Mackey-Glass Time Series Forecasting by Nanowire Networks

Mackey-Glass Time Series Forecasting by Nanowire Networks

Gianluca Milano: Advanced Materials Metrology and Life Sciences Division, INRiM (Istituto Nazionale di Ricerca Metrologica), Torino, Italy

Tushar Chakrabarty: Department of Applied Science and technology, Politecnico di Torino, Torino, Italy

Carlo Ricciardi: Department of Applied Science and technology, Politecnico di Torino, Torino, Italy

Abstract:

Physical reservoir computing is a brain-inspired computational framework that allows information processing by exploiting the complex dynamics of high-dimensional physical systems. In this context, self-organizing memristive systems composed of interacting nano-objects have been proposed as multipurpose platforms for the hardware implementation of reservoir computing (RC). Here, we report on Mackey-Glass time series prediction with memristive nanowire (NW) networks. Besides showing that emergent memristive dynamics of these networks modeled through a graph theoretical approach can be exploited for time series prediction, it is shown that the accuracy of the system can be tailored through appropriate configuration of the multiterminal NW network. Results show that NW networks can be exploited for in materia implementation of reservoir computing paradigm towards the realization of brain-inspired neuromorphic systems based on low-cost self-organizing nanomaterials.

Keywords—physical reservoir, reservoir computing, timeseries prediction, Mackey-Glass time series, nanowire networks

Introduction

In the era of Big Data and machine learning, the ever-growing demand of computing power is hampered by current computing technologies. In this scenario, neuromorphic computing architectures inspired by biological concepts associated to the human brain have been proposed as energy-efficient alternatives to conventional computing architectures. [1], [2]. Indeed, neuromorphic architectures could enable to overcome the von Neumann bottleneck, i.e., the continuous and intensive exchange of data in between memory and processing units that is responsible for a large part of the power consumption.

While neuromorphic chips were originally associated to analogue silicon technology [3], current neuromorphic computing devices are exploring a wide range of emerging materials and concepts [1]. Among such new technologies, memristive devices are emerging as ideal candidates for biologically inspired neuromorphic architectures and in-memory computing systems. These are two terminal devices where the internal resistance state can be analogically tuned depending on the history of input voltage and current [4]. Similarly to any

biological system but differently from common solid state electronic devices, the dynamics of such memristive states is ruled by ionic transport, while electronic motion typically plays a minor role. By coupling ionics with electronics, these devices have been demonstrated to be able to emulate a wide range of functionalities typical of biological neurons and synapses [5], [6]. For this reason, large arrays of memristive devices organized in the so-called crossbar architecture have been exploited for hardware implementation of brain-inspired computing [7].

As an alternative to memristive crossbar architectures, self-assembled memristive nanonetworks have been demonstrated for *in materia* implementation of neuromorphic type of data processing [8]–[17]. Differently from crossbar architectures where a fine tuning of each single element composing the network is required, functionalities of self-assembled systems rely on the collective emergent behavior due to the non-linear interaction of a huge number of nano objects [18]. In this context, nanowire (NW) networks have been demonstrated to possess typical brain-like functionalities like homo- and heterosynaptic plasticity [8].

On the other hand, progresses in neuromorphic hardware have been accompanied by the development of new computational models and computing paradigms inspired by biological neural networks. Derived from recurrent neural network models such as echo state networks (ESNs) [19] and liquid state machines (LSMs) [20], reservoir computing (RC) has recently attracted a growing attention as a bio- inspired unconventional computing paradigm able to perform temporal/sequential information processing with fast learning and reduced training cost. At the same time, RC is more and more employed as hardware implementation in a wide range of physical systems and devices [21], [22]. Thanks to their non-linear complex emergent dynamics, self-assembled memristive networks have been proved as ideal platforms for such so-called “physical” reservoir computing [23]–[27].

