1 Résumé du projet (maximum 1 page)

1.1 Résumé en Français (maximum 1500 caractères)

Les instabilités Magnéto-Hydro-Dynamique, appelées Edge Localized Mode (ELM), sont régulièrement observées dans les scenarios standard des plasmas sur un tokamak. Les pertes d'énergie induites par ces ELMs dans les plasmas du réacteur ITER sont un réel problème. De plus, la compréhension actuelle des quantités d'énergie perdues a cause des ELMs est extrêmement limitée. Dans la littérature, aucune simulation numérique ne permet la prise en compte de ces instabilités ELM, depuis son apparition, en passant par son évolution non-linéaire, jusqu'à sa disparition. Récemment, des résultats encourageants sur la simulation d'un cycle d'instabilité ELM ont été obtenus à l'aide du code JOREK développé au CEA mais avec une résolution toroïdale réduite. Le code JOREK dispose d'un schéma d'évolution en temps complètement implicite et utilise le solveur PaStiX pour la résolution du système linéaire creux associé.
Dans ce projet, nous proposons de développer et d'implémenter des méthodes pour améliorer le code MHD afin de permettre la simulation des instabilités ELM pour des résolutions élevées. La simulation de ces instabilités correspond à un besoin urgent de compréhension de ces phénomènes pour permettre d'évaluer un mécanisme de contrôle de ces fuites d'énergie.
Ces améliorations passent par la prise en compte de techniques de type raffinement de maillages, par la mise en œuvre de schémas numériques MHD robustes et par l'utilisation d'éléments finis cubiques d'Hermite raffinables. Ces développements doivent être compatibles avec l'utilisation d'un schéma d'évolution en temps implicite et avec l'adaptation du solveur PaStiX. De part les très grandes différences d'échelle de temps, il est en effet nécessaire d'utiliser un schéma implicite dans les simulations MHD.
Ces nouvelles méthodes seront implémentées et évaluées dans le code FluidBox, développé dans l'équipe INRIA ScAlApplix et dans le code JOREK afin d'optimiser les échanges d'expertises sur les schémas numériques et les simulations MHD.

1.2 Résumé en Anglais (maximum 1500 caractères)

The magneto-hydro-dynamic instability called ELM for Edge Localized Mode is commonly observed in the standard tokamak operating scenario. The energy losses the ELM will induce in ITER plasmas are a real concern. However, the current understanding of what sets the size of these ELM induced energy losses is extremely limited. No numerical simulations of the complete ELM instability, from its onset through its non-linear phase and its decay, exist in literature. Recently, encouraging results on the simulation of an ELM cycle have been obtained with the JOREK code developed at CEA but at reduced toroidal resolution. The JOREK code uses a fully implicit time evolution scheme in conjunction with the PaStiX sparse matrix library.
In this project it is proposed to develop and implement methods to improve the MHD simulation code to enable high-resolution MHD simulations of ELMs. The ELM simulations are urgently needed to improve our understanding of ELMs and to evaluate possible mechanism to control the energy losses.
The improvements include adaptive mesh refinement, a robust numerical MHD scheme and refinable cubic Hermite finite elements. These developments need to be consistent with the implicit time evolution scheme and the PaStiX solver. The implicit scheme is essential due to the large variety of time scales in the MHD simulations.
The new methods will be implemented and evaluated in the code FluidBox, developed by the ScAlApplix team and the JOREK code to optimize the exchange of expertise on numerical methods and MHD simulations.

2 Description courte du projet (maximum 2 pages)

2.1 *Contexte et motivation du projet*

The operational limits with respect to the maximum pressure and current in tokamak fusion plasmas are determined by large-scale instabilities of the plasma. These instabilities are well described by the magneto-hydro-dynamic (MHD) model: the instabilities are commonly called MHD instabilities. Even away from the operational limits in the standard operating scenarios, as in the case of the plasma scenarios foreseen in ITER, MHD instabilities are commonly observed. Examples include the so-called sawtooth instability, which causes a periodic relaxation of the pressure in the very center of the plasma. At medium to high plasma pressures, magnetic island-like structures can form in the bulk of the plasma leading to a local loss of the energy confinement properties of the magnetic field.
One MHD instability, the so-called Edge Localized Mode (ELM), is of particular concern for the operation of ITER. As its name implies, this instability is located at the edge of the plasma. Its driving force comes from a locally very large pressure gradient which forms due to a small region of several centimeters of improved energy confinement (the H-mode operating regime). The ELM instability limits the maximum pressure gradient at the edge by periodic (typically 1-100Hz) expulsions of plasma energy in very short bursts (~200 μs). Extrapolation to ITER of the energy lost during an ELM suggests that these energy losses, (10-30MJ on a contact surface of 3 m^2 in 300 μs) could be causing important damage to the tokamak walls in ITER. However, this extrapolation is based on experimental measurements combined with simple model assumptions. At present no theory exists on which to base such an extrapolation. The underlying MHD instabilities have been identified but at present no numerical MHD simulations exist of a full cycle of the ELM instability. A recent overview of the theory and modeling of ELMs can be found in [Huysmans]. The details of the mechanisms through which the energy is lost and what determines the amplitude of the energy losses are not known in enough detail to make predictions nor to compare with existing experiments.
The MHD simulation of a full ELM cycle is one of the important challenges to the modeling of fusion plasmas. ELM simulations are required not only to improve our understanding but also to be able to confidently predict the ELM energy losses in ITER. In addition, ELM simulations are essential to device and verify proposed methods for the control of the ELM losses by external means (such as external magnetic field perturbations [Bécoulet]). At present no non-linear MHD code exists that can simulate the complete ELM instability.

The objective of this project is the high resolution MHD simulation of a complete cycle of the ELM instability, from its onset, the highly non-linear phase and its decay. The nonlinear MHD code JOREK, under development at CEA/DRFC, will be used as the simulation code. Very recently, first simulations of the ELM have been obtained with the JOREK code (but at reduced toroidal resolution). The code uses a fully implicit time evolution scheme leading to large sparse matrices which are solved using the PastiX library developed by INRIA ScAlApplix team. The same ScAlApplix team also develops a compressible fluid solver, FluidBox that has been closely coupled with the PaStiX library. FluidBox is a 2D and 3D solver which is able to run on a wide variety of flow configurations, in particular when large gradient develops with the flow or with complex EOS. It included a fully implicit version similar to the JOREK numerical scheme. Further developments are needed to run MHD configurations.

