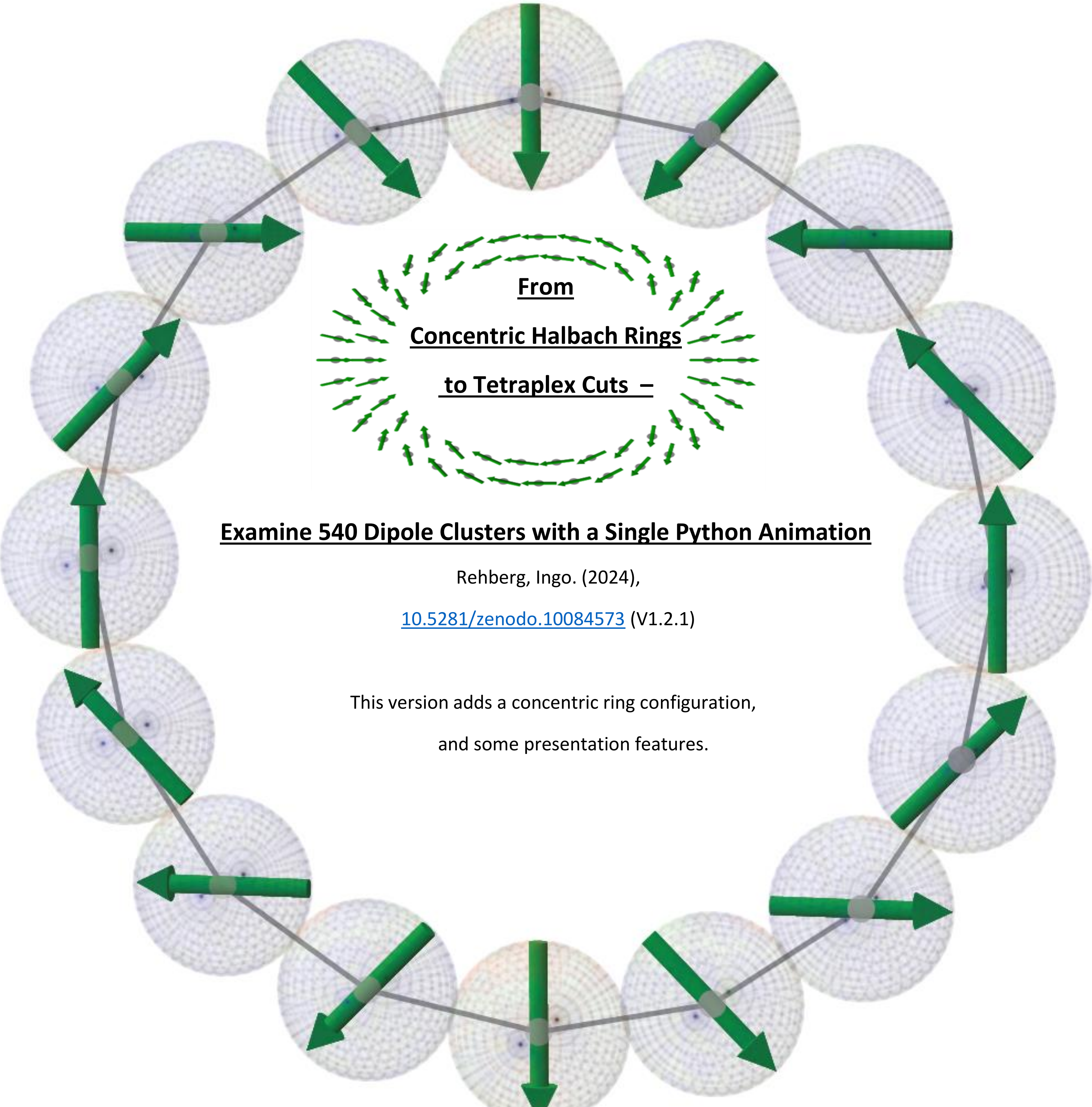


From

Concentric Halbach Rings to Tetraplex Cuts –

Examine 540 Dipole Clusters with a Single Python Animation

Rehberg, Ingo. (2024),

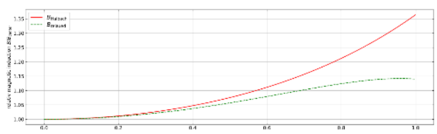
10.5281/zenodo.10084573 (V1.2.1)

This version adds a concentric ring configuration,

and some presentation features.