Here, we report on the simulation of physical reservoir computing in memristive NW networks for Mackey-Glass time series forecasting. The simulation framework is composed as follows: the NW network topology is modelled through graph theory, while the memristive interaction in between nano objects is analytically defined through a potentiation-depression rate balance equation deduced from physical arguments. In this framework, the emergent spatio-temporal memristive dynamics of NW network is revealed and exploited for the realization of a “physical reservoir” for *in-materia* implementation of time-dependent computing tasks. In particular, the influence of the multiterminal NW network configuration on computing performances has been analyzed by implementing Mackey-Glass time series forecasting. Results show that memristive NW networks represent suitable substrates for *in-materia* implementation of reservoir computing, towards the realization of neuromorphic computing base on self-assembled systems.

Results and Discussion

A. Physical Reservoir Computing

A schematization of the physical RC concept is reported in Figure 1. Here, a physical system or device acts as a "reservoir" able to nonlinearly project an input signal *u(t)* into a feature space *x(t)* that represents the reservoir internal state. After this nonlinear transformation enabled by internal complex dynamics of the physical system/device, features can be analyzed by a readout algorithm, where output weights *Wout* are the only weights to be trained by comparing the output *y^(t)* with the desired output. Since training occurs only at the readout and the training phase is typically the most expensive in terms of runtime and power consumption, this computing paradigm is usually associated to low -cost training and fast learning [21], [22].

B. Memristive Nw Networks as Physical Reservoirs

NW networks are complex systems of highly interconnected NW s, characterized by macroscale electronic paths supported by the high number of memristive NW junctions [28], [29]. Under electrical stimulations, emerging spatiotemporal memristive dynamics of NW networks in multiterminal configuration has been demonstrated to be exploitable for the realization of a physical reservoir able to process multiple input signals [23], [24]. The emergent behavior of these networks can be modeled by means of a graph-theoretical approach [13], [30]. For this purpose, the process of NW network self-assembly can be mimicked by randomly dispersing 1D objects on a 2D surface [13], [31]. According to experimental results obtained with Ag NW networks, where the morphology was assessed by SEM imaging [13], the length of simulated NWs was chosen from a normal distribution with mean value of *40μm* and a standard deviation of *14μm*. These NWs were randomly dispersed on a $170\times170\mu m^2$ plane, as reported in Figure 2a. Here, red dots correspond to the geometric NW center, while blue dots represent a junction formed at the interconnection among NWs. The obtained network can be then mathematically represented as a graph *G=(V,E)* where *V* and *E* are the set of nodes and edges, respectively. In this framework, each NW is mapped as a node, while each junction is mapped as an edge. Figure 2b reports the graph representation of the NW network topology simulated in Figure 2a.

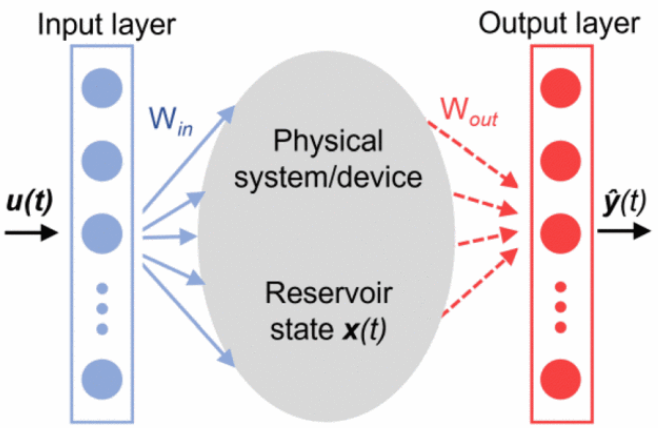

Fig. 1.
Conceptual schematization of the physical RC paradigm where a physical system/device acting as a reservoir projects an input signal *u(t)* into a feature space *x(t)* that is then analysed through a readout function to give the predicted output *y^(t)* after training of readout weights *Wout*.

