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ComFiT: a Python library for computational field theory with topological defects

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Statement of need

Field theories described by partial differential equations (PDEs) are the backbone of many areas in physics. Examples of such field theories include the Navier-Stokes equations, which describe how air flows around the wing of an airplane; the Schrödinger equation, which governs how microscopic particles behave; Maxwell's equations, which explain the behavior of electromagnetic fields; and the Nobel Prize-winning Ginzburg-Landau theory, which explains how superconductors work. Despite their importance, simulating field theories often requires specialized software and programming expertise. Even though there exist specialized software packages like FEniCS (Alnaes et al., 2015) for solving PDEs, these are often focused on numerical efficiency at the cost of legibility or user-friendliness and fall short in offering functionalities for visualizing and analyzing outcomes. In particular, in the realm of many field theories, the study of topological defects - small structures like vortices in fluids - is essential for understanding phenomena such as phase transitions, turbulence and pattern formation. Due to the shared mathematical structures of these topological defects, recent research has shown that a common computational framework can be used to study them across different physical systems, ranging from Bose-Einstein condensates to nematic liquid crystals and crystalline solids (Skogvoll et al., 2023). However, a unified computational framework that brings all these systems together is lacking. ComFiT aims to close this gap, catering to both researchers and educators in physics, by providing a user-friendly, object-oriented framework for setting up a physical system, solving PDEs in one, two and three dimensions, visualizing results, and tracking topological defects. In so doing, ComFiT also brings advanced models of phase-field crystal modeling and nematic liquid crystals to the Python ecosystem, which are currently scarcely available in the open-source community, especially for three dimensions.

ComFiT sets itself apart from existing open-source Python software for solving PDEs in these ways:

- **Spectral Methods**: Like Dedalus (Burns et al., 2020), ComFiT employs spectral methods for differentiation and integration, which is more accessible for those familiar with Fourier analysis, unlike more complex finite element/volume approaches common in performance-driven libraries, e.g., FEniCS (Alnaes et al., 2015), PyClaw (Ketcheson et al., 2012), and Firedrake (Ham et al., 2023).
- **Built-in Visualization**: Unlike the aforementioned libraries, ComFiT includes tailored plotting tools for physical systems, saving users the effort of integrating with external libraries.
- **Topological Defect Analysis**: ComFiT's defect identification and tracking algorithms provide unique insights crucial for studying physical phenomena. To the best of our knowledge, no other integrated Python library for PDEs offers this functionality.

Summary

The core functionality of ComFiT is provided in the `BaseSystem` class, which defines a computational domain, auxiliary quantities, methods for time evolution, visualization tools and algorithms for identifying and tracking topological defects. To simulate a physical system, a user can create a class inheriting from `BaseSystem` and implement the specific equations and parameters of the model. The library also provides a range of predefined models, which inherit from the `BaseSystem` class, such as `QuantumMechanics`, `BoseEinsteinCondensate`, `NematicLiquidCrystal`, and `PhaseFieldCrystal`, each tailored to a specific field theory, which may be used to quickly get started with simulations for research or educational purposes.

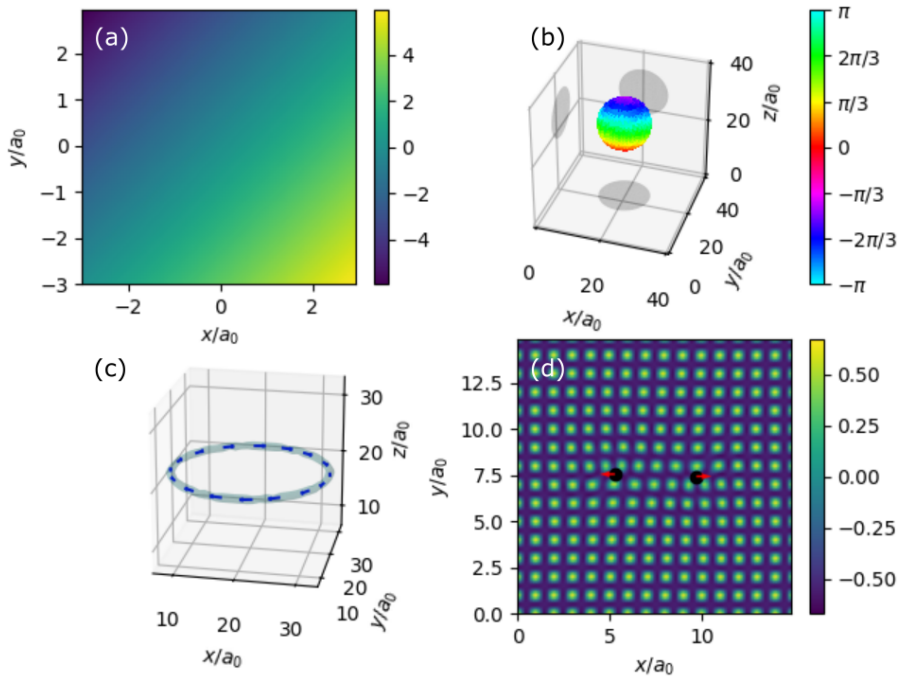

Figure 1: Four example setups of the ComFiT library. (a) The function $f(x, y) = x/a_0 - y/a_0$ where a_0 is a length scale, (b) a quantum mechanical wavepacket with a nonzero velocity in three dimensions, (c) a Bose-Einstein condensate vortex ring in three dimensions with vortex nodes identified and (d) a square phase-field crystal simulation containing a dislocation dipole. More details of the systems are given in the package documentation, and the code used to make these figures is given in the appendix.

