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MARIE SKŁODOWSKA-CURIE ACTIONS

Individual Fellowships (IF) Call: H2020-MSCA-IF-2014

PART B

"Cosmological Simulations of Radio Bright Plasmas"

This proposal is to be evaluated as:

[GF]

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List of Participants

Participants	Legal Entity Short Name	Academic	Non-Academic	Country	Dept./Division/ Laboratory	Supervisor	Role of Partner Organisation
Beneficiary							
Istituto Nationale di Astrofisica	INAF	1		Italy	IRA^{a}	G. Brunetti	
Partner Organisations							
University of Minnesota	UMN	1		USA	MSI/MIA^b	T. Jones	Outgoing host
Cray Inc.	Cray		✓	USA	Softw. Dev.	P. Mendygral	Training host

^aIstituto di Radioastronomia

 $^b\mathrm{Minnesota}$ Supercomputing Institute / Minnesota Institute for Astrophysics

1 Summary

Mergers of galaxy clusters are among the most energetic events in the Universe. The interaction generates shocks and turbulence in the ionised cluster medium, driving the amplification of magnetic fields and the acceleration of relativistic particles. This leads to the formation of large diffuse radio sources in clusters, whose origin is sparking a lively theoretical debate in the community. The ongoing leap in radio instrumentation, lead by the European LOFAR observatory, will revolutionize the field and unveil the increasingly complex picture expected at unexplored low radio frequencies.

In recent years, simulations have played an important role in the field, providing first steps towards complete models of non-thermal sources. However, we still lack the advanced numerical models required to match the capabilities of leading instruments and to uncover the underlying physics. This roots in the physical as well as algorithmic complexities of the modelling, which are challenging to even the largest computers available to date.

In this project, we aim to meet these challenges and to build the first comprehensive numerical model of the non-thermal components in clusters and their observational signature. Recent progress in numerical models for particle acceleration by the researcher now demands substantially improved scalable methods for MHD-cosmology, which are available solely at the outgoing host and will be transferred to the beneficiary by the researcher. In particular,

- **Goal 1:** we will run a nested-grid cosmological MHD simulation with 2 kpc resolution inside the virial radius of a few clusters. This will, for the first time, resolve the turbulent MHD-dynamo in these clusters and reveal the evolution of turbulence and magnetic fields in the inter-cluster-medium.
- **Goal 2:** we will, for the first time, include a self-consistent description for the acceleration and transport of cosmic-ray protons and electrons in this simulation, thus deriving direct constrains on the non-thermal components in clusters and the cosmic web.
- **Goal 3:** we will simulate the predicted population of non-thermal radio sources in galaxy clusters for LO-FAR key science. The results will guide the interpretation of observations of galaxy clusters from radio to gamma-rays and neutrino and are of paramount importance for our understanding of the intra-cluster-medium.

This project will not only provide eagerly awaited predictions for the next generation of cluster observations, but reveal an unprecedented view on the micro-physics in hot weakly-collisional plasmas. We will achieve our ambitious goals in collaboration with experts for particle acceleration and Eulerian-MHD at the University of Minnesota and for high performance computing at Cray Inc.

During the *outgoing-phase*, the researcher will be trained in Eulerian methods for cosmological simulations, he will for the first time in his career use world-class grid methods for MHD (WOMBAT-code) and adapt his algorithms for cosmic-ray physics to the method in collaboration with the code-authors. He will collaborate with experts of diffuse shock acceleration and contribute his complementary expertise in particle acceleration by turbulence, the cosmic MHD-dynamo and numerical models for dark matter. Under supervision of software engineers at the leading manufacturer of supercomputers (Cray Inc.), he will then run a cosmological simulation with unprecedented resolution and sub-grid modelling of particle acceleration, showcasing the capabilities of modern supercomputers.

During the *return-phase*, the researcher will work with leading observers and theorists at the beneficiary to compare his unique simulation with ground-breaking new radio data and constrain the efficiency of cosmicray acceleration by shocks and turbulence in galaxy clusters, thereby shedding light on the micro-physics governing the dynamics of the intra-cluster-medium.

These advances in numerical modelling will deliver influential results and establish the researcher as a leading numerical scientist in a transformational science case, paving the way to the era of the Square Kilometer Array.

2 Excellence (50%)

2.1 Quality, innovative aspects and credibility of the research

Galaxy clusters, junctions in the cosmic web: It is now accepted that the observed structure of our Universe is well described by the presence of cold dark matter and dark energy. Within the framework of this " Λ CDM" cosmology, the matter distribution evolves in a hierarchical bottom-up fashion by infall and merging through gravitational interaction. Clusters of galaxies evolve in the junctions of the resulting cosmic web in a highly dynamic process driven by the gravitational instability.

In clusters, dark matter forms a deep potential well into which diffuse baryonic matter is advected, bound and heated by shocks, turbulent motions and compression to temperatures of hundreds of millions of Kelvin. This intra-cluster-medium (ICM) makes clusters luminous sources in the X-rays through the emission of thermal bremsstrahlung (figure 1, colors). Additionally, radio observations of galaxy clusters discovered large-scale synchotron emission from the ICM proving that magnetic fields and relativistic particles are present in these systems. These components are a powerful independent probe of the properties of the ICM plasma and their origin and evolution is an active field of astrophysical research.

Non-thermal radio emission on the largest scales: The present picture of non-thermal emission from galaxy clusters is mainly based on data from radio observations that identify diffuse large-scale radio sources in many massive merging galaxy clusters. This emission implies the presence of ultra-relativistic, cosmic-ray (CR) electrons that emit synchrotron radiation while spiraling in the cluster magnetic field. These sources are usually classified into two main categories:

Radio relics are elongated polarised arcs at the cluster outskirts, Mpcs long, but only few hundred kpc thin. Figure 1 shows a double relic in contours, with the two arcs 1.5 Mpc apart. There is consensus that radio relics are caused by giant shocks in the ICM. These merger-driven shocks can accelerate relativistic electrons and can lead to a local amplification of the magnetic field. However the details of this process, including the role of relativistic protons, are still poorly constrained¹.

Radio halos are diffuse emission around the cluster centre that extends for more than a Mpc (figure 1, diffuse emission/radio contours in the center). A popular model for the origin of radio halos is based on the hypothesis that relativistic particles can be accelerated in gigantic turbulent regions during cluster-cluster mergers. Still the details of this process and the possible connection between halos and relics are unclear¹. Following this approach, our numerical simulations of merging galaxy clusters have recently and for the first time demonstrated how radio halos can be generated by merger-induced turbulence in the cluster medium².



Figure 1: X-rays (colors) and radio halo & double radio relic (contours), in the merging cluster MACS-JJ1752.0 (van Weeren et al. 2012, MNRAS, 425).

These models for the generation of relics and halos successfully reproduce the connection of the radio sources with cluster mergers¹. However a unified numerical model explaining the phenomenology of halos and relics and their connection in the framework of structure formation is still missing. In particular, the physical mechanisms produce highly transient, spatially irregular and frequency dependent radio patterns in clusters, whose complexity requires advanced numerical simulations to be adequately modelled. A unified model would also yield first firm expectations for the high-energy emission from clusters.

Numerical simulations have driven the development of models for the non-thermal cluster emission in recent years. Cosmological simulations of galaxy clusters follow the collisionless dynamics of the dark matter

¹Brunetti G., Jones T. W., 2014, International Journal of Modern Physics D, 23, 30007

²Donnert J., Dolag K., Brunetti G., Cassano R., 2013, MNRAS, 429, 3564

and evolution of baryons in a fluid approach³. This presents a challenging numerical problem, because of the high dynamic range in densities and velocities. Lagrangian (particle-) based simulations are still limited by their algorithmic treatment of magnetic fields and subsonic turbulence⁴, while Eulerian (grid-) based simulations have so far failed to resolve the turbulent MHD-dynamo in clusters, due to limited spatial resolution and diffusivity. Regardless of the technique, simulators only partially implemented the necessary CR physics to model either radio halos or radio relics⁵. Hence, we are still lacking a complete numerical model of non-thermal radio sources in clusters that would allow a self-consistent view on the micro-physical processes that dissipate gravitational energy on small scales. Our research aims to build this new numerical model, which is eagerly awaited by the radio observer community and will also have considerable impact on the design of the next generation of high-energy telescopes like CTA.

