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Multiscale computational strategy with time and space homogenization: a radial-type approximation technique for solving micro problems

Anthony Nouy∗, Pierre Ladevèze∗

∗LMT-Cachan (ENS Cachan / CNRS / University Paris 6)
61, avenue du Président Wilson, F-94235 Cachan CEDEX, France

ABSTRACT

A new multiscale computational strategy for the analysis of structures (such as composite structures) described in detail both in space and in time was introduced recently. This strategy is iterative and involves an automatic homogenization procedure in space as well as in time. At each iteration, this procedure requires the resolution of a large number of linear evolution equations, called the "micro" problems, on the micro scale. In this paper, we present a robust approximate resolution technique for these micro problems based on the concept of radial approximation. This very general technique, which leads to the construction of a relevant reduced basis of space functions, is particularly suitable for the analysis of composite structures.

KEY WORDS

Homogenization, Multiscale, Domain decomposition, Radial approximation
1. INTRODUCTION

The behavior of heterogeneous structures, such as composite structures, often results from complex phenomena taking place on the microscale. Attempts to predict the behavior of such structures have led to the development of increasingly sophisticated models describing the material on a very fine scale compared to the scale of the structure. Therefore, the numerical simulation of these problems requires the development of efficient computational strategies taking into account these multiscale aspects. For the description of local phenomena with short lengths of variation in space as well as in time to be accurate, the calculations must be performed on a fine discretization of the structure and of the time interval being considered. This condition leads to problems with very large numbers of degrees of freedom, whose computation costs with standard calculation codes are generally prohibitive. One of the main objectives in the last few decades has consisted in developing efficient and robust computational strategies suitable for this type of problem. One of these efficient strategies uses the theory of the homogenization of periodic media [18, 3, 1, 19]. Other developments and the associated computational approaches can be found in [2, 8, 21, 7, 20, 6, 9, 5]. These strategies, however, have some limitations. Besides periodicity, these strategies rely on the fundamental assumption that the ratio between the small-scale length and the large-scale length is small. Moreover, the boundary zones require specific treatment because in these zones the material cannot be homogenized.

A new multiscale computational strategy for nonlinear evolution problems was introduced recently. This strategy involves an automatic homogenization technique in space as well as in time [15, 12, 16] which is an extension of previous works limited to space [13, 14]. This strategy, developed in a general framework, makes no a priori assumption on the form of the solution and, therefore, does not have the limitations of standard homogenization techniques. Until now, it has been developed in the framework of small disturbances of (visco)plastic structures under possible contact conditions with or without friction.

The first characteristic of this strategy consists in partitioning the structure into substructures and interfaces, each of these entities having its own variables and equations. The change of scale takes place only at the interfaces, where forces and displacements are split into “macro” and “micro” contributions. The macro quantities are some mean values of the forces and displacements over space and time. The second characteristic of this strategy is the use of the LATIN method [11], an iterative resolution technique taking into consideration the whole time interval being studied. At each iteration, one must solve a homogenized macro problem defined over the whole space-time domain, and a set of independent micro problems, which are linear evolution problems defined within each substructure, at their boundaries, and over the time interval being studied.

The resolution of a large number of micro problems at each iteration can lead to prohibitive calculation costs if classical incremental techniques are used. Moreover, when dealing with composite structures containing a large number of similar substructures, the operators and right-hand sides of the micro problems may vary only slightly from one resolution to the next, but classical techniques are unable to take advantage of this characteristic.

A possible answer to this problem is an alternative resolution technique based
on the concept of generalized radial approximation [11]. This technique, which is often used in the context of the LATIN method, consists in approximating the solution defined over the space-time domain by a sum of radial functions, each of which is the product of a scalar function of the time variable by a function of the space variable. First of all, this approach reduces the computation cost drastically by transforming an evolution problem defined over the space-time domain into a series of uncoupled problems defined either over the space domain or over the time domain. It also reduces the storage cost for the variables defined over the space-time domain. Last but not least, it enables the construction of a relevant reduced basis of space functions which turns out to be particularly suitable for composite structures containing families of many identical substructures.

Of course, the radial approximation is not defined uniquely. The classical approach is to define this approximation using an orthogonality criterion associated with a primal or dual formulation of the evolution equation [11]. This definition leads to the “best” approximation only for particular cases, and it provides no simple and systematic way to evaluate the quality of this approximation. Still, this classical approach is efficient in the single-scale framework. However, in some special situations, it may lead to non-convergence of the LATIN method. This lack of robustness is particularly notable for the multiscale computational strategy.

In this paper, we introduce a new and extremely robust approach which maintains a completely mixed vision of the evolution problem. This approach is based on a minimization problem and it now provides a simple and relevant error criterion to evaluate the quality of the radial approximation. This new approximation technique leads to significant savings in terms of computational and storage costs without affecting the efficiency and the robustness of the multiscale computational strategy.

2. THE REFERENCE PROBLEM ON THE MICRO SCALE

Sections 2 to 4 present a brief review of the main aspects of the multiscale computational strategy. Further details can be found in [14, 16].

2.1. Description of the problem

Let us consider, assuming small perturbations and a quasi-static isothermal state, the equilibrium of a structure defined in the spatial domain $\Omega$. At each time $t$ of the interval $(0, T)$ being studied, this structure is subjected to volume forces $f_{d}$ and surface forces $F_{d}$ on a part $\partial_{2}\Omega$ of the boundary. On the complementary part $\partial_{1}\Omega$, the displacement $u_{d}$ is prescribed. All the quantities with subscript “d” are known. The displacements, strains and stresses are subject to initial conditions at $t = 0$.

