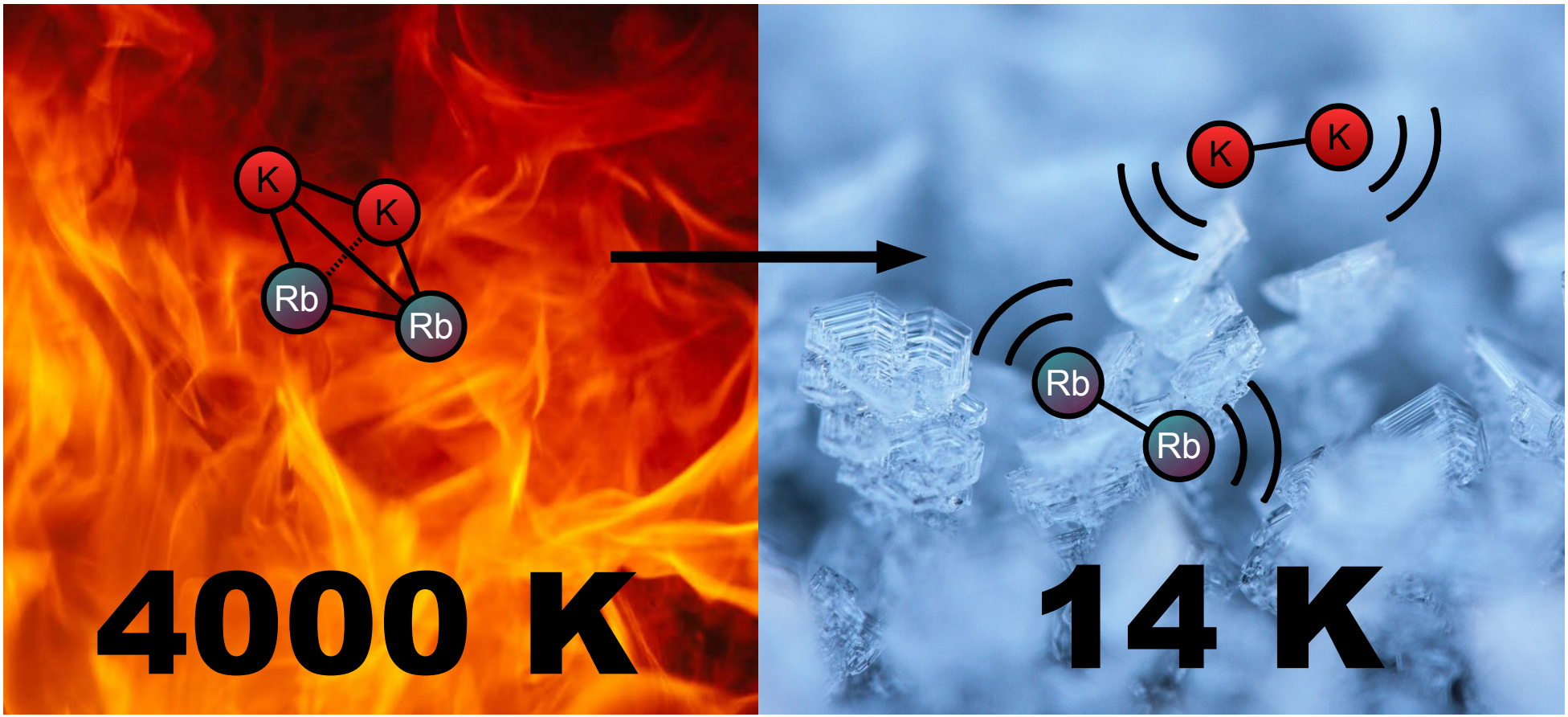
I use Blue Waters to simulate an ultracold inferno.

