Activity report based on CPU time and storage used on PDC and NSC of 2020/2021

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In this activity report, we describe and list some highlights of the 44 papers that all acknowledge SNAC. Out of those, 4 are in press, 13 are published in 2021, and another 17 are published in 2020. For the calculations, we use the code Runko and the Pencil Code, both of which are hosted on github (`https://github.com/natj/runko` and `https://github.com/pencil-code`).

The Pencil Code Collaboration consists of currently 38 developers who have published their effort in JOSS, the Journal of Open Source Software [412].

412. Pencil Code Collaboration: Brandenburg, A., Johansen, A., Bourdin, P. A., Dobler, W., Lyra, W., Rheinhardt, M., Bingert, S., Haugen, N. E. L., Mee, A., Gent, F., Babkovskaia, N., Yang, C.-C., Heinemann, T., Dintrans, B., Mitra, D., Candelaresi, S., Warnecke, J., Käpylä, P. J., Schreiber, A., Chatterjee, P., Käpylä, M. J., Li, X.-Y., Krüger, J., Aarnes, J. R., Sarson, G. R., Oishi, J. S., Schober, J., Plasson, R., Sandin, C., Karchniwy, E., Rodrigues, L. F. S., Hubbard, A., Guerrero, G., Snodin, A., Losada, I. R., Pekkilä, J., & Qian, C.: 2021, "The Pencil Code, a modular MPI code for partial differential equations and particles: multipurpose and multiuser-maintained," *J. Open Source Softw.* **6**, 2807

Here and below, the 3-digit numbering of the papers coincides with that of Brandenburg's full list of publications on `http://www.nordita.org/~brandenb/pub`. Those preceded by the letter B are also in that list, but under invited conference proceedings. All the papers quoted below acknowledge SNIC, PDC, and/or NSC.

1 Shocks and turbulence in collisionless astrophysical plasmas

Many astrophysical plasmas are extremely diluted and, hence, appear almost collisionless. In order to investigate such plasmas that are beyond the validity regime of MHD, we in Nordita have developed a new open-source particle-in-cell (PIC) simulation code Runko [1]. The main focus of the code is to perform self-consistent fully-kinetic studies of non-thermal particle acceleration in collisionless plasmas.

Turbulence in astrophysical plasmas is ubiquitous, appearing in systems such as the solar wind all the way to galaxy cluster scales. By using massively-parallel PIC simulations, we have studied the formation and evolution of turbulence in magnetically-dominated diluted plasmas. This work helped us, for the first time, understand how the large-scale energy in the plasma is transferred from one state (large magnetic field perturbations) to other forms (small turbulent motion and subsequently non-thermal particle populations).

Under a strong radiation field (such as close to black holes) the turbulence dynamics is altered due to strong radiative cooling. In order to understand the non-linear behavior of turbulent plasma in such a strong radiation environment, we have performed pioneering radiative kinetic turbulence simulations [2]. This in turn, will help us understand, for example, particle acceleration and heating of diluted plasmas near black holes and neutron stars.

The kinetic turbulence is also known to depict a copious creation of intermittent, very energetic, and localized space regions with strong currents. By using our first-principles simulations, we are, for the first time, starting to trace the statistics and dynamics of these sheet-like structures (forthcoming paper [3]). Such understanding is important as it can be used to parameterize the efficiency of particle acceleration and dissipation strength of diluted plasmas.

In recent years, particle-in-cell simulations have allowed to study particle acceleration in relativistic shocks from first principles. They showed, notably, that relativistic shocks with no or low magnetizations lead to efficient particle acceleration through Fermi acceleration while for highly magnetized shocks, no substantial particle energization was reported.

However, in realistic astrophysical environments, one can expect the upstream plasma not to be homogeneous as assumed in these studies but, to present perturbations or even to be turbulent. How upstream turbulence affects the shock properties and particle acceleration is to date an open question. Using the Runko code, we have studied how a relativistic magnetized shock responds to upstream density perturbations and found, unlike previous works, evidence of particle acceleration [2].

The following papers presenting our results are in preparation:

[1] Nättilä, J., & Belobodorov, A.: 2021, “Radiative turbulent flares in magnetically-dominated plasmas,” arXiv:2012.03043

[2] Bussov, M., & Nättilä, J.: 2021, “Segmentation of turbulent computational fluid dynamics simulations with unsupervised ensemble learning,” arXiv:2109.01381

[3] Demidem, C., Nättilä, J., & Veledina, A.: 2021, ”Particle acceleration in corrugated relativistic collisionless shocks”, in prep.