Some observations from the exploration of Halbach rings:

The Halbach ring configuration denoted dipole is not a stable state. In the animation the magnets are allowed to rotate, and you might let them relax into an equilibrium configuration with a remarkable homogenous field inside the ring.



- The field of the Halbach configuration is larger than that of the relaxed configuration.
- The Halbach configuration has no total magnetic moment.
- The field inside the relaxed ring is more homogenous.
- There is no torque acting on the individual dipoles in the relaxed state.

Version 1.2.1 adds a concentric ring configuration (which cannot be interactively changed yet, however). Other features added allow a faster presentation and a better documentation of the results:

- The dipole configuration can be saved in a csv-file for further examination with other programs.
- In addition, a screenshot of this configuration is saved with the same name as the data file, in the same directory.
- Additional Buttons to control
  - the viewing angle of the 3d-plot.

Version 1.2.0 added the 3d-cuts of the tetraplex to the list of animated clusters. Other features added:

- Halbach configurations as starting condition.
- Stopping the cluster rotation produces a file with an image of the cluster configuration.
- Additional sliders to control
  - the direction of the field examination and
  - the location of the second cluster.

Version 1.1.1 also added technical animation features:

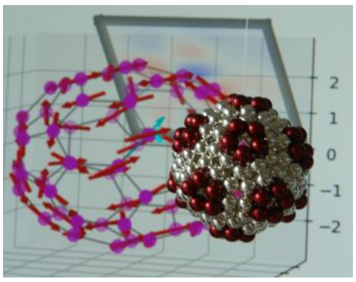
- Visualization tools:
  - A continuous rotation of the 3d-cluster turned on or off.
  - Axes visible or invisible.
  - Dipole moments visible or invisible
- The scalar magnetic potential can be shown along the same line as the field.
- Feedback to judge the timing of the actions triggered by the interactive steering.

Version 1.1.0 added the rhombicuboctahedron to the list of animated clusters. Other features added:

- Interactive tuning of the magnetic moment of selected dipoles, used for demonstrating:
  - The circular-dipolar transition in the filled hexagon geometry [4].
  - The radial-axial transition in magnetic tubes [5].
- An indicator for the toroidal magnetic moment.
- Orientation-dependent colours to emphasize the radial-axial transition in tubes.
- A switch between triangular and cubic tubes.

Version 1.0.1 erased some trouble of the former version with the sliders of Matplotlib 3.8.0.

General Motivation: The dipole-dipole interaction is a substantial part of the force that holds matter together. Since the electric and magnetic dipole-dipole interactions are mathematically equivalent, this fundamental interaction can be experimentally examined with magnetic spheres. For a numerical investigation the software package "dipole_clusters.py" allows an interactive examination of



- the dipole arrangement,
- the field,
- and the interaction

for more than 500 dipole clusters.

