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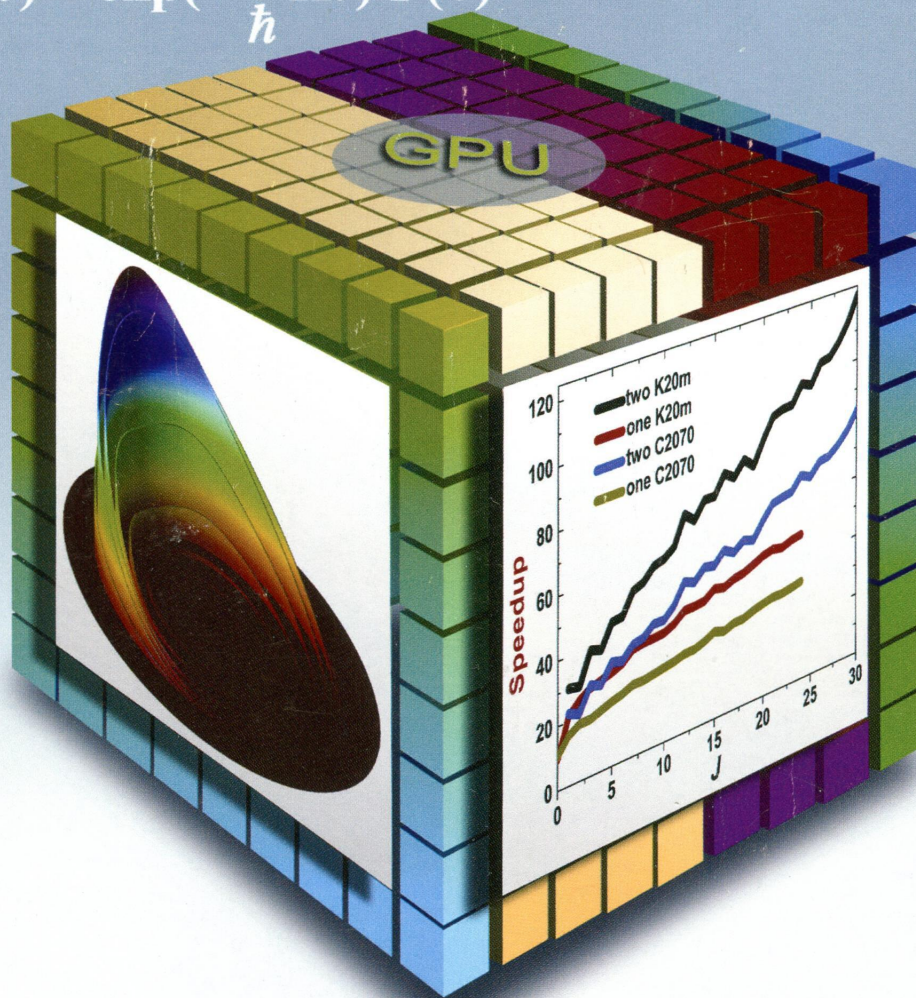
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A

$$\Psi(t) = \exp\left(-\frac{i}{\hbar} \hat{H}t\right) \Psi(0)$$



GPU-Based
State-to-State
Reactive Scattering
Dynamics
(see page 8929)

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ON THE COVER: A parallel code for state-to-state quantum dynamics with propagation of a time-dependent wave packet in reactant coordinates has been developed on GPUs. In the computation of the differential cross sections of the H + HD reaction, the average speedups are 57.0 and 83.5 for the parallel computation on two C2070 and K20m GPUs relative to serial computation on the Intel E5620 CPU, respectively. Cover art created by Keli Han and Pei-Yu Zhang. The speedup graph (right) is from Han, K. L.; Zhang, P. Y. Reactant Coordinate Based State-to-State Reactive Scattering Dynamics Implemented on GPUs. *J. Phys. Chem. A*, 2014, DOI: 10.1021/jp5009779. This special issue was organized by Guest Editors Keli Han and Jin Zhong. See page 8929.

SPECIAL ISSUE: INTERNATIONAL CONFERENCE ON THEORETICAL AND HIGH PERFORMANCE COMPUTATIONAL CHEMISTRY SYMPOSIUM

Guest Editors: Keli Han and Jin Zhong

Special Issue Preface

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Zhong Jin and Keli Han*

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