Computing the demagnetising tensor for finite difference micromagnetic simulations via numerical integration

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Summary

- In finite difference micromagnetic simulations, the demagnetising field is computed as a convolution of magnetisation with the demagnetising tensor
- The demagnetising tensor is the multidimensional integral of the potential function $1/|r|$ over the interacting cells
- Usually computed using an analytical formula
- At distances far from the originating cell, the analytical formula is inaccurate
- We compute the demagnetising tensor using numerical integration
- Compare the accuracy and performance to the explicit formula and to an asymptotic expansion for large R

Demagnetising tensor

The magnetostatic energy of a uniformly magnetised cuboid cell τ due to the field of a uniformly magnetised cuboid cell τ' is a bilinear function (i.e. a rank 2 tensor) of the cell magnetisations $\mathbf{M}$ and $\mathbf{M}'$:

$$E = -\frac{1}{2}\mu_0 \tau \, \mathbf{M} \cdot \mathbf{N} \cdot \mathbf{M}' \quad (1)$$

where $\mathbf{N}$ is the demagnetising tensor

$$\mathbf{N} = -\frac{1}{4\pi\tau} \int_{\tau} dr \int_{\tau'} \nabla_r \nabla_{r'} \frac{1}{|r - r'|} dr' \quad (2)$$

The demagnetising tensor is dimensionless, and if the cells are congruent, symmetric. In finite difference micromagnetic simulations, the values of $\mathbf{N}$ are precomputed for each possible offset between the interacting cells τ and τ' of the mesh.

Smolyak quadrature

The demagnetising tensor integral (2) can be computed analytically [1]. However, if the distance between the cells is large, numerical computation using the analytical formula loses precision [2]. As shown on the right, if a mesh has more than ~ 100 divisions in a certain dimension, the computed result may be inaccurate even in the most significant digit.

In this work we compute the demagnetising tensor numerically using Smolyak quadrature [3] and compare the result with the analytical calculation. The 6d multidimensional integral can either be computed directly or first converted to a 4d integral using the Gauss formula.

Smolyak quadrature computes the multidimensional integral

$$I^d[f] = \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} \quad (3)$$

using a family of quadrature rules Q_n^d derived from a family of one-dimensional quadrature rules Q_n according to:

$$Q_n^d[f] = \sum_{|\mathbf{i}| \le d+n} (\Delta_{i_1} \otimes \ldots \otimes \Delta_{i_d})[f] \quad (4)$$

where

$$\Delta_i = Q_i - Q_{i-1} \quad (5)$$

For a certain number of integrand evaluation points, Smolyak quadrature obtains a good (and in some sense optimal) order of approximation for the desired multidimensional integral.

Several options are available for the choice of the one-dimensional quadrature rule sequence Q_n. The currently popular choice is the so-called delayed Kronrod-Patterson sequence described in [4].

The best results are obtained when the 4d integral is used in conjuction with the quadrature formula based on the delayed Kronrod-Patterson rule. The accuracy in the intermediate range of intercell distances is significantly higher compared to the analytical formula or the asymptotic expansion.