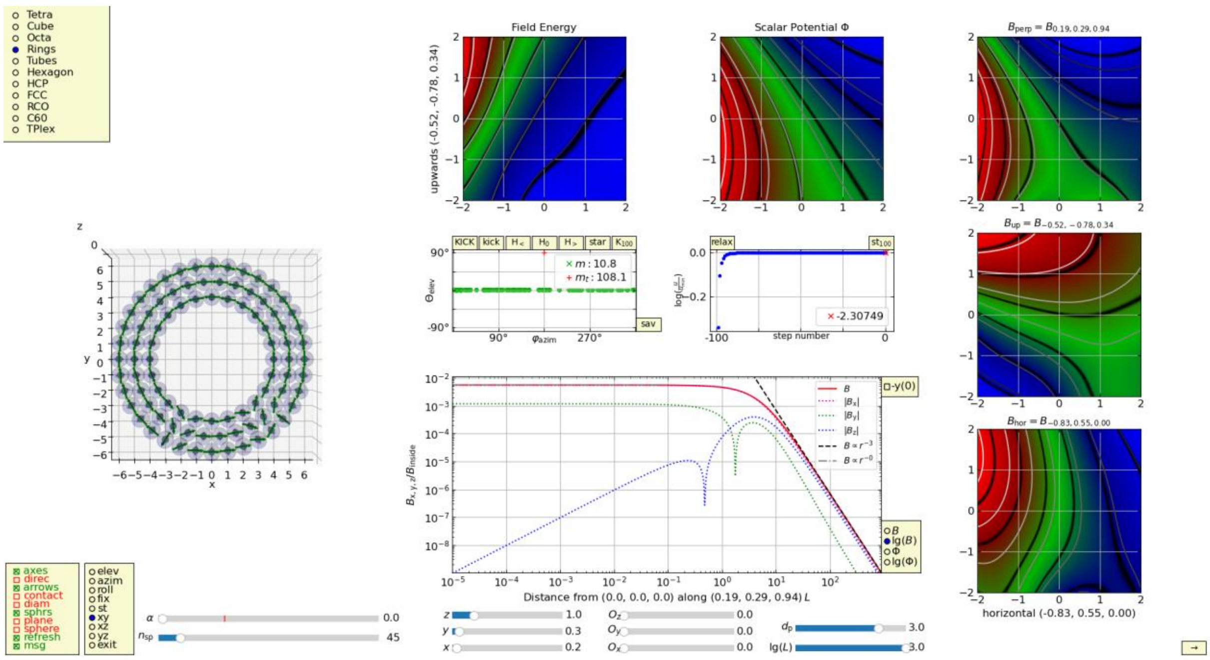
Using the software:

The program "dipole_clusters.py" comes as a Python script [1]. It is tested with Python 3.11.7, as downloaded from: https://www.anaconda.com/download/#windows. To get started, unzip the files in “dipole_clusters_1_2_0.zip”, and run “dipole_clusters.py”, which is located in the upper directory, e.g. by typing “python -i dipole_clusters.py”.

The animation acts on 2 pages shown in 2 different windows. It is organized in three parts:

1. You first choose the geometry of the cluster configuration. It is initialized with a random orientation of the dipoles.
2. Subsequently, you let the orientation relax into a local minimum of the magnetic energy for a fixed position.
3. Whenever you find the cluster sufficiently interesting, you can study the interaction of two such clusters in a second window.

The actions of part 1 and 2 are controlled from the first page. A screenshot of that is provided below:

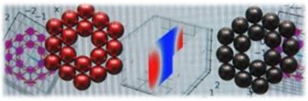


- The 11 “Tetra, Cube, …”- RadioButtons in the left upper corner allows to choose from 10 different types of clusters: the 5 Platonic solids (tetrahedron, cube [2], octahedron; the dodecahedron and icosahedron are obtained as 3d-cuts from the tetraplex), concentric rings (Rings) [3] and stacked rings of dipoles (Tubes), stacked hexagons filled with a center dipole (Hexagon) [4], the hexagonal close packed configuration of 13 dipoles (HCP), the face centered cubic lattice (FCC), the rhombicuboctahedron (RCO), and the C_{60} buckyball (C60). Five of these cluster types (Cube, Ring_{st}, Hexagon, FCC, TPlex) represent whole families and allow for variations via sliders (which pop up in consequence of the cluster selection). They provide the flexibility to create more than 500 different clusters.

