COVER PAGE

Title of Proposal: MathVRE: Open Virtual Research Environment Kit for Pure Mathematics and Applications

Date of preparation: December 19, 2014

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2	Logilab	FR
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8	University of Southampton	UK
9	University of St Andrews	UK
10	University of Warwick	UK
11	Jacobs University Bremen	DE
12	University of Kaiserslautern	DE
13	University of Silesia	PL
14	Universität Zürich	СН
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EC Commentary: Please follow the structure of this template when preparing your proposal. It has been designed to ensure that the important aspects of your planned work are presented in a way that will enable the experts to make

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an effective assessment against the evaluation criteria. Sections 1, 2 and 3 each correspond to an evaluation criterion for a full proposal.

Please be aware that proposals will be evaluated as they were submitted, rather than on their potential if certain changes were to be made. This means that only proposals that successfully address all the required aspects will have a chance of being funded. There will be no possibility for significant changes to content, budget and consortium composition during grant preparation.

Page limit: The cover page, and sections 1, 2 and 3, together should not be longer than 70 pages. All tables in these sections must be included within this limit. The minimum font size allowed is 11 points. The page size is A4, and all margins (top, bottom, left, right) should be at least 15 mm (not including any footers or headers). If you attempt to upload a proposal longer than the specified limit, before the deadline you will receive an automatic warning, and will be advised to shorten and re-upload the proposal. After the deadline, any excess pages will be overprinted with a 'watermark', indicating to evaluators that these pages must be disregarded.

Please do not consider the page limit as a target! It is in your interest to keep your text as concise as possible, since experts rarely view unnecessarily long proposals in a positive light.

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Outline of Project (for Proposers)

♦TO DO: *This is the place for various READMEs not included in the final submission***♦** An internal attempt at specifying our vision through short (unsubstantiated) answers.

> 1) Who are we?

Lead or core developers of some of the major open source components for pure mathematics and applications:

- Computational components: GAP, Linbox, MPIR, Pari, Sage, Singular
- Databases: LMFDB (findstat as well)
- Knowledge management: MathHub

Together with, in a larger scientific domain, lead developers for:

- Collaborative user interfaces (IPython, SageMathCloud)
- Database and Scientific Computing for the industry (Logilab)
- Numerical code optimization/parallelisation (Pythran)
- > 2) What is our goal?

Building blocks with a sustainable development model that can be seamlessly combined together to build versatile high performance VRE's, each tailored to a specific need in pure mathematics and application.

> 2.5) What is our strategy?

Maximize sustainability and impact by reusing and improving existing building blocks, and reaching toward larger communities whenever possible. E.g. factoring out our common user interface needs at the level of IPython/Jupyter will save us time (sustainability), and impact the larger scientific computing community. The improvements to the building blocks will impact all their users, whether they use the VRE or not.

- > 3) From where do we start?
- Building blocks with a sustainable development model
- Proof-of-concept prototypes of VRE (SMC, Simulagora)
- Experience on combining together some of the building blocks
- > 4) How do we connect or differ from other projects?

The other projects focus on either one or a few of the building blocks, or on a specific VRE.

We articulate our work with each of them.

> 5) Why are we excellent?

The consortium puts together recognized experts in all areas and most building blocks that are relevant to the goal. There is

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simultaneously a variety of point of views and a record of past experiences collaborating together at smaller scale (e.g. GAP-Singular). The approach is bottom up. Most joint tasks consist in bringing together people with a common need. There is experience in community building. Most participants are simultaneously users and developers of their tools.

All of this makes me confident that we will indeed be able to productively collaborate. And do stuff that is first class and useful.

On Sat, Dec 13, 2014 at 11:18:10PM +0100, Wolfram Decker wrote:

- > 0) What precisely is our starting point and why are we the right people to
- > achieve what we promise to do? Are we leaders in the area touched
- > by the proposal? How do we connect? Is there some past
- > collaborative success?
- > 1) You still do not say what we actually will provide. What precisely will
- > the VRE offer to its users?

I more or less answered those points above. Let me know if I should elaborate.

- > Who will be its users? Will those already familiar with the involved
- > CAS use it? Will it make the CAS more attractive for a much larger
- > community?

One objective is definitely to make CAS and others more attractive by lowering a lot the entry barrier to access the soft (and db, ...). A typical situation that most of us ran into is, when collaborating with other less tech-savvy mathematicians, to have trouble sharing code, data, and in-the-writing papers with them. SMC was launched with this idea in mind, and the success proves the concept.

At the same time, the improvements in the building blocks will also impact CAS users that are happy with their current user interface / work-flow.

Improvements to IPython will impact a much larger community.

- > 2) You motivate what we wish to do by the success of SageMathCloud.
- > But why do we than need another VRE? How do we differ from
- > SageMathCloud?

There is no one-size-fits-all VRE. One might want to run a VRE on one's own computer resources for a variety of reason (speed of access, specific resources, privacy, independence, ...). One might want a different combination of software (e.g. a lightweight VRE with only Singular). One might want to focus on data with LMFDB-style database searches, or on interactive computing, or on document writing, or some combination thereof.

> Do we have a chance to compete? Or will we rather join forces? In
> which way?

/ WILLCII way:

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We join forces (the plan is to have William/UW in the consortium, as non funded participant). SMC focuses on one specific cloud based VRE. We focus on the building blocks and the glue. Both project are mutually beneficial. See the language p. 14 of the proposal.

- > 3) You motivate what we wish to do by the success of LMFDB. But what
- > are our connections to this database? Will we enhance it? Will we connect
- > it to other stuff we do? Will we create other databases?

LMFDB is a prototype of large scale database. We want to make it easier for other groups of mathematicians to setup similar databases in their area. Reciprocally, like SMC, the LMFDB with benefit back from the improved building blocks.

- > 4) Why is Europe in the lead if there is already SageMathCloud?
- > Where precisely is Europe in the lead?

Europe is the lead in many of the building blocks.

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1 Excellence

MathVRE focuses on delivering tools that will make it easy to setup Virtual Research Environments, customized to meet the diverse needs of collaborative research in pure mathematics and applications, and built out of a sustainable ecosystem of community-developed open software, databases, and services.

The remarkable emergence and success in the last decade(s) of a large ecosystem of community-developed computational software like e.g. GAP, LinBox, PARI/GP, Sage, or Singular and of interactive scientific computing environments like IPython showcase the viability of community development models for such components.

The recent successes of the Virtual Research and Teaching Environment SageMathCloud (hosting more than 10k users and 100k projects after just one year) and of the online number theory database LMFDB showcase the strong need for **integrated solutions** enabling large-scale collaboration on **software**, **knowledge**, and **data**.

Yet setting up infrastructures like those mentioned above currently requires massive ad-hoc efforts. Challenges include portability, compatibility, performance, usability, reproducibility, not to mention the many social aspects involved in communities and ecosystems thereof.

♦TO DO: Better explain the specific needs in maths, and why we focus on VRE building blocks rather than VRE themselves, in the DIY spirit.**♦**

A specific challenge in mathematics comes from the vast yet tightly connected array of concepts involved. Different groups of researchers may have radically different needs, workflows, and resources, calling for a highly modular and customizable VRE infrastructure.

MathVRE will attack all those challenges upfront, while consolidating Europe's leading position in this field.

1.1 Objectives

♦EC Commentary: 1-2 pages **♦EC Commentary**: Describe the specific objectives for the project, which should be clear, measurable, realistic and achievable within the duration of the project. Objectives should be consistent with the expected exploitation and impact of the project (see section 2). **♦**

The specific aims of MathVRE are:

- **Aim** 1: Improve the productivity of researchers in pure mathematics and applications by promoting collaborations based on mathematical **software**, **data**, and **knowledge**.
- **Aim** 2: Make it easy for teams of researchers of any size to setup custom collaborative Virtual Research Environments tailored to their needs and workflows, supporting the entire life-cycle of computational work in mathematical research, from initial exploration to publication, teaching and outreach.
- Aim 3: Identify and promote best practices in computational mathematical research, including making results easily reproducible, making software sustainable, reusable and easily accessible and sharing data in a semantically sound way. •TO DO: insert the ecosystem keyword•
- Aim 4: Maximize sustainability as well as impact in mathematics, neighbor fields, and scientific computing.

Our research will cover a wide variety of aspects, ranging from software development models, user interfaces **TO**DO: virtual environments? , deployment frameworks and novel collaborative tools, component architecture, design, and standardization of software TO DO: system? and databases, to links to publication, data archival and reproducibility of experiments, development models and tools, and social aspects.

The concrete objectives of MathVRE are:

Objective 1: To develop and standardise an architecture allowing a range of mathematical and data and software components to be combined with off-the-shelf non-mathematical infrastructure to produce specialised VREs for different research communities. The architecture will take the form of standards documents and APIs equipped, where appropriate, with formal or informal mathematical semantics to ensure interactions are mathematically sound. This primarily addresses aim 2, thereby contributing to aims 1 and 3.

TO DO: This is a bit long.

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- **Objective** 2: To develop open source core components for such VREs where existing software is not or not suitable. These components should support VREs running on a variety of platforms, including standard cloud and cluster platforms. This primarily addresses Aim 2, thereby contributing to Aim 1 and 3.
 - **♦TO DO**: SL Write detailed description**♦**
- **Objective** 3: Community building

Bring together the communities (IPython, Sage, Singular, GAP)

- **♦TO DO**: NT expand and write detailed description**♦**
- **Objective** 4: Update a range of existing open source mathematical software systems for seamless deployment and efficient execution within the VRE architecture of objective 1. This fulfills part of Aim 2.
 - **♦TO DO**: *SL*: write detailed description**♦**
- **Objective** 5: Foster a sustainable ecosystem of interoperable open source components developed by overlapping communities, in particular by identifying and promoting software development best practices, and outsourcing development to larger communities whenever suitable. This fulfills part of Aim 3 and 4.
- **Objective** 6: Explore the social aspects: how do researchers collaborate in Mathematics? What can be the role of Virtual Research Environments? This addresses part of Aim 3 and 2. ◆**TO DO**: *UM: write detailed description*◆ ◆**TO DO**: *SL: semantics from mathematical text?*◆
- **Objective** 7: Identify and extend ontologies and standards to allow easy, safe and efficient storage, reuse, interoperation and sharing of rich mathematical data taking account of provenance and citability. This fulfills parts of Aim 2 and 3. ◆TO DO: POD write detailed description◆
- **Objective** 8: Demonstrate the effectiveness of Virtual Research Environment built on top of **MathVRE** components for a number of real-world use cases taken from different domains, or crossing previously little connected domains. This addresses part of Aim 2.
- **Objective** 9: Effective Dissemination ◆**TO DO**: *VP write detailed description*◆

Detailed Descriptions of Objectives

Objective 1: Virtual Research Environment Kit

Computational techniques have become a core asset for research in pure mathematics and its applications in the last decades. Mathematics communities have come together to develop powerful computational tools, such as GAP, PARI/GP, SAGE or Singular, and valuable on-line services such as the Encyclopedia of Integer Sequences and the ATLAS of Group Representations. **TO DO**: cite In building these systems, mathematicians have gained strong experience in collaborative software development, with pioneering work and continuing leadership of Europe.

A number of approaches to linking these resources have been developed, such as the SCSCP protocol from the Framework 6 SCIEnce project, and the incorporation of a variety of free software tools in the SAGE system, but the overall model is still that of a single mathematician running programmes or interacting with a "notebook" page. The software provides little or no support for other aspects of mathematical research: collaboration, archival, reproducibility or linkage between programmes, data and publication. Databases are updated mainly by mathematicians directly, retaining no record of the source of new entries, and providing no way of refering to the actual version of the data used in a particular computation.

The first objective of this project is to design an architecture which will allow existing mathematical software systems (suitably updated), off-the shelf non-mathematical tools and a small number of new components to be flexibly combined to produce a VRE that will effectively support collaborative mathematical research throughout it's entire life-cycle. This will include software APIs and standards, frameworks for assuring the semantic consistency of similar mathematical objects in different systems. It will be informed by the outputs of objective 6, ensuring that the VREs fit the ways that mathematicians actually work.

♦TO DO: Keyword: flexible/versatile virtual environment. Does this belong here**♦**

Our research will cover a wide variety of aspects, ranging from software development models, user interfaces **TO**DO: virtual environments? deployment frameworks and novel collaborative tools, component architecture, design,

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and standardization of software components and databases, to links to publication, data archival and reproducibility of experiments, development models and tools, and social aspects. It will build on the remarkable success of the open source ecosystem and consolidate Europe's leading position in computational mathematics.

Following the call specifications, all software, data, and publications resulting from this proposal will be open.

Objective 2: Core components

Most of the direct mathematical capabilities of our software will come from existing or updated open source mathematical systems. For instance we will use the power of the GAP Library for computational group theory or PARI/GP for number theory. Generic services such as storage, version control, authentication and resource accounting will come from off-the-shelf components building on standard infrastructures.

Nevertheless some new or adapted tools will be needed. One example is a general infrastructure for mathematical databases, covering some of the types of data values and search criteria common in mathematics, but rare outside, and issues such as provenance and citation that are common to most mathematical databases. Other examples include adapting user interface and collaboration tools to support mathematical notations.

Objective 3: ♦TO DO: TITLE: COMMUNITY ♦ ◆TO DO: NT detailed description ♦

Objective 4: Updates to Mathematical Software Essential to our vision is leveraging the communities massive decades-long investment in a range of open source mathematical software systems. These systems are complex, widely used and powerful, but generally designed for operation as stand-alone programs, not as part of an integrated VRE. Many are also not well-suited for modern platforms, needing work to better support parallel programming, virtualisation and HPC platforms. We will update these systems to work together seamlessly and comply with best practice for portability and platform integration.

Objective 5: A sustainable ecosystem of software components

The success of large specialized software like PARI/GP, Singular or GAP in the last decades has shown the viability of the academic open source development model for such. For a long time, it was bitterly debated whether this model would have any chance to scale to general purpose systems for pure mathematics. The rapid takeoff of Sage in the last decade has proven the viability of the "developed by users for users" model: despite its large international community of about 150 active developers, it's running on a tiny specific budget, with most activities being funded indirectly by research grants that require specific development.

This was made possible by reusing existing components whenever possible (e.g. hundreds of specialized open source math libraries, or the Python programming language with its developers tools and huge library), by spinning off software development (e.g. the Cython compiler) to larger communities whenever possible, and by carefully designing the development workflow.

Yet, long term critical non mathematical features like portability, modularization, packaging, user interfaces, large data, parallelism, or outreach toward related software, have been lagging behind. Indeed they can hardly be implemented as a side product of research projects, and **need to be assigned to a few full time developers**. Regular funding is also needed to better structure the computational mathematics community in Europe and support its upcoming major widening through training, development workshops, exchanges, ...

One purpose of this grant is to initiate this process and invest on the long run to reduce the recurrent needs.

The principle is that, with the growth of the user base, a tiny number of institutions or companies will hire a full-time developer to support critical needs of their in-house research or development. Opportunities for such hiring are for example actively investigated at the Laboratoire de Recherche en Informatique. It should be noted that, at the scale of a large university, the cost of licenses for analogous commercial software can reach the same order of magnitude as that of a developer.

To reduce the number of required full time developers **MathVRE** will invest toward, factoring out joint needs, and outsourcing or spinning off more components to larger communities. For example, **MathVRE** will save much recurrent efforts to the mathematics community by providing a temporary boost to outsource the development of the user interface of each computational component to IPython and make IPython stand to the stringent needs of the community. Later on, thanks to its large user base both in academia and industry, IPython will continue to thrive without specific funding or major contributions from the mathematics community.

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MathVRE will also foster the productivity within the ecosystem by investigating better collaboration processes between components, and identifying, sharing, and promoting software development best practices.

Objective 6: ♦TO DO: *TITLE: SOCIAL* ♦**TO DO**: *UM detailed description* ♦

Objective 7: Next generation mathematical databases

TO DO: POD detailed description

Objective 8: ♦TO DO: *TITLE: DEMO* **♦TO DO**: *detailed description* **♦**

The success of any research software or service is strongly related to its ability to attract and convince a great amount of users. Our different communities (Sage, Gap, PARI/GP, Singular...) have developed a solid experience and network. As an example, Sage has gathered thousands of users in less than 10 years. This was achieved thanks to a very strong community building philosophy, especially through the organization of Sage-Days all over the world. The first Sage-days happened in 2006, today we count 63 of them, including 10 for 2014 only, and also Sage Education days, Sage Bug days, Sage Doc days and more. Most of us, **MathVRE** project members, have been involved in these events either as organizers or participants and it appears as the most efficient way to promote our software. More precisely, our objective is to create constant dialogue with the different communities: frequent workshops, conferences, user groups, mailing lists. By building on existing tools, we intend to involve the communities in the development process itself in the spirit of open-source software.

We also intend to reach a larger crowd of researchers by cutting down non-research technical issues to access existing tools: building better documentation and tutorials, developing easy-to-install distributions, easy web and cloud access, better user interfaces, better interactions between different software. Doing so, our objective is to help the communities to grow themselves and interact together using our work.

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1.2 Relation to the Work Programme

- **♦EC Commentary**: 1-2 pages; Eugenia will help there**♦**
- **♦EC Commentary**: Indicate the work programme topic to which your proposal relates, and explain how your proposal addresses the specific challenge and scope of that topic, as set out in the work programme. ♠
- **♦EC Commentary**:

This is a synthesis of Antonios Barbas' slides describing the Call 3
Topic 9-2015 EINFRA-9: e-Infrastructure for Virtual Research Environment

See file:../Documentation/VirtualEnvironmentsWorkProgramme2014-2015.ppt

- ** Suggested EU contribution per proposal: 2 to 8 M euros ; Total budget: 42 Meuros
- ** Dates: 14/01/2015
- H2020-EINFRA-2014-1 15/04/2014
- H2020-EINFRA-2014-2 02/09/2014
- H2020-EINFRA-2015-1 14/01/2015(tbc)
- ** European contacts: Antonios Barbas See file:Documentation/Contacts.docx
- ** Definition:
- Groups of researchers, typically widely dispersed, who are working together
- through ubiquitous, trusted and easy access to services for scientific data, computing and networking
- in a collaborative, virtual environment:
 - > the e-Infrastructures
- ** Characteristics:
- Address the needs of specific scientific communities { in support of e-Science;
- Have users from both academia and industry;
- Involve bottom-up research and develop user-oriented services;
- Are based on e-infrastructures
- ** Specific challenge:
- Capacity building in interdisciplinary research
- through community-led development and deployment of service-driven digital environments
- for large-scale cross-disciplinary research collaboration and data interoperability
- ** Expected impact:
- More effective collaboration between researchers and increased take-up of collaborative research by new disciplines;
- Easier discovery, access and re-use of data, resulting in higher productivity of researchers;
- Accelerate innovation via access to integrated digital research resources across disciplines;
- *** Scope: Proposals are expected to

Notations: [X]: easy to argue; [?]: we have some lead, but that will take some arguing

- [?] Integrate resources across all layers of the e-infrastructure (networking, computing, data, software, user interfaces) to foster cross-disciplinary data interoperability
- [?] Build on requirements from real use cases, i.e. integrate heterogeneous data from multiple sources and re-use tools and services from existing infrastructures
- [X] Target any area of Science and Technology, especially

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- interdisciplinary ones, including ICT, mathematics, web science and social sciences and humanities
- [X] Use standardised building blocks and workflows, well-documented interfaces and interoperable components;
- [?] Define semantics, ontologies and metadata to enable data citation and promote data sharing, as to ensure interoperability;
- [X] Target easy-to-use functionalities; and indicate the number of researchers they target as potential users;
- ** Specific conditions for the Call on e-Infrastructures:
- [X?] Proposals should be structured around Networking, Service and Joint Research Activities
- [X] The Software to be developed needs to be open source
- [] A Data Management Plan to be developed enabling data preservation, on-line discoverability, authorisation and re-use of data
- [X] Clear Metrics (KPIs) to be proposed and used;
- [?] Open Access to Publications resulting from the project;
- [X] Usefulness of services to the end user community and financial sustainability to be ensured;
- ** Where should the emphasis be?
- [?] Services
- [X] Thinking innovation
 With both suppliers or users
- [X] Mainstreaming skills development
- [] Integration between data and computing
- [X] Business plans for financial sustainability
 - ...and partnerships with the private sector
- [] Supporting policies
- [X] open data and software
- [X] Sharing basic operations services and building blocks
- [X] Monitoring performance (KPIs)
- ** Simplified funding model
 - Up to 100% for Research and Innovation
 - Flat 25% rate for indirect costs (overhead?)

