Magnetization Normalization Methods for Landau-Lifshitz-Gilbert

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Introduction

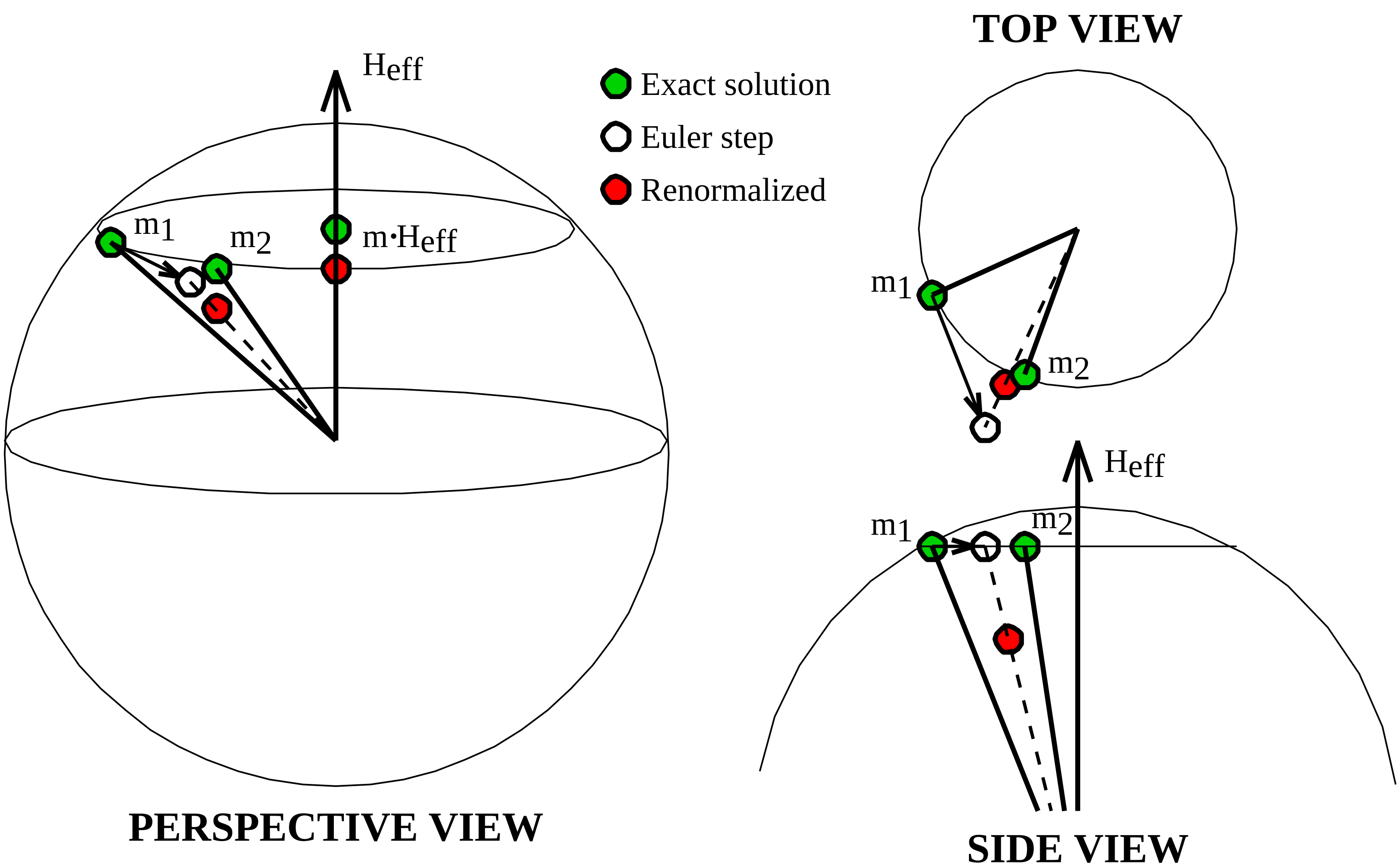
- Exact solutions of LLG,

$$\dot{m} = \frac{dm}{dt} = \frac{\gamma}{1+\alpha^2} m \times H_{\text{eff}} - \frac{\alpha\gamma}{1+\alpha^2} m \times H_{\text{eff}} \times m \qquad (1)$$

  satisfy $|m| = 1$.