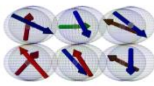
<u>For the tubes you control:</u>

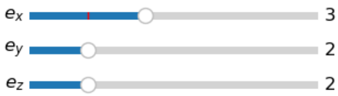
- The length of the ring L_r,
- The number of rings stacked n_s.

- The “tri, sqr”-RadioButton allows to choose between a triangular and square lattice arrangement of the spheres.
- The strength of the outer dipole moments m [5], as selected by “mom” in the “mom, dst”-RadioButton.
- The distance d between the two halves of the tube (selected by “dst”). Both parameters, d and m, might serve as a bifurcation parameter for the radial-axial transition.

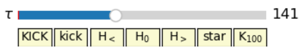
<u>The parameters of the FCC cluster</u>  <u>family are:</u>

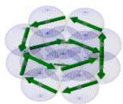
- The number of spheres along the 3 axes (e_i, e_j, e_k) of the triangular lattice.
- The inner and outer distance (r_i, r_o , measured from the center) of dipoles to be included in the cluster assembly. This is used, e.g., to create the plane ring configuration shown here.

<u>Parameters of the cube</u>  <u>family are:</u>

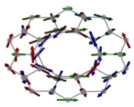


- The number of spheres along the 3 axes (e_x, e_y, e_z) of the cubic lattice.
- Adjustment of the angle in the continuous ground state of the 2×2×2-cube.



<u>Parameters of the filled hexagon</u>  <u>family are:</u>

- The number n_s of filled hexagons stacked.
- The dipole moment of the center dipole m].

<u>The parameter of the tetraplex family</u>  <u>is:</u>

- The number of those values of the fourth dimension which produce sufficiently rich 3d-cuts.

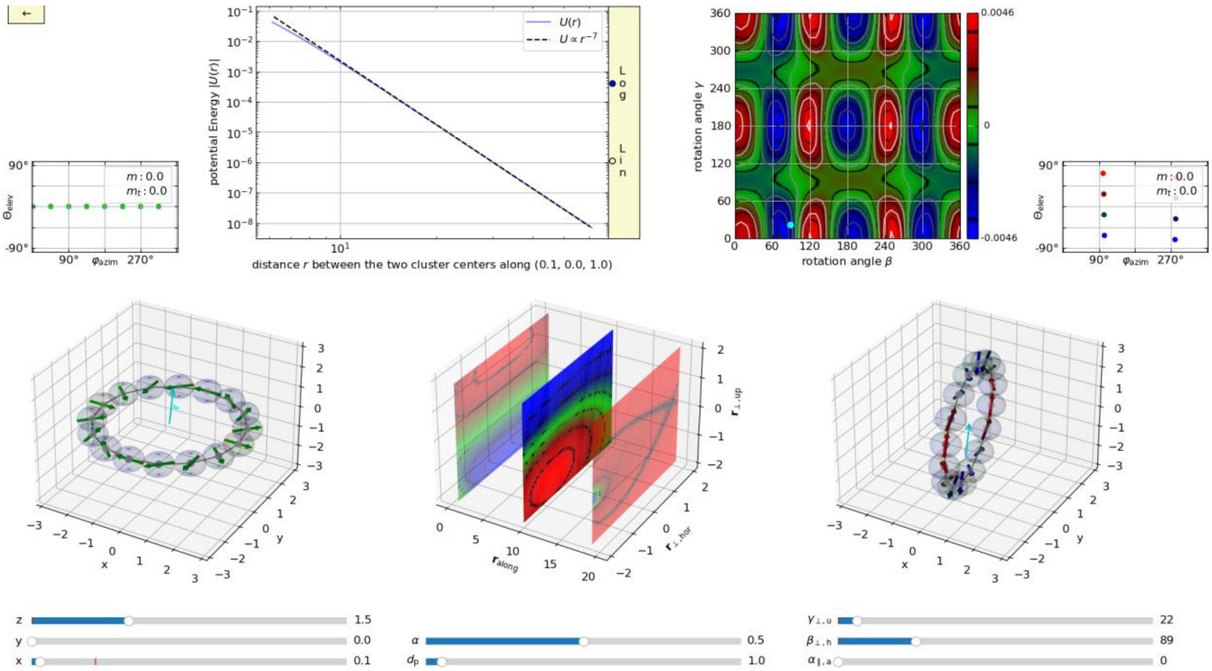
- The 3d-figure on the left hand side shows the location and orientation of the dipoles (here an example for a stable configuration of the RCO-cluster). Whether this stable state is the ground state is unknown, however. Additional observation tools can be integrated in this figure with the “axes, direc, arrows, contact, diam, sphrs, plane, sphere, refresh, msg”-CheckButtons:
  - axes toggles the 3d-axes between an and off.
  - direc turns the vector for the direction of the line, along which the field is calculated, on or off. The planes to display the field are perpendicular to this direction.
  - arrows indicate the direction of the dipoles. Their color is chosen according to the z-component: positive (negative, horizontal) direction red (blue, green).
  - Contact between spheres is indicated by grey lines connecting their centers.
  - Diam connects dipoles with the largest distance – the diameter – in the cluster.