At the beneficiary, the researcher has recently pioneered numerical models that connect CR electrons to cluster turbulence. This unique approach can be extended to a first self-consistent treatment of all processes relevant to the formation of radio halos and relics. However his models are limited by the underlying numerical methods for MHD and their treatment of turbulence. To proceed, it is imperative for him to seek improved numerical models for cluster MHD-turbulence.

Cosmological MHD-simulations with WOMBAT: Simulating cosmic baryons using *Eulerian grids* is highly advantageous for modelling turbulence, non-viscous flows and it provides manifestly divergence free magnetic fields. So far, this approach was limited by low effective resolution, which stems from code complexity and available computational resources. The new WOMBAT code, recently developed at the University of Minnesota and Cray Inc., is for the first time able to exploit the full computational power of the new generation of supercomputers, featuring *flat* (< 2%) *linear weak scaling to* 10⁵ *processors*⁶. WOMBAT employs new and sophisticated domain decomposition and load balancing methods to reach scalability to peta-scale HPC environments. Combined with the researchers unique sub-grid models for CR electron and proton evolution⁷, proper numerical models of turbulence and the non-thermal radio emission in clusters now becomes for the first time feasible. This project aims to run the first simulation of this kind. In a nested grid approach (not AMR) we will perform cosmological simulations with uniform spatial resolution of 2 kpc inside the virial radius of pre-selected clusters (sect. 4.1) and thereby reveal turbulence and magnetic field structure in the ICM with unprecendented accuracy (**Goal 1**). This simulation will unlock the full potential of the researchers approach and provide the first faithful model of non-thermal processes in galaxy clusters (**Goal 2**).

At the same time, LOFAR will conduct the first high-sensitivity exploration of galaxy clusters at low radio frequencies (< 200 MHz). These observations enter unexplored territory, where cluster-scale radio sources are expected to be brigher and more common⁸, hence challenging our current understanding of their formation and the underlying mechanisms in the ICM. The researchers simulations will be the first ones aimed at a self-consistent treatment of these mechanisms and their observational signature (Goal 3). Consequently it will be of paramount importance to guide observers in the interpretation of their data. This comparison marks a unique opportunity for the researcher and the beneficiary to constrain the physics of the intra-cluster-medium and its interplay with the cosmic web. Such an outstanding contribution to the field will boost the career of the researcher and provide the beneficiary priority access to top-level numerical research.

2.2 Clarity and quality of transfer of knowledge/training for the development of the researcher in light of the research objectives

During the outgoing-phase, supervision and training will be shared among T. Jones (UMN) and the main code author P.Mendygral (Cray Inc). The researcher will use the state-of-the art WOMBAT code, featuring collisionless dynamics via a highly scalable multi-grid solver and TVD constrained transport magneto-

³Borgani S., Kravtsov A., 2011, Advanced Science Letters, 4, 204

⁴Bauer A., Springel V., 2012, MNRAS, 423, 2558

⁵Vazza et.a. 2014, MNRAS 439; Pfrommer et al. 2008, MNRAS, 385; Miniati et al. 2002, MNRAS, 337

⁶see http://www.astro.umn.edu/groups/compastro/?q=node/112

⁷Donnert J., Brunetti G., 2014, MNRAS, 443, 3564

⁸Brunetti et al. 2008, Nature, 455, 944

hydrodynamics (MHD). He is an expert in particle methods for dark matter and MHD, experience he will contribute at the outgoing-host. For this project he will for the first time use an Eulerian MHD approach in his career. In Jones' group, the researcher will be trained in models for diffusive shocks acceleration, CR proton dynamics and in constrained transport MHD grid methods, instructed by leading experts in the field. He will extend his existing code base to CR protons and implement the scheme into the WOMBAT code, supporting accelerators. This will provide hands-on training in these techniques and introduce him to accelerator methods for high performance computing though software engineers at Cray. In this unique environment, researcher and computer scientists at Cray will mutually benefit from each others view on core astrophysics and computer science problems. This will enable the researcher to develop a deep understanding of the algorithmic issues related to peta-scale computation. This inter-sectoral inter-disciplinary experience will provide him with unique skills and deliver important insight and connections to a leading vendor for supercomputers. This will be a unique competitive advantage in his future career. The interaction with professionals at a US American company will broaden his understanding for project management and communication and provide important action alternatives for an own future management position.

Upon return, the researcher and the host supervisor will leverage the new simulation to interpret unique European radio data in a completely new way and provide unprecedented modelling opportunities to the community of radio astronomers. This will yield influential publications and put the researcher in a strong position in his career. It will also strongly benefit the scientists at the beneficiary institute (IRA), which otherwise do not have access to this kind of simulation and numerical expertise.

2.3 Quality of the supervision and the hosting arrangements

Outgoing-phase

The Minnesota Supercomputing Institute at the University of Minnesota has over three decades of history in high performance computational research. It currently provides free and substantial access for its faculty and their collaborators to multiple large-scale computer systems (30.000 Cores), along with over a PB of storage, software support and training and a visualisation studio. The University also has a strong tradition of promoting high standards of teaching and communications, so maintains regular programs to train potential faculty in teaching and communication methods based on the latest research. All of these resources will be available to the researcher while at the University, since he will receive an adjunct research appointment during his stay. The researcher will receive a J-1 research visa, which allows unlimited travel to and from the USA. Staff will support the researcher in finding adequate accomodation near the university campus upon arrival in Minneapolis. Secretary staff at MSI and MIA will support him in formal questions regarding paper work in the US. The researcher has lived in the US for a year during his undergraduate and has recently visited UMN.

Cray Inc. is a leading vendor of supercomputers, a Cray XK7 system is currently the second fastest system in the world. The researcher will be directly trained by the Cray's Programming Environment group, housed nearby in St Paul and accessible by frequent public transit within 30 minutes. The group is responsible for the development of the Cray compiler, MPI library, scientific libraries and performance tools. It is focused on developing tools and libraries that maximize application performance at scale. This group consists of experts in optimizations on the latest CPU and GPU architectures as well as Cray's innovative interconnect technology. The researcher will regulary interact with developers in the Programming Environment group to learn techniques for obtaining the best possible performance with Cray solutions. Cray has numerous internal HPC systems and will provide the researcher with access to partnership network systems.

Return-phase

The Instituto di Radioastronomia Bologna (IRA) is among the worlds leading institutes for radioastronomy. The hosting group is leading in the observational and theoretical aspects of non-thermal components in galaxy clusters and large scale structure. It is widely known through highly influencial models and observational discoveries that truly guided the scientific research in the field⁹. This research line, now requires extensive numerical simulations, for which the institute seeks strongs partners. With this strategic goal in mind, experts at the beneficiary work with the researcher since the beginning of his PhD¹⁰. IRA has a strong interest in the successful development of this research line and thus the researchers career. In the last years the researcher has developed his prize-winning numerical approach for the simulation of CR acceleration and evolution in collaboration with experts at IRA¹¹, a cornerstone of this proposal. With its long-standing experience and competences, IRA is thus the natural place to optimize the analysis of the simulations of this project, in particular the properties of turbulence, shocks and CRs.

Through memberships in the core management team of the LOFAR "Survey Key Project" (SKP), IRA scientists routinely collaborate with the European LOFAR network of research groups collecting about 80 researchers and students. This allows a tight connection of the project with this new observational facility. The hosting group, has a long record of supervising students and postdocs, including early-stage Marie Curie Fellows. In Bologna, IRA maintains a close link to the university and its observatory. The institute has its own public outreach program at the Medicina facilities, where the researcher is expected to present the project to the public in talks and contribute posters and videos to the permanent exhibition.

2.3.1 Qualifications and experience of the supervisor(s)

Gianfranco Brunetti (IRA) is internationally renown for theoretical models of the acceleration and propagation of high energy particles in galaxy clusters and the interpretation of non-thermal radio data. His results pioneered the theoretical picture in the field and his expertise triggered numerous independent studies and science cases for the next generation of observational facilities, including radio telescopes such as LOFAR and the SKA precursors. He has solid experience in the coordination of research groups/projects and in the supervision of students and post-docs, including Marie Curie Fellows.