- Cartesian numerical solvers allow $|m| \neq 1$.
- Renormalization required to put solvers back on track.
- Different renormalization techniques influence results.

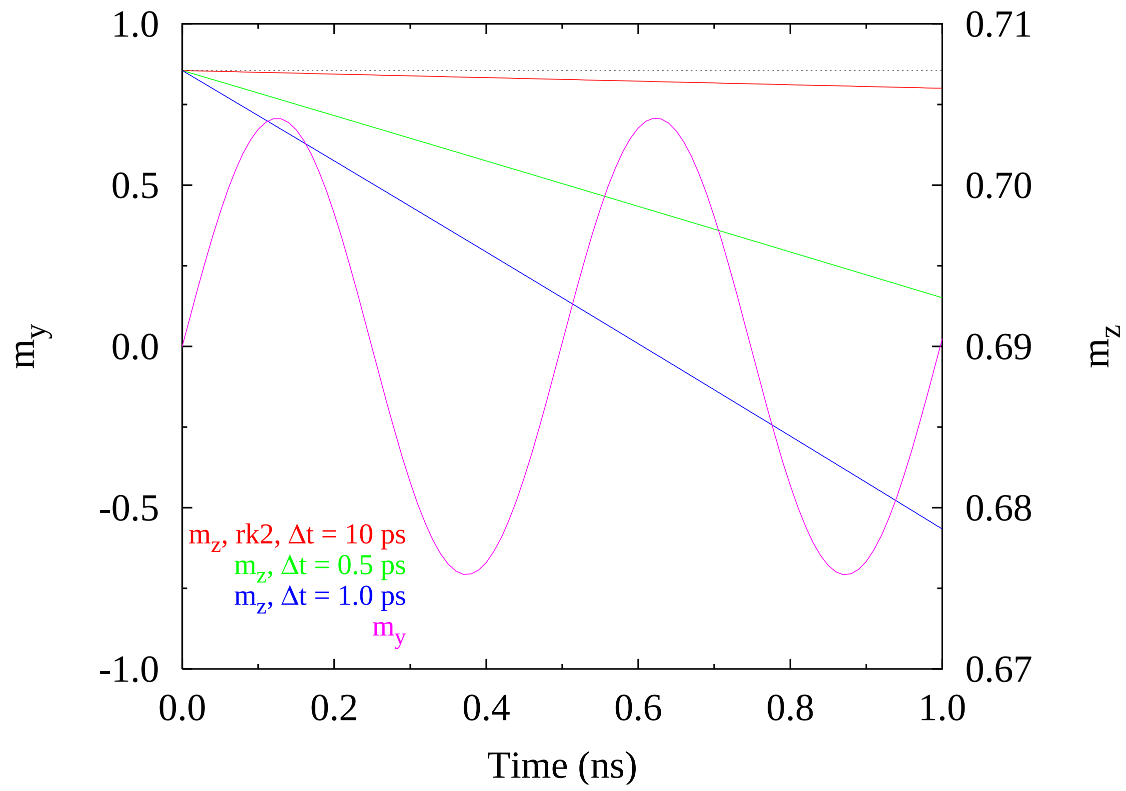
Example: Single Spin Undamped Precession



