**CUED - Engineering Tripos Part IIB 2024-2025** **Module Coursework**

| Module | 4C11 | Title of report | 4C11 Coursework 3 |
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# 4C11 Coursework 3

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## 1 Introduction

This report investigates the application of Recurrent Neural Operators (RNOs) to learn mappings between the complete history of macroscopic strain and the resulting homogenized stress in a one-dimensional viscoelastic model. Focusing on a unit cell composed of three distinct material phases, the study outlines both the theoretical foundation - drawing on operator theory and homogenization concepts - and the practical implementation of two RNO variants: the Standard RNO and the Viscoelastic RNO. The report details the formulation of the microscale and macroscale problems, the network architectures, discretization strategies, and the training protocols, including hyperparameter tuning.

## 2 Unit Cell Problem (1D Viscoelastic Model)

We consider a one-dimensional domain $x \in [0, 1]$ that represents a unit cell (or Representative Volume Element, RVE) composed of three distinct material phases, as shown in Figure 1. Each phase is characterized by its own elastic and viscous properties.

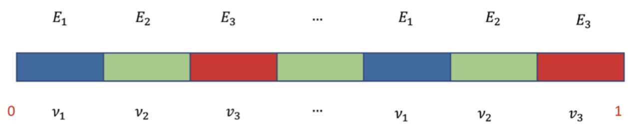



Figure 1: The unit cell that has three phases.

### 2.1 Microscopic Problem

At the microscale, within the RVE, the material behavior is described by:

1. **Kinematics:** The strain is defined as the spatial derivative of the displacement:
$$\epsilon(x,t) = \frac{\partial u(x,t)}{\partial x}.$$

2. **Equilibrium:** With no body forces present, the stress is constant throughout the RVE:
$$\frac{\partial \sigma(x,t)}{\partial x} = 0.$$

3. **Constitutive Model (Viscoelasticity):** The stress is the sum of an elastic response and a viscous contribution:
$$\sigma(x,t) = E(x)\,\epsilon(x,t) + v(x)\,\frac{\partial u(x,t)}{\partial t},$$
where $E(x)$ is the Young's modulus and $v(x)$ is the viscosity, both of which are piecewise constant across the three phases.

4. **Initial and Boundary Conditions:** The initial state is quiescent:
$$u(x,0) = 0, \quad \frac{\partial u(x,0)}{\partial t} = 0,$$
and the boundary conditions are:
$$u(0,t) = 0, \quad u(1,t) = \bar{\epsilon}(t),$$
where the prescribed displacement at $x = 1$ corresponds to the macroscopic strain $\bar{\epsilon}(t)$.

### 2.2 Macroscopic Problem

Since the equilibrium condition enforces a uniform stress $\sigma(x,t)$ throughout the domain, this constant stress directly represents the macroscopic stress $\bar{\sigma}(t)$. The macroscopic strain $\bar{\epsilon}(t)$ is defined by the displacement imposed at the right boundary (x=1).

Thus, the macroscopic constitutive model seeks to establish a mapping from the entire history of the macroscopic strain at $x = 1$ to the macroscopic (homogenized) stress:

$$\Psi^* \ : \ \{\bar{\epsilon}(\tau)\colon \tau \in [0,t]\} \longrightarrow \bar{\sigma}(t), \quad t \in [0,T].$$

Here, $\Psi^*$ encapsulates the effective behavior of the heterogeneous microstructure by linking the strain history $\{\bar{\epsilon}(\tau)\}$ (input) to the macroscopic stress $\bar{\sigma}(t)$ (output).

## 3 Recurrent Neural Operator (RNO)

### 3.1 Architecture

Our goal is to approximate the operator $\Psi^*$, which maps the entire macroscale strain history to the current homogenized stress, using a recurrent neural operator (RNO).