The dynamics of the system is provided by the memristive interaction between NWs (nodes) responsible for a reconfiguration of the network under external electrical stimulation. In this context, the graph representation of the NW network can be represented as an electrical circuit where edges are represented by memristive elements, as schematically represented in Figure 2c.

More in particular, the NW network can be mathematically represented as a *memristive graph* where the conductivity of edges evolves over time depending on the spatial location and temporal sequence of external electrical stimulation [32]. Memristive dynamics of memristive edges have been modeled with one equation for memory state and one for electron transport, as detailed in ref. [33].

The memory state *gij* of the edge connecting nodes *i* and *j* is represented by the normalized edge conductance and is described by means of a physics-based potentiation-depression rate balance equation that models short-term memory effects:

$$\frac{dg_{ij}}{ar} = k_{P,ij}(1 - g_{ij}) + k_{D,ij}g_{ij} \qquad (1)$$

where *κP,ij* and *κD,ij* are the potentiation and depression coefficients, respectively, of the edge *ij*. These coefficients are defined as a function of the applied voltage through the relationships:

$$\kappa_{P,ij}(V_{ij}) = \kappa_{P0}exp(+\eta_P V_{ij}) \qquad (2)$$
$$\kappa_{D,ij}(V_{ij}) = \kappa_{D0}exp(-\eta_D V_{ij}) \qquad (3)$$

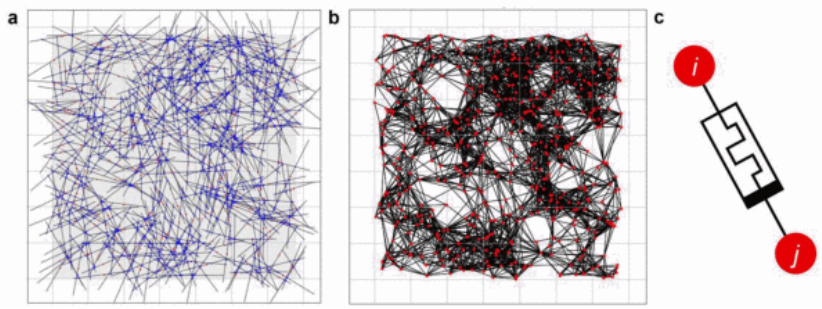

Fig. 2.
Memristive NW network as a memristive graph. (a) NW network topology simulated by dispersing 1D objects on a 2D plane. 500 NWs with an average length of *40 μm* (standard deviation of *14 μm*) are randomly dispersed on a *170×170μm²* plane. Red dots represent the NW geometrical center while blue dot represent NW junctions (b) Graph representation of the NW network reported in panel a where each NW is represented as a node while NW junctions are represented by edges. (c) Conceptual schematization of the memrsitive edge interaction in between NW nodes.

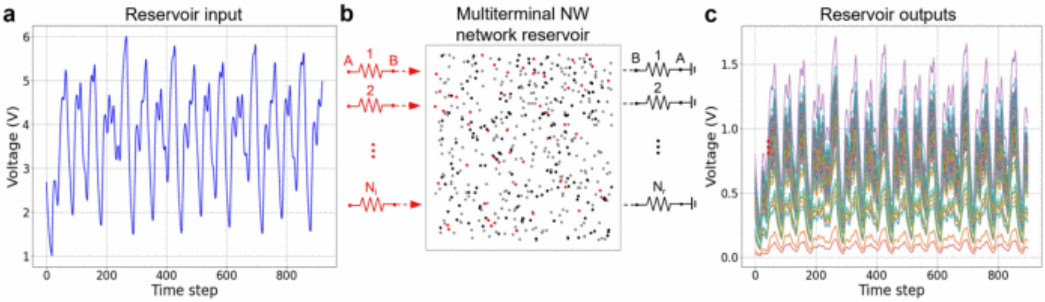

Fig. 3.
NW network as a multiterminal memristive reservoir. (a) Mackey-Glass input voltage signal obtained by transforming and normalizing the time series signal in the range 1–6 V. (b) NW network reservoir where the Mackey-Glass input voltage signal is applied at terminals A of resistances ($R=82\ \Omega$) connected at terminals B to multiple input nodes N_i (red nodes). Reservoir outputs are collected at terminals B of resistances ($R=82\ \Omega$) connecting reading nodes N_r (black nodes) and ground. Hidden nodes of the NW network are represented in grey. The schematization refers to a NW network with 500 NWs, N_i=50 and N_r=150(c) Reservoir output voltage signals.

