Particle simulation of hydraulic fracture and sustainable geothermal reservoir fluid flow: towards realisation of a new green energy industry

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SUMMARY

Realising the potential of geothermal energy as a cheap, green, sustainable resource to provide for the planet's future energy will demand that a key geophysical problem be solved first: how to develop and maintain a network of multiple fluid flow pathways for the time required to deplete the heat within a given region. Without this pre-requisite, the enormous investment in research wells and networks of exploitation wells, establishment of above-ground infrastructure, and applied research for efficient stream-driven power plants would simply be wasted. In this paper, we propose that the key breakthroughs can be achieved by constructing a suitable micro-scale particle-based numerical model. Such a model will enable development of fracture systems to be simulated in discontinuous media, and studies to be conducted of the granular dynamics, elastic stress release, and grinding that occurs as fluid-injected joint surfaces slip; the consequent frictional heat generation and heat flow within the hot rocks; the heat exchange between the hot rocks and water within flow pathways; hydraulic fracturing; and fluid flow through complex, narrow, compact and gouge- or powder-filled fracture and joint systems. We propose further developing and applying the Lattice Solid Model for this purpose. Here, we focus on demonstrating the ability of this computational model to simulate the listed fundamental processes, which are all components of the geophysical problem that is crucial for realising this new green energy resource.

1. INTRODUCTION TO THE LATTICE SOLID MODEL

The Lattice Solid Model (LSM), was first developed by Peter Mora in 1992 at Institute de Physique du Globe (Mora, 1992; Mora & Place, 1993). The LSM was motivated by molecular dynamics principles with either particle interactions via Lennard-Jones potential functions or elastic-brittle bonds. The software shares similarities with the Discrete Element Model, but involves a different computational approach that is based on the use of large-scale supercomputer simulation via domain decomposition and parallel programming. The model was initially developed to study fracture, friction, rock rheology, tectonic processes and earthquake dynamics (Mora, 1992; Mora & Place, 1993; Mora & Place, 1994) As more physics was incorporated including heat flow, thermo-porous coupling, thermo-mechanical feedback, and additional degrees of freedom in 3D (tension, shear, torsion and bending) to ensure realistic fracturing behaviour, it became more powerful and was calibrated with laboratory experiments and used to study outstanding scientific research questions and the complex nonlinear behaviour of discontinuous solids including the Heat Flow Paradox in geophysics (), The LSM has since been developed as a parallel open-source C++ software system called ESyS_Particle. The initial team working on the LSM consisted of Peter Mora and his Ph.D. student (David Place), but rapidly grew into a major particle research group at Earth Systems Science Computational Centre (ESSCC) that was directed by P. Mora at the University of Queensland. Major contributors included Steffen Abe, Yucang Wang, Fernando Alonso-Marroquin, and Shane Latham, among others. The development of the ESyS-particle software infrastructure became funded by the Australian Computational Earth Systems Simulator Major National Research Facility established by P. Mora and a national group of solid earth systems simulation scientists. The ESyS-Particle software is available at: https://launchpad.net/esys-particle/ESyS-particle, which is a site maintained by Dion Weatherley with software developments contributed from around the world and by present and past ESSCC researchers. The initial particle simulation program of 1992 was written by Peter Mora in Connection Machine Fortran (CMF was a precursor to HPF and F90) at the IPG in Paris France and was called LSMearth. David Place worked on an accurate way to simulate inter-particle friction for his Ph.D. (Place & Mora, 1999), and Peter Mora then added frictional heating and heat flow. Subsequently, Peter Mora, David Place and Steffen Abe added random particle sizes (Place & Mora, 2001), thermo-porous and thermo-mechanical coupling effects (Abe et al, 2000), and proposed an efficient scheme to model arbitrary shaped angular particles (Abe & Mora, 2003).