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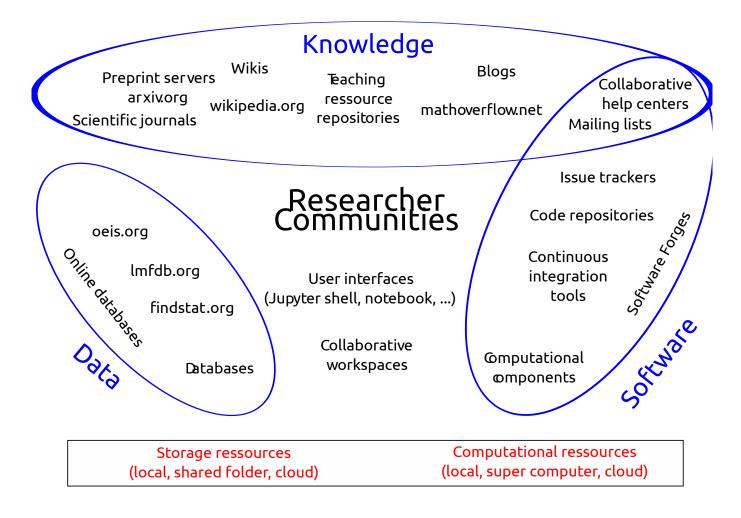


Figure 1: Virtual Research Environments for research in pure mathematics and applications.

1.3 Concept and Approach

- **♦EC Commentary**: 5-8 pages **♦EC Commentary**: Describe and explain the overall concept underpinning the project. Describe the main ideas, models or assumptions involved. Identify any trans-disciplinary considerations; Describe and explain the overall approach and methodology, distinguishing, as appropriate, activities indicated in the relevant section of the work programme, e.g. Networking Activities, Service Activities and Joint Research Activities, as detailed in the Part E of the Specific features for Research Infrastructures of the Horizon 2020 European Research Infrastructures (including e-Infrastructures) Work Programme 2014- 2015;
- Describe how the Networking Activities will foster a culture of co-operation between the participants and other relevant stakeholders.
- Describe how the Service activities will offer access to state-of-the-art infrastructures, high quality services, and will enable users to conduct excellent research.
- Describe how the Joint Research Activities will contribute to quantitative and qualitative improvements of the services provided by the infrastructures.
- As per Part E of the Work Programme, where relevant, describe how the project will share and use existing basic operations services (e.g. authorisation and accounting systems, service registry, etc.) with other e-infrastructure providers and justify why such services should be (re)developed if they already exist in other e-infrastructures. Describe how the developed services will be discoverable on-line.
- Where relevant, describe how sex and/or gender analysis is taken into account in the project's content.♠
- **◆TO DO**: NT: the purpose of Figure 1 is to give a quick sense of what Virtual Research Environments can be in our context, and a "big picture" for the project. A graphic artist friend of mine is going to help me improve it. I have collected here some material for her.

What we would like the "big picture" in Figure 1 to highlight:

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This is a human centered project: *At the core: researchers and communities thereof.*

The three types of information: Software, Knowledge, Data (currently in blue)

How they interact:

- *Knowledge help structure data and software (e.g. through ontologies)*
- Software produce data
- Data is used by researchers to build knowledge

Physical resources: (currently in red)

Virtual Research Environments

- Researchers in Math have a long tradition of collaborating on Software, Knowledge, and, up to some point, Data
- For this they use a variety of collaborative tools which form a loosely knit Virtual Research Environment.
- Aim 2: make it easy for subcommunities of researchers to setup custom collaborative work spaces / Virtual Research Environments tailored to their needs, by combining:
 - Computational resources
 - Storage resources
 - Computational software components
 - Databases
 - User interfaces
 - Wikis-Knowledge bases (true for findstat, LMFDB): quicker cycle for consolidation of information spread over papers/brains

Such VRE shall help them:

- collaboratively develop software (e.g. specialized libraries), data and knowledge (e.g. articles) for their research projects.
- contribute back this information to the larger community whenever relevant.

Processes:

It would be interesting to depict the following processes. They are indeed about collaboration and sharing (and quality control), that is what **Aim 1** is to promote.

Software development

- bug reports and enhancement requests emerge from the community, typically through collaborative help centers, and are posted on issue trackers.
- Design discussions occur on mailing lists and issue trackers.
- Researchers submit code to the code repositories.
- Quality control: the code is reviewed and tested by continuous integration tools.
- Finally the code integrated within computational components, and used by the community.

Researchers (as well as other users: teachers, engineers, ...) interact at each step of the process.

Scientific publication

- researchers submit articles to journals and post them on preprint servers;
- the articles get reviewed by other researchers;
- finally they are distributed back to the community

Improvements to implement:

- the findstat link does not work for me, kerning looks extremely weird POD
- lmfdb, oeis, and findstat have a strong knowledge component as well, with knowls and wikis, references, ...

• arxiv is not far from a database of knowledge

A collection of links that might give some idea of the look and feel of our universe:

Examples of (computational) components:

- *IPython:* http://ipython.org/
- *GAP*: http://www.gap-system.org/
- Singular: http://www.singular.uni-kl.de/
- Sage: http://sagemath.org/
- PARI/GP: http://pari.math.u-bordeaux.fr/
- Linbox: http://www.linalg.org/

Examples of online collaborative tools

- Issue tracker: http://trac.sagemath.org/timeline/
- Code repository: https://github.com/
- Collaborative help center: http://ask.sagemath.org/
- Collaborative math site: http://mathoverflow.net/

Examples of online databases

- Online databases: http://oeis.org/?language=french
- LMFDB: http://www.lmfdb.org/EllipticCurve/Q/14.a3
- Findstat: http://www.findstat.org/

Example of graphical material

• http://boxen.math.washington.edu/home/nthiery/main2014.pdf

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1.3.1 Importance of experimental tools in pure mathematics and applications

From their early days, computers have been used in pure mathematics, either to prove theorems (e.g. the four color theorem) or, like the telescope for astronomers, to explore new theories. By now the experimental method, based on exact computer aided calculations, has now been added to the standard toolbox of the pure mathematician, and its usage has grown to the point that certain areas of mathematics now completely depend on it.

Experiments lead to new conjectures which may have a deep impact on the future development of mathematics. An outstanding example is the Birch and Swinnerton-Dyer conjecture which is one of the Clay Millenium Problems. Databases relying on computer calculations such as the Small Groups Library or the Modular Atlas in group and representation theory provide indispensible tools for researchers. A constructive way of understanding proofs of deep theorems yields algorithmic tools to deal with highly abstract concepts. These tools make the concepts available to a broader class of researchers, with many potential applications. A prominent example from algebraic geometry is the desingularization theorem of Hironaka, for which Hironaka won the Fields Medal, and its algorithmization by Villamayor.

Spectacular theoretical breakthroughs such as the recent complete resolution of Serre's conjectures, directly inspired by Wiles' proof of Fermat's last theorem, are based on interdisciplinary approaches. Current developments on the algorithmic side allow one to conquer crossconnections between different areas of mathematics also computationally and, thus, to arrive at cutting-edge applications which previously were inconceivable.

The field of computational mathematics allows us to compute in and with a multitude of mathematical structures. It is interdisciplinary in nature, with links to quite a number of areas in mathematics, with applications in mathematics and other branches of science and engineering, and with constantly new and often surprising developments. Quite a number of these developments, in fact the creation of whole subareas of the field, have been initiated by European researchers who made crucial contributions at all levels. These include the design of fundamental algorithms, the development of major computer algebra systems (*TO DO: this is a bit redundant with below*), applications of the computational methods in various fields, and the creation of widely used databases.

Particularly fruitful interactions unfold between computer algebra and algebraic geometry, number theory, combinatorics and group theory. Algebraic algorithms open up new ways of accessing subareas of these key disciplines of mathematics, and they are fundamental to practical applications of the disciplines. Conversely, challenges arising in algebraic geometry, number theory, combinatorics and group theory quite often lead to algorithmic breakthroughs which, in turn, open the door for new theoretical and practical applications of computer algebra.

1.3.2 A long track of collaboration on software, data, knowledge

Supporting the experimental method requires spending major efforts on software development. As the sophistication of the required computations increased, supported by the boom of the available computational power, it became vital to share those efforts at the scale of large research communities. European mathematicians have been pioneers and have grown a steady tradition of collaborative open source software development, with specialized systems like GAP, Singular, or PARI/GP playing a major role for decades.

The next scale was reached in the last decade with the advent of the general purpose mathematical system Sage which proved the viability and sustainability of the "developed by users for users" development model at the international level.

- **◆TO DO**: This is somewhat redundant with the language in Objective 5; see where this belongs best to.◆
- **◆TO DO**: *Develop* **◆** Similarly, mathematicians have been building and sharing databases for a long while; the needs for such is growing tremendously, and the process needs to be streamlined.
- **♦TO DO**: *Develop*♠Mathematicians have a strong tradition of sharing knowledge openly (arxiv, Wikipedia, ...).

1.3.3 Early VRE's

♦TO DO: Motivate the relevance of VRE's, in particular by the success of SageMathCloud or Simulagora. Mention as well LMFDB.◆

♦TO DO: Highlight some other deployed VRE's that would benefit to the sorts of improvements you suggest. You could include Wakari.io and also the tmpnb thing in Nature magazine: http://www.nature.com/news/ipython-interactive-demo-7.21492**♦**

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1.3.4 Key concept: bringing communities together toward a VRE kit

♦TO DO: Focus on VRE kit and building blocks**♦**

◆TO DO: Why this focus? variability of needs, sustainability, ... **◆**

♦TO DO: Bringing communities together**♦**

1.3.5 Linked research and innovation activities

♦EC Commentary: Describe any national or international research and innovation activities which will be linked with the project, especially where the outputs from these will feed into the project;**♦**

♦TO DO: For each item below, write a paragraph describing the project and one describing how it connects with this proposal**♦**

DFG Priority Project SPP 1489 computeralgebra.de

The SPP1489 "Algorithmic and Experimental Methods in Algebra, Geometry, and Number Theory" is a nationwide Priority Project of the German Research Council DFG which commenced in July 2010 and will end in June 2016. The focus of the programme is on the interactions between computer algebra and algebraic geometry, number theory, and group theory. It combines expertise at all levels of research in computer algebra, be it the design of algorithms, the implementation of algorithms, the application of algorithms, or the creation of mathematical databases. The goal of SPP1489 is to considerably further the algorithmic and experimental methods in the afore mentioned disciplines, to combine the different methods across boundaries between the disciplines, and to apply them to central questions in theory and praxis. A fundamental concern of the programme is the further development of open source computer algebra systems with origins in Germany, which in the framework of different projects will be crosslinked on different levels. Of particular interest are interactions with application areas inside and outside of mathematics such as system-and control theory, coding theory, cryptography, CAD, algebraic combinatorics, and algebraic statistics as well as hybrid methods which combine numerical and symbolic approaches.

The work in the SPP1489 has established effective communication channels between the core developers of different computer algebra systems. It is a showcase project for several objectives of this proposal (such as community building and fostering a sustainable ecosystem of interoperable open source components). The experience made in parallelizing mathematical software will be crucial for Workpackage WP5.

IPython/Jupyter grant from the Alfred P. Sloan foundation http://ipython.org/sloan-grant.html ♠IPython [WRITE HERE: Proofread description of the Sloan grant and link to this project]♠

The IPython project received a \$1.15M grant from the Alfred P. Sloan foundation that is supporting IPython development for two years (1/1/2013-12/31/2014), in particular at the University of California, Berkeley and California Polytechnic State University, San Luis Obispo. This grant enabled the project to focus on developing the IPython Notebook as a general tool for scientific and technical computing that is open, collaborative and reproducible. This goes a long way toward Aim •TO DO: ... and ...• of MathVRE, especially given the current rapid evolution of IPython toward its language agnostic avatar Jupyter.

MathVRE will build on the outcome of the Sloan grant, and further develop the critical IPython/Jupyter component in close collaboration with the IPython/Jupyter team. In particular, we plan to hire some of the European developers that are currently funded by the Sloan grant to work in California and wish to later return to Europe.

NSF SI2-SSE OCI-1147247 The OCI-1147247 Collaborative Research grant "Sage-Combinat: Developing and Sharing Open Source Software for Algebraic Combinatorics" is a project funded by the National Science Foundation from June 2012 to May 2015. The grant supports the development of Sage-Combinat, on the USA side and in areas relevant to the ongoing research of the participants (symmetric functions, Macdonald polynomials for arbitrary Cartan types, crystals, rigged configurations and combinatorial R-matrices, affine Weyl groups and Hecke algebras, cluster algebras, posets, ...), together with relevant underlying infrastructure. The project includes three Sage Days workshops, and cofunded one at ICERM and another in Orsay. The grant also funds a dedicated software development and computation server for Sage-Combinat, hosted in the Sage computation farm in Seattle. Emphasis is placed on the development of thematic tutorials that make the code accessible to new users. The proposal also funds graduate student RA support, curriculum development, and other mentoring.

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The workshops and outreach actions pursued by this NSF grant have proven to be a potent tool for connecting researchers and recruiting Sage users and developers. One of the role of this proposal is to support similar community building in Europe.

This NSF grant also funded

Two of the proposers, Stein and Thiéry, are respectively PI and foreign senior participant to this NSF grant which This NSF grant,

also funded some of the development of SageMathCloud and of the category framework in Sage which are key assets for this proposal.

HPAC grant from the A.N.R. The french national research agency ANR has funded a 4 years project on High Performance Algebraic Computing (HPAC) focused on the development of parallel exact linear algebra. The consortium gathers research groups from LIP6 (Paris 6), LIRMM (Montpellier), LIP (Lyon) and LIG and LJK (Grenoble). The main goals of the project is to first develop high performance exact linear algebra kernels with dedicated parallel runtime, propose a domain specific language for the parallelization of exact linear algebra libraries and their composition, invent new algorithmic solutions for large scale parallelizations. The output of the project is then twofolds: new computational challenges arising in algebraic cryptanalysis will be addressed, and the open-source libraries maintained by each group will not only integrate these advances, but will expose them in a close integration to high level computer algebra softwares. In this process, Sage will start benefitting from the new shared-memory parallel code of LinBox for the linear algebra over a finite field. The scope of this project is mostly focused on shared memory parallelism (except for some challenge computations). Addressing distributed and heterogeneous infrastructures is the next step after this project, that is be addressed in work-package 5 of the this proposal.

Logilab: simulagora, cubicweb, ... ◆Logilab [WRITE HERE: One paragraph description of simulagora, cubicweb, ...] ◆ ◆Logilab [WRITE HERE: How does it relate to this project] ◆

SageMathCloud https://cloud.sagemath.com/

♠NT/SL/WS [WRITE HERE: Proofread section about SMC]♠

Sage and with each other. It has Sage and IPython worksheets, powerful MEX editing features and a full Linux computer, all accessible from a standard web browser. Its main design feature is to enable and promote collaboration between groups of users. It is for example a natural place to host a course, allowing teachers to collaborate with their students using modern tools like Sage and MEX, with facilities for real-time communication through chat, video, and shared editing of documents, programs and worksheets; course material can be provided as worksheets, assignments can be distributed, collected, and returned as well. Launched in 2013, SageMathCloud presently hosts over 100,000 projects and 10,000 weekly active users. This fast adoption by a wide variety of users demonstrates the relevance and the long term impact this kind of collaborative environments can have.

Technically speaking, SageMathCloud is a specific open-source cloud-based Virtual Research and Teaching Environment for mathematics developed since 2013 under the lead of William Stein, with funding from the NSF, and Google's Education Grant program. It's currently deployed at the University of Washington at Seattle, with a business plan in the work for commercial support for massive on line courses, subsidizing a free service for all other academic usage and some further Sage development.

In comparison MathVRE focuses on open source building blocks and architecture to easily setup and deploy custom Virtual Research Environments. On the one hand, SageMathCloud will serve as prototype for MathVRE, paving the way and showcasing important features from the users perspective. On the other hand, basically each and every task undertaken in MathVRE will benefit back SageMathCloud.

FLINT grant?

LMFDB grant The L-functions and Modular Forms Database (LMFDB) project originated at a meeting at The American Institute for Mathematics (AIM) in 2007. L-functions are ubiquitous in number theory, and have applications to mathematical physics and cryptography. The simplest example of an L-functions is the Riemann zeta function. Two of the seven Clay Mathematics Million Dollar Millennium Problems deal with properties of these

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functions, namely the Riemann Hypothesis and the Birch and Swinnerton-Dyer Conjecture, that were conjectured following computational exploration. As well as providing a central repository of data as a resource for researchers, through its website www.lmfdb.org, the LMFDB provides a modern handbook, including tables, formulas, links and references, concerning particular specific L-functions and their sources. Between 2008 and 2012 the LMFDB was funded through a US National Science Foundation (NSF) Focussed Research Grant (FRG) of around \$1M. Since 2013, the funding of the LMFDB has passed to Europe through a six year £2.2M Programme Grant from the UK Engineering and Physical Sciences Research Council (EPSRC), held at the universities of Warwick and Bristol, with Professor John Cremona (Warwick) as its Principal Investigator (see http://www2.warwick.ac.uk/fac/sci/maths/people/staff/john_cremona/lmf). This grant supports six three-year postdoctoral research fellows, mathematical researchers who work on the mathematical aspects of the project full-time, biannual workshops, equipment and a portion of the investigators' own time.

Almost all contributors to the LMFDB project, including those directly supported by the EPSRC grant and the larger world-wide team of 30-50 contributors of data and code, are pure mathematicians. Most of these have good computational skills, but are not professional programmers or software developers. The LMFDB has a great need to broaden the support it can call upon from software developers, to enhance the project in several ways, including the computation of number-theoretic data but more specifically in supporting the database management and website user interface, in order to make the data more accessible and useful to others. The codebase of the LMFDB project is entirely open source and hosted at github (https://github.com/LMFDB/lmfdb), written in python with specialist modules such as flask and pymongo to manage the website and database interface, and Sage for higher-level mathematical computations. The LMFDB project would therefore benefit greatly from collaboration with MathVRE as it would connect the project with a pool of experts. Joint workshops between the LMFDB and MathVRE will stimulate and develop such collaboration: the LMFDB places great importance on its workshops, which are small gatherings of around 30 invited participants who work throughout one week on certain specific aspects of the project, coming together in plenary sessions to make decisions, plan and collectively approve of proposed developments. As a leading example of the use of databases in mathematical research, the LMFDB will provide MathVRE with a real large-scale prototype around which to develop new ideas about the design and implementation of such databases and their associated software. The feasibility of such collaboration was successfully tried at a workshop at the ICMS in Edinburgh in January 2013 on "Online databases: from L-functions to combinatorics", sponsored by the NSF, AIM and the ICMS.

Findstat?

Kwarc group

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1.4 Ambition

♦EC Commentary: 1-2 pages**♦**

♦EC Commentary: − Describe the advance your proposal would provide beyond the state-of-the-art, and the extent the proposed work is ambitious. Your answer could refer to the ground-breaking nature of the objectives, concepts involved, issues and problems to be addressed, and approaches and methods to be used.

