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ISSUES 13 (SEPTEMBER - DECEMBER 2023)

Welcome to the Newsletter e-Science Putra. This issue presents the research activities from September to December 2023 which highlight the latest research findings by the selected faculty members.

HIDDEN GEMS OF GENTING HIGHLANDS: UNVEILING THE ELUSIVE MYCOHETEROTROPIC ORCHID – EPIPOGIUM ROSEUM (D.DON) LINDL

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Genting Highlands is home to various species of fascinating orchids including the recently recorded species of Epipogium roseum found in one of the trails of Awana Bio Park, a private land managed by the Awana Resort World Genting Highlands. Epipogium roseum belongs to the Orchidaceae family and it is part of the Epidendroideae subfamily. Due to its leafless characteristic, it is frequently referred to as the 'ghost orchid' and is found in many parts of Tropical Africa, Tropical and Subtropical Asia, and the South West Pacific (POWO, 2023). The absence of leaves causes it to be achlorophyllous (not having chlorophyll) hence, unable to undergo photosynthesis process. Being one of the fully mycoheterothrophic angiosperm plant species, E. roseum is primarily found in humid and shaded areas. It lives in symbiotic association with a variety of microbial communities, including mycorrhizal fungi, which act as a substitute for photosynthesis and provide additional nutrients. The fungi are directly connected to the roots of the orchid, and they use the roots of other plants or decaying organic matters in the soil as their source of nutrients (Tom, 2011). The flower stalk that bears almost translucent delicate white flowers can reach up to 60 cm (Seidenfaden & Wood, 1992). On close observation, purple spots can be seen scattering on the lip.

According to the Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES), E. roseum is placed under Appendix II which includes a list of species that are not necessarily now threatened with extinction but that may become so unless trade is closely controlled, meanwhile the conservation status of E. roseum according to the International Union for Conservation of Nature Red List of Threatened Species (IUCN Red List), is yet to be evaluated. Threats like urban development, land conversion, and logging activities can lead to habitat loss and cause detrimental effects on the population of the E. roseum. In addition, being one of the biggest environmental concerns, climate change can also affect the moisture and temperature of the exclusive conditions required for the survival of the ghost orchids. Through this finding, E. roseum is undoubtedly regarded as a mysterious and an elusive orchid in the nature known for its unique characteristics that have captivated researchers as well as orchids enthusiasts from all over the world to further study and contribute to the survival of this unique species.

The flowers of Epipogium roseum show purple spots on the lip

Matured Epipogium roseum found in the wild

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EXPLORING QUANTUM CIRCUIT COMPLEXITY WITH LIE GROUPS AND RIEMANNIAN GEOMETRY

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In quantum mechanics, a quantum state describes an object on a tiny scale, typically representing the motion of particles. This state is mathematically represented by what is called a wave function. The states are just vectors which are elements in a vector space, known as the Hilbert space. Thus, vectors are well-known objects in linear algebra, making linear algebraic methods a powerful tool in quantum mechanics that seamlessly integrates geometry and algebra. With a solid grasp of the formulation and mathematical tools of quantum mechanics, several advanced problems in quantum science and technology can be reduced to more established and efficient methods in linear algebra.

One illustrative example is the transformation of a quantum circuit complexity problem into a geometry problem, which can then be studied through the lens of Riemannian geometry [1,2]. Quantum circuit complexity is a challenging issue in quantum computing, focusing on enhancing and advancing quantum algorithms to design efficient quantum circuit models. Here, quantum states transform into qubits, the carriers of quantum information, operated on by quantum gates within specialized algorithms. In this pursuit, the qubit replaces the classical bit of traditional computing.

Our work has successfully delved into the quantum circuit complexity within the framework of Riemannian geometry, particularly in the context of the three-qubit quantum Fourier transform (QFT) (Figure 1). We computed and proposed the Hamiltonian and Riemannian metric for the three-qubit QFT and formulated its geodesic equation in differential form. The resolution of this equation suggests that an efficient QFT of this kind can be realized.