LSMearth was redeveloped in C++ by David Place, and subsequently parallelised by Steffen Abe (Abe et al, 2004) and Shane Latham (Latham et al, 2005) using MPI into a highly efficient and usable tool, with various new micro-physics being added by a group of researchers and computational scientists under the direction of Peter Mora as part of the ACcESS MNRF. Around 20 researchers worldwide are currently contributing to ESyS-particle. Some of the most critical recent developments have been made by Yucang Wang and Fernando-Alonso Marroquin respectively to model the full set of degrees of freedom (six kinds of independent relative movements are transmitted between two 3-D interacting particles) needed to accurately simulate observed fracture patterns (Wang et al, 2006, Wang & Mora, 2008b; Wang, 2009; Wang & Mora, 2009; Wang & Allonso-Marroquin, 2009), and how to efficiently simulate complex particle shapes (Abe & Mora, 2003; Alonso-Marroquin et al, 2007; Alonso-Marroquin & Wang, 2009).. One of the major advantages of the discrete (LSM) model over the continuum models is that the large deformation and dynamics process associated with fracture phenomena can be easily modelled. It has been successfully utilised to the study of physical process such as rock fracture (Mora, 1992, Mora & Place, 1993; Place & Mora, 2001, Place et al., 2002, Wang & Mora, 2008b, Wang & Alonso-Marroquin, 2009), the stick-slip frictional instability and earthquake dynamics (Mora & Place, 1993; 199), the Heat-Flow Paradox (Mora & Place, 1996a; 196b;1997;1998;1999, Alonso-Marroquin et al, 2006), accelerating acoustic emmisions/energy release, Load-Unload-Response-Ratio and critical sensitivity prior to catastrophic failure and simulated earthquakes (Mora et al, 2000; Mora et al, 2002), earthquake physics and predictability (Mora & Place, 2002), , earthquake physics and predictability (Mora et al, 2000; Mora & Place, 2002), localisation phenomena (Mora et al, 1997; Mora & Place, 1999, Place & Mora, 2000), fault gouge evolution (Mora & Place, 1997;1999, Mora et al, 2000, Alonso-Marroquin et al 2006; 2007, Mair & Abe, 2008) and comminution in shear cells (Mair & Abe, 2008).

2. ELASTIC BEHAVIOUR OF REGULAR LATTICES

In the original Lattice Solid Model (Mora, 1992, Mora & Place, 1993;1994), the force between particles was specified by tensile and compressional interactions and can be written as

$$F_i = \sum_\alpha F_i^\alpha = \sum_\alpha k^\alpha ((\mathbf{x} - \mathbf{x}^\alpha) \cdot \mathbf{e}^\alpha - r) e_i^\alpha \ . \qquad (1)$$

Expanding in terms of a continuous differentiable displacement field yields

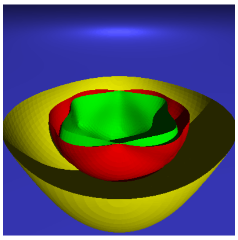
$$u_i^\alpha = u_i + \sum_k r e_k^\alpha \frac{\partial u_i}{\partial x_k} + \sum_k \sum_\ell \frac{r^2}{2!} e_k^\alpha e_\ell^\alpha \frac{\partial^2 u_i}{\partial x_k \partial x_\ell} \ldots , \qquad (2)$$

and using the relations $\sum_\alpha e_i^\alpha e_j^\alpha = \begin{cases} 3\delta_{ij} & \text{2D - Lattice} \\ 4\delta_{ij} & \text{3D - Lattice} \end{cases}$ and $\sum_\alpha e_i^\alpha = 0$ yields for the particle acceleration

$$a_i = \frac{F_i}{m} = \frac{c_{ijk\ell}}{\rho} \frac{\partial^2 u_j}{\partial x_k \partial x_l} \qquad (3)$$

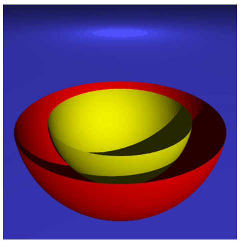
in the macroscopic limit where ρ is the medium density and the Hooke tensor is given by $c_{ijkl} = \frac{1}{\rho} \sum_\alpha k^\alpha \frac{r^2}{2!} e_i^\alpha e_j^\alpha e_k^\alpha e_\ell^\alpha$ which leads to isotropic elastic waves in a Face-Centered-hexagonal-cubic FCHC lattice with compressional and shear wave speeds given by

$$v_p = \sqrt{\frac{9}{8}} r \sqrt{\frac{k}{M}} \quad \text{and} \quad v_S = \frac{1}{\sqrt{3}} v_P \qquad (4)$$