- Describe the innovation potential which the proposal represents. Where relevant, refer to products and services already available, e.g. in existing e-Infrastructures.♠

For most pure mathematicians using computational tools in their research, the state of the art in 2014 is still a collection of programs each of which must be installed individually on their desktop or laptop computer, respecting a complicated graph of dependencies. Alternatively software may be installed on a departmental server or cluster and used via text-based remote login. The software performs computations (using excellent implementations of extremely sophisticated algorithms) with inputs and outputs usually in a bespoke text-based format. The results of computations are incorporated into publications by cut-and-paste and collaboration is through exchange of programs and data by email, shared general-purpose fileservers or, rarely, a service such as GitHub. Multiple computations involved in producing a mathematical result must be managed by editing, naming and filing multiple scripts or programs, and there is no automatic support for rerunning computations to check for human or algorithmic error.

♦TO DO: Work out best order for these topics**♦**

There are commercial "symbolic computation systems" such as Mathematica [®]. or Maple [®]. which offer somewhat more modern frameworks, but they lack the specialised algorithms for research work in fields such as algebra, number theory or algebraic geometry and are not well-suited to support them.

The need for a more modern, more productive and less error-prone environment for this kind of mathematical research computing is widely acknowledged, but the separate groups developing the systems have indvidually, neither the time nor the expertise to develop it. There have been a number of interesting projects which have explored different aspects of what is needed: **TO DO**: SCIEnce, SageMathCloud, MathOverflow, Polymath, SAGE itself, SAGE notebooks, HPCGAP, recomputation and we will build on the experiences, and where useful the software, of all of these.

Our ambitious plan in this project is to learn from, and leapfrog, these piecemeal developments and provide a toolkit of software and interfaces, which supports the whole mathematical research process in a way which is **modern**, **seamless**, **collaborative**, mathematically **rigourous** and **adaptable** to the diverse needs of different mathematical research areas and of different mathematicians and collaborations.

♦TO DO: Explain all the highlighted words in the para above **♦**

♦TO DO: Some examples here – what will we deliver to individuals; small "single-problem" collaborations; longer-lived data- or algorithm- centred teams; massive "flagshsip" projects. Think "User Stories" **♦**

1.4.1 Challenges specific to mathematics

Mathematical research, especially pure mathematics presents some unique challenges to the realisation of this ambition

♦TO DO: Evidence this in more detail, clean up the language**♦**

- Community mainly made of individuals or *very* small groups (1 PI + a few students). Few formal or structured research groups such as you might find in an equipment-intensive science. Large scale collaborations happen (CoFSG, Polymath), but still driven by individuals, not formal structures or money.
- Much top quality research has little or no formal research funding. So computational resources are limited to what is available anyway personal laptops, departmental clusters...
- Many mathematical computations are highly irregular and complex. Traditional HPC paradigms coming from simulation and linear algebra do not apply.
- Mathematical notations have been refined over many centuries for use by humans with pen, paper and black-board. Even such simple problems as selecting a sub-expression are hard to handle well on a computer. For instance a + c is naturally seen as a subexpression of a + b + c by a human.
- The mathematical correctness of widely used algorithms hinges on quite complex chains of reasoning. Subtle coding errors may easily produce plausible, but wrong, answers.

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- Mathematical data different in several ways from tyopical scientific data
 - More often than not data is the result of a computation (and not a measurement of the real world). The
 role of databases is thus primarily to store results for later reuse (persistent caching), and enable searches.
 Because of this, many issues (semantic, ontologies, reproducibility, ...) are to be treated upstream at the
 level of software rather than data.
 - extreme reification in mathematics makes classical ontologies techniques/RDF impractical ◆TO DO:
 Someone explain this ◆
 - interlinking very high
 - several alternate and defining description of same objects

1.4.2 Challenges of a community built around multiple existing software projects

Another source of unique challenges for this project is the need to interact with several large and diverse ecosystems of software developers. For instance the GAP package development community, the SAGE development community, the wider Python community, the developers of key open-source libraries on which we rely and so on.

These communities exist in a delicate balance between collaboration and competition. For instance the SCIEnce project and SAGE were simultaneously exploring two different approaches to linking open-source mathematical software. Many technical developments (better IO handling in GAP, for instance) could usefully be shared, and at the end of the day we all want to do better mathematics, but a certain degree of competition is both natural and healthy.

In this project we need to build a sustainable "meta-ecosystem" in which systems may compete to have the best designs or algorithms, but all agree to cooperate on interfaces, bug reporting, testing, etc. to keep the final user experience seamless and reliable.

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2 Impact

♦TO DO: Orsay's grant services will help here in December**♦**

2.1 Expected Impacts

EC Commentary: Please be specific, and provide only information that applies to the proposal and its objectives. Wherever possible, use quantified indicators and targets.

Describe how your project will contribute to:

- the expected impacts set out in the work programme, under the relevant topic (including key performance indicators/metrics for monitoring results and impacts);
- improving innovation capacity and the integration of new knowledge (strengthening the competitiveness and growth of companies by developing innovations meeting the needs of European and global markets; and, where relevant, by delivering such innovations to the markets;
- any other environmental and socially important impacts (if not already covered above).

Describe any barriers/obstacles, and any framework conditions (such as regulation and standards), that may determine whether and to what extent the expected impacts will be achieved. (This should not include any risk factors concerning implementation, as covered in section 3.2.).

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2.2 Measures to Maximise Impact

2.2.1 Dissemination and Exploitation of Results

♦EC Commentary: − Provide a draft 'plan for the dissemination and exploitation of the project's results'. The plan, which should be proportionate to the scale of the project, should contain measures to be implemented both during and after the project.

Dissemination and exploitation measures should address the full range of potential users and uses including research, commercial, investment, social, environmental, policy making, setting standards, skills and educational training. The approach to innovation should be as comprehensive as possible, and must be tailored to the specific technical, market and organisational issues to be addressed

- Explain how the proposed measures will help to achieve the expected impact of the project. Provide a draft business plan for financial sustainability as stated in the Part E of the Specific features for Research Infrastructures of the Horizon 2020 European Research Infrastructures (including e-Infrastructures) Work Programme 2014-2015.
- Where relevant, include information on how the participants will manage the research data generated and/or collected during the project, in particular addressing the following issues: What types of data will the project generate/collect? What standards will be used? How will this data be exploited and/or shared/made accessible for verification and re-use (If data cannot be made available, explain why)? How will this data be curated and preserved?
- Include information about any open source software used or developed by the project. You will need an appropriate consortium agreement to manage (amongst other things) the ownership and access to key knowledge (IPR, data etc.). Where relevant, these will allow you, collectively and individually, to pursue market opportunities arising from the project's results.
- The appropriate structure of the consortium to support exploitation is addressed in section 3.3.
- Outline the strategy for knowledge management and protection. Include measures to provide open access (free on-line access, such as the "green" or "gold" model) to peer-reviewed scientific publications which might result from the project.

Open access publishing (also called 'gold' open access) means that an article is immediately provided in open access mode by the scientific publisher. The associated costs are usually shifted away from readers, and instead (for example) to the university or research institute to which the researcher is affiliated, or to the funding agency supporting the research.

Self-archiving (also called "green" open access) means that the published article or the final peer-reviewed manuscript is archived by the researcher - or a representative - in an online repository before, after or alongside its publication. Access to this article is often - but not necessarily - delayed ("embargo period"), as some scientific publishers may wish to recoup their investment by selling subscriptions and charging pay-per-download/view fees during an exclusivity period.

Long term sustainability By design (Objective 1), the VRE's promoted by **MathVRE** will consist of a thin layer on top of an ecosystem of components. Hence, the long term sustainability of those VRE is guaranteed by the sustainability of the ecosystem of components, that is by Objective 5.

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2.2.2 Communication activities

♦EC Commentary: Describe the proposed communication measures for promoting the project and its findings during the period of the grant. Where appropriate these measures should include social media and public events with user participation. Measures should be proportionate to the scale of the project, with clear objectives. They should be tailored to the needs of various audiences, including groups beyond the project's own community. Where relevant, include measures for public/societal engagement on issues related to the project. ♠

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3 Implementation

◆TO DO: Typical granularity: 5-8 work packages with 3-5 tasks and one deliverable per task; 10 milestones**◆**

3.1 Work Plan — Work packages, deliverables and milestones

EC Commentary: *Please provide the following*:

- brief presentation of the overall structure of the work plan;
- timing of the different work packages and their components (Gantt chart or similar);
- detailed work description, i.e.:
 - a description of each work package (table 3.1a);
 - a list of work packages (table 3.1b);
 - a list of major deliverables (table 3.1c);
- graphical presentation of the components showing how they inter-relate (Pert chart or similar).

•

Overall Structure of the Work Plan

The work plan is broken down into XX workpackages as shown in Figure ??: WP2 deals with ... In addition, there is one management work package (WP1) and one general dissemination work package (??). The Gantt chart on Page 21 illustrates the timeline for the various tasks for these work packages, including inter-task dependencies.

How the Work Packages will Achieve the Project Objectives

♦ALL [WRITE HERE: This needs to explain that we're actually going to meet the objectives. Needs to be done after objectives and WPs.]♠

The project objectives (Section 1.1, page 2) and the corresponding work packages that contribute to achieving those objectives are:

Objective	Purpose	WPs
Objective 1	XX	WPX

Work Programme for Objective 1: Objective 1 is covered by WPX, which will ...

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Work package list

Work	Work package title	Lead	Lead	Person	Start	End
package		partic	short	months	month	month
No		no.	name			
WP1	Project Management	1	UPS		1	60
WP2	Community Building and Engagement	1	UPS			
WP3	Component Architecture	3	UVSQ			
WP4	User Interfaces	15	Simula			
WP5	HPC and massively parallel components	4	UJF			
WP6	Next generation mathematical databases	11	JU			
WP7	Social Aspects	6	UO			
WP8	Dissemination, Exploitation and Communication	9	USTAN			
Total				XXX		

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List of Deliverables

Del.	Deliverable name	WP	Lead	Type	Dissemi-	Delivery
no.		no.			nation	date
					level	

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List of milestones

Milestone	Milestone name	Related work	Estimated	Means of verification
number		package(s)	date	(deliverables shown
				here + success criteria
				below)
MS1	Completed initial requirements analysis.	WPX	1	??.
MS3		WPX		

Milestone	Success Criteria	Contributes
		to Objec-
		tive(s)
MS1	Completed requirements analysis (Deliverable ??).	1, 3.
MS3	XX	XX

[♦]EC Commentary: KEY Estimated date Measured in months from the project start date (month 1) Means of verification Show how you will confirm that the milestone has been attained. Refer to indicators if appropriate. For example: a laboratory prototype that is 'up and running'; software released and validated by a user group; field survey complete and data quality validated. **♦**

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Work package description (WP1)

Work package number	WP1		Start date or starting event:			Month 1		
Work package title	Project Management							
Participant number	1	9						
Participant short name	UPS	USTAN						
Person-months per participant:	48	48						

Objectives: Objectives: The objectives of WP1 are to undertake all project management activities, including:

- monitoring the overall progress of the project and the use of resources;
- ensuring the timely production of deliverables and other project outputs;
- reporting to the European Commission on financial matters;
- preparing for and attending the annual project review meetings; and
- managing the project Advisory Board.

Description of work:

This workpackage will perform all the activities related to monitoring of progress towards the project milestones shown on Page 3.1 and the deliverables listed on Page 3.1, assuring the quality of the deliverables, ensuring the collation and distribution of the required reports, questionnaires and deliverables including the annual reports to the European Commission, arranging project management meetings, tracking the project budget in terms of expenditure and person-months, obtaining financial certificates as required, convening project management meetings, ensuring that important project documents such as the project contract and the consortium agreement are properly maintained and amended as necessary, ensuring that contractual details are complied with, monitoring compliance with the grant agreement, preparing for the annual review meetings, and reviewing research results against the aims and objectives of the project. It also involves managing and supporting the project Advisory Board, including supporting attendance at project meetings, convening Advisory Board meetings, and obtaining feedback on the project direction and results.

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Deliverables:

Deliverable 1.1 (Month 1) Create tickets for all relevant tasks / deliverables

- **♦TO DO**: Rewrite everything below using the WPDeliverable macro**♦**
 - D1.1Month 1): Internal and external mailing lists.
 - D1.3Month 1): Internal software repository. TO DO: Needed? •
 - D1.3Month 1): Internal software repository. TO DO: Needed? •
 - D1.4Month 12): Project Periodic Report (first year).
 - D1.5Month 24): Project Periodic Report (second year).
 - D1.6Month 36): Project Periodic Report (third year).
 - D1.7Month 48): Project Periodic Report (fourth year).
 - D1.8Month 48): Project Final Report

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Work package description (WP2)

Work package number	WP2		Start date or starting event:			Month 1			
Work package title	Communi	Community Building and Engagement							
Participant number	9								
Participant short name	USTAN								
Person-months per participant:	1								

Objectives: The objective of WP2 is to further develop the community at the European scale, foster cross teams collaborations, spread the expertise, and engage the greater community to participate to the definition of the needs, and the implementation and use of the produced solutions.

Description of work:

We will organize regular open workshops (e.g. Sage Days, Pari Days, summer schools, etc.); some of them will be focused on development and coding sprints, and others on training.

This work package will also provide general travel budget to fund short to long term visits between the participants, to collaborate on specific features. A typical such visit would bring together an IPython developer with a GAP developer for a couple of days to implement a first prototype of notebook interface to GAP.

This work package will complement and lean on a parallel COST network whose role is to build and animate the greater community.

Deliverables:

- ?? (Month 12): Report on community needs
- Workshop 1 ...
- Workshop 2 ...
- Workshop 3 ...
- **♦TO DO**: make a list**♦**

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Work package description (WP3)

Work package number	WP3		Start date or starting event:			Month 1		
Work package title	Component Architecture							
Participant number	1	3	9					
Participant short name	UPS	UVSQ	USTAN					
Person-months per participant:	24	1	1					

Objectives: The objective of this work package is to develop and demonstrate a set of API's enabling components such as database interfaces, computational modules, separate systems such as GAP or Sage to be flexibly combined and run smoothly across a wide range of environments (cloud, local, server, ...).

Description of work:		

Task 3.1 Portability

In order to achieve maximum availability and accessibility, mathematical software must be developed and tested for a wide range of computer architectures and operating systems. However most of open source development happens in POSIX environments (usually Linux or OSX), and almost exclusively on x86 platforms. The vast majority of the developers of mathematical software does not have the expertise, nor the access to appropriate hardware and software, to insure appropriate testing and porting of components. The best incarnation of this issue is the involved installation procedure for Sage on Windows, a major adoption barrier and common source of complaints by end-user.

In this task we will address the common needs of the community in terms of portability layers, building and testing infrastructure.

- Best practices adopted by the larger open source community will be investigated and leveraged, and existing expertise will be shared between the component developers.
- Windows being largely dominant in the desktop/laptop market, a specific focus will be placed on the port of Sage, and therefore all the components included in its distribution (in particular PARI/GP, GAP, Singular, LinBox) to this platform (D 3.2, D 3.3).
- The deployment of a common infrastructure for multi-platform continuous integration (testing, building and distribution) will be addressed.

Task 3.2 Interfaces between systems

In this task we will investigate patterns to share data, ontologies, and semantics across computational systems, possibly connected remotely. We will leverage the well established semantics used in mathematics (categories, type systems, . . .) to give powerful abstractions on computational objects.

Through well defined APIs, we will enable discovery of subsystems, functionality, documentation and computational resources. The user interfaces shall be enabled to automatically choose the best available algorithms and resources to perform a required computation, as well as clearly and intuitively present the available choices to the expert user. As a first concrete test bed, we will consider the Sage interface to GAP, or more precisely libGAP (Deliverable 3.4). Like most Sage interfaces, this uses the now classical handle design pattern, whereby one can manipulate from Sage an object created and stored in GAP, through a handle (a.k.a. remote objects). By introspection, one can discover available GAP functions on this object and access the related GAP documentation. In a few cases, for example when the object is a group, one can further wrap the handle with an adapter that makes it behave like a native Sage group. By mapping GAP's categories to Sage's categories (as a rough approximation, both can be thought of as hierarchies of abstract classes), we will:

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- Implement a modular infrastructure for adapters, based on the category hierarchy, in order to let the implementation of adapters scale to a large variety of objects.
- Refactor the existing adapters, using this infrastructure to generalize their features. This step by itself will provide adapters for larger categories like semigroups or monoids.
- Merge the adapters into the handles, so that a handle to a GAP group will automatically behave like a native Sage group.

A specific challenge will be performance; indeed low level method adapters, e.g. for arithmetic, need to be compiled when most of the interface infrastructure is dynamic by nature.

♦*TO DO*: Other deliverables: generalization to other interfaces, factorization of the adapter code through standardized API's, semantic-enabled remote objects in SCSCP, reports, ...♦

Task 3.3 Modularization and packaging

In this task we will investigate best practices for composing, sharing and interfacing computational components and data for connected mathematical systems.

We will start with a comparative study of the practices adopted in various open source projects, both inside and outside of this project. This will include reviewing non-mathematical systems, e.g.: operating systems, platforms, web frameworks, cloud and HPC infrastructures.

We will address the current shortcomings to promote a new generation of mathematical software that is capable of scaling to large code bases, large datasets, and massively distributed infrastructures. This task also needs to consider the results of work package WP7n social issues regarding distributed development, community management, acknowledging contributions, etc.

As an example, Sage has a long history of integrating and distributing large mathematical libraries/software as a whole, with relatively few attention given to defining and exposing interfaces. Component re-usability is not a main focus for the Sage community, at the same time the non-standard and relatively underused package system discourages writing and maintaining autonomous libraries. These factors have contributed to make the Sage distribution what is usually described as a "monolith" (Sage library code alone, not counting included libraries, makes up for 1.5M lines of code and documentation), hard to distribute, to maintain, to port, and to develop with.

On the opposite side, GAP has been distributing community-developed "GAP packages" for a long time, but faces now fragmentation issues, at the code and at the community level. The rudimentary package system adds more technical difficulties to GAP's development model.

Both models reach the limits of their scalability, and a synthesis is very much needed.

Task 3.4 Deployment and distribution

♦*TO DO*: NT: what did you have in mind?**♦**

Task 3.5 Component architecture for High Performance Computing and Parallelism

As in all other areas of science, properly supporting massively parallel architecture is a major challenge. Many of the computational components have already gone a long way in this direction, and further work will happen there within WorkPackage T5.1.

In this task we will investigate and implement parallelism-friendly ways of combining components together, so that calling components can benefit from the parallelism features of called components, with self-adaptation to the environment and cooperative sharing of resources. **TO DO**: details+deliverables

Task 3.6 Improving the development workflow, in Sage and elsewhere.

♦TO DO: **♦**

Deliverables:

Deliverable 3.2 (Month 12) one-click install Sage distribution for Windows with Cygwin 32bits

Deliverable 3.3 (Month 24) one-click install Sage distribution for Windows with Cygwin 64bits

Deliverable 3.4 (Month 12) Semantic-aware Sage interface to GAP.