2 Gravitational waves and early universe magnetic fields

An important activity involves the computation of the stochastic gravitational wave background from the Big Bang. Those can be measured in future with LISA and the pulsar timing array. Our first paper on the numerical method is described in Ref. [394]. In [410], we compare the resulting primordial gravitational wave signal with the sensitivity curves for LISA.

We have continued studying the chiral magnetic effect [393] and have now calculated the resulting GW production [416]. We have also studied new aspects of decaying turbulence in the early universe with magnetic helicity [405].

428. Roper Pol, A., Mandal, A., Brandenburg, A., & Kahniashvili, T.: 2021, “Polarization of gravitational waves from helical MHD turbulent sources,” *J. Cosmol. Astropart. Phys.*, submitted (arXiv:2107.05356)

422. Brandenburg, A., He, Y., & Sharma, R.: 2021, “Simulations of helical inflationary magnetogenesis and gravitational waves,” *Astrophys. J.*, in press (arXiv:2107.12333)

421. Brandenburg, A., & Sharma, R.: 2021, “Simulating relic gravitational waves from inflationary magnetogenesis,” *Astrophys. J.* **920**, 26

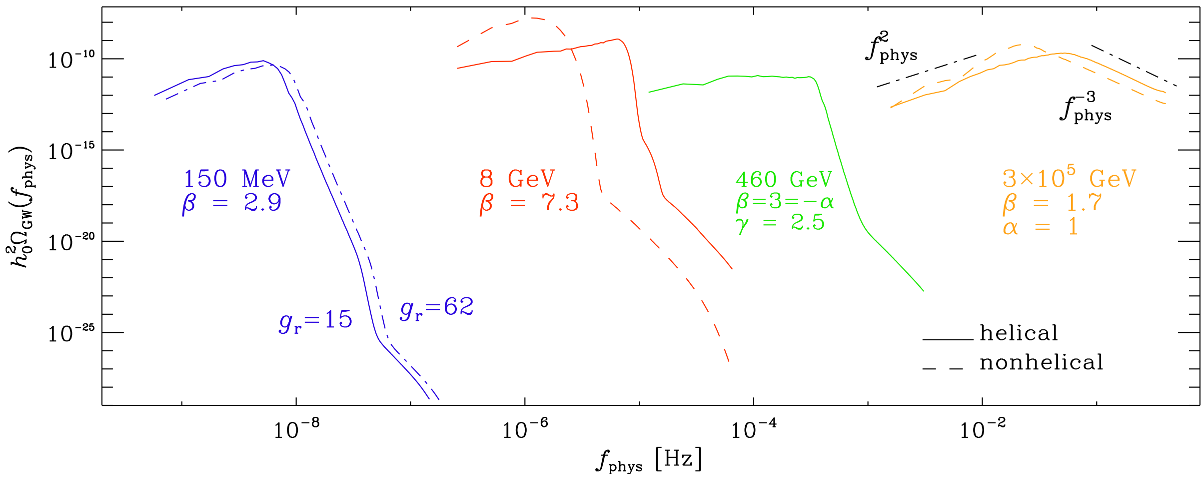

Figure 1: $h_0^2\Omega_{\rm GW}(f_{\rm phys})$ for runs with reheating temperatures $T_{\rm r}$ ranging from 150 MeV to 3×10^5 GeV. Dashed lines denote nonhelical runs and dashed-dotted show the result for $g_{\rm r}=62$.

419. Brandenburg, A., Clarke, E., He, Y., & Kahniashvili, T.: 2021, "Can we observe the QCD phase transition-generated gravitational waves through pulsar timing arrays?" *Phys. Rev. D* **104**, 043513

418. He, Y., Brandenburg, A., & Sinha, A.: 2021, "Spectrum of turbulence-sourced gravitational waves as a constraint on graviton mass," *J. Cosmol. Astropart. Phys.* **07**, 015

417. Brandenburg, A., Gogoberidze, G., Kahniashvili, T., Mandal, S., & Roper Pol, A., & Shenoy, N.: 2021, "The scalar, vector, and tensor modes in gravitational wave turbulence simulations," *Class. Quantum Grav.* **38**, 145002