He has supervised parts of the PhD work of the researcher, he is also the scientist in charge of the current Marie Curie project of the researcher "Giant Radio Halos". They have published five papers together. His leadership and the numerical models of the researcher have recently lead to a important change in the interpretation and modelling of giant radio halos¹². The host scientist is actively supporting and promoting the career development of the researcher.

Tom Jones (UMN) is internationally known for his theoretical and computational studies in astrophysical plasmas in several environments, acceleration of high energy particles at collisionless shocks and astrophysical magneto-hydrodynamics, especially of turbulent flows. He has a long-standing collaboration with the host scientist¹³. His PhD students include Dr. Mendygral, now at Cray and a partner in this proposed research. His success in his scientific efforts have allowed him to obtain regular, annual computational allocations of several million CPU hours, experience which he will contribute to the project. He knows the researcher and his work from conferences and a recent visit at UMN. He will actively support the career development of the researcher during the outgoing part of the project and introduce him to the US American astrophysics community. He will share project management with G. Brunetti during the out-going phase.

Peter Mendygral (Cray) has 8 years of HPC experience developing scientific applications and optimizing to use in libraries on Cray solutions. His PhD work, supervised by the project partner Dr. Jones, focused on the development of the high performance MHD application WOMBAT and its application to a number of astrophysical problems. His publications include high resolution simulations of AGN jets and their environments. As an engineer at Cray, Dr. Mendygral focuses on performance analysis of a very wide range of customer applications with Cray solutions. He is a technical lead on internal automation and optimization tools at Cray and manages interns assisting with these projects. He will introduce the researcher to his group

 $^{^9}$ Giovannini et al. 1993, ApJ 406, 399 ; Giovannini et al. 1999, NewA, 4, 141; Brunetti et al. 2001, NewA, 6, 1B; Brunetti & Lazarian 2007, MNRAS, 378, 245; Brunetti et al. 2008, Nature, 455, 944; Cassano et al. 2010, ApJ, 721L, 82

¹⁰Donnert J., Bonafede A., Dolag K., Cassano R., Brunetti G., 2010, MNRAS, 401, 47; Donnert J., Dolag K., Cassano R., Brunetti G., 2010, MNRAS, 407, 1565

¹¹e.g. Donnert J., Brunetti G., 2014, MNRAS, 443, 3564

¹²Donnert J. M. F., 2013, Astronomische Nachrichten, 334, 515

¹³Brunetti G., Jones T. W., 2014, International Journal of Modern Physics D, 23, 30007

at Cray, manage the collaborative effort with the group leaders and be the contact person for the intersectoral part of the project.

2.4 Capacity of the researcher to reach and re-enforce a position of professional maturity in research

This project aims at the simulation of cosmic magnetic fields and particle acceleration in galaxy clusters and to model the non-thermal radio emission from the large scale structure of our Universe. The researcher is an expert in cosmological magneto-hydrodynamic (MHD) simulations with particle methods (SPH) and modelling of non-thermal processes in galaxy clusters. He has made key contributions to magnetic fields in structure formation, and the modelling of giant radio halos in galaxy clusters. He is aspiring a leadership position in the numerical astrophysics.

The cosmic magnetic dynamo: He has demonstrated that the current picture of magnetic fields on cosmological scales can be explained by an outflow driven bottom-up seeding process from early star-bursting galaxies. He has conducted the first simulation with truly physically motivated magnetic fields in galaxy clusters. This provided the first meaningful observational test of where magnetic fields originate in the Universe¹⁴. His Diploma work has been cited over 60 times.

In the past four years, he has investigated two popular models for the diffuse non-thermal radio emission from galaxy clusters. When he started this work, two models for the origin of the underlying relativistic electrons were competing in the field. His research revealed substantial shortcomings of one model, and highlighted the predictive power of the other. Combined with new γ -ray data this lead to a fundamental change in our understanding of how galaxy clusters accelerate particles.

He received the 2011 prize for the best PhD thesis in German astronomy for his work, with the comment from the assessment panel: "His work [...] has found great recognition in the field".

Cosmic accelerators: He has for the first time used state-of-the-art cosmological MHD simulations and a popular model for the in-situ injection of cosmic-ray electrons by cosmic-ray proton collisions to compare expected emission with observations. He has demonstrated that this model is incompatible with observations. In the last four years this work has been cited more than 60 times¹⁵.

He has pioneered re-acceleration models in high-resolution astrophysical simulations. He revealed that re-energisation of cosmic-ray electrons by turbulence predicts correct spectral shapes and transient behaviour of diffuse extragalactic radio sources. This discovery has made a substantial contribution to the on-going paradigm shift in how we see the ionised cosmic medium: not as a collisional fluid, but as a weakly collisional plasma¹⁶. He was awarded a Marie Curie fellowship by the European Research Council, with the comment from the assessors that he has "... demonstrated independent thinking and autonomy ...", and that he has "... demonstrated clear evidence of his potential for acquiring new knowledge". For his work he has been competitively awarded one million CPU hours on the FERMI supercomputer at the Italian centre for supercomputing, CINECA.

Numerical tools for cosmic-rays: The researcher has developed crucial numerical tools for the integration of CR electron physics in Lagrangian astrophysical simulations¹⁷. He demonstrated these tools to be highly scalable, and has shown that his approach is transferable to graphics processors with limited memory. This presents the researcher with a unique advantage in the numerical modelling non-thermal radio sources.

¹⁴Donnert J., Dolag K., Lesch H., Müller E., 2009, MNRAS, 392, 1008; Stasyszyn F., Nuza S. E., Dolag K., Beck R., Donnert J., 2010, MNRAS, 408, 684

¹⁵Donnert J., Bonafede A., Dolag K., Cassano R., Brunetti G., 2010, MNRAS, 401, 47; Donnert J., Dolag K., Cassano R., Brunetti G., 2010, MNRAS, 407, 1565

¹⁶Donnert J., Dolag K., Brunetti G., Cassano R., 2013, MNRAS, 429, 3564

 $^{^{17} \}rm{Donnert}$ J., Brunetti G., 2014, MNRAS, 443, 3564

3 Impact (30%)

3.1 Enhancing research- and innovation-related human resources, skills, and working conditions to realise the potential of individuals and to provide new career perspectives

During this project, the researcher will learn from long-standing experts in the field of CR acceleration (Jones, Brunetti), who will provide him with a solid theoretical foundation for the project. He will be introduced to simulations of Eulerian magneto-hydrodynamics, an approach he has not used so far, thus broadening his numerical experience significantly. He will gain access to the unique code base currently used at UMN and Cray Inc. in this subject, which he can use in his future career. He will be trained in HPC techniques at Cray, where he will have continuous access to the Cray software engineers maintaining the Cray Software Environment, i.e. C/FORTRAN compiler, MPI library, OpenACC compiler. This will provide him with a unique in-depth view of the challenges and solutions in high performance scientific computing at petascale, such as scaling, node-communication, data handling and accelerators. The researcher will participate in the "Preparing Future Faculty" programme at the UMN to strengthen his soft skills in management and communication and prepare him for a leadership position in science (figure 2, violet).

At the host institute and in collaboration with observers there, he will provide much anticipated models to lead predictions and interpretation of the new low-frequency radio data from the European LOFAR telescope. This is expected to yield unique scientific publications, as this frequency range is largely unexplored and LOFAR is expected to detect a completely new population of steep radio sources in clusters. Considering that the project is very relevant for the upcoming Square Kilometer Array, the researcher, the beneficiary and the European radio astronomy community will benefit from spearheading the development in the field. The outstanding science will put the researcher into a very strong position to apply for long-term positions at the end of the project. Finally, the project will build a new independent collaboration of the beneficiary with the out-going host and, through Cray Inc., will provide new excellent opportunities for training of IRA students and staff in the future.