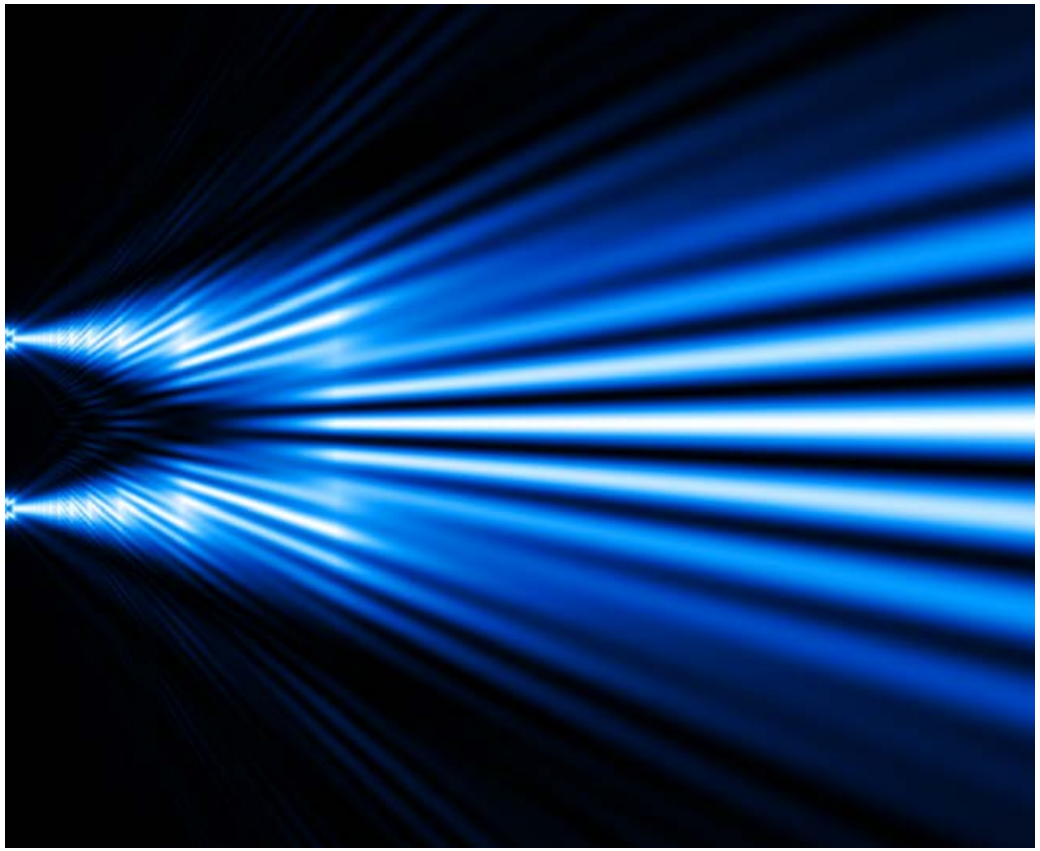
Micheline Soley



Goal: To introduce the concept of an ultracold inferno in order to make investigation of ultracold reactions possible.