- The spheres are shown only when the sphrs-option is checked, their transparency is controlled with the α-slider.
- Additionally, a component of the magnetic induction is shown on a plane, or spherical surface (as determined by the "plane, sphere"-CheckButtons). More precisely, it is the field component perpendicular to that surface.
  - Sphere: Its spatial resolution of the can be adjusted with the n_{sp}-Slider at discrete values within the range 10 to 360 (not shown in this screenshot). This number has to be chosen as a compromise between the artistic impression and the speed of the calculation.
  - Plane: It is chosen perpendicular to the cyan arrow shown inside the cube. Its direction and origin is changed with the 6 "x, y, z, O_x, O_y, O_z"-sliders in the lower middle part. The distance of the plane from the origin is set with the "d_p"-slider.
  - The α-slider sets the transparency of both surfaces, and of the individual spheres.
- When refresh is turned off, 6 figures are turned unvisible and are not updated. This speeds up the presention of the cluster geometry.
- msg controls the printing of some messages, which are helpful to judge the speed of the program. Many seconds might be needed to calculate all the measures provided in the plots for the larger clusters. Observing the messages might help you not to press too many buttons or sliders too quickly.

- Additional control of the 3d-plot is provided by the "elev, azim, roll, fix, st, xy, xz, yz, exit"-radioButtons:
  - elev, azim, roll change the viewing angle continously .
  - fix stops the rotation of the 3d-orientation. That should be done before leaving the animation.
  - st, xy, xz, yz switch to fixed viewing angles of the 3d-plot.
  - Exit stops the rotation and closes the animation.

- The figure in the lower middle shows the three ***B***-field components, or the scalar magnetic potential ψ, along the direction ***r*** as indicated by the cyan arrow, for a distance set by the lg(*L*)-Slider. They are shown on either a linear or a loglog-scale, switchable with the "*B*, lg(*B*), *ψ*, lg(*ψ*)"- RadioButtons. The asymptotic slope of the absolute value B_a or *ψ* is shown as a dashed line, and the slope near the center of the cluster is indicated by a dash-dotted line.
- The Figs. 3-7 on the upper and right hand side show aspects of the magnetic field (field energy density, scalar potential *ψ*, field component perpendicular to the plane, along the horizontal and vertical axis of that plane) within the plane perpendicular to the ***r*** direction, at a finite distance d_p determined by the d_p -slider. The same blue-green-red color map (legend on page 2) is used here.
- The figure "azimuthal angle" (x-axis) indicates the orientations of the dipoles in spherical coordinates as dots in the same color as the corresponding arrows. If the configuration has a magnetic moment *m*, its direction is indicated with a cross. Its strength is given in the legend (*m*=10.8 in the case shown here). The toroidal magnetic moment m_t is indicated by a ''+'' (m_t =108.1 in the case shown here).
- The "save"-button writes the current configuration into a csv-file and save the current figure under the same name in the same subdirectory named "config".

