Preprints.org

Communication

Not peer-reviewed version

On the Help of Mathematical-Analytical Modeling for Present and Future Advances in Current Engineering

Paolo Di Sia *

Posted Date: 28 August 2025

doi: 10.20944/preprints202508.2064.v1

Keywords: engineering; advances; nanotechnology; nano-bio-materials; devices performance; mathematical (analytical) modeling; DS model

Communication

On the Help of Mathematical-Analytical Modeling for Present and Future Advances in Current Engineering

Paolo Di Sia [1,2,3]

[1] School of Engineering & School of Medicine, University of Padova, 35131 Padova, Italy; paolo.disia@unipd.it or paolo.disia@univr.it or paolo.disia@gmail.com

[2] School of Medicine, Engineering for Innovation Medicine, University of Verona, 37134 Verona, Italy

[3] "Primordial Dynamic Space" Research, 37134 Verona, Italy

Abstract

The challenges that engineering has to face in the present and near future are increasingly linked to nano-bio-technologies, one of the most significant mainstreams of current research. Improvements in the enhancement of devices performance are a principal objective of pure and applied research. The devices sensitiveness, directly correlated to the diffusion process at the (micro-)nano-level, is a crucial characteristic for controlling a high increase in their quality. In this direction, mathematical modeling has always played a fundamental role at the experimental and theoretical level, not only by the numerical viewpoint, but also by the analytical one. Developments in this direction are desirable and will give fruitful results.

Keywords: engineering; advances; nanotechnology; nano-bio-materials; devices performance; mathematical (analytical) modeling; DS model

---

1. Introduction

In last years the ability to handle matter, combined with advances in structures synthesis and assembly at micro- and nano-scale, resulted in considerable goals in scientific and technological areas. In order to capitalize on nano-scale phenomena in devices, a better comprehension of the electronic, magnetic and photonic interactions at this size scale is required, across experiments, phenomenology, theory, and modeling [1,2].

The use of innovative methodologies, based on advanced bottom-up and top-down approaches, is allowing to design and synthesize new organic, organic/inorganic hybrid, and inorganic materials, aimed at a controlled assembly in active (micro-)nano-structured devices with applications in all technological sectors of benefit for human being [3].

Through the study and development of new technologies and methodologies, the functionalities of innovative devices can be explored for an ever-increasing range of applications. All fundamental studies are making possible the exploration of new techniques and methodologies in the most diverse engineering fields.

Present and future challenges concern in particular:

a) Civil engineering: solving complex problems typical of the construction of large infrastructures, in relation to the principles of structural modeling and the most advanced digital tools to support the engineer [4–6];

b) Energy engineering: the energy transition from fossil to synthetic fuels, renewable energy technologies, micro- and macro-conversion (energy harvesting and controlled nuclear fusion); these are scenarios that humanity is called to face in the transition towards a sustainable use of energy resources [7–9];

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 28 August 2025 doi:10.20944/preprints202508.2064.v1

c) Electronic and biomedical engineering: light technology for bio-medicine and human health, nano-devices between electronics and nano-technologies, the new frontiers of digital twin, "learning by doing", also through advanced software tools used for modeling and simulation, in parallel with the development of e-noses [10–22];

d) Computer engineering: questions of computer security, advances in programming for mobile devices, visual programming of applications for IoT. We also think about programming of applications for mobile devices, with particular attention to the aspects of creating the user interface [23–25];

e) The soil ecosystem: a network of relationships in the fabric of life. Soil is a very complex living system, extraordinarily rich in biodiversity, in which a wide range of biochemical and biophysical processes occur, including decomposition, a key process for the functioning of ecological systems, that transforms organic fractions into real nutrients for the living community. This leads to the need to monitor the health of the arboreal component of the ecological network, through the collection of parameters related to the physiology of plants, environmental conditions and the structural stability of plant elements inserted in the urban fabric [26–28].