3.2 Effectiveness of the proposed measures for communication and results dissemination

3.2.1 Communication and public engagement of the action

The researcher will publish results alongside videos and renderings of the simulation, on a website at the host institute, specifically setup for the project. He will prepare 3D fly-throughs for the visualisation lab at MSI. He will provide public outreach at IRA in Medicina with talks, posters, images and videos for the permanent public exhibition. He will present the project at the European researchers night in Bologna (Notte dei ricercatori), where he will collaborate with the local IT staff at IRA to provide interactive fly-thoughs through the simulation, thereby making it explorable for the general public. Cray Inc. will use the simulation to showcase the capabilities of their hardware and software environment to the computer science community and the private sector. The company will be required to sign a legally binding agreement to ensure proper credit to the researcher, the host institute and the Horizon 2020 programme of the European Research Council.

3.2.2 Dissemination of the research results

All publications during this project will be made in top journals. We plan to publish a first paper on numerical methods after 10-12 months (**paper I**). We will then submit the main simulation paper to Nature, since this simulation will be the first resolving the MHD dynamo in clusters with a robust treatment magnetic fields and turbulence and a self-consistent model of CR proton and electron physics (**paper II**). Towards the last year of the project we will analyse the properties of CRs and the resulting radio emission from the run to predict the steep low frequency radio emission targeted by LOFAR key science (**paper III & IV**). We will also investigate the neutrino signal from hadronic interactions of CR protons with the thermal gas in clusters(**paper IV**).

The results will be communicated at top-level conferences for turbulence, plasma physics and cosmology, throughout the project (see figure 2). Meta-data from the simulations, like a catalog of the simulated clusters at different wave lengths, will be made available on European servers hosted at IRA or CINECA. Raw data of the simulations will be too large to be meaningfully interpreted by external researchers.

3.2.3 Exploitation of results and intellectual property

The simulations proposed here will be exploited beyond the three years of the project by the scientists involved. The rights will remain with the host institute / researcher in Europe. Cray Inc. will not assume any rights on the intellectual property build for the project. The data will be available to the researcher at the UMN beyond the duration of the project. Coarse versions of the data snapshots will be transferred to IRA for further exploitation.

4 Implementation (20%)

4.1 Overall coherence and effectiveness of the work plan, including appropriateness of the allocation of tasks and resources

During an initial 3 month advanced training phase at Cray Inc. the researcher will be introduced to the numerical techniques and the WOMBAT code, running simple code tests. Under the supervision of Jones, he will familiarise himself with the technique and its theoretical aspects. Afterwards, the researcher will independently work on the following items (see also fig. 2):

Algorithm Implementation ($\approx 10 \text{ months}$)

The first part of the project will be concerned with implementation details and will yield one paper on the CR algorithm and numerical methods employed (**paper I**). During this time we will also acquire the computation time needed for the project. We expect the involvement of Cray to be beneficial in this process.

CR physics: The existing Fokker-Planck solver for CRs dynamics will be ported into the WOMBAT code. Under supervision of Jones & Brunetti, it will be extended to CR protons. Infrastructure to split the spatial diffusion from the momentum diffusion of CRs is already present in WOMBAT and will be reused. This includes on-the-fly estimation of turbulence and a shock finder. At Cray Inc. the researcher will then port and optimize his part of the code to accelerators (GPUs) via OpenACC. The Cray compiler offers world leading performance in OpenACC. This part of the project is fundamentally new, hence has the highest risk associated. *Risk: High*

FoF Halo Finder & Magnetic field Seeding: The researcher will implement an on-the-fly friends-offriends halo finder into WOMBAT, a standard technique to find virialised halos in collisionless simulations. The FoF algorithm reduces to a simple neighbour search, which the researcher knows very well from his past research. He has access to an existing implementation. The FoF groups will be used to seed magnetic fields at high redshift, an approach the researcher has pioneered at the beginning of his career¹⁸. *Risk: Medium*

Cosmological Initial Conditions: The researcher will write a scalable IC generator suitable to setup cosmological simulations based on the second order Zeldovich approximations, for WOMBAT. The researcher does have prior experience with all numerical techniques involved (FFTs, power spectra, displacement fields), but has never generated ICs of that size before. Several public codes are available online, which can be in principle be adapted.

Synthetic Observations: The necessary emission functions required to produce mock radio, X-ray, γ -ray, and SZ observations from the simulation will be implemented into the GRIZZLYEYE code. The researcher has written such a code for his previous project and has extensive experience in the topic from his PhD work. Risk: Low

¹⁸Donnert J., Dolag K., Lesch H., Müller E., 2009, MNRAS, 392, 1008



Figure 2: Gantt chart of the project

Cosmological simulation (\approx 11 months)

Preparations: A series of cosmological simulations will be run with increasing resolution. Scalability and correctness of the code base and initial conditions will be tested. Computing time will come from the local computer at the University of Minneapolis (30.000 cores). Risk : Medium

Main Run: We aim at a large cosmological simulation with 3 levels of nested grids, centered on 2-5 large galaxy clusters, all grids with 4096^3 resolution elements. This is different from an AMR approach as the refinement is set a priori, WOMBAT already supports this nested grid approach very efficiently to > 100.000CPUs. The same infrastructure is used to efficiently handle DM particles. We require a spatial resolution of $\approx 2 \,\mathrm{kpc}$, which we want to approach over the whole cluster volume. This high resolution in the whole cluster volume is necessary to faithfully track the evolution of turbulence over a wide range of scales and allow the analysis of the inertial range (Goal 1, paper II). To find sufficiently large clusters, we will need a 256 Mpc^3 root grid, with two refinements at 64 Mpc^3 and at 10 Mpc^3 , centered on a few previously found clusters, with a spatial resolution of 2.44 kpc inside the virial radius. This requires the largest Cray machines available today. We aim to keep initial storage below 2 PByte, which is a reasonable number for the largest machines available in 2017. We need 180 Byte per resolution element using the CR spectrum compression developed in Donnert & Brunetti 2014. This means a snapshot size of 12 TB per cluster and time slice. For 5 clusters and 20-30 time slices, we reach 1-2 PByte of raw storage, we will not save the DM particles.

Risk : High

Initial Analysis & First results regarding turbulence, cosmic-rays and radio brightness from this simulation will be submitted to Nature, as this simulation represents a significant step forward in the treatment of non-thermal cluster physics as well as computational science (Goal 1, paper II). Risk : Low

Analysis & Comparison with observations (12 months)

At IRA we plan to start full exploitation of our simulation. We will use the simulation to perform unprecedented studies of turbulence & shocks in clusters and beyond (paper II+III). Upon return to Italy, LOFAR is expected to provide the first all sky survey at low frequencies. The researcher will use his unique numerical simulation to predict observations and interpret the fundamentaly new data (paper IV). We will for the first time derive an expectation for the neutrino brightness of the large scale structure from CR proton hadronic interaction.

4.2 Appropriateness of the management structure and procedures, including quality management and risk management

The risky implementation work (CRs, scaling, accelerators) will be done with optimal support by experts in CR dynamics (Jones), grid codes (Mendygral) and HPC (Cray Inc). These will ensure timely execution of the work plan and management of the early phase of the project. In the event of serious problems with the code implementation or acquisition of computing time, the details of the main run can then be flexibly adjusted to available resources in computing time and storage. If necessary the initial analysis part for paper II can be moved into the return phase to free more time in the US, even though we allocated a generous amount of time for the main run in our schedule. Similary, the neutrino study could be postponed until after the end of the project. Even in the catastrophic event of complete failure of scalability of the code, a reasonably sized Eulerian cluster simulation, including self-consistent CR physics, would be a unique contribution to the field. It would yield influencial papers and it would allow an, albeit limited, comparison to LOFAR key science. The analysis of the simulation is then low risk and should be done in Europe, where the researcher can directly benefit from the theoretical expertise at IRA and the new LOFAR data.