Renormalization Artifiacts

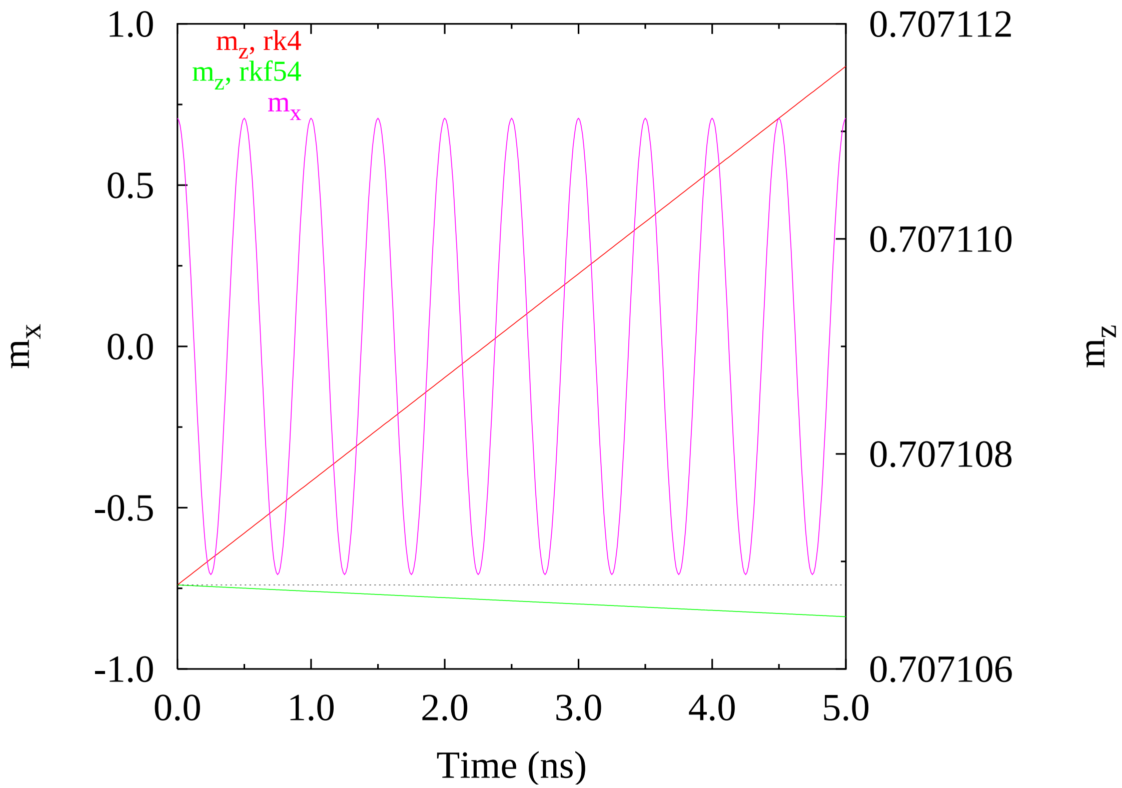
- Traditional (naive) renormalization
  - Keep direction
  - Reset magnitude to 1.
  - Nearest point on sphere.
- Produces error in $m \cdot H_{\text{eff}}$.
- Therefore, error in energy, dissipation rates, etc.