To arrive at the ambitious goal, further developments and improvements of the MHD codes are envisaged on several fronts. In this project, it is proposed to develop adaptive mesh refinement (AMR) consistent with the fully implicit time evolution scheme used in the JOREK code. It is also proposed to construct new finite elements with high order approximations for increasing the quality of the solutions.

Since several strategies are possible (least square and non-linear stabilization), this will be done in the JOREK and FluidBox codes, exchanges of modules will occur. The developments in the JOREK and FluidBox codes will be done in conjunction with the extension of the PaStiX spare matrix library, in particular for what matters the time stepping and the AMR. The AMR is particularly suited to the ELM MHD problem where the perturbations become very localized.
Another improvement foreseen in the project is the application of refinable cubic Hermite finite elements based on Bezier patches. This will reduce the number of degrees of freedom needed to obtain a given accuracy (as compared to the linear finite elements which are use at the moment in the JOREK and FluidBox codes.) This reduction in combination with the optimized representation with the adaptive mesh refinement is particularly relevant to reduce the size of the large sparse matrices which result from the fully implicit method.
The initial ELM simulations with the JOREK code have been obtained using a reduced MHD model. For quantitative predictions of the ELM energy losses, which are the aim of this project, the full MHD model will need to be implemented. This will be done in JOREK and FluidBox.
In addition, improvements to the numerical scheme for the evolution of the full MHD equations will be investigated. Using an equal order finite element scheme for the MHD simulations will encounter similar as occurring in fluid dynamics simulations. A modification of the weak form description of the MHD equations is required, with for example additional least square or non linear stabilization terms in fluid dynamics these solutions are well known, their applicability in MHD needs to be verified.

The project is a collaboration between two teams at the CEA/DRFC (research department on fusion) and at the ScAlApplix project from INRIA Futurs (University Bordeaux 1, LaBRI and MAB). This brings together two teams with the expertise on parallel numerical solution methods (INRIA) and the expertise on MHD simulations in tokamak plasmas and their application to ELMs (CEA/DRFC).

2.2 *Retombées scientifiques et techniques attendues*

The goal of the project, high resolution MHD simulations of the complete ELM cycle, would result in the physics understanding of the non-linear evolution of the ELM. Especially the clarification of the mechanisms that determine the size of the energy losses due to the instability will be an important result. This information is vital to know which are the relevant parameters for the extrapolation of the current experimental results to ITER. It will also enable the search for plasma scenario regimes with small energy losses and mechanism to control the size of the ELMs by external means.

Given that the MHD simulation of ELMs is one of the most challenging tasks in MHD simulations in tokamaks, the resulting MHD simulation code can very well be applied to the other MHD stability problems in tokamaks like, for example, sawteeth and tearing modes. The MHD simulation code will be made available to the plasma physics community.

From the developments of the numerical scheme we expect the following results: a better understanding of how residual distribution schemes can handle MHD problem, in particular the div.B=0 constraints. This problem has already been tackled by De Sterk, but his scheme was first order accurate. Here we intend to reach second order accuracy or more. We also expect a general improvement of the schemes by dealing with more general than standard P1 elements. These results will also benefits to other problems we are interested in, such as standard compressible flow problems.

The high resolution simulation of ELMs requires the development of adaptive finite elements consistent with the implicit time evolution scheme and parallel solution of sparse matrices. These developments will be of interest to the wider community of fluid and MHD simulations. The adaptive mesh refinement techniques will be implemented as an extension to the PaStiX library.

2.3 *Retombées industrielles et économiques escomptées (le cas échéant)*

2.4 *Principaux "délivrables"*

	Libellé	Type[1]	Partenaire pilote	Partenaires participants	Date[2]
1	Hybrid direct/iterative version of sparse matrix library PaStiX including the adaptive mesh refinement extension	software (open source) publication	P. Ramet	Postdoc_1 O. Coulaud G. Huysmans	+24
2	Implicit parallelized MHD simulation code JOREK with adaptive finite elements (AMR).	software publication	G. Huysmans	Postdoc_2 R. Abgrall P. Ramet O. Czarny	+24
3	Implicit parallelized MHD simulation modules of FluidBox with high order adaptive finite elements (AMR)	software, publication	R. Abgrall	Thesard_1 B. N'Konga G. Huysmans	+36
4	Investigation of the physics of the ELM and quantitative prediction of energy losses due to the Edge localized Modes in tokamak plasmas	publication	G. Huysmans	M. Becoulet Thesard_2	+36

1 *Rapport, logiciel, publication de logiciel en open-source, proceedings, …*
2 *T0+x mois où T0 désigne la date de lancement du projet.*

3 Description scientifique et technique détaillée du projet

Cette partie peut être rédigée en langue française ou anglaise.

3.1 But du projet (2 pages maximum)

The aim of the project is the high resolution simulation of the Edge-Localized-Mode (ELM) instability in tokamak fusion plasmas. The ELM is a magneto-hydro-dynamic (MHD) instability which occurs at the boundary of the plasma. The ELMs occur only in the plasma regime with high energy confinement (the so-called H-mode) which will be the standard operating regime in ITER. This regime is characterized by an extremely large pressure gradient at the edge of the plasma in a region with a width of the order of 5% of the radius of the plasma. The large pressure gradient is accompanied by a large current density due to the so-called bootstrap current. The pressure gradient and the current density are the two driving forces for MHD instabilities. In H-mode plasmas the large edge pressure gradient and the large edge current density are the cause of the ELM. The instability is thought to develop when the edge pressure gradient or the edge current density grow too large and cross the MHD stability limit. The resulting kink-ballooning mode leads to the energy losses.

An important feature of the H-mode regime is that this regime and the ELMs occur only in plasmas where the plasma boundary is determined by a magnetic separatrix and an X-point. The magnetic geometry consists in a main plasma where the magnetic field lines wrap around the torus and lie on closed surfaces. Outside the main plasma the field lines are open and intersect the wall of the tokamak vacuum chamber. This complicated magnetic geometry has an important influence on the MHD stability properties of the plasma. It is therefore essential that the simulation take the exact magnetic geometry into account.

