Geophysical Research Abstracts,
Vol. 10, EGU2008-A-02428, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-02428
EGU General Assembly 2008

The method for efficient calculation of phase diagrams and in situ rock properties based on 3D adaptive wavelet approach.

Y. Mishin (1), O. Vasilyev (2) and T. Gerya (1)

(1) Department of Earth Sciences, ETH Zurich, Switzerland, (2) Department of Mechanical Engineering, University of Colorado, Boulder, USA (yury.mishin@erdw.ethz.ch / Fax: +41 44 6331065)

Calculation of phase diagrams for the Earth's materials exerts a growing impact in studying of core and mantle dynamics. Recently, the method for calculation of phase diagrams and related in situ properties of rocks (e.g. density, enthalpy, seismic velocity, etc.) in space of two variables (P, T) by using second generation 2D wavelets was proposed (Vasilyev et al., EPSL, 2004). Here we present further generalization of this approach to three dimensions. We employ combination of adaptive wavelet-based meshing technology and efficient "phase diagram function" designed as a Gibbs free energy minimization. The proposed automated strategy allows one to obtain equilibrium phase assemblages and related physical properties depending on three arbitrary variables (e.g. P, T, water activity). The use of this strategy captures very small details of phase diagram morphology allowing both acceleration of the calculations and efficient compression of the results.