

## A Simulation-Based Non-Destructive Framework for Assessing Polymer Chain Flexibility

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### INTRODUCTION & AIM

#### Background

- Polymer chain flexibility strongly influences mechanical adaptability and dynamic material behavior.
- Conventional characterization often relies on destructive mechanical testing.
- Emerging non-destructive testing (NDT) increasingly incorporates computational and simulation-assisted methodologies.

#### Motivation & Aim

- Develop a simulation-assisted framework for non-destructive evaluation of polymer chain flexibility.
- Extract statistical response descriptors including:
  - End-to-end distance distribution
  - Mean-square displacement (MSD)
- Enable indirect inference of polymer dynamic behavior without physically damaging real materials.
- Combine stochastic random-walker modeling with molecular dynamics simulations

### METHOD

#### Polymer Chain Model

- Polymer chains represented using a stochastic random-walker framework.
- Thermal motion simulated through probabilistic chain evolution.
- Both equilibrium and force-driven conformational behavior were investigated.

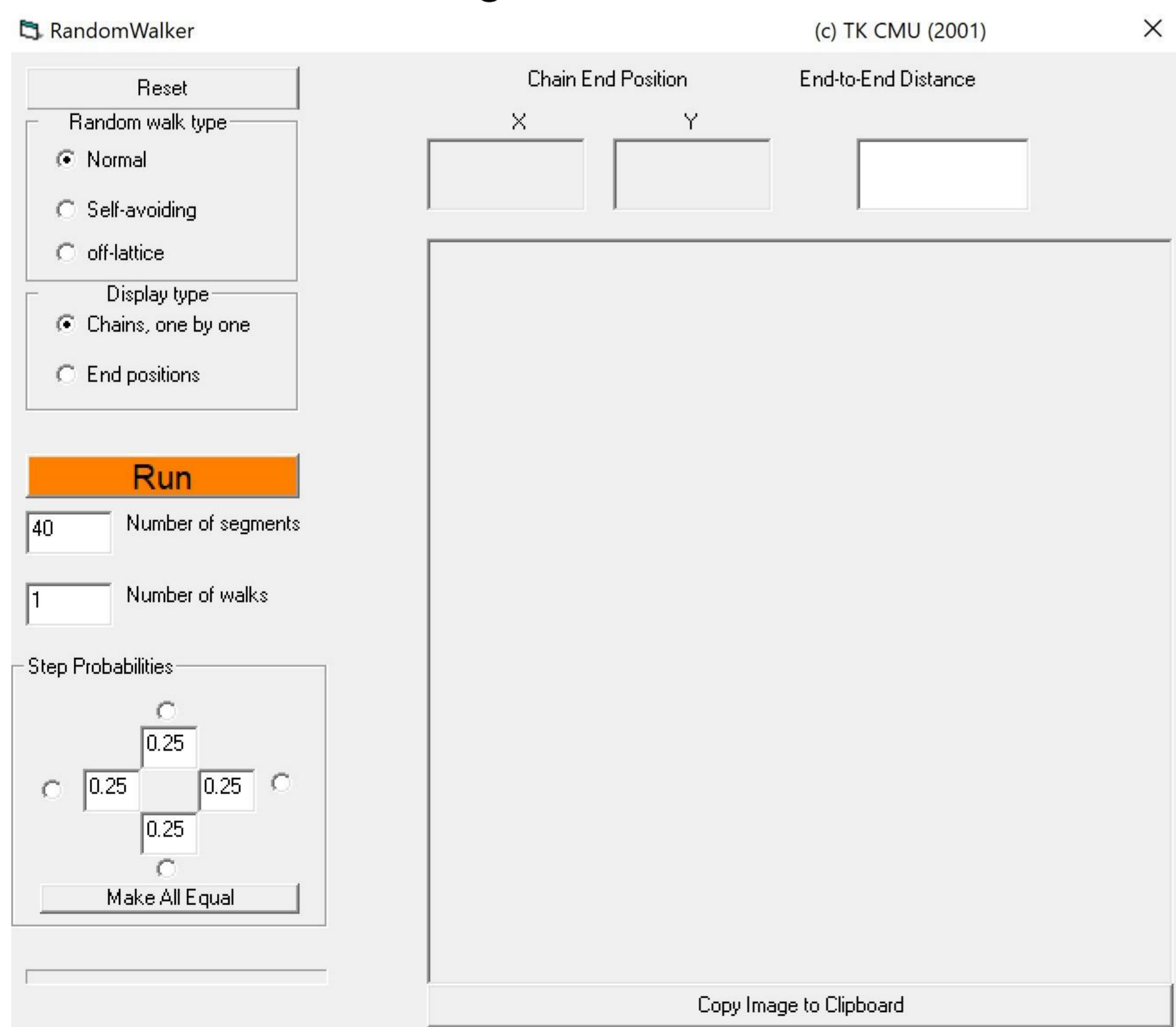
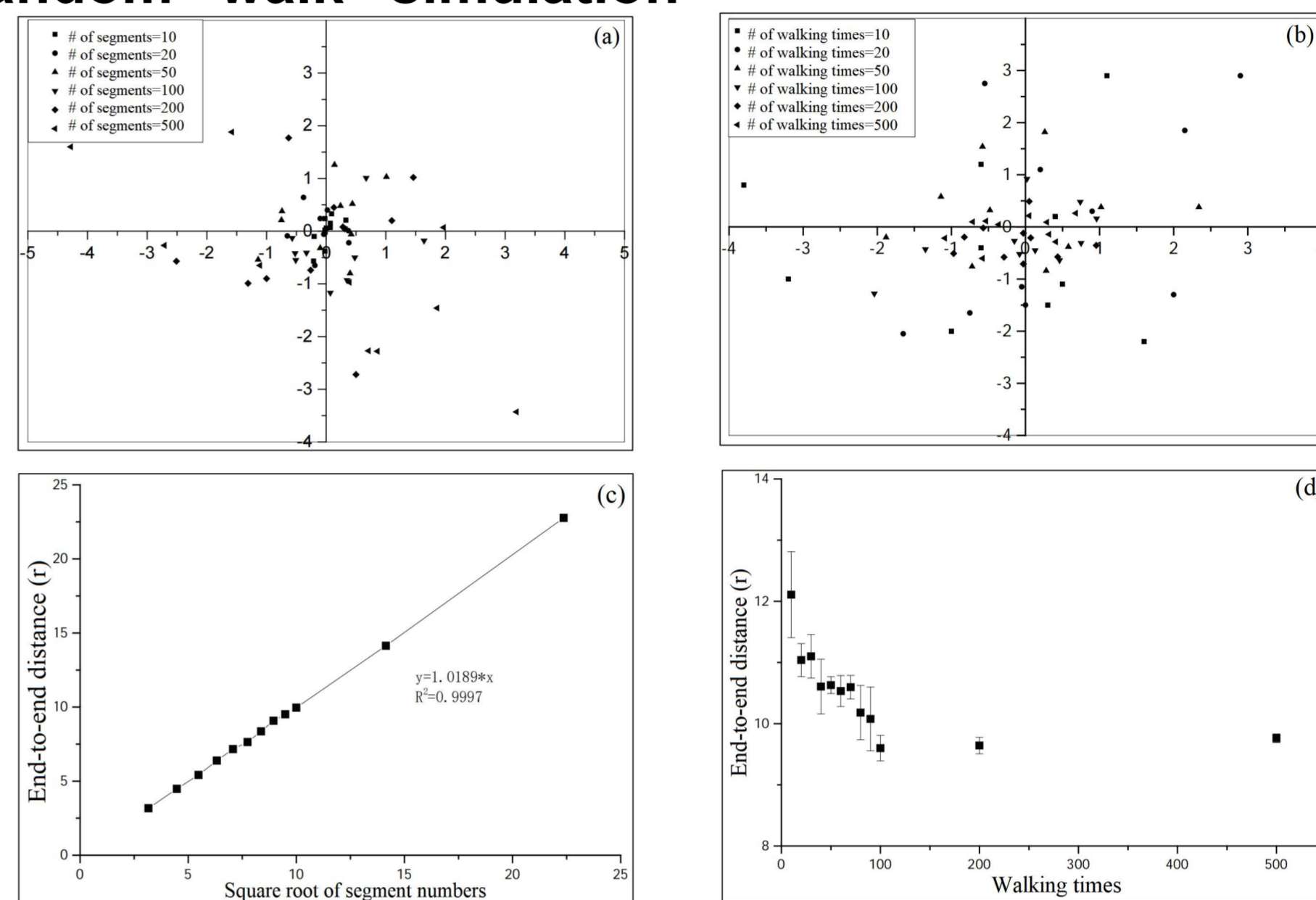