2.2. Constitutive relation model with internal state variables

The inelastic strain $\epsilon_{p}$ is treated independently of the other internal variables, which are denoted $X$. The conjugate variable of $X$ is $Y$; thus, the dissipation rate is:

$$\sigma : \dot{\epsilon}_{p} - Y \circ \dot{X} \overset{def}{=} \begin{bmatrix} \sigma \\ Y \end{bmatrix} \circ \begin{bmatrix} \dot{\epsilon}_{p} \\ \dot{X} \end{bmatrix}$$
where \( \odot \) designates a scalar product between dual quantities. From the free energy \( \rho \Psi(\varepsilon, X) \), under the usual decoupling assumptions, one obtains the following “normal” formulation of the state equations (see [11]):

\[
\sigma = \rho \frac{\partial \Psi}{\partial \varepsilon_e} = \mathbf{K} \varepsilon_e \quad \text{and} \quad \mathbf{Y} = \rho \frac{\partial \Psi}{\partial X} = \Lambda \mathbf{X}
\]

(2.1)

where \( \Lambda \) and the Hooke’s tensor \( \mathbf{K} \) are linear, constant, symmetric and positive definite operators characterizing the material. The advantage of such a model lies in the simplicity of the corresponding constitutive relation which, except for (2.1), can be written as a differential equation:

\[
\begin{bmatrix}
\dot{\varepsilon}_p \\
-\dot{X}
\end{bmatrix} = \mathbf{B} \begin{bmatrix}
\sigma \\
\mathbf{Y}
\end{bmatrix}
\]

(2.2)

where \( \mathbf{B} \) is a monotonous operator characterizing the material.

2.3. Decomposition of the structure into substructures and interfaces

The structure is viewed as an assembly of simple components: substructures and interfaces [11]. Each component has its own variables and equations. A substructure \( \Omega_E, E \in \mathbf{E} \), is subjected to the action of its environment (the neighboring interfaces) defined by a force distribution \( \mathbf{F}_E \) and a displacement distribution \( \mathbf{W}_E \) at its boundary \( \partial \Omega_E \). An interface \( \Gamma_{EE'} \) between two substructures \( E \) and \( E' \) transfers the distributions of both the displacement and the force: \( \mathbf{W}_E, \mathbf{W}_{E'} \) and \( \mathbf{F}_E, \mathbf{F}_{E'} \) (Figure 1).

![Figure 1: Decomposition into substructures and interfaces](image)

2.4. Approximation spaces

The displacements \( \mathbf{W} \) and the forces \( \mathbf{F} \) at the interface \( \Gamma_{EE'} \) belong to spaces \( \mathbf{W}^{(0,T)}_{h,E,E'} \) and \( \mathbf{F}^{(0,T)}_{h,E,E'} \) respectively. These spaces, extended to the set of the neighboring interfaces of \( \Omega_E \), lead to spaces \( \mathbf{W}^{(0,T)}_{h,E} \) and \( \mathbf{F}^{(0,T)}_{h,E} \). The stress \( \sigma_E \) and the displacement \( \mathbf{u}_E \) in a substructure \( \Omega_E \) belong to spaces \( \mathbf{S}^{(0,T)}_{h,E} \) and \( \mathbf{U}^{(0,T)}_{h,E} \) respectively. The strains \( \varepsilon_E, \varepsilon_{eE} \) and \( \varepsilon_{pE} \) belong to space \( \mathbf{E}^{(0,T)}_{h,E} \). The variables \( \mathbf{X}_E \) and \( \mathbf{Y}_E \) belong to spaces \( \mathbf{X}^{(0,T)}_{h,E} \) and \( \mathbf{Y}^{(0,T)}_{h,E} \) respectively. We will designate by \( s_E = (\varepsilon_{pE}, \mathbf{X}_E, \mathbf{W}_E, \sigma_E, \mathbf{Y}_E, \mathbf{F}_E) \) the set of the variables associated with substructure \( \Omega_E \) and its boundary. The corresponding space is denoted \( \mathbf{S}^{(0,T)}_{h,E} \).

In practice, the interfaces and substructures are discretized in space, classically, using finite elements. On the time scale, one uses the discontinuous Galerkin
method [4]. The time interval $(0, T)$ being considered is decomposed into $T_h = \{t_i = (t_i, t_i+1)\}_{i=0}^{N-1}$, $t_0 = 0 < t_1 < ... < t_N = T$. Let us denote $\mathcal{P}_r(I; S)$ the space of the polynomial functions of degree $r$ defined over $I$ with coefficients in $S$. Then, let us introduce the space $Z_r(T_h; S)$, $r \in \mathbb{N}^N$, defined by:

$$Z_r(T_h; S) = \{ v | v_{[i]} \in \mathcal{P}_r(I; S), \forall i \in \{0, ..., N-1\} \}$$

To simplify the notations, let $Z_r^{(0,T)} = Z_r(T_h; \mathbb{R})$. A space $S^{(0,T)}$ is said to be of type $Z_r^{(0,T)}$ if $S^{(0,T)} = Z_r(T_h; S)$. On the time scale, all spaces will be considered to be of type $Z_r^{(0,T)}$.

2.5. Reformulation of the reference problem

$E^{(0,T)}_{h,E,ad} \subset E^{(0,T)}_{h,E} \times W^{(0,T)}_{h,E}$ designates the space of the kinematically admissible variables $(\varepsilon_E, W_E)$. $E^{(0,T)}_{h,E,ad} \subset S^{(0,T)}_{h,E} \times F^{(0,T)}_{h,E}$ designates the space of the statically admissible variables $(\sigma_E, F_E)$ (i.e. the variables which verify the equilibrium equations) and $F^{(0,T)}_{h,E,0}$ designates the associated vector space.

Definition 2.1. $s_E = (\varepsilon_p, X_E, W_E, \sigma_E, Y_E, F_E) \in S^{(0,T)}_{h,E}$ is said to be $E$-admissible if it verifies:

- the static admissibility of $(\sigma_E, F_E)$,
- the kinematic admissibility of $(\varepsilon_E, W_E)$,
- the state equations (2.1),

The corresponding space is designated by $S^{(0,T)}_{h,E,ad}$. $S^{(0,T)}_{h,E,0}$ is the associated vector space.

Then, the reference problem consists in finding $s = \{s_E\}_{E \in E}$ which verifies:

- $s_E$ $E$-admissible, $\forall E \in E$,
- the constitutive relation describing the state evolution (2.2),
- the behavior at the interfaces, of which the boundary conditions on $\partial_i \Omega$ and $\partial_2 \Omega$ are particular cases,
- the initial conditions.

3. DESCRIPTION OF THE VARIABLES ON THE MACRO SCALE

3.1. Definition of macro quantities

The distinction between the micro level and the macro level is made only at the interfaces. For space, the macro scale is defined by the characteristic length of the interfaces. For time, the macro scale is associated with a coarse subdivision $T_{h'} = \{t_i' = (t_i', t_{i+1}')\}_{i=0}^{N'-1}$, $t_0' = 0 < t_1' < ... < t_{N'}' = T$, of the time interval being studied.