- **♦TO DO**: Make all those deliverables one-liners, and move the material to the task descriptions**♦**
 - ?? Make sure that Sage and therefore all the components it depends on (including GAP, Linbox, PARI/GP, Singular, ...) have standard packages in the main Linux distributions: Debian/Ubuntu, Redhat, Gentoo, ...
 - **♦TO DO**: Get feedback from our experts, and make this precise; what can we actually promise to achieve? how much work is this? Do we have personnel for this? There is strong expertise in Logilab with a Debian developer working there; he could advise someone on this. Logilab is interested in this because it's meeting similar issues with some of its clients software like Salomé. ♠
 - ?? (Month 12): Creation, deployment, and distribution of preconfigured virtual machines (and/or Docker images) for PARI/GP, Sage, ... as a cloud service, in particular within the StratusLab infrastructure. This includes build bots and test bots for continuous integration over a variety of operating systems.
 - ?? Modularization of the Sage distribution
 - Separation of the different components of Sage (communication with third-party softwares, build system, Sage native code). This is a prerequisite for easier packaging and integration in standard Linux distributions and Imonade, native integration within the IPython notebook and other interfaces (larcheny, Spyder, ...) and collaboration with sister projects.
 - ?? Add support for the SCSCP interface protocol to all relevant components (e.g. Sage, ...). •SL/AK [WRITE HERE: Brief description of what SCSCP is, reference to previous grant, relevance to the goals of this grant; maybe this should go in the work package description]•

SCSCP (Symbolic Computation Software Composability Protocol) is a remote procedure call protocol by which a computer algebra system (CAS) may offer services to a variety of possible clients, including e.g. another CAS running on the same computer system or remotely; another instance of the same CAS (in a parallel computing context); a simplistic SCSCP client (e.g. C/C++/Python/etc. program) with a minimal SCSCP support needed for a particular application; a Web server which passes on the same services as Web services, etc. A distinctive feature of the protocol is that both instructions and data are represented in the OpenMath format (http://www.openmath.org/; previously supported by the EU JEM Thematic Network; EU project 24969 "ESPRIT" and other projects); moreover, OpenMath support is not limited by existing official OpenMath content dictionaries - private encodings may be easily embedded into SCSCP messages.

SCSCP has been developed in the EU FP6 project 26133 "SCIEnce – Symbolic Computation Infrastructure for Europe" (TODO: fix and insert URL) and by now is supported by a number of computer algebra systems, including GAP, Macaulay2, Maple, TRIP and others. To facilitate SCSCP implementations, there are also APIs for Java, C and C++, and a simple Python SCSCP client (for a full overview, see SCIEnce website).

TODO: more on the relevance to to the goals of this grant. This is useful to exchange information between systems for problems that can not be solved within any single system; for storing and retrieving information (in databases) immediately into the CAS session; for organising distributed computations.

- Some IPython/Jupyter deliverables here. ◆TO DO: review what it can already do in term of choice of computational resource and storage back-end. ◆ ◆TO DO: cross link to Task 4.7◆
- Contribution by Kaiserslautern: libSingular, pySingular?, GAP-Singular, Singular-Sage. Moving code from Sage into Singular when relevant
- ?? (Month ...) Configure the components of Sage's distribution (e.g. Atlas, Linbox, GAP, Singular, ...) to be systematically HPC-enabled, and make sure that Sage's calls to such components indeed enable HPC.

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- Implementation of a transparent abstraction over mpi.
- Develop or integrate existing solutions for MapReduce operations over big data.

Raw material:

Component Architecture

Recomputation connection belongs here?

Collaboration with unreliable (or restricted!) networking connections (peer-to-peer, opportunistic syncing, 3rd world). This is technically interesting, and gets in support for non-networked working. Not sure if it belongs here or not.

- Security concerns

Goal: Fostering collaborations/integration between components in an open source ecosystem

- How to make systems "cooperate" rather than "predate each other".
- E.g. reduce the version issues
- Foster collaboration with upstream libraries by sharing the development and maintenance of the interfaces, typically as standalone upstream Python bindings (e.g. py-Singular).
- How to make it easy to develop simultaneously two interdependent components (e.g. Sage+Singular)
- Foster communication
- Social aspect:
 Credit, Citations, Recognition, Funding

Documentation system

In which package?

Improvements to Sphinx

Sage heavily customizes the Sphinx documentation system, hacking deep in it in some cases, with quite some duplication in some cases. Refactor the whole thing, generalizing and contributing back upstream as much as possible (e.g. parallel compilation).

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Work package description (WP4)

Work package number	WP4		Start dat	e or startin	Month 1			
Work package title	User Inte	User Interfaces						
Participant number	1	2	9	12	5	8		
Participant short name	UPS	Logilab	USTAN	UK	UB	USO		
Person-months per participant:	1	1	1	1	1	25		

Objectives: The objective of this work package is to provide a modern, robust, and flexible user interface for computation, supporting real-time sharing, integration with collaborative problem-solving, multilingual documents, paper writing and publication, links to databases, etc.

Description of work:

♦TO DO: What is a notebook interface**♦**

♦IPython [WRITE HERE: improve this draft presentation of IPython]♦

IPython is a leading notebook interface in the world of interactive computations, and use massively by biologists, physicists, **TO DO**: *and outside academia!* •. Originally tailored for Python, it has been language agnostic, and can communicate through a standardized interface to various computation kernels •TO DO: *cite a few* •. It can transparently run kernels locally or remotely (e.g. on the cloud), and has built in support for parallel computing and HPC.

The last tasks in this work package is focused on an *application of the IPython Notebook technology to a simulation package* that is actively used in materials research by a wide range of scientists and engineers, in academia and industry. We will develop a state-of-the art IPython Notebook interface and fronend and demonstrate the power that this approach delivers to accelerate computational science, deliver better value for money and make computational science more robust. We have chosen the Object Oriented MicroMagnetic Framework (OOMMF) simulation package [1] as the target tool which is used to simulate magnetic nanostructures in over 1800 publications [2]. We use OOMMF-NB (for OOMMF NoteBook) as an identifier for this case study.

Task 4.7 Uniform notebook interface for all interactive components

In this task, we will implement Jupyter interfaces for the interactive computation components of **MathVRE**, including GAP, Pari, Sage, and Singular. A first release D 4.5 will focus on basic functionality, and a second release D 4.6 will cover advanced features like 3D graphics or transparent documentation browsing (as live worksheets whenever relevant).

Sage itself will require a specific treatment as it already has a notebook interface. Its development started about at the same time as the IPython notebook, with similar target features but a different agenda: the Sage notebook had to be available very quickly to solve pressing needs of the Sage community; instead the IPython notebook was to take its time and build robust foundations from the ground up. The two projects have exchanged a lot, and the IPython notebook, which benefits from a much larger user base and thus developer pool, has mostly caught up with the Sage notebook in terms of functionality. It's thus time for the Sage community to outsource this key but non disciplinary component and phase out the Sage notebook in favor of the IPython notebook.

The Sage and IPython convergence D 4.7 will require:

- Robust migration path and tools for Sage worksheets,
- Support for math, 2D, and interactive 3D output.,
- Import (and export?) of ReST documents, with full support for Sage's specific roles (math, ...),

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- Support for remote Sage kernel, typically on the cloud, or running with a different Python version (Sage as a library),
- A migration path for interactive widgets implemented with Sage's @interact functionality.

Joint meetings and visits between the developers of Jupyter and of the computing components will be a key asset for this task.

♦*TO DO*: convergence with TeXmacs?**♦**

Task 4.8 Notebook interface usability

In this task, we will further improve Jupyter as a uniform user interface for interactive computation and database query.

▶IPython [**WRITE HERE**: Split off the work into an appropriate list of deliverables]*▶*

- Collaborative and shared worksheets.
- Multilingual notebooks?
- Improved 2D/3D graphics: maybe architecture for integrating VPython, vispy, ...? 3D visualization of algebraic surfaces (in collaboration with Singular)
- *Native folding support for sections and the like, with mouse and keyboard commands.*
- Version control
- ?? (Month ???) Heavyweight (e.g. QT based and not web based) user interface with docking support in the style of Spyder https://code.google.com/p/spyderlib/. Can possibly be implemented by extending the QT IPython console, or by letting Spyder use the IPython protocol (*TO DO: If that's not yet the case*).

Task 4.9 Using Notebooks for verification tests

In this task, we will develop tools that allow to re-execute stored notebooks. The computed output will be compared against the stored output, and deviations reported as assertion errors. This allows to use any notebook for automated regression testing.

• Reproducibility: ?? Support for tested notebooks. The writer specifies the expected outputs, e.g. in text format, and can check at any point that the full execution of the notebook yields exactly the expected output, as can be done with e.g. ReST files in Sage: sage -t notebook.rst

Task 4.10 Dynamic documentation and exploration system

Introspection has become a critical tool in interactive computation, allowing user to explore on the fly the properties and capabilities of the objects under manipulation. This becomes particularly acute in systems like Sage where large parts of the class hierarchy is built dynamically, and static documentation builders like Sphinx cannot anymore render all the available information.

In this task, we will investigate how to further enhance the user experience. This will include:

- On the fly generation of Javadoc style documentation, through introspection, allowing e.g. the exploration of the class hierarchy, available methods, etc.
- Logilab [WRITE HERE: Inclusion of database queries and views]
- ?? (Month 36) Exploratory support for semantic-aware interactive widgets providing views on objects represented and or in databases

Preliminary steps are demonstrated in the Larch Environment project (see demo vidéo on http://www.larchenvironment.com/) and sage-explorer.

Ultimate goal: automatically generated LMFDB-style interfaces. Mention Knowls, as dynamic context-free items of knowledge

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Whenever possible, those features will be implemented generically for any computation kernel by extending the Jupyter protocol with introspection and documentation queries.

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Task 4.11 Structured documents

Support for writing interactive structured documents, and in particular papers, books, experimentation log books and reports, presentations, course notes, etc, with the following features:

- Static printed/PDF/HTML version and interactive version.

 Achieved by either importing or exporting document files in some standard format (LaTeX, ReST, Markdown, ...).
- Tests (see above).
- Collaborative edition.
- Version control.

♦TO DO: include here everything about this topic in Needs.rst**♦**

◆TO DO: Wherever relevant, create tickets with details, and refer to them here. **◆**

Deliverable 4.5 (Month 12) Basic Jupyter interface for GAP, Pari, Sage, Singular

Deliverable 4.6 (Month 12) Full featured Jupyter interface for GAP, Pari, Singular

Deliverable 4.7 (Month 12) Sage notebook / IPython notebook convergence

Task 4.12 OOMMF case study: Create Python interface to OOMMF code

We split creation of the Python interface to OOMMF into two different layers of abstraction and corresponding tasks: **Task A**: Select and implement appropriate Python-C++ interface

We will identify best option for interfacing from Python to OOMMF core routines. The technical options include CTypes, Cython, Swig, and Boost-Python, all with particular advantages/disadvantages. Following analysis of the current OOMMF code layout and compilation model, we will use the most suitable tool, bearing in mind our ambition not to modify the OOMMF code so that the python interface we create remains functional and maintainable with minimal effort while the OOMMF core code is developed further by the OOMMF authors.

The interface will expose the raw C++ objects in Python, and for clarity we will refer to this interface as OOMMF-py-raw, to annotate that this gives access to OOMMF from PYthon but in a RAW way. Creation of this OOMMF-py-raw is technically doable as OOMMF had been written allowing to do this from Tcl.

Task B: The OOMMF-py-raw library for Python provides access to the OOMMF functionality but requires some care from the user. In this second task, we will create a user friendly Python library that combines the OOMMF-RAW capabilities we expect to become the main user interface to OOMMF in the medium term future. This will make use of object orientation to assist users in efficient and safe exploitation of the available facilities, following the design of the well-received Nmag simulation package [5].

Once this is completed, several new features will be available to OOMMF users: (i) ability to drive OOMMF from Python, (ii) computational steering, and (iii) combination of OOMMF simulation with the existing Python eco-system of computational tools.

We illustrate the advantage of (iii) through an example: to solve the micromagnetic standard problem 3 [3], traditionally multiple OOMMF simulation runs would have to be conducted, and for each of those a new configuration file as to be written. Between these the size of the simulated geometry needs to be modified until two particular values of energy are the same. Given the new interface developed in this work package, this whole process can be replaced by

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one Python script that creates multiple OOMMF simulations, combined with a root finding method for the automatic iterative determination of the required simulation geometry.

Parallel in developing this, a set of unit tests is created that can be run periodicly as regression tests. For all tasks relating to OOMMF-NB, documentation and tests are created simultaneously with the code.

We anticipate to start this task 4.12 in month 4.

Deliverables:

Deliverable 4.8 (Month 9) Basic Python Interface to OOMMF

Task 4.13 OOMMF case study: Extend OOMMF-py with IPython notebook attributes and GUI templates

The web server based Notebook environment (Jupyter) allows to host, execute and document the Python-based OOMMF simulation in an executable document. In this interactive environment, the representation of objects can be overloaded, and can include representation of objects as text, as bitmaps or svg files. We will create this functionality so that magnetisation vector field objects can be presented as a rendered 3d and 2d-view of the magnetisation field, and similar features for scalar fields such as field components and energies. This allows the interactive exploration and computational steering of the behaviour of magnetic nanostructures. Depending on the development of 3d packages such as vispy, it may be possible to provide interactive data objects in the notebook.

Beyond that, the Jupyter Widgets allow the creation of graphical user interface (GUI) like elements, and we will generate code to display these widgets on demand to (i) set up micromagnetic simulation using a GUI, and (ii) assist in post-processing simulation results. Not all OOMMF users are keen on using GUIs for simulation set up or post processing, but in particular new or infrequent users benefit significantly from this. Recent pilot work has shown that it is possible to make IPython Widgets interact with the python interpreter session and this allows to activate a GUI-like (widget based) interface when desired but to quickly return to the interpreter prompt, taking forward the results (data) from the GUI session [6] and providing a continuous path from scripting to GUI. We believe that having the ability to mix and match GUI-based and command driven analysis combines the best of both approaches and provides significant additional value.

Deliverables:

Deliverable 4.9 (Month 15) IPython Notebook Interface for OOMMF (OOMMF-NB)

Task 4.14 OOMMF case study: OOMMF-NB tutorial and documentation

We will create documentation and a new tutorial on usage of OOMMF that introduces micromagnetic modelling in the new framework of OOMMF-NB, combined with complete documentation of the OOMMF-Py library. The documentation will be provided in form of executable IPython notebooks.

The tutorial, in terms of content, will take guidance from the tutorial provided for Nmag [4] but tailored for the special simulation capabilities of OOMMF, and will introduce the special capabilities of the new IPython interface for OOMMF.

The output of this activity will provide multiple benefits: providing a systematic introduction to OOMMF-py suitable for both those users (i) new to micromagnetic modelling and those (ii) new to the OOMMF-py interface. Because the documentation is developed in an IPython notebook, the documents are executable. For new learners this is a great simplification because they can skip through the given document and execute the given examples there and then: at the moment, this is a process of manually writing a script, or locating it in the directory structure of files, then executing this, subsequently opening and processing the data files, etc. In the new model, this end-to-end simulation will start from specifying the material parameters in the notebook (all of this is given in the tutorial), to running the simulation in the notebook to processing of computed data while the simulation runs (or subsequently) in the notebook; thus providing one virtual research environment, with all the associated benefits of making best use of the scientist's time using the tool and environment.

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The documentation and tutorial will include a number of typical micromagnetic case studies that (i) demonstrate the correctness of the code by executing some of the micromagnetic standard problems and (ii) demonstrate the additional power gained by the IPython-based OOMMF interface.

Deliverables:

Deliverable 4.10 (Month 21) OOMMF-NB executable tutorial and documentation

Task 4.15 OOMMF case study: OOMMF-NB virtual environments

Recently, a TeMPorary ipython NoteBook has been made available at http://tmpnb.org, that allows anybody to go to this URL and use their very own IPython Notebook for quick calculations and tests online. We will provide similar functionality but for a server that provides the OOMMF-NB software and OOMMF-NB documentation and tutorials so that the tutorial can be executed immediately on that web server; thus removing the barrier of having to install code before being able to interactively drive and test a simulation system.

We will further provide as open source the scripts that allow creation of virtual environments (such as vagrant scripts to generate VirtualBox images, and Docker containers). These virtual environments underpin the web hosted temporary OOMMF-NB service but are also of use to those users who want to download a complete virtual machine to run their simulations within that machine.

We request 3100 EUR (ex VAT) to purchase a machine to provide these services (shared memory, 16 cores, 64GB RAM, small solid state drive to make the system more responsive). This machine will also provide the regression testing and continuous integration (see task 8.36). Setup and maintenance of the machine is part of this work task.

Deliverables:

Deliverable 4.11 (Month 24) OOMMF-NB dynamic web service available

Deliverable 4.12 (Month 24) OOMMF-NB virtualmachine images available for download

Task 4.16 OOMMF case study: Evaluation and refinement

We will make the OOMMF-NB open source code available to micromagnetic research groups as early as possible to gather feedback over a period as long as achievable. A questionnaire will be developed and used to gather user feedback on usefulness of the provided capibilities, with particular focus on (i) where OOMMF-NB enables new and better science, (ii) where it allows to do work more effectively, (iii) more reproducibly. We will further gather suggestions for improvements, and this feedback will be evaluated continuously. Time permitting, additional features and changes can be implemented, based on the user feedback. We will target OOMMF-NB users that attend workshops (see task XXX). Towards the end of the project, all results and insights will be summarised in a report to share the lessons learned from this user interface application example, and be made publicly available. Where possible, we will report our findings at relevant workshops/conferences.

Deliverables:

Deliverable 4.13 (Month 48) OOMMF-NB evaluation report

About the availability of people to hire, I have a full-time, experienced developer whose contract runs out in fall 2015, he would be ideal for the project. I also have a doctoral student who needs employment after the MathSearch project (until 10/2015) runs out. So I do have people who would directly be available.

Michael

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Task 4.10. Structured Documents (12 PM total, 3 PM per deliverable)

-> This existing task we could just take over based on our MathHub.info system, which would need to be adapted to the task.

Deliverables:

D1: Active Documents based on sTeX

D2: Distributed, Collaborative, Versioned Editing of Active Documents in MathHub.info

D3: Notebook Import into MathHub.info (interactive display)

D4: in-place computation in active documents (context/computation). Comments:

MathHub.info is a portal for reading and interacting with "active documents"

- (i.e. documents that have an additional semantic layer that supports semantic services like
- definition lookup, type-inference, unit conversion, ...)
 Notebooks are essentially "programs with documentation", whereas

Notebooks are essentially "programs with documentation", wherea active documents are

documents with a semantic knowledge layer. Regular publications are an important

boundary case: Active Documents look like papers, but are web-standards compatible

and interactive.

sTeX is a semantic variant of LaTeX that we can transform into OMDoc/MMT, which is the native knowledge representation format for active documents and machine-actionable knowledge about math and symbolic programs.

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Task K-4.11 Math Search Engine (10 PM total; 2 each for D1/2, 3 each for D3/4)

D1: Full-text search (formulae + Keywords) over LaTeX-based documents (e.g. arXiv subset)

D2: Full-text search (F+K) over Notebooks (in the format determined in task 4.7)

D3: Formula search in CAS programs and Software Modules

D4: Search from Notebooks/Active Documents (for local context to inform search)

Comments:

We already have a search engine, therefore we only need to build harvesters for D1/2;

D3/4 are more speculative.

I am going to get some sushi now, I have 2 or 3 tasks for WP6 in mind, but not written up.

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Work package description (WP5)

Work package number	WP5		Start dat	e or startin	Month 1		
Work package title	HPC and massively parallel components						
Participant number	1	1 2 9 12 5 4					
Participant short name	UPS Logilab USTAN UK UB UJF						
Person-months per participant:	1	12	1	1	1	12	

Objectives: The objective of this work package is to improve the performance of the computational components of **MathVRE**, in particular on massively parallel architectures. This includes notably:

- Fine grained High Performance Computing on many-cores architectures.
- Coarse grained or embarrassingly parallel computing on grids or on the cloud.
- Compilation of high level interpreted code to optimized parallel native code.
- Develop novel HPC infrastructure in the context of combinatorics.

A key aspect will be to foster further sharing expertise and best practices between computational components.