416. Brandenburg, A., He, Y., Kahniashvili, T., Rheinhardt, M., & Schober, J.: 2021, "Gravitational waves from the chiral magnetic effect," *Astrophys. J.* **911**, 110

413. Kahniashvili, T., Brandenburg, A., Gogoberidze, G., Mandal, S., & Roper Pol, A.: 2021, "Circular polarization of gravitational waves from early-universe helical turbulence," *Phys. Rev. Res.* **3**, 013193

[410] Roper Pol, A., Mandal, S., Brandenburg, A., Kahniashvili, T., & Kosowsky, A.: 2020, "Numerical Simulations of Gravitational Waves from Early-Universe Turbulence," *Phys. Rev. D* **102**, 083512

[405] Brandenburg, A., Durrer, R., Huang, Y., Kahniashvili, T., Mandal, S., & Mukohyama S.: 2020, "Primordial magnetic helicity evolution with a homogeneous magnetic field from inflation," *Phys. Rev. D* **102**, 02353

[394] Roper Pol, A., Brandenburg, A., Kahniashvili, T., Kosowsky, A., & Mandal, S.: 2020, "The timestep constraint in solving the gravitational wave equations sourced by hydromagnetic turbulence," *Geophys. Astrophys. Fluid Dyn.* **114**, 130–161

[393] Schober, J., Brandenburg, A., & Rogachevskii, I.: 2020, "Chiral fermion asymmetry in high-energy plasma simulations," *Geophys. Astrophys. Fluid Dyn.* **114**, 106–129

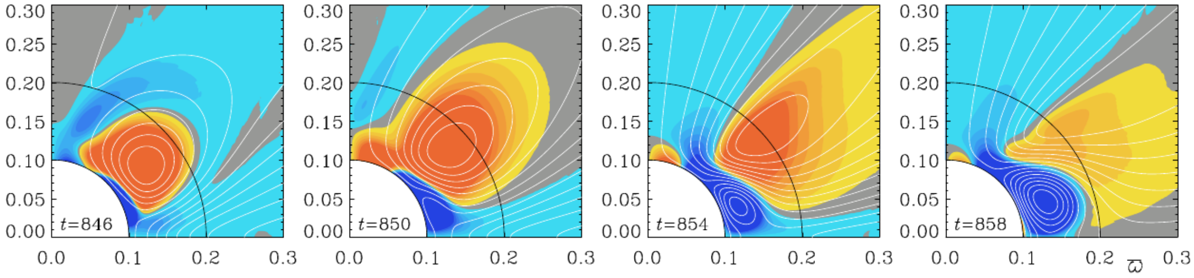

Figure 2: Color representation of $B_\phi(r,\theta)$ for different times for a model combining the dynamo region with the outer wind. Only the region close to the star is shown. Note the occurrence of V-shaped field lines during certain times at $822 \leq t \leq 834$, and 846. The field shows radial outward migration during certain times: negative B_ϕ at low latitudes for $814 \leq t \leq 826$, and positive B_ϕ at midlatitudes for $834 \leq t \leq 854$.

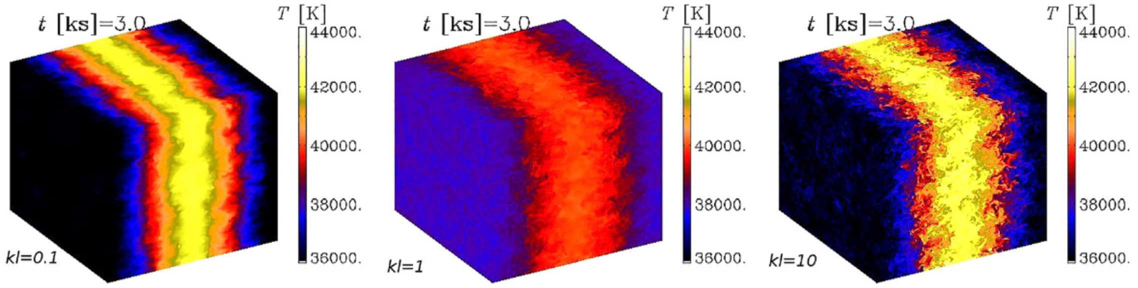

Figure 3: Temperature on the periphery of the computational domain for $k\ell = 0.1$ (left), $k\ell = 1$ (middle), and $k\ell = 10$ (right) for $t = 3\,$ks. The (x, y, z) coordinates are indicated in the first panel and the approximate 1 Mm scale is shown in the second panel.