Let us consider the interface $\Gamma_{EE'}$ between two substructures $E$ and $E'$ and choose the spaces in which the macro displacements and forces will be sought, i.e. $W^{(0,T)}_{h,E,EE'}$ and $Z^{(0,T)}_{h,E,EE'}$. Classically, for space, one takes affine functions over $\Gamma_{EE'}$. For displacements, this corresponds to translations, rotations and expansions of the interface (4 functions in 2D). For forces, this corresponds to
the resultants, moments and expansions at the interface. Regarding time, one chooses for the grid $T_h'$ functions of the type $Z_{p}^{(0,T)}$, $p \in \mathbb{N}^n$.

The macro parts $(W^M, F^M)$ of $(W, F)$ are defined as the best approximations in the sense of the work’s bilinear form (see [16]). The micro forces and displacements are simply defined by:

$$E^{m} = E - E^{M} \quad \text{and} \quad W^{m} = W - W^{M}$$

Thus, one ends up with uncoupled macro and micro works at the interface:

$$\int_{\Gamma_{E,E'} \times [0,T]} F \cdot W \, ds \, dt = \int_{\Gamma_{E,E'} \times [0,T]} (E^{M} \cdot \dot{W}^{M} + E^{m} \cdot \dot{W}^{m}) \, ds \, dt$$  \hspace{0.5cm} (3.1)

Extended to the set of the interfaces, this decomposition leads to the spaces $W_{h}^{(0,T), M}$ and $F_{h}^{(0,T), M}$.

### 3.2. Admissibility of the macro quantities

Another important aspect of the multiscale computational strategy consists in the choice of the admissibility conditions for the macro quantities: the macro forces are required to verify the transmission conditions, including the boundary conditions. These conditions remain unchanged under unilateral contact. The corresponding space is designated by $F_{h, ad}^{(0,T), M}$.

### 4. MULTISCALE COMPUTATIONAL STRATEGY WITH TIME AND SPACE HOMOGENIZATION

#### 4.1. Principle

The partial verification *a priori* of the transmission conditions at the interfaces leads to the following reformulation of the reference problem: find $s = \{s_E\}_{E \in \mathcal{E}}$, with $s_E \in S_{h,E}^{(0,T)}$, which verifies:

$$A_d \| - \text{the E-admissibility of } s_E, \ E \in \mathcal{E}$$

$$- \text{the admissibility of } E^{M}$$

$$- \text{the initial conditions}$$

$$\Gamma \| - \text{the constitutive relation describing}$$

$$\text{the state evolution (2.2)}$$

$$- \text{the behavior at the interfaces}$$

$$- \text{the initial conditions}$$

$\Gamma$ constitutes a set of (possibly nonlinear) equations which are local in space and in time. $A_d$ is a set of global linear equations. With this decomposition, it is possible to apply the LATIN method [11], a general computational strategy for time-dependent nonlinear problems which operates globally over the entire time-space domain. Figure 2 shows the scheme for one iteration, which consists of two stages, called the local stage and the linear stage.
4.2. The local stage at iteration \( n \)

The problem consists in constructing \( \hat{s}_{n+1/2} \in \Gamma \) knowing \( s_n \in A_d \). \( \Delta \hat{s} = (\hat{s}_{n+1/2} - s_n) \) must follow a search direction \( E^+ \); more precisely, for each substructure \( \Omega_E \), \( \Delta \hat{s} \) must verify:

\[
\begin{align*}
H^+ \begin{bmatrix}
\Delta \hat{\sigma}_E \\
\Delta \hat{Y}_E 
\end{bmatrix} + \begin{bmatrix}
\Delta \hat{\varepsilon}_{pE} \\
-\Delta \hat{X}_E 
\end{bmatrix} &= 0 \quad (4.1) \\
h^+ \Delta \hat{F}_E - \Delta \hat{W}_E &= 0 \quad (4.2)
\end{align*}
\]

\( H^+ \) is a positive definite operator which is a classical parameter of the method. \( h^+ \) is another parameter of the method which can be interpreted as a “viscosity” effect at the interface. The problems in the substructures and at the interfaces are independent of one another. Moreover, these problems are local in space and in time and, therefore, they lend themselves to the highest degree of parallel computing.

4.3. The linear stage at iteration \( n \)

The problem consists in constructing \( s_{n+1} \in A_d \) knowing \( \hat{s}_{n+1/2} \in \Gamma \). \( (s_{n+1} - \hat{s}_{n+1/2}) \) must follow a search direction \( E^- \). Because of the admissibility of the macro forces, this search direction is global. Let us introduce a Lagrange multiplier \( W^M \) to guarantee the admissibility of the macro forces in a weak sense (see [16]). \( W^M \in W^{(0,T), M}_{h,0} \), the space of the macro displacements which are continuous at the interfaces and zero on \( \partial_1 \Omega \). Let us denote \( \Delta s = (s_{n+1} - s_n) \). Then, the search direction can be written as follows: for each substructure \( \Omega_E \),

\[
\begin{align*}
H^- \begin{bmatrix}
\Delta \sigma_E - \Delta \hat{\sigma}_E \\
\Delta Y_E - \Delta \hat{Y}_E 
\end{bmatrix} + \begin{bmatrix}
\Delta \hat{\varepsilon}_{pE} - \Delta \hat{\varepsilon}_{pE} \\
-\Delta \hat{X}_E - \Delta \hat{X}_E 
\end{bmatrix} &= 0 \quad (4.3) \\
h^- \left( \Delta \hat{F}_E - \hat{F}_E \right) + \left( \Delta \hat{W}_E - \hat{W}_E \right) &= W^M \quad (4.4)
\end{align*}
\]

The resolution of the linear stage can be split into two parts: the resolution of a set of micro problems defined in each substructure, and the resolution of a global macro problem defined over the entire space-time domain.
4.3.1. The micro problem defined in substructure $\Omega_E$ and its boundary $\partial \Omega_E$, and over $(0, T)$

The micro problem associated with substructure $E$ is a linear evolution equation which can be expressed as: find $\Delta s_E \in S_{h,E,0}^{(0, T)}$ which verifies:

- the $E$-admissibility to zero: $\Delta s_E \in S_{h,E,0}^{(0, T)}$
- the search directions (4.3) and (4.4).