Description of work:

As in all other areas of science, properly supporting massively parallel architecture is a major challenge. Many of the computational components in **MathVRE** have already gone a long way in this direction. For example, an adaptation of the GAP kernel for HPC was developed during the 2009-2013 EPSRC project. The expertise gained there was then transferred to the ongoing Singular-HPC project, in particular through the rehiring of one of the developers of GAP-HPC. The French ANR HPAC project (2012-2015) has also widely contributed to design parallel exact linear algebra kernels which is a core component for most HPC applications. The LinBox library, used in sage, has benefited from this experience on the multi-core processing aspects.

In this work package, we will build on this momentum to further implement HPC support in the components Tasks 5.17, 5.19, and 5.21.

♦TO DO: transition**♦**

Many of the computational components of **MathVRE** use a high level interpreted language for their library. This is notably the case of Sage. Performance is achieved by compiling critical sections using the Cython Python-to-C compiler, to the expense of a lower level implementation. In Tasks 5.23 and 5.24, we will also boost performance by further developing and applying such compilation tools, while keeping a high-level approach.

Task 5.17 PARI

PARI is a C library mainly oriented toward arithmetic and number theory.

It currently lacks interfaces for parallelism (POSIX threads or MPI). More precisely, it should be possible from an external package or software (e.g. Sage) to better exploit PARI parallel features.

On the other hand, many basic algorithms in PARI (e.g. integer factorization) are currently implemented using only one core. One can take better use of multi-core architecture and more generally parallel architectures.

Task 5.18 *GAP*

◆SL/AK [WRITE HERE: Task around HPC/parallelism/perf in GAP]◆

♦*TO DO*: deliverable**♦**

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Task 5.19 Linbox

♦JGD/CP [WRITE HERE: Task around HPC/parallelism/perf in Linbox] ♦

♠TO DO: deliverable*♠*

Task 5.20 Singular

The unique challenge of parallelizing Singular has been that it is a decades-old project, with a codebase exceeding 300,000 lines of code and an enormous existing investment of development effort. This makes a wholesale manual rewrite or reengineering approach infeasible.

We therefore use a multi-pronged approach: First, we have created automated source-to-source translation tools that take existing C/C++ code as input and generate threadsafe code as output. Secondly we are also adding facilities to the C/C++ code and the Singular interpreter to safely access shared memory. These facilities ensure in particular that common pitfalls of concurrent programming, such as data races and deadlocks, cannot occur. For this, we leverage approaches that have already been successfully used for HPC-GAP and whose principles are well-understood.

To supplement the above existing work, we propose to add very fine-grained parallelism to some key components of Singular. These include writing a multi-threaded implementation of the Singular multivariate polynomial arithmetic, of the main quadratic sieve implementation for integer factoring and parallelisation of the FFT based integer and dense polynomial multiplication algorithm. These key components are used extensively for Singular's overall workload, including in the Groebner basis engine and polynomial subsystems. Performance increases through fine-grained parallelisation of key components such as these will provide extensive benefits to virtually all users of Singular on multi-core machines.

Deliverables:

Deliverable 5.14 (Month 3) Parallelise the relation sieveing component of the Quadratic Sieve

Deliverable 5.15 (Month 9) Implement a parallel version of Block-Wiederman linear algebra over GF2 and the triple large prime variant.

Deliverable 5.16 (Month 12) Take advantage of multiple cores in the matrix Fourier Algorithm component of the FFT for integer and polynomial arithmetic, and include assembly primitives for SIMD processor instructions (AVX, Knight's Bridge, etc.), especially in the FFT butterflies

Deliverable 5.17 (Month 12) Parallelise the Singular sparse polynomial multiplication algorithms

Deliverable 5.18 (Month 12) Parallel versions of the Singular sparse polynomial division and GCD algorithms.

Task 5.21 MPIR

MPIR (Multiple Precision Integers and Rationals) is the core library in Sage for bignum arithmetic. It is used extensively by a majority of the core C/C++ libraries in Sage, and by Sage directly via Cython. MPIR is a fork of the GMP (Gnu Multi-precision) library, with many independent implementations of the core algorithms (including a faster FFT and division code, better superoptimisation on some common 64 bit processors and native MSVC support). It consists of around 250,000 lines of code, much of which is assembly primitives and very low level, highly optimised C code.

Maintainence of MPIR is not merely a matter of updating the build system. Rather, every time a new processor is released by AMD, Intel, Sparc or ARM, significant development has to be invested in hand-optimising and then superoptimising assembly code for the new processors. This gives up to a 12x performance increase over optimised C code, due to the specialised nature of bignum arithmetic, which is in some sense a worst case for C compilers. Indeed without continuous effort, MPIR would not even run on new operating systems and processors, let alone run fast. This is a unique problem that assembly libraries have.

As a successful and key component of Sage, we believe it is time to invest in maintenance and improvement of MPIR by hiring an assembly expert who can work full time on the project after MPIR's lead assembly expert sadly passed away recently. Significant challenges exist, such as optimising for SIMD instruction sets. Without investment into maintenance, assembly superoptimisation, processor support, fat binary support, etc. this key component of Sage will fall behind, to the detriment of Sage as a whole and the numerous other standalone libraries that make use of MPIR.

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Deliverables:

Deliverable 5.19 (Month 12) Extend the existing assembly superoptimiser for AVX and upcoming Intel processor extensions

Deliverable 5.20 (Month 24) Ongoing support of Intel, AMD, ARM, Sparc processors and new Operating System versions

Deliverable 5.21 (Month 12) Provide FAT binary support for all new x86_64 processors, build system maintenance and improvements to tuning, profiling and testing subsystems

Task 5.22 HPC infrastructure for combinatorics

♦FH [**WRITE HERE**: Task around HPC infrastructure for combinatorics]**♦**

Several members of the projects are experts in combinatorics a field where Sage is clearly a world leader. This particular research field has several specific features which makes it interesting from the HPC point of view:

- The main obstacle is combinatorial explosion which stop many experiment very early. Algorithm of exponential complexity are extremely common.
- Embarrassingly parallel problem are extremely common.
- Problem that are not embarrassingly parallel very often reduce to a large tree exploration.

To help the researcher, it is crucial to minimalize the extra work needed to get a parallel program from a serial one in these simple situations. Through this task we will provide a practical and concrete as well as highly demanding use case for the infrastructure developed. In particular, we aim to test on real problems the benefit of tasks 5.23, 3.3, 3.4, and 3.5.

In a second and more exploratory direction, some experiments shows that the large tree exploration problem is very easily solved in C++ using the new Intel Cilk++ technology. We would like to explore the possibility to interface smoothly Pythran, Cython and Cilk++.

Deliverables:

Deliverable 5.22 (Month 3) Turn the Python prototypes for tree exploration into production code, integrate to Sage.

Deliverable 5.23 (Month 12) Explore the possibility to interface smoothly Pythran, Cython and Cilk++.

Deliverable 5.24 (Month 24) Refactor the existing combinatorics **Sage** code using the new developed Pythran and Cython features.

Task 5.23 Pythran-Cython convergence

Pythran is a Python to C++ compiler for a subset of the Python language. It is meant to efficiently compile scientific programs, and takes advantage of multi-cores and SIMD instruction units. Thanks to type inference, it requires little annotations. Its rutime supports a subset of the Numpy package.

Cython is a Python to C compiler that was originally developed for Sage and is now a thriving project of its own. It can handle essentially any Python code, and in particular classes, but relies heavily on annotations for producing optimized code.

Therefore, Pythran and Cython are similar in spirit but have complementary feature sets: Pythran can heavily optimize high level Numpy constructs and Cython has broader Python support. In this task, we will investigate the opportunity and feasibility of a convergence between Cython and Pythran: depending on the code at hand, one strategy or the other would be automatically selected, eventually using Pythran generated called from Cython when relevant D 5.25. This would result in compiler-runtime cooperation driven by the Cython compiler thanks to part of the Pythran-runtime and the extra typing information provided by Cython. An effort will be made to improve more and more the parallelism in the Pythran runtime D 5.26.

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This work will be achieved through a close collaboration between the Pythran developers hired for MathVRE and Cython developers involved in the Sage project. It should quicken Sage execution time at least on Numpy centric codes, while not putting an extra burden on the developers. Preleminary dicussions with the Cython community have already taken place and received a very favorable feedback.

Task 5.24 Pythran for Sage and Sage Users

Currently, Sage doesn't provide facilities to improve user written Python code without the modifications implied by the use of the Cython compiler. As Pythran doesn't need these codes to be rewriten, a notebook interface to compile Pythran compilant code will he added in Sage to improve user kernels using the Pythran compiler D 5.27.

In a similar perspective, testing and improving the integeration between mpi4py and Pythran could provide an efficient toolchain for HPC while keeping full backward compatibility with pure Python code. This will required a continuous integration of Pythran to ensure its capabilities D 5.28.

Internally, Sage uses Cython for compiling the critical sections of its libraries. In this task, we will explore opportunities to benefit from Pythran compilation within the Sage library, in particular toward better support for parallelism. A specific challenge is that the Sage library uses quite heavily object-oriented programming.

This task will strongly benefit from Task 5.23, while providing in return a real life large-scale use case for it.

A first step to support object-oriented programming will be to make Pythran type inference more accurate, which will also improve error feedback provided for the user D 5.29.

Task 5.25 Explorative task: Add support for classes in Pythran.

Classes support is a real challenge for Pythran as it requires a more accurate typing information but also invalidates some compiler optimisations.

As it will need a full rework of the aliases analysis in Pythran, which is the keystone of Pythran, we are not sure it could really be integrated but it would be a proof of scalability for Pythran. Thanks to this typing and this better aliaing analysis, we could add more optimizations like the ones from Cython enabled with decorator annotation.

Deliverables:

Deliverable 5.25 (Month 6) Implement Pythran runtime support in Cython when they are implemented instead of using default implementation.

Deliverable 5.26 (Month 3) Improve Pythran runtime support to automatically take advantage of multi-cores and SIMD instruction units.

Deliverable 5.27 (Month 2) Facility to compile Pythran compliant user kernels.

Deliverable 5.28 (Month 1) Ensure inteoperability of Pythran with Python and its packages.

Deliverable 5.29 (Month 12) Make Pythran typing better to improve error information.

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Work package description (WP6)

Work package number	WP6		Start date or starting event:			Month 1	
Work package title	Next generation mathematical databases						
Participant number	14						
Participant short name	UZH						
Person-months per participant:	1						

Objectives: The objectives of WP6 are: to design and implement interfaces that can be used for a wide range of mathematical data and to standardise metadata allowing for interoperability, searching, documentation, versioning and visualisation.

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Description of work:

Mathematics is the only science that has not yet benefitted greatly from the systematic interchange of data. At the same time, mathematics has a richer notion of data than other disciplines. Indeed, "mathematical data" consists of three kinds of objects:

[D]: proper (numeric/symbolic) data

[K]: the knowledge about the mathematical objects given as statements (definitions, theorems or proofs; either formal or rigorously informal)

[S]: software that computes (with) the mathematical objects

All three kinds of "data" are equally important for mathematics and are tightly interlinked:

- [D] serves as examples for [K] or as counterexamples for conjectures in [K];
- [S] computes [D] and establishes properties of [D] (given as [K]);
- [D] tests [S], [S] is verified with respect to [K];

theorems and proofs in [K] induce and justify algorithms for [S];

[D] induces conjectures and guides proofs in [K].

Many mathematical databases now exist, but their internal structure does not reveal this richness. This weakness prevents the formulation of new conjectures, the testing of new hypotheses, and generally an exploratory approach to mathematical data. The past has shown that such an approach can be fruitful:

- both the Riemann Hypothesis and the Birch and Swinnerton-Dyer conjectures resulted from exploratory *L*-function computations, and now stand among the seven Clay Millenium Problems;
- the Monstrous Moonshine conjecture finds its origin in a numerical coïncidence between dimensions of representations of the Monster group and coefficients of the *j*-function, and its conclusion eventually led to Borcherds' Fields medal.

Therefore to facilitate future advances, we need ways to represent DKS in the same systems, and – since current computational/experimental mathematics involve extensive DKS – we need a new kind of "database", which we will call Mathematical Data/Knowledge/Software-bases.

This complexity is on vivid display in the *L-functions and Modular Forms database* project (LMFDB): while the general shape of the functional equation of an *L*-function is dependent on a lot of theoretical knowledge, it also requires parameter data and the coefficients of the associated Dirichlet series. Once this is obtained, highly optimised (and heavily parallelizable) algorithms can be run to compute values of this function.

We propose in this work package to design and build an infrastructure that would make it easy for either individual mathematicians or a distributed collaboration to manage and use such interlinked mathematical data. This work would provide part of the backend to Work Packages •TO DO: work package on interfaces, and???•, and would draw on previous work with the LMFDB and FindStat (which will be treated as prototypes for our purposes, to serve as exemplars to other projects) and in return will substantially enhance their capabilities. Prerequesites should be kept to a minimum (depending on contributors' and users' needs and goals), and in particular would not require any background in databases to contribute new data or perform queries.

Task 6.26 Survey of existing databases

All the systems considered in this proposal (GAP, Sage, PARI, Singular) include data as part of their regular distribution. In this task, we will survey existing databases, the technology used to implement them, how they were linked to the rest of the existing infrastructure and the functionalities offered. We will also select additional external data and projects to add to this effort, aiming to maximise the impact of our work.

Task 6.27 Design of new infrastructure, formulation of requirements

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Ontologies are the canonical method used to implement databases that require significant data interchange. However, because of extreme reification in mathematics, this is not entirely suitable for our goals. We will design a new infrastructure for **MathVRE**, drawing on existing emerging standards.

We will organise a workshop associated to this task.

Task 6.28 Triform Theories in OMDoc/MMT

OMDoc/MMT is a representation language for mathematical knowledge and documents. Carette and Farmer have developed the notion of biform theories (K/S) in a uniform representational approach; our work here would extend this along the data axis, which will require a specialised but integrated treatment.

Task 6.29 Computational Foundation for Python/Sage (or some CAS)

In the OMDoc/MMT world a foundation is a logical base language that gives the formal meaning to all objects represented/formalized in it. We have created a very initial computational foundation for Scala and implemented it in the MMT API. This can be used to execute (or verify) computations directly in OMDoc/MMT and thus forms the basis for various integration tasks for OMDoc/MMT biform theories that integrate Scala computations. Here we propose to develop a somewhat more complete computational foundation for Python and/or parts of Sage (coverage to be determined). Bi/Triform theories come in three parts:

- syntax: what operators/types are there, how do they nest,
- computation: what does the computation relation look like (sometimes called operational semantics). The declarative semantics of a computational foundation can be given as an OMDoc/MMT theory morphism into another foundation (e.g. a set theory);
- ??? three parts

Task 6.30 OEIS Case Study (Coverage and automated import)

In this case study we test the practical coverage of the trifunctional modules, by transforming an existing, high-profile database (the Online Sequence of Integer Sequences http://www.oeis.org) into OMDoc/MMT. The OEIS has about 250 thousand sequences, with formulae, descriptions, definitions, references, software, etc. in a structured text file (but no standardized format for formulae and references), so we expect to get 250 k theories. Having the OEIS in OMDoc/MMT form allows to do Knowledge Management services (presentation, definition lookup, formula search, ...) in MathHub.info (see WP4.?). The OEIS is a good case study, since the DKM are licensed under a CC license which allows derived works. The large size will allow statistically significant semantic cross-validation of the heuristic transformation process and thus achieve a significant DKS community resource.

Task 6.31 FindStat Case Study (triformal theories)

In this task we would develop triformal theories for the FindStat project to test the design from 6.29. Similarly to the previous task, in this case study, we first develop a thorough OMDoc/MMT model, which should only involve a handful of MMT theories (combinatorial collections, maps, statistics,...), each with a few hundred realisations. Together with \$\times POD [WRITE HERE: WP4] \&\times\$, this will again allow for easier knowledge management services, and in particular improved search services.

This Task will be co-developed with 6.29, it will validate the design of triformal theories and be iterated to test the design changes.

Task 6.32 LMFDB Case study (triformal theories)

In this task we would develop triformal theories for an exemplary part of the LMFDB project to test the design from 6.29. We will identify a fragment of the LMFDB that we want to model and design the model. Then we will perform cross-validation of the three model parts against each other (essentially model-based testing of software and inference). Finally, we will pick an algorithm from the LFMDB and verify it against its specification and the computational foundation developed in 6.29. (decrease importance of verification as opposed to interoperability)

Task 6.33 Memoization and production of new data

Many CAS users run large and intensive computations, for which they want to collect the results while simultaneously working on software improvements. Sage currently has a limited cached_method, that is not persistent across

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sessions and does not enable to publish the result or share it with a smaller group of collaborators. We propose to use, extend and contribute back to some established persistent memoization infrastructure, such as python-joblib, redis-simple-cache or dogpile.cache. The caching should apply recursively to lower level functions, and should be trivial to setup and configure for the end user: in a single line, the user only needs to select an existing function and maybe provide some additional semantic information, and has the option to change the defaults for a few parameters, such as the backend (shared dropbox folder, remote directory, database, git repository, ...). The interface could be through a Python decorator. Additionally, it should be easy to launch a data-bot to populate the database, all the versioning and provenance tracking should be handled (user, algorithm, software version, ...), and the system should have useful data properties (atomicity, merging, and error detection).

Deliverables:

- Conversion of existing and new databases to unified interoperable system:
 - Polytopes in Polymake
 - graphs, graph properties
 - Finite groups (Max)
 - Lattices
- **♦TO DO**: *Make this a task*
 - ?? (Month X): Shared persistent memoization library for Python/Sage.
- Recomputation?
- Ease of publishing, importing, ...
- **♦TO DO**: Use the WPdeliverable macro; see e.g. UserIntefaces.tex**♦**
 - D6.2: workshop report
 - D6.3.1: Design of Triform (DKS) Theories (Specification/RNC Schema/Examples) # 12 PM
 - D6.3.2: Implementation of Triform Theories in the MMT API.
 - D6.4.1: Python/Sage Syntax Foundation Module in OMDoc/MMT # 12PM
 - D6.4.2: Python/Sage Computational Foundation Module in OMDoc/MMT
 - D6.4.3: Python/Sage Declarative Semantics in OMDoc/MMT
 - D6.5.1: LMFDB deep modelling: Fragment Identification & Initial Model Design # 12PM
 - D6.5.2: LMFDB Data vs. Knowledge vs. Software Validation
 - D6.5.3: LMFDB Algorithm verification wrt. a Triformal theory
 - D.6.5.4: LMFDB full integration of algorithms, data and presentation (not so much verification)
 - D6.6.1: Heuristic Parser for the OEIS
 - D6.6.2: Cross-Validation for OEIS DKS-Theories.

Another connection: on several occasions, we found that software was the best way to represent certain databases of mathematical

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knowledge. E.g. in Algebraic Combinatorics we have a whole zoo of Hopf algebras. Many of them are implemented in MuPAD/Sage by specifying the objects that index the basis together with computation rules for the product and coproduct. When we want to retrieve information about such algebras, it's usually much more convenient to look at the code than to search through the literature. Especially since the code is usually more correct than the literature because it's *tested*.