Where $\kappa P0$ and $\kappa D0>0$ are constants, $\eta P,\eta D>0$ are the transition rates while V_{ij} is the voltage across the junction. The rate balance equation with this exponential voltage dependance typical of ionic transport can be analytically solved through a recursive method, as detailed in ref. [33]. Electronic transport can be modeled through the equation:

$$I(t) = [G_{min}(1 - g(t)) + G_{max}(g(t))]V(t) \tag{4}$$

where G_{min} and G_{max} are the minimum and maximum of conductance of each edge, respectively. Model parameters were extracted from experimental data [23]. Modified voltage analysis was exploited to calculate voltages at each network node and current flowing in network edges at each timestep. In agreement with experimental results, this modeling approach allows to simulate the emergent short-term dynamics of memristive NW networks, as detailed in ref. [13].

C. Mackey-Glass Time Series Forecasting

The time series prediction task was implemented by considering the Mackey-Glass time-delayed differential equation:

$$\frac{dx}{dt} = \beta \frac{x(t-\tau)}{1 + (x(t-\tau))^n} - \gamma x(t) \tag{5}$$

with parameters β=0.2, γ=0.9, n=10 and τ=18 corresponding to chaotic dynamics. In this case, the equation represents a chaotic system that has a deterministic form but is difficult to predict with standard machine-learning techniques [34]. In a preprocessing step, the time series was normalized and transformed to an input voltage signal in the range

1 −6V (Figure 3a). As schematized in Figure 3b, the time-dependent input signal is applied to a set of input network nodes (N_i) through series resistances R (terminals A), while the reservoir output is represented by voltages measured on resistances R (terminals B) connecting a set of reading nodes (N_r). A resistance value of 82 Ω was considered for simulations. A detailed description of the RC implementation strategy can be found in ref. [24]. Figure 3c reports temporal evolution of reading node voltages representing nonlinear transformations of the input signal. These multiple outputs are then passed to the readout that perform autonomous forecasting by exploiting the virtual node method for delayed feedback systems [35].

Initially, a teacher signal was applied to the set of input nodes Ni while output dynamics was exploited to train the readout. Training of the readout was performed by linear regression. Figure 4a reports the target and the predicted signal by considering a network with 500 NW, N_i=50, N_r=150 and a set of 20 virtual nodes. As can be observed, the target and predicted values well matches with an accuracy of ≈95%, revealing that the trained readout can forecast the next time step signal based on reservoir outputs. Note that the accuracy was evaluated as 1- RMSE, where RMSE is the root mean square error. After training, autonomous and continuous prediction can be performed by feeding a new input to the reservoir in a closed feedback loop. Because of the chaotic time series dependence on the initial conditions, an initialization step was needed: a true input (without training) was sent to excite the network from its pristine state. After that, the readout output is sent as reservoir input in a closed feedback loop to perform autonomous forecasting, as reported in Figure 4b. As shown, an accuracy of 88 % over 100 time steps is achieved during the autonomous forecasting with the expected ground truth plotted as a reference. As prediction goes forward, accumulation of small errors in the forecasting results in phase shifts with consequent deviations from the ground truth, even if main features of the Mackey-Glass time series are maintained in the output signal. However, the unavoidable divergence from the ground truth with time can be mitigated by periodically updating the reservoir with the truth signal, allowing to achieve long-term time series forecasting [23].