4.3 Appropriateness of the institutional environment (infrastructure)

The combination of MSI and Cray Inc. provides a unique environment for the project, with world-leading industry experience in HPC and theoretical expertise in the numerical simulations of CR protons and MHD-grid methods, complementary to the researchers approach. MSI and Cray also provide access to large amounts of computational infrastructure as well as profound experience in obtaining large amounts of computing time at top five supercomputers in the US, such as the Blue Waters machines through NSF grants. Worldwide, only IRA Bologna hosts decades of experience in radio astronomy, access to the ground-breaking new radio data from LOFAR and the theoretical expertise to meaningfully connect new observational results through theoretical interpretation with the results from this project.

4.4 Competences, experience and complementarity of the participating organisations and institutional commitment

The host institution (IRA) is leading in the theoretical interpretation and observations of diffuse radio sources in galaxy clusters for over two decades. The advent of LOFAR and the complexity of the involved physics now require detailed numerical modelling of these sources, in parts provided by the researcher during his last IEF fellowship at IRA. However, to make a step forward in these models, the hosting group requires the researcher to tap into significant numerical expertise in Eulerian MHD simulations of cluster turbulence, shocks, and peta-scale simulations. These competences are currently not available to them in the EU. To our knowledge, no European group employs a code with the required scaling properties in a complementary scientific environment, as supercomputers are mostly designed in the USA by Cray¹⁹, IBM, SGI. Only the outgoing host (UMN) provides these top-level competences in Eulerian MHD simulations and cosmic-ray acceleration (Jones), widely complementary to the prior work of the researcher. Moreover, the Eulerian code developed by P. Mendygral features the performance characteristics required to faithfully simulate cluster radio sources. The size of the numerical problem will require significant input from computational scientists, which is provided first hand by Mendygral and the software development group at Cray Inc. Hence the partner organisations in the USA are a *unique complementary match* to the competences brought in by the beneficiary and the researcher, connecting complementary astrophysical expertise (Donnert, Brunetti, Jones) with computer science expertise at a company (Mendygral, Cray).

⁽stop page count, max 10 pages)

¹⁹Top 2 supercomputer is currently "Titan" an Cray XK7 at Oakridge Nation Lab USA (http://top500.org)

5 CV of the Experienced Researcher (max 5 pages)

Istituto di Radioastronomia	Tel: +39 051 639 9364
Via P. Gobetti 101	Email: donnert@ira.inaf.it
40129 Bologna, Italy	Date of Birth : 14th April 1981
Nationality: German	German, English, Italian (B1), Japanese (JLPT4)

Experience

I am currently a Marie Curie Fellow at the Istitute di Radiostronomia in Bologna. My research has focused on the simulation of non-thermal components in the large scale structure of the Universe: Magnetic fields, cosmic rays, turbulence - their interplay and observational signatures.

Motivated by my experience as a working student at MPE Garching and as exchange student at the University of Hawai'i prior to graduation I decided to start my Diploma project in astrophysical simulations with K. Dolag at the MPA in Garching. During this project I gained knowledge in and access to the development branch of the simulation code GADGET-3 including its MHD extension. It performs simulations of magnetic fields in astrophysical plasmas in a cosmological context. Using this code and a semi-analytical model of galactic outflows, I was able to show that the current observational picture of magnetic fields on cosmological scales is compatible with purely outflow driven seeding processes. I made predictions to guide future observations of Faraday rotation measurements in filaments and voids. This work provided me with the first cosmological simulation with truly physically motivated magnetic fields in galaxy clusters.

This gave me a great advantage in my PhD project on the non-thermal emission from galaxy clusters. Magnetic fields are a key variable in the formation process of radio halos and so my Diploma work was an excellent basis to build on. When I started my PhD, hadronic models in simulations had received a lot of attention, but new systematic observations led me to question the validity of these models: in particular their predictions of radio spectra, statistics and spatial distribution of and in radio halos. I used the simulation from my diploma work together with a synchrotron solver I developed to show that these models actually fail at a number of points when compared in detail to observations. Assuming my well-motivated magnetic fields and fitting radio observations, the CR proton density had to become > 10% of the thermal energy density in the cluster outskirts. The corresponding non-thermal pressure was then not compatible with observations. Furthermore I found that hadronic models neither recover the transient behaviour nor the spectral shape of observed radio halos. I predicted the γ -ray flux from these models, which was not detected by FERMI in the nearest clusters thus confirming my expectation that hadronic models for radio halos are oversimplified.

This work required the development of numerical methods to efficiently extract synthetic observations using a variety of emission processes from SPH simulations. I developed SMAC-2, a MPI-parallelised, modular projection code that properly handles irregular particle distributions as found in SPH calculations. It features a variety of analysis techniques and emission mechanisms: the numerical solver for polarised synchrotron emission of arbitrary CR spectra mentioned above; Faraday rotation including relativistic corrections; γ -ray emission from hadronic CR proton interactions; and a wide variety of thermal processes. Facing the apparent problems of simple hadronic models for the radio halos and the non-detections by FERMI, I focused my research on a reacceleration approach. It required a complete numerical description of the underlying CR electron spectrum and its non-linear dynamics. Its evolution is governed by a Fokker-Planck equation, which describes the stochastic momentum diffusion of the particle population induced by turbulence and energy gains and losses. I implemented a Fokker-Planck solver in C. It uses the efficient Chang & Cooper algorithm to evolve particle spectra, coupled to turbulence. The performance of this code greatly exceeds the performance of other particle codes used before. Using this code and a simple idealised non-cosmological model for two colliding galaxy clusters I was for the first time able to show that magnetosonic reacceleration models predict correct spectral and spatial shapes of the diffuse radio halo emission in simulations. These models also show the transient behaviour seen in the observations and require significantly less CR protons in clusters.

In my first postdoc, I turned to realistic models for idealised cluster mergers, which offer the unique opportunity to simulate models taylored to specific observed systems. As LOFAR was delayed it became clear to me that observers would continue to find radio halos and relics by pointed observations, so this approach offered a "smoking gun" to constrain models for CR acceleration in the ICM. Unfortunately I found that idealised models had never been compared to real cluster correlations in the literature. I then build my own model, which for the first time compares very well with observed cluster properties. I published a paper with my new approach to isolated cluster mergers, featuring the first model for the El Gordo cluster. El Gordo is of particular interest, because it shows a radio halo at a redshift of z = 0.89, where IC losses are so high, that nobody expected a halo. An ideal target for my CR model. Unfortunately I found that the particular appearance of El Gordo and thus the non-thermal emission cannot be reproduced by simple binary mergers. Substructure plays a major role in this cluster. So I extended my model to include substructure, for which I had to use very advanced techniques to setup initial conditions. Because the cluster cannot be relaxed anymore, I had to use weighted Voronoi tesselations to set the SPH particle distribution, a technique for which a had to implement an OpenMP parallel neighbour tree. I also had to numerically solve Eddingtons equation to compute the equilibrium distribution function for the dark matter particles in the combined potential of gas and DM in the cluster. I used the model of C. Giocoli, a fellow postdoc at the observatory in Bologna, to implement substructure in my cluster merger. I am currently working on the numerical model for El Gordo to finally simulate its radio halo. In the meantime, I also implemented CRe shock acceleration into my Fokker-Planck solver to model El Gordos double relic. I published a numerical method paper on the Fokker-Planck solver, in which I also present a novel compression algorithm for CR spectra based on splines.

One year into my postdoc, I encountered severe problems with our SPH code, especially in modeling turbulence and shocks in low viscosity environments, key ingredients of my research ! The standard numerical approach was so viscous, it was not a good model for the ICM, which likely has Reynolds number of $> 10^4$. Popular low viscosity shock capturing schemes did not work well enough to faithfully track turbulence in cosmological environments. Simulations were plagued by particle noise, particle setup and relaxation was incredibly difficult to get acurately right. I was surprised people actually used the method so extensively. Unfortunately, this was a major set-back for my Marie Curie project, for which I wanted to use our code to simulate radio halo populations in a cosmological environment. My input on these problems eventually lead to a complete overhaul of the SPH algorithms in MHD-GADGET-3 by a PhD student of my former supervisor in Munich (Beck et al. in prep., I am providing the testing against decaying turbulence). The code now works much better and is well tested, it is the best SPH code on the market. I hope to publish a first cosmological study with this version next year, however the properties of SPH regarding turbulence remain not well defined, at best the code converges incredibly slowly in the subsonic regime.