We may also think of providing an interface to \LMFDB via SCSCP protocol (http://www.symbolic-computing.org/scscp) so it may be accessed by a variety of other systems (see their current list at http://www.symbolic-computing.org/scscp)

database access to \LMFDB as a python library

♦DP/UM [**WRITE HERE**: Workpackage Social Aspects]**♦**

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Work package description (WP7)

Work package number	WP7		Start date or starting event:			Month 1	
Work package title	Social As _l	pects					
Participant number	6						
Participant short name	UO						
Person-months per participant:	1						

Objectives: The objectives of WP7 are to:
•
•
 Development models for an academic free software ecosystem
Supporting the Mathematical Process
Description of work:
This workpackage
This workpackage
Deliverables:
Deliverable 7.30 (Month 12)

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Work package description (WP8)

Work package number	WP8		Start date or starting event:			Month 1	
Work package title	Dissemination, Exploitation and Communication						
Participant number	9	8					
Participant short name	USTAN	USO					
Person-months per participant:	1	7					

Objectives: The objective of this work package is to organize and optimize the communication with the larger community. This includes:

- reviewing emerging technologies;
- disseminating research results to the scientific community;
- ensuring awareness of the results in the user community;
- raising general public awareness of the MathVRE project;
- defining individual exploitation plans; and,
- managing existing and new intellectual property.

Description of work:

Dissemination: software, APIs, technologies, research results, ...

Task 8.34 Reviewing emerging technologies

In this task, we will produce periodic reviews of emerging technologies and relevant developments elsewhere, and implications for our plans. This include the review of standard components and service for storage and sharing, computational resources, authentication, package management, etc. This may further include negotiating access or shared development when appropriate. This information will be fed to the other work packages, in particular Work Package WP3omponent Architecture.

Task 8.35 Dissemination and Communication activities

♦*TO DO*: scale this down as appropriate**♦**

This task comprises all forms of direct dissemination and public communication activities such as press releases, creation of the project web-site including visitor analysis and monitoring tools (8.32), scientific and technical publications, outreach activities (seminars, keynote talks, media interviews, press releases), pro-motion through social media (e.g. twitter, facebook, linkedin), technical workshop organisation, creation of advertisement materials such as flyers, posters, and electronic feeds as well as their distribution.

At least two press releases will be generated in the course of the project (8.31, ??), and the project will organise at least one open technical workshop each year.

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Deliverables:

Deliverable 8.31 (Month 3) Press release announcing start of MathVRE.

Deliverable 8.32 (Month 3) Project web site

Deliverable 8.33 (Month 12) Year 1 report

Deliverable 8.34 (Month 24) Year 2 report

Deliverable 8.35 (Month 36) Year 3 report

Deliverable 8.36 (Month 48) Year 4 report

Task 8.36 Dissemination of OOMMF-NB virtual environment

OOMMF-NB is build on top of MathVRE and demonstrates the power of the environment in a production environment of active OOMMF users. The source code of OOMMF-NB will be made available as open source on public repository hosting sites (such as github/bitbucket), and announced to the community via the mumag mailing list. We will encourage participation of the micromagnetic community in the maintenance and development of the tools, and allow time to train users to join the OOMMF-NB project to drive towards a self-sustained OOMMF-NB project at the end of the funding period.

To underpin this process, we will set up a publicly accessible Jenkins/Travis-CI system (see Task 4.15) to (i) run regression tests routinely when the OOMMF-NB code changes or OOMMF core code changes and (ii) re-execute notebooks and use as regression test (making using of task 4.9). This will test user-contributions automatically, and can automatically create virtual environments for download containing the latest versions.

We will create a manuscript for journal publication, summarising the approach taken and experience gathered so far. An important point of this publication is to provide a reference that can be cited by publications making use of the new OOMMF-NB, allowing tracking of uptake of this technology in the medium and long run.

Deliverables:

Deliverable 8.37 (Month 15) OOMMF-NB available online as open source

Deliverable 8.38 (Month 18) Public continuous integration system set up

Deliverable 8.39 (Month 36) Submitted OOMMF-NB manuscript

Task 8.37 OOMMF-NB dissemination workshops

In this task, we run a series of workshops at major international meetings to disemminate the open source OOMMF-NB tool in the micromagnetic community.

We will prepare the software stack for the workshops, develop teaching materials, and do the planning (location, advertising, registration) and delivery of workshops at the 4 major international meetings taking place in the appropriate time frame¹ each of which tends to attract around 1000 attendees. Depending on demand, multiple workshops can be given per conference. We anticipate to travel with two people (Hans Fangohr and PDRA or other support staff) to be able to teach effectively and deliver hands-on training as part of the workshop. We request 500 EUR room hire per meeting.

Deliverables:

Deliverable 8.40 (Month 48) Delivered OOMMF-NB workshops at major international meetings

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¹Anticipated major meetings are 61st Conference on Magnetism and Magnetic Materials October 31-November 4, 2016, New Orleans, Louisiana; 62nd Conference on Magnetism and Magnetic Materials November 6-10, 2017, Pittsburgh, Pennsylvania; 21st International Conference on Magnetism (ICM 2018) July 16–20, 2018, San Francisco, California; 14th Joint MMM-Intermag Conference January 14-18, 2019, Washington, DC)

Raw material:

- Documentation improvements: overview, cross links, overview of recent improvements
- Thematic tutorials
- Collections of pedagogical documents

 E.g. a complete collection of interactive class notes with computer lab projects for the "Algèbre et Calcul formel" option of the French math aggregation (starting from 2014-2015, only open-source systems will be supported, and Sage is a major player).
- Localization of the Sage user interface and key documents in various European languages.
- Distribution of the documents either in the main distribution of Sage or through the online repository (see collaborative tools).
- Massive online introduction course to Sage, drawing on the sage tutorial/notebooks. Could be "First year Sage course in a box".
- Taking the opportunity of Python courses to propose Sage as a natural extension for mathematics; an example is French's "Classes préparatoires", where Python has been recently selected as the language to learn programming³.

♦TO DO: Milestones need to be discussed and then described here. **♦**

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 $[\]label{thm:posterior} $$ ^2http://en.wikipedia.org/wiki/Classe_pr\unhbox\voidb@x\bgroup\let\unhbox\voidb@x\setbox\@x\ent0ex=\label{thm:posterior} $$ accent0ex=\acc$

³See the "Annexe" at http://www.education.gouv.fr/pid25535/bulletin_officiel.html?cid_bo=71586

3.2 Management Structure and Procedures

- **♦EC Commentary**: Will get help from Orsay's grant services**♦**
- **♦EC Commentary**: Describe the organisational structure and the decision-making (including a list of milestones (table 3.2a)).

Explain why the organisational structure and decision-making mechanisms are appropriate to the complexity and scale of the project.

Describe, where relevant, how effective innovation management will be addressed in the management structure and work plan.

Describe any critical risks, relating to project implementation, that the stated project's objectives may not be achieved. Detail any risk mitigation measures. Please provide a table with critical risks identified and mitigating actions (table 3.2b).

3.3 Consortium as a Whole

♦EC Commentary:

- Describe the consortium. How will it match the project's objectives? How do the members complement one another (and cover the value chain, where appropriate)? In what way does each of them contribute to the project? How will they be able to work effectively together?
- If applicable, describe the industrial/commercial involvement in the project to ensure exploitation of the results and explain why this is consistent with and will help to achieve the specific measures which are proposed for exploitation of the results of the project (see section 2.3).
- Other countries: If one or more of the participants requesting EU funding is based in a country that is not automatically eligible for such funding (entities from Member States of the EU, from Associated Countries and from one of the countries in the exhaustive list included in General Annex A of the work programme are automatically eligible for EU funding), explain why the participation of the entity in question is essential to carrying out the project

◆TO DO: The participants are core developers of the involved components**◆**

♦TO DO: Experience in community building and engagement**♦**

Writing interfaces between computer algebra systems from different areas and collaboritive software development are important themes within the DFG Priority Project SPP1489. As in the SAGE community, networking measures include the regular exchange of developers and the regular organization of software workshops (coding sprints) which bring whole teams together for solution finding and intense code writing. Particular tight collaborations exist between the GAP and the SINGULAR communities, with major GAP-SINGULAR developers meetings taking alternately place at St. Andrews, Kaiserslautern, and Aachen. See http://www.computeralgebra.de/.

♦TO DO: User interfaces: recruitement of IPython developers**♦**

♦TO DO: Pythran and HPC: a key asset will be the recruitment of two of the lead developers of the Pythran Python-to-C compiler.**♦**

♦JGD/CP [WRITE HERE: Linbox: recruitement of previous ANR developper]♦

♦TO DO: Explanation of why we want to include Seattle (sage-math cloud, is a key component; access to IP).

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3.4 Resources to be Committed

- **♦EC Commentary**: Will get help from Orsay's grant services**♦**
- **EC Commentary**: *Please provide the following*:
 - a table showing number of person/months required (table 3.4a)
 - a table showing 'other direct costs' (table 3.4b) for participants where those costs exceed 15% of the personnel costs (according to the budget table in section 3 of the administrative proposal forms)

Summary of staff effort

◆EC Commentary: Please indicate the number of person/months over the whole duration of the planned work, for each work package, for each participant. Identify the work-package leader for each WP by showing the relevant person-month figure in bold.◆

♦TO DO: Update this once the list of parthers and the WPs are finalised.**♦**

Partic.	Partic.		Work package								
no.	short	WP1	WP2	WP3	WP4	WP5	WP6	WP7	WP8	WP9	PMs
	name										
1	UPS										
2	Logilab										
3	UVSQ										
4	UJF										
5	UB										
6	UO										
7	USHEF										
Tot	tal PM										

♦EC Commentary: Please complete the table below for each participant if the sum of the costs for' travel', 'equipment', and 'goods and services' exceeds 15budget table in section 3 of the proposal administrative forms). ♠

Other direct cost items

	Cost (€)	Justification
Travel		
Equipment		
Other goods and services		
Total		

Management Level Description of Resources and Budget

♦TO DO: This needs to be updated in line with the rest of the project.**♦**

The project will employ XX person-months of effort over YY years, comprising ...

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♦EC Commentary: *This section is not covered by the page limit. The information provided here will be used to judge the operational capacity.*•

4 Members of the Consortium

4.1 Participants

- **EC Commentary**: *Please provide, for each participant, the following (if available):*
 - a description of the legal entity and its main tasks, with an explanation of how its profile matches the tasks in the proposal;
 - a curriculum vitae or description of the profile of the persons, including their gender, who will be primarily responsible for carrying out the proposed research and/or innovation activities; this includes a description of the profile of the to-be-recruited personnel
 - a list of up to 5 relevant publications, and/or products, services (including widely-used datasets or software), or other achievements relevant to the call content;
 - a list of up to 5 relevant previous projects or activities, connected to the subject of this proposal;
 - a description of any significant infrastructure and/or any major items of technical equipment, relevant to the proposed work;
 - any other supporting documents specified in the work programme for this call.

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University of St Andrews

The Centre for Interdisciplinary Research in Computational Algebra (CIRCA) fosters research at the interface of Mathematics and Computer Science including abstract and algorithmic algebra and combinatorics, formal languages and automata, mathematical software and constraint programming. Our success is founded on the close integration of theoretical and algorithmic research and the development and use of state-of-the-art software.

In 1997, CIRCA became the centre of the development of GAP after the retirement of under Prof. J. Neubüser who initiated the system in mid-1980s in Aachen. This move was supported by EPSRC, EU and Leverhulme grants. Nowadays, as one of the centres of GAP development, CIRCA has excellent contacts with developers and users worldwide. CIRCA's output includes first class results in Pure Mathematics and in Computer Science, recognised by our highly-cited publications in top international venues in both disciplines and our widely used research software. Beyond the individual international connections of the investigators and research staff, CIRCA as a centre has national importance and international standing. CIRCA has been selected to host major conferences such as CP 2010, BCC 2009, PP 2007, and the "Groups St Andrews" series in 2005 and 2013.

Curriculum vitae

Steve Linton is a Professor of Computer Science at St Andrews. He has worked in computational algebra since 1986 and has helped coordinate the development of GAP since its move from Aachen in 1997. He personally wrote key features of GAP, such as workspaces and exception handling, and has overseen the development and releases of the whole system. He directed CIRCA from 2000–2013. He is an editor of AAECC⁴. He has been PI of four major EPSRC grants and coordinated the EU project SCIEnce. He is the general chair of ISSAC 2015, the main conference in computer algebra.

Alexander Konovalov is a Senior Research Fellow in CIRCA and has worked on GAP for more than 10 years. After holding the fellowship at the Vrije Universiteit Brussel in 2006, researching computational group ring theory, he moved to St Andrews in 2007 to join EU project SCIEnce. He leads many aspects of the GAP project, including release preparation, regression testing and liaison with package authors. He has authored 38 papers and 8 GAP packages, and co-organised a number of events, most recently the LMS/EPSRC Short Instructional Course in Computational Group Theory, the HPC-GAP workshop (2013), and the Summer School on Experimental Methodology in Computational Science Research (2014). He is an editor of Journal of Software for Algebra and Geometry and a Fellow of the Software Sustainability Institute.

Publications, products, achievements

1. S. Linton, K. Hammond, A. Konovalov, C. Brown, P.W. Trinder, H.-W. Loidl, P. Horn and D. Roozemond, Easy Composition of Symbolic Computation Software using SCSCP: A New Lingua Franca for Symbolic Computation. J. Symbolic Computation, 49 (2013), 95–119.

Previous projects or activities

- 1. Multidisciplinary Critical Mass in Computational Algebra and Applications EP/C523229 2005–2010.
- 2. SCIEnce: Symbolic Computation Infrastructure for Europe (FP6 eRII3-CT-026133) 2006–2011.
- 3. **HPCGAP: High Performance Computational Algebra and Discrete Mathematics** EP/G055181 2009–2014, four sites.

Significant infrastructure

CIRCA provides hosting for the GAP website and ftp-servers, runs the automated system to check, fetch and test updates of GAP packages, uses the Jenkins continuous integration system to run regression tests for the development version and release candidates on its computer infrastructure, and manages GAP releases preparation.

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⁴Applicable Algebra and Error Correcting Codes

Université Paris Saclay

♦TO DO: INRIA or INRA below? – sorry to jump in, Paul**♦**

University Paris-Sud is among the 40 top universities worldwide in the 2013 Shanghai ranking, and is one of the two best French research universities. With about 27000 students, 1800 permanent teaching staff and 1300 permanent research scientists from national research organisations (CNRS, Inserm, INRA), it is the largest campus in France. Since 2006, scientists from the University were awarded two Fields medals, one Nobel Prize and a number of other international (European Inventor Award 2013, Wolf Prize 2010, Holweck Prize 2009, Japan prize 2007) and national prizes. The Université Paris-Sud has a complete array of competences, ranging from the purest of exact sciences to clinical practices in medicine, covering life and health sciences, legal sciences and economics. Research at the Université Paris-Sud, an essential part of academic understanding, is complemented by research activities with a high valorisation potential. Research contracts and partnership with companies make the Université Paris-Sud a key actor and a major player in French research. The University is located close to the Plateau de Saclay, the largest cluster of public and private R&D institutions in France (with ca. 16000 research staff), and is one of the core members of the University Paris Saclay – a world class university and a world-renowned research and innovation hub.

In the context of this project, the Université Paris Saclay is the home of one of the largest group of Sage developers worldwide. It's a member of the Open Source Thematic Group of the Systematic Paris Region Systems and ICT Cluster. The University also hosts a major research group working on proof assistants (Coq), which naturally opens the door for reaching toward this neighbor community.

Curriculum vitae of the investigators

Florent Hivert Professor at the Laboratoire de Recherche en Informatique, Florent Hivert is a senior researcher in Algebraic Combinatorics with 29 papers in international journals and 15 communications in international conferences. With 100 tickets (co)authored and as many refereed, Hivert is himself a core Sage developer, with contributions including key components of the Sage infrastructure (documentation, automated test, combinatorics infrastructure, paralellism, ...), specialized research libraries.

Viviane Pons Maître de Conférences at the Laboratoire de Recherche en Informatique, Viviane Pons is a young researcher in Algebraic Combinatorics. She defended her thesis in 2013 and has 3 papers in international journals and 3 communications in international conferences. Before committing herself to research, she spent two years working in industry as a Java and web developer.

She discovered Sage during her first sage-days in 2010 and has since been an active user and contributor with 10 (co)authored tickets improving the support of combinatorial objects into Sage. She is very involved in the promotion of Sage, participating in Sage-Days and proposing Sage introduction tutorials or Sage presentations in various conferences. She is also one of the main developers of the project FindStat dedicated to databases in combinatorics.

Nicolas M. Thiéry Professor at the Laboratoire de Recherche en Informatique, Nicolas M. Thiéry is a senior researcher in Algebraic Combinatorics with 15 papers published in international journals. Among other things, he is a member of the permanent committee of FPSAC, the main international conference of the domain, and has collaborators in Canada, India, and in the US where he spent three years (Colorado School of Mines, UC Davis); he also coorganized fourteen international workshops, in particular Sage Days, and the semester long program on "Automorphic Forms, Combinatorial Representation Theory and Multiple Dirichlet Series" hosted in Providence (RI, USA) by the Institute for Computational and Experimental Research in Mathematics.

Algebraic combinatorics is a field at the frontier between mathematics and computer science, with heavy needs for computer exploration. Pioneer in community-developed open source software for research in this field, Thiéry founded in 2000 the Sage-Combinat software project; with 50 researchers in Europe and abroad, this project has grown under his leadership to be one of the largest organized community of Sage developers, gaining a leading position in its field, and making a major impact on one hundred publications⁵. Along the way, he coauthored part of the proposal for NSF Sage-Combinat grant OCI-1147247.

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 $^{^5} http://sage math.org/library-publications-combinat.html, \\ http://sage math.org/library-publications-mup ad.html$

With 150 tickets (co)authored and as many refereed, Thiéry is himself a core Sage developer, with contributions including key components of the Sage infrastructure (e.g. categories), specialized research libraries (e.g. root systems), thematic tutorials, and two chapters of the book "Calcul Mathématique avec Sage".

Publications, achievements

♦TO DO: *Il faut être plus formel dans la description des projets antérieurs : Acronyme, titre, agence de financement, durée. Pareil pour les publi - auteurs, titre exact, année etc.***♦**

- 1. Lead of the Sage-Combinat software project.
- 2. Coauthoring of the open source book "Calcul Mathématique avec Sage", the first of its kind comprehensive introduction to computational mathematics in Sage for education.
- 3. XXX tickets contributed to Sage.

Previous projects or activities

- 1. Home of six one week-long Sage Days workshops.
- 2. Co-Organizer of **♦TO DO**: XXX**♦** Sage Days.
- 3. Founder and regular organizer of a bimonthly Sage User Group meeting in the greater Paris area.
- 4. Expertise exchanges with Logilab
- 5. **♦TO DO**: *XXX***♦**

Significant infrastructure

The Université Paris Sud hosts the lead developers of the open source cloud infrastructure Stratuslab and its reference infrastructure (*TO DO: XXX cores*). The participants are regular users of this infrastructure, and in close contact with the developers.

◆TO DO: Comments by Olivier Chapuis◆ Paris Sud also hosts the WILDER platform, an experimental wall-sized high-resolution interactive touch-screen for conducting research on collaborative human-computer interaction and the visualization of large datasets.

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4.1.1 University of Kaiserslautern

Principal investigator Prof. Dr. Wolfram Decker Wolfram Decker is a professor of mathematics at TU Kaiserslautern. He formerly was a research fellow at Berkeley with a NATO grant, a visiting researcher at Kyoto with a JSPS grant, and a professor at Saarbrücken, Germany. Decker has more than thirty publications including two books on computational algebraic geometry and papers in Compositio, Crelle, and Mathematische Annalen. He has held several grants in four different priority programmes of the German Research Council DFG and is now coordinator of the priority programme SPP 1489 "Algorithmic and Experimental Methods in Algebra, Geometry, and Number Theory". He was also coordinator of the European algebraic geometry network EuroProj (1996–1999) and Chair of the programme management committee of the European algebraic geometry network EAGER (2000–2004). He held seven grants for EU Highlevel Scientific Conferences and (co-)organized about 50 conferences, summer schools, workshops, and coding sprints. He was Chair of the Minisymposium on Computer Algebra during the third ECM. Decker has supervised 13 PhD students. He has been a frequent lecturer at the African Institute of Mathematics (AIMS) at Cape Town, and he has run 8 schools on computational algebraic geometry in different countries.