Since Relation (4.4) is local at boundary $\partial \Omega_E$, the micro problems in each substructure are independent of one another. If $H^-$ and $h^-$ are positive definite operators, the micro problem defined in substructure $\Omega_E$ and at its boundary has a unique solution such that:

$$\Delta s_E = s_E^{(1)} + s_E^{(2)} (\tilde{W}_E^M) \quad (4.5)$$

where $s_E^{(1)}$ depends on $\Delta s_E$ and $s_E^{(2)}$ depends linearly on $\tilde{W}_E^M$. In particular, one has:

$$\Delta F_{E|0,T}^M = F_{E|0,T}^{(1)} + L_E (\tilde{W}_{E|0,T}^M) \quad (4.6)$$

$L_E$ is a linear operator which can be interpreted as a homogenized behavior operator over the space-time substructure $\Omega_E \times (0, T)$. This operator can be calculated by solving a set of micro problems over $\Omega_E \times (0, T)$ in which one takes successively for $\tilde{W}_E^M$ the macro basis functions of $W_{h,E}^{(0, T), M}$.

4.3.2. The macro problem defined over $\Omega \times (0, T)$

The macro problem consists in finding $\Delta F^M$ and $\tilde{W}^M$ which verify:

- $\Delta F^M \in F_{h,0}^{(0, T), M}$ (static admissibility to zero),
- $\tilde{W}^M \in W_{h,0}^{(0, T), M}$ (kinematic admissibility to zero),
- the homogenized behavior relation (4.6).

This problem can be formulated in terms of the macro displacements $\tilde{W}^M$. If the number of macro space-time substructures is large, an approximation technique based on the introduction of a third scale can be used [17, 16].

4.3.3. Resolution of the linear stage

To solve the linear stage, one proceeds as follows: first, one solves a series of micro problems defined over $\Omega_E \times (0, T)$, $E \in E$, in which one considers only the data $\Delta s_E$ of the previous stage. This leads to $s_E^{(1)}$. Then, one solves the macro problem to obtain $\tilde{W}_E^M$. Finally, in order to calculate $s_E^{(2)}$, one solves a second series of micro problems with the Lagrange multiplier as the only data.

Remark 4.1. If the search direction operators $H^-$ and $h^-$ are updated in substructure $E$, one must also update the homogenized operator $L_E$. The calculation of this operator requires the resolution of a set of micro problems. The approximation technique presented further on can also be applied to this calculation.
5. RESOLUTION OF THE MICRO PROBLEMS: THE CLASSICAL RADIAL APPROXIMATION TECHNIQUE

At each iteration of the computational strategy and for each substructure, one must solve two micro problems which represent evolution equations defined over $\Omega_E \times (0, T)$, $E \in \mathcal{E}$. The resolution of these micro problems with standard incremental methods can lead to prohibitive computation costs, especially if the search direction operators $H^-$ and $h^-$ are time-dependent. Moreover, in the case of composite structures containing large numbers of identical substructures, the operators and right-hand sides of the micro problems vary only slightly from one resolution to another. The classical approaches are unable to take advantage of this particularity.

The radial loading approximation, commonly used in the framework of the LATIN method [11], is a possible answer to this problem. In this section, we present the classical radial approximation technique [11] based on the dual variational formulation of the micro problem.

5.1. Dual variational formulation of the micro problem

Let us write a micro problem defined over $\Omega_E \times (0, T)$ formally as follows:

\[\begin{align*}
\text{Problem 5.1.} & \quad \text{Find } s_E \in S_{h,E,0}^{(0,T)} \text{ which verifies } \\
& \quad H^- \left[ \begin{bmatrix} \sigma_E - \bar{\sigma}_E \\ Y_E - \bar{Y}_E \end{bmatrix} - \begin{bmatrix} \dot{\varepsilon}_{pE} - \bar{\varepsilon}_{pE} \\ -\dot{\varepsilon}_{pE} - \bar{\varepsilon}_{pE} \end{bmatrix} \right] = 0 \\
& \quad h^- \left( F_E - \bar{F}_E \right) + \left( \bar{W}_E - \bar{W}_E \right) = 0
\end{align*}\]

where $s_E = \Delta \hat{s}_E$ for the first set of micro problems, and $s_E = (0, 0, \bar{W}_M^E, 0, 0, 0)$ for the second set.

To simplify the notations, let us drop the subscript $E$. Let us also introduce the following notations:

\[\Delta = H^- \begin{bmatrix} \sigma \\ Y \end{bmatrix} - \begin{bmatrix} \dot{\varepsilon}_{pE} \\ -\dot{\varepsilon}_{pE} \end{bmatrix} \quad \text{and} \quad \Delta = h^- F + \bar{W}\]

By injecting relations (5.1) and (5.2) into the weak expressions of the kinematic admissibility and of the state equations, we obtain the following dual formulation of the micro problem:

\[\begin{align*}
\text{Problem 5.2.} & \quad \text{Find } \left( \sigma, F \right) \in F_{h,E,0}^{(0,T)} \text{ and } Y \in Y_{h,E}^{(0,T)} \text{ which verify: } \forall (\sigma^*, F^*) \in F_{h,E,0}^{(0,T)} \forall Y^* \in Y_{h,E}^{(0,T)}, \\
& \quad \int_{\Omega_E \times [0,T]} \begin{bmatrix} \sigma^* \\ Y^* \end{bmatrix} \circ \left( \begin{bmatrix} K^{-1} & 0 \\ 0 & \Lambda^{-1} \end{bmatrix} \right) \begin{bmatrix} \sigma \\ Y \end{bmatrix} + H^- \begin{bmatrix} \sigma \\ Y \end{bmatrix} \right) \, dx \, dt + \int_{\partial \Omega_E \times [0,T]} h^- F \cdot F^* \, ds \, dt = \\
& \quad \int_{\partial \Omega_E \times [0,T]} \Delta \, F^* \, ds + \int_{\Omega_E \times [0,T]} \Delta \circ \begin{bmatrix} \sigma^* \\ Y^* \end{bmatrix} \, dx \, dt
\end{align*}\]

Remark 5.1. Problem 5.2 is a classical parabolic evolution equation. In fact, the following developments could be applied to any evolution problem of this type.
5.2. The concept of radial approximation

The classical radial approximation technique consists in searching an approximate solution \((\tilde{\sigma}, \tilde{F}, \tilde{Y})\) to the dual problem 5.2 as a sum of radial functions, which are products of scalar functions of time by functions of space:

\[
(\tilde{\sigma}, \tilde{F})(x, t) = m \sum_{i=1}^{m} c_i(t)(C_i, C_i^*)(x)
\]

\[
\tilde{Y}(x, t) = m' \sum_{i=1}^{m'} d_i(t)D_i(x)
\]

where \(\forall i, c_i \in Z_{r(0,T)}, (C_i, C_i^*) \in \mathbf{F}_{h,E,0}\) and \(D_i \in \mathbf{Y}_{h,E}\). The inelastic strain and other kinematic internal variables can be deduced from Relations (5.1) and (5.2).