The project aims to be highly community-driven, continuously improving the code stability, efficiency and usability, and to be a platform for sharing and developing new models and methods for field theories and topological defects. The documentation is hosted with MkDocs and contains a range of theoretical backgrounds for all the subclasses, tutorials, and examples to guide users through the process of setting up and running simulations, as well as visualizing and analyzing the results.

Research projects

ComFiT is a synthesized code base that was originally written in Matlab and used to fuel research into projects exploring the statistical properties and similarities between the dynamics

of topological defects between Bose-Einstein condensates and phase-field crystals (Skaugen, 2018). It was built on the framework for evolving stiff numerical systems described by Cox & Matthews (2002) and the methods for tracking defects developed by Mazenko (1997), Mazenko (1999), and Angheluta et al. (2012). The code base was further improved, stabilized and extended in the PhD projects of the paper authors (Rønning, 2023; Skogvoll, 2023). ComFiT has been used for research into a range of physical systems, including active matter (Rønning et al., 2023), stirred Bose-Einstein condensates (Rønning et al., 2020; Rønning & Angheluta, 2023), and phase-field crystals (Skogvoll, Skaugen, Angheluta, & Viñals, 2021; Skogvoll, Skaugen, & Angheluta, 2021; Skogvoll, Angheluta, et al., 2022; Skogvoll, Salvalaglio, et al., 2022). In all of these applications, the role of topological defects is central to understanding the critical dynamics and the statistical properties of the systems. For example, in Bose-Einstein condensates, the formation of vortices marks the transition to quantum turbulence, whereas in crystals, the formation of dislocations is central to understanding how materials buckle. The library is, at the time of publication, being used to research turbulence in 3D active nematics and the dynamics of 3D vortex structures in Bose-Einstein condensates. The phase-field crystal framework is currently under exploration at the Njord Centre at the University of Oslo for modeling crack propagation in Earth's upper crust and the basic framework is used as a foundation for several projects in the theoretical physics group at Porelab at the University of Oslo.

Appendix

The code used to produce the illustration is given below.

```
!pip install comfit==1.5.0
import comfit as cf
import matplotlib.pyplot as plt

fig = plt.figure(figsize=(10, 10))

# Base System class instance
bs = cf.BaseSystem(2, xlim=[-3,3], ylim=[-3,3])
field = bs.x - bs.y
ax1 = fig.add_subplot(2, 2, 1)
bs.plot_field(field, ax=ax1)

# # Quantum Mechanical System
qm = cf.QuantumMechanics(3, xRes=41, yRes=41, zRes=41)
qm.conf_initial_condition_Gaussian(initial_velocity=[0,0.1,0.3])
qm.evolve_schrodinger(200)
ax2 = fig.add_subplot(2, 2, 2, projection='3d')
qm.plot_complex_field(qm.psi, ax=ax2)

# Bose Einstein Condensate System
bec = cf.BoseEinsteinCondensate(3, xRes=41, yRes=41, zRes=41)
bec.conf_initial_condition_Thomas_Fermi()
bec.conf_insert_vortex_ring()
bec.evolve_relax(100)
vortex_nodes = bec.calc_vortex_nodes()
ax3 = fig.add_subplot(2, 2, 3, projection='3d')
bec.plot_field(abs(bec.psi), alpha = 0.2, ax=ax3, colorbar=False)
bec.plot_vortex_nodes(vortex_nodes,ax=ax3)

# Phase-field crystal system
pfc = cf.PhaseFieldCrystal2DSquare(15,15)
```

```
eta = pfc.calc_amplitudes_with_dislocation_dipole()
pfc.conf_PFC_from_amplitudes(eta)
pfc.evolve_PFC(100)
dislocation_nodes = pfc.calc_dislocation_nodes()
ax4 = fig.add_subplot(2, 2, 4)
pfc.plot_field(pfc.psi,ax=ax4)
pfc.plot_dislocation_nodes(dislocation_nodes,ax=ax4,grid=False)
```

References

Alnaes, M. S., Blechta, J., Hake, J., Johansson, A., Kehlet, B., Logg, A., Richardson, C. N., Ring, J., Rognes, M. E., & Wells, G. N. (2015). The FEniCS project version 1.5. *Archive of Numerical Software*, *3*. https://doi.org/10.11588/ans.2015.100.20553