To better elucidate the computing capabilities of the system as a function of the number of reservoir outputs, the system accuracy evaluated by considering 100 time steps of time series prediction is reported in Figure 5 for different values of N_r/N ‘ Here, a multiterminal NW network with 500 NW, a set of input nodes N_i=50 and a set of 20 virtual nodes have been considered, where box plots have been realized by considering results obtained on 10 different NW topologies realized by dispersing NWs with a different random seed.

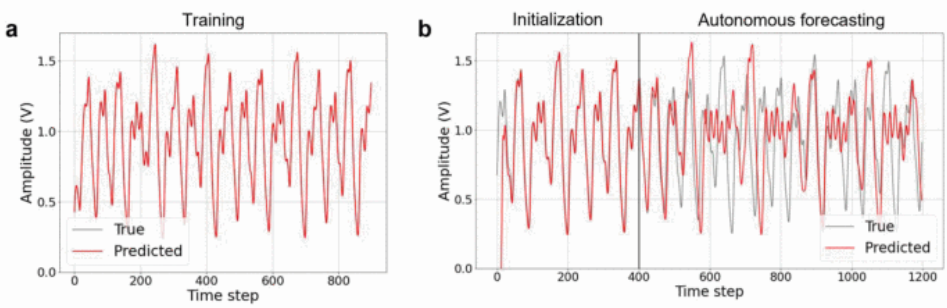

Fig. 4.
Mackey-Glass time series prediction with a NW network physical reservoir. (a) Training and (b) autonomous forecasting of the Mackey-Glass time series. Results have been obtained by considering a NW network with 500 NWS, N_i=50, N_r=150, and 20 virtual nodes.

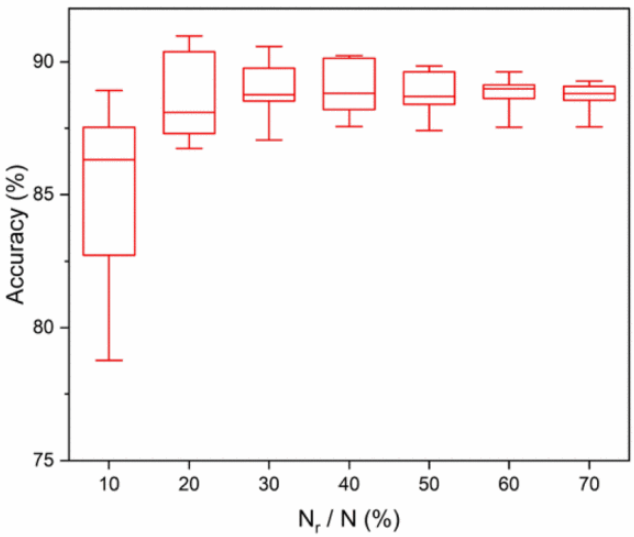

Fig. 5.
Accuracy of the system for Mackey-Glass time series prediction as a function the the percentage of reading nodes N_r. The accuracy was evaluated by considering 100 timesteps of autonomous time series prediction after training of the readout *mathrmin* a NW network with 500 NWs, by fixing N_i=50 and by considering 20 virtual nodes. Box plots were obtained by considering 10 different NW topologies, where midline represent median value, boxes the 25th and 75th percentiles and whiskers the 10th and 90th percentiles.

As can be observed, the median accuracy of the system tends to increase by increasing the percentage of reading nodes up to about 30 %, while saturation of median accuracy can be observed by further increasing the reading node percentage. Notably, a larger distribution of accuracy values can be observed for lower values of N_r/N suggesting that the peculiar network topology in this case plays a more relevant role in determining the network accuracy. In this context, it is worth noticing that an appropriate tailoring of the network topology allows to achieve even larger values of accuracies for lower values of N_r/N. For example, results shows that a peculiar network topology can achieve an accuracy of 91% in case of N_r/N =20, even if the median value of accuracies over different network topologies is in this case lower than median values obtained with higher N_r/N percentages. In this context, it is worth mentioning that the model does not considers *i*) junction-to-junction variability of the memrsitive response experimentally reported by considering single NW junction devices [8] and the possible presence of inhomogeneous areas over the network experimentally discussed through electrical resistance tomography [28], [29]. Despite the effect of these unavoidable non-idealities will require further investigation, it is worth mentioning that variabilities that can led to different nonlinear responses of different network areas can be even beneficial for the extraction of relevant features of the input signal [36]. In this context, further work will be necessary to elucidate the relationship in between peculiar network topologies and computing capabilities.