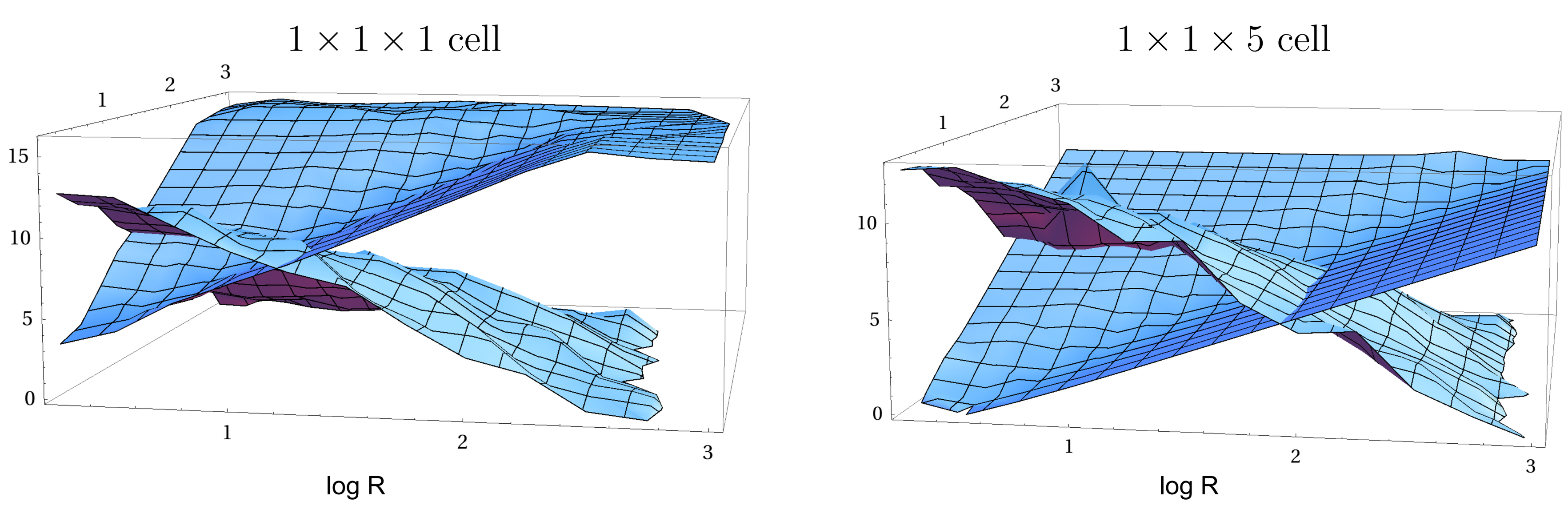
Future work

- Devise an error estimation scheme that can be used to select the appropriate algorithm (analytical, numerical, asymptotic)
- Investigate how the added accuracy influences the calculation of the demagnetising field as well as the precision of micromagnetic simulations in general
- Perform the measurements in single precision floating point (commonly used for GPU calculations)