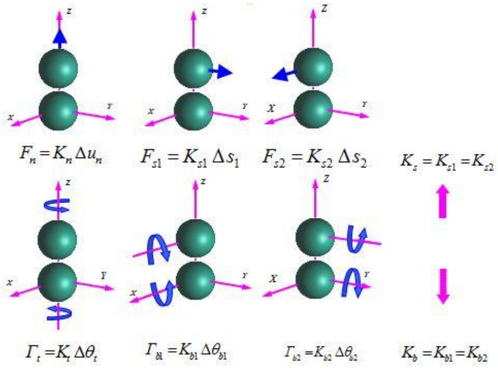
For a Face Centered Cubic (FCC) lattice, the wave speeds are anisotropic which can be obtained by using the unit vectors in the α–direction of the lattice denoted by the $\mathbf{e}^\alpha$ that specify an FCC instead of an FCHC lattice.

Phase velocity surfaces
for an FCC lattice.



Phase velocity surfaces
for an FCHC lattice.

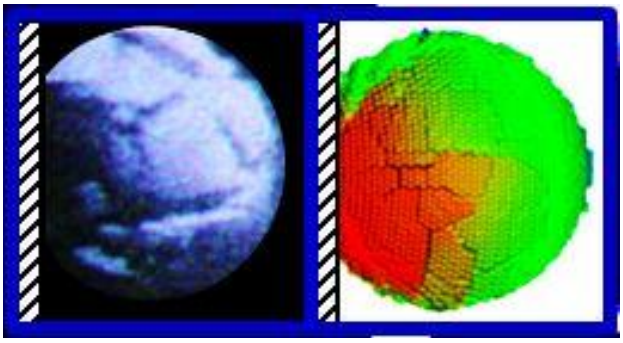
3. TENSION, SHEAR, TORSION AND BENDING DEGREES OF FREEDOM



The accurate modelling of realistic fracturing behaviour that matches with experimental laboratory data was only possible by including rotational dynamics as new degrees of freedom. This is illustrated in the Figure to the left. Details of the contact model are provided in the literature (Wang & Mora, 2008b, Wang & Mora 2009, Wang, 2009). Elastic properties in regular lattices have been derived in these cases (Wang & Mora, 2008a). As a test of fracture behaviour, we have accurately reproduced “wing cracks” that are observed in the laboratory (Wang & Mora, 2008b). ESyS_Particle has unique capabilities to model such wing cracks as all six degrees of freedom per particle are modelled to include contact forces, bending and twisting moments (Wang & Mora, 2009; Wang, 2009). The 2D example of wing cracks to the right is from Wang & Mora, 2008b.