Of course, this approximation is not unique. Therefore, the following question arises: how can one obtain the “best” radial approximation?

5.3. Seeking the “best” approximation

5.3.1. Definition of the “best” approximation

The classical choice consists in injecting into the variational formulation 5.2 the following test functions:

\[
(\sigma^*, F^*) = \sum_{i=1}^{m} c_i^*(C_i, C_i^*) + c_i(C_i^*, C_i^*)
\]

\[
Y^* = \sum_{i=1}^{m'} d_i^*D_i + d_iD_i^*
\]

Thus, the approximation is defined by an orthogonality criterion.

5.3.2. The problem to be solved and the resolution technique

To simplify the presentation, let us consider only the case with no internal variable, in which one seeks a first-order approximation (i.e. \(m=1\)). Let \(u = (\sigma, F) \in \mathbf{F}_{h,E,0}(0, T), v = (\varepsilon, W) \in \mathbf{E}_{h,E,0}(0, T)\) and

\[
< v, u >_{(0, T)} = \int_{\Omega \times [0,T]} \varepsilon : \sigma \, dx \, dt + \int_{\partial \Omega \times [0,T]} W : F \, ds \, dt
\]

The variational problem can be written formally as follows: find \(u \in \mathbf{F}_{h,E,0}(0, T)\) such that

\[
< \mathcal{L}(u), u^* >_{(0, T)} = < f, u^* >_{(0, T)} \quad \forall u^* \in \mathbf{F}_{h,E,0}(0, T)
\]

where \(\mathcal{L}\) is the linear differential operator defined by \(\mathcal{L}(u) = (K^{-1} \dot{\sigma} + H^{-1} \sigma, hF)\), \(f = (\Delta, \Delta)\) is the right-hand side. The problem consists in finding \((c, U) \in \mathbf{F}_{h,E,0}(0, T)\) that optimizes the following functional:

\[
J(c, U) = \frac{1}{2} \left( \int_{\Omega \times [0,T]} \varepsilon : \sigma \, dx \, dt + \int_{\partial \Omega \times [0,T]} W : F \, ds \, dt \right)
\]
Equation (5.3) is a "space" problem whose operators depend on time functions. Equation (5.4) is a simple differential equation in time whose parameters depend on the space functions.

The classical technique for building these radial functions is iterative. It consists in calculating successively the space functions (with fixed time functions) and the time functions (with fixed space functions).

5.4. Limitations of the classical approach

Frequently, within the framework of the multiscale computational strategy, one observes that the classical algorithm for the construction of the approximation does not converge. Actually, this construction technique is unsuitable for the definition adopted for the approximation. Indeed, the problem defined by (5.3) and (5.4) can be interpreted as a generalized eigenvalue problem. Since operator \( L \) is not self-adjoint, this problem can have complex eigenvalues. Therefore, the proposed iterative algorithm, which can be viewed as a simple power method, generally does not converge. In order to circumvent this problem, the definition of the approximation could be extended to the complex domain. A more sophisticated resolution technique for the eigenvalue problem, inspired by Krylov-type techniques, could also be used. This type of technique constitutes an effective way to build a set of radial functions and could be used when an accurate solution of the evolution problem is necessary. However, the classical approach does not solve the true problem which is to find the best approximation. Moreover, it does not offer a simple criterion to evaluate the quality of the approximation. Sometimes, because of the lack of robustness of this approach, the LATIN method fails to converge; this tendency is particularly notable in the context of the multiscale computational strategy.

6. RESOLUTION OF THE MICRO PROBLEMS: A NEW RADIAL APPROXIMATION TECHNIQUE

In order to circumvent the problems encountered with the classical radial approximation technique, one idea consists in defining the approximation \( \tilde{u} \) through the minimization of the residue:

\[
\|\| f - L(\lambda U) \|\|^2
\]

This approach, based on the symmetrization of the variational problem, leads to a proper definition of the best approximation. It is appropriate for the spatial discretization framework. However, it is not easily transposable to the continuous framework. Indeed, in the case of partial derivative equations, it is not always easy to use the adjoint operator. Moreover, this formulation of the approximation requires a higher degree of regularity of the functions. This tends to make the \textit{a posteriori} spatial discretization more expensive.

In order to apply the radial approximation, we propose to maintain a completely mixed vision of this evolution problem. Then, a natural approach consists in formulating the micro problem as the minimization of the constitutive relation error associated with the search directions. With this new approach,
the approximation relates only to the search directions, which are the parameters of the strategy. Compared to the classical method, this approach certainly increases the computational cost, but it also improves the effectiveness and the robustness of the strategy.

6.1. The mixed formulation of the micro problem

The search directions can be interpreted as linear constitutive relations. Therefore, one can introduce the concept of constitutive relation error associated with the search directions. Thus, the micro problem 5.1 can be reformulated as the minimization of this error in the space $S_{h,E,0}^{(0,T)}$ of the functions which are $E$-admissible to zero. The micro problem is expressed as follows:

**Problem 6.1.** Find $s \in S_{h,E,0}^{(0,T)}$ which minimizes the constitutive relation error $e^2_{C.R.E}(s - \bar{s})$ associated with the search directions, defined by:

$$e^2_{C.R.E}(s - \bar{s}) = \|h^{-1}(F - \bar{F}) + (\dot{W} - \bar{W})\|^2_{E,m} + \|\mathbf{H}^{-1} \begin{bmatrix} \sigma - \bar{\sigma} \\ \mathbf{Y} - \bar{\mathbf{Y}} \end{bmatrix} - \begin{bmatrix} \dot{\xi}_p - \bar{\xi}_p \\ -(\dot{\mathbf{X}} - \bar{\mathbf{X}}) \end{bmatrix} \|^2_{E,M}$$

with

$$\|\Delta\|^2_{E,M} = \int_{\Omega_{E} \times [0,T]} \Delta \circ \mathbf{M}(t) \Delta \, dx \, dt$$

$$\|\Delta\|^2_{E,m} = \int_{\partial\Omega_{E} \times [0,T]} \Delta \cdot \mathbf{m}(t) \Delta \, ds \, dt$$

where $\mathbf{M}$ and $\mathbf{m}$ are linear, symmetric, positive definite operators.