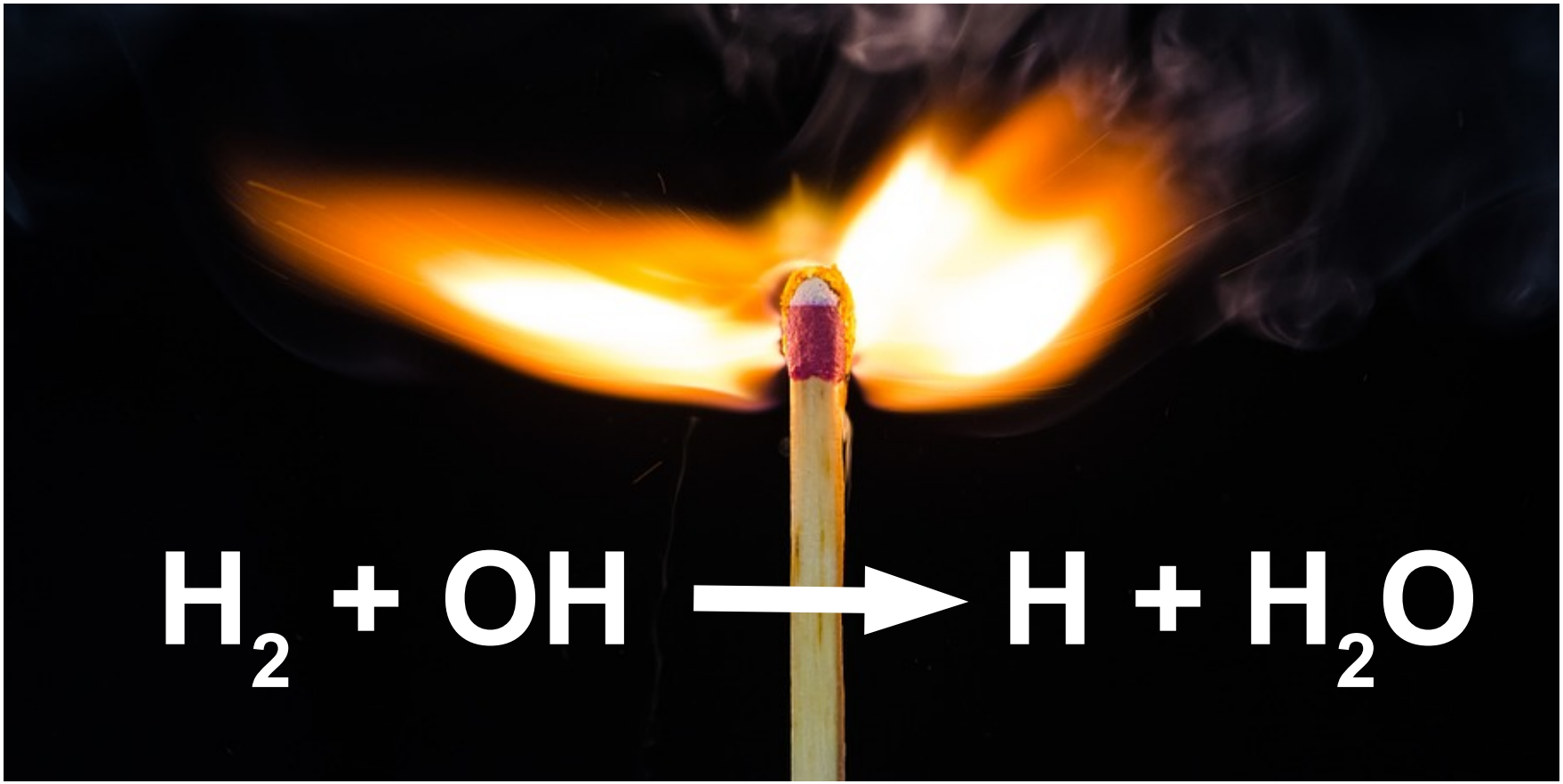
Standard Approach

Typically, quantum mechanics is used for precise simulation of chemical reactions.



Standard Approach

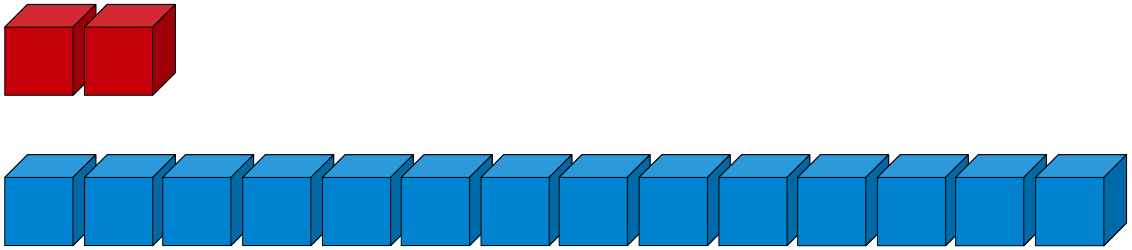
However, time-dependent quantum mechanics is computationally intensive and has only been used for a few high-temperature reactions