During a workshop on the simulation of astrophysical turbulence in Stockholm, I gained new insight in how different numerical techniques model turbulence and low viscous flows. It became clear to me that only grid methods provide the unambiguous dissipation scale at the resolution limit needed to track turbulence properly. I found moving mesh techniques to address the issues I had encountered with SPH before perfectly. Unfortunately, only two codes exist, both are not public, do not have MHD and both do not scale well enough for my needs. Surprisingly, the fixed mesh code WOMBAT in Minneapolis was the first code that was able to handle all the demands I and my group in IRA have at cosmological simulations. This was achieved by a major step in scalability and implementation, not fundamentally new algorithms, Eulerian MHD is very mature. I visited the institute and Cray Inc. and found a productive, inspiring environment and communicative people; perfect for me to learn Eulerian methods, CR proton acceleration and bleeding-edge HPC. This environment would allow me not only to finally do a ground-breaking simulation of turbulence, CRs, radio halos and relics, but let me learn implementation of hybrid parallel programs directly from the source, the people who actually build the computers, compilers, libraries and communication infrastructure. These techniques are one of my main interests. Currently all but one cosmological codes are struggling to get proper scaling to more than a few 10^4 cores, mostly because astrophysists lack the computer science knowledge. This project is my chance to get ahead in the game. The obvious overlap of this opportunity with the goals of the Marie Curie GF then lead to the submission of this proposal.

Research Interests

- Cosmological magnetic fields: origin and amplification
- Non-thermal emission and particle acceleration in the cosmic web
- Cosmological simulations of structure formation
- Isolated models for galaxy clusters
- Particle methods for collisionless dynamics (Dark Matter)
- Smoothed Particle Hydrodynamics (SPH)

Positions & Education

- 2012 pres. Marie Curie Fellow, INAF-Istituto di Radioastronomia Bologna, Italy
- 2011 2012 Postdoc, INAF-Istituto di Radioastronomia Bologna, Italy
 - 2011 **Postdoc**, Max Planck Institute for Astrophysics, Garching, Germany
- 2007 2011 PhD, Ludwig Maximilians University, Munich, Germany summa cum laude
- 2001 2007 **Diploma**, *Technical University*, Munich, Germany General physics with focus on astrophysics and computational physics
- 2005 2006 Visiting student, University of Hawai'i at Manoa, Honolulu, USA Focus on astronomy & astrophysics

Prizes. Grants & Fellowships

- Jul. 2012 PhD Award, German Astronomical Society Best PhD in German Astronomy 2011
- Mar. 2012 Marie Curie Fellowship, European Research Council "Giant Radio Halos", 94.2 / 100 points
- Dec. 2013 **CAASTRO Exchange Grant**, *CAASTRO* Collaboration with B.Gaensler Sydney Institute for Astronomy, C.Power ICRAR Perth, Australia
- Sept. 2008 ASTROSIM Exchange Grant #2065, Computational Astrophysics and Cosmology, Supporting visit at IRA Bologna, Italy.

PhD Thesis

title	On the Diffuse Non-thermal Emission from Galaxy Clusters
supervisors	K. Dolag (MPA), G. Brunetti (IRA), H. Lesch (LMU)
description	We investigate the validity of hadronic and reacceleration models of giant radio
	halos by means of astrophysical simulations.

Diploma Thesis

title	A Numerical Study on the Origin of Cluster Magnetic Fields
supervisors	K. Dolag (MPA), E. Mueller (TU/MPA), H.Lesch (LMU)
description	We use MHD simulations to predict the magnetic field in galaxy clusters, as-
	suming field seeding by galactic outflows at high redshifts.

Other Relevant Experiences

Aug. 2014	Visiting scientist , University of Minnesota, Minneapolis, MN, USA. Collaboration with T. Jones & P. Mendygral
Mar. 2014	Visiting scientist , <i>SIfA & ICRAR</i> , Australia. Collaboration with B. Gaensler & C. Power
Sept. 2010 & Fall 2008	Visiting scientist , <i>Instituto di Radioastronomia</i> , Bologna, Italy. Collaboration with G. Brunetti & R.Cassano
July 2009	Summer School , <i>Institute for Advanced Study</i> , Princeton, USA. Prospects in Theoretical Physics, Computational Astrophysics.
Spring 2005	Seminar <i>Technical University</i> , Munich, Germany Intercultural Business Communication
Fall 2004	Working student Max Planck Institute for Extraterrestrial Physics, Garching, Germany Testing of a calibration source for future X-ray observatories & Software devel- opment

Conferences & Workshops

Mar 2013	Conference, SnowCluster, Salt Lake City, USA
	Contributed talk: Radio Haloes in isolated Galaxy Cluster Simulations

- Aug 2012 Workshop, Simulating Astrophysical Turbulence, Stockholm, Sweden Contributed talks: Reviews on Smooth Particle Hydro- and Magnetohydrodynamics
- May 2010 **Conference**, *Magnetic fields on scales of kpc to km*, Cracow, Poland Contributed talk: Constraining CRs in galaxy clusters using radio halos and simulations
- Nov 2009 Workshop, KAW 5: Shock waves, turbulence and particle acceleration, Pohang, South Korea Contributed talk: Radio halos in simulated galaxy clusters
- June 2009 **Conference**, *Cosmological magnetic fields*, Ascona, Switzerland Contributed talk: Radio halos from secondary CR models in cosmological MHD simulations

Refereed Publications

J. Donnert, G. Brunetti. An Efficient Fokker-Planck Solver and its Application to Stochastic Particle Acceleration in Galaxy Clusters. *MNRAS* accepted

J. Donnert. Initial conditions for idealized clusters mergers, simulating 'El Gordo'. *MNRAS*, 438:1971-1984 March 2013

J. Donnert, K. Dolag, G. Brunetti, and R. Cassano. Rise and fall of radio haloes in simulated merging galaxy clusters. *MNRAS*, 429:3564–3569, March 2013.

J. Donnert, K. Dolag, G. Brunetti, R. Cassano, and A. Bonafede. Radio haloes from simulations and hadronic models - I. The Coma cluster. *MNRAS*, 401:47-54, January 2010.

J. Donnert, K. Dolag, R. Cassano, and G. Brunetti. Radio haloes from simulations and hadronic models - II. The scaling relations of radio haloes. *MNRAS*, 407:1565-1580, September 2010.

J. Donnert, K. Dolag, H. Lesch, and E. Mueller. Cluster magnetic fields from galactic outflows. . Lesch, and E. Mueller. Cluster magnetic fields from galactic outflows. *MNRAS*, 392:1008-1021, January 2009.

H. Kotarba, H. Lesch, K. Dolag, T. Naab, P. H. Johansson, J. Donnert, and F. A. Stasyszyn. Galactic menage a trois: Simulating magnetic fields in colliding galaxies. ArXiv e-prints, sub. *MNRAS*, November 2010.

F. Stasyszyn, S. E. Nuza, K. Dolag, R. Beck, and J. Donnert. Measuring cosmic magnetic fields by rotation measuregalaxy cross-correlations in cosmological simulations. *MNRAS*, pages 1287-+, September 2010.

Proceedings

J. Donnert. Modelling giant radio halos. Doctoral Thesis Award Lecture 2012. Astronomische Nachrichten, 334:515, June 2013.

K. Dolag, F. Stasyszyn, J. Donnert, and R. Pakmor. Magnetic fields and cosmic rays in galaxy clusters and large scale structures. In *IAU Symposium, volume 259 of IAU Symposium*, pages 519-528, April 2009.