Single Spin, Euler Integration



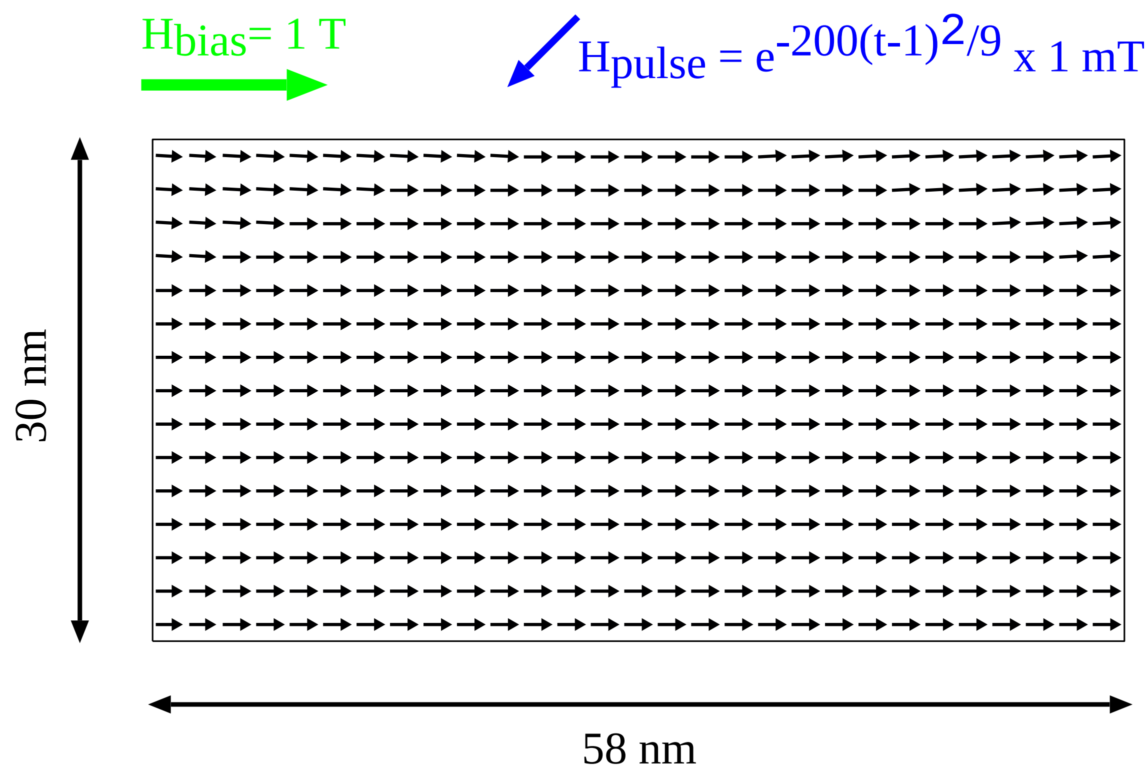
- Damping $\alpha = 0 \Rightarrow m_z$ (= -energy) should be constant.
  (rk2 is second order Runge-Kutta, others are 1st order Euler.)

Single Spin, Runge-Kutta Integration



- Similar (but smaller) errors. Time step = 10 ps.
  (rk4 = 4th order; rkf54 = 5 + 4th order Runge-Kutta-Fehlberg.)