**Standard RNO:** In our formulation, the standard RNO is defined by

$$\begin{cases} \bar{\sigma}(t) = f\Big(\bar{\epsilon}(t),\ \{\xi_\alpha(t)\}_{\alpha=1}^k\Big), \\ \dot{\xi}_i(t) = g_i\Big(\bar{\epsilon}(t),\ \{\xi_\alpha(t)\}_{\alpha=1}^k\Big), \quad i = 1,\dots,k, \end{cases} \tag{1}$$

where $\{\xi_\alpha(t)\}_{\alpha=1}^k$ represents $k$ internal variables capturing the material's microstructural memory, and $f$ and $g_i$ are constitutive and evolution functions, respectively. In our approach, both $f$ and each $g_i$ are approximated using fully-connected neural networks (FCNNs).

We discretize the continuous equations using the forward Euler method:

$$\begin{cases} \bar{\sigma}^n = f\Big(\bar{\epsilon}^n,\ \{\xi_\alpha^{n-1}\}_{\alpha=1}^k\Big), \\ \xi_i^n = \xi_i^{n-1} + \Delta t \cdot g_i\Big(\bar{\epsilon}^n,\ \{\xi_\alpha^{n-1}\}_{\alpha=1}^k\Big), \quad i = 1,\dots,k. \end{cases} \tag{2}$$

**Viscoelastic RNO:** Since the RVE exhibits purely viscoelastic behavior (with no elasto-viscoplastic effects), we follow the approach of [2] by incorporating an explicit dependence on the strain rate $\dot{\bar{\epsilon}}(t)$ in the constitutive model:

$$\begin{cases} \bar{\sigma}(t) = f\Big(\bar{\epsilon}(t),\ \dot{\bar{\epsilon}}(t),\ \{\xi_\alpha(t)\}_{\alpha=1}^k\Big), \\ \dot{\xi}_i(t) = g_i\Big(\bar{\epsilon}(t),\ \{\xi_\alpha(t)\}_{\alpha=1}^k\Big), \quad i = 1,\dots,k. \end{cases} \tag{3}$$

Its forward Euler discretization is given by:

$$\begin{cases} \bar{\sigma}^n = f\Big(\bar{\epsilon}^n,\ \frac{\bar{\epsilon}^n - \bar{\epsilon}^{n-1}}{\Delta t},\ \{\xi_\alpha^{n-1}\}_{\alpha=1}^k\Big), \\ \xi_i^n = \xi_i^{n-1} + \Delta t \cdot g_i\Big(\bar{\epsilon}^n,\ \{\xi_\alpha^{n-1}\}_{\alpha=1}^k\Big), \quad i = 1,\dots,k. \end{cases} \tag{4}$$

**Network Approximation & Loss Function:** The functions $f$ and $g_i$ are approximated by FCNNs. We define the training loss as the mean-squared error (MSE) between the normalized ground-truth stress and the predicted stress, averaged over both time and samples.

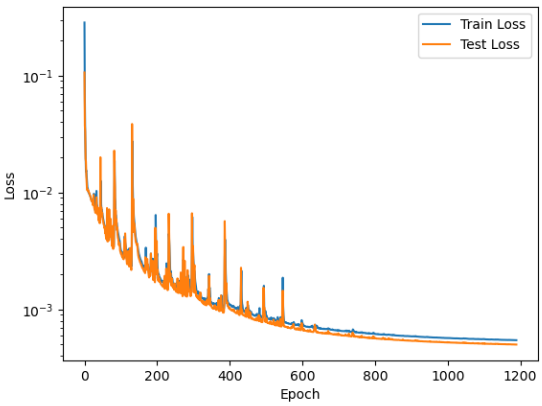
### 3.2 Hyperparameter Tuning and Training

The dataset consists of 400 samples, where each sample contains 1001 time-series data points of macro strain and macro stress. The data was downsampled to 251 time points (with a time step of $ft = 0.004$ s) and normalized. A total of 320 samples were used for training and 80 for testing, with a fixed batch size of 80.