2. Discussion

These challenges have a common denominator, i.e. nano-bio-technologies, which today allow the creation of miniaturized devices on a micro- and nanometric scale that, integrated with electronics, become intelligent nano-devices with multiple capabilities and surprising functionalities.

One of the most important aspects at the nano-scale affects the charge transport, which can be guided by particles dimensions and takes different features with respect to those of bulk. From a theoretical point of view, several techniques can be used for the knowledge of transport phenomena, both numerical and analytical ones, based on transport equations. The numerical approaches are important, but not able to provide an overall vision, instead typical of analytical approaches; these latter are of high mathematical interest and lead to newsworthy results and predictions, implemented via experimental literature data and obtained at any time by experiments [29].

The most used formulations are as follows:

A) The "Tight-Binding" Method (T-BM), semi-empirical method mainly preferred when the computational calculation is considerable [30];

B) The "ab-initio" formulations, that produce accurate results, although dependent by the initial choices;

B_1) The "Density Functional Theory" (DFT), that gives the total energy of the system through the functional of the electrons total density [31];

B_2) Local Density Functional Theory (LDFT).

Other approaches include:

C) Non-Local Functional Approach (N-LFA);

D) Car-Parrinello Molecular Dynamic Method (C-PMDM) [32];

E) Conjugate-Gradient Method (C-GM) [33];

F) Augmented Plane Wave Method (APWM) [34];

G) Korringa-Kohn-Rostoker Method (K-K-RM) [35];

H) Linearized-Muffin-Thin-Orbital Method (L-M-T-OM) [36];

I) Full Potential Linearized Augmented Plane Wave Method (FPLAPWM) [37];

J) "Drude-Lorentz-type" models: they are basically improvements of Drude model [38]. The "Smith model" contains a parameter c_n accounting for the scattering anisotropy upon the first scattering event [39]. In the "Effective Medium Theories" (EMTs) the electromagnetic interactions among pure materials and host matrixes are roughly taken into account. Among EMTs, we remember in particular the "Maxwell-Garnett model" (MG) and the "Bruggeman model" (BR) [40,41].

About new generalizations, the "DS model" fits significantly well with experimental data and provides also new predictions of several peculiarities at nano-level. It is structured on the analytical form of three most important functions describing the charge transport, namely the velocities

 doi:10.20944/preprints202508.2064.v1

correlation function $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_T$, the mean square deviation of position $R^2(t)$ and the diffusion coefficient $D(t)$. This approach embraces classical and quantum-relativistic aspects [42–45]; it studies the dynamics of transport from sub-pico- to macro-level, thanks to a gauge factor.

It is based on the total Fourier transform of the frequency-dependent complex-valued far-infrared photo-conductivity $\sigma(\omega)$, as deduced by the linear response theory, considering the Cauchy integration on the entire time axis (-∞, +∞), using the residue theorem in the plane of complex numbers.

3. Future Perspectives

Tuning on every physical-chemical, systemic and model-intrinsic parameter, namely the temperature *T*, values of relaxation times τ_i and frequencies ω_i , the carrier density *N*, the effective mass m^* , the chiral vector, the quantum weights of modes, the speed of carriers, we can conduct a fine tuning of $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_T$, $R^2(t)$ and $D(t)$, in order to gauge the work of nano-bio-devices, with "a-priori" and "a-posteriori" use of the model [46].

Drude-Lorentz-type models are very promising tools from every point of view, because they involve ("DS model" in particular) quantum and relativistic effects too. The totally analytical form of DS model looks very elegant; it is giving notable confirmations, and new knowledge on the dynamics at the nano-scale, properly tested with experimental time-resolved techniques, as TRTS, Photon-Induced Near-Field Electron Microscopy and Graphene based Plasmonics [47–60].

Author Contributions: Conceptualization, methodology, software, validation, formal analysis, investigation, resources, data curation, writing-original draft preparation, writing-review and editing, visualization, supervision, project administration, P.D.

