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Exploration of a 2D Material Monte Carlo Simulator: Parallelization Strategy and Noise Characterization of MoS_2

E. Pascual(1), J. M. Iglesias(1), M. J. Martín(1), R. Rengel(1), and K. Kalna(2)
(1) Applied Physics Dept. **Universidad de Salamanca**, Salamanca, SPAIN
(2) Nanoelectronic Devices Computational Group, College of Engineering, **Swansea University**, Swansea, U.K.

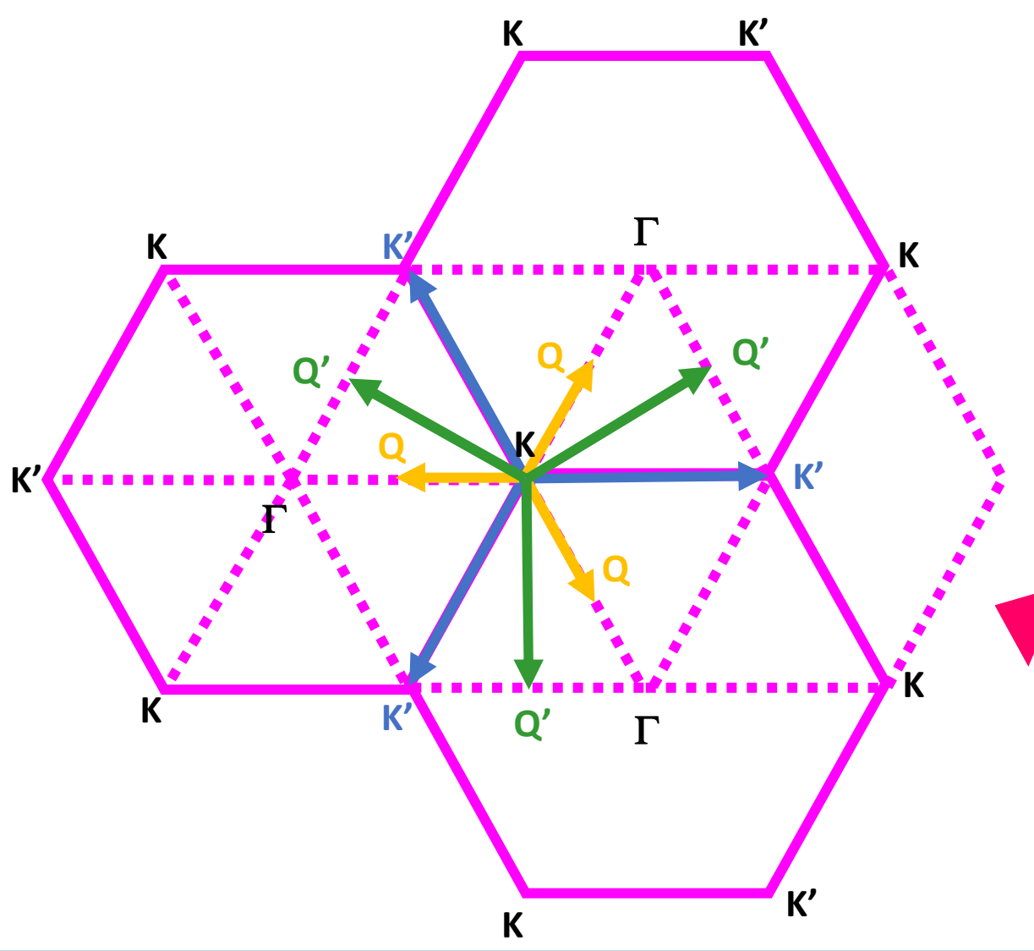
INTRODUCTION

Two dimensional (2D) metal dichalcogenides are under an intensive research which is mainly motivated by their inherent bandgap and their feasible applications beyond gapless graphene [1]. The dichalcogenides possess fascinating properties such as a direct bandgap, promising novel optical and electronic properties [2]. An exhaustive study of electronic transport of these materials is essential to assess their application by advanced physically-based models as an ensemble Monte Carlo (MC) technique which present well-recognised benefits to model the stochastic and quantum-mechanical transport processes at nanoscale.

