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SEPRAN: A Versatile Finite-Element Package for a Wide Variety of Problems in Geosciences

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ABSTRACT: Numerical modelling of geological processes, such as mantle convection, flow in porous media, and geothermal heat transfer, has become quite common with the increase in computing and the availability of usable software. Today modelling these dynamical processes entails the solving of the governing equations involving the mass, momentum, energy and chemical transport. These equations represent partial differential equations and must be solved on powerful enough computers because they require sufficient spatial and temporal resolution to be useful. We describe here the salient and outstanding features of the SEPRAN software package, developed in the Netherlands, as a case study for a robust and user-friendly software, which the geological community can utilize in handling many thermal-mechanical-chemical problems found in geology, which will include geothermal situations, where many types of partial differential equations must be solved at the same time with thermodynamical input parameters.

KEY WORDS: SEPRAN, finite element package, geodynamic and planetary modelling, geothermal, groundwater flow.

0 INTRODUCTION

Today modelling dynamical processes in geological sciences is generally carried out by solving the governing equations involving mass, momentum and energy transport. These are partial differential equations and must be solved on the computer. There is available software for solving individual equations such as the heat equation for analyzing the thermal state of the crust and mantle or the momentum equation for mountain collision or the development of folding in nappes, such as PDE/Protran developed by Sewell (2005) and ABAQUS by the group at Brown University. Much effort has been expended in providing software for geodynamicists, e.g., CITCOM (Moresi and Solomatov, 1995), and underworld software (http://www.underworldproject.org/models.html) (Moresi et al., 2007), and more recently, ASPECT (Kronbichler et al., 2012). There is clearly a market for robust codes in solving diverse situations encountered in geological or hydrological sciences. In this paper we discuss the features of the SEPRAN package as a case study for a robust code, which the geological community can employ in solving many thermal-mechanical-chemical problems found in geology.

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0.1 History of the SEPRAN Finite Element Package

The finite element package SEPRAN was developed as the succesor of the package AFEP by SEPRA engineering company in cooperation with the department of applied mathematics of Delft Technical University (TUD). AFEP was developed in the 1970's to have a flexible research tool to investigate the finite element method at TUD. At that time (around 1975) no packages were available that gave the user the opportunity to create his own element matrices and element vectors, nor was it possible to include user algorithms. Interest from commercial users and their need for support resulted in the development of the more user friendly package SEPRAN built on the ideas of AFEP but with a completely new code and user interface, starting in the early 1980s (version 1.0 in 1982). There have been continual upgrades of the SEPRAN package since the early versions, such as extensions to the library of supported finite elements, introduction of parallel computation through domain decomposition and extensions of the syntax of the scripting tool.

SEPRAN code is written mostly in Fortran 77. The source code is included in the SEPRAN package distribution. SEPRAN manuals including examples of applications can be downloaded from the website (http://ta.twi.tudelft.nl/nw/sepran).

The SEPRAN package has been applied to a wide range of problems related to mechanical and transport models including the following industrial and medical applications; flow models of molten glas in the glass industry for example in simulations of construction of TV tubes, modelling of extrusion processes (aluminum, plastics), computation of dissolution of particles in multi-component alloys, simulation of flow processes (blood, oil), flow in bearings for electric tools like CD and DVD play-

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ers, computation of the melting component of the mark formation model in optical recording, groundwater flow modelling.

The package has been used for over 25 years in the education and research program of the Geophysics Department at Utrecht University and many students have used the package in their work dealing with numerical modelling in geosciences. Other geoscience institutes where SEPRAN has been applied in research and teaching include, University of Michigan, Charles University Prague, University of Durham, China University of Geosciences, Wuhan.

