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Mathematics and Computers in Simulation 80 (2010) 1578-1588

www.elsevier.com/locate/matcom

Efficient computer implementation of coupled hydro-thermo-mechanical analysis

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Received 3 November 2008; accepted 6 November 2008 Available online 27 November 2008

Abstract

Hydro-thermo-mechanical analysis of reactor vessels based on the finite element method is a very demanding task due to its complexity as well as the large number of unknowns. This contribution deals with efficient computer implementation of the coupled analysis and attention is also devoted to domain decomposition methods which enable utilisation of parallel computers. The parallel processing leads to very good speedup and it also enables to solve significantly large problems in acceptable time. The proposed strategy is demonstrated on a coupled analysis of an existing reactor vessel. © 2008 IMACS. Published by Elsevier B.V. All rights reserved.

Keywords: Coupled problem; Domain decomposition; Parallel computing

1. Introduction

At this time, many nuclear power plants in Europe are approaching the end of their service life. Construction of new power plants is extremely expensive and difficult and therefore a prolongation of the service life is the most simple way to produce electric energy. The prolongation of service life comes into question only if all requirements on reactor vessels are satisfied. Therefore, detailed analyses of vessels have to be done.

This article deals with a coupled analysis of prestressed concrete reactor vessels. One of the most important requirements is the integrity of the vessel, i.e. absence of cracks or existence of microcracks, which does not cause a leakage during an accident. Another important requirement, related to the previous one, is the limit to the internal pressure which can be developed inside the vessel and which does not cause a damage. There are, of course, additional requirements but only the mentioned ones were taken into account.

In order to estimate the overall behaviour of a vessel, hydro-thermo-mechanical analysis of the whole life of the vessel has to be done. The coupled analysis is necessary because concrete is a developing material and temperature with moisture have a considerable influence on its mechanical properties. The applied mechanical load which is represented by its weight, prestress and internal pressure occurring during service of the reactor has of course influence on concrete properties. The material properties of concrete at the present time with respect to its whole history is necessary for the limit state analysis as well as the analysis of damage and resistance against leakage.

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The existing vessels are approximately 30 years old and it means that the coupled hydro-thermo-mechanical analyses have to cover such a long period. A pure mechanical analysis of a vessel would use a time step which could grow significantly because selfweight and prestress are applied at the beginning of the service life and afterwards they are more or less constant. Unfortunately, it is not true for the coupled analysis, where the time step is influenced by changes of mechanical load, temperature and moisture. Finally, the time step has to be approximately one day which means that, at a rough estimate, 12,000 time steps are necessary for the whole service life.

The number of time steps together with the number of degrees of freedom used for spatial discretization of the vessel lead to huge time consumption and computer requirements. A single processor computer is able to execute only two-dimensional model of the vessel. If a three-dimensional model is required, a parallel computing is the only way to solve it. Parallel computing needs some modifications in comparison with the single processor computer code which has to be modified. It is an important advantage because finite elements, material models, algorithms connected with material models and integration points (e.g. stress update algorithms in plasticity) can be used without any modification.

There are two modifications needed. The first one is based on a mesh partitioning. It means that the original finite element mesh is partitioned into smaller submeshes and each submesh is assigned to one processor. Each submesh can be viewed as a small problem which is connected to other problems through a system of algebraic equations. The system of algebraic equations is not assembled on a processor but it is distributed on many processors. Therefore, the classical solvers cannot be used which is the second modification needed.

At this time, domain decomposition methods are suitable and very efficient tools for solution of systems of algebraic equations on parallel computers. The Schur complement method was selected because some material models used in coupled analyses may lead to non-symmetric matrices. Other domain decomposition methods are formulated especially for symmetric systems and their reformulation for non-symmetric ones becomes complicated.

This article is organised as follows. Section 2 summarises formulation of hydro-thermo-mechanical analysis and solution strategy for a nonlinear system of algebraic equations is indicated. Section 3 describes the Schur complement method which is used for parallelisation of the problem. Efficient computer implementation of the coupled analyses and parallelisation is discussed in Section 4. Section 5 describes the analysed vessel as well as the performed analyses. Several results are depicted in figures.