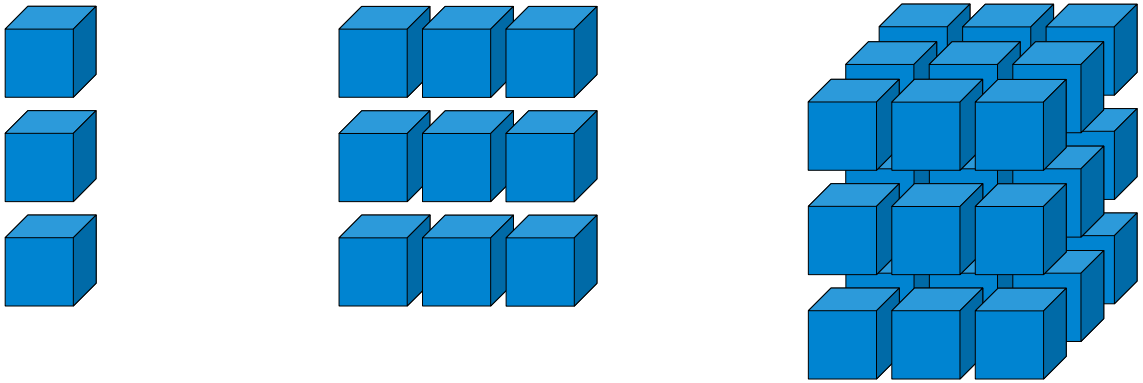
Key Challenges

Ultracold reactions cannot be studied with existing quantum techniques because:

- Vectors scale as $T^{-1/2}$ with temperature T



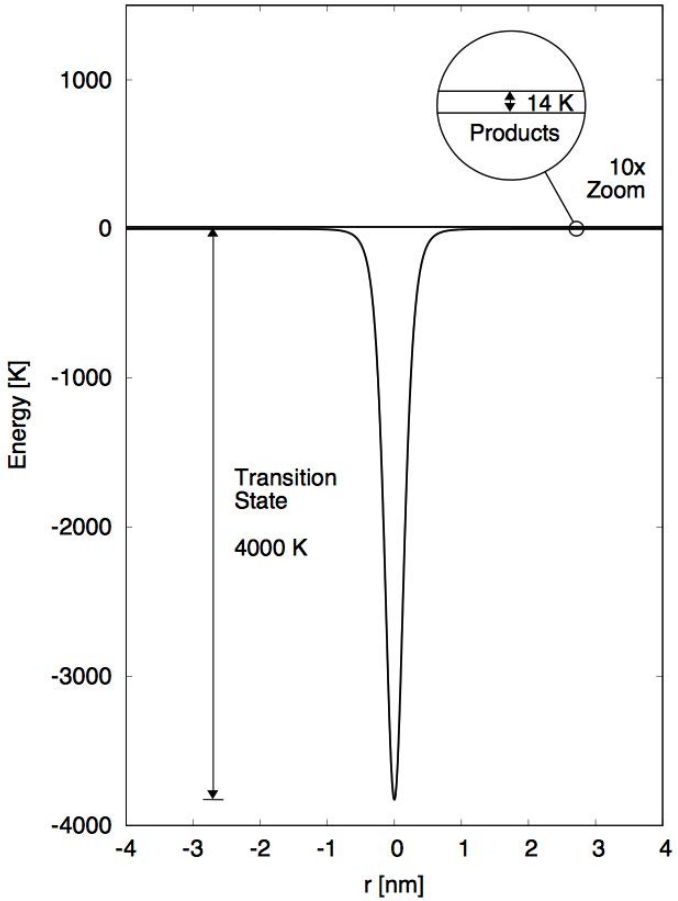
- Arrays scale as N^D with system size D



In contrast, classical mechanics is free of exponential scaling

...but still limited to high temperatures.

Solution



To make simulation of the ultracold KRb dimer reaction possible, we recognize that it acts like an ultracold inferno.