SEPRAN is available for a range of platforms including Linux/Unix and Microsoft Windows. The package has the following capabilities. (a) It contains a mesh generator with a flexible scripting interface for general 2D and 3D mesh configurations. Mesh objects like lines, surfaces and volumes can be generated and combined into larger objects. A range of element geometries in 1D, 2D and 3D is available with several options for the type of basis functions involved. SEPRAN includes graphics tools for plotting meshes and computational results. Furthermore results can be output in a format suitable for visualization with ParaView (http://www.paraview.org). A complete list of the implemented options is given in the SEPRAN user manual (see below). (b) Coupled problems formulated by multiple partial differential equations (PDEs) and related boundary conditions can be solved simultaneously. The maximum number of simultaneous problems has been set, by a single parameter in the code, to an arbitrary value of one hundred. Typical examples of geo-applications dealing with simultaneous problems include transport problems like thermal convection and coupled heat and mass transport processes in porous media. (c) Application building is greatly facilitated by using high level scripting tools as for example with PDE2D (Sewell, 2005), escript (Gross et al., 2007). SEPRAN includes a flexible scripting language interface for problem specification in terms of coupled PDE's and their coefficients and boundary conditions and for the computational steps of the model computations. Experience shows that the scripting tool helps to shorten the learning curve for working with the SEPRAN package. Students doing computer lab assignments learn to use the tool quickly, including writing their own user defined extensions to the code, by making use of the SEPRAN interfaces to user written, Fortran procedures. (d) The SEPRAN package is extensively documented in the following manuals available at the web site (http://ta.twi.tudelft.nl/nw/sepran).

1. The Introduction Manual (intro.pdf). This gives a general introduction on setting up numerical modelling experiments with SEPRAN discribing the mesh generation, the organization of the computational part and the available postprocessing options.

2. The User Manual (um.pdf). Besides a more general introduction this manual contains comprehensive overview of the SEPRAN mesh generator and scripting commands for development of SEPRAN applications built on the toolkit library.

3. The Standard Problems Manual (sp.pdf). This manual describes the list of PDE's and options for boundary conditions with corresponding finite elements in the SEPRAN element library. Besides the available standard elements users can develope their own element routines to be linked with the SEPRAN library in application code development.

4. The Programmers Guide Manual (pg.pdf). Besides using the SEPRAN scripting tool, in combination with a precompiled standard executable file, users can develop their own programs based on the SEPRAN library. Such user codes will include calls to the Fortran procedures—subroutines and functions of the SEPRAN library. Interface descriptions and explanation of how to use the main procedures of the library can be found in the programmers guide.

(i) Parallel computing based on MPI is supported using domain decomposition, where each parallel proces represents a separate subdomain. SEPRAN includes alternative direct and iterative matrix solvers for the solution of the finite element equations and besides this an interface to the PETSC library (Portable, Extensible Toolkit for Scientific Computation), containing advanced algebraic multigrid solvers that allow for large scale parallellisation with optimal scaling characteristics for very large problem size (Geenen et al., 2009).

(ii) The package provides tools for a wide range of applications in science and engineering, including second order elliptic, parabolic and hyperbolic equations, suitable for mechanical problems dealing with linear elasticity and for flow problems for both incompressible and compressible viscous media (van Kan et al., 2005; Cuvelier et al., 1986).

(iii) Transport problems can be handled in several ways: typically diffusive transport is modeled using a separate PDE for the convection-diffusion equation as in thermal convection models. Non-diffusive material transport has been modelled in several ways: first SEPRAN includes facilities for level set methods (Hillebrand et al., 2014). Besides this several alternative methods have been applied as extensions to SEPRAN such as: (1) marker chain methods similar to Christensen and Yuen (1984) were used in van Keken et a1. (1997) and Lin and van Keken (2006); (2) a characteristics based method similar to Malevsky and Yuen (1991) has been applied in de Smet et al. (2000) to model reactive transport in models for the petrological evolution of continental roots; (3) particle tracer methods using particle in cell techniques have used extensively in planetary and geoscience problems (Asgari and Moresi, 2012; Chertova et al., 2012; Cizkova et al., 2012; de Vries et al., 2010; van Summeren et al., 2009; van Hunen and van den Berg, 2008; van Thienen et al., 2005; Schott et al., 2001).

In the applications of item (3) so called active tracers were used providing feedback between material properties transported by tracers and the flow velocity field. Passive tracers without feedback were used for monitoring evolution of model properties such as local temperature and mineral phase (van den Berg et al., 2010).

(iv) Geothermal modelling problems can be solved by SEPRAN using an elliptic (potential type) equation for porous flow coupled to a convection-diffusion equation for energy transport. Several time integration methods for time dependent problems are available in SEPRAN, including Crank-Nicolson, Runge-Kutta and Newmark. A complete list of the methods implemented is given in the forementioned user manual and in the standard problems manual.