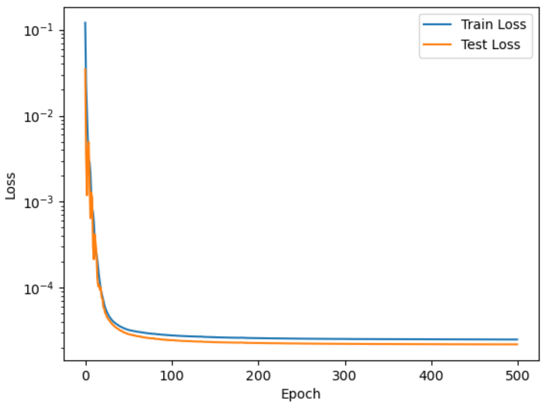
For both the Standard RNO and the Viscoelastic RNO, the hidden state dimension was set to 10 to maximize the model performace. However, due to the different network architectures, the hyperparameters were tuned individually. In particular, the Standard RNO required a longer training period with early stopping applied, while the Viscoelastic RNO converged much faster and achieved lower error. Table 1 summarizes the hyperparameters used for the two models:

| **Hyperparameter** | **Standard RNO** | **Viscoelastic RNO** |
|---|---|---|
| Hidden Dimension | 10 | 10 |
| Input Dimension | 1 | 1 |
| Output Dimension | 1 | 1 |
| Input Layers | [1+10, 20, 20, 1] | [2+10, 20, 20, 1] |
| Hidden Layers | [1+10, 10, 10] | [1+10, 10, 10] |
| Epochs | 5000 | 500 |
| Learning Rate | $3 \times 10^{-2}$ | $3 \times 10^{-2}$ |
| Step Size | 50 | 50 |
| Gamma | 0.8 | 0.7 |
| Early Stop Patience | 100 | – |
| Min Delta | $1 \times 10^{-5}$ | – |

Table 1: Hyperparameter settings for the Standard and Viscoelastic RNOs.




(a) Standard RNO training history

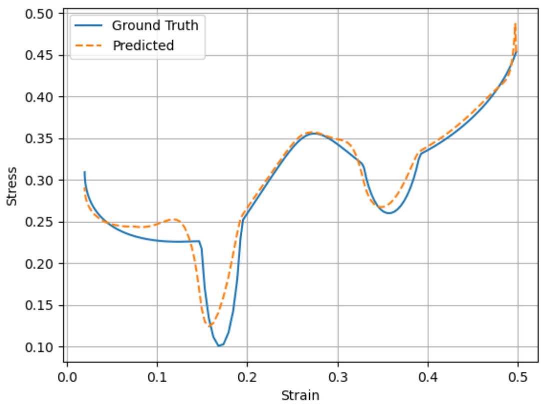



(b) Viscoelastic RNO training history

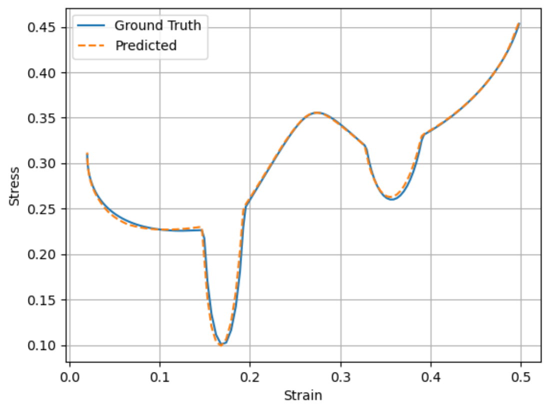
Figure 2: (a) Training history for the Standard RNO, (b) Training history for the Viscoelastic RNO.

The **Standard RNO** yielded a final training loss of $5.46 \times 10^{-4}$, a test loss of $5.00 \times 10^{-4}$, and a test error of 2.24% (see Figure 2a). In contrast, the **Viscoelastic RNO** converged much faster, reaching a final training loss of $2.51 \times 10^{-5}$, a test loss of $2.20 \times 10^{-5}$, and a test error of 0.47% (see Figure 2b). In addition, Figures 3a and 3b present the corresponding prediction visualizations for the Standard and Viscoelastic RNOs, respectively.

In summary, the Viscoelastic RNO not only converged more rapidly but also achieved lower error rates compared to the Standard RNO, indicating its superior suitability for addressing the Unit Cell problem.