2. Coupled hydro-thermo-mechanical analysis

Detailed description of a general hydro-thermo-mechanical analysis is not in the centre of attention of this article and it can rather be found in monographs such as [6], than in articles. This section is devoted to description of selected general relationships which play a significant role in an efficient computer implementation.

There are many possibilities of unknown selection in coupled problems. The estimation of the properties of presstressed concrete used in the reactor vessel was based on the following set of unknowns: displacements, pore pressures and temperature. The subscript u denotes the displacements, the subscripts p_1 and p_2 denote the pore pressures and the subscript T denotes the temperature. Conservation equations after space discretization have the form

$$\begin{pmatrix} C_{uu} & C_{uT} & C_{up_1} & C_{up_2} \\ C_{Tu} & C_{TT} & C_{Tp_1} & C_{Tp_2} \\ C_{p_1u} & C_{p_1T} & C_{p_1p_1} & C_{p_1p_2} \\ C_{p_2u} & C_{p_2T} & C_{p_2p_1} & C_{p_2p_2} \end{pmatrix} \begin{pmatrix} \dot{d}_u \\ \dot{d}_T \\ \dot{d}_{p_1} \\ \dot{d}_{p_2} \end{pmatrix} + \begin{pmatrix} K_{uu} & K_{uT} & K_{up_1} & K_{up_2} \\ K_{Tu} & K_{TT} & K_{Tp_1} & K_{Tp_2} \\ K_{p_1u} & K_{p_1T} & K_{p_1p_1} & K_{p_1p_2} \\ K_{p_2u} & K_{p_2T} & K_{p_2p_1} & K_{p_2p_2} \end{pmatrix} \begin{pmatrix} d_u \\ d_T \\ d_{p_1} \\ d_{p_2} \end{pmatrix} = \begin{pmatrix} f_u \\ f_T \\ f_{p_1} \\ f_{p_2} \end{pmatrix}.$$
 (1)

Eq. (1) represents a system of nonlinear ordinary differential equations, where K denotes the stiffness or conductivity matrices, C denotes the capacity matrices and f denotes the prescribed nodal forces or prescribed nodal fluxes. The stiffness and conductivity matrices (denoted by K with appropriate subscripts) have generally the form

$$\boldsymbol{K}_{ij} = \int \boldsymbol{B}_i^T \boldsymbol{D}_{ij} \boldsymbol{B}_j \mathrm{d}\Omega, \qquad (2)$$

where B_i and B_j denote the gradient matrices, D_{ij} denotes the matrix of stiffness or conductivity of the material and the subscripts *i* and *j* substitute any of subscripts *u*, *T*, p_1 or p_2 . Similarly, the capacity matrices (denoted by *C* with appropriate subscripts) have generally the form

$$\boldsymbol{C}_{ij} = \int \boldsymbol{N}_i^T \boldsymbol{H}_{ij} \boldsymbol{N}_j \mathrm{d}\Omega, \tag{3}$$

where N_i and N_j denote the matrices of base functions and H_{ij} denotes the matrix of material parameters.

For better understanding, the following extension of the mechanical analysis is presented. Let an elastic material be assumed. The constitutive equation (Hook's law) has the form

$$\boldsymbol{\sigma} = \boldsymbol{D}_{\boldsymbol{u}\boldsymbol{u}}\boldsymbol{\varepsilon}(\boldsymbol{u}) \tag{4}$$

and it relates the strains ε and stresses σ . It should be noted that the strains depend on displacements u which are discretized and the nodal displacements are denoted by d_u . The mechanical problem with negligible inertial forces can be written in the form

$$K_{uu}d_u = f_u, (5)$$

where K_{uu} denotes the stiffness matrix and f_u denotes the vector of prescribed nodal forces. Eq. (5) expressed the equilibrium condition.