Micromagnetic Example: Instabilities



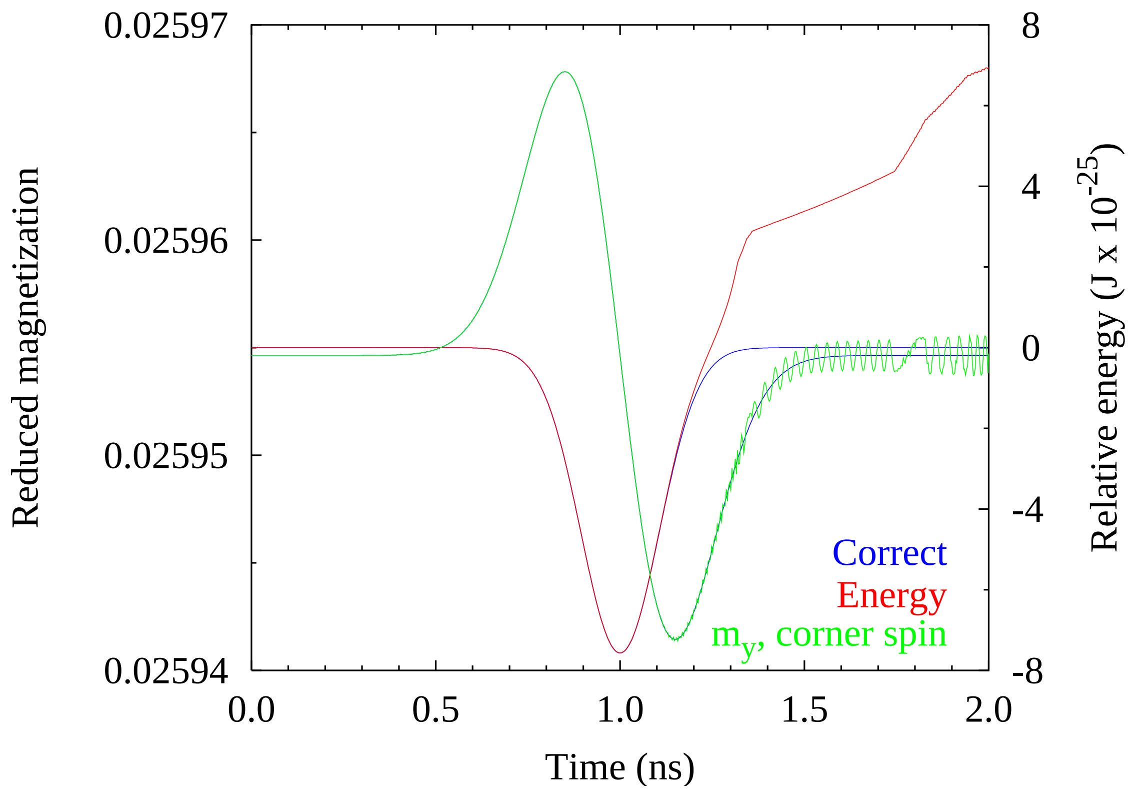
Thickness = 2 nm

Py material parameters

Simulation cellsize = 2nm