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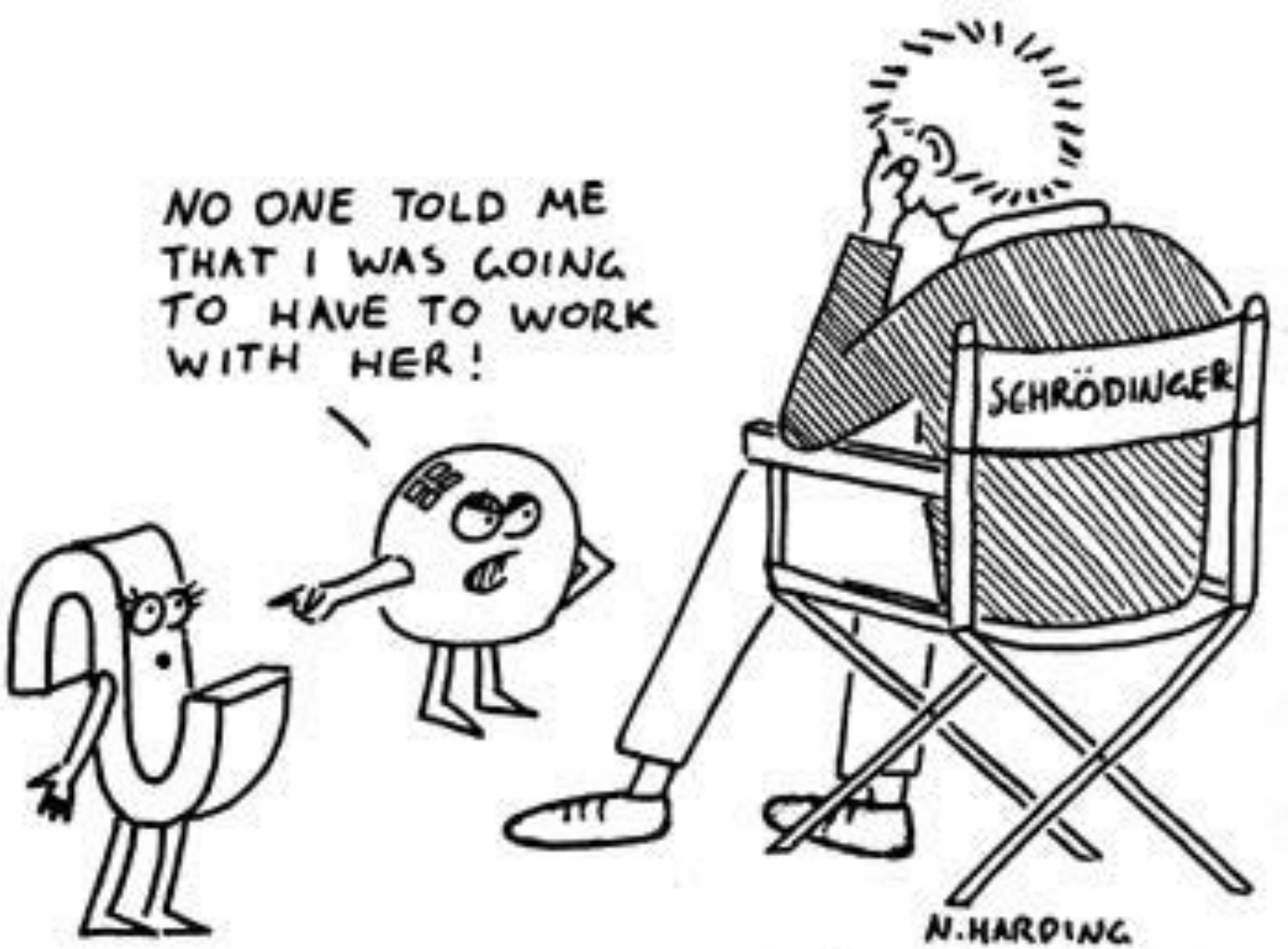
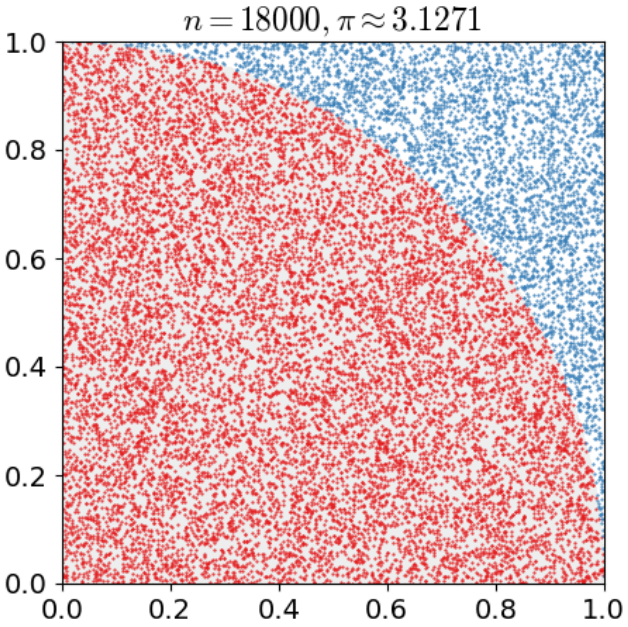
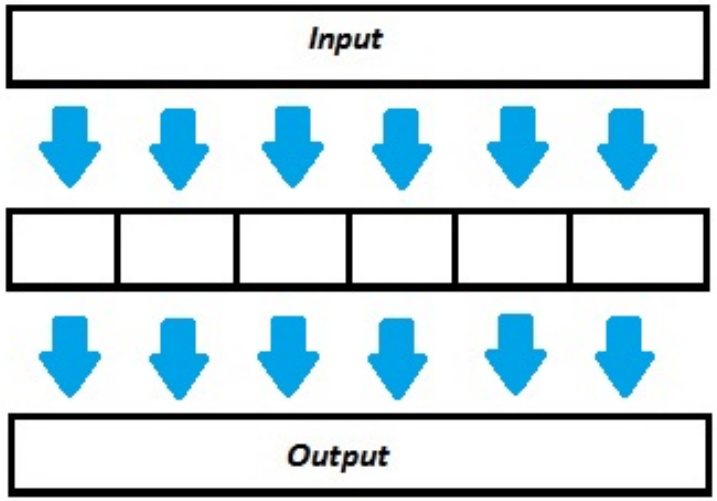
The ultracold inferno enables simulation of the the reaction through semiclassical treatment of the hot intermediate and quantum treatment of the cold products.