Funding: This research received no funding.

Data Availability Statement: No new data were created.

Conflicts of Interest: The author declares no conflicts of interest.

References

1. Abraham, T.R., Ganesh, K.M., Bhaskar, S., Thomas, S. Chapter 19 - Nanoscale engineering for biomedical applications. Nano-Engineering at Functional Interfaces for Multi-Disciplinary Applications - Electrochemistry, Photoplasmonics, Antimicrobials, and Anticancer Applications - Micro and Nano Technologies, 473-489 (2025). https://doi.org/10.1016/B978-0-443-21691-6.00020-2 .
2. Ellis, G.F.R., Di Sia, P. Complexity Theory in Biology and Technology: Broken Symmetries and Emergence. Symmetry 15, 1945 (2023). https://doi.org/10.3390/sym15101945.
3. Bai, X., Zhang, X. Artificial Intelligence-Powered Materials Science. Nano-Micro Letters 17, 135 (2025). https://doi.org/10.1007/s40820-024-01634-8.
4. Chen, L., Chen, S. Civil Engineering Quality Monitoring System Based on Big Data. In: Al-Turjman, F. (eds). Smart Infrastructures in the IoT Era. Sustainable Civil Infrastructures. Springer, Cham (2025). https://doi.org/10.1007/978-3-031-72509-8_24.
5. Gao, Y., Qiu, Z., Zhao, J., He, H., Wang, B. A comprehensive review on the applications of carbon dots in civil engineering materials. Journal of Materials Science 60, 3227-3252 (2025). https://doi.org/10.1007/s10853-025-10656-5.
6. Ramesh, M., Selvan, M.T., Saravanakumar, A. 4 - Evolution and recent advancements of composite materials in structural applications. Applications of Composite Materials in Engineering - Woodhead Series in Materials, 97-117 (2025). https://doi.org/10.1016/B978-0-443-13989-5.00004-8.
7. Behera, U.S., Sangwai, J.S., Byun, H.-S. A comprehensive review on the recent advances in applications of nanofluids for effective utilization of renewable energy. Renewable and Sustainable Energy Reviews 207, 114901 (2025). https://doi.org/10.1016/j.rser.2024.114901.