Decker's research interests lie in areas of algebraic geometry and computer algebra. In addition to writing theoretical papers, he is a leader in mathematical software development and has written thousands of lines of code himself. He has made contributions to the systems Macaulay2 and, much more substantially, Singular. Since 2009 he is the head of the Singular development team. Current tasks of the team include crosslinking Singular to other systems, most notably to GAP, and parallelizing Singular. These tasks are fundamental to the **MathVRE** project.

Dr. William Hart William Hart is a postdoctoral researcher at the University of Kaiserslautern. He is the lead developer of the Flint and MPIR projects as well as the main author and maintainer of the BSDNT bignum library, the Nemo and ANTIC libraries and a contributor to various other software packages.

Before coming to Kaiserslautern, held a prestigious five year Career Acceleration Fellowship "Algorithms in Algebraic Number Theory" at Warwick University in the UK. He has been involved in a number of high performance computing records, including computation of congruent numbers (subject to the BSD conjecture) up to a trillion (10¹²).

William is the main author of the FFT code for multiplication of large integers and polynomials in both MPIR and Flint, which are used extensively by the Sage, Singular and Macaulay 2 computer algebra systems.

The main focus of William's research has been in algorithms for fast arithmetic, fast integer and polynomial factorisation and to algebraic number theory, including computation of modular equations and class invariants.

Publications, products, achievements

- 1. Singular computer Algebra system.
- 2. Wolfram Decker is coordinator of the DFG Priority Project SPP1489 *Algorithmic and Experimental Methods in Algebra, Geometry, and Number Theory*'.
- 3. FLINT AND MPIR C libraries for number theory and bignum arithmetic.
- 4. William Hart held an EPSRC Career Acceleration Fellowship EP/G004870/1 from 2008-2013, *Algorithms in Algebraic Number Theory*

Previous projects or activities

1. Member of the DFG Priority Project Algorithmic Number Theory and Algebra.

Significant infrastructure Excellent computing infrastructure (high end servers), access to different types of compute clusters through the IT-Center of the TU Kaiserslautern.

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University of Oxford

♦DP/UM [WRITE HERE: Description of the university of Oxford] ♦

Curriculum vitae

Ursula Martin Professor Ursula Martin has recently joined the University of Oxford, where she holds a Professor-ship, in conjunction with a Senior EPSRC Fellowship, on a joint arrangement between the Department of Computer Science and the Mathematical Institute. Her current research concerns social and computational techniques for creating mathematics, building on a significant track record at the interface of mathematics and computing. Prior to this she worked at Queen Mary University of London, where as Vice Principal for Science and Engineering she led strategic change, and was active in knowledge transfer activities and developing young staff.

Her work is characterized by strongly interdisciplinary collaboration in new problem domains at the interface of mathematics and computer science, identifying novel interactions between theory and practice, with real-world problems inspiring scientific advance. Major achievements include results linking randomness and symmetry, new unifying explanations of the power of computational logic, and new practical techniques for using computational logic and algebra in industry.

The work to be undertaken in the Work Package 5 (Social Aspects) fits very well into her current project, which concerns crowdsourced mathematics: the overarching goal is to understand and extend the human and computer creation of mathematics. It is mostly funded by her 2014 EPSRC Advanced Fellowship (EPSRC awards only one or two of these annually in Computer Science) is a partnership of industry, government and international academia.
•UM [WRITE HERE: CV Ursula Martin]•

First name Last name to be added. ◆DP [WRITE HERE: CV Edith Elkind]◆

Dmitrii Pasechnik is a Senior Research Fellow at the Department of Computer Science of the University of Oxford, where he also holds a Lectureship at Pembroke College. Before moving to Oxford in 2013, he taught mathematics for 8 years in Nanyang Technological University (Singapore). While there, he was successful in receiving individual grant funding totalling over 500K, graduated 2 PhD students, supervised post-doctoral researchers, and co-organized a 2-months research program at Singapore Institute for Mathematical Sciences on a range of topics in computational mathematics, involving over 100 participants.

He works on a wide area of interconnected topics, related to computational algebra and optimization, combinatorics, algorithm, symbolic computing, and game theory, and authored over 70 papers on these topics, several of them using Sage and/or its components, such as GAP.

He is an active Sage developer, and regularly contributes, himself or together with his undergraduate or graduate students, new or improved Sage interfaces to various mathematical packages and databases. He has good understanding of the overall Sage development process, as well as of development of other open-source sofware and databases, including their social/community aspects. ◆DP [WRITE HERE: CV Dima Pasechnik]◆

Publications, products, achievements

1. ♠DP/UM [WRITE HERE: Publications Oxford]♠

Previous projects or activities

1. ◆DP/UM [WRITE HERE: Projects and activities in Oxford] ◆

Significant infrastructure

♦DP/UM [WRITE HERE: Significant infrastructure in Oxford] ♦

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Université de Bordeaux

- INRIA, LaBRI, IMB
- journal de théorie des nombres
- Plafrim and a mesocentre Avakas
- Several softwares developped in Bordeaux: pari/GP, tulip, etc

Curriculum vitae

Vincent Delecroix CNRS researcher at the Laboratoire Bordelais de recherche en informatique, Vincent Delecroix is a junior researcher in Number theory, Combinatorics and Dynamical systems.

X publications. He has several international collaboration (England, Mexico, United-States).

- Bobo - cours Sage Bordeaux

Delecroix is a major developer of Sage in various components: - integers - combinatorics - dynamical systems

Karim Belabas Karim is One of the main pari developer.

Bill Allombert CNRS Ingénieur de Recherche. One of the main pari developer.

Publications, products, achievements

Some recent Publications:

- 1. Belabas, Karim; Friedman, Eduardo; Computing the residue of the Dedekind zeta function. Math. Comp. 84 (2015), no. 291, 357–369.
- 2. The PARI Group; PARI/GP version 2.7.0, Bordeaux, 2014, http://pari.math.u-bordeaux.fr/.
- 3. Belabas, Karim et al. Explicit methods in number theory. Rational points and Diophantine equations, 179 pages, Panoramas et Synthèses 36, 179p., 2012.
- 4. Allombert, Bill; Bilu, Yuri and Pizarro-Madariaga, Amalia;) CM-Points on Straight Lines, to appear in "Analytic Number Theory" (dedicated do H. Maier), Springer.

Previous projects or activities

Current grants:

- 1. ANR PEACE (2012-2015) Goal: The discrete logarithm problem on algebraic curves is one of the rare contact points between deep theoretical questions in arithmetic geometry and every day applications. On the one side it involves a better understanding, from an effective point of view, of moduli space of curves, of abelian varieties, the maps that link these spaces and the objects they classify. On the other side, new and efficient algorithms to compute the discrete logarithm problem would have dramatic consequences on the security and efficiency of already deployed cryptographic devices.
- 2. ERC starting grant ANTICS (2011-2016) Goal: "Rebuild algorithmic number theory on the firm grounds of theoretical computer science". Challenges: complexity (how fast can an algorithm be?), reliability (how correct should an algorithm be?), parallelisation.

Significant infrastructure

♦VD [WRITE HERE: this still needs to be done]♦

Two center for computations: Plafrim and Avakas.

Université de Grenoble

♦JGD/CP [WRITE HERE: Description of UJF]**♦**

Curriculum vitae

Jean-Guillaume Dumas Professor at the Laboratoire Jean Kuntzmann, Jean-Guillaume Dumas is a senior researcher in Computer Algebra with 40 papers published in international journals or refereed international conferences. Among other things, he is vice-president of ACM Special interest group on symbolic and algebraic manipulations (SIGSAM), department chair within his Laboratoire (6 research teams, 130 members) and has collaborators in USA, Canada, Ireland, Germany and Luxembourg; he has also co-organized fifteen international conferences.

Computer Algebra is a field at the frontier between mathematics and computer science, with heavy needs for computer exploration. Jean-Guillaume Dumas is the main developer of the LinBox and Givaro C++ libraries (libgivaro1, libgivaro-dev, libgivaro-doc, liblinbox0, liblinbox-dev in Debian) used, e.g., by Sage respectively as its exact linear algebra and its finite fields.

Along the way, he coauthored part of the proposal for NSF-INRIA grant QOLAPS on Quantfier elimination, Optimization, Linear Algebra and Polynomial Systems and he is the director of the French ANR program on High-Performance Algebraic Computations.

Clément Pernet Associate Professor at the joint Inria-LIG research group MOAIS, Clément Pernet is a junior researcher in Computer Algebra, parallel computing and coding theory with 16 papers published in international journals or refereed international conferences. He is associate editor of the ACM transactions on Mathematical Software and has co-organized 10 conferences, including 2 sage-days and the 2012 edition of ISSAC, the leading conference in computer algebra.

Since he was a post-doc at University of Washington, under the supervision of William Stein, head of the Sage project, he has had many contributions to Sage on the exact linear algebra and the symbolic computation tools. He co-authored the book "Calcul Mathématique avec Sage" with the chapter on Linear algebra. Clément Pernet is the founder and lead developper of the fflas-ffpack library, kernel for dense linear algebra over a finite field, delivering high performance computation to LinBox and Sage. He is a core contributor to the LinBox library and contributed to the m4ri library.

Pierrick Brunet Junior Research and Development Engineer at INRIA Grenoble, Pierrick Brunet is working on compilation of C/C++ OpenMP program to C/C++ programs with calls to specific OpenMP runtimes.

With about 25% of commits in the Pythran project, Pierrick is one of the core devs of this project which compile a subset of the Python language to native Python modules.

Publications, products, achievements

Software projects

fflas-ffpack: An open-source C++ library offering dense linear algebra kernels over a finite field. In the same spirit as the numerical BLAS (Basic Linear Algebra Subroutines), and LAPACK libraries, it delivers high performance for the most commonly used routines of scientific computing: matrix multiplication, solving linear systems, computing echelon forms, determinants, characteristic polynomials, etc. This library has set the standard approach for high performance exact dense linear algebra. It is currently used in Sage, and has inspired the design of similar routines in most commercial computer algebra softwares: maple, magma, etc.

LinBox: An open-source C++ middleware library for exact linear algebra. It uses fflas-ffpack for its dense finite field linear algebra part and extends its functionalities to other computation domains (integers, rationals, polynomial rings) and type matrices (sparse and structures matrices, black-box matrices). **LinBox** is integrated in Sage.

Pythran: An open-source Python-to-C++ optimizing compiler offering an high performance runtime for Scientific Python kernels. Dynamicity of the Python language is not compliant with static compilation. That's why only a subset of the Python language is supported by Pythran. Thanks to these restrictions, Pythran generate code up to 3000 faster than original module.

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Selected Publications

- 1. Coauthoring of the open source book "Calcul Mathématique avec Sage", the first of its kind comprehensive introduction to computational mathematics in Sage for education.
- 2. Parallel computation of echelon forms (with J-G. Dumas, T. Gautier and Z. Sultan). *In Proc. Euro-Par'14* (2014), LNCS 499–510. DOI: 10.1007/978-3-319-09873-9_42.
- 3. Pythran: Enabling static optimization of scientific python programs (Serge Guelton, Pierrick Brunet, Alan Raynaud, Adrien Merlini, and Mehdi Amini.) *Proceedings of the Python for Scientific Computing Conference (SciPy)* June 2013.
- 4. Fast Computation of Hermite Normal forms of random integer matrices (with W. Stein). *J. of Number Theory* **130.7** (2010), 1675–16833. DOI: 10.1016/j.jnt.2010.01.017
- 5. Dense Linear Algebra over Word-size Prime Fields (with J.-G. Dumas and P. Giorgi). *Trans. on Math. Software* **35.3** (2008), 1–42. DOI: 10.1145/1391989.1391992.
- 6. Faster Computation of the Characteristic Polynomial (with A. Storjohann). *In Proc. ISSAC'07* (2007), 307–314. DOI: 10.1145/1277548.

Previous projects or activities

- 1. Direction of the ANR program on High-Performance Algebraic Computations 2012-2015.
- 2. Participation to the NSF-Inria associate teams QOLAPS (with NCSU, USA)
- 3. Coordination of a CNRS PEPS grant (parallel computer algebra)
- 4. Organization of the ISSAC'12 conference, the main international conference in computer algebra, and of PASCO'15 a satelitte conference on parallel computer algebra.

Significant infrastructure

♦JGD/CP [WRITE HERE: Significant infrastructure in Grenoble (or remove section)]♦

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Logilab

Logilab (http://www.logilab.fr/) is a french SME focused on using the web and free software to help scientists. It has been in business since 2000 and counts over 20 engineers and PhDs proficient in software engineering, knowledge representation, design and management of IT infrastructure, etc.

Logilab invests 15% of its turnover in research and development and has been part of several R&D projects at the national and european levels, always to provide technical expertise and support to the other partners.

In the context of this project, Logilab will innovate to support the partners with tools and infrastructure, including open databases to flexibly store mathematical objects, user interfaces to visualize complex mathematical properties, fluid workflow tools to ease large-scale collaboration, etc.

Logilab's PIC number is 948455525.

Curriculum vitae

Publications, products, achievements

- 1. ♦XXX [**WRITE HERE**: ...]♦
- 2. CubicWeb (mention of prize at DataConnexion#3)
- 3. publi Brainomics

Previous projects or activities

- 1. **♦**XXX [**WRITE HERE**: ...]**♦**
- 2. ASWAD (eu)
- 3. KIDDANET (eu)
- 4. PYPY (eu)
- 5. OpenHPC (fr/FUI)
- 6. BRAINOMICS (fr/ANR)
- 7. Mention Debian development experience

Significant infrastructure

♦XXX [WRITE HERE: ...]♦

University of Warwick

The Mathematics Institute at the University of Warwick was ranked 23rd worldwide in the 2013 QS world university subject rankings. Five members of the Department are Fellows of the Royal Society, and one, Regius Professor Martin Hairer, was awarded a Fields Medal in 2014. Mathematics and Statistics at Warwick currently hold £35.8M in research grants from EPSRC (the next highest in the UK being Cambridge at £22.8M and Oxford at £24.2M). Nine members of the department currently hold ERC grants.

Curriculum vitae

John E. Cremona Professor of Mathematics. DPhil (Oxford, 1981) under Birch. Previous posts: Michigan, Dartmouth (US), Exeter, and Nottingham (as chair and Head of Pure Mathematics). Cremona has around 50 publications, including a book and papers in Compositio and Crelle. He has held grants from EPSRC and other UK sources worth £2.5M as well as €2.5m from the EU for Marie-Curie Research Training Networks in 2000-2004 and 2006-2010. He was a Scientist in Charge of one of twelve teams in both of these networks, and leader of the research project "Effective Cohomology Computations" in the second. He has been on the Scientific Committee of 30 international conferences (including several Sage Days), and given many invited lecture series. He co-organised semester-long research programmes at IHP Paris (2004) and MSRI (2011). He has been an editor for five journals. He has supervised 16 PhD students, a dozen Masters students, two EU-funded postdoctoral fellows and currently has three EPSRC-funded postdoctoral research assistants. Cremona has given over 30 invited conference addresses and seminars in 9 countries in the last 10 years.

Cremona's research includes areas of particular relevance to the current project. His methods for systematically enumerating elliptic curves, which are the subject of a book and numerous papers, have been used to compile a definitive database of elliptic curves which is very widely cited, and now forms part of the LMFDB. Cremona's experience in managing such computations and the management, publication and electronic dissemination of the resulting large datasets set a standard which large-scale number-theoretical database projects such as the LMFDB now seek to match. Cremona's experience and reputation in this field have been important for the successful management of the LMFDB project.

Cremona has been the leading computational number theorist in the UK since his PhD thesis in 1981, following in the tradition of Birch and Swinnerton-Dyer. He has written thousands of lines of code in his C++ library eclib (one of the standard packages included in Sage since its inception) which includes his widely-use program mwrank for computing ranks of elliptic curves. As well as writing thousands of lines of new python code for Sage, he has also contributed to the active number-theoretical packages Pari/GP and Magma.

Publications, products, achievements

- 1. The Number Theory research group at Warwick was started only in 2006, but has rapidly risen to international status and one of the largest and most vibrant groups in Europe, comprising 25 members (professors, lecturers, postdoctoral researchers and early stage researchers). Of the group's members, two (Loeffler and Dokchitser) hold Royal Society Research Fellowships and one (Bartel) a Royal Commission 1851 Fellowship. Loeffler won a Leverhulme Foundation Prize jointly with Zerbes.
- 2. Several members of the Number Theory group at Warwick are Sage developers, including John Cremona, who has contributed thousands of lines of code to Sage since 2006 both through his eclib C++ library and through original Python code which forms part of the Sage library; David Loeffler, who has contributed substantially to the modular forms module in Sage; and postdoc Marc Masdeu, who has worked on the Sage-Flint interface.

Previous projects or activities

1. In 2013 Professors John Cremona and Samir Siksek, together with co-investigators at Bristol, were awarded a six-year major grant of £2.2M from the UK Engineering and Physical Sciences Research Council (EPSRC) to support the L-functions and Modular Forms Database (LMFDB) project. This grant funds three postdoctoral researchers at Warwick, computer equipment to host its database and website, and regular LMFDB workshops.

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2. Each year Warwick hosts a year-long Warwick EPSRC Symposium focussing on one area of mathematical research. The 2012-13 Number Theory Symposium included six research workshops and a summer school "Number Theory for Cryptography" and raised the international profile of the number theory group substantially.

Significant infrastructure

Computing infrastructure available to the group is excellent, with seven dedicated machines (over 300 cores) as well as access through Warwick's Centre for Scientific Computing which hosts a 6000-core linux cluster and a 3500-core cluster of workstations.

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Jacobs University Bremen

Jacobs University is a private Anglo-Saxon style research university. It opened in 2001 and has an international student body (1320 students from 115 nations as of 2011). The KWARC (KnoWledge Adaptation and Reasoning for Content [?]) Group headed by *Prof. Dr. Michael Kohlhase* specializes in knowledge management for STEM. Formal logic, natural language semantics, and semantic web technology provide the foundations for the research of the group.

Curriculum vitae

Michael Kohlhase Dr. Michael Kohlhase is full professor for Computer Science at Jacobs University Bremen and an associate adjunct professor at Carnegie Mellon University.

He studied pure mathematics at the Universities of Tübingen and Bonn (1983 - 1989) and continued with computer science, in particular higher-order unification and automated theorem proving (Ph.D. 1994, Saarland University).

His current research interests include knowledge representation for mathematics, inference-based techniques for natural language processing, and computer-supported education. He has pursued these interests during extended visits to Carnegie Mellon University, SRI International, and the Universities of Amsterdam, Edinburgh, and Auckland.

Michael Kohlhase is recipient of the dissertation award of the Association of German Artificial Intelligence Institutes (AKI; 1995) and of a Heisenberg stipend of the German Research Council (DFG 2000-2003). He was a member of the Special Research Action 378 (Resource-Adaptive Cognitive Processes), leading projects on both automated theorem proving and computational linguistics. Michael Kohlhase was trustee of the Conference on Automated Deduction (CADE), Mathematical Knowledge Management (MKM), and the CALCULEMUS conference, he is a member of the W3C Math working group, president of the OpenMath Society, and the general secretary of the Conference on Intelligence Computer Mathematics (CICM).

Florian Rabe ***** to be written *****

Relevant previous experience: The KWARC group is the lead implementor of the OMDoc (Open Mathematical Document) format for representing mathematical knowledge [?] and redeveloped its formal core in the OMDoc/MMT format [?]. The latter has been implemented in the MMT system [?,?] which provides efficient implementations of the computational primitives such as type checking, flattening, and presentation at a logic/foundation-independent level. The group has developed services powered by such semantically rich representations, different paths to obtaining them, as well as platforms that integrate both aspects. *Services* include the adaptive context-sensitive presentation framework provided by the MMT API and the semantic search engine MathWebSearch[?, ?].