0.2 An Example SEPRAN Application for Groundwater Flow

To illustrate the ease of use of the scripting interface to the

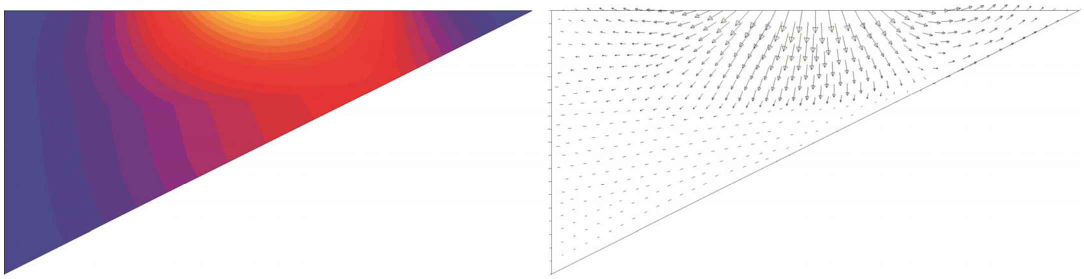

Figure 1. Dynamic pressure Δp from SEPRAN solution of equation (2) (left), and corresponding Darcy flow vector field (right).

software package for a relevant problem we present an application to a simple 2D model for steady state groundwater flow. The triangular wedge shaped computational domain, including three layers of contrasting hydraulic conductivity, is illustrated in Fig. l, showing the driving pressure and the corresponding Darcy velocity. Fluid is infiltrating through the top boundary. The bottom boundary is impermeable and the lefthand boundary is implemented as an open boundary. The model is based on a Darcy flow equation for a constant density fluid ($\Delta\rho= 0$)

$$\boldsymbol{q} = -\frac{k}{\mu}(\nabla p - \rho g e_z) = -\frac{k}{\mu}(\nabla \Delta p - \Delta \rho g e_z) = -\frac{k}{\mu}\nabla \Delta p \qquad (1)$$

where $\boldsymbol{q}$ is the Darcy flow velocity vector, k, μ are the permeability of the porous medium and the viscosity of the fluid respectively. p respresents the total pressure and Δp is the dynamic (total minus hydrostatic) pressure. Assuming an incompressible porous matrix and fluid material and applying the constraint from mass conservation we have

$$\nabla \cdot \boldsymbol{q} = -\nabla \cdot (\frac{k}{\mu}\nabla \Delta p) = 0 \qquad (2)$$

A generalized Poisson equation for the dynamic pressure involving variable hydraulic conductivity k/μ. Applying impermeable boundary conditions to the bottom boundary, we have there $\boldsymbol{q} \cdot n = 0 \Rightarrow \nabla \Delta p \cdot n = 0$. Inflow conditions are fixed on the top boundary by a functional description of the dynamic pressure there, $\Delta P(x,y) = f(x), (x,y) \in C_{\text{in}}$. The vertical outflow boundary is treated as an open boundary characterized by zero valued dynamic pressure, $\Delta p(x,y) = 0, (x,y) \in C_{\text{out}}$.

0.2.1 The SEPRAN problem definition script

The specification of the above groundwater flow problem for the SEPRAN application and the necessary computational steps in the numerical solution are defined in the script file listed below. The example script consists of a leading definition part followed by an execution part in the structure … end block.

The definition part consists of: (1) A declaration block constants ... end specifying user defined variable names and parameter value settings. (2) A problem definition block problem … end defining a single FE type, from the library of standard elements, that corresponds to the PDE for a general convection-diffusion problem. This is done for all three element groups corresponding to the three layers of contrasting hydraulic conductivity. This block also specifies the parts of the boundary with essential boundary conditions, referring to mesh boundary segments that correspond to in- and outflow boundaries. The impermeable condition for the bottom boundary, $\nabla\Delta\, p{\cdot}n$=0, is implicitly assumed. (3) A block of further specification of the essential boundary conditions. Integer switch values, func=2 are passed by the code to a user defined Fortran function with an implementation of the functional description of the boundary conditions. (4) A coefficient definition block specifying the non-zero diagonal elements of a 2×2 hydraulic conductivity tensor for the general anisotropic conductivity model corresponding to the standard element applied. The example specifies contrasting values for the 3 layers, represented by 3 element groups, corresponding to a piecewise uniform conductivity model.

The computational part in the structure block contains the following executable commands.

(1) Prescribe_boundary_conditions, pressure results in evaluation of the essential boundary conditions.

(2) Solve_linear_system pressure results in building the system of FE equations and subsequent solving of the system for the unknown dynamic pressure. For the matrix solver the default option, a direct method for the symmetric matrix is applied. Several alternatives including Krylov iterative methods are available in SEPRAN.

(3) Plot_colored_ levels pressure produces a color plot of the pressure field shown in Fig. 1.