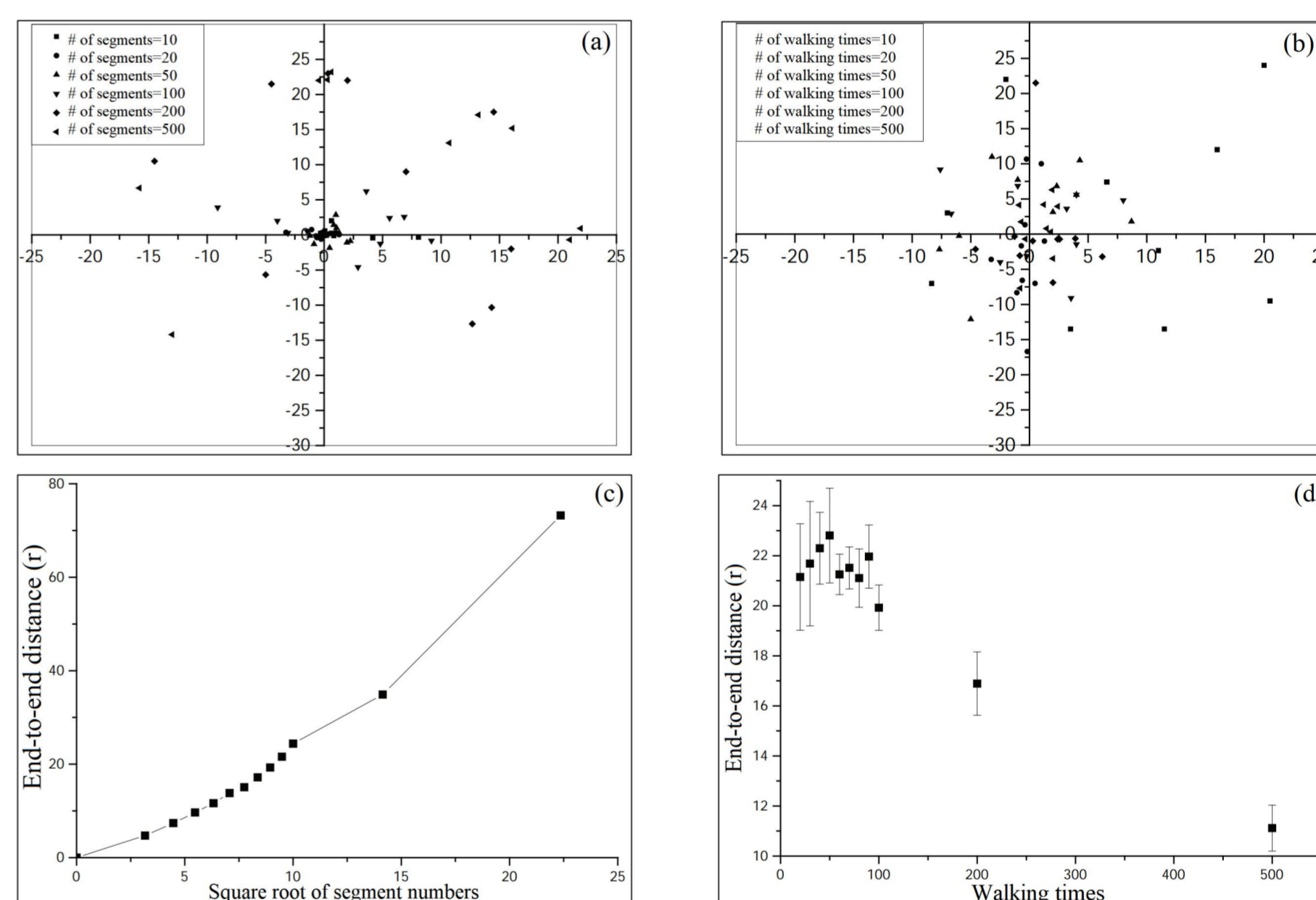
Figure 1. Interface of the stochastic random-walker simulation framework used to model polymer chain conformational evolution