If the temperature plays a role, the constitutive relationship (4) has to be replaced by the following constitutive equation

$$\boldsymbol{\sigma} = \boldsymbol{D}_{\boldsymbol{u}\boldsymbol{u}}\boldsymbol{\varepsilon}(\boldsymbol{u}) + \boldsymbol{D}_{\boldsymbol{u}\boldsymbol{T}}\nabla\boldsymbol{T},\tag{6}$$

where the temperature T occurs. Moreover, the constitutive relationship between the heat flux q and the temperature gradient is needed and it has the form

$$\boldsymbol{q} = \boldsymbol{D}_{TT} \nabla T. \tag{7}$$

It is usually accepted that the heat flux is independent of the displacements u. Equilibrium condition (5) is therefore extended with the heat balance equation and the system of equations has the form

$$\begin{pmatrix} K_{uu} & K_{uT} \\ \mathbf{0} & K_{TT} \end{pmatrix} \begin{pmatrix} d_u \\ d_T \end{pmatrix} = \begin{pmatrix} f_u \\ f_T \end{pmatrix}.$$
(8)

The first equation in the system (8) expresses the equilibrium condition while the second equation in the system (8) expresses the heat balance condition. The zero block in the heat balance equation determines the independence of the heat transfer on the mechanical problem, but on the contrary, the mechanical problem is coupled with the heat transfer.

Additional variables can be introduced in the constitutive equations and additional balance equations can be added to the system. The thermo-mechanical problem (8) extended by the pore pressures and capacity terms result in the form of (1).

The matrices K and C generally depend on nodal values and this dependency results in nonlinear feature of the system. The system of differential Eq. (1) can be written more compactly as

$$C(d)d + K(d)d = f. (9)$$

The solution of the system of Eq. (9) cannot be obtained explicitly due to the nonlinearity and has to be found by a suitable numerical method. Time discretization is based on the v-form of generalised trapezoidal method [4] defined by the relationships

$$\boldsymbol{d}_{n+1} = \boldsymbol{d}_n + \Delta t \boldsymbol{v}_{n+\alpha},\tag{10}$$

$$\boldsymbol{v}_{n+\alpha} = (1-\alpha)\boldsymbol{v}_n + \alpha \boldsymbol{v}_{n+1},\tag{11}$$

where d denotes the nodal values and v denotes the first derivatives of nodal values with respect to time. The subscript n denotes the time step.

Substitution of expressions defined in Eqs. (10) and (11) to the system of differential Eq. (9) leads to relationship

$$(\boldsymbol{C}(\boldsymbol{d}) + \Delta t \boldsymbol{\alpha} \boldsymbol{K}(\boldsymbol{d})) \boldsymbol{v}_{n+1} = \boldsymbol{f}_{n+1} - \boldsymbol{K} (\boldsymbol{d}_n + \Delta t (1 - \boldsymbol{\alpha}) \boldsymbol{v}_n).$$
⁽¹²⁾

The system of algebraic Eq. (12) is nonlinear and the Newton–Raphson method [1,2] has to be used at each time step.

1580

The trial solution $v_{n+1,0}$ of the system of Eq. (12) is used for computation of the trial nodal values $d_{n+1,0}$. Substitution of the trial solution back to the system of Eq. (12) with modified matrices does not generally lead to equilibrium. Residuum is computed from the relationship

$$\mathbf{r}_{n+1,0} = \mathbf{f}_{n+1} - \mathbf{K} \left(\mathbf{d}_n + \Delta t (1 - \alpha) \mathbf{v}_n \right) - \left(\mathbf{C} (\mathbf{d}_{n+1,0}) + \Delta t \alpha \mathbf{K} (\mathbf{d}_{n+1,0}) \right) \mathbf{v}_{n+1,0}$$
(13)

and additional nodal time derivatives are computed from the equation

$$(C(d_{n+1,0}) + \Delta t \alpha K(d_{n+1,0})) \Delta v_{n+1,0} = r_{n+1,0}$$
(14)

It has to be noted that the permanent recalculation of matrices K and C with respect to actual nodal values is very computationally demanding. Furthermore, the matrix of the system of equations $C(d) + \Delta t \alpha K(d)$ has to be factorized during every iteration at every time step. Speedup of the described computation is therefore very desirable. In this analysis, the speedup was based on parallelisation of the problem.