(4) Flow=derivatives (pressure, icheld=3) results in computation of the Darcy flow vector field from the pressure field, that is plotted with the subsequent command plot_vector.

(5) The output command results in writing of the results, nodal point values of pressure, flow to an output file for post-processing.

```
constants
  reals
    xwidth=2
    pmax_inflw=10
    psigma_inflw=0.5
    kperm1=1
    kperm2=10
    kperm3=kperm1

   vector_names                  #        |  |  |  |  |  |  |
    pressure                     #        V  V  V  V  V  V  V
    flow                         #      *--------------------*
end                              # <-  |          c11        /
problem 1    #pressure problem   # <-  |                    /
  types                          # <-  | c4               /
    elgrp 1 to 3 (type=800)      # <-  |               /
  essboundcond                   # <-  |            /
   curves (c4) # inflow bound.   # <-  |         /
   curves (c11) # outflow bound. #      * /
end                              # x=0                x=1
essential boundary conditions, problem=1
```

```
  degfd1curves (c4), (func=2) # inflow boundary p=x–functional description
  degfd1curves (c11), (func=2) # outflow boundary p=x–functional description
end
coefficients, sequence_number=1, problem=1 # coefficients pressure equation
  elgrp1
    coef 6=kperm1    # a11
    coef 9=kperm1    # a22                      "
  elgrp2
    coef 6=kperm2    # a11
    coef 9=kperm2    # a22                      "
  elgrp3
    coef 6=kperm3    # a11
    coef 9=kperm3    # a22                      "
end
structure # computational part
  prescribe_boundary_conditions, pressure
  solve_linear_system pressure, seq_coef=1, problem=1
  plot_colored_levels pressure
  flow=derivatives (pressure, icheld=3) # f= -grad p
  plot_vector flow
  output
end
end_of_sepran_input
```

1 SEPRAN APPLICATIONS TO GEODYNAMICAL PROBLEMS

In the geophysics group at the University of Utrecht especially SEPRAN problem types have been applied that deal with the general convection diffusion equation in the single dependent variable c, typically mass concentration or temperature

$$\rho c_p(\frac{\partial c}{\partial t} + u \cdot \nabla c) - \nabla \cdot (a \nabla c) + \beta c = f \tag{3}$$

and the (Navier)Stokes equation for (in)compressible flow field u

$$\rho\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u\right) + \nabla P - \nabla \cdot \tau = \rho f \tag{4}$$

which simplifies in the geodynamically relevant case of an infinite Prandtl number, where the inertial term can be neglected, into $\nabla P - \nabla \cdot \tau = \rho f$. Here the shear stress tensor τ is related to the velocity field u and the viscosity η, by the constitutive equation for a purely viscous medium $\tau = \eta(\nabla u + \nabla u^T - 2/3(\nabla \cdot U)I)$.

A flexible and extensible code is important for a research environment (this may not always be availabale with commercial software). In SEPRAN this is supported, more so than in community codes such as CITCOM, by a high level scripting tool and user interfaces to the main routines of the sepran code library.

This way it is, for instance, easy to interface new implementations of material properties such as viscosity and thermal conductivity, to typical geodynamic convection codes or codes written for geothermal modeling—see for instance (van den Berg et al., 2010, 2005, 1993; Hofmeister, 1999).

Another application of this flexible interfacing facility in SEPRAN is the implementation of completely general material properties, density, thermal expansivity and specific heat, derived from separate self-consistent thermodynamic models, both from Ab initio and semi-empirical lattice dynamics methods (van den Berg et al., 2012; Jacobs and van den Berg, 2011; Umemoto et al., 2006).

This set up allows us to include results from frontier mineral physics in our convection models applied to planetary mantles but it is also applicable in other possible application domains such as reactive transport in porous media and geothermal modelling where thermodynamic properties play a role that may be tabulated in P, T space.

