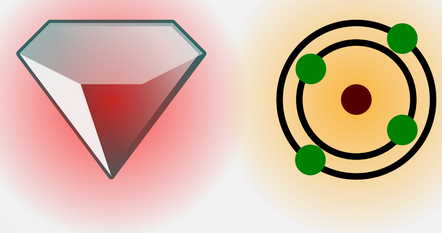
Optimised numerical simulation of quantum sensors with rich time dependence,

or...

We made the time-dependent Lindblad equation much faster to simulate

1 Design an atomic/ defect system.



Our **python** interface includes helper functions to construct arbitrary spin systems under time-dependent control.

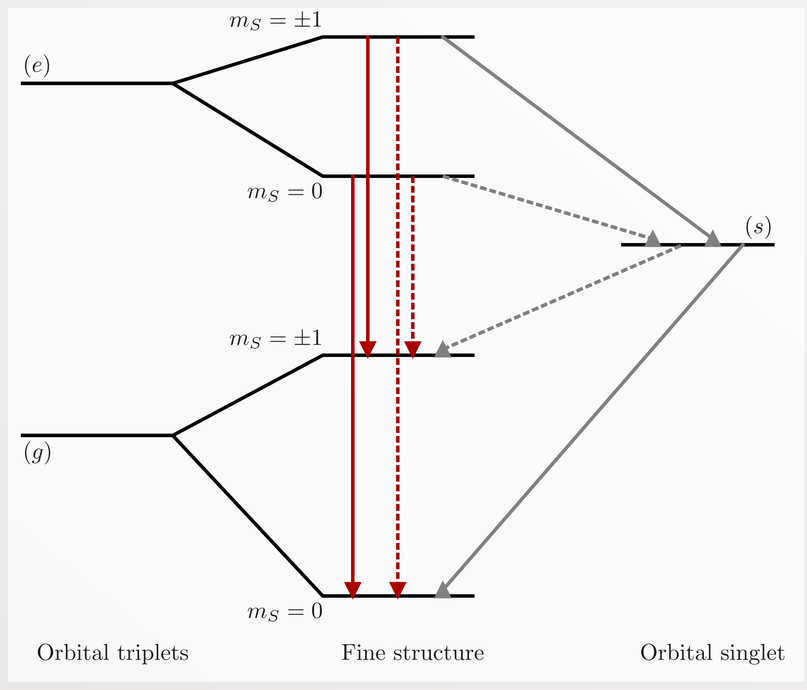
2 Vectorise Lindblad equation.

We express density matrices as vectors, and time evolution superoperators as matrices.

$$\frac{\mathrm{d}\hat{\rho}(t)}{\mathrm{d}t} = \hat{\hat{\mathcal{L}}}(t)\,\hat{\rho}(t) = [\hat{\hat{\mathcal{H}}}(t) + \hat{\hat{\mathcal{D}}}(t)]\,\hat{\rho}(t).$$

3 Transform problem to avoid numerical errors and remove redundancies.

The spin/optical model for nitrogen-vacancy centres in diamond (below) says that there is no coherence between orbitals; only within triplets. We ignore these degrees of freedom.



We used quantum control theory to prove that the NV model cannot be further compressed.

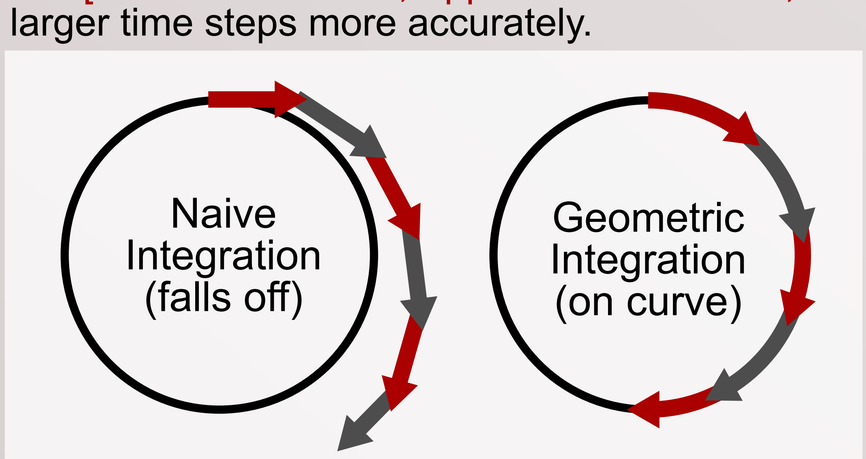
4 Calculate time steps in parallel on a GPU.