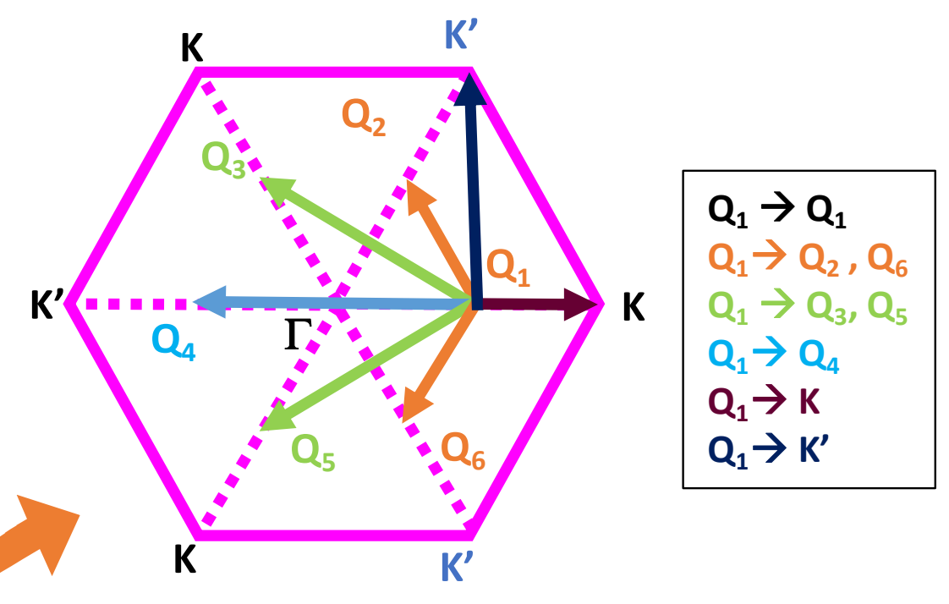
In this work, an in-house ensemble Monte Carlo (MC) simulator has been developed and widely tested for the study of different 2D materials such as graphene, silicene, molybdenum disulfide (MoS_2) and other transition metal dichalcogenides [3, 4, 5, 6]. We have focused on exploiting the advantages that this tool offers to characterize the microscopic noise sources in MoS_2 due to charge fluctuations and also in developing a parallelization strategy under Message Passage Interface (MPI) in order to upgrade our purely sequential MC simulator.

MC: Noise Characterization of MoS_2

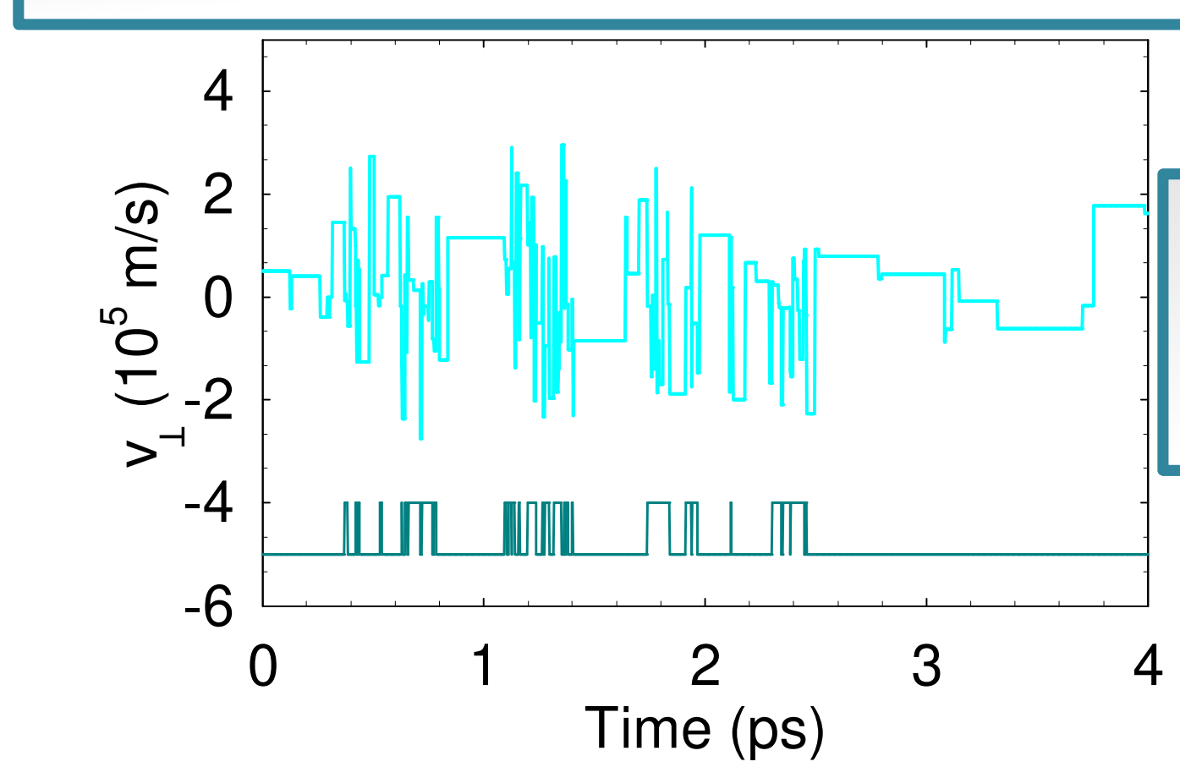
- **Non-degenerate conditions** considered (**50.000** super-particles).
- Phonon branches considered [2]:
  - ✓ Intravalley acoustic phonons.
  - ✓ Intervalley acoustic phonons.
  - ✓ Optical phonons.
- Aggregated phonon modes to account for:
  - ○ **TA** and **LA**.
  - ○ **TO(E')**, **LO(E')** and **A1** (homopolar).
- Deformation potentials for valley transitions, effective masses and K-Q valley separation are collected in [2].