(a) Standard RNO prediction visualization




(b) Viscoelastic RNO prediction visualization

Figure 3: (a) Prediction visualization for the Standard RNO, and (b) Prediction visualization for the Viscoelastic RNO.

# 4 Internal variables

## 4.1 Theorem: Existence of Exact Parameterization

According to Theorem 3.6 in [1], for a one-dimensional viscoelastic problem with piecewise-constant material properties in the unit cell (i.e., when the RVE is divided into L regions), the homogenized constitutive model can be exactly parameterized using a finite set of internal variables. Specifically, the theorem states that there exists a set of internal variables $\{\xi_\ell(t)\}_{\ell=1}^{L-1}$ (i.e., $L-1$ internal variables) along with corresponding evolution equations such that the macroscopic stress is given by

$$\bar{\sigma}(t) = \Psi\Big(\bar{\epsilon}(t)\Big) = \; E_0\bar{\epsilon}(t) + \nu_0\dot{\bar{\epsilon}}(t) - L_0\sum_{\ell=1}^{L-1}\xi_\ell(t), \tag{5}$$

where $E_0$ and $\nu_0$ represents the macroscopic effective stiffness and viscosity coefficient. Each internal variable $\xi_\ell(t)$ satisfies

$$\dot{\xi}_\ell(t) = \beta_\ell\,\bar{\epsilon}(t) - \alpha_\ell\,\xi_\ell(t), \quad \xi_\ell(0) = 0. \tag{6}$$

This means that although the microscopic behavior might exhibit complex history dependence (i.e., non-Markovian memory effects), by introducing $L-1$ internal variables the homogenized constitutive relation can be reformulated as a Markovian process that depends only on the current state rather than the entire history.

In our unit cell problem, where the cell comprises three distinct phases ($L = 3$), t**he theorem indicates that only two internal variables ($L-1 = 2$) are needed in addition to the strain and strain rate.**

## 4.2 Experiment: Required Internal Variable Number

We conducted experiments to compare the performance of the Standard RNO and the Viscoelastic RNO models under varying numbers of internal variables, as shown in Figure 4. For the Standard RNO, where the network input consists solely of the macroscopic strain at the current time step, $\bar{\epsilon}^n$, the results indicate that a single internal variable is sufficient to capture the required temporal derivative effects. In contrast, the Viscoelastic RNO receives as input both the current macroscopic strain, $\bar{\epsilon}^n$, and an approximation of the strain rate given by $\left(\bar{\epsilon}^n - \bar{\epsilon}^{n-1}\right)/\Delta t$; consequently, no additional internal variables are required.

Thus, **apart from the strain and its time derivative, no extra internal variables are needed in our specific problem setup**. At first glance, this observation might appear to conflict with the discussion in Section 4.1 - which posits the necessity of extra internal variables - but this discrepancy can be resolved by examining the role of body forces.

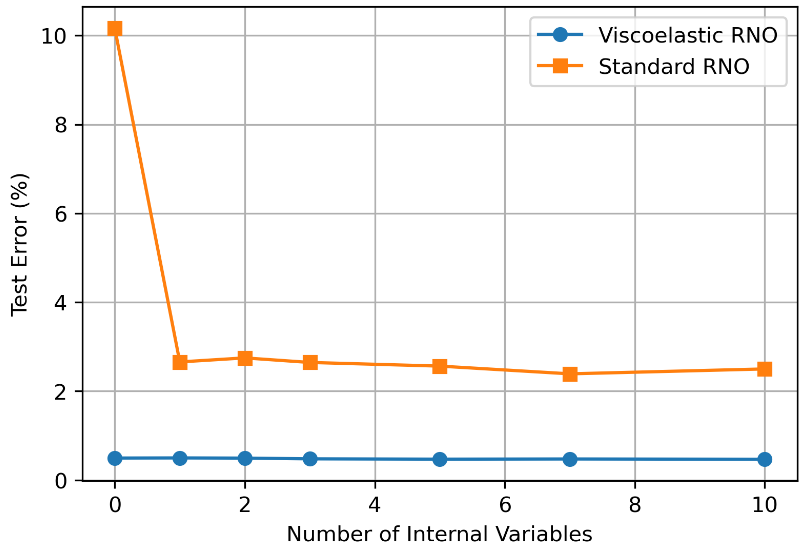



Figure 4: Test error for Standard RNO and Viscoelastic RNO with varying numbers of internal variables.