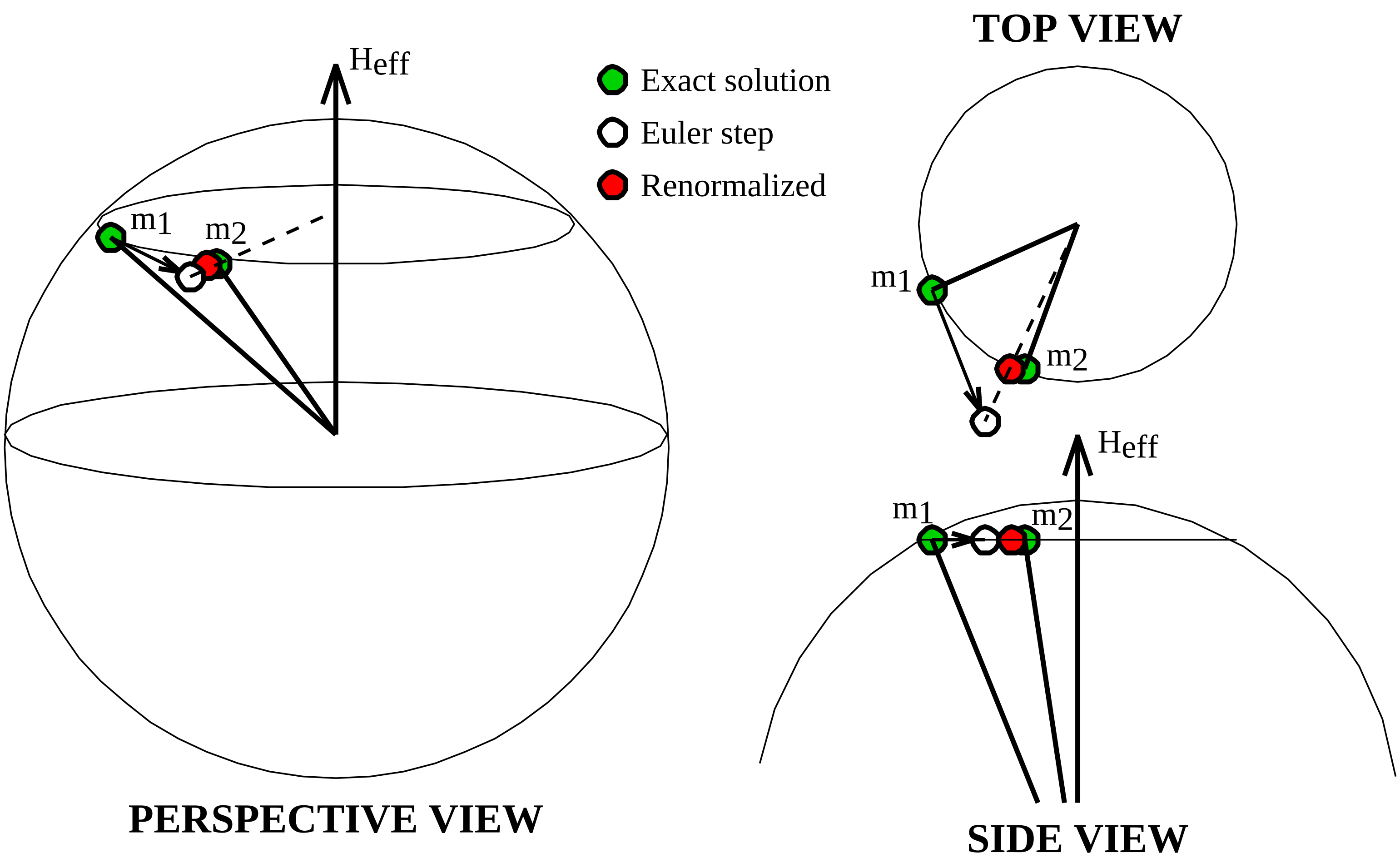
Damping $\alpha = 0.001$

Renormalization Induced Instability



- rkf54 method, variable stepsize.

