit. A feasible adoptive exact solution is also required for the problem with a degenerate boundary. Since the jump behavior can not be described by the adoptive exact solution using the Cartesian coordinates for the corresponding collocation point on the slit, we adopt the harmonic basis function in the elliptical coordinates to construct the new adaptive exact solution. After comparing available exact solutions of conduction shape factor, the present data are consistent with those in the literature. However, the numerical instability due to the degenerate scale of an outer boundary is also observed. Regularized techniques are proposed to suppress the appearance of numerical instability. Moreover, the boundary layer effect is also treated in the present method.

Keywords： conduction shape factor, meshfree boundary integral equation method, adaptive exact solution, degenerate boundary, degenerate scale.

# 向量式有限元理之論發展與工程應用回顧

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## 摘 要

本文主要回顧介紹向量式有限元素理論發展與工程應用，在向量式有限元素理論主要兩部分，分別為元素類型與材料非線性介紹。在元素類型部分，包含桁架元素、剛架元素與固體元素及版殼元素，元素理論推倒都已考慮扣除剛體位移後計算出之純變形量來計算元素內力，因此各類元素均可用來模擬結構幾何非線性變形。材料性質介紹內容，包括鋼材與混凝土及鋼筋混凝土非線性材料。在結構桿件斷面分析方法，包括塑性鉸與纖維斷面分析方法兩種。工程上應用方面則包括，橋梁與軌道及結構工程，例如車軌橋互制非線性力分析、斜張橋倒塌分析、鋼筋混凝土結構倒塌分析、橋梁倒塌分析與混凝土裂縫拓展分析及鋼結構火害分析等，在向量式有限元破壞模擬分析，亦考慮變形體元素之間接觸碰撞偵測與接觸力計算方法，透過本文介紹可完整了解目前向量式有限元歷史發展與實際應用相關成果。

關鍵字：向量式有限元、幾何非線性、材料非線性、接觸碰撞

# An Efficient Solver for Fractional Diffusion Equations

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## Abstract

The fractional order differential operators have attracted considerable attention recently as an essential tool for developing more sophisticated mathematical models that can accurately describe complex anomalous systems. Since the fractional order differential operators are nonlocal, the corresponding linear system involves a dense, structured Toeplitz matrix. Many research activities are devoted to developing robust and efficient solvers for such linear systems.

In this talk, we propose a numerical method for the fractional diffusion equations based on a new preconditioner that can be used to develop direct and iterative solvers for fractional diffusion equations with total O(N log N) operations per time step. Numerical results suggests the new method is a competitive alternative to existing methods.

Keywords： fractional、differential、precondition、equations、direct、iterative

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