3 Solar wind and radiation transport

We have studied turbulent radiative diffusion and the new concept of turbulent Newtonian cooling and found a surprisingly weak scale dependence [418]. In an earlier study of this type, we have determined the time step constraint for radiation hydrodynamics [395]. We have also now combined a solar dynamo with a Parker wind [414]. Moreover, we have studied the formation of magnetic bipoles in rotating turbulence with coronal envelope [379].

420. Brandenburg, A., & Das, U.: 2021, "Turbulent radiative diffusion and turbulent Newtonian cooling," *Phys. Fluids* **33**, 095125

414. Jakab, P., & Brandenburg, A.: 2021, "The effect of a dynamo-generated field on the Parker wind," *Astron. Astrophys.* **647**, A18

[395] Brandenburg, A., & Das, U.: 2020, "The time step constraint in radiation hydrodynamics," *Geophys. Astrophys. Fluid Dyn.* **114**, 162–195

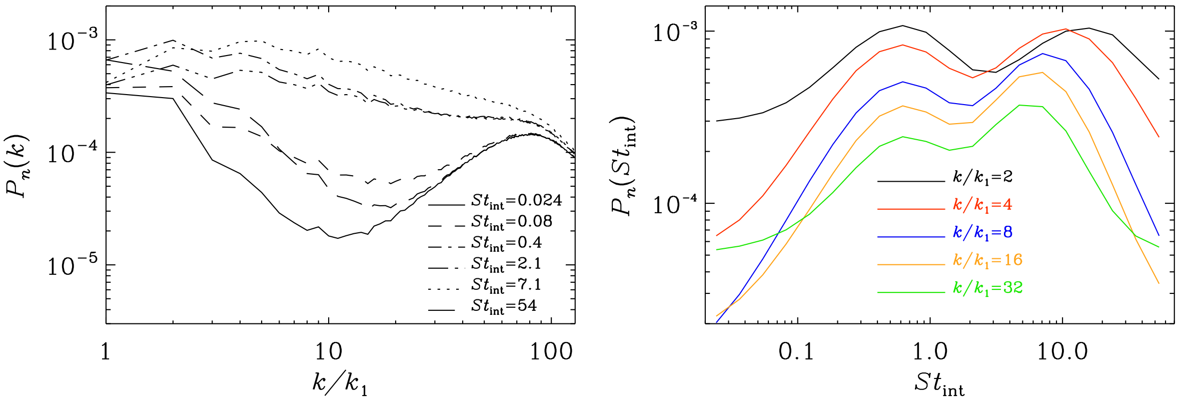

Figure 4: $P_n(k)$ and $P_n(St_{\rm int})$ for a run with spherical expansion wave driving for 20 different particle sizes. The different line types in the left panel, marked in the legend, correspond to the line types of the short vertical lines on the upper abscissa of the right panel. Likewise, the different colors in the right panel, indicated in the legend, correspond to the colors of the short vertical lines in the left panel.

4 Dynamo action in the Sun and Galaxies

Linear polarization, as characterized by the Stokes Q and U parameters, is coordinate-dependent. A coordinate-independent characterization is provided by the parity-even and parity-odd E and B mode polarizations that are routinely used in cosmology [402]. Their cross-correlation can also reveal information about magnetic helicity, but only if the system is inhomogeneous.

We have also continued using simulations to reveal subsurface properties of the Sun's magnetic field using simulations [396]. We have now extended these studies to our Galaxy [402] and to edge-on galaxies [404].