A natural definition for the constitutive relation error consists in choosing

$$\mathbf{M}(t) = (1 - \frac{t}{T})\mathbf{H}(t)^{-1}_{sym}$$

$$\mathbf{m}(t) = (1 - \frac{t}{T})\mathbf{h}(t)^{-1}_{sym}$$

6.2. Radial decomposition of the variables

Here, the idea is to define a radial approximation $\tilde{s}$ compatible with the definition of $S_{h,E,0}^{(0,T)}$, i.e.:

$$(\tilde{\sigma}, \tilde{F})(x, t) = \sum_{i=1}^{m} c_i(t)(\mathbf{C}_i, \tilde{\mathbf{C}}_i)(x)$$

$$\tilde{\mathbf{Y}}(x, t) = \sum_{i=1}^{m'} d_i(t)\mathbf{D}_i(x)$$

$$(\tilde{\xi}, \tilde{W})(x, t) = \sum_{i=1}^{m''} e_i(t)(\mathbf{E}_i, \tilde{\mathbf{E}}_i)(x)$$

where $\forall i, (c_i, d_i, e_i) \in \mathbb{Z}_{h,E,0}^{(0,T)} \times \mathcal{F}_{h,E,0} \times \mathcal{Y}_{h,E,0} \times \mathcal{E}_{h,E,0}$. 

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The inelastic strain and the kinematic internal variables are deduced from the state equations:

\[
\tilde{\varepsilon}_p = \sum_{i=1}^{m'} e_i E_i - \sum_{i=1}^{m} c_i K^{-1} C_i
\]

\[
\tilde{X} = \sum_{i=1}^{m'} d_i \Lambda^{-1} D_i
\]

This choice implies that the radial approximation \( \tilde{s} \) belongs to the space \( S^{(0,T)}_{h,E,0} \).

Since \( K \) and \( \Lambda \) are constant operators, \( \tilde{\varepsilon}_p \) and \( \tilde{X} \) also have radial decompositions. Indeed, all the variables, static as well as kinematic, have radial decompositions. Thus, the new approach yields significant savings in terms of storage cost.

6.3. Search for the best approximation

6.3.1. Definition of the best approximation

The definition of the best radial functions is simply that they minimize the constitutive relation error \( e^2_{CR,E} \). Let us recall that with this new approximation technique, the search directions alone, which are the parameters of the algorithm, are approximated. The approximate solution verifies static and kinematic admissibility as well as the state equations, which was not the case of the classical approach.

Then, the best first-order approximation (i.e. \( m = m' = m'' = 1 \)) is defined by the following problem:

**Problem 6.2.** Find an approximation \( \tilde{s} \), defined by functions \( (c, d, e) \) and \( (C, C', D, E, E') \) belonging to \( F_{h,E,0} \times Y_{h,E} \times E_{h,E,0} \) and \( (c, d, e) \in \left[ Z^{(0,T)}_f \right]^3 \), which minimizes the constitutive relation error

\[
e^2_{CR,E}(\tilde{s} - s) = \|ch\mathbf{C} + \mathbf{E} - \Delta\|_{E,m}^2 + \int_{\Omega_{E}\times[0,T]} \left\{ \left[ \begin{array}{cc} K^{-1} & 0 \\ 0 & \Lambda^{-1} \end{array} \right] \left[ \begin{array}{c} \dot{c} \mathbf{C} \\ \dot{d} \mathbf{D} \end{array} \right] + \mathbf{H} \left[ \begin{array}{c} c \mathbf{C} \\ d \mathbf{D} \end{array} \right] - \left[ \begin{array}{c} \dot{c} \mathbf{E} \\ 0 \end{array} \right] \right\} \circ \mathbf{M} \Delta \, ds \, dt
\]

6.3.2. Property of the approximation

**Proposition 6.1.** If \((c, d, e)\) and \((C, C', D, E, E')\) constitute the solution of Problem 6.2, then they have the following properties:

- the space functions are obtained in terms of \((c, d, e)\) and of the data by expressing the stationarity of \( e^2_{CR,E} \) with respect to the space functions;
- the functions \((c, d, e)\) are such that the Rayleigh quotient \( R(c, d, e) \) defined by

\[
R(c, d, e) = \int_{\Omega_{E}\times[0,T]} \{ch\mathbf{C} + \mathbf{E} + \mathbf{M} \mathbf{A}\} \cdot \mathbf{M} \Delta \, ds \, dt + \int_{\Omega_{E}\times[0,T]} \left\{ \left[ \begin{array}{cc} K^{-1} & 0 \\ 0 & \Lambda^{-1} \end{array} \right] \left[ \begin{array}{c} \dot{c} \mathbf{C} \\ \dot{d} \mathbf{D} \end{array} \right] + \mathbf{H} \left[ \begin{array}{c} c \mathbf{C} \\ d \mathbf{D} \end{array} \right] - \left[ \begin{array}{c} \dot{c} \mathbf{E} \\ 0 \end{array} \right] \right\} \circ \mathbf{M} \Delta \, dx \, dt
\]
is stationary;
• \( e_{CR,E}^2(\tilde{s} - \bar{s}) = e_{CR,E}^2(\bar{s}) - R(c, d, e) = \|\Delta\|_{E,M}^2 + \|\Delta\|_{E,m}^2 - R(c, d, e) \)

Proposition 6.1 constitutes a significant tool for the estimation of the error associated with a set of radial functions.

6.3.3. Technique of construction of the radial approximation

Table 1 presents the iterative scheme used to build the radial approximation. This scheme consists in carrying out the minimization on the time functions and on the space functions alternatively. The value of the Rayleigh quotient is an indicator of the convergence of the algorithm.