8. Ock, I.W., Yin, J., Wang, S., Zhao, X., Baik, J.M., Chen, J. Advances in Blue Energy Fuels: Harvesting Energy from Ocean for Self-Powered Electrolysis. Advanced Energy Materials 15(2), 2400563 (2025). https://doi.org/10.1002/aenm.202400563.
9. Zhang, Q., Soham, D., Liang, Z., Wan, J. Advances in wearable energy storage and harvesting systems. Med-X 3, 3 (2025). https://doi.org/10.1007/s44258-024-00048-w.
10. Mamidi, N., Delgadillo, R.M.V., Sustaita, A.O., Lozano, K., Yallapu, M.M. Current nanocomposite advances for biomedical and environmental application diversity. Medicinal Research Reviews 45(2), 576-628 (2025). https://doi.org/10.1002/med.22082.
11. Ma, Y., Liang, Z., Chen, Y., Wang, J. Advances in precise cell manipulation. Droplet 4(1), e149 (2025). https://doi.org/10.1002/dro2.149.
12. Yang, Z., Song, H., Ding, H. Advancements in implantable temperature sensors: Materials, mechanisms, and biological applications. Journal of Semiconductors 46(1), 011609 (2025). 10.1088/1674-4926/24100003.
13. Ahmad, B., Shareef Masoud, M., Ali Ashfaq, U., Ansari, M.-ur-R., Nahid, N., Qasim, M. Chapter 13 - Smart E-noses for medical and clinical applications. Advanced Sensors for Smart Healthcare, 231-242 (2025). https://doi.org/10.1016/B978-0-443-24790-3.00014-4.
14. Zhang, J., Dai, Y., Hwan Lee, C. Chapter 30 - Healthcare with smart contact lenses: innovations, challenges, and future perspectives. Advanced Sensors for Smart Healthcare, 521-545 (2025). https://doi.org/10.1016/B978-0-443-24790-3.00031-4.
15. Wang, Z., Zhang, L., Li, Z., Duan S., Yan, J. Improving E-Nose Performance: A Novel ELM-Based Dual-Level Joint Domain Adaptation Method for Sensor Drift Data. IEEE Transactions on Instrumentation and Measurement 74, 1-11 (2025). 10.1109/TIM.2025.3540144.
16. Gil, M., Rudy, M., Duma-Kocan, P., Stanisławczyk, R. Electronic Sensing Technologies in Food Quality Assessment: A Comprehensive Literature Review. Applied Sciences 15(3), 1530 (2025). https://doi.org/10.3390/app15031530.
17. Yadav, S., Singh, A., Kumar, N. Electronic panel for sensory assessment of food: A review on technologies integration and their benefits. Journal of Food Science 90(3), e70128 (2025). https://doi.org/10.1111/1750-3841.70128.
18. Glöckler, J., Mitrovics, J., Beeken, S., Leja, M., Welearegay, T., Österlund, L., Haick, H., Shani, G., Di Natale, C., Murillo, R., Flores-Rangel, G., Bricio-Arzubide, F., Pinilla, R., Vargas, R., Saboya, C., Mizaikoff, B., Díaz de León-Martínez, L. Infrared Spectroscopic Electronic Noses: An Innovative Approach for Exhaled Breath Sensing. ACS Sensors 10(1), 427-438 (2025). https://doi.org/10.1021/acssensors.4c02725.
19. Chen, C.-D., Zheng, Y.-X., Lin, H.-F., Yang, H.-Y. Development of Electronic Nose as a Complementary Screening Tool for Breath Testing in Colorectal Cancer. Biosensors 15(2), 82 (2025). https://doi.org/10.3390/bios15020082.
20. Qu, C., Zhang, Z., Liu, J., Zhao, P., Jing, B., Li, W., Wu, C., Liu, J. Multi-scenario adaptive electronic nose for the detection of environmental odor pollutants. Journal of Hazardous Materials 489, 137660 (2025). https://doi.org/10.1016/j.jhazmat.2025.137660.
21. Heng, Y., Zhou, Y., Nguyen, D.H., Nguyen, V.D., Jiao, M. An electronic nose drift compensation algorithm based on semi-supervised adversarial domain adaptive convolutional neural network. Sensors and Actuators B: Chemical 422, 136642 (2025). https://doi.org/10.1016/j.snb.2024.136642.
22. van der Aart, T.J., Visser, M., van Londen, M., van de Wetering, K.M.H., Ter Maaten, J.C., Bouma, H.R. The smell of sepsis: Electronic nose measurements improve early recognition of sepsis in the ED. The American Journal of Emergency Medicine 88, 126-133 (2025). https://doi.org/10.1016/j.ajem.2024.11.045.
23. Alzubi, T.M., Alzubi, J.A., Singh, A., Alzubi, O.A., Subramanian, M. A Multimodal Human-Computer Interaction for Smart Learning System. International Journal of Human-Computer Interaction 41(3), 1718-1728 (2023). https://doi.org/10.1080/10447318.2023.2206758.
24. Shahin, M., Frank Chen, F., Hosseinzadeh, A., Bouzary, H., Shahin, A. Robotics multi-modal recognition system via computer-based vision. The International Journal of Advanced Manufacturing Technology 136, 3989-4005 (2025). https://doi.org/10.1007/s00170-024-13164-z.
25. Khumsikiew, J., Netthong, R., Yingngam, B. Chapter 5 - Research advancements in quantum computing and digital twins, 103-125 (2025). https://doi.org/10.1016/B978-0-443-28884-5.00005-1.