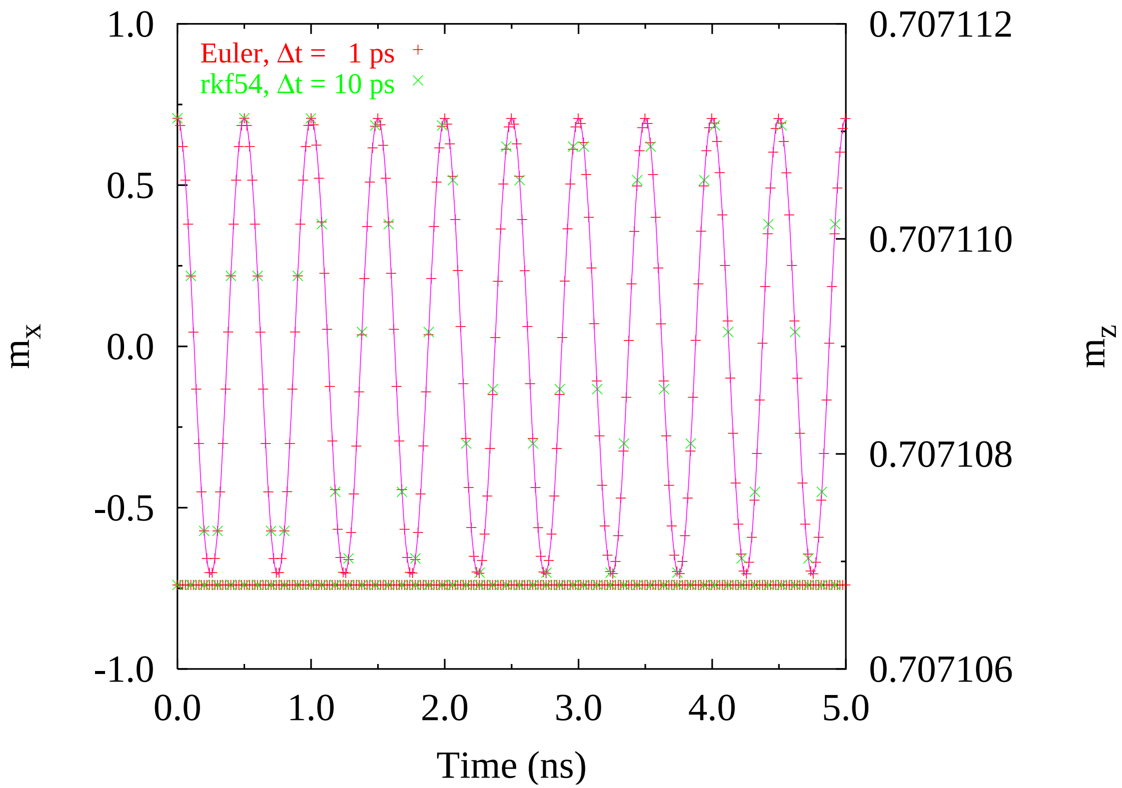
Revised Example: Modified Normalization



Revised Example: Modified Normalization

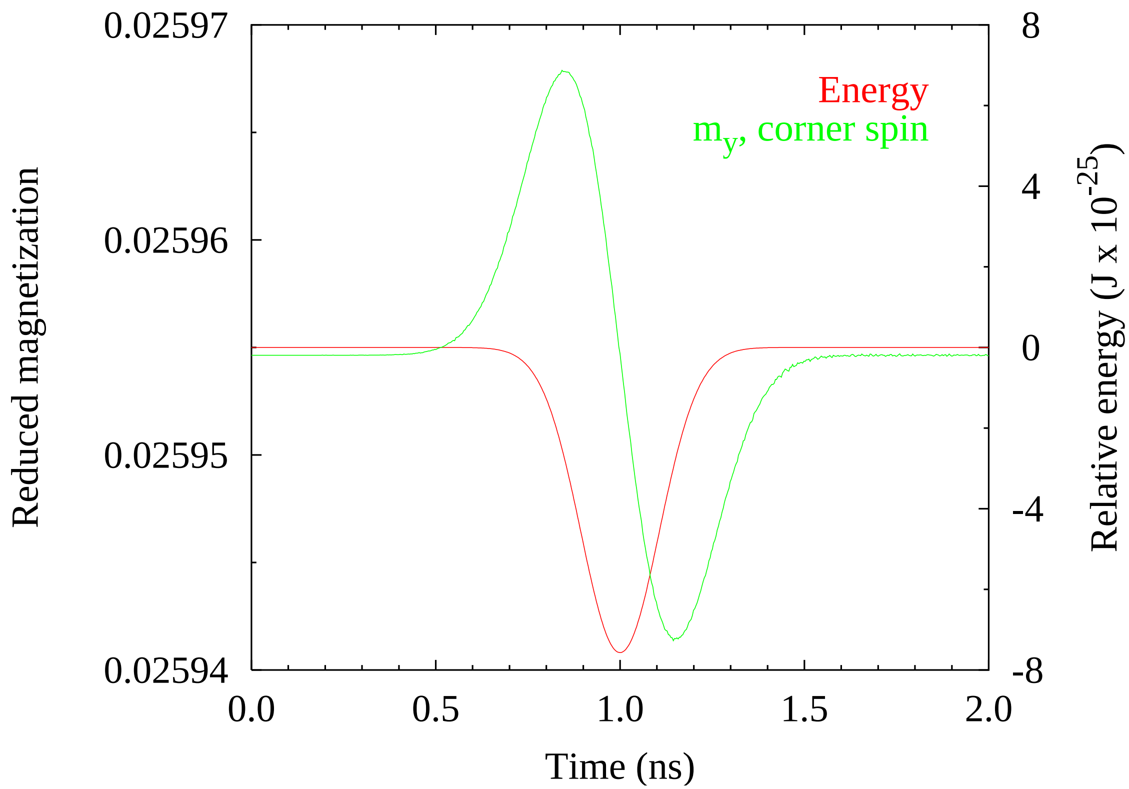
- Modified renormalization
  - Adjust both direction and magnitude.
  - Nearest point on "orbit of precession".
  - Generalized orbit: Nearest point on intersection of sphere and plane through unnormalized value perpendicular to $\dot{m}_1 \times \dot{m}_2$.
  - Generalized orbit accounts for non-zero damping and for dependence of H_{eff} on m.
- Greatly reduced errors.

Modified Normalization, Single Spin



- Revised normalization improves all integration techniques. (Data points are subsampled.)