- The orientation can be disturbed by the 9 buttons named “KICK”, “kick”, “$H_<$”,“H_k”,“$H_>$”, “star”, “K_100”, “relax”, and “st_{100}”.
    - Clicking on the “KICK”-button will orient all dipoles randomly.
    - A smaller disturbance is provided by the “kick”-Button, which will add a small (10%) random distortion to the current configuration (this is useful for checking the stability).
    - The “H_k”-button produces a Halbach configuration with *k* rotations. It produces known results for rings, and interesting starting scenarios for the other clusters.
    - The “$H_<$”- and “$H_>$”-buttons decrease or increase the number of rotations *k*.
    - The “star”-button will create a cluster where all dipole point away from the center. If there is a center dipole, its direction will point along the x-axis.
    - The “K_100”-button will perform a “KICK”, followed by a “relax”-procedure described below. If the result has a lower energy as the former one, that new configuration will replace the old one and the search procedure stops. If the energy is not lower, the procedure will be repeated up to 100 times.
    - The “relax”-button will trigger a variable number of relaxation steps lowering the potential magnetic energy of the cluster configuration. After a few hundred relaxation steps that energy will appear as constant due to the finite numerical resolution, at this point the calculation stops. That state is stable, but not necessarily the ground state. The result is shown in the figure “step number”. The value of the potential Energy *U* after the last step is indicated by the label.
    - The “st_{100}”-button will trigger 100 relaxation steps.
    - The “sav”-button writes the current configuration into a file, together with a screen shot.
- The figure “step number” (x-axis) shows the magnetic potential energy of the configuration for the last 100 iteration steps. If no relaxations steps have been performed, it will show the current value 100 times.
    - The “st_100”-button start 100 relaxation steps.
    - The “relax”-button start relations steps, which will finish, when numerical convergence is reached.
    -
- The →-button on the lower right hand side sends the current cluster configuration to a further analysis with respect to the mutual interaction between two such clusters. It is displayed in a second page shown below. The calculation takes some seconds up to several minutes, depending on the number of dipoles.



A screenshot from the second page showing aspects of the interaction of two Halbach rings.

The coordinate systems of the two identical clusters are parallel to each other. For the animation, the center of the second cluster is located at a fixed distance of 20 along the ***r*** –direction, which is indicated in cyan color. ***r*** can be manipulated with the y, z-sliders. The interaction between both clusters is characterized by the potential *U(r)* shown in the upper plot on a logarithmic or linear scale, as chosen by the "log, lin"-RadioButtons. The asymptotic decay is indicated by the dashed line. The example shown here indicates that the interaction potential between two Halbach rings composed of 16 dipoles decays with the 7^{th} power of the distance, i.e. the repelling (red line) or attracting (color changes to blue) force decays with the 8^{th} power.

While that power is robust for all orientations of the second cluster, both the sign and the prefactor are a function of its rotation, which is manipulated with the "α-, β-, γ"-Sliders. The first rotation is around ***r***, the second around the horizontal perpendicular to ***r***, the third around the vertical perpendicular to ***r***. The "rotation angle β"-figure indicates *U(*β, γ*)*, with α fixed to the value of the corresponding slider.

The lower middle plot illustrates that interaction further for a fixed distance of *r*=20 between the cubes centers measured along the direction of the cyan arrow ***r***. In this figure the coordinate system is chosen such that the x-axis is parallel to the cyan arrow ***r*** shown in the center of the left cube. The planes on the left and right hand side indicate the scalar potential from the corresponding cube. The plane in the middle denotes the component of the Maxwell stress tensor, such that the integral over this plane (extended to infinity) gives the strength of the force component $\boldsymbol{F}_{along}$ measured along ***r***.