 doi:10.20944/preprints202508.2064.v1

26. Sharma, U.C., Datta, M., Sharma, V. Recent Advances and Future Challenges. In: Soil Acidity. Progress in Soil Science. Springer, Cham, 523-580 (2025). https://doi.org/10.1007/978-3-031-76357-1_6.
27. Tripathi, M., Singh, P., Pathak, S., Manimekalai, R., Garg, D., Dashora, K. Strategies for the Remediation of Micro- and Nanoplastics from Contaminated Food and Water: Advancements and Challenges. Journal of Xenobiotics 15(1), 30 (2025). https://doi.org/10.3390/jox15010030.
28. Nene, A., Sadeghzade, S., Viaroli, S., Yang, W., Uchenna, U.P., Kandwal, A., Liu, X., Somani, P., Galluzzi, M. Recent advances and future technologies in nano-microplastics detection. Environmental Sciences Europe 37, 7 (2025). https://doi.org/10.1186/s12302-024-01044-y.
29. Di Sia, P. Present and Future of Nanotechnologies: Peculiarities, Phenomenology, Theoretical Modelling, Perspectives. Reviews in Theoretical Science 2(2), 146-180 (2014). https://doi.org/10.1166/rits.2014.1019.
30. Holman, J., Parsons, A., Pilling, G., Price, G. Chemistry^3: Introducing Inorganic, Organic and Physical Chemistry. Oxford University Press, Oxford (2013).
31. Engel, E., Dreizler, R.M. Density Functional Theory: An Advanced Course. Springer, New York (2011).
32. Car, R., Parrinello, M. Unified Approach for Molecular Dynamics and Density-Functional Theory. Physical Review Letters 55(22), 2471 (1985). https://doi.org/10.1103/PhysRevLett.55.2471.
33. Avriel, M. Nonlinear Programming: Analysis and Methods. Courier Dover Publications, New York (2003).
34. Thijssen, J. Computational Physics. Cambridge University Press, Cambridge (2007).
35. Mizutani, U. Introduction to the Electron Theory of Metals. Cambridge University Press, Cambridge (2001).
36. Bland, J.A.C., Bretislav, H. Ultrathin Magnetic Structures I: An Introduction to the Electronic, Magnetic and Structural Properties. Springer, New York (2005).
37. Wandelt, K. Surface and Interface Science. John Wiley & Sons, Hoboken, Vols 1-2 (2012).
38. Drude, P. Zur Elektronentheorie der metalle. Annalen der Physik 306(3), 566 (1900). https://doi.org/10.1002/andp.19003060312.
39. Smith, N.V. Classical generalization of the Drude formula for the optical conductivity. Physical Review B 64, 155106 (2001). https://doi.org/10.1103/PhysRevB.64.155106.
40. Choy, T.C. Effective Medium Theory: Principles and Applications. Oxford University Press, Oxford (1999).
41. Kuzyk, M.G. Polymer Fiber Optics: Materials, Physics, and Applications. CRC Press, Boca Raton (2010).
42. Di Sia, P. Overview of Drude-Lorentz type models and their applications. Nanoscale Systems: Mathematical Modeling, Theory and Applications 3, 1-13 (2014). https://eudml.org/doc/267041.
43. Di Sia, P. Quantum-Relativistic Velocities in Nano-Transport. Applied Surface Science 446, 187-190 (2018). https://doi.org/10.1016/j.apsusc.2018.01.273.
44. Di Sia, P. Symmetry and the Nanoscale: Advances in Analytical Modeling in the Perspective of Holistic Unification. Symmetry 15(8), 1611 (2023). https://doi.org/10.3390/sym15081611.
45. Di Sia, P. Quantum-Relativistic Diffusion in Nano-Transport. Preprints 2024, 2024100982. https://doi.org/10.20944/preprints202410.0982.v1.
46. Di Sia, P. About the Influence of Temperature in Single-Walled Carbon Nanotubes: Details from a new Drude-Lorentz-like Model. Applied Surface Science 275, 384-388 (2013). https://doi.org/10.1016/j.apsusc.2012.10.132 .
47. Park, S.T., Lin, M., Zewail, A.H. Photon-induced near-field electron microscopy (PINEM): theoretical and experimental. New Journal of Physics 12, 123028 (2010). 10.1088/1367-2630/12/12/123028.
48. Park, S.T., Zewail, A.H. Relativistic Effects in Photon-Induced Near Field Electron Microscopy. The Journal of Physical Chemistry A 116(46), 11128-11133 (2012). 10.1021/jp304534n.
49. Th Hassan, M. Attomicroscopy: from femtosecond to attosecond electron microscopy. Journal of Physics B: Atomic, Molecular and Optical Physics 51, 032005 (2018). 10.1088/1361-6455/aaa183.
50. Grigorenko, A.N., Polini, M., Novoselov, K.S. Graphene plasmonics. Nature Photonics 6, 749-758 (2012). 10.1038/nphoton.2012.262.
51. Koppens, F.H.L., Chang, D.E., García de Abajo, F.J. Graphene Plasmonics: A Platform for Strong Light-Matter Interactions. Nano Letters 11(8), 3370-3377 (2011). 10.1021/nl201771h.
52. Huang, S., Song, C., Zhang, G., Yan, H. Graphene plasmonics: Physics and potential applications. Nanophotonics-Berlin 6(6), 1191-1204 (2017). 10.1515/nanoph-2016-0126.