Modified Normalization, Stability



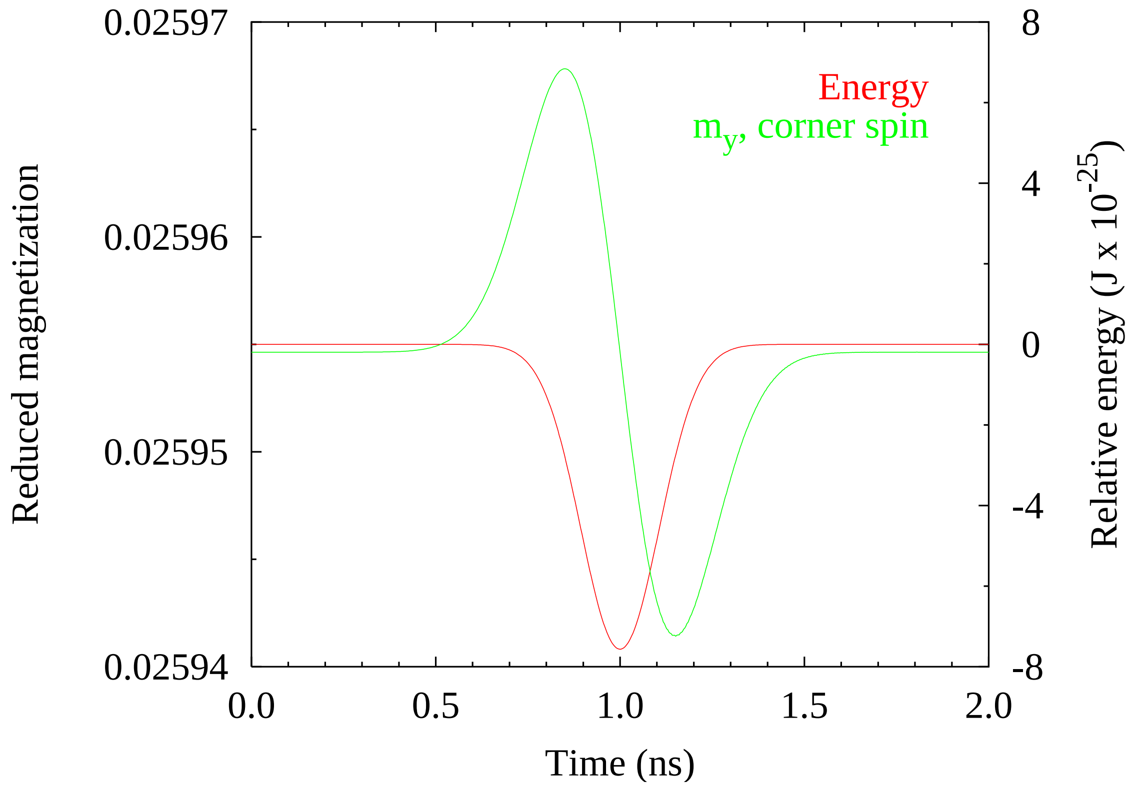
- Revised normalization greatly reduces instability.

Revised Equation

$$\dot{m} = \frac{\gamma}{1+\alpha^2} m \times H_{\text{eff}} - \frac{\alpha\gamma}{1+\alpha^2} m \times H_{\text{eff}} \times m + u(|m|-1)V(m) \quad (2)$$

- $u(\cdot)$ is scalar weighting function, output from PID controller. Initially, $u(0) = 0$.
- $V(m)$ is vector in same direction as modified normalization.
- Exact solutions of (2) are same as exact solutions of (1).
- Correction term in the equation itself has advantages:
  - More direct use by solvers with automatic step size control
  - Multi-step solvers do not require resets at normalization points.

Modified LLG, Stability



- No instability with modified LLG.
- Also fixes single spin precession (not shown).

Summary

- Cartesian solvers employ renormalization when solving LLG.
- Simple renormalization choice introduces artifacts.
  - Energy calculation errors compared with analytical solution.
  - Numerical instabilities in more complex problems.
- Modified renormalization techniques yield improved results
  - Normalization to “orbit of precession”
  - Modified equation that self-corrects to normalized values.