Monte Carlo integration is used to determine the number of ways that atoms can be arranged in the hot intermediate semiclassically.





Blue Waters enables the use of quintillions of sampling points via data paralellism.

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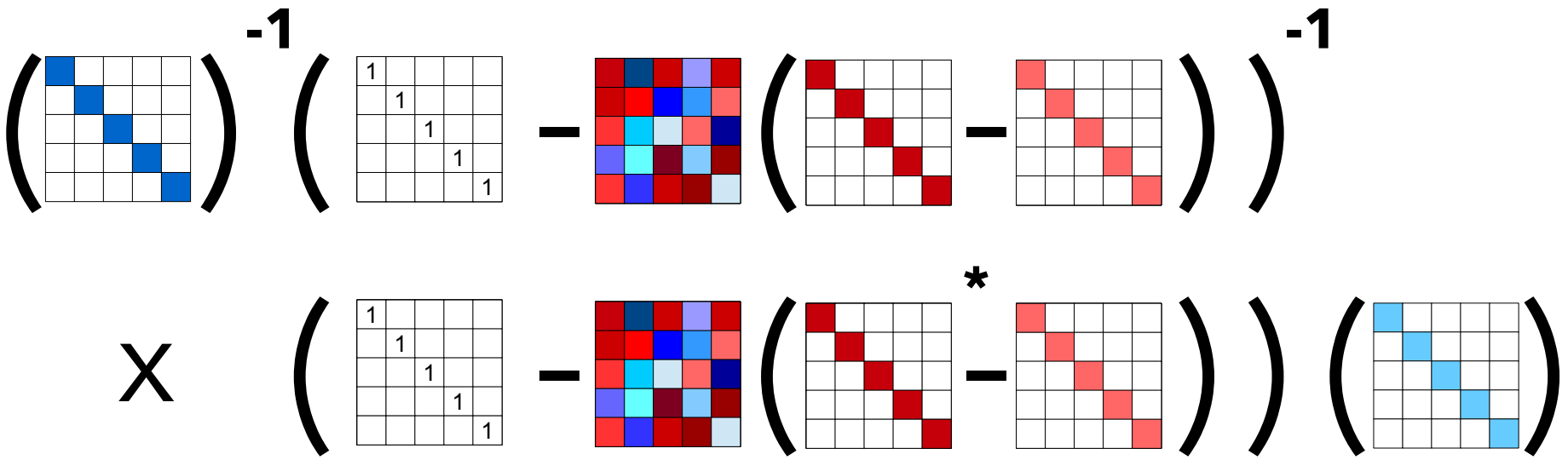
Random matrix theory and *R*-matrix theory are used to analyze the cold products quantum mechanically.