The non-linear MHD simulation code JOREK is under development at the CEA to study the evolution of the ELM instability. The code is using finite element in the (poloidal) cross-section of the torus. This allows the accurate representation of the magnetic geometry: the finite elements are aligned with the structure of the magnetic field. In the periodic (toroidal) direction of the torus, finite elements can be used to form a 3D finite element grid or Fourier harmonics can be used. It is at this moment not clear what the best choice is for the representation of the toroidal direction. The initial phase of the instability can be described with a small number of harmonics but in the non-linear evolution of the mode the complicated structures may possibly be better represented by finite elements.

The team ScAlApplix of INRIA develops simulation code FluidBox which may run 2D and 3D configurations for Euler and Navier Stokes fluid problems. The fluid may be perfect or have more complex equations of states. It uses state-of-the art numerical techniques ranging from now standard finite volume methods to the more recent genuinely multidimensional Residual Distribution schemes. In Residual Distribution schemes, the stabilization mechanisms bear lots of similarities with the least square stabilization. The main difference is that the choice of the stabilization parameters is parameter free; this enables to run very different situations. The mesh are fully unstructured with triangular/quads or tetrahedrons in 3D. Extension to hexahedrons should be no problem. It is fully parallel and has already been coupled with the PaStiX library. A wide variety of flow simulations can be run ranging to very low Mach numbers flows (where the times scales of the different waves are very different) to hypersonic problems.

The MHD equations exhibit a wide variation of time scales ranging from the fast waves, Alfven waves and slow waves to relatively slow growing MHD instabilities. Typical time scales are from 10^{-7}s to 10^{-9}s for the fast waves, 10^{-6}s for Alfven waves, 10^{-4}s for slow waves and from 10^{-5}s to 10^{-3}s for the MHD instabilities. In contrast the evolution of the equilibrium pressure gradient is determined by the energy confinement time which is of the order of 1s in today largest tokamaks. The duration of the ELM

instability, after its onset, is about 200-300 μs.
To simulate the complete cycle of the ELM instability, a large range of time scales need to be resolved. The evolution of the equilibrium pressure gradient needs to be resolved to study the onset of the instability and the energy losses induced by the ELM instability. The growth time of the ELM is typically several tens of microseconds. In addition to these time scales of interest, there are the even faster timescales which are present in the system but are not interesting for the ELM simulations. However the numerical scheme for the time evolution needs to take the presence of these time scales into account.
For this reason, a fully implicit time evolution scheme is used in the JOREK code. At each time step the non-linear system of equations is linearized and the Crank-Nicholson scheme is used for the time advance. This time stepping strategy is also used in FluidBox. This leads to a large sparse matrix system to be solved at every time step. The fully implicit scheme allows for very large time steps in the absence of an MHD instability to follow the equilibrium pressure gradient evolution and to adapt the time scale to the instability time scale when the instability develops. The faster time scales are not resolved but do not pose a problem using the fully implicit time evolution scheme.
This scheme has only become feasible due to the recent advances made in the parallelized direct (i.e. non-iterative) solution of general sparse matrices. Both in the JOREK and FluidBox codes, the library PaStiX is used to solve the sparse system of equations.

Recently, initial simulations of the non-linear evolution of the ELM using the JOREK code has shown that the fully implicit time evolution scheme is sufficiently robust to allow the simulation of the ELM all the way until it has decayed away. However these initial simulations are at a reduced resolution in the toroidal direction with very few Fourier harmonics and using a reduced MHD model where the fast waves are removed from the model.

To progress these early simulations towards the high resolution simulations which are needed for the understanding of the ELM and quantitative predictions of the energy losses due to the ELMs, advances are required on several fronts.

The fully implicit method leads to very large sparse matrices. To achieve the high resolution simulations the number of degrees of freedom will need to be optimized. Due to the localized nature of the 'Edge Localized Mode' at the boundary of the plasma the use of adaptive mesh refinement (AMR) is ideally suited to minimize the number of elements required for a given accuracy. The high resolution is only required where large gradients develop which is on a surface which is deforming in time. At a later stage during the ELM evolution, blobs of plasma are disconnected from the main plasma for which an adaptive mesh refinement also appears to be an optimal solution.

To reduce the large memory requirements of the sparse matrix solve, the PaStiX library is being extended to include an iterative solver which uses an incomplete decomposition of the original matrix as a preconditioner. The resulting solver is a hybrid solution method which can greatly reduce the memory requirements compared to the direct solver. This recent addition to the PaStiX library still needs further development and its suitability for the application to MHD simulations needs to be more firmly established. It should be noted that iterative solvers are difficult to apply to the system of equations that result from the MHD simulation due to the extremely large condition number of the matrices. Initial tests of the PaStiX solver in the JOREK code show that the hybrid solver can solve the MHD matrices in the relevant regime of very high magnetic and fluid Reynolds numbers.

An additional optimization of the degrees of freedom needed to represent the solution is the use of higher order finite elements. At the CEA/DRFC, a new formulation of isoparametric cubic Hermite finite elements has been developed (by O. Czarny and G. Huysmans) based on so-called Bezier patches. The result is a finite element representation in which both the variable and its derivative are continuously known through space. The advantage of the Bezier patches is that, in contrast to the traditional Hermite finite elements, they can be easily refined. This is of course a prerequisite for the development adaptive mesh refinement using finite elements. The isoparametric elements, meaning the space coordinates are represented with the same finite elements, are ideally suited to accurately represent the shaped interior of the tokamak vessel and the magnetic geometry of the field lines. The Bezier patches approach has been tested in a code that solves the magnetic equilibrium equations and in a 2D MHD simulation code where it has been shown that a significant gain in both the number of degrees of freedom and also computing time can be achieved using the Bezier patches as compared to standard linear finite elements. The Bezier finite elements now need to be incorporated into the JOREK 3D MHD simulation code.

The ScAlApplix team is also working on higher order elements. Some preliminary results with second and third order Lagrange elements have been obtained with the Residual Distribution framework. The order of accuracy is third and fourth in practice, and there is no problem in simulating problems with discontinuities and very large gradients. Problems with parabolic terms (such as physical dissipation) have also been considered. The coupling between the convective and dissipative terms has been studied with lots of attention because this is a key element for the accuracy. Several solutions have been found where the expected order of accuracy is reached for parabolic problems. More recently, a preliminary version of FluidBox with P2 Lagrange elements, for fluid problems, have been written and tested. Further developments are needed to make the scheme efficient: algorithm choices, type of elements (for example what about Lagrange versus Hermite), etc.