3. Domain decomposition method

Application of parallel computers to the numerical analysis based on solution of systems of algebraic equations requires some changes in comparison with the classical single processor (sequential) computation. Domain decomposition methods create a suitable framework for efficient parallel computations. Only the Schur complement method, sometimes also called the method of substructuring, is used in this article and its main features are described in this section. For more details about domain decomposition methods see references [3,5,7–9]

The Schur complement method is discussed in connection with the finite element method. Let a domain (structure) be discretized by finite elements. The system of algebraic equations can be written in the form

$$Ad = f. (15)$$

Consider decomposition of the generated mesh into *m*submeshes. A special ordering of unknowns (see references [5,8]) leads to a rearranged system of algebraic equations in the special form

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$$\begin{pmatrix} A_{ii}^{(1)} & \mathbf{0} & A_{ib}^{(1)} \\ A_{ii}^{(2)} & A_{ib}^{(2)} \\ \mathbf{0} & A_{ii}^{(3)} & A_{ib}^{(3)} \\ \vdots & \ddots & \vdots \\ & & A_{ii}^{(m)} & A_{ib}^{(m)} \\ A_{bi}^{(1)} & A_{bi}^{(2)} & A_{bi}^{(3)} & \dots & A_{bi}^{(m)} \\ A_{bi}^{(1)} & A_{bi}^{(2)} & A_{bi}^{(3)} & \dots & A_{bi}^{(m)} & A_{bb} \end{pmatrix} \begin{pmatrix} d_i^{(1)} \\ d_i^{(2)} \\ d_i^{(3)} \\ \vdots \\ d_i^{(m)} \\ d_b \end{pmatrix} = \begin{pmatrix} f_i^{(1)} \\ f_i^{(2)} \\ f_i^{(3)} \\ \vdots \\ f_i^{(m)} \\ f_b \end{pmatrix},$$
(16)

where the subscript *i* denotes the inner quantity and the subscript *b* denotes the quantity defined on boundary between two subdomains. The superscript denotes number of subdomain. All subvectors $d_i^{(j)}$, except the last subvector d_b , may be expressed in the form

$$\boldsymbol{d}_{i}^{(j)} = \left(\boldsymbol{A}_{ii}^{(j)}\right)^{-1} \left(\boldsymbol{f}_{i}^{(j)} - \boldsymbol{A}_{ib}^{(j)} \boldsymbol{d}_{b}\right).$$
(17)

Substitution of expressions from Eq. (17) to the last equation of the system (16) gives

(1)

$$Sd_b = s, \tag{18}$$

where the following notation is used

$$S = A_{bb} - \sum_{j=1}^{m} A_{bi}^{(j)} \left(A_{ii}^{(j)} \right)^{-1} A_{ib}^{(j)},$$
(19)

$$s = f_b - \sum_{j=1}^m A_{bi}^{(j)} \left(A_{ii}^{(j)} \right)^{-1} f_i^{(j)}.$$
(20)

The system of equations from (18) is called a coarse or reduced problem. The number of unknowns is significantly smaller than the number of unknowns in the original system of Eq. (16).

The reduced system (18) can be solved by a direct or iterative method which depends on the number of processors used. In the case of a small number of processors, the reduced system (18) can be assembled on the master processor and solved by a direct method, e.g. the matrix S can be factorized by LU factorization. On the other hand, if many processors are employed, the matrix S is distributed on those processors and an iterative method has to be used, e.g. the bi-conjugate gradient method.

4. Efficient computer implementation with respect to the future

This section contains two subsections which describe an efficient implementation of a computer code for coupled problems and parallelisation of this code.

4.1. Computer code for coupled problems

A general coupled problem can be described by a system of differential equations in the form the (9). The matrices K and C and the vectors v and f are composed from several submatrices and subvectors similarly to the Eq. (1). If new variables and balance equations are added to the model, new submatrices and subvectors will arise. The extension of the mechanical problem to a thermo-mechanical and later to a thermo-hydro-mechanical problem is described in Section 2.

An efficient and extensible computer code has to enable simple implementation of these new submatrices and subvectors. A close study of the system (1) reveals its three main parts. If the coupling submatrices K_{uT} , K_{up_1} , K_{up_2} , K_{Tu} , K_{p_1u} , K_{p_2u} , C_{uT} , C_{up_1} , C_{up_2} , C_{Tu} , C_{p_1u} and C_{p_2u} are replaced by zero matrices, the original system split into a mechanical problem and a transport problem which are independent. They are two main parts of the coupled problem. The transport problem is still coupled because there is common transfer of heat and moisture. There are similarities between the mechanical and transport problems (the governing equations are the balance equations, the balance of momentum is used in mechanics while the balance of heat or moisture is used in transport processes) but there are also differences (the mechanical problems are vector problems while the transport processes are scalar problems so the solution algorithms differ because transport processes sometimes require a stabilisation method, etc.).