Conclusions

In conclusion, we reported on the implementation of physical reservoir computing in NW networks through simulations based on a graph theoretical approach. Results show that the NW network in multiterminal configuration acts as a physical reservoir able to map the input time series signal in a high dimensional feature space that, after readout training, can be exploited for autonomous time series prediction. Besides showing that the accuracy of the

system can be tailored by appropriate selection of reservoir reading nodes, results suggest that computing capabilities rely also on the network topology. More generally, simulations reveal that randomly dispersed NW networks can be exploited for the realization of neuromorphic systems capable of performing computing tasks involving time series forecasting.

Acknowledgment

This work was supported by the European project MEMQuD, code 20FUN06. This project (EMPIR 20FUN06 MEMQuD) has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.

References

1. D. V. Christensen et al., "2022 roadmap on neuromorphic computing and engineering", *Neuromorphic Computing and Engineering*, vol. 2, no. 1, pp. 0-31, Jan. 2022.

2. K. Berggren et al., "Roadmap on emerging hardware and technology for machine learning", *Nanotechnology*, vol. 32, no. 1, pp. 012002, Jan. 2021.

3. C. Mead, "Neuromorphic electronic systems", *Proceedings of the IEEE*, vol. 78, no. 10, pp. 1629-1636, 1990.

4. Z. Wang et al., "Resistive switching materials for information processing", *Nat Rev Mater*, vol. 5, no. 1, pp. 173-195, Mar. 2020.

5. J. Tang et al., "Bridging Biological and Artificial Neural Networks with Emerging Neuromorphic Devices: Fundamentals Progress and Challenges", *Advanced Materials*, vol. 31, no. 49, pp. 1902761, Dec. 2019.

6. G. Milano et al., "Self-limited single nanowire systems combining all-in-one memristive and neuromorphic functionalities", *Nat Commun*, vol. 9, no. 1, pp. 5151, Dec. 2018.

7. Q. Xia and J. J. Yang, "Memristive crossbar arrays for brain-inspired computing", *Nat Mater*, vol. 18, no. 4, pp. 309-323, Apr. 2019.

8. G. Milano et al., "Brain-Inspired Structural Plasticity through Reweighting and Rewiring in Multi- Terminal Self-Organizing Memristive Nanowire Networks", *Advanced Intelligent Systems*, vol. 2, no. 8, pp. 2000096, Aug. 2020.

9. Z. Kuncic and T. Nakayama, "Neuromorphic nanowire networks: principles progress and future prospects for neuro- inspired information processing", *Adv Phys X*, vol. 6, no. 1, Jan. 2021.

10. H. G. Manning et al., "Emergence of winner- takes-all connectivity paths in random nanowire networks", *Nat Commun*, vol. 9, no. 1, pp. 3219, Dec. 2018.

11. A. Diaz-Alvarez et al., "Emergent dynamics of neuromorphic nanowire networks", *Sci Rep*, vol. 9, no. 1, pp. 14920, Dec. 2019.

12. G. Milano, S. Porro, I. Valov and C. Ricciardi, "Recent Developments and Perspectives for Memristive Devices Based on Metal Oxide Nanowires", *Adv Electron Mater*, vol. 5, no. 9, pp. 1800909, Sep. 2019.

13. G. Milano, E. Miranda and C. Ricciardi, "Connectome of memristive nanowire networks through graph theory", *Neural Networks*, vol. 150, pp. 137-148, 2022.