For these compressible models we apply an anelastic liquid approximation as described in (Jacobs and van den Berg, 2011). For the Stokes equation an integrated method is applied retaining velocity and pressure as the degrees of freedom (dof). This is combined with a direct solver for the symmetric profile matrix. Renumbering of the dof's is necessary to avoid problems related to the zero diagonal block of the Stokes matrix (Ur Rehman et al., 2008). Direct solvers for the Stokes problem applied here are robust and reasonably efficient for problem size up to about 10^7 degrees of freedom (Thieulot, 2014; Ur Rehman et al., 2008). For larger problems iterative solvers become indispensible. SEPRAN has several options for iterative solvers, including well known Krylov methods and ILU preconditioners (Ur Rehman et al., 2008). Conventional ILU type preconditioners break down for even larger problems because the number of solver iterations increases with the problem size. For this reason modern block preconditioners, with convergence characteristics independent of the problem size have been made available by interfacing SEPPRAN to the PETSc (Portable, Extensible Toolkit for Scientific Computation) library package (www.mcsmanl.gov/petsc). Geenen et al. (2009) have shown that the latter approach results in superior scaling characteristics for problem size up to at least 10^8 degrees of freedom, and that these solvers scale well with the number of processors in parallel computations up to at least 500 processors.

For the energy transport equation we have used a direct solver for the non-symmetric matrix. Upwinding methods, available with several options in SEPRAN, were not applied for the examples shown.

An example of an extension to SEPRAN is the library of routines supporting the use of lagrangian particle tracers. This is typically used in non-diffusive transport problems that occur in thermo-chemical convection studies (de Vries, 2012; de Vries et al., 2010; van Summeren et al., 2009; van Thienen et al., 2005). The tracers can be applied either as passive monitor tracers that register the spatial and temporal evolution of the problem solution or as so-called active tracers that represent material properties. In the latter case these material properties can be either time invariant or they can evolve in a reactive environment.

The routines from the tracer library are interfaced to SEPRAN such that, for instance, the convective velocity computed by the SEPRAN solvers is applied to advect the tracer coordinates over an integration time step. Vice versa the material properties defined on the tracer locations are passed to the SEPRAN routines that compute the matrix-vector coefficients of the finite element equations of the numerical model (van Summeren et al., 2009; van Hunen and van den Berg, 2008; van Keken et al., 1993).

2 EXAMPLE APPLICATION: A LUNAR THERMO-CHEMICAL EVOLUTION MODEL

As an example of the above, combining both the tracer setup and the thermodynamic interface, we show some recent results of evolution models of the moon. This is an example of a model computation for compressible convection including compositional heterogeneity related to contrasting mineral assemblages in a convection model for lunar evolution (de Vries, 2012). The model for this Rayleigh-Taylor type problem starts from a gravitationally unstable layering that collapses and that is shown to dominate the subsequent evolution of the moon.

The model is started directly after the complete solidification of the early magma ocean in the moon's mantle, from the unstable layering shown in Fig. 2a and a temperature profile closely below the melting temperature. Corresponding density profiles for time zero and after a model time of about 4 Gyr are shown in Fig. 2b.

The composition vector field in this example is represented on 5. 10^5 particle tracers and the material properties of the different mineral assemblages indicated schematically in the initial layering shown in Fig. 2a have been computed with a self-consistent thermodynamics model based on P, T tabular representation. Time evolves from the bottom row upwards in Fig. 3. The results show an initial overturn of the layering with dense layers of (grey) ilmenite and (red) clinopyroxene on top, followed by smaller scale mixing during the 4 billion year

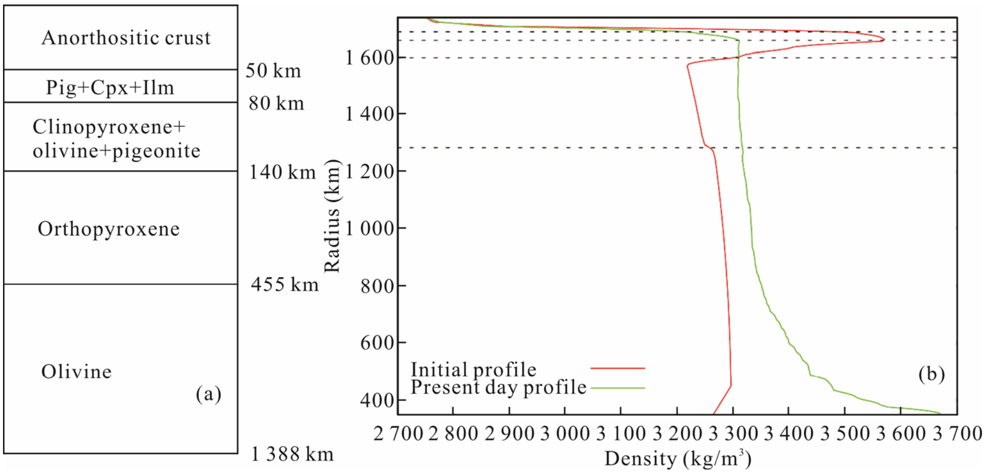

Figure 2. (a) Initial compositional layering of the mantle model derived from (Snyder et al., 1992); (b) radial density profiles illustrating the instable initial layering (red) characterized by a dense ilmenite bearing layer at shallow depth, the profile after some 4 Gyr of convective mixing is shown in green.