### 4.3 Intuition of the Theorem

Within the homogenization framework, the microscale solution is approximated by an asymptotic expansion in the small parameter $\delta$ (which represents the ratio of the microscale length to the macroscale length):

$$u(x,t) \approx u_0 + \delta\, u_1 + \delta^2\, u_2 + \cdots\,, \tag{7}$$

where:

- $u_0$ (Leading-Order Term): **This term represents the macroscopic (homogenized) displacement field ($u_0 = \bar{u}$).** During homogenization, the rapidly oscillating microscale variations are averaged out, and $u_0$ is obtained as the solution to the effective (macroscopic) problem. In essence, the macroscopic displacement $u_0$ captures the overall behavior of the material and eliminates all higher-order corrections associated with microscale heterogeneities.

- $\delta\, u_1$ (First-Order Correction): This term captures the first-order effects of the microscale fluctuations. Although $u_0$ is sufficient to describe the average behavior, $u_1$ contains vital information about local variations that are lost during the averaging process. **Such local variations typically give rise to memory effects or history dependence in the effective constitutive model.**

- $\delta^2\, u_2$ (Second-Order Correction) and Higher-Order Terms: These higher-order corrections further refine the approximation by incorporating subtle effects of the microscale heterogeneities. They provide additional detail on how local variations influence the macroscopic response; however, their contribution diminishes as $\delta$ becomes small. In practice, the influence of these terms is often neglected.

Since the macroscopic solution $u_0$ is obtained via spatial averaging, it omits the detailed information in the higher-order terms $u_1, u_2, \ldots$. Internal variables are introduced to parameterize the effect of the first-order correction $\delta\, u_1$ and thus capture the resulting history dependence.

Moreover, when the material is composed of $L$ distinct phases, each phase would nominally contribute its own first-order term. However, because the material is connected, ensuring continuity of the displacement field across phase boundaries, one of these degrees of freedom is redundant. Consequently, only $L-1$ independent internal variables are necessary. This discussion provides intuitions to the exact parameterization theorem.

### 4.4 Absence of Body Force

In the special case where the body force $f$ vanishes, the equilibrium condition forces the microscopic stress to be uniform across the RVE (as in our problem setup). Consequently, the leading term $u_0$ is spatially constant and entirely characterizes the macroscopic behavior. In this setting, no residual effects or additional memory arise; hence, no extra internal variables are required to account for higher-order corrections.

In summary, when $f = 0$, the homogenized model is fully determined by the leading-order term, and the macroscopic stress equals the spatial average of the microscopic stress. Therefore, the Markovian parameterization relies solely on the strain and strain rate, reconciling the experimental observations with the theoretical framework and confirming that, under zero body force conditions, the absence of additional internal variables does not conflict with the theorem of the existence of exact parameterization.

## 5 Summary

The experimental results demonstrate that the Viscoelastic RNO, which explicitly incorporates the strain rate, converges faster and achieves a lower error rate compared to the Standard RNO. This efficiency underscores the importance of including dynamic effects in the constitutive model. Additionally, theoretical insights confirm that, under zero body force conditions, the macroscopic behavior can be fully captured by the strain and its time derivative, eliminating the need for extra internal variables. Overall, the report provides a comprehensive examination of RNOs and their effectiveness in approximating complex, history-dependent material responses in heterogeneous viscoelastic systems.

## References

[1] Kaushik Bhattacharya, Burigede Liu, Andrew M. Stuart, and Margaret Trautner. Learning markovian homogenized models in viscoelasticity. *Multiscale Modeling & Simulation*, 21(2):641–679, 2023.

[2] Burigede Liu, Eric Ocegueda, Margaret Trautner, Andrew M. Stuart, and Kaushik Bhattacharya. Learning macroscopic internal variables and history dependence from microscopic models. *Journal of the Mechanics and Physics of Solids*, 178:105329, May 2023.