Parallelization on Blue Waters with ScaLAPACK enables manipulation of large, non-sparse matrices.

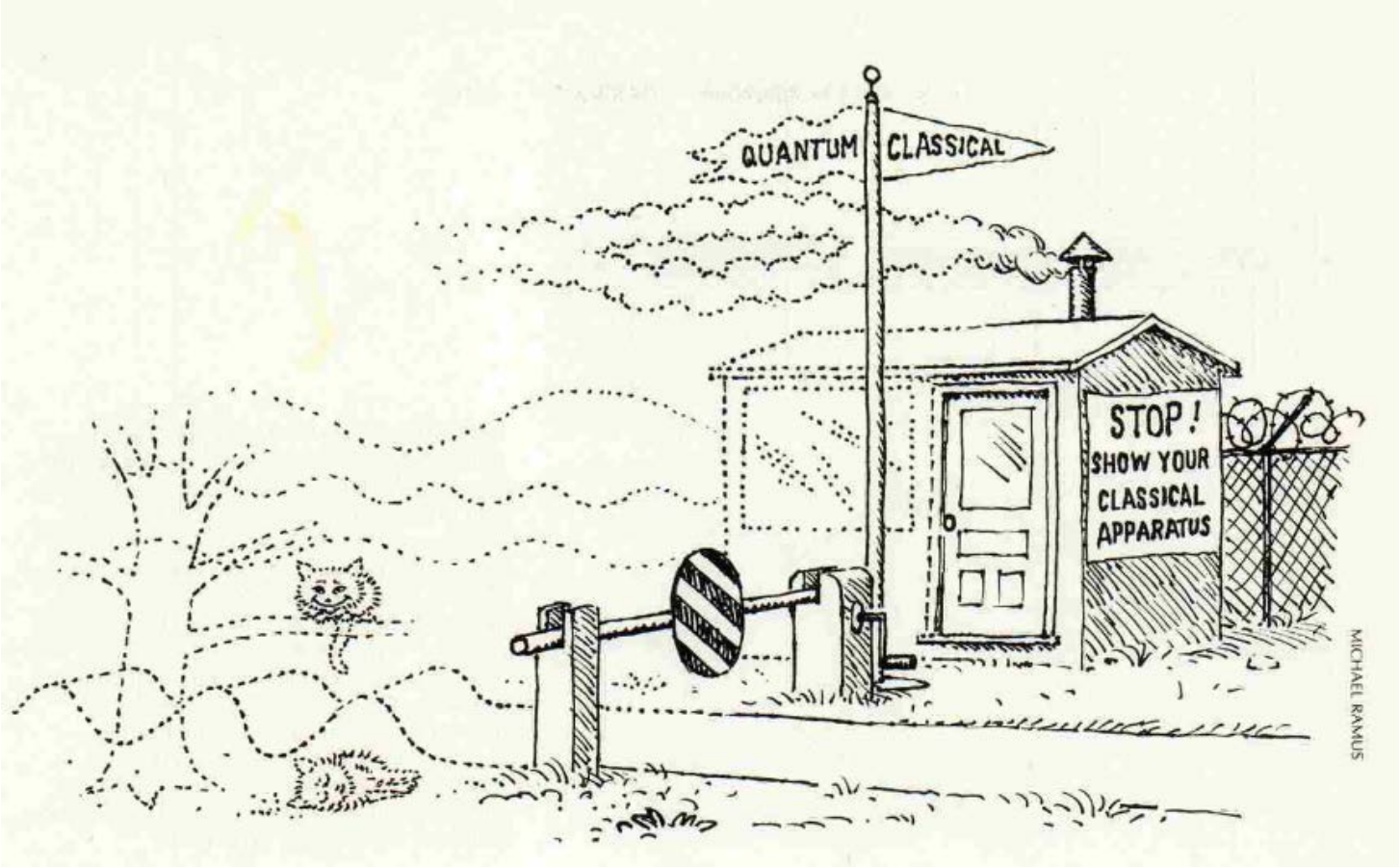
Accomplishments

Preliminary results suggest semiclassical mechanics is not only computationally efficient, but also nearly exact for the hot intermediate.

Type	Molecules	Semiclassical	Quantum	Analytic
Rigid Rotors	K_2	$1.224 \cdot 10^5$	$1.225 \cdot 10^5$	$1.224 \cdot 10^5$
	Rb_2	$3.06 \cdot 10^5$	$3.058 \cdot 10^5$	$3.063 \cdot 10^5$
	K_2, Rb_2	$1.875 \cdot 10^{10}$	$1.874 \cdot 10^{10}$	$1.874 \cdot 10^{10}$

Why It Matters

The combination of classical and quantum mechanics makes possible computational simulation of systems previously considered off-limits.