[404] Brandenburg, A., & Furuya, R. S.: 2020, "Application of a helicity proxy to edge-on galaxies," *Mon. Not. Roy. Astron. Soc.* **496**, 4749–4759

[402] Brandenburg, A., & Brüggen, M.: 2020, "Hemispheric handedness in the Galactic synchrotron polarization foreground," *Astrophys. J. Lett.* **896**, L14

[396] Singh, N. K., Raichur, H., Käpylä, M. J., Rheinhardt, M., Brandenburg, A., & Käpylä, P. J.: 2020, "*f*-mode strengthening from a localized bipolar subsurface magnetic field," *Geophys. Astrophys. Fluid Dyn.* **114**, 196–212

5 Particles in Turbulence

We have started a new project on the spectral characterization of inertial particle clustering in turbulence. We have found spectra to be an excellent tool to identify *different* and *new* mechanisms of particle clustering in supersonic turbulence [426]. We have also now completed several papers on the subject of multi-dimensional condensation and coagulation. We also have performed work that includes the effects of condensation, in addition to coagulation [424]. Finally, we have characterized the importance of fluctuations in dilute systems [412]. This work has now been extended to the astrophysical context [5,6] and applied to stellar wind [7].

426. Haugen, N. E. L., Brandenburg, A., Sandin, C., & Mattsson, L.: 2021, "Spectral characterisation of inertial particle clustering in turbulence," *J. Fluid Mech.*, submitted (arXiv:2105.01539)

424. Li, X.-Y., Mehlig, B., Svensson, G., Brandenburg, A., & Haugen, N. E. L.: 2021, "Collision fluctuations of lucky droplets with superdroplets," *J. Atmos. Sci.*, submitted (arXiv:1810.07475)

[5] Li, X.-Y., & Mattsson, L.: 2021, "Coagulation of inertial particles in supersonic turbulence," *Astron. Astrophys.* **648**, A52

[6] Li, X.-Y., & Mattsson, L.: 2020, "Dust growth by accretion of molecules in supersonic interstellar turbulence," *Astrophys. J.* **903**, 148

[7] Sandin, C. & Mattsson, L.: 2020, "Three-component modelling of C-rich AGB star winds V. Effects of frequency-dependent radiative transfer including drift," *Mon. Not. Roy. Astron. Soc.* **499**, 1531–1560

6 Small-scale dynamo turbulence, ambipolar diffusion, Hall cascade

In an attempt to clarify the nature of large-scale dynamo action, we have discovered efficient quasi-kinematic large-scale dynamo growth as the small-scale dynamo saturates [413]. We have studied the Hall cascade and applied it to neutron star crusts [408]. Using kinetic simulations, we have shown that the dynamo effect in weakly collisional nonmagnetized plasmas is strongly impeded by Landau damping of magnetic fields [403]. Our work on hydromagnetic turbulence has also led to the understanding that the spectrum of the resulting stress is the same as that of the underlying field, provided the spectrum is not bluer than white noise [400]. We have also discovered the existence of negative turbulent magnetic diffusion in three classes of optimal dynamos [399]. We have compared magnetic helicity conservation with the PENCIL CODE and with `FLASH` and found that the latter produces spurious magnetic helicity [398]. We have conducted two investigations of dynamos and MHD systems at large magnetic Prandtl number: one that can be applied to galaxy clusters and the solar corona where we now argue that heating occurs not on current sheets, as usually believed, but viscously [387]. In the cooler interstellar medium, ambipolar diffusion becomes important and we have now conducted two-fluid simulations [386]. As an additional off-spring of earlier work, we have completed this year a detailed investigation on varying the forcing scale in low Prandtl number dynamos [367]. It will provide an important benchmark for future studies.

[408] Brandenburg, A.: 2020, "Hall cascade with fractional magnetic helicity in neutron star crusts," *Astrophys. J.* **901**, 18

[403] Pusztai, I., Juno, J., Brandenburg, A., TenBarge, J. M., Hakim, A., Francisquez, M., & Sundström, A.: 2020, "Dynamo in weakly collisional nonmagnetized plasmas impeded by Landau damping of magnetic fields," *Phys. Rev. Lett.* **124**, 255102

[400] Brandenburg, A., & Boldyrev, S.: 2020, "The turbulent stress spectrum in the inertial and subinertial ranges," *Astrophys. J.* **892**, 80

[399] Brandenburg, A., & Chen, L.: 2020, "The nature of mean-field generation in three classes of optimal dynamos," *J. Plasma Phys.* **86**, 905860110