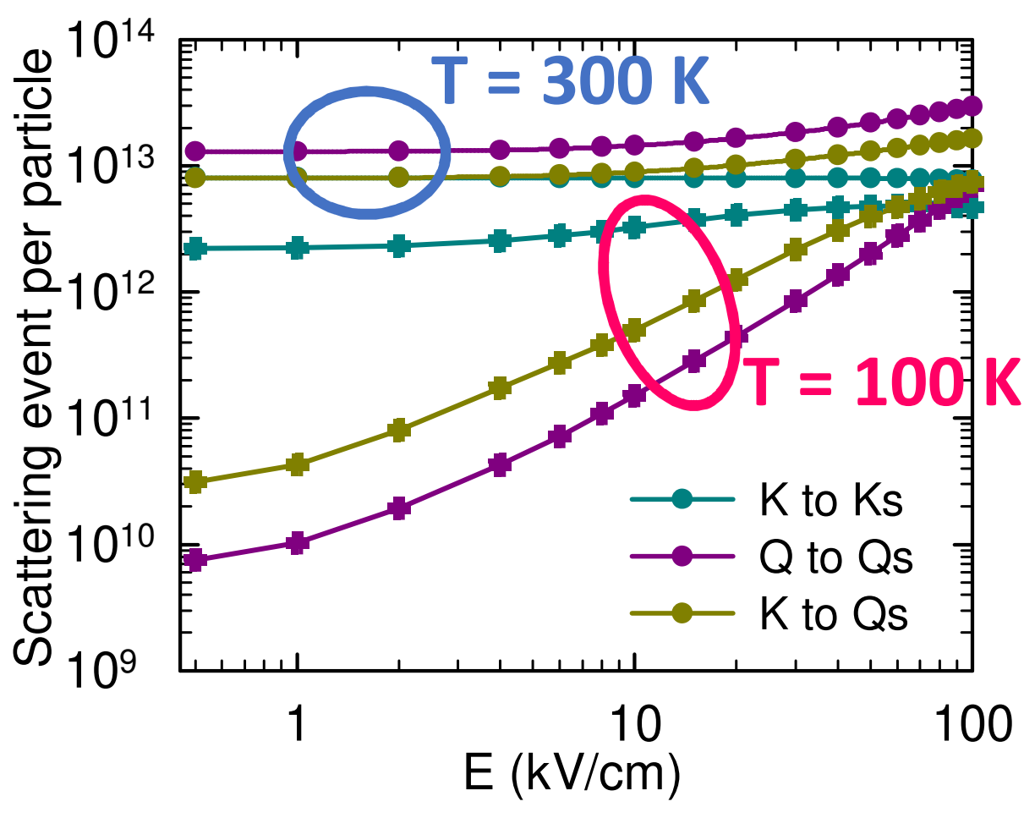
- Possible intervalley transitions for electrons:
  - ○ in **K valleys.**
  - ○ in **Q valleys.**