### RESULTS & DISCUSSION

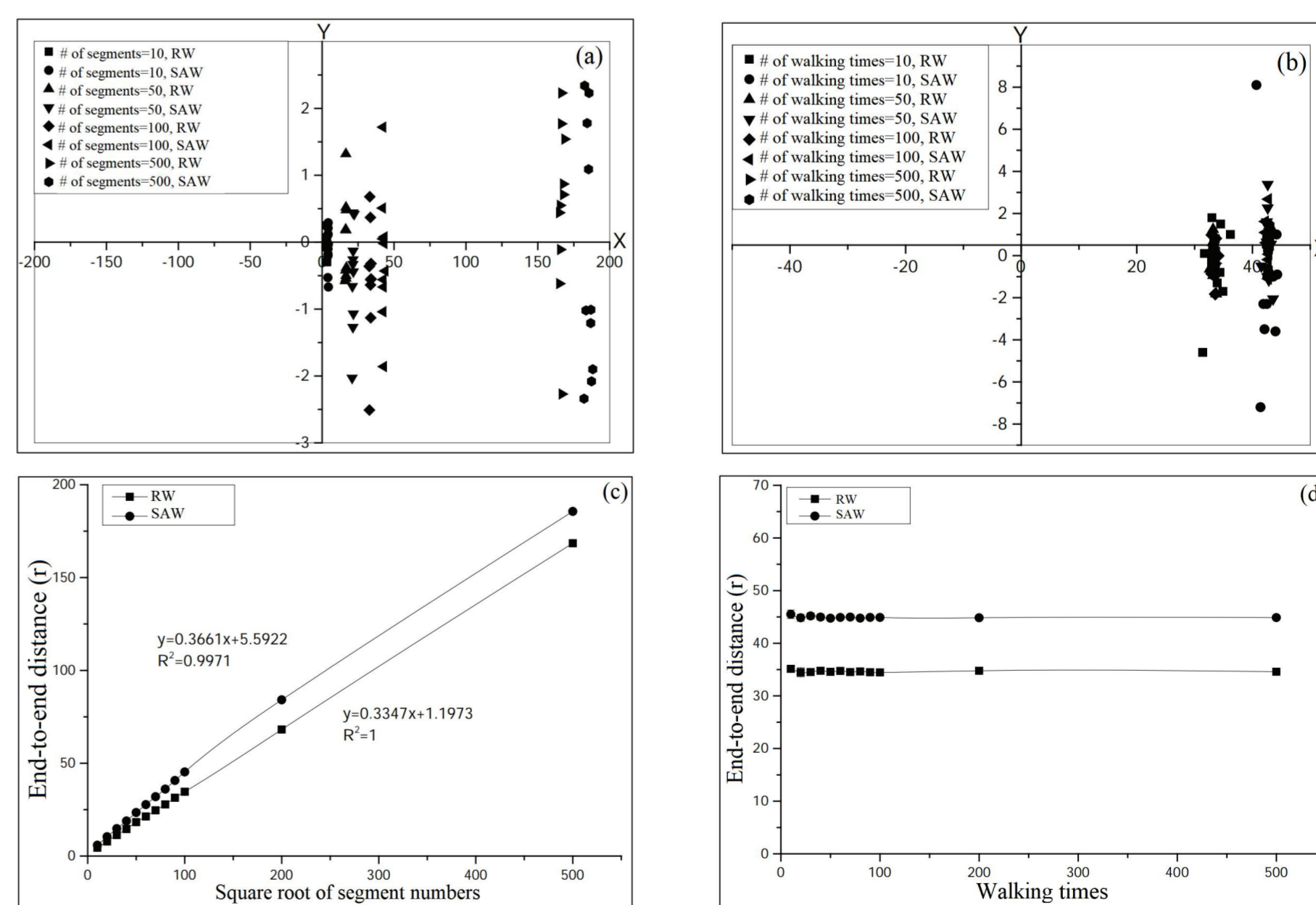
#### Random “walk” simulation



#### Self-avoid “walk” simulation



#### External force-driven “walk” simulation



### CONCLUSION

- The framework enables indirect inference of polymer dynamic behavior without damaging materials.
- Computational modeling demonstrates strong potential for emerging simulation-assisted NDT methodologies.