In the early simulations of the ELM instability with the JOREK code, a reduced MHD model has been used (this removes the 'fast waves' from the system and simplifies the numerical problems). For the quantitative prediction the full MHD model needs to be implemented. This introduces challenges to the current numerical scheme, notably the weak form of the finite element method similar to the problem encountered in fluid dynamics when using equal-order finite elements for all variables. In addition, early tests of adaptive mesh refinement in the JOREK code has shown the importance of possible noise introduced by the AMR. Thus, further investigations of the numerical scheme used for the evolution of the full MHD equations are necessary. Solutions successfully applied in fluid dynamics, like stabilized finite element methods and non linear stabilizations, will be tested for their application to MHD equations.

The developments on the JOREK and FluidBox codes, and the PaStiX library, will enable the high-resolution MHD simulations of the complete cycle of the ELM instability from its onset, the non-linear evolution and its decay. The simulations of the ELMs will be essential to improve our understanding of the energy losses caused by the ELM and where this energy is deposited. The aim of the simulations is to be able to make quantitative predictions of the energy losses in ITER type plasmas.

3.2 *Contexte et état de l'art (2 page maximum)*

MHD simulation codes

One of the major difficulties in the numerical simulations of MHD instabilities in tokamak plasmas is the wide variety of time-scales present in the system. The shortest time scales set by the fast and Alfven waves (< 1 μs) in the plasma do not need to be resolved for the study of MHD instabilities but the numerical time stepping schemes must take care of these time scales. Typical values of the growth rates of the instability are of the order of 50μs to 1ms. The instabilities need to be simulated on (a significant fraction of) the time scale of the energy confinement time (~1s).
Additional complications in the simulations of MHD instabilities in tokamaks result from the very high magnetic Reynolds numbers ($S \sim 10^6 - 10^9$) and the large anisotropy of the directions parallel and perpendicular to the magnetic field (energy conduction: $\kappa_{//}./\kappa_{\perp} \sim 10^8 - 10^{10}$)
Well-established MHD simulation codes like XTOR [Lutjens] and NIMROD [Sovinec] use a semi-implicit time integration schemes to deal with the disparate time scales. This scheme uses a semi-implicit operator based on the linear ideal MHD operator of the initial magnetic geometry. The standard semi-implicit scheme works less well when the MHD instabilities cause a large deformation of the magnetic geometry (as may be expected in the simulation of ELMs) and in the presence of large flows.
To represent the complex magnetic and material geometry of the inside of a tokamak, necessary for the simulation of ELMs, finite elements are a common choice for the discretization of the 2 non-period directions of a torus (NIMROD, M3D). Additional complications arise from the very localized layers of current induced by the MHD instabilities. The current layers are extremely thin at the low magnetic Reynolds numbers typical in fusion plasmas. Adaptive finite elements would be well suited to represent the localized current layers induced by the MHD instabilities but at present adaptive mesh refinement is not commonly used in the simulation of MHD instabilities in fusion plasmas.

In Europe, there is only one well-established code for non-linear simulations of MHD instabilities in tokamak plasmas. The XTOR code by Lutjens and Luciani from the Ecole Polytechnique Paris [Lutjens] is a highly advanced code but is adapted towards instabilities in the centre of the tokamak. It does not take into account the region between the main plasma and the wall with its specific magnetic geometry (magnetic separatrix and x-point). This part of the geometry is essential for the simulation of ELMs.
In the USA, there are 3 MHD simulation codes for tokamaks that can in principle be applied to the problem of ELMs: NIMROD [Sovinec], BOUT [Xu] and M3D [Chen, Sugiyama]. However, the ELMs simulations published do not go beyond the early non-linear stage due to numerical problems. The total energy losses due to the ELMs require the simulation of the complete ELM event. This vital step has not yet been achieved by anyone.

Sparse matrix solvers
Solving large sparse systems of linear equations is a crucial and time-consuming step, arising in many scientific and engineering applications. Due to their robustness, direct resolutions are often used in industrial codes despite their memory consumption. In addition, the factorizations used in nowadays direct solvers are able to take advantage of the superscalar capabilities of the processors by using blockwise algorithms and BLAS primitives. Consequently, many parallel techniques for sparse matrix factorization have been studied and implemented.

There are two main approaches for numerical factorization algorithms: the *multifrontal* approach, and the *supernodal* approach. Both can be described by a computational tree whose nodes represent computations and whose edges represent transfer of data. In the case of the multifrontal method, at each node, some steps of Gaussian elimination are performed on a dense frontal matrix and the remaining Schur complement, or contribution block, is passed to the parent node for assembly. In the case of the supernodal method, the distributed memory version uses a right-looking formulation which, having computed the factorization of a column-block corresponding to a node of the tree, then immediately sends the data to update the column-blocks corresponding to ancestors in the tree.
In a parallel context, one can locally aggregate contributions to the same block before sending the contributions. This can significantly reduce the number of messages.

The PSPASES solver [jkkgg] is based on a multifrontal approach without pivoting for symmetric positive definite systems. It uses METIS for computing a fill-reducing ordering, a ``subtree to subcube''-like algorithm is applied to build a static mapping before the numerical factorization.
The MUMPS solver [adlk] uses a multifrontal approach with dynamic pivoting for stability while the SuperLU solver [Li] is based on a supernodal technique with static pivoting.

In [hrr] the authors have proposed some efficient algorithms for high performance sparse supernodal factorization without pivoting. These techniques yield a static mapping and scheduling algorithm based on a combination of 1D and 2D block distributions. Very good performances are obtained by taking into account all the constraints of the problem as well as the specifics (communication and computation) of the parallel architecture. The implementation of these algorithms is called PaStiX that manages $L.L^t$, $L.D.L^t$ factorizations and more generally L.U factorization when the symmetrized pattern $A+A^t$ is considered. The PaStiX library has been successfully used in industrial simulation codes to solve systems of several million of unknowns.

These works have been recently extended to provide a method which exploits the parallel blockwise algorithmic approach used in the framework of high performance sparse direct solvers in order to develop robust parallel incomplete factorization based on preconditioners for iterative solvers.

Adaptive Mesh Refinement (AMR)
Numerical modelling of disparate spatial and temporal scales presents a formidable challenge to computational physics. There has been a rapid development in numerical algorithms that can efficiently cope with such problems. Adaptive Mesh Refinement (AMR) is becoming a standard tool for resolving many orders of spatial scales since the early work by [Berger] et al. and then [Quirk].