Additionally, we described quantum gates in a quantum circuit as elements of the SU(2) Lie group in operator representation and proposed a refined version of the three-qubit quantum Fourier transform within SU(3) (Figure 2). The frequency of the structure constant for the Lie algebra of su(8) in the Pauli basis is analyzed, confirming that all quantum circuits can essentially be generated using one-qubit gates and CNOT gates [3]. This provides insight into the relationship between the quantum circuit model and Lie Algebra.

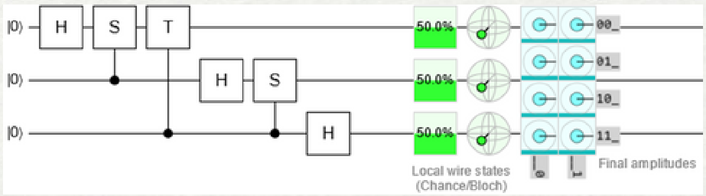

Figure 1: A quantum circuit of three-qubit quantum Fourier transform with Hadamard (H), S and T gate.

$$e^{\frac{\pi i}{8}} e^{\frac{\pi i}{16}} * \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & e^{\frac{i\pi}{4}} & i & ie^{\frac{i\pi}{4}} & -1 & -e^{\frac{i\pi}{4}} & -i & -ie^{\frac{i\pi}{4}} \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & ie^{\frac{i\pi}{4}} & -i & e^{\frac{i\pi}{4}} & -1 & -ie^{\frac{i\pi}{4}} & i & -e^{\frac{i\pi}{4}} \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -e^{\frac{i\pi}{4}} & i & -ie^{\frac{i\pi}{4}} & -1 & e^{\frac{i\pi}{4}} & -i & ie^{\frac{i\pi}{4}} \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -ie^{\frac{i\pi}{4}} & -i & -e^{\frac{i\pi}{4}} & -1 & ie^{\frac{i\pi}{4}} & i & e^{\frac{i\pi}{4}} \end{pmatrix}$$

Figure 2: Matrix representation for corrected three-qubit quantum Fourier transform.

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THE INDIVIDUAL DIPOLE MOMENT EFFECTS ON THE FLUCTUATION OF VOLUME DIPOLE MOMENT IN BULK POLAR SOLVENTS

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Designing a material from the chemical structure of the molecules that form the material is difficult because there are not many bulk material properties that have known relation to the structure of the molecules that constitute the material. Among the exception is the static dielectric constant, ε [1]. ε describes the ability of a material to screen the force between two charged plates. ε can be related to the dipole moment, μ using the classical molecular dynamics simulation employing force field method by an equation derived by Neumann [2]:

$$\varepsilon = (4\pi/3)(k_B TV)(\langle M^2\rangle - \langle M\rangle^2) + 1 \text{------------- eq1}$$

In this equation, ε is the static dielectric constant, k_B is the Boltzmann Constant, T is the temperature, and V is the volume of the bulk solvent. M is the said volume dipole moment, where it is defined as: $M = \sum \mu_i$ (Figure 1). Here, μ is the individual dipole moment of each molecule in the volume. Since M depends on μ, μ also affects the static dielectric constant of the bulk solvent. In addition, because the molecules are free to move in the bulk solvent, understanding the effect of μ can help predict the value of M and thus ε.

Molecular dynamics simulations were performed on a polar organic solvent, tetrahydrofuran (THF). In each simulation of 500 molecules, the partial charges and Van der Waals parameters were carefully parametrized such that the simulation matches the experimental static dielectric constant and bulk density. From the simulation, μ are oriented in parallel to- and in the opposite direction to M. However, there are more μ oriented in parallel to the M. Plotting the net number of μ that are oriented parallel to M, against M shows that M can be predicted by only looking at the number of μ (Figure 2).