- **Initialization** \((c^{(0)}, d^{(0)}, e^{(0)})\)
- **Loop on** \(k = 0...k_{\text{max}}\)
  - With the time functions \((c^{(k)}, d^{(k)}, e^{(k)})\) fixed, one seeks \((C^{(k+1)}, C^{(k+1)}, D^{(k+1)}, (E^{(k+1)}, E^{(k+1)})\) which minimizes \(e_{CR,E}^2(\tilde{s} - \bar{s})\)
  - Normalization of the space functions
  - With the space functions \((C^{(k+1)}, C^{(k+1)}, D^{(k+1)}, (E^{(k+1)}, E^{(k+1)})\) fixed, one seeks \((c^{(k+1)}, d^{(k+1)}, e^{(k+1)})\) which minimizes \(e_{CR,E}^2(\tilde{s} - \bar{s})\)
  - Ending criterion based on the convergence of \(R(c^{(k+1)}, d^{(k+1)}, e^{(k+1)})\)

Table 1: Algorithm for searching a set of radial functions

The algorithm of Table 1 converges very rapidly. In practice, one limits the number of iterations to \(k_{\text{max}} = 2\) or 3.

The resolution of the minimization problems with respect to the time and space functions does not present any particular difficulty. However, it can result in higher computational costs than with the classical approach.

- **Minimization with respect to the space functions:**
  In practice, a standard displacement finite element approach is used. The minimization with respect to the space functions is partially dualized, which leads to seeking two finite element displacement fields simultaneously. Therefore, the size of the problem is twice that of a standard finite element calculation. In general, however, the resolution cost is not prohibitive because the sizes of the micro problems are small. Nevertheless, one can introduce an alternative resolution technique which consists in minimizing with respect to \((C^{(k+1)}, C^{(k+1)}, D^{(k+1)}, (E^{(k+1)}, E^{(k+1)})\) and \((E^{(k+1)}, E^{(k+1)})\) successively rather than over \((C^{(k+1)}, C^{(k+1)}, D^{(k+1)}, E^{(k+1)}, E^{(k+1)})\) simultaneously.

- **Minimization with respect to the time functions:**
  The minimization with respect to the time functions leads to a global problem in time. In practice, this problem is assembled. Its size may be larger than that of the spatial problem, especially if the number of time functions being calculated simultaneously and the number of time steps are large. However, this problem leads to a symmetric block-tridiagonal linear system in which a block is associated with all the unknowns on
an interval of the partition $T_h$. Such a system can be solved relatively inexpensively using a block-Cholesky technique.

6.4. Resolution of the micro problems

6.4.1. Relative error criterion

This new approximation technique comes with a natural error criterion which can be used to estimate the quality of the approximation $\tilde{s}$. This criterion is based on the constitutive relation error $e_{CR,E}^2(\tilde{s} - \bar{s})$. Let us define the following norm on $S_{h,E}$:

$$\|\|s\|\|_E^2 = \|H\left[\begin{array}{c} \sigma \\ Y \end{array}\right]\|_{E,M}^2 + \left\| \left[\begin{array}{c} \varepsilon_p \\ -X \end{array}\right]\right\|_{E,M}^2 + \|hF\|_{E,m}^2 + \|W\|_{E,m}^2$$

One can define a relative error criterion $\xi_{CR,E}$ based on the norm of the previous iterate $s_n$ as follows:

$$\xi_{CR,E}^2(\tilde{s} - \bar{s}; s_n) = \frac{e_{CR,E}^2(\tilde{s} - \bar{s})}{\|\|s_n\|\|_E^2}$$ (6.1)

6.4.2. Reutilization of the space functions: initialization step

The construction of the space functions is by far the most expensive step. Therefore, it can be interesting to store and reuse these functions. The space functions constructed at each iteration can be reused systematically during the subsequent iterations. Moreover, in the case of composite structures, the basis of the space functions is shared by a large number of identical substructures. Therefore, the initialization step of a micro problem on a particular substructure can reuse the space functions defined in other substructures during the previous iterations (or even the current iteration).

Then, the resolution of a micro problem begins with an initialization step which consists in seeking a set of time functions associated with an already existing basis of space functions. This initialization consists in minimizing the constitutive relation error over all the time functions while keeping the space functions fixed. The operators and the right-hand sides of the micro problems vary little from one iteration to the next, and even from one substructure to another. Therefore, this initialization step is often sufficient to obtain a good approximation of the solution of the micro problem. As we will see in the examples, only a few space functions are necessary to solve a problem with a large number of substructures.

The initialization step leads to an initial approximate solution $\tilde{s}$. To find out whether new sets of functions are necessary, one can use the error criterion $\xi_{CR,E}$ defined by (6.1).

Remark 6.1. The solutions of micro problems in identical substructures can be very similar in terms of forces, stresses, strains and, possibly, internal variables. The solutions in terms of displacements can also be similar, except for the rigid body modes. Therefore, it is essential to add to the basis of functions of the initialization step the space functions corresponding to the rigid body modes of the boundary $\partial \Omega_E$. In order for the criterion $\xi_{CR,E}$ to be consistent among substructures, the norm of the interface’s displacements in the denominator
must be replaced by a norm of \( \{W\} \), the part of \( W \) with zero resultant and moment over \( \partial \Omega_E \).

6.4.3. Construction of new sets of radial functions

One chooses a criterion \( \xi_{CR} \) for the verification of the search directions. If this criterion is not matched at the end of the initialization step, new sets of functions must be constructed. Usually, these functions are built one by one. When a new approximation \( \tilde{s} \) is obtained, if \( \xi_{CR,E} > \xi_{CR} \), a new set of functions is calculated using the algorithm of Table 1 with updated data. In practice, in order to reduce the calculation cost (and since a coarse approximation of the search directions is generally sufficient), one can limit the number of new sets of radial functions calculated for the resolution of a micro problem to 1 or 2.

7. EXAMPLE: COMPOSITE GANTRY

7.1. Description of the problem

Let us consider the 2D problem of a composite structure containing cracks (unilateral contact with Coulomb’s friction characterized by parameter \( f = 0.2 \)) (Figure 3). The structure is fixed on the bottom and subjected to forces \( F_1 \) and \( F_2 \) (Figure 4). The in-plane dimensions are 120 mm × 120 mm. We make the plane strain assumption. The structure consists of two types of cells denoted I and II. The materials are viscoelastic with Young’s modulus \( E_i \), Poisson’s ratio \( \nu_i \) and viscosity \( \eta_i \). Their constitutive relations are such that \( B_i = \frac{1}{\eta_i} K_i^{-1} \).