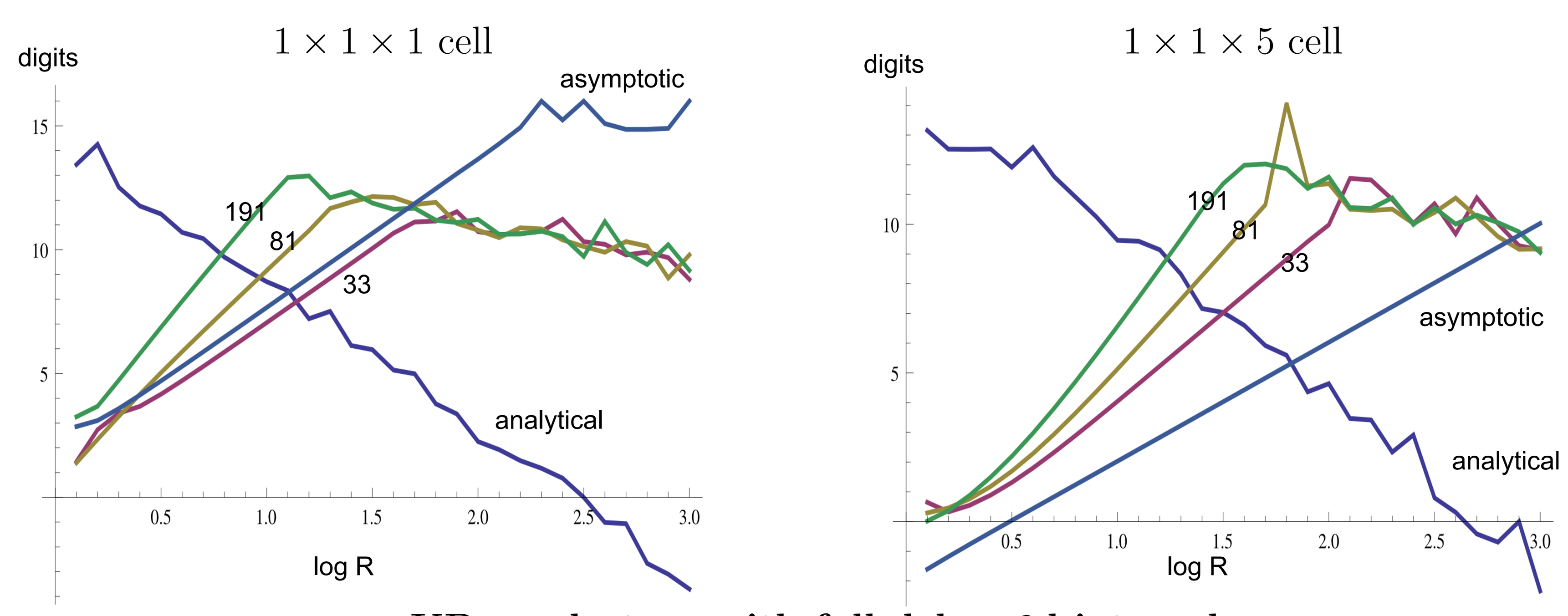
References

1. Newell A.J., Williams W., Dunlop D.J. A Generalization of the Demagnetizing Tensor for Nonuniform Magnetization. *Journal of Geophysical Research.* **98** (B6) 1993.
2. Accurate computation of the demagnetization tensor, M.J. Donahue, *6th International Symposium on Hysteresis Modeling and Micromagnetics*, Naples, Italy 2007.
3. Smolyak S.A., Quadrature and interpolation formulas for tensor products of certain classes of functions, *Soviet Math. Dokl.* **4** 1963
4. Petras K., Smolyak cubature of given polynomial degree with few nodes for increasing dimension, *Numerische Mathematik.* **93** (4) 2003

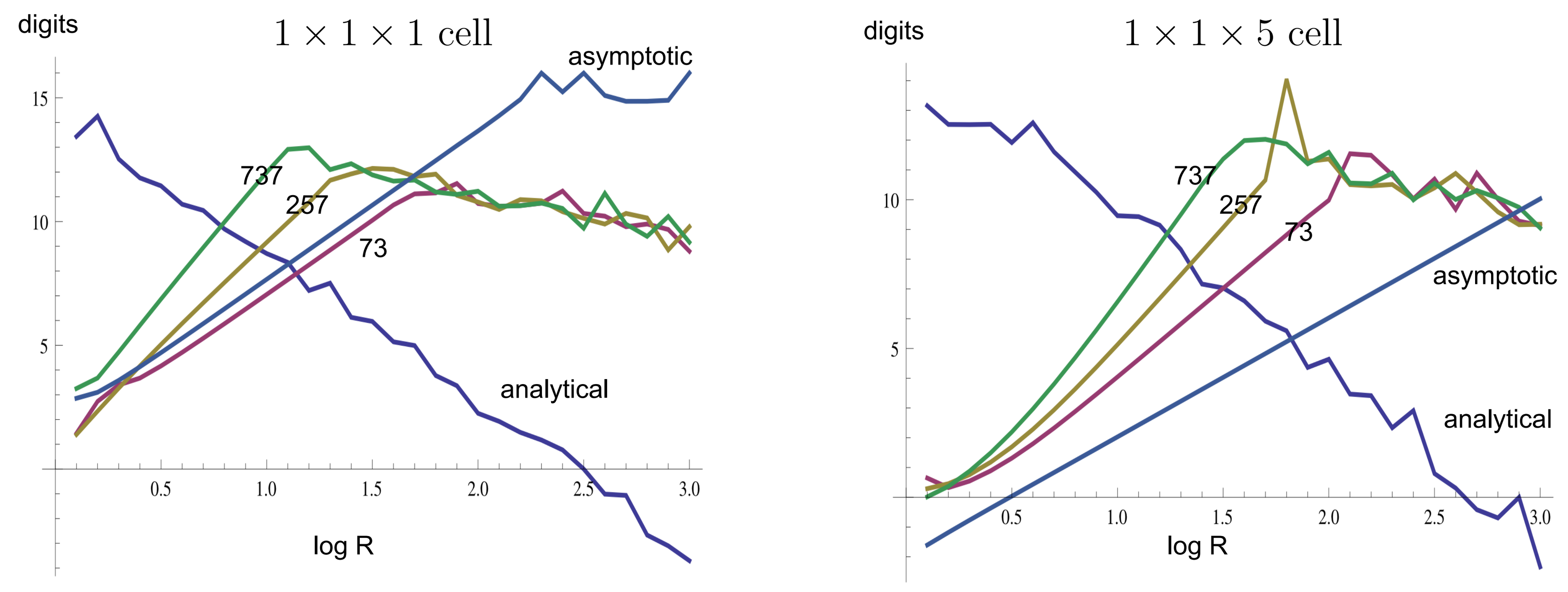
Accuracy of analytical and asymptotic computation