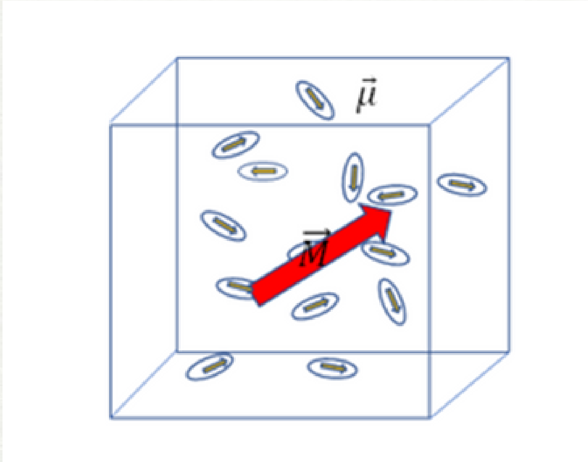

Figure 1: The relation between M and μ

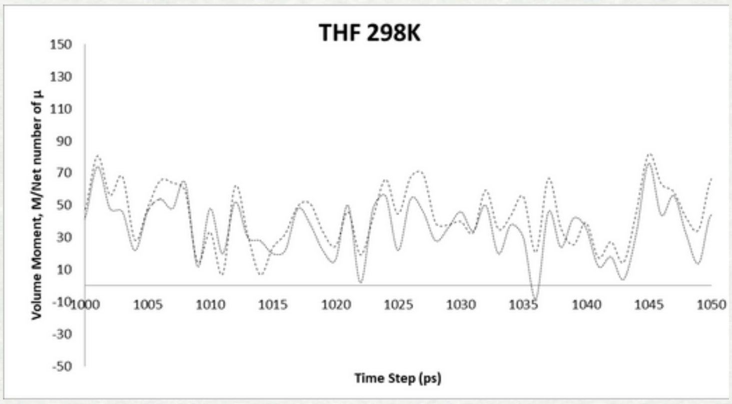

Figure 2: The plot of volume dipole moment, M and net number of dipole moment μ against simulation time. The similarity between the plot suggests that M can be predicted by predicting the number of μ

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TRANSFORMING AGRICULTURAL WASTE INTO ENVIRONMENTAL SOLUTIONS AND SUSTAINABLE CHEMISTRY

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In an era where sustainability is paramount, the creative repurposing of agricultural waste materials is emerging as a powerful approach to combat pollution and foster cleaner chemical processes. One significant advancement in this field involves the use of natural or chemically modified agricultural waste materials as biosorbents for removing pollutants, including pharmaceuticals, dyes, and heavy metals from water and wastewater. This approach not only aids in mitigating the adverse environmental impacts of these contaminants but also transforms agricultural waste into a valuable resource, contributing to a circular economy. Researchers are exploring the potentials of agricultural waste materials such as rice husks, plant stems, bagasse, coconut shells, oil palm wastes, and fruit peels. These materials exhibit remarkable adsorption capabilities when properly treated and engineered, serving as highly effective adsorbents. The agricultural waste capture and remove pollutants, resulting in cleaner and safer water sources for communities and ecosystems.

Furthermore, there is a growing interest in utilizing agricultural waste materials as catalysts, catalyst supports, and feedstocks in various chemical reactions, especially in the production of biofuels and biodiesel. Waste materials such as rice husks, oil palm wastes, bagasse, shells, and peels have found valuable applications in the production process of biofuels. This approach reduces the reliance on energy-intensive and environmentally harmful processes while converting waste materials into valuable resources. These innovations are propelling the green chemistry revolution, contributing to cleaner fuel and chemical production, reducing our ecological footprint.

By embracing these practices, we are paving the way for a greener, more sustainable future where agriculture, industry, and the environment coexist harmoniously, leading to a cleaner and healthier environment for all.