There are several variants of AMR grids: cell-based mesh refinement, block-based mesh refinement, and hierarchical patches.

In the cell-based AMR technique each cell can be refined individually. This technique is the most flexible in terms of adapting the grid to the features of interest in the computational domain. On the other hand the resulting unstructured grid is not optimal for loop optimization, it is difficult to handle numerical schemes with wide stencils, and achieving good load balancing is complicated.

The hierarchical patch algorithm combines cells of the same refinement level into regular subgrids and patches. The equations are solved at all levels of the grid and the time step is usually taken to be proportional to the grid resolution. The patches interact via ghosts cells and possibly via prolongation and restriction operators (e.g. to obtain error estimates, or in multi-grid solvers). Due to the regularity of the patches, this algorithm can use almost all schemes developed for uniform grids. On the other hand, the varying size of the patches and the interaction of the overlapping coarse and fine patches can make load balancing somewhat complicated.

The block adaptive grid approach is very similar to the cell-base AMR, except that the smallest unit that can be refined is a block with a fixed number of cells.

In each case, one of the main algorithmic difficulties is the control of the chronology. In order to have optimal phase error on each level, the standard compromise is to have a CFL number that is as close as possible to unity. Hence, there is a ratio of 4 in 2D and 8 in 3D between two adjacent patches. This leads to complicated interface conditions which are at the chore of the algorithm. Moreover, in problems with solid boundary conditions, the handling of the geometry leads to rather complex techniques.

Depending on the physical problem, the time stepping strategy will be different. If in a problem coexist phenomena with very heterogeneous times scales, like in low Mach number problems, combustion problems or MHD problems, an implicit or semi-implicit strategy can be of interest.

There are several issues in developing a parallel, fully implicit algorithm, which are all related to the time stepping strategy and the coupling between the different grids.

There exists few parallel implementations of the AMR methodology, and among these parallel implementations, even fewer use an implicit time stepping. Among the few, one can mention the work of [Keyes] et al. and that of [Collela] et al. in Livermore. The first reference deals with the computation of interface by the immersed boundary method, the second one deals with combustion and MHD problems. A more recent work is that of [Toth] et al. about astrophysical flow problems, involving MHD.

Simulations of ELMs

As mentioned in the context, no complete simulations of the ELM instability exist at present. The linear MHD stability properties relevant to ELMs are well known (see for example [Huysmans]). Simulations of the initial non-linear phase of the instability have been published [Snyder] but existing codes struggle to simulate a complete cycle. Predictions of the energy losses due to ELMs based on numerical simulations are not available.

Recently, a first version of the JOREK code has shown promising results in that it allows to follow the evolution ELM from the linear phase all the way to its disappearance (at a reduced resolution in the toroidal direction). The present version of the JOREK code is using a 2D finite element/ Fourier representation combined with a fully implicit method for the time evolution. The sparse matrix library PaStiX is used to solve the resulting sparse matrix systems using the direct solver. At present, the use of the direct solver limits the resolution of the simulations.

references

[Huysmans] G.T.A. Huysmans, *ELMs: MHD instabilities at the transport barrier*, Plasma Phys. Control. Fusion **47** (2005) B165-B178.

[Bécoulet] M. Bécoulet et al., *Edge localized modes control by stochastic magnetic fields, Nucl. Fusion* **45** No 11 (November 2005) 1284-1292

[Lutjens] Lutjens H. and Luciani J. F., 2005 Phys. of Plasmas 12 080703
Lerbinger K. and Luciani J. F., 1991 J. Comp. Phys. 97 444

[Sovinec] Sovinec et al., *NIMROD: A computational laboratory for studying nonlinear fusion magnetohydrodynamics,* Physics of Plasmas, Vol. 10, no. 5 (2003) 1727 (http://www.nimrodteam.org)

[Snyder] P.B. Snyder et al., *Progress in the peeling-ballooning model of edge localized modes: Numerical studies of nonlinear dynamics* Physics of Plasmas Vol. 12 (2005) 56115

[adlk] P. R. Amestoy and I. S. Duff and J. Koster and J.-Y. L'Excellent, *A Fully Asynchronous Multifrontal Solver Using Distributed Dynamic Scheduling*, SIAM Journal on Matrix Analysis and Applications}, Vol. 23, no 1, (2001), p.15-41.

[Li] X. S. Li and J. W. Demmel, SuperLU_DIST: *A Scalable Distributed-Memory Sparse Direct Solver for Unsymmetric Linear Systems*, TOMS, Vol. 29, No. 2, 2003.

[jkkgg] Joshi, M. and Karypis, G. and Kumar, V. and Gupta, A. and Gustavson F., *PSPASES: Scalable Parallel Direct Solver Library for Sparse Symmetric Positive Definite Linear Systems*, University of Minnesota and IBM Thomas J. Watson Research Center, 1999.

[hrr] Henon, P. , Ramet, P. and Roman, J., *PaStiX: A High-Performance Parallel Direct Solver for Sparse Symmetric Definite Systems*, Parallel Computing, Vol. 28, no. 2, p. 301-321 (2002).

[Abgrall1] R. Abgrall and P.L. Roe *High-order fluctuation schemes on triangular meshes*. J. Sci. Comput. 19(1-3):3--36, 2003.

[Abgrall2] R. Abgrall and M. Mezine. *Construction of second order accurate monotone and stable residual distribution schemes for unsteady flow problems*. J. Comput. Phys., 188(1):16--55, 2003

[Abgrall3] R.Abgrall, N. Andrianov, and M. Mezine. T*owards very high-order accurate schemes for unsteady convection problems on unstructured meshes*. Int. J. Numer. Methods Fluids, 47(8-9):679--691, 2005.

[Abgrall4] R. Abgrall and F. Marpeau. *Residual distribution schemes on quadrilateral meshes*. J. Scientific Computing, 2006. in press.

[Abgrall5] R. Abgrall, B. Nkonga, and R. Saurel. *Efficient numerical approximation of compressible multi-material flow for unstructured meshes*. Comput. Fluids, 32(4):571--605, 2003

[Xu] Xu X.Q. *et al* 2002 *New J. Phys.* **4** 53

[Chen] Computer physics communication 164, pp. 468-471 (2003) (http://w3.pppl.gov/~jchen/)

[Sugiyama] L. E. Sugiyama and W. Park, *A nonlinear two-fluid model for toroidal plasmas*, Phys. Plasmas **7**, 4644 (2000).