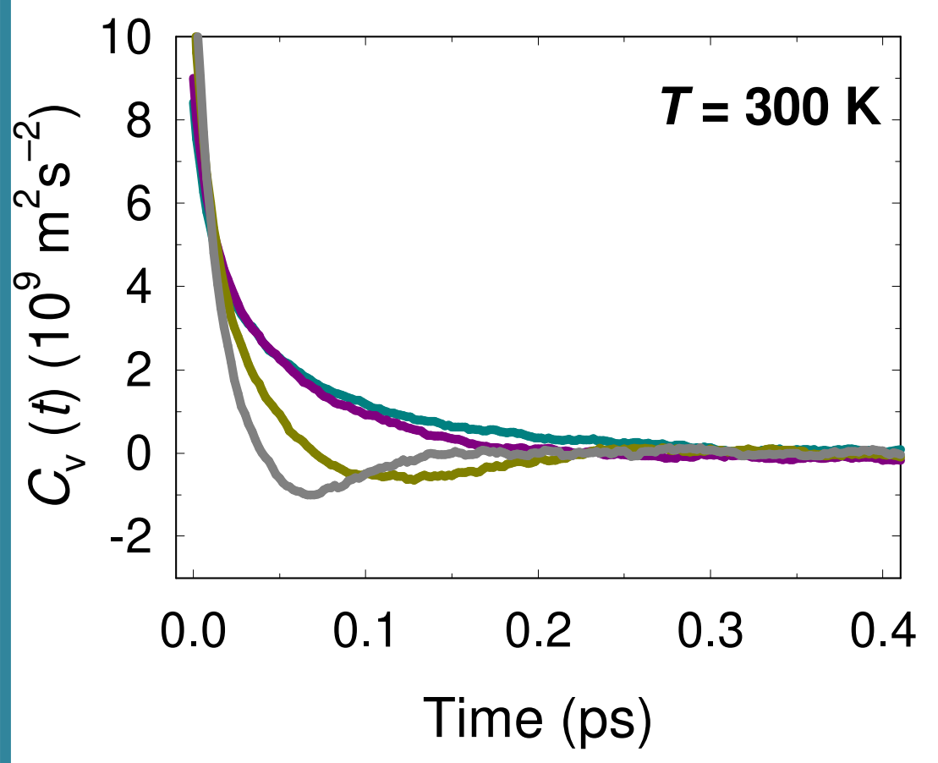


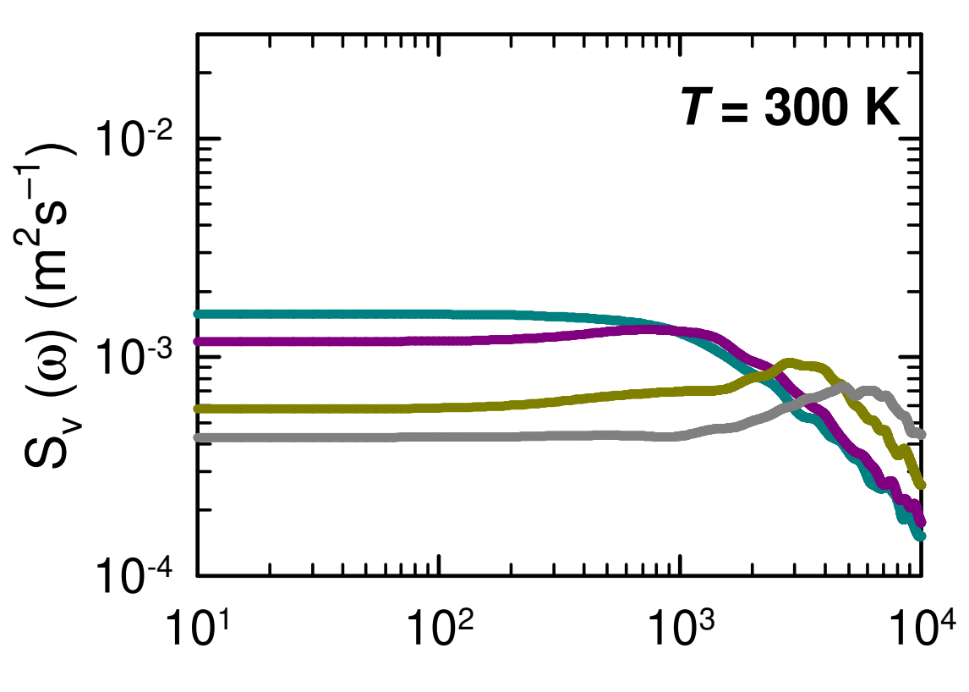
Stochastic microscopic history of a single particle:

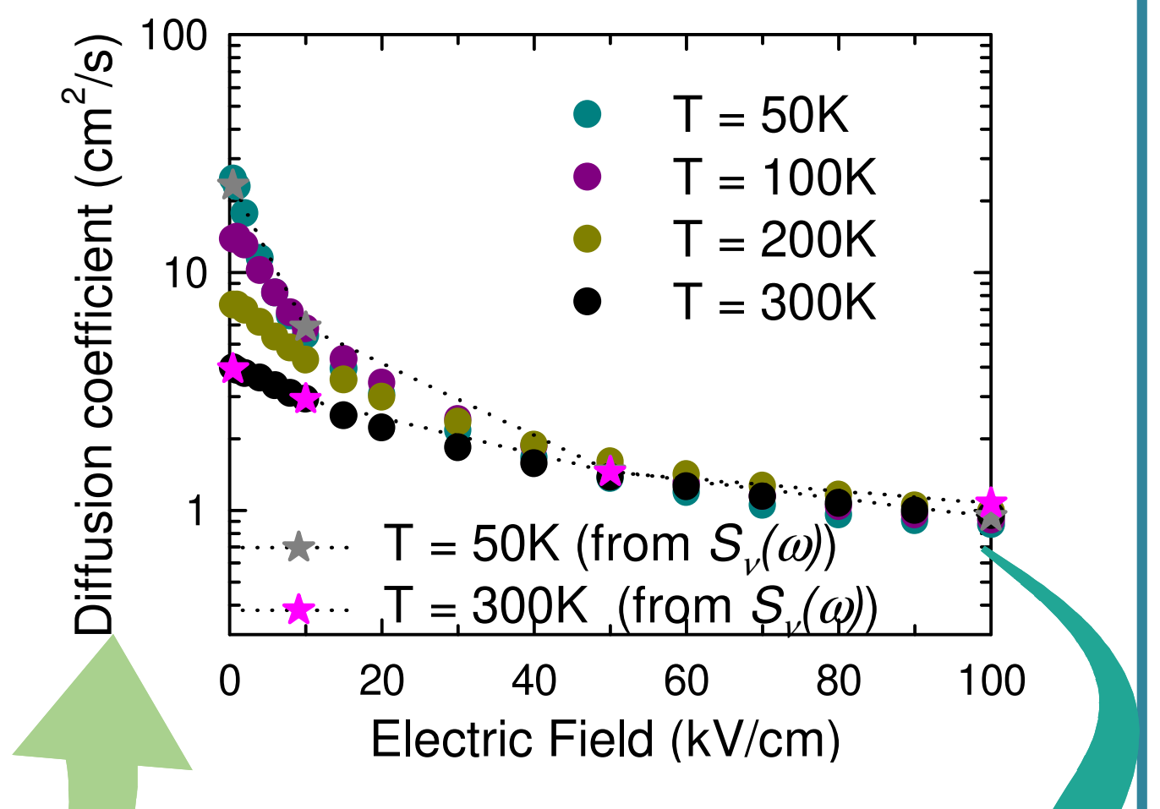


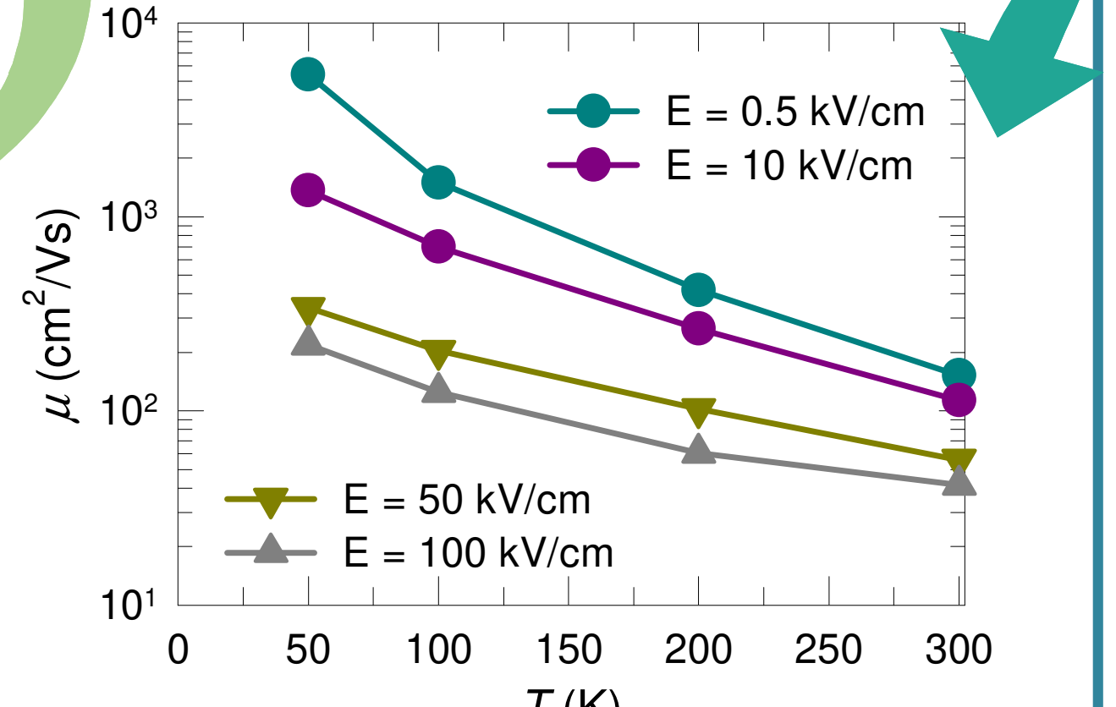
Velocity fluctuations as the primary source of thermal noise.