![Figure 3: Description of the problem](image-url)

Each cell is a substructure of the partitioned problem. The type-II cell is homogeneous, with a Type-I material whose characteristics are \( E_1 = 50 \) Pa, \( \nu_1 = 0.3 \) and \( \eta_1 = 10 \) s. It was meshed with 138 TRI3 elements. The type-I cells consists of a matrix of Type-1 material with inclusions of Type-2 material whose characteristics are \( E_2 = 250 \) Pa, \( \nu_2 = 0.2 \) and \( \eta_2 = 1000 \) s. It was meshed with 262 TRI3 elements. Each interface was meshed with 8 elements. The time interval being considered is \((0, 10)\). Partition \( T_h \) contains 60 intervals \((N = 60)\) while \( T_{h'} \) contains 3 intervals \((N' = 3)\). The micro spaces are of type \( Z^{0,T}_{0} \) on the micro grid \( T_h \). The macro spaces contain affine functions on the space level (4
functions per interface) and functions of type $Z_2^{(0,T)}$ on macro grid $T_h'$ on the time level.

### 7.2. Description of the resolution procedure

Since the constitutive relation is linear, the natural search directions in the substructures are $H^+ = H^- = B$. The characteristic length of the cells is $L_M = 4\, mm$. At the interfaces, we chose the same scalar search direction for all the interfaces: $h^+ = h^- = \frac{1}{2}(\frac{1}{h} + \frac{1}{h'}) \frac{L_M}{E}$. The structure contains two families of cells. The space functions built by the radial approximation technique generated two common bases which were systematically reused for the initialization step of the micro problems. These bases were orthonormalized using the following scalar product:

$$
((C^*, C^*), (C, C))_{F_{h,E,0}} = \int \Omega_E C^* : K^{-1} C \, dx
$$

$$
((E^*, E^*), (E, E))_{E_{h,E,0}} = \int \Omega_E E^* : K E \, dx
$$

**Remark 7.1.** A more consistent procedure than a simple orthonormalization could have been used for sorting the space functions.

**Remark 7.2.** It is possible to solve the linear stage incrementally over the macro intervals (see [16]). Therefore, the radial approximation consists in seeking a set of radial functions for each macro interval. In this case, the basis of the space functions is shared by all the macro intervals.

As we will see further, the criterion $\xi_{CR}$ conditions the accuracy of the approximate solution obtained by the strategy. During the first iterations, $s_n$ is only a coarse approximation of the solution (error much greater than ten percent). Greater accuracy would be unnecessary for the verification of the search directions and would lead to the construction of too many new sets of radial functions. Therefore, one can use an adaptive technique which consists in increasing the accuracy $\xi_{CR}$ as the iterations progress. Here, we took $\xi_{CR} = 0.3$ for the first 4 iterations. Then, we took $\xi_{CR} = 0.05$. If $\xi_{CR,E} > \xi_{CR}$ after the initialization step, we calculated a new set of radial functions using the algorithm of Table 1 with parameters $k_{max} = 3$ and an ending criterion of $10^{-2}$ for the convergence of the Rayleigh quotient.
7.3. Effectiveness of the new method

7.3.1. Convergence of the algorithm

To evaluate the convergence of the algorithm, we calculated the distance between the $s_n$ and $\hat{s}_{n+1/2}$. Then, we introduced the following convergence criterion:

$$err_n^2 = \frac{\sum_{E \in \mathcal{E}} \|\hat{s}_{n+1/2} - s_n\|^2_E}{\sum_{E \in \mathcal{E}} \|s_n\|^2_E}$$  \hspace{1cm} (7.1)

Figure 5 shows the convergence curves of the iterative strategy with and without radial approximation of the micro problems. The algorithm with approximation had the same convergence rate as the reference algorithm during the first iterations, and converged towards an error of $2.5\%$, equivalent to the criterion $\xi_{CR}$ chosen. If better accuracy were needed, one could, of course, modify criterion $\xi_{CR}$ accordingly.

![Figure 5: Error $err_n$ vs iteration with and without radial approximation](image)

7.3.2. Construction of the radial functions

Figure 6 shows that very few new sets of radial functions were built at each iteration. Moreover, this number decreases as the iterations progress. Figure 7 shows the evolution of the error with respect to the number of radial functions constructed.

Figure 8 shows the number of new sets of radial functions constructed per iteration and per substructure. During the first iterations, new functions were built primarily near the boundary and the edges, and around the high-gradient zones (near the cracks). After a few iterations, new sets of radial functions were constructed only near the cracks. These results account for the relevance of the new approximation technique and for the quality of the proposed error criterion.

7.3.3. Cost of the algorithm

Let us recall that at each iteration two micro problems must be solved for each substructure. The use of a classical incremental technique would have required the resolution of $468 \times 60 \times 2 = 56,160$ “space” problems per iteration. Here,
the radial approximation technique required the construction of 72 sets of radial functions to reach an error of 2.5%. Since \( k_{\text{max}} = 3 \), at most 216 space problems were solved. Thus, the number of space problems which had to be solved, although their size was indeed twice that of a classical finite element calculation on a cell, was divided by 3,000 for the same accuracy.

Assembling the space and time problems, however, can be rather expensive, since this requires the computation of many integrals over time and space. To reduce this cost, it could be interesting to perform a radial decomposition of \( \tilde{s} \) and of the operators \( \mathbf{H} \) and \( \mathbf{h} \). Indeed, if both the variables and the operators are decomposed radially, the integrals over the space-time domain can be split into products of integrals over space by integrals over time. A simplified construction technique for these radial decompositions can be found in [10].

8. CONCLUSION

A new radial approximation technique for the resolution of the micro problems of the multiscale computational strategy with time and space homogenization introduced in [15, 12, 16] has been presented. This new technique does not have the drawbacks of the classical radial approximation technique [11]. Here, the
Figure 8: Number of new sets of radial functions per iteration and per substructure

approximation is based on the minimization of the constitutive relation error associated with the search directions of the computational strategy. This new approach comes with a simple and relevant error criterion to evaluate the quality of the approximation. It also leads to the construction of a relevant reduced basis of space functions which can be systematically reused. It is particularly suited to the case of composite structures containing many similar cells. This new technique drastically reduces the calculation and storage costs of the computational strategy without affecting its robustness and effectiveness.

Another possible improvement of the computational strategy consists in approximating the macro problem by introducing a third scale [17, 16]. Together, these improvements enable the analyst to deal with structures containing very large numbers of cells.

References