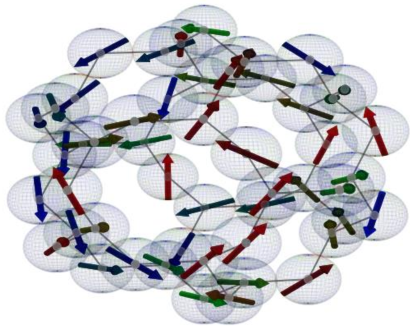
The d_p-Slider controls the distance between the outer planes. The transparency of both planes is set with the α-Slider from the first page, while the middle "Maxwell"-plane is fixed to α=1.

Acknowledgements:

I gratefully acknowledge – and highly recommend –
the use of Spyder IDE! (Spyder: 5.5.1 (conda); Python 3.11.7 64-bit; Qt version: 5.15.2; PyQt5 version: 5.15.10; OS: Windows 10).

- It is a pleasure to thank Matthias Schroeter for constructive criticism concerning the organization of this text.
- Eric Aderholt gave useful hints concerning the presentation and storage of the 3d-cluster.
- I am grateful to Peter Blümler, who introduced me to Halbach rings,
- and Jan Lellmann, who led me to the beauty of four-dimensional Platonian solids.
- Special thanks to René Messina, Boyd Edwards, Johannes Schönke, Kyongwan Kim, and Ivan Novikau for encouraging comments.

Any comments and suggestions for expanding this software project will be appreciated.



Remarks & Literature

[1] The inner structure of the program is adapted to the dipole cluster relaxation code described in T. Friedrich, I. Rehberg, R. Richter, Comment on "Self-assembly of magnetic balls: From chains to tubes", Phys. Rev. E 91 (2015) 057201 . The relaxation gains acceptable speed for clusters with less than 100 dipoles by calculating geometrical factors of a given cluster only once. It is thus restricted to fixed geometries, i.e. the dipoles are free to rotate, but do not translate. The Python version makes use of Numpy, and is provided in the package “dipole_clusters.zip” within the module “dipole_cluster.py”.

[2] The ground state of the cube deserves special attention. It can be animated with another Python program:
   a. Python code for the animation of a cubic dipole cluster (Version 1.2). Zenodo. Rehberg, Ingo. (2023).
   b. That animation is based on: J. Schönke, T. M. Schneider, and I. Rehberg, Infinite geometric frustration in a cubic dipole cluster, PhysRevB **91**, 020410 (2015).
   c. The interactive gallery of the dipole cube cited there moved to formaldesign.
   d. Additional images can be found at: Magnetkugeln – Ein 10-Euro-Labor.
   e. For experimental details see: Phys. Rev. B 98, 214424 (2018), or the preprint.

[3] Soares, Y. B., Graeser, M., Ackers, J., Bakenecker, A., Friedrich, T., Schumacher, J., Lüdtke-Buzug, K., Blümler, P., & Buzug, T. M. (2022). High gradient nested Halbach system for steering magnetic particles. *International Journal on Magnetic Particle Imaging*, *8*(1), [2203012]. https://doi.org/10.18416/ijmpi.2022.2203012

[4] The filled hexagon configuration contains a remarkable bifurcation scenario described in:
   a. Simeon Völkel, Stefan Hartung, and Ingo Rehberg, Comment on: Hysteretic transition between states of a filled hexagonal magnetic dipole cluster, Journal of Magnetism and Magnetic Materials **559**, 169520 (2022), or the preprint.
   b. The corresponding animation software is available at: Python code for the animation of a magnetic catastrophe machine, V1.2.3, Zenodo. Rehberg, I. (2024).
   c. A movie of the experiment showing the bifurcations is provided here: Magnetic Dipole Clusters - Resurrection of Catastrophe Machines. Zenodo. Rehberg, I., & Völkel, S. (2024, February 3).

[5] Ingo Rehberg, Magnetic Tubes – Instability of a Drug Deliverer (2024, March 21). The slides (V1.0.2) and movies (in Version V1) for this talk are available here.