14. J. B. Mallinson, S. Shirai, S. K. Acharya, S. K. Bose, E. Galli and S. A. Brown, "Avalanches and criticality in self-organized nanoscale networks", *Sci Adv*, vol. 5, no. 11, pp. eaaw8438, Nov. 2019.

15. A. Loeffler et al., "Neuromorphic learning working memory and metaplasticity in nanowire networks", *Sci Adv*, vol. 9, no. 16, 2023.

16. A. Z. Stieg, A. V. Avizienis, H. O. Sillin, C. Martin-Olmos, M. Aono and J. K. Gimzewski, "Emergent Criticality in Complex Turing B- Type Atomic Switch Networks", *Advanced Materials*, vol. 24, no. 2, pp. 286-293, Jan. 2012.

17. G. Milano and C. Ricciardi, "Nanowire memristor as artificial synapse in random networks" in Intelligent Nanotechnology, Elsevier, pp. 219-246, 2023.

18. M. Aono and K. Ariga, "The Way to Nanoarchitectonics and the Way of Nanoarchitectonics", *Advanced Materials*, vol. 28, no. 6, pp. 989-992, Feb. 2016.

19. H. Jaeger, *The "echo state" approach to analysing and training recurrent neural networks*, Dec. 2001, [online] Available: https://linkinghub.elsevier.com/retrieve/pii/S1471595301900356.

20. W. Maass, T. Natschläger and H. Markram, "Real-Time Computing Without Stable States: A New Framework for Neural Computation Based on Perturbations", *Neural Comput*, vol. 14, no. 11, pp. 2531-2560, Nov. 2002.

21. G. Tanaka et al., "Recent advances in physical reservoir computing: A review", *Neural Networks*, vol. 115, pp. 100-123, Jul. 2019.

22. K. Nakajima, "Physical reservoir computing-an introductory perspective", *Jpn J Appl Phys*, vol. 59, no. 6, pp. 060501, Jun. 2020.

23. G. Milano et al., "In materia reservoir computing with a fully memristive architecture based on self-organizing nanowire networks", *Nat Mater*, vol. 21, no. 2, pp. 195-202, Feb. 2022.

24. G. Milano, K. Montano and C. Ricciardi, "In materia implementation strategies of physical reservoir computing with memristive nanonetworks", *J Phys D Appl Phys*, vol. 56, no. 8, pp. 084005, Feb. 2023.

25. S. Lilak et al., "Spoken Digit Classification by In-Materio Reservoir Computing With Neuromorphic Atomic Switch Networks" in Frontiers in Nanotechnology, vol. 3, pp. 1-11, May 2021.

26. G. Milano, M. Agliuzza, N. de Leo and C. Ricciardi, "Speech recognition through physical reservoir computing with neuromorphic nanowire networks", *2022 International Joint Conference on Neural Networks (IJCNN) IEEE*, pp. 1-6, Jul. 2022.

27. H. O. Sillin et al., "A theoretical and experimental study of neuromorphic atomic switch networks for reservoir computing", *Nanotechnology*, vol. 24, no. 38, Sep. 2013.

28. G. Milano et al., "Mapping Time-Dependent Conductivity of Metallic Nanowire Networks by Electrical Resistance Tomography toward Transparent Conductive Materials", *ACS Appl Nano Mater*, pp. acsanm.0c02204, Oct. 2020.

29. A. Cultrera, G. Milano, N. De Leo, C. Ricciardi, L. Boarino and L. Callegaro, "Recommended implementation of electrical resistance tomography Nanowire-Based Memristors Using a Potentiation-Depression Rate Balance Equation", *IEEE Trans Nanotechnol*, vol. 19, pp. 609-612, 2020.

30. K. Montano, G. Milano and C. Ricciardi, "Grid-graph modeling of emergent neuromorphic dynamics and heterosynaptic plasticity in memristive nanonetworks", *Neuromorphic Computing and Engineering*, pp. 0-22, Jan. 2022.