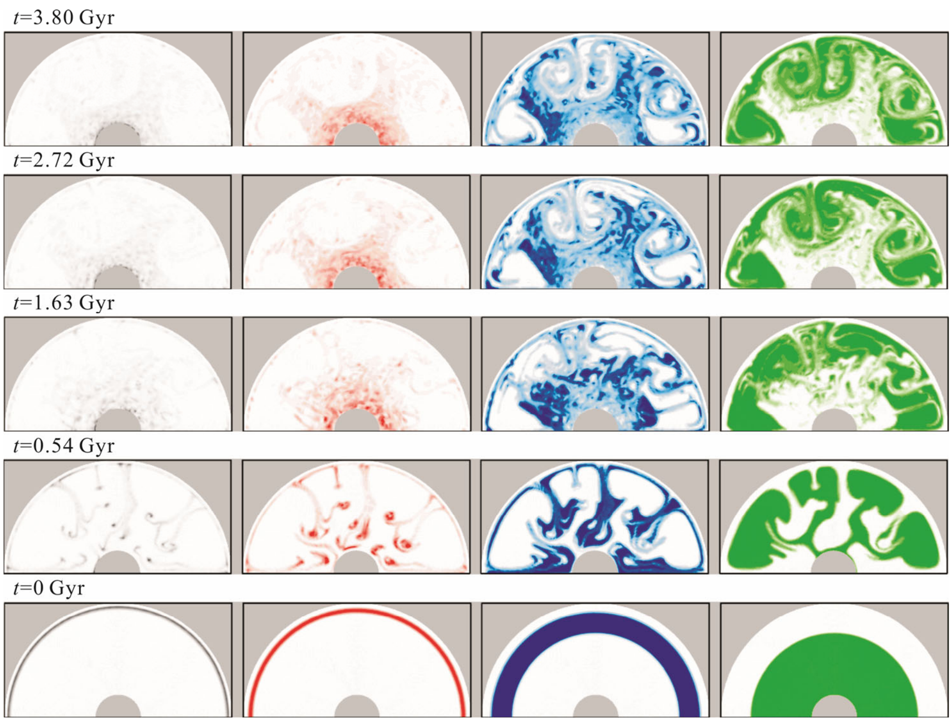

Figure 3. Evolution of the lunar compositional layering. Each row represents a snapshot of the distribution, of the individual mineral components, labeled with the model time. The different columns represent from, left to right 1) high density ilmenite bearing layer enriched in, radiogenic elements that have a strong impact on, lunar thermal evolution, 2) dense clinopyroxene, 3) orthopyroxene and 4) olivine.

model evolution. The denser material, that is also enriched in radiogenic isotopes accumulates on the core-mantle boundary and plays a key role in the thermal evolution of the lunar core and mantle.

3 CONCLUDING REMARKS

After 30 years of continual improvement and progress made by SEPRAN, we see the following accomplishments: (1) a robust FE package has become available for a wide range of applications in science and engineering, (2) flexibility and extensibility are main characteristic's, coupled problems formulated in simultaneous PDE's can be solved, combining an in principle arbitrary number of available SEPRAN standard problems and user defined problems. (3) a versatile meshgenerator with a scripting interface is available for 1D, 2D and 3D computational domains, (4) a flexible high end scripting tool can be used for both the problem specification, through selection of the types of PDE's and their coefficients and the choice of boundary conditions, as well as for specifications of computational tasks, (5) FE meshes and computational results can be visualized either using integrated graphics or by output of files in a suitable format for visualization with the PARAVIEW visualization program. (6) mpi-based parallel computations are facilitated using domain decomposition.

Future development will be directed by the arising needs of the user community, including university and commercial research and development institutes. Some foreseeable directions include: (1) extension in massively parallel computing to more than 1 000 cores, (2) larger sets of simultaneous problems for example required for geodynamo computations, 3) improvements in pre- and postprocessing like mesh generation and visualization.

In the above we have illustrated the great versatility of the SEPRAN finite element package for a variety of situations relevant for the geo- and environmental sciences and related areas of engineering, including flow in porous media and geothermal energy transport problems.

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