6 Capacity of Participating Organisations (1 + 1/2 + 1/2 pages)

INAF - Istituto di Radioastronomia Bologna			
General Description	IRA is one of 19 research institutes coordinated by INAF (National Institute for Astro-		
	physics), and the main interlocutor for radioastronomy research in Italy. The institute		
	combines top-level competences in theoretical and observational astrophysics with major re-		
	search focuses in the field of extragalactic astrophysics, from radiogalaxies and quasars to		
	clusters of galaxies. This research is carried out through intensive European and interna-		
	tional collaborations and exchanges of scientists. Researchers at IRA have access to the most		
	important observational international facilities in the field and are deeply involved in key		
	projects and collaborations with the most important telescopes (ongoing and future) such		
	as LOFAR, MeerKAT, ASKAP, SKA, FERMI, CTA, EVN, VLBI, ALMA,.		
Role and Commitment	The research interests of Dr. Brunetti cover a broad area of important topics, from radio		
of key persons (supervi-	galaxies to galaxy clusters, and fundamental astrophysical processes, including the acceler-		
sor)	ation and propagation of high energy particles and radiative processes in astrophysics. Dr.		
	Brunetti is internationally reknown primarily for his seminal studies on the acceleration of		
	relativistic particles and non-thermal emission in galaxy clusters. Nonetheless, one of his		
	most notable works is the derivation of original solutions to the problem of anisotropic in-		
	verse Compton scattering and its application to the X-ray emission of radio galaxies and		
	quasars ("Brunetti mechanism"). Brunetti published about 110 papers in refereed journals,		
	including Nature and Science, and several reknown review papers. He has 4500+ citations		
	(H factor = 39), 1400 + normalized citations and 1600 + citations as first author and a strong		
	record of top-ranked and high-ranked papers.		
Key Research Facili-	IRA operates three radio telescope facilities for use by the scientific community in Medicina		
ties, Infrastructure and	and Noto (Sicily). A new 64-m antenna, the SRT, is under construction in Sardinia. The		
Equipment	antennas are part of the VLBI global network for about 150 days a year. IRA is a member		
	of the Joint Institute for VLBI in Europe (JIVE) and participates in Consortia such as		
	the European VLBI Network (EVN) and the International VLBI Service for Geodesy and		
	Astronomy (IVS), as well as in the Committee for Radio Astronomial Frequencies (CRAF).		
	IRA is also part of the INAF network of 19 research institutes in Italy focus on astrophysics,		
	sharing common goals and long term programme.		
Independent research	IRA is located in the "C.N.R. Campus of Research" in Bologna. This is a special environment		
premises?	that comprises six research institutes from CNR (National Council of Research), two research		
	Equipment institutes from INAF and a conference center. The campus hosts about 1000		
	researchers in different fields of physics and chemistry, and provides an excellent environment		
	to develop inter-disciplinary collaborations.		
Previous Involvement in	IRA has been a node for several European networks for training and mobility. Among others,		
Research and Training	the "Consortium for European Research on Extragalactic Surveys" (CERES) funded by the		
Programmes	EU through TMR programme, and the "EU Marie Curie Early Stage Training Network for		
	long-wavelength Astronomy" (ESTRELA).		
Current involvement in	Currently IRA is hosting an ALMA regional center, and a Marie Curie Fellow. Personel at		
Research and Training	IRA trains about 10 degree students and 3 PhD per year		
Programmes			
Relevant Publica-	• Donnert J., Brunetti G., 2014, MNRAS, 443, 3564 ; • Brunetti, G., Giacintucci, S.,		
tions and/or re-	Cassano, R., Lane, W., Dallacasa, D., Venturi, T., Kassim, N. E., Setti, G., Cotton, W. D.,		
search/innovation	Markevitch, M., 2008, Nature, 455, 944; • Brunetti G., Jones T. W., 2014, International		
products	Journal of Modern Physics D, 23, 30007		

Cosmo Plasmas - GF

University of Minneso	ota - Minnesota Supercomputing Institute
General Description	The University of Minnesota is one of the top research universities in the US. It maintains
	highly ranked programs in physical sciences, mathematics, engineering and computer science.
	For 30 years it has fostered high performance scientific computation through the Minnesota
	Supercomputing Institute (MSI). The MSI provides free access for its faculty and their
	collaborators to multiple large-scale computer systems, along with storage, software support
	and training. The University is also home to a national Institute for Mathematics and Its
	Application, several of whose faculty are renowned for innovation in computational methods
	relevant to the effort of this proposal.
Role and Commitment	T. Jones is a full professor at the Minnesota Institute for Astrophysics (MIA), staff member
of key persons (supervi-	at the Minnesota Supercomputing Institute (MSI) and a Fellow of the American Physical
$\mathbf{sor})$	Society. He has published more than 150 papers in refereed journals with an H-index of
	48 and presents several invited/review talks at international meetings each year. He has
	supervised more than 10 PhD dissertations.
Key Research Facili-	Itasca cluster, 30.000 CPUs + accelerators, > 100 TB storage, visualisation laboratory,
ties, Infrastructure and	$dedicated \ workstation \ / \ server \ environment, \ dedicated \ hardware \ and \ software \ support \ groups$
Equipment	
Independent research	MSI is located on the main campus of the University of Minnesota.
premises?	
Previous Involvement in	We are not aware of previous involvement of MSI in European research and training pro-
R&T Programmes	grammes.
Current involvement in	We are not aware of current involvement of MSI in European research and training pro-
R&T Programmes	grammes.
Relevant Publications	• Ryu D., Miniati F., Jones T., Frank A. 1998, ApJ, 509; • Mendygral P. J.; Jones T. W.;
	Dolag K., 2012, ApJ, 750; •

Cray Inc.	
General Description	Cray Inc. is a global leader in supercomputing with 40 years of experience developing the
	world's most advanced supercomputers. It provides solutions to government, industry and
	academic sectors that enable scientists and engineers to make breakthrough discoveries. As
	of the June, 2014 Top500 list of the fastest supercomputers in world, 18 of the top 100
	are Cray systems. Cray Inc. has been central to the development of a number of innovative
	software technologies such as OpenACC and Chapel, and it is an active member of numerous
	standards committees including MPI, Fortran, and OpenMP.
Role and Commitment	P. Mendygral is a software engineer in the Cray Programming Environment division. He will
of key persons (supervi-	coordinate interactions between the researcher and Cray developers as well as provide one
sor)	on one training. As the primary developer of WOMBAT he will work with the researcher to
	enhance the code's capabilities and performance on Cray solutions.
Key Research Facili-	Cray employs over 1000 people worldwide, with research and manufacturing facilities in
ties, Infrastructure and	Seattle, Minnesota, Texas and Wisconsin and many sales and service locations around the
Equipment	world.
Independent research	Cray software support is located in an office building in St. Paul, reachable within 30 min
premises?	by public transport from UMN.
Previous Involvement in	None
R & T Programmes	
Current involvement in	None
R & T Programmes	
Relevant Publica-	The Cray XE, XK and XC supercomputers and Cray Programming Environment provide a
tions and/or re-	complete solution for optimized performance of real-world HPC applications at scale. The
search/innovation	Cray Compiling Environment includes OpenACC, directives-based programming for enabling
products	accelerators in hybrid HPC systems.

7 Ethics Issues

There are no ethics issues associated with this project.

8 Letters of Commitment

We attach the letters of commitment from:

- 1. Prof. T. Jones, Minnesota Institute for Astrophysics, University of Minnesota, USA
- 2. Prof. J. Vinals, Supercomputing Institute for Advanced Computational Research, University of Minnesota, USA
- 3. Dr. L. DeRose, Programming Environment Director, Cray Inc., USA

UNIVERSITY OF MINNESOTA

Twin Cities Campus

Minnesota Institute for Astrophysics School of Physics and Astronomy College of Science and Engineering 116 Church St. SE Minneapolis, MN 55455 Office: 612-624-4811 Fax: 612-626-2029 www.astro.umn.edu

September 2, 2014

Dear Sir or Madam:

I am very pleased to support and partner in the research and training activities for Dr. Julius Donnert as outlined in his Marie Skłodowska-Curie Actions proposal, "Cosmological Simulations of Radio Bright Plasmas." His research plan very nicely complements my own ongoing and planned computational astrophysics research funded by the National Science Foundation (NSF) at the University of Minnesota. This work has included pioneering efforts to simulate astrophysical plasma flows and the acceleration of high energy charged particles in these environments, especially in collisionless shocks. That research has spanned several astrophysical contexts. Most recently it has focused on the diffuse plasmas in galaxy clusters, which is the topic of Dr. Donnert's proposal. By combining his strengths with ours I am confident we can substantially strengthen each of our efforts and accomplish uniquely valuable scientific goals that will have major and lasting impact on important studies of large scale structure formation in the universe and fundamental plasma physics. In addition, I expect his presence in Minnesota to enhance our ongoing efforts to develop the world class computational tools needed to address current and future challenges in these areas. That work is carried out in collaboration with Dr. Peter Mendygral at Cray Inc. in St Paul, Minnesota. So, Dr. Donnert's planned interactions with Cray and time on their site during his time in Minnesota will be much to our benefit on this effort.