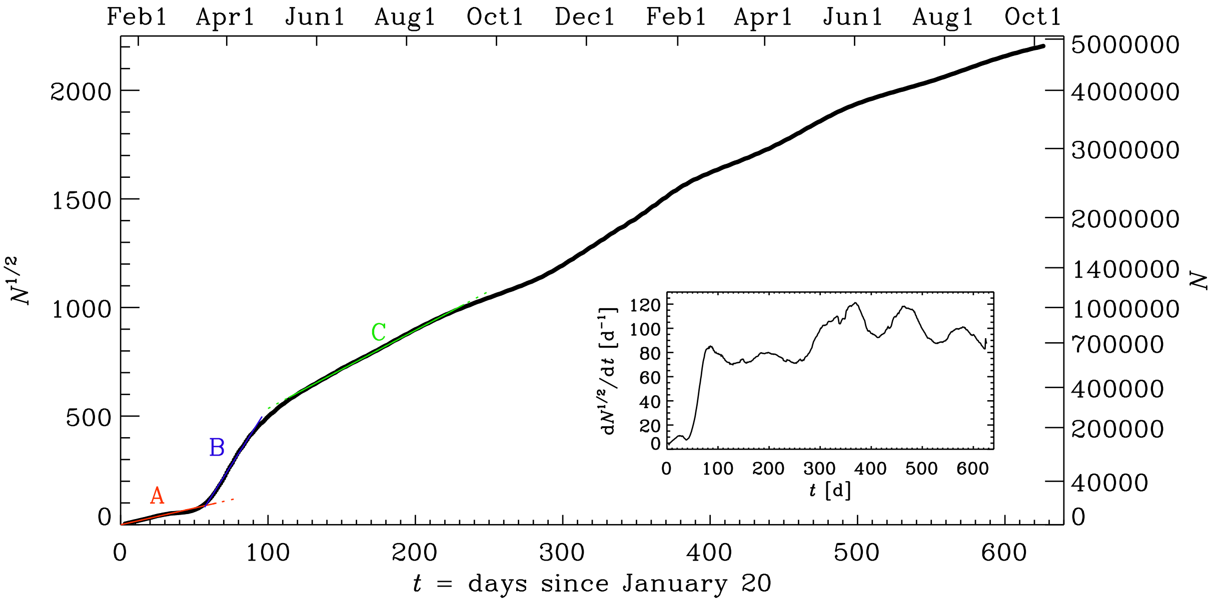

Figure 5: Square root of the number N of deaths, which is regarded as a proxy of the number of infected that is more reliable than the reported number of SARS-CoV-2. Note the piecewise linear growth in $N^{1/2}$, corresponding to a piecewise quadratic growth. Adopted from [B.42].

[398] Brandenburg, A., & Scannapieco, E.: 2020, "Magnetic helicity dissipation and production in an ideal MHD code," *Astrophys. J.* **889**, 55

7 Astrobiology and chemical reactions

With the Pencil Code, we can perform simulations of chemical reactions. The spreading of COVID-19 is in principle one such example. This led us to understand why the spreading of COVID-19 follows a piecewise quadratic growth [409,B.42]; see Figure 5. One important application is hydrogen combustion which can lead to detonation. In [392], we have produced high-resolution studies of this process. Chemical reactions also play a role in origin-of-life studies. In [B.41], we have studied the effect of fluctuations in accomplishing reactions that drive the system toward a homochiral state without the explicit effects of autocatalysis or enantiomeric cross-inhibition.

[B.42] Brandenburg, A.: 2021, "Chirality in Astrophysics" in *Proceedings to Nobel Symposium 167: Chiral Matter*, ed. E. Babaev, D. Kharzeev, M. Larsson, A. Molochkov, & V. Zhaunerchyk, World Scientific, in press

[B.41] Brandenburg, A.: 2021, "Homochirality: a prerequisite or consequence of life?" in *Prebiotic Chemistry and the Origin of Life*, ed. A. Neubeck, & S. McMahon, Springer, in press (arXiv:2012.12850)

[409] Brandenburg, A.: 2020, "Piecewise quadratic growth during the 2019 novel coronavirus epidemic," *Infectious Disease Modelling* **5**, 681–690

[392] Qian, C., Wang, C., Liu, J., Brandenburg, A., Haugen, N. E. L., & Liberman, M.: 2020, "Convergence properties of detonation simulations," *Geophys. Astrophys. Fluid Dyn.* **114**, 58–76

Academic achievements

In July 2020, Dr Alberto Roper Pol successfully defended his PhD thesis at the University of Colorado with Axel Brandenburg as the main supervisor. This project was supported by a grant from the National Science Foundation in the US, with Axel Brandenburg as the PI.