Angheluta, L., Jeraldo, P., & Goldenfeld, N. (2012). Anisotropic velocity statistics of topological defects under shear flow. *Phys. Rev. E*, *85*(1), 011153. https://doi.org/10.1103/PhysRevE.85.011153

Burns, K. J., Vasil, G. M., Oishi, J. S., Lecoanet, D., & Brown, B. P. (2020). Dedalus: A flexible framework for numerical simulations with spectral methods. *Physical Review Research*, *2*(023068), 023068. https://doi.org/10.1103/PhysRevResearch.2.023068

Cox, S. M., & Matthews, P. C. (2002). Exponential Time Differencing for Stiff Systems. *Journal of Computational Physics*, *176*(2), 430–455. https://doi.org/10.1006/jcph.2002.6995

Ham, D. A., Kelly, P. H. J., Mitchell, L., Cotter, C. J., Kirby, R. C., Sagiyama, K., Bouziani, N., Vorderwuelbecke, S., Gregory, T. J., Betteridge, J., Shapero, D. R., Nixon-Hill, R. W., Ward, C. J., Farrell, P. E., Brubeck, P. D., Marsden, I., Gibson, T. H., Homolya, M., Sun, T., … Markall, G. R. (2023). *Firedrake user manual* (First edition) [Manual]. Imperial College London and University of Oxford and Baylor University and University of Washington. https://doi.org/10.25561/104839

Ketcheson, D. I., Mandli, K. T., Ahmadia, A. J., Alghamdi, A., Quezada de Luna, M., Parsani, M., Knepley, M. G., & Emmett, M. (2012). PyClaw: Accessible, extensible, scalable tools for wave propagation problems. *SIAM Journal on Scientific Computing*, *34*(4), C210–C231. https://doi.org/10.1137/110856976

Mazenko, G. F. (1997). Vortex velocities in the O(n) symmetric time-dependent ginzburg-landau model. *Phys. Rev. Lett.*, *78*(3), 401–404. https://doi.org/10.1103/PhysRevLett.78.401

Mazenko, G. F. (1999). Velocity distribution for strings in phase-ordering kinetics. *Physical Review E*, *59*(2), 1574–1584. https://doi.org/10.1103/PhysRevE.59.1574

Rønning, J. (2023). *Topological Defects and Flows in BECs and Active Matter* [PhD thesis]. https://www.duo.uio.no/handle/10852/104678.

Rønning, J., & Angheluta, L. (2023). Precursory patterns to vortex nucleation in stirred Bose-Einstein condensates. *Physical Review Research*, *5*(2), 023108. https://doi.org/10.1103/PhysRevResearch.5.023108

Rønning, J., Renaud, J., Doostmohammadi, A., & Angheluta, L. (2023). Spontaneous flows and dynamics of full-integer topological defects in polar active matter. *Soft Matter*, *19*(39), 7513–7527. https://doi.org/10.1039/D3SM00316G

Rønning, J., Skaugen, A., Hernández-García, E., Lopez, C., & Angheluta, L. (2020). Classical analogies for the force acting on an impurity in a Bose–Einstein condensate. *New Journal of Physics*, *22*(7), 073018. https://doi.org/10.1088/1367-2630/ab95de

Skaugen, A. (2018). *A unified perspective on two-dimensional quantum turbulence and plasticity*

[PhD thesis]. The University of Oslo; https://www.duo.uio.no/handle/10852/66179.

Skogvoll, V. (2023). *Symmetry, topology, and crystal deformations: A phase-field crystal approach* [PhD thesis]. https://www.duo.uio.no/handle/10852/102731.

Skogvoll, V., Angheluta, L., Skaugen, A., Salvalaglio, M., & Viñals, J. (2022). A phase field crystal theory of the kinematics of dislocation lines. *Journal of the Mechanics and Physics of Solids*, *166*, 104932. https://doi.org/10.1016/j.jmps.2022.104932

Skogvoll, V., Rønning, J., Salvalaglio, M., & Angheluta, L. (2023). A unified field theory of topological defects and non-linear local excitations. *Npj Computational Materials*, *9*(1), 1–13. https://doi.org/10.1038/s41524-023-01077-6

Skogvoll, V., Salvalaglio, M., & Angheluta, L. (2022). Hydrodynamic phase field crystal approach to interfaces, dislocations and multi-grain networks. *Modelling and Simulation in Materials Science and Engineering*. https://doi.org/10.1088/1361-651X/ac9493

Skogvoll, V., Skaugen, A., & Angheluta, L. (2021). Stress in ordered systems: Ginzburg-Landau-type density field theory. *Physical Review B*, *103*(22), 224107. https://doi.org/10.1103/PhysRevB.103.224107

Skogvoll, V., Skaugen, A., Angheluta, L., & Viñals, J. (2021). Dislocation nucleation in the phase-field crystal model. *Physical Review B*, *103*(1), 014107. https://doi.org/10.1103/PhysRevB.103.014107