It is reasonable to have a computer code which deals with mechanical problems and a different computer code which deals with the transport processes. Both codes can be developed absolutely independently of each other.

The code for transport processes has to be designed with respect to an arbitrary number of transported variables and balance equations. The key point is hidden in assembling of the conductivity and capacity matrices as well as in assembling of the right hand side which expresses prescribed nodal fluxes. The system of differential equations or the system of algebraic equations after discretization is formally identical and therefore the same solution method can be used.

The computer subroutine for the conductivity matrix of a finite element in one problem with one balance equation contains a loop over the integration points. In the case of one balance equation, one set of integration points is needed because information about the material model is accommodated in the integration points. In each integration point, the gradient matrix B and the constitutive matrix D are assembled and the product $B^T DB$ is computed. Let such subroutine have declaration conductivity_matrix (long ri, long ci), where ri and ci are dummy integer variables.

In the case of *n* balance equations, a new subroutine is needed which contains a double loop over the original subroutine conductivity_matrix (long ri, long ci), where ri and ci indicate any of the subscripts u, p_1, p_2 or *T*. Each finite element needs n^2 sets of integration points, where appropriate material models are defined. For example, the set of integration points (1,3) contains a material model defining the matrix D_{up_2} . The matrix K_{up_2} is obtained from the subroutine conductivity_matrix (1,3).

As was mentioned earlier, a computer code for mechanics and a code for transport problems are two basic parts of the computer code for coupled analyses. The remaining third part has to couple the previous two codes together. The coupling code has to deal with submatrices K_{uT} , K_{up_1} , K_{up_2} , K_{Tu} , K_{p_1u} , K_{p_2u} , C_{uT} , C_{up_1} , C_{up_2} , C_{Tu} , C_{p_1u} , C_{p_2u} and appropriate subvectors. It has a similar structure as the code for transport processes.

The proposed implementation enables independent development of the code for mechanics and for transport processes. A code coupling the mechanics with transport processes can be built by adding only those subroutines which are responsible for coupling the submatrices and subvectors between u and the set of p_1 , p_2 , T. All features implemented in the mechanical and transport codes are already available.

4.2. Parallelisation

Parallelisation focuses especially on the part of a code which deals with the solution of systems of algebraic equations. Domain decomposition methods enable parallelisation and particularly, the method of Schur complement has been used.

Implementation of the Schur complement method used in the code for coupled problems was based on combination of direct and iterative methods. The inverse matrices in relationship (17) were not computed explicitly because the \mathbf{LDL}^T or \mathbf{LU} factorization were used. Factorizations of matrices $A_{ii}^{(j)}$ can be done simultaneously. The coarse problem (16) was solved by an iterative method (bi-conjugate gradient method) and therefore the matrix S was not assembled on the master processor.

The Schur complement method was applied to the system of algebraic Eq. (12). Therefore, the matrix A used in Eq. (15) has the form

$$A = C(d) + \Delta t \alpha K(d) \tag{21}$$

and the vector f from Eq. (15) has the form

$$\boldsymbol{f} = \boldsymbol{f}_{n+1} - \boldsymbol{K} \left(\boldsymbol{d}_n + \Delta t (1 - \alpha) \boldsymbol{v}_n \right).$$
⁽²²⁾

It has to be emphasized, that only the subroutine for solution of the system of equations has been replaced by a new subroutine while all other subroutines have been untouched. This is a significant advantage because development of new solvers of systems of equations in parallel environment and development of the mechanical and transport codes are independent and these parts may be simply connected.

5. Analysis of prestressed concrete nuclear vessel

As was mentioned in the introduction, complex analyses of existing nuclear vessels become important in connection with intended prolongation of serviceability of nuclear power plants. The described analyses were conducted within MAECENAS project supported by EU. A real reactor vessel of an existing nuclear power plant was analysed. All necessary information about the vessel (geometry, lengths, thicknesses, forces, pressures, temperatures, material properties, etc.) were given as a part of the project.