Broader Impact

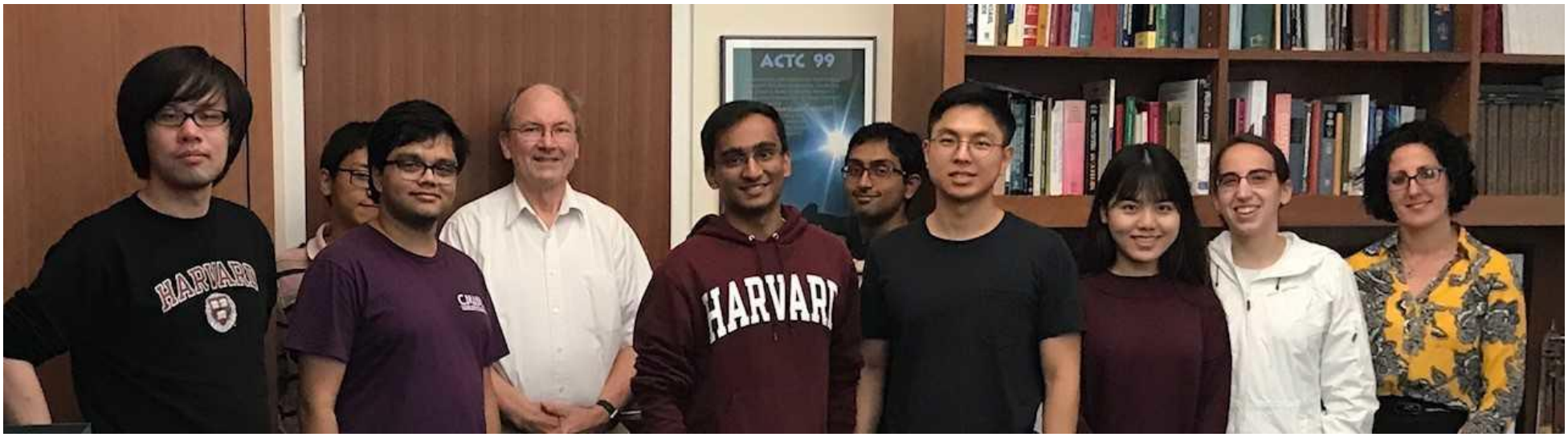
Simulation of the ultracold KRb dimer reaction on Blue Waters has the power to impact a wide range of fields.

- Theoretical ultracold chemistry
- Experimental ultracold chemistry
- Computational chemistry
- Physics, chemistry, and computer science communities

Blue Waters Contributions

- Education on supercomputing techniques
- Computational support and resources not otherwise available
- Discussion with researchers from other fields

Acknowledgments



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And you, for your attention!