As a Professor at the University of Minnesota I have at no cost ready access to substantial high performance computing resources, especially through the University-based Minnesota Supercomputing Institute for Advanced Computational Research (MSI), of which I am a major user, Fellow and a past Interim Director. MSI provides and supports access to multiple computing platforms to carry out large parallel computations and to store and analyze the output. Given the scope of the hardware likely to be present in MSI during Dr. Donnert's two year Minnesota stay (including systems with sustained performance of several hundred TF, plus multiple GPU accelerators for suitable operations) and my consistent success in obtaining allocations of multiple millions of CPU hours on these systems, I am confident I can commit to providing access for Dr Donnert to local resources sufficient for the development and exploration efforts in the proposed research. For the final, very large scale production simulation effort outlined in the proposal, which will require systems larger than individual universities can provide, I will propose to NSF-funded centers in the US, where much larger allocations are available, for example on the Blue Waters system at NCSA. As additional, local infrastructure, I also maintain a cluster of dedicated workstations and have under construction more than 100 TB of dedicated storage space acquired through NSF funds that are beyond MSI-based storage and would be available for use by Dr. Donnert.

In addition to outstanding computational research opportunities and access to highly ranked faculty in physical sciences, mathematics and engineering, the University of Minnesota can offer Dr. Donnert valuable training opportunities. These include an outstanding, regularized program

Driven to Discover^{ss}

in higher education teacher training ("Preparing Future faculty") and frequent, informal teaching workshops taught by experienced, award-winning faculty. These are available to individuals with postdoctoral-level appointments at the University. In my role as Faculty Principal Investigator I can and will obtain such an appointment for Dr. Donnert during his stay at the University of Minnesota.

The proposed research partnership will have several components. The research centers on extension and application of a very high performance magnetohydrodynamic (MHD) code originally developed in our group under the leadership of Dr. Mendygral, now at Cray. Current versions of the code include the transport and energization (acceleration) of energetic charged particles in shocked flows, but exclude their acceleration through stochastic, turbulent interactions. A critical new extension of the code is one that removes that limitation, enabling it follow the acceleration of energetic particles interacting with plasma turbulence. Dr. Donnert's recent, ground-breaking work in Bologna on this topic uniquely qualifies him to lead that effort. This will be carried out at the University of Minnesota and at Cray Inc. Dr. Donnert will also participate in other extensions of the code that are underway to enable it to follow the formation of galaxy clusters, and to study the hot plasmas they contain at a level of detail previously not possible. He will also be a key player in carrying out and analyzing the simulations, as well as publishing the results.

In summary, Dr. Donnert's proposed extended visit in Minnesota is a winning proposition for everyone and an exciting opportunity to solve some key astrophysical problems. We will welcome him and support his efforts in every way we can.

Sincerely,

Thomas he gones

Thomas W. Jones, Professor, Fellow of the Minnesota Supercomputing Institute, Fellow of the American Physical Society

UNIVERSITY OF MINNESOTA

Supercomputing Institute for Advanced Computational Research 117 Pleasant Street S.E. Minneapolis, MN 55455 Office: (612) 624-0528 Fax: (612) 624-8861 www.msi.umn.edu

August 4, 2014

Dear Sir or Madam,

On behalf of the Minnesota Supercomputing Institute for Advanced Computational Research (MSI) I am pleased to support the Marie Sklodowska-Curie Actions proposal, "Cosmological Simulations of Radio Bright Plasmas," by Dr. Julius Donnert. In particular, I confirm, as outlined in the accompanying letter by Professor Jones, that MSI expects during his proposed stay at the University of Minnesota to have available the kinds and levels of resources and support needed to pursue the proposed research plan. As pointed out in that letter, Professor Jones is an MSI Fellow, and is a long-time investigator and major user of our resources. We certainly welcome the proposed collaboration with Dr. Donnert and will strive to help it succeed. MSI has a distinguished, 30 year history of supporting high performance computational research by University faculty and their collaborators. The most relevant computer systems expected to be available through MSI in 2015 include the currently installed Itasca cluster (a 11,000+ core Intel Xeon-based cluster from HP) and a new HP cluster to be installed in late 2014 with (18000+ Xeon cores plus a substantial number of GPUs). In addition, MSI provides users with access to over a PB of on-line data storage, as well as several computational laboratories for analysis, including high performance visualization. MSI also offers access to PhD-level technical support staff, plus excellent training opportunities through its extensive series of hands-on tutorials presented by that staff. Current tutorials include several relevant topics in high performance computing, such as Message Passing optimization. All these resources would be accessible to Dr. Donnert during his time in Minnesota.

MSI is dedicated to providing competitive research computation opportunities to its research community. Support for unique collaborative efforts of the kind represented in Dr. Donnerts proposal clearly benefit that community substantially, so contribute directly to MSI's mission. In addition, the kind of research to be carried out promises to have high visibility, and, because of the nature of the simulations to be done, should provide good opportunities for public outreach.

Sincerely,

Jorge Viñals Professor and Director



Dr. Luiz DeRose Cray Inc. 380 Jackson Street Suite 210 St. Paul, MN 55101 Phone: +1 651-605-8925 www.cray.com

To Whom It May Concern:

Cray Inc. is pleased to support the research and training activities of Dr. Julius Donnert for the proposal entitled "Cosmological Simulations of Radio Bright Plasmas." As a leading vendor in High Performance Computing (HPC), Cray Inc. engages with research groups that use Cray solutions to achieve scientific breakthroughs and to perform cutting edge science. In addition, we encourage feedback on our products as the HPC community prepares for exascale class systems. The proposed work is well positioned to realize significant scientific gains and demonstrate effective use of Cray products, especially the Cray Programming Environment, at the largest scale. The application work included in this proposal can leverage the unique capabilities and features within the Cray Programming Environment through the use of the Cray Compiling Environment (CCE) and Cray MPICH.

Dr. Peter Mendyaral is the lead developer of the simulation code WOMBAT as well as a Crav Software Engineer. Dr. Mendygral's key role in this project provides a unique opportunity for Cray, to interact with the scientific community and exchange knowledge on this important scientific application. The primary avenue for support and training of Dr. Donnert on Cray solutions will be through the Cray software engineer and training host Dr. Peter Mendygral who will train and work with Dr. Donnert in implementing all new features and capabilities required to achieve the scientific goals. Dr. Mendygral's participation will last throughout the life of the project. In addition to regular interaction with Dr. Mendygral, the applicant will have access to other Cray engineers within the Cray Programming Environment and Benchmarking organizations. During the first three months of the project, Dr. Donnert will be trained in techniques for realizing the optimal performance with CCE on x86 architectures as well as accelerators using OpenACC. He will also be trained in optimizing communication within parallel applications using Cray MPICH. Finally, access to Cray Benchmark Engineers will ensure that Dr. Donnert is exposed to the techniques required to realize the best overall application performance at scale. Since the personnel included in these groups are all located in Cray's offices in St. Paul, MN, it is required that Dr. Donnert is resident in St. Paul for the discussion/training sessions to be effective.

It is expected that this project will broaden Cray's exposure throughout the astrophysical and wider scientific community while demonstrating the achievements made possible with Cray solutions. In exchange, Dr. Donnert will gain knowledge of the techniques necessary to achieve extreme scalability and sustained application performance.

Best regards,

Ohin, A. Le Rore

Dr. Luiz DeRose Programming Environment Director

END PAGE

MARIE SKŁODOWSKA-CURIE ACTIONS

Individual Fellowships (IF) Call: H2020-MSCA-IF-2014

PART B

"Cosmo Plasmas"

This proposal is to be evaluated as:

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