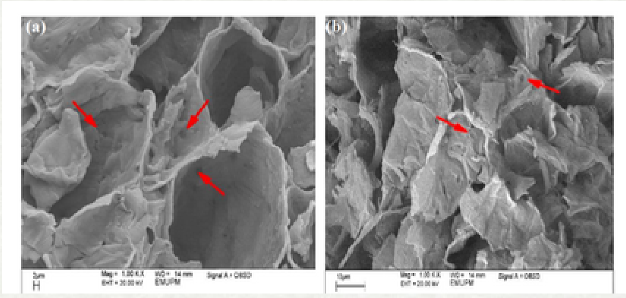

Figure 1: SEM micrographs of (a) Pineapple plant stem (PPS) (b) Oxalic acid modified PPS at 1,000X magnification

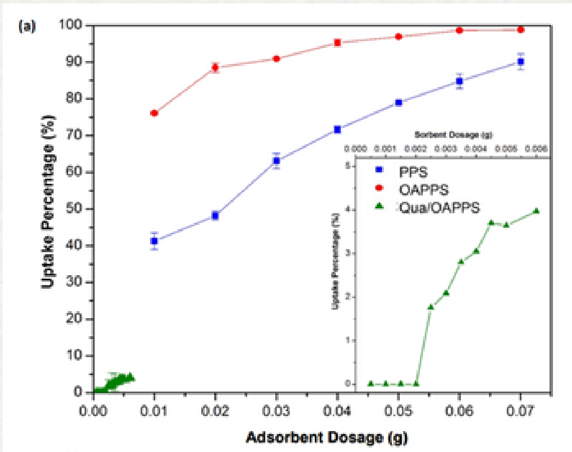

Figure 2: Effects of adsorbent dosage on the uptake percentage of Basic Blue 3 (BB3) in single dye solution using pineapple plant stem (PPS), oxalic acid modified PPS (OAPPS) and quaternized OAPPS (Qua/OAPPS)

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p-ADIC ORDERS OF ZEROS OF A POLYNOMIALS

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Let $f(x,y)$ be a polynomial in $Z_p[x,y]$ and p be a prime. For $\alpha > 1$, the exponential sums associated with f modulo a prime p^α is defined as $S(f;q) = \sum e^{\frac{2\pi i f(x)}{q}}$, where the sum is taken over a complete set of residues modulo p^α. It has been shown that the exponential sums are depends on the cardinality of the set of solutions to the congruence equation associated with the polynomial $f(x,y)$. The information of p-adic sizes of common zeros need to be obtained, in order to estimate the cardinality of the set $N(f_x, f_y; p^\alpha)$. p-adic methods and Newton polyhedron technique is used to estimate the p-adic sizes of common zeros of partial derivative polynomials by constructing and analyzing the indicator. The "p" in p-adic refers to a prime number. The notation of Z_p denote as the ring of p-adic integers, Ω_p is the completion of the algebraic closure of Q_p the field of rational p-adic numbers and $ord_p x$ as the highest power of p which divide x and the definition is as follow.

Definition 1
Let p be prime number. For any nonzero integer a, let the p-adic ordinal of a, denoted by $ord_p a$, be the highest power of p which divides a. If $a = 0$, we define $ord_p 0 = \infty$.
For examples, $ord_5 250 = ord_5(5^3 \cdot 2) = 3$ and $ord_7 90 = 0$.

Newton polyhedron is an analogue of the Newton polygon concept. It is two-variable polynomials case $f(x,y) = \sum_{i,j} a_{ij} x^i y^j$ in $\Omega_p[x,y]$. The relationship between the p-adic orders of zeros of a polynomial and Newton polyhedron are shown by using the following definitions and theorem.

Definition 2 (*Newton Polygon*): Let $f(x,y) = \sum a_{ij} x^i y^j$ be a polynomial of degree n in $\Omega_p[x,y]$. By mapping the terms $T_{ij} = a_{ij} x^i y^j$ of $f(x,y)$ to the points $P_{ij} = a_{ij} x^i y^j$ in the three-dimensional Euclidean space R^3. The set of points P_{ij} is defined as the Newton diagram of $f(x,y)$.