In order to estimate the behaviour and actual state of the vessel after more than 30 years of service, coupled hydrothermo-mechanical analyses and limit state mechanical analyses were performed. The coupled analyses were computed first and several stages at selected times were stored. The limit state analyses of saved stages from the coupled analyses were performed later.

The reactor vessel has a cylindrical shape and it is made from prestressed concrete with an inner steel liner. The diameter of the cylinder is approximately 30 m and the height is approximately 36 m. Thickness of walls is about 5 m.

The coupled hydro-thermo-mechanical analysis consists of concurrent moisture transfer, heat transfer and creep analysis. Therefore, there are two pore pressures, temperature and two or three displacements (it depends whether 2D or 3D model is used) defined at each node. Five or six variables at each node lead to extremely large systems of algebraic equations with relatively dense matrices. With respect to the mentioned extreme computational demands of the coupled analyses, an axisymmetric two-dimensional model was used. The cross-section of the vessel is depicted in Fig. 1.

The whole period of service of the reactor vessel had to be modelled. Combinations of several effects led to a small time step which was one day and during significant heating or cooling the time step had to be reduced to one hour. Therefore, more than 12,500 time steps were necessary for computation.

In order to speed up the computation, parallel algorithms were used. Namely, the Schur complement method (one type of domain decomposition methods) was applied and computation was executed on a cluster of PC. The



Fig. 1. Finite element mesh and decomposition into 8 subdomains.



Fig. 2. Prestress forces during life time.



Fig. 3. Internal pressure during life time.



Fig. 4. Vertical displacement of selected point during life time.



Fig. 5. Deformed shape of the vessel caused by all load cases in comparison with undeformed shape.



Fig. 6. Decomposition of three-dimensional model into 20 subdomains.

number of processors was established as the minimum number of processors available to all teams associated in the MAECENAS project. The finite element mesh was therefore decomposed into eight submeshes and one example of such decomposition is depicted in Fig. 1.

There were two groups of effects, which had to be modelled. The first group contained the mechanical effects and the second group contained the heat and moisture transfer effects. Prestress of the vessel is an important load case influencing especially creep of the structure. History of prestress is depicted in Fig. 2. Prestress tendons were in the vertical as well as in the horizontal direction and they were modelled as nodal forces multiplied by time function from Fig. 2. Gravity load was applied gradually during the first 150 days. The last mechanical load case was the internal pressure whose history is depicted in Fig. 3.

Fig. 4 shows vertical displacement of a selected point over time. There are several loading and unloading steps during the life of the vessel and they are clearly visible in this figure. Fig. 2 shows deformation of the vessel caused by prestress only. This result was obtained separately from the hydro-thermo-mechanical analysis in order to check the material model and the prescribed load. The total deformation of the vessel obtained from the hydro-thermo-mechanical analysis at time 6000 days is depicted in Fig. 5.

The two-dimensional axisymmetric model was later replaced by a three-dimensional model. While the twodimensional model contained 17,021 nodes (each node contained 5 unknowns), the three-dimensional model contained 50881 nodes (each node contained 6 unknowns). Such a large number of unknowns cannot be executed on a single processor computer but the parallelisation allows solving the coupled problem on the given mesh (Fig. 6).

6. Conclusion

Complex hydro-thermo-mechanical analyses and following limit state mechanical analyses were performed for an existing nuclear vessel made of prestressed concrete with an inner steel liner. All analyses were computed by authors software developed during the MAECENAS project. Distribution of displacements, strains, stresses, pore pressures, temperatures and damage parameters were computed. Simply extensible code architecture has been introduced and three computer codes have been implemented. The codes are continuously developed and additional features are further implemented.

Computationally very demanding analyses were parallelised with help of the Schur complement method and a homogeneous cluster of PCs was utilized. Parallelisation speed the computation up because it reduced computational time for solution of the system of algebraic equations as well as it reduced time for evaluation of complicated relationships in the material models which were executed on thousands of integration points. The behaviour of the vessel during 33 years described by the hydro-thermo-mechanical analysis formulated as an axisymmetric problem took only several hours on a cluster of eight PCs in comparison with several days on a single-processor computer without parallelisation.

Acknowledgement

Financial support for this work was provided by the Ministry of Education, Youth and Sports of the Czech Republic, project VZ 03 CEZ MSM 6840770003. The financial support is gratefully acknowledged.

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