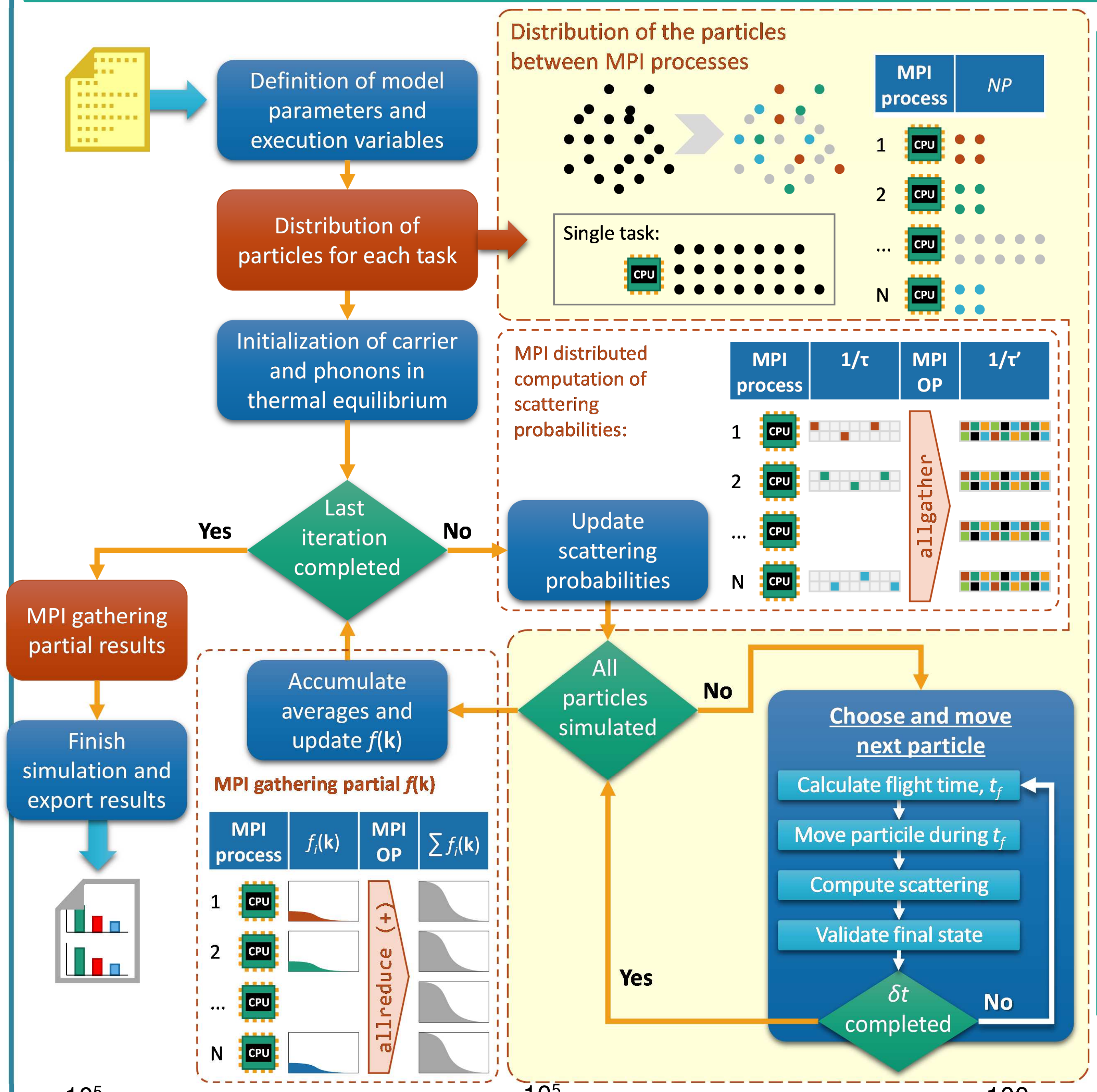


* **Correlation function** has a slow decay in a low electric field. Decay times reduce with both E and T. →**Spectral density** presents its maximum at larger frequencies.

* Larger decay of **diffusion coefficient** with the electric field for lower temperatures.

Parallelization Strategy of MC - MPI

The motion of **simulated particles** in the ensemble MC technique depends on their previous history probabilistically governed by **Boltzmann Transport Equation** using classical free flights interrupted by quantum-mechanical scattering events.