Definition 3 (*Newton Diagram*): Let $f(x,y) = \sum a_{ij} x^i y^j$ be a polynomial of degree n in $\Omega_p[x,y]$. By mapping the terms $T_{ij} = a_{ij} x^i y^j$ of $f(x,y)$ to the points $P_{ij} = a_{ij} x^i y^j$ in the three-dimensional Euclidean space R^3. The set of points P_{ij} is defined as the Newton diagram of $f(x,y)$.

Definition 4 (*Newton Polyhedron*): Let $f(x,y) = \sum a_{ij} x^i y^j$ be a polynomial of degree n in $\Omega_p[x,y]$. By mapping the terms $T_{ij} = a_{ij} x^i y^j$ of $f(x,y)$ to the points $P_{ij} = a_{ij} x^i y^j$ in the Euclidean space, the Newton polyhedron of $f(x,y)$ is defined to be the lower convex hull of the set S of points P_{ij}, $0 \le i,j \le n$. It is the highest convex connected surface which passes through or below the points in S. If $a_{ij} = 0$ for some (i,j) then $ord_p a_{ij} = \infty$.

Definition 5 (*Indicator Diagram*) : The set of lines associated with the Newton polyhedron, denoted by N_f. Let $(\mu_i, \lambda_i, 1)$ be the normalized upward-pointing normals to the faces F_i of N_f, of a polynomial $f(x,y)$ in $\Omega_p[x,y]$. The point $(\mu_i, \lambda_i, 1)$ is mapping to the point (μ_i, λ_i) in the $x - y$ plane. If F_r and F_s are adjacent faces in N_f, sharing a common edge, we construct the straight line joining (μ_r, λ_r) and (μ_s, λ_s). If F_r shares a common edge with a vertical face F say $\alpha x + \beta y = \gamma$ in N_f, we construct the straight line segment joining (μ_r, λ_r) and the appropriate point at infinity that corresponds to the normal F, that is the segment along a line with a slope $-\alpha/\beta$.

Theorem 1: Let p be a prime. Suppose f and g are polynomials in $\mathbb{Z}_p[x,y]$. Let (μ, λ) be a point of intersection of the indicator diagrams associated with f and g at the vertices or simple points of intersections. Then, there are ξ and η in Ω_p^2 satisfying $f(\xi,\eta) = g(\xi,\eta) = 0$ and $ord_p \xi = \mu_1, ord_p \eta = \mu_2$.

The construction of Newton Polyhedron is by using Definiton 2 to Definiton 4. The example of Newton polyhedron associated with $f(x,y) = 9x^2 - 3xy + 3y^2 - 18$, $p = 3$ as in Figure 1.

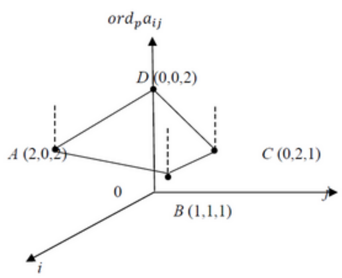

Figure 1: The Newton polyhedron of polynomial $f(x,y) = 9x^2 - 3xy + 3y^2 - 18$ with $p = 3$.

The construction of indicator diagram associated with $f(x,y) = 9x^2 - 3xy + 3y^2 - 18$, $p = 3$ as shown in Figures 2 is by using Definition 5 and Theorem 1.

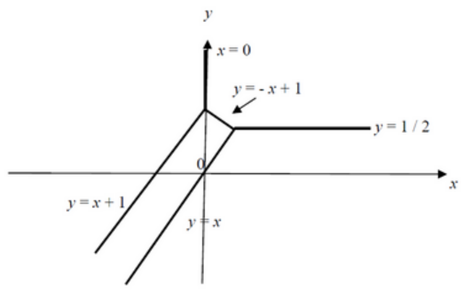

Figure 2. Indicator diagram associated with the Newton polyhedron of $f(x,y) = 9x^2 - 3xy + 3y^2 - 18$, $p = 3$.

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