Quasiclassical trajectory computations of elementary processes in air hypersonic flows

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Collision processes of heavy particles

**Inelastic processes**
\[ A + BC(v, j) \rightarrow A + BC(v', j') \]

**Reactive processes**
\[ A + BC(v, j) \rightarrow B + AC(v', j'), C + AB(v', j') \]

**Dissociation/recombination**
\[ A + BC(v, j) \rightarrow A + B + C \]
Reactivity of $O+N_2 \rightarrow NO+N$

Relaxation of $O+N_2(v=1)\rightarrow O+N_2(v'=0)$


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A classification of collisions

Purely inelastic event, a weak *two-body* interaction

Quasi-reactive event, a strong three-body interaction, *inelastic*

Reactive event, a strong three-body interaction with rearrangement

Classical vibrational distribution for O+N₂(ν=5)
**Relaxation of He+H$_2$**

Comparison of QCT with QM Close Coupling calculations


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Reaction of $H+HeH^+(v=0,j=0)\rightarrow He+H_2^+$

Comparison of QCT with accurate QM calculations

Reaction of $H+HeH^+(v=0,j=0)\rightarrow He+H_2^+$

Comparison of QCT with accurate QM calculations: final vibration

Reaction of $H + HeH^+ \rightarrow He + H_2^+$

Comparison with other QM calculations

**Reaction of $H^+ + \text{HeH}^+ \rightarrow \text{He} + \text{H}_2^+$**

Normalized computational load in QCT and QM calculations

![Graph showing normalized computational load vs collisional energy](image)

F. Esposito, C.M. Coppola, and D. De Fazio, JPCA 119, 12615—12626 (2015).

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Quasiclassical Performance

Extreme computational efficiency on parallel machines

![Graph showing speedup on the FERMI machine at CINECA](image)

- real calculations
- ideal case

speedup

n.of nodes

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Reactivity of $O+N_2 \rightarrow NO+N$


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Relaxation of $O+N_2(v=1)\rightarrow O+N_2(v'=0)$


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Relaxation of $O+N_2(v=1,j=0)$: work in progress...

- In collaboration with George McBane, Grand Valley State University
Monoquantum vibrational deexcitation of N+N$_2$ and O+O$_2$


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Recombination of $H+H+H \rightarrow H+H_2(\nu,j)$

Comparison with QM Coupled States calculations

Final Remarks

- Computing datasets for heavy particle vibrational kinetics needs more than one dynamical method.

- Quantum mechanical calculations are fundamental for assessing the level of accuracy of other methods, but can be used only for quite restricted ranges of total energy.

- Quasiclassical method is particularly suited for the task, if used in combination with other accurate methods.

- Approximations of quantum mechanical treatments are not necessarily more reliable than quasiclassical results.