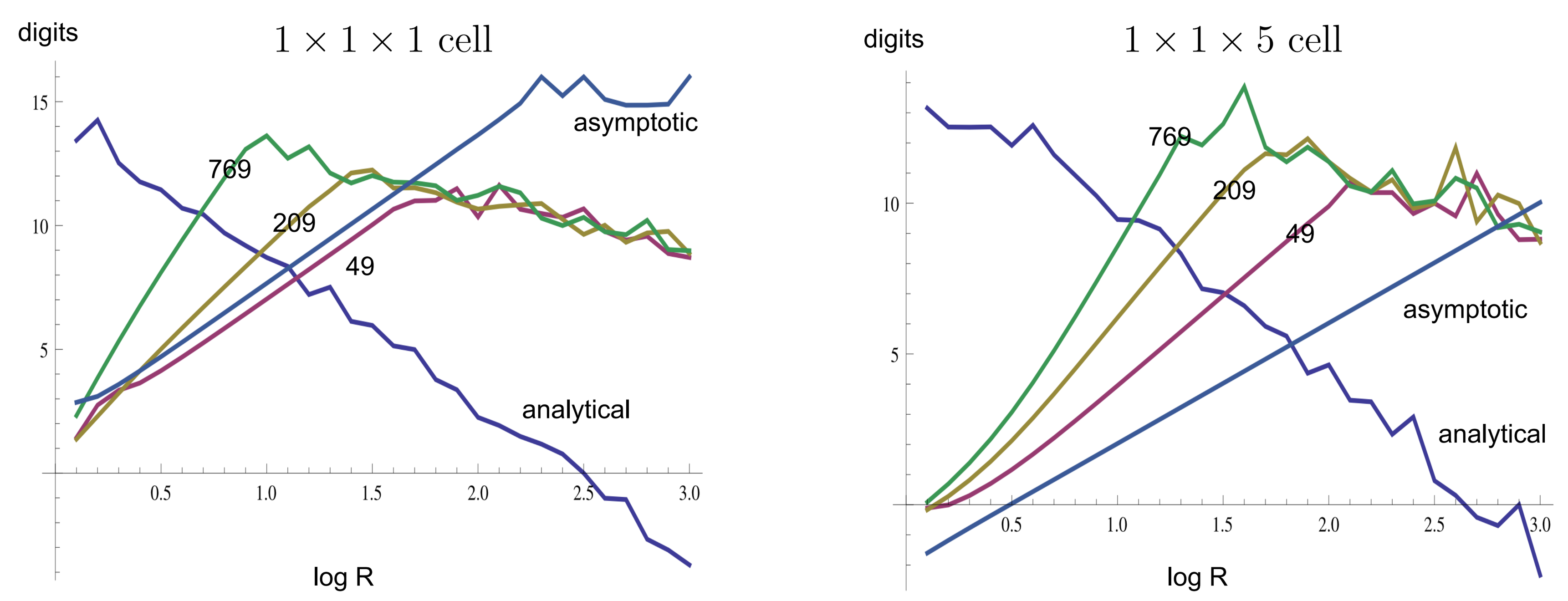
Kronrod-Patterson quadrature with full delay



KP quadrature with full delay, 6d integral



Kronrod-Patterson quadrature, no delay



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