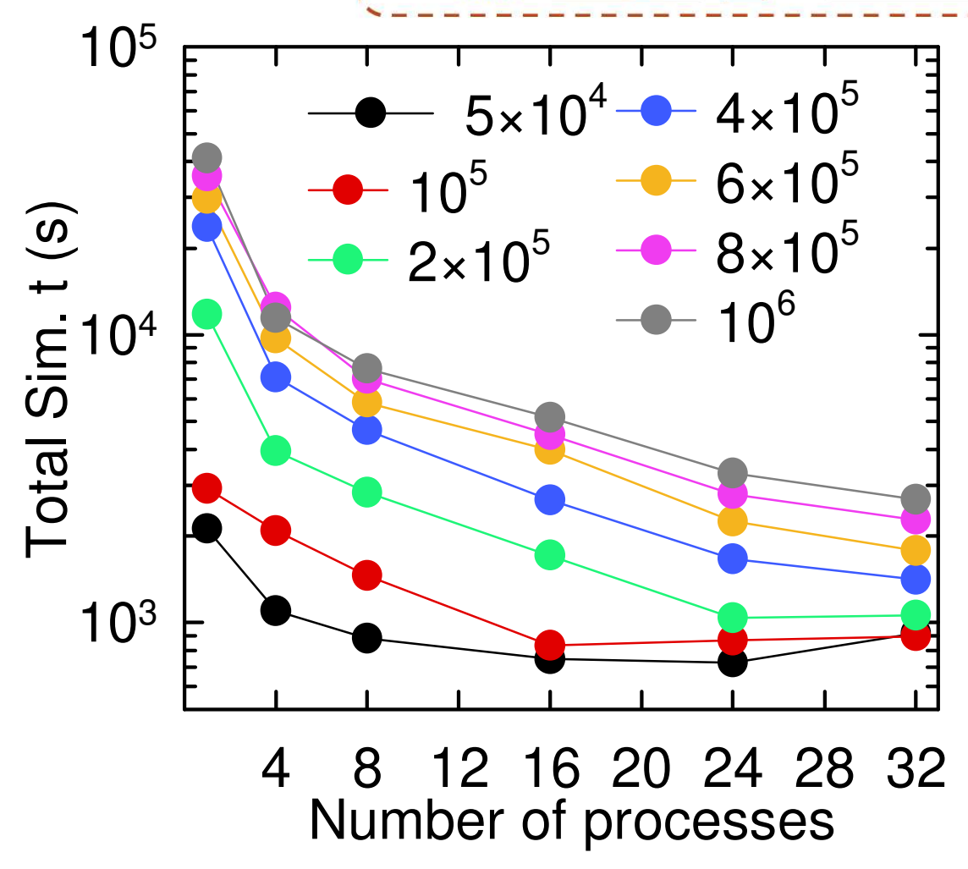


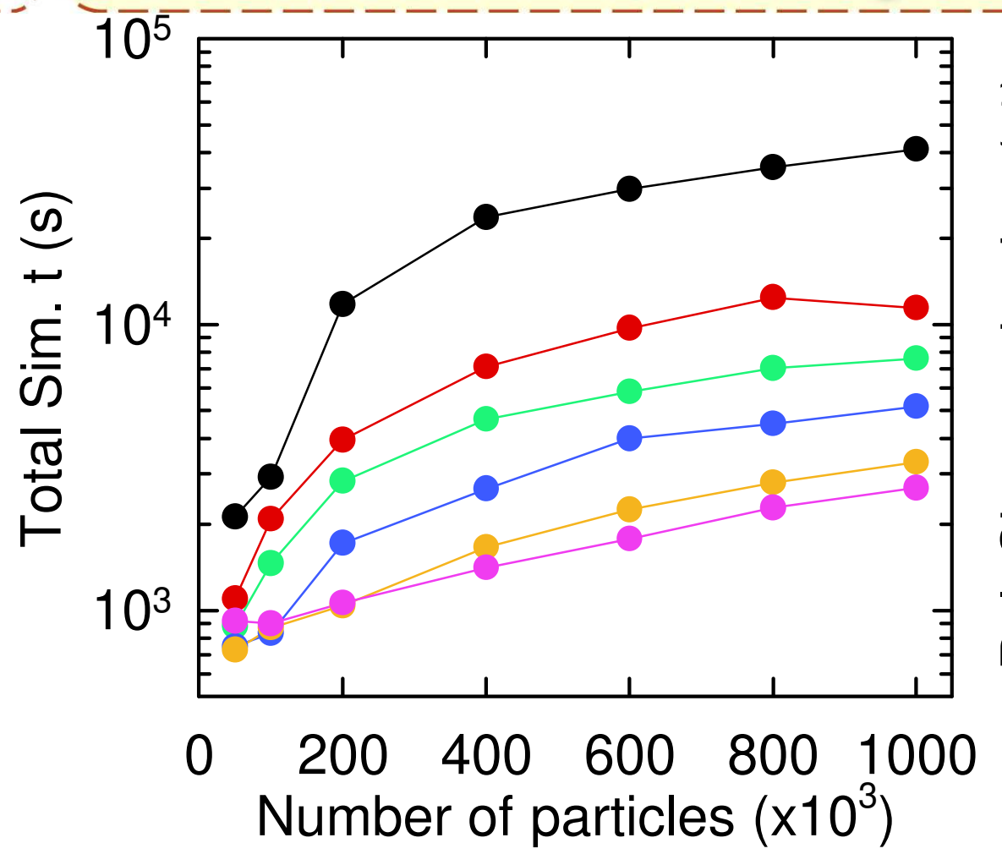
Message Passing Interface (MPI):