Semantic services can be integrated into the documents generated from OMDoc/MMT representations, making them into "active documents", i.e. documents that are interactive and adaptive to the user and situation. For *obtaining* rich content, the group investigates assisted manual editing [?] as well as automatic annotation using linguistic techniques [?]. Finally, KWARC has developed the MathHub.info portal a community-based library and knoweldge management system for flexiformal libraries, which can be used for semantic publishing and eLearning [?, ?, ?].

The OMDoc/MMT knowledge representation format and the MathHub.info system will an important basis for the developments Work Packages 4 and 6.

Michael Kohlhase has initiated and led the CALCULEMUS! IHP-Research and Training Network and participated in the FP6 IST MoWGLI (Mathematics on the Web: Get it by Logic and Interfaces) project, the FP6 CSA Once-CS (Open Network of Centres of Excellence in Complex Systems), The FP7 EDC project WebALT (Web Advanced Learning Technologies).

Specific expertise:

- Modeling formal structures of mathematical knowledge in a web-scalable way
- Transforming large collections of legacy scientific publications to semantically structured markup
- Designing user interfaces for authoring and interacting with mathematical knowledge

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University of Zürich

The University of Zurich consistently ranks among the top 15 research institutions in Europe. It is the largest university in Switzerland, with over 26000 students, and offers the most comprehensive academic program of the country. It has close to 600 professors and over 5000 academic staff.

Switzerland ranks high in innovation, competitiveness and research spending, and much of this is enthusiasm for research is concentrated around Zurich. UZH also benefits from synergies with the ETH Zurich.

The Mathematics Institute has 17 professors and around 60 PhD students, part of a graduate school run jointly with ETH Zurich. Also joint is a Computational Science program uniting 47 researchers, mostly in the sciences, who make use of computational methods.

Curriculum vitae

Paul-Olivier Dehaye Paul-Olivier Dehaye is a Swiss National Science Foundation Assistant Professor at the University of Zurich. After his Phd at Stanford (2006), he has also worked in Oxford, at the Institut des Hautes Etudes Scientifiques and at ETH Zurich. He currently has 13 papers published in international peer-reviewed journals. He is currently supervising three PhD students and one post-doc.

His main research is at the intersection of Number Theory and Combinatorics, and in particular in Random Matrix Theory conjectures. He has additional interests in FLOSS, semantic tools, massive online education and crowdsourcing, all with the view of enabling larger scale mathematical and scientific collaborations. He is also member of the program committee of CICM 2015 (Conference on Intelligent Computer Mathematics).

He is a contributor to the Sage, LMFDB and OpenEdX projects, and has organised two conferences relating to these projects. The first was held in 2013 in Edinburgh, and organised jointly with Nicolas Thiery. Its official title was *Online databases: from L-functions to combinatorics*, and it served as a precursor to some aspects of this grant, by bringing the Sage-Combinat and LMFDB communities together. The second was held in June 2014 in Zurich and organised jointly with Stanford. It aimed at building a community around the open source python-based MOOC platform OpenEdX, and opened a series of conferences now held twice annually.

Dehaye has also taught for two years now a python course using OpenEdX, which aims to bring first year students to the level of potential contributor to Sage. This course also has a project-based component. It is now run locally for a small audience, but could be scaled up in various ways.

Publications, products, achievements

- 1. Dehaye is editor for the LMFDB, and has contributed to the project since its inception (2007). His students are also contributors.
- 2. For several of his papers, Dehaye used extensive computer-assisted experimentation (using mostly the combinatorial components of Sage) to inform the formulation of the eventual theorems, including for instance:
 - Combinatorics of lower order terms in the moments conjecture for the Riemann zeta function, arXiv:1201.4478
 - Integrality of hook ratios, arXiv:1111.5959, in Proceedings of the Formal Power Series and Algebraic Combinatorics 2012 (Nagoya) conference.
 - *A multiset hook length formula and some applications*, with Guoniu Han, in *Discrete Mathematics*, (311) 23–24, pp. 2690–2702, 2011.
 - A note on moments of derivatives of characteristic polynomials, in DMTCS Proc. Formal Power Series and Algebraic Combinatorics 2010, vol. 12.
 - Joint moments of derivatives of characteristic polynomials, in Algebra and Number Theory Journal 2 (2008), no. 1, pp. 31–68.
- 3. Dehaye has been extensively involved in teaching Python and Sage at UZH, through an online platform called OpenEdX. This has led him to organise the first community-driven conference around this (open-source) software, and to develop (together with students) additional tools, such as edx-presenter.

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Previous projects or activities

Swiss National Foundation PP00P2/138906: Combinatorics of partitions and number theoretic aspects This grant covers research at the intersection of number theory and combinatorics. Some of its aims are to uncover combinatorial structures that lurk in complicated formulaes for moments of *L*-functions (such as the Riemann zeta function). As such, it is simultaneously a heavy user of numerical methods from analytic number theory and of combinatorial techniques implemented in Sage.

Significant infrastructure

- 1. The Faculty of Sciences of the UZH benefits from very strong specialized IT support in the form of the S3IT group. They operate for instance a research cloud and a local supercomputer, and provide further assistance for the design of hardware and software systems to further research. They have a pool of software engineers that can be hired on projects such as this one for shorter periods.
- 2. UZH has a stake in Piz Daint, currently the sixth largest (and most energy-efficient) supercomputer in the world. This supercomputer is now currently expanded.

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Simula Research Laboratory

Dedicated to tackling scientific challenges with long-term impact and of genuine importance to real life, Simula Research Laboratory (Simula) offers an environment that emphasizes and promotes basic research. At the same time, we are deeply involved in research education and application-driven innovation and commercialisation.

Simula was established as a non-profit, limited company in 2001, and is fully owned by the Norwegian Ministry of Education and Research. Its research is funded through competitive grants from national funding agencies and the EC, research contracts with industry, and a basic allowance from the state. Simula?s operations are conducted in a seamless integration with the two subsidiaries Simula School of Research and Innovation and Simula Innovation.

At its outset, the laboratory was given the mandate of becoming an internationally leading research institution within select fields in information and communications technology. These fields are (i) communication systems, including cyber-security; (ii) scientific computing, aiming at fast and reliable solutions of mathematical models in biomedicine, geoscience, and renewable energy; and (iii) software engineering, focusing on testing and verification of mission-critical software systems, and on planning and cost estimation of large software development projects. Recent evaluations state that Simula has met its challenge and is an acknowledged contributor to top-level research in its focus areas. Specifically, in the 2012 national evaluation of ICT research organized by the Research Council of Norway and conducted by an international expert panel, Simula received the highest average score (4.67) on a 1-5 scale among all evaluated institutions. In comparison, the national average was 3.38. Only five of the 62 research groups evaluated were awarded the top grade (5), and two of these five groups are located at Simula.

Simula is currently hosting one Norwegian Centre of Excellence, Center for Biomedical Computing (2007-2017), and one Norwegian Centre for Research-based Innovation, Certus (2011-2018). In addition, we participate as research partner in another Centre for Research-based Innovation, Centre for Cardiological Innovation (2011-2018), hosted by Oslo University Hospital. These two center-oriented schemes are the most prestigious funding instruments offered by the Research Council of Norway.

Curriculum vitae

Hans Petter Langtangen is director of Center for Biomedical Computing at Simula Research Laboratory, a Norwegian Center of Excellence doing inter-disciplinary research in the intersection of mathematics, physics, computer science, geoscience and medicine. Langtangen is on 80% leave from a position as professor at the Department of Informatics, University of Oslo.

Langtangen received his PhD from the Department of Mathematics, University of Oslo, in 1989, and then worked at SINTEF before being hired as assistant professor at the University of Oslo in 1991. After being promoted to full professor of mechanics at the Department of Mathematics in 1998, he moved in 1999 to a professorship in computer science. In the period 1999-2002 he also held an adjunct professor position at the Department of Scientific Computing at Uppsala University in Sweden. The Simula Research Laboratory was formed in 2001, and Langtangen has since then worked with research and management at this laboratory. The scientific computing activity at Simula has been awarded the highest grade, Excellent, by five panels of top-ranked international scientists in the period 2001-2012.

Langtangen's research is inter-disciplinary and involves continuum mechanical modeling, applied mathematics, stochastic uncertainty quantification, and scientific computing, with applications to biomedicine and geoscience in particular. He has also been occupied with developing and distributing scientific software to make the research results more widely accessible and help accelerate research elsewhere. For over three decades he has been very active with teaching and supervision.

The scientific production consists of 4 authored books, 3 edited books, about 60 papers in international journals, about 60 peer-reviewed book chapters and conference papers, and over 130 scientific presentations. The publications cover fluid flow, elasticity, wave propagation, heat transfer, finite element methods, uncertainty quantification, and implementation techniques for scientific software. Langtangen is on the editorial board of 7 journals and serves as Editor-in-Chief of the leading SIAM Journal on Scientific Computing. He is also a member of the Norwegian Academy of Science and Letters.

Publications, products, achievements

1. A. Logg, K.-A. Mardal, G. N. Wells et al. Automated Solution of Differential Equations by the Finite Element Method, Springer (2012). [doi:10.1007/978-3-642-23099-8]

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- 2. P. E. Farrell, D. A. Ham, S. W. Funke, and M. E. Rognes. Automated Derivation of the Adjoint of High-Level Transient Finite Element Programs. SIAM J. Sci. Comput. 35-4 (2013), pp. C369-C393
- 3. H.P. Langtangen. A Primer on Scientific Programming with Python. Texts in Computational Science and Engineering, Springer (2014), 792 pp..

Previous projects or activities

- 1. The Centre for Biomedical Computing, a Norwegian Centre of Excellence, awarded by the Research Council of Norway. Duration: 2007-2017. Budget: 75 MNOK (10 MEUR).
- 2. The FEniCS Project (www.fenicsproject.org) Duration: 2007–on-going.

Significant infrastructure

The fully owned Simula subsidiary Simula Innovation handles pre-commercial innovation projects, creation and follow-up of company spin-offs, and general support for entrepreneurs.

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University of Southampton

The University of Southampton (UoS) is one of the leading universities in the United Kingdom, was founded in 1952 and is a member of prestigious Russell Group of UK Universities. UoS has more than 19,000 undergraduate students and 4,000 postgraduates and is an excellent venue for conducting cutting-edge research and for providing high quality education. The university is truly international, drawing students from over 130 different countries and benefiting from a wide and varied culture. It is ranked in the top 1% of universities worldwide (QS world university rankings 2014-15) and in the top 15 of research led universities in the UK, and is participating in a high number of collaborative research projects and related initiatives. UoS has a successful track record of industrial collaborations and is at the centre of a cluster of local high technology companies. It has an enviable track record in the generation of patentable work, with a portfolio of over 350 patents. To ensure the impact of its research projects, University of Southampton's Research & Innovation Services (R&IS) is responsible for professional protection of IP and supporting commercial development with industry. R&IS has had considerable success, licensing annual revenue in excess of 1€million and launching twelve successful spin-out companies since 2000. UoS has a strong track record of working in European projects, especially within the Framework Programme. The EC 6th FP7 Monitoring Report ranked UoS 17th out of all higher and secondary education organisations for number of FP7 participations during 2007-2012. Throughout the FP7 UoS has received 132M € in research grants and has been involved in 319 projects, including 63 ICT and 8 INFRASTRUCTURES Collaborative Projects. In 2013/14 alone UoS has received over €181.5M in research grants and contracts, including over €16.3M from the European Commission.

The Faculty of Engineering and the Environment (FEE) is one of the lead engineering faculties in Europe, educating a range of professionals and generating research of the highest quality. In the 2008 Research Assessment Exercise(RAE), FEE was ranked second in the UK in terms of research power for both civil engineering and mechanical/aero/production engineering. FEE brings together a wide range of disciplines, offering undergraduate and postgraduate programmes in audiology and environmental science as well as acoustical, civil and environmental, mechanical, and aeronautical/astronautical engineering and ship science. It consists of 370 research postgraduate students and 340 academic and research staff. FEE also hosts the University Technology Centres and Research Framework Agreements with key partners including: Airbus, Rolls-Royce, Lloyd's Register, Microsoft and Network Rail. FEE has a strong background in working on international research projects, including 84 EU FP7 projects worth over €28M. In 2013/14 only FEE has received about €50M in research grants and contracts, of which over €1.7M from EU funding programmes.

Curriculum vitae

Principal Investigator Prof Hans Fangohr Hans Fangohr is Professor of Computational Modelling at the University of Southampton. He heads the University's interdisciplinary Computational Modelling Group (http://cmg.soton.ac.uk), and has more than 100 publications on applied computer simulation in magnetism as well as development of computational methods. He has attracted over 12 €m as investigator and co-investigator for teaching, research and research infrastructure grants.

In 2013, he attracted 5€m from the UK's Engineering and Physical Sciences Research Council (EPSRC) to fund the only Centre for Doctoral Training in Next Generation Computational Modelling (ngcm.soton.ac.uk) in the UK. This flagship activity will train about 75 PhD students (10 to 15 starting every year, beginning in September 2014) in the state-of-the-art and best-practice in computational modelling, the programming of existing and emerging parallel hardware and to apply these skills and tools to PhD research projects across a range of topics from Science and Engineering. The centre has chosen IPython as a key tool to deliver this teaching, document and communicate computational exploration and drive reproducible computation to push for excellent computational science.

Hans Fangohr has led the development of the Open Source Nmag software (http://nmag.soton.ac.uk), which prodives a finite-element micromagnetic simulation suite to a community of material scientists, engineers and physicists who research magnetic nanostructures in academia and industry. He has designed the package in 2005 so that it has an IPython-compatible Python interface, to make the workflow of using the simulation package as accessible as possible to scientists without substantial computational background. He has extensive experience in micromagnetic simulation use and development.

Publications, products, achievements

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1. **♦**XXX [**WRITE HERE**: ...]**♦**

Previous projects or activities

1. **♦**XXX [**WRITE HERE**: ...]**♦**

Significant infrastructure

♦XXX [WRITE HERE: ...]♦

Université de Versailles - Saint-Quentin-en-Yvelines

PRISM Laboratory. The research teams of the PRiSM laboratory (Parallélisme, Réseaux, Systèmes et Modélisation) are involved in two main scientific themes of UVSQ: Mathematics and Computer science on one hand, "Design, Modelization and Implementation of Systems" on the other hand. These two directions are not separated from each other, as shown by many collaborations with other labs, and the participation of many PRiSM teams to both directions. Within the "Mathematics and Computer Science" theme, the PRiSM teams study cryptology and security, models for algorithms and operational research. All the teams also participate to the "Design, Modelization and Implementation of Systems" theme, with a particular focus on communication systems (networks and telecommunication), embedded systems, mobile systems, high speed networks, and database systems.

PRiSM is home to the "Cryptology and Information Security". In its research activities, the cryptography team aims at widely covering the various themes of academic research in cryptology, public key and secret key cryptography, cryptanalysis, security of implementations, number theory, multivariate cryptography, hash functions, etc. The cryptology team brings its specificity in the computer science courses at UVSQ and, since several years, the university offers several teaching programs with a part devoted to cryptology and information security. In particular, the research graduate program "Applied Algebra" offers a full course in cryptology. It has been complemented by a professional graduate program, called SeCReTS (Security of Contents, Networks, Telecommunications and Systems). Many activities of the team, require the use of advanced computer algebra. For this, the team has a long history of using computer algebra systems (GAP, Pari, Maple, Magma, ...). In recent years, with the arrival of young researchers, and with the affirmation of Sage in research and teaching, the team has moved from a pure user perspective to a contributor one, taking active part in the development of computer algebra software.

Curriculum vitae of the investigators

Luca De Feo got his PhD in 2010 at Ecole Polytechnique. He was appointed Maître de Conférences at Versailles-St-Quentin-en-Yvelines University in 2011. His research interests cover Algorithmic Number Theory, Computer Algebra, Cryptology and Automated deduction, and he has already published 8 papers in international journals or refereed international conferences.

He is an active Sage contributor, with a dozen of tickets co-authored and about as much reviewed. He is also active in promoting the use of Sage for research and for teaching: most of his papers feature a publicly available Sage implementation, he teaches Sage to undergraduate and graduate students, he participates and organizes various events for the introduction of Sage to beginners and young researchers.

Publications, achievements

Recent publications:

- 1. L. De Feo, J. Doliskani, É. Schost; Fast arithmetic for the algebraic closure of finite fields. ISSAC '14. ACM, 2014. pp 122-129.
- 2. L. De Feo, É. Schost; Transalpyne: a language for automatic transposition. ACM SIGSAM Bulletin, 2010, 44 (1/2), pp. 59-71.

Software:

1. FAAST, a C++ library for Fast Arithmetic in Artin-Schreier Towers. http://github.com/defeo/FAAST.

Previous projects or activities

Current grants:

- 1. ANR CLE (2013-2017): Cryptography from Learning with Errors.
- 2. DIGITEO project ARGC (2013-2016): "Fast arithmetic for geometry and cryptology". The project explores fast algorithms and implementations for algebraic geometry and curve-based cryptography.

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attice reduction.			

3. DIGITEO project IdealCodes (2014-2016): IdealCodes (http://idealcodes.github.io/) spans the three

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◆MK [WRITE HERE: Description of University of Silesia] ◆ ◆MK [WRITE HERE: PIC for University of Silesia] ◆ ◆WS [WRITE HERE: Description of University of Washington, CV] ◆ ◆TO DO: Reorder partners accordingly to the list on the front page? ◆ [?]

4.2 Third Parties Involved in the Project (including use of third party resources)

♦EC Commentary: Please complete, for each participant, the table (see page 27 of "VRETemplate.PDF"), or simply state "No third parties involved", if applicable.◆

No third parties involved.

♦TO DO: Or Seattle?**♦**

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5 Ethics and Security

♦EC Commentary: *This section is not covered by the page limit.* **♦**

5.1 Ethics

- **EC Commentary**: If you have entered any ethics issues in the ethical issue table in the administrative proposal forms, you must:
- *submit an ethics self-assessment, which:*
- describes how the proposal meets the national legal and ethical requirements of the country or countries where the tasks raising ethical issues are to be carried out;
- explains in detail how you intend to address the issues in the ethical issues table, in particular as regards: research objectives (e.g. study of vulnerable populations, dual use, etc.), research methodology (e.g. clinical trials, involvement of children and related consent procedures, protection of any data collected, etc.), the potential impact of the research (e.g. dual use issues, environmental damage, stigmatisation of particular social groups, political or financial retaliation, benefit-sharing, malevolent use, etc.)
- provide the documents that you need under national law(if you already have them), e.g.:
- an ethics committee opinion;
- the document notifying activities raising ethical issues or authorising such activities

If these documents are not in English, you must also submit an English summary of them (containing, if available, the conclusions of the committee or authority concerned).

If you plan to request these documents specifically for the project you are proposing, your request must contain an explicit reference to the project title.

5.2 Security

Please indicate if your proposal will involve:

- activities or results raising security issues: NO
- 'EU-classified information' as background or results: NO

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References

- [1] http://math.nist.gov/oommf/.
- [2] http://math.nist.gov/oommf/oommf_cites.html.
- [3] http://www.ctcms.nist.gov/ rdm/spec3.html.
- [4] Nmag guided tour. http://nmag.soton.ac.uk/nmag/0.2/manual/html/guided_tour.html.
- [5] Nmag micromagnetic simulation suite. http://nmag.soton.ac.uk.
- [6] Notebook based interactive gui for common simulation requirements, 2014. https://www.youtube.com/watch?v=RhMHgQbP__A.

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