[Berger] M.J. Berger and P. Collela, *local adaptive mesh refinement for shock hydrodynamics*, J. Comput. Phys., vol 82, 64, 1989

[Keyes] K. Germaschewski, R. Grauer, D. Keyes, B. Smith, *Using Krylov-Schwarz methods in an adaptive mesh refinement environment*. Plewa, Tomasz (ed.) et al., Adaptive mesh refinement - theory and applications. Proceedings of the Chicago workshop on adaptive mesh refinement methods, Chicago, IL, USA, September 3-5, 2003. Berlin: Springer. Lecture Notes in Computational Science and Engineering 41, 115-124 (2005).

[Quirk] J.J. Quirk, *An alternative to unstructured grids for computing gas dynamic flows around arbitrarily complex geometries*, Computer and Fluids, vol 23 (1), 1994

[Collela] R. Samtaney, S.C. Jardin O. Colella and D.F. Martin, *Adaptive mesh refinement for MHD fusion applications*. Plewa, Tomasz (ed.) et al., Adaptive mesh refinement - theory and applications. Proceedings of the Chicago workshop on adaptive mesh refinement methods, Chicago, IL, USA, September 3-5, 2003. Berlin: Springer. Lecture Notes in Computational Science and Engineering 41, 491-503 (2005).

[Toth] G. Toth, D. L de Zeeuw, T.I. Gombosi and K.G. Powel, *A parallel explicit/implicit time stepping scheme on block-adaptive grids*, J. Comput. Phys, in press, 2006.

3.3 Organisation du projet - description des sous-projets (6 à 10 pages)

Work package I : Improvement of existing solvers

Over the past few years, parallel sparse direct solvers have made significant progress. They are now able to solve efficiently real-life three-dimensional problems having in the order of several millions of equations.

Nevertheless, the need of a large amount of memory is often a bottleneck in these methods. On the other hand, the iterative methods using a generic preconditioner like an ILU(k) factorization require less memory, but they are often unsatisfactory when the simulation needs a solution with a good precision or when the systems are ill-conditioned. The incomplete factorization technique usually relies on a scalar implementation and thus does not benefit from the superscalar effects provided by the modern high performance architectures. Furthermore, these methods are difficult to parallelize efficiently.

We have provided a method which exploits the parallel blockwise algorithmic approach used in the framework of high performance sparse direct solvers in order to develop robust parallel incomplete factorization based on preconditioners for iterative solvers.

The aim of this task is to add numerical criteria to improve the efficiency of our preconditioners (which are only based on the sparse pattern of the matrix) in the context of MHD simulations.
Our preconditioners also have to be adapted to the 2D finite elements and Fourier discretization used the JOREK MHD simulation code.

Indirectly, this task has as additional role to identify and better understand the difficulties in order to prepare for the workpackage 3.

Man power:
Dr. Pierre Ramet (40%)
Dr. G. Huysmans (10%)
Postdoc_1 (100%)

Expected time required:
6 months (first year of project)

Work package II : Fluid solvers

2.1 Development of the FluidBox Simulation code

Using the know-how of the CEA team as well as the existing literature on compressible MHD ([Powell, Balsara, Rossmanith, DeSterck] to quote just a few which fits in our framework), we will first upgrade the FluidBox code so that it can run MHD flows.

The second task that is conducted in parallel is to increase the resolution of the existing FluidBox solver. We intend to explore two possibilities: Lagrange elements and Hermite elements. We already have some experience on the high order Lagrange elements, but the schemes are not yet mature.
The stabilization we use bears lots of analogy with the least square scheme, especially for the lowest order elements. The analogy for P2 and P3 elements is less clear. The stabilisation we develop is parameter free so that it is possible to use the same code, with no user input, on very different flow regimes. The solution is oscillation free even when large gradient exist in the flow: note that the flow regime the project want to study may develop very steep gradients at the border of the plasma. Accuracy is mandatory since the flow regimes are unstable.
Our experience on high order element will help on developing for the Hermite elements the proper non linear stabilisation so that the scheme will be monotonicity preserving. The experience of the CEA group has developed on Bezier patches will also be incorporated in FluidBox in order to better represent

boundaries: it is well known that a proper treatment of the boundary geometry is mandatory to get accurate results.
We will also work on the time stepping strategy in coordination with the CEA group. Our current experience is on fully implicit time stepping, this choice has to be confirmed for MHD flow regimes.

One challenge of the project is about AMR. This meshing strategy leads to non conformal meshes; we plan to study how to adapt our high order methods to this context. One promising method to match different grids is the mortar element technique developed by Bernardi et al. in Paris VI

As already said, regular interactions with the CEA group are planned to guaranty that the correct physical phenomena are considered. Exchanges of modules are planned.

References:

[Powell] Powell, Kenneth G. and Roe, Philip L. and Linde, Timur J. and Gombosi, Tamas I. and De Zeeuw, Darren L., A solution-adaptive upwind scheme for ideal magnetohydrodynamics. J. Comput. Phys., volume 154(2), 284-309, 1999.

[Balsara] Balsara, Dinshaw, Divergence-free adaptive mesh refinement for magnetohydrodynamics. J. Comput. Phys., volume 174(2), 614-648, 2001.

[Rossmanith] J.Rossmanith, A high-resolution constrained transport method with adaptive mesh refinement for magnetohydrodynamic flows. Comp. Phys. Comm., 164:128-133, 2004.

[DeSterck] H. De Sterck, `Multi-Dimensional Upwind Constrained Transport on Unstructured Grids for `Shallow Water' Magnetohydrodynamics', AIAA Computational Fluid Dynamics Paper 2001-2623

Man power:

Dr. Rémi Abgrall (20%)
Dr. Boniface N'Konga (30%)
Thesard_1 (100%)

Title: High order accurate compact and stable schemes for MHD problems
Resp: Abgrall and N'Konga

Expected time required:

3 years

2.2 Development of the JOREK MHD simulation code

This task consists of the implementation of the improved methods ready to be included in the JOREK code and the implementation of new methods and solvers to be developed in this project.