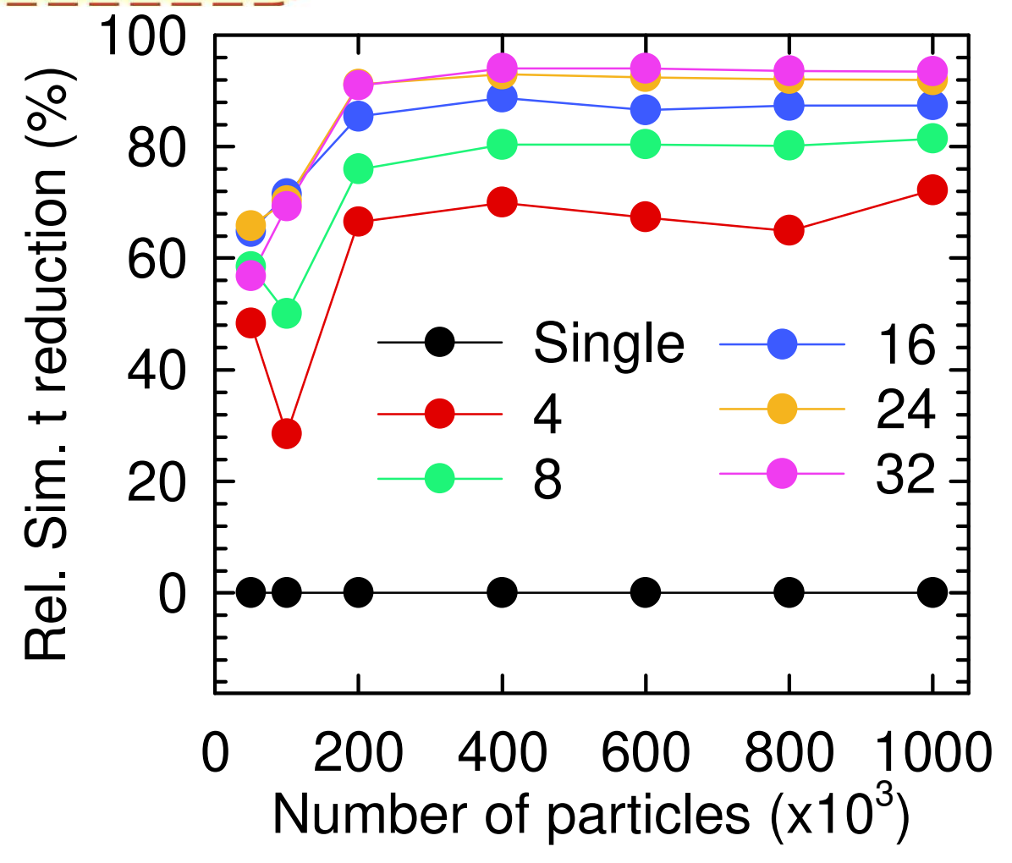
- First message-passing interface standard
- Provides source-code portability
- Allows efficient implementation

Implementation approach:

- Computation distribution of scattering probabilities calculation and particle flights







At **50.000** simulated particles, the optimum number of processes is 8 increasing the number of processes improves only slightly conditions: High relative intercommunication overhead. Simulations **with a large number of particles** decrease the relative computational burden of communications: **the best parallelization candidate.**

A greater reduction of the simulation time when passing from 1 to 4 processes, communication between them may interfere: A relative sim. time reduction of a 60% when the number of particles is larger than 200.000 for 4 processes and of 95% for 32 processes.

Conclusions

- Transfer to the upper Q valleys: important dependence on T and E.
- Diffusion coefficient is determined for the first time using a MC simulator.
- Mobilities in the range of 150 cm^2/Vs to 4100 cm^2/Vs at a low electric field.
- Parallelization strategy under Message Passage Interface (MPI) in our sequential MC simulator is profitable under certain conditions: a large number of particles and more complex probability simulations.
- Substantial improvements are expected with MPI in device simulations.

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MINISTERIO DE ECONOMÍA, INDUSTRIA Y COMPETITIVIDAD
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CONTACT PERSON

Elena Pascual
elenapc@usal.es

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