Each of the time evolution superoperators for different time intervals are independent, meaning they can be calculated in parallel on separate GPU threads.

$$\hat{\rho}(t_N) = \underbrace{\hat{\hat{\mathcal{V}}}(t_N, t_{N-1})}_{\text{Thread } N-1} \cdots \underbrace{\hat{\hat{\mathcal{V}}}(t_2, t_1)}_{\text{Thread 1}} \underbrace{\hat{\hat{\mathcal{V}}}(t_1, t_0)}_{\text{Thread 0}} \hat{\rho}(t_0).$$

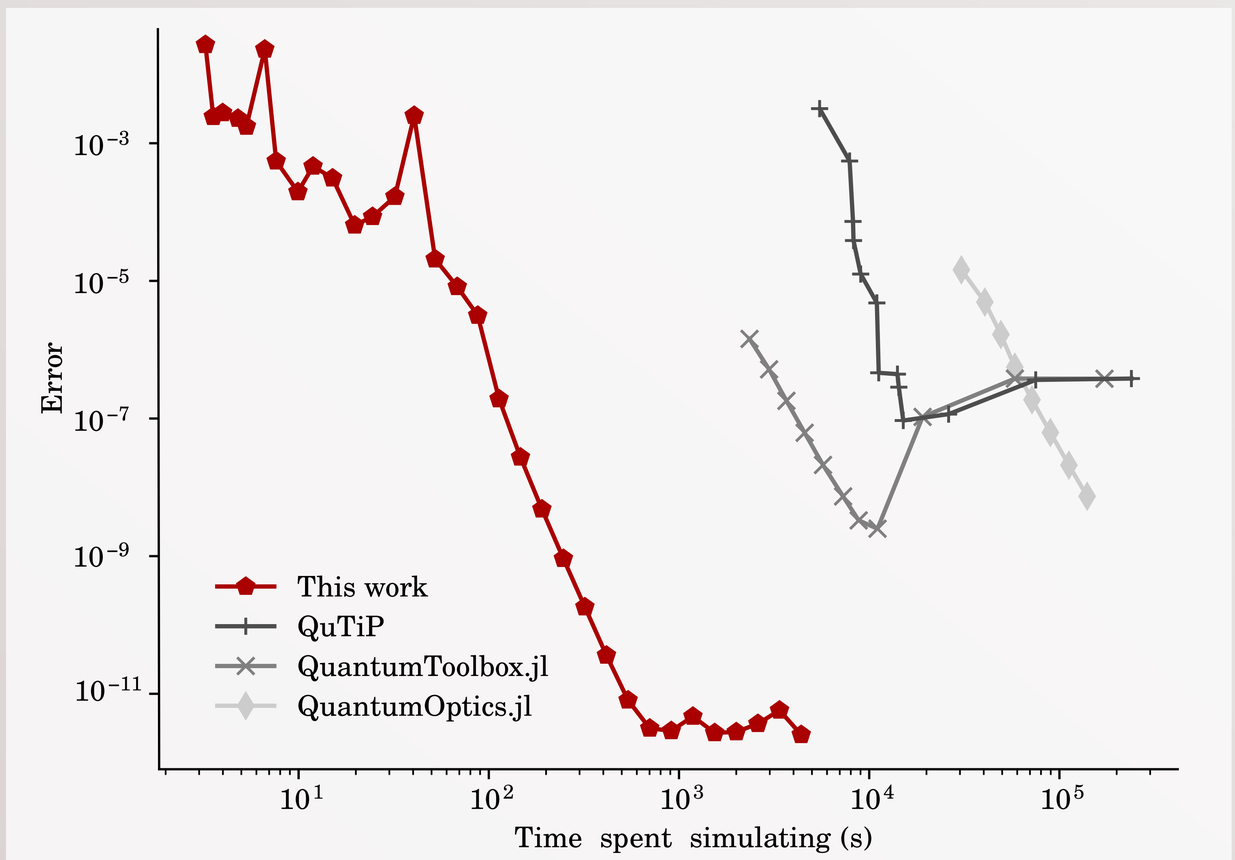
5 Respect geometry while integrating.

We use a commutator-free Magnus integrator - a geometric integrator - [Blanes and Moan, Appl.Numer.Math. 56, 12 (2006)] to take larger time steps more accurately.



6 Profit! (Simulations complete faster)

Below is a comparison of our simulation technique against standard packaged simulators. We simulate the 7-level spin/optical model of an NV-centre in diamond under an ODMR sweep, with the oscillations of the microwave chirp fully-rendered in time.



Scan for the GitHub repository for the **python** package, which is a **work-in-progress**.

```
pip install superspinsim
uv install superspinsim
```

Manuscript detailing techniques used also in progress.

See also: [Tritt et al., Comput.Phys.Commun. 287,108701 (2023)]

Alex Tritt[1], Lyryl H. C. Vaecairn[2], Charles Marrder[2], Michael S. J. Barson[1]

[1]School of Physics and Astronomy, Monash University, Victoria 3800, Australia
[2]JILA and Department of Physics, University of Colorado, Boulder, Colorado, USA

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