2.2a Implementation of cubic Bezier finite element in JOREK

This task involves the implementation of cubic finite element using Bezier patches in the JOREK code**.** A new cubic Hermite finite element has been developed at the association Euratom-CEA. This new method is based the use of Bezier patches which are widely used in the area of Computer aided design. The new elements are of 3^{rd} order (although they can be generalised to higher order) with a continuous representation of both the variable and its first derivatives. The Bezier elements allow a refinement of the size of the element either in two or in four smaller elements.
The efficiency of these new elements and their refinement has been tested on model problems in 2D geometry. A gain up to an order of magnitude has been demonstrated in both the required number of degrees of freedom and in the total computing time for the non-linear MHD test case in 2D. The finite element routines and the routines for the refinement of the grid need to be included in the 3D JOREK code.
In addition to the finite element routines, also the grid generation routines will need to be adapted to the new isoparametric Bezier finite elements. At the moment the grid is constructed using linear finite elements. The elements are distributed such that the elements are aligned to the magnetic field (in the poloidal plane on the so-called flux surfaces). The construction of grid will become more complicated (but also much more accurate) with the Bezier finite elements. In addition to the position of the grid

points also the direction of the variation of the flux surfaces is represented by the isoparametric elements.

Man power:

Dr. O. Czarny, postdoc at CEA/DRFC until 31-12-2006 (100%)
Dr. G. Huysmans (10%)
Postdoc_2 (100%)

Expected time required:

4 months (first year of project)

2.2b Implementation of developments of numerical scheme and AMR in JOREK

In the second part of this task, the developments of the adaptive mesh refinements and of the robust numerical scheme for MHD (which will be mostly developed in Fluidbox) will be implemented in the JOREK code. The improvements will then need to be evaluated for their application for typical tokamak MHD stability problems and specifically on the problem of the ELM simulations.

Man power:

Dr. G. Huysmans (10%)
Dr. Rémi Abgrall (5%)
Postdoc_2 (100%)

Expected time required:

2 years

Work package III : AMR method based on numerical implicit schemes

The large scale applications which we study are increasingly complex in the sense that they require some simulations at a very large scale; several tens or hundreds teraflops of computation using several terabyte of data are often needed, and they use multi-physics or multi-scales modelling giving place to fine couplings. To carry out these more and more accurate full-scale simulations without increasing the number of unknowns in a uniform way, the AMR technique consists in handling a finer grid where the solution varies abruptly and a coarser grid at other places accordingly to quite specific criteria. These new finer grids are regarded as patches to the initial grid. One can thus obtain a hierarchy of grids by repeating this procedure.

This approach is broadly used when explicit numerical schemes are considered. In the case of numerical implicit schemes (as implemented in JOREK and FluidBox), the difficulty is to take into account the additional unknowns due to the hierarchy of grids in the modified linear system that must be solved at each time step of the simulation.

The aim of this task is at first to make a state of the art of the AMR methods based on numerical implicit schemes in particular for irregular grids.

A specific study of the error estimators adapted to the problem of MHD instabilities needs to be carried out, in particular in connection with the discretization with cubic Hermite (Bezier) finite elements used in JOREK. A first step will be to use the error estimates to construct an grid adapted to the solution. In this approach no information of a previous step is used and the solution will be calculated as a new problem at each refinement, i.e. not using parts of a previous solutions. This induces a large cost, in particular for the parallel execution.

In a second step, a hierarchy of grids will be used to capture the small scales in order not to reconstruct the grid and the matrix at each iteration of the AMR. The difficulty will be to define the hierarchy of solvers coupled to the hierarchy of the finite element grids to solve the linear problem.

Finally, in the context of high performance computing, we then have to study within a parallel framework the principal difficulties encountered in these methods such as: management of the hierarchy of the grids which themselves are distributed, criteria of “refinement/unrefinement”, management of the versatility of the parallel solvers. The efficiency of such a method will therefore require the use of dynamic load balancing methods over the set of processors to compensate the variability of the grid during the simulation.

Man power:
Dr. Pierre Ramet (40%)
Dr. Olivier Coulaud (20%)
Dr Pascal Hénon (10%)
Postdoc_1 (100%)

Expected time required:
2 years

Work package IV : Application of the methods developed in the project to advance the simulation of ELMs in ITER plasmas

With all the envisaged improvements to the JOREK and FluidBox codes and the sparse matrix library PaStiX high resolution simulations of the complete ELM cycle will become feasible. At this moment many open questions remain to be answered. Examples are :

0 How can a plasma significantly cross a linear MHD stability limit such that a violent instability develops?
1 What is the non-linear saturation mechanism of the instability?
2 What is determining the size of the ELM, i.e. how to extrapolate the energy losses due to an ELM to ITER?
3 Is the MHD model sufficient to describe the ELM in sufficient detail to be able to compare with experimental observations?
4 Can one identify the different type of ELMs that have been identified experimentally also in the simulations.

The initial simulations of the ELM instability will aim to answer at least some of these fundamental questions. The questions above probably represent several years of work, their answers would greatly advance the understanding and eventual control of this instability.

The validation of the simulation results through a comparison with the increasingly detailed measurements of the ELM instability are an important aspect of the simulations. Only through a confrontation with experimental results can one gain confidence in the validity of the simulations and the predicted ELM energy losses. This will require simulations starting from experimentally obtained plasmas from for example the JET tokamak and comparison with available measurements of the magnetic, temperature and density perturbations and the energy losses.

Manpower:
Dr. G. Huysmans (70%)
Dr. M. Becoulet (35%)
Dr. P. Ramet (10%)
Thesard_2 (100%)
Title: non-linear MHD simulations of Edge Localised Modes
Resp: G. Huysmans, M. Becoulet

expected time required:
36 months

On présentera, si possible sous forme graphique, un échéancier des différentes tâches identifiées au paragraphe *précédent ainsi que des dépenses pour chacun des partenaires, en indiquant les principaux points de rendez-vous, les points bloquants ou alea qui risquent de remettre en cause l'aboutissement du projet ainsi que les revues de projet prévues.*

<table>
<tr><th colspan="3">First year</th><th>Second year</th><th colspan="2">Third year</th></tr>
<tr><td colspan="2">WP1
Postdoc_1</td><td colspan="3">WP3
Postdoc_1</td><td></td></tr>
<tr><td colspan="6">WP2.1
Thesard_1</td></tr>
<tr><td>WP2.2a
Postdoc_2</td><td colspan="3">WP2.2b
Postdoc_2</td><td colspan="2"></td></tr>
<tr><td colspan="6">WP4
Thesard_2</td></tr>
</table>

Si des doctorants sont présents dans le projet, on explicitera leur sujet de thèse et les conditions de leur encadrement

On listera les membres permanents des laboratoires impliqués dans le projet avec pour chacun d'eux la quotité de temps consacrée au projet en moyenne sur sa durée. On joindra en annexe un mini-CV de ceux-ci.