53. Kuzmin, D.A., Bychkov, I.V., Shavrov, V.G., Temnov, V.V. Plasmonics of magnetic and topological graphene-based nanostructures. arXiv:1711.10777v1 [cond-mat.mes-hall] (2017).
54. Kovalev, S., Green, B., Golz, T., Maehrlein, S., Stojanovic, N., Fisher, A.S., Kampfrath, T., Gensch, M. Probing ultra-fast processes with high dynamic range at 4th-generation light sources: Arrival time and intensity binning at unprecedented repetition rates. Structural Dynamics-US 4, 024301-(1-7) (2017). https://doi.org/10.1063/1.4978042.
55. Bennett, K., Rouxel, J.R., Mukamel, S. Linear and nonlinear frequency- and time-domain spectroscopy with multiple frequency combs. The Journal of Chemical Physics 147, 094304 (2017). https://doi.org/10.1063/1.5000375.
56. Hafez, H.A., Chai, X., Sekine, Y., Takamura, M., Oguri, K., Al-Naib, I., Dignam, M.M., Hibino, H., Ozaki, T. Effects of environmental conditions on the ultrafast carrier dynamics in graphene revealed by terahertz spectroscopy. Physical Review B 95, 165428 (2017). https://doi.org/10.1103/PhysRevB.95.165428.
57. Mitra, S., Avazpour, L., Knezevic, I. Terahertz conductivity of two-dimensional materials: a review. Journal of Physics: Condensed Matter 37(13), 133005 (2025). 10.1088/1361-648X/adab6a.
58. Ji, S., Guo, J., Li, Z., Tong, L., Guo, J., Liu, J., Deng, Y., Liu, C., Sun, Z., Chen, X., Gao, C., Liu, F., Feng, M., Fu, X. Development of a femtosecond analytical electron microscopy based on a Schottky field emission transmission electron microscope. Review of Scientific Instruments 96, 033701 (2025). https://doi.org/10.1063/5.0226913.
59. Ruimy, R., Karnieli, A., Kaminer, I. Free-electron quantum optics. Nature Physics 21, 193-200 (2025). https://doi.org/10.1038/s41567-024-02743-2.
60. Fuad, M.H., Nayan, M.F., Mahmud, R.R. Advances in Surface Plasmon Resonance-Based PCF and MIM Sensors. Plasmonics (2025). https://doi.org/10.1007/s11468-025-02796-w.