Nom Prénom	WP1 6 months	WP2.1 36 months	WP2.2 24 months	WP3 24 months	WP4 36 months
Rémi Abrall (Prof, Univ. Bdx1)		**20%**	**5%**		
Marina Bécoulet (CR, CEA/DRFC)					**35%**
Olivier Coulaud (DR INRIA)				**20%**	
Pascal Hénon (CR INRIA)				**10%**	
Guido Huysmans (CR, CEA/DRFC)	**10%**		**10%**		**70%**
Boniface N'Konga (MdC, Univ Bdx1)		**30%**			
Pierre Ramet (MdC, Univ Bdx1)	**40%**			**40%**	**10%**

Un tableau de l'ensemble des « délivrables » du projet sera inclus sous la forme indiquée ci-avant (1.4). Ce tableau reprend les principaux déjà listés ci-avant et les complète d'éventuels autres livrables.

	Libellé	Type	Partenaire pilote	Partenaires participants	Date
1	Hybrid direct/iterative version of sparse matrix library PaStiX		P. Ramet	Postdoc_1	+6
2	Adaptive mesh refinement methods consistent with the implicit time evolution scheme.		P. Ramet	Postdoc_1 G. Huysmans	+24
3	Implementation of cubic Bezier finite elements in JOREK		O. Czarny	G. Huysmans Postdoc2	+4
4	Implicit parallelised MHD simulation code JOREK with adaptive mesh refinement using finite elements		G. Huysmans	Postdoc_2	+36
5	Robust implicit numerical scheme for MHD consistent with AMR		R. Abgrall	Thesard_1 G. Huysmans	+36
6	MHD simulations of a full ELM cycle. Quantitative prediction of energy losses due to the Edge localized Modes in tokamak plasmas		G. Huysmans	Thesard_2 M. Becoulet	+36

3.4 Résultats escomptés – perspectives (1 à 2 pages)

3.4.1 Retombées scientifiques et techniques

The main objective of the project is the development of a high resolution non-linear MHD simulation code for tokamak plasmas as required for the simulation of the Edge Localized Modes in tokamaks.
The final criterion for the evaluation of the project will be the validation of the simulation results with the experimental observations. Even before this validation exercise, there will be fundamental physics questions that can be answered with the code as at has been developed in this project. The results of the physics studies will be published in the conventional literature for fusion plasma physics (such as the journals Nuclear Fusion or Plasma Physics and Controlled Fusion). The success of the physics simulations part of the project can be evaluated by the publications produced. The physics results will also be presented at the relevant plasma physics conferences and workshops, the EPS conference on Plasma Physics and the IAEA conference on Controlled Nuclear Fusion. The ELM simulations will also be presented at the regular ITER physics working group meetings (ITPA) on the physics of the plasma edge transport barrier.
The MHD simulation code JOREK will be made available to the European fusion plasma physics community (the Euratom Associations of the national fusion laboratories) and its use by a wider community will be actively encouraged. The code JOREK will be contributed to the European Integrated Tokamak Modeling taskforce (ITM) which has as its objective to provide an integrated set of codes for the complete simulation of tokamak fusion plasmas. The full tokamak simulations are essential in order to prepare for the exploitation of ITER and the design of the next generation reactor called DEMO.

The developments of the numerical methods and tools foreseen in the project include:

Adaptive mesh refinement methods, compatible with the parallel implicit time evolution scheme and the PastiX sparse matrix library.

One of the goals is to improve the quality of generic preconditioners based on the sparse solver PaStiX and to validate those algorithms on MHD simulations area. The developments on solvers to allow AMR techniques with numerical implicit scheme will be available as open-source software. The design of solvers coupled to the hierarchy of finite elements grids could be applied on applications from other areas. The main contributions developed in our project will be published in international conferences or journals.
The high performance implementation of parallel solver should allow us to realize complete MHD simulations of ELM instabilities.

Robust numerical scheme for the evolution of the MHD equations compatible with equal order cubic finite elements and the adaptive mesh refinement

As we expect to better understand how residual distribution schemes can handle the div.B=0 constraints, and since we expect to be able to handle high order accurate elements (i.e. more than second order accurate), this schemes will be used to applied to simulate complex, unstable configurations that occur in ITER.

Implementation of the cubic Bezier finite element method in the JOREK code.

The validation of the Bezier elements will be a comparison of the required number of degrees of freedom and the CPU time between linear finite elements and the new Bezier finite elements. When successful an improvement of at least one order of magnitude in the number of degrees of freedom is expected with the use of the cubic Bezier finite elements.

Implementation of the full MHD equations (including the heat and particle transport) in the JOREK code.

When the developed methods have been successfully integrated into the JOREK code, the details of the numerical methods used in the JOREK code and the validation of the code will be published in a suitable journal (such as Journal of Computational Physics).

The JOREK code can also be used to study the methods to stabilize the ELM instability through the use of small non axi-symmetric external magnetic field perturbations. This stabilization method has been successfully demonstrated in the DIII-D tokamak. Simulations are required to establish in order to understand the stabilization mechanism. Also, design studies are under way to apply this stabilization method to the JET and ITER tokamaks. MHD simulations will be important to evaluate the effectiveness of the designs.

When the numerical methods developed in this project are successful, their application can be envisaged more widely in the simulations of fluids in fusion plasmas. Fluids simulations are very often used in fusion plasmas to study the turbulent transport of energy and particles. The physics models used to study the fluid turbulence commonly neglect the effect of magnetic field perturbations, thereby excluding the MHD instabilities. Similarly, the current MHD simulations neglect the physics of plasma turbulence which would require the inclusion of additional physics in the MHD equations.

The challenge in the coming years will be to combine the physics of the turbulence and MHD in the same simulations to study their mutual interaction. Since the physics model for the combination of turbulence and MHD includes all the problems of the current MHD simulations, the method developed for the JOREK code may form a good basis for the next challenge in fluid simulations in fusion plasmas.

3.4.2 Retombées industrielles et économiques escomptées (le cas échéant)

3.5 <u>Propriété intellectuelle</u>