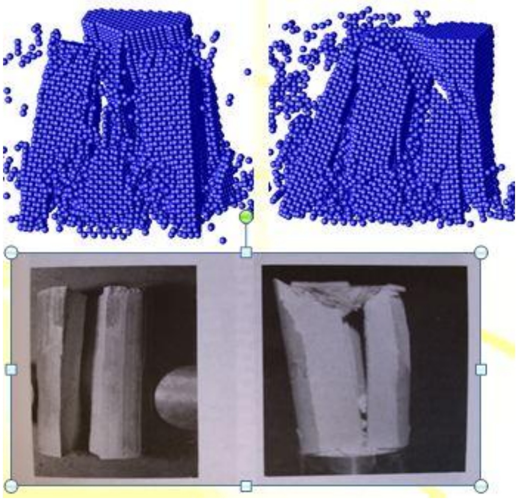
4. SIMULATION OF REALISTIC FRACTURING BEHAVIOUR

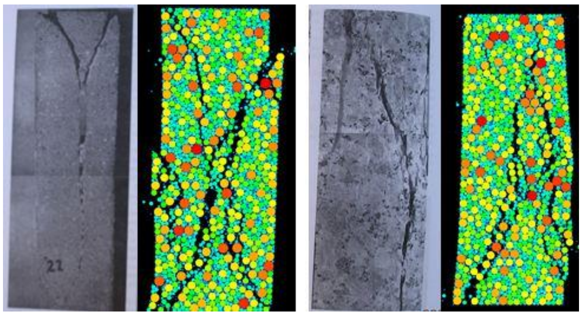
The examples below show 3D complex fracturing behaviour of a leftwards travelling impacting ball in a laboratory experiment (left plot, left panel) compared to a simulation (left plot, right panel). The right plot represents a 3D simulation result showing axial breakage (top right plot) compared to a laboratory experiment of axial breakage (bottom right plot) – see also Wang & Alonso-Marroquin 2008 and Wang & Alonso-Marroquin, 2009.



Lab result, from
M. Khanal, 2008.

Numerical result, from
Wang, 3D simulation
of brittle rock failure.





The examples shown on the right provide additional examples of the simulation of the development of brittle fracture systems and their close match to the patterns observed in laboratory experiments (Wang & Mora, 2008; Wang and Mora, 2009), and provides a further illustration that the Lattice Solid Model software system, ESyS-Particle, is capable of matching fracture patterns seen in laboratory experiments. Hence, implementations of the Lattice Solid Model including thermo-porous flow, frictional heat generation and heat flow, thermo-mechanical coupling effects and hydraulic fracturing, provide a unique platform for scientific breakthroughs on how to create and sustain the multiple fluid flow pathways required for proof of concept and development of the new geothermal green energy industry.

5. THERMO-PORO-MECHANICAL-COUPLING

ESyS_Particle allows calculation of heat produced by frictional dissipation. The heat flow equation is given by

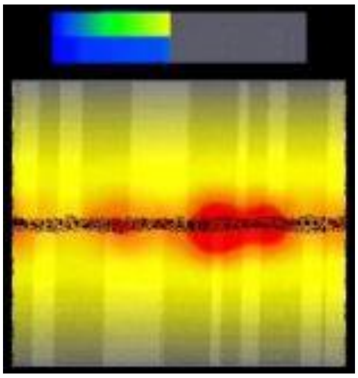
$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial \vec{x}^2} + \frac{1}{\rho c_p} H(\vec{x}, t), \qquad (5)$$

where H is the local heat production, κ is the thermal diffusivity, T is the temperature, ρ is the density and c_p is the specific heat of the rocks. Temperature is included within the lattice by using a two-step process. First we add the heat source term to each particle's temperature as

$$T_i(t) = T_i(t) + \frac{1}{\rho c_p} H_i(t) \qquad (6)$$

Then we transfer a fraction of the heat to adjacent particles in contact using

$$T_i(t + \Delta t) = T_i(t) + \xi \kappa \sum_j \frac{T_j(t) - T_i(t)}{r_{ij}^2} \qquad (7)$$



This two-step approach yields the heat-flow equation in the macroscopic limit (see Abe et al, 2000). An illustration of heat being generated on a fault surface as it slips due to the shear pre-stress exceeding the strength of the granular fault gouge zone (ie. the effective friction of the fault) is shown in the figure above (from Mora & Place, 1997; 1998). Frictional heat generated along the fault as it slips flows though the lattice and is depicted by yellows (warm) through to reds (hot). The upper rectangular bars represent temperature bars, with the upper one being the total theoretical heat within the model assuming the effective fault friction equals the inter-particle or intrinsic friction. The lower temperature bar is the measured total heat in the numerical model during the simulation, which shows a blue reading which is cool (cf. the upper bar shows a yellow reading half way through the simulation = warm). Hence, the effect of rolling and rotation of the angular gouge particles in the fault zone substantially decrease the heat generated along the fault, thus, together with other results, provide a possible explanation for the Heat Flow Paradox (Mora & Place, 1998; 1999).

The effect of temperature on pore fluid pressure can be modelled as Darcy flow using

$$\frac{\partial P}{\partial t} = \frac{\gamma}{\beta} \frac{\partial T}{\partial t} + \alpha_p \frac{\partial^2 P}{\partial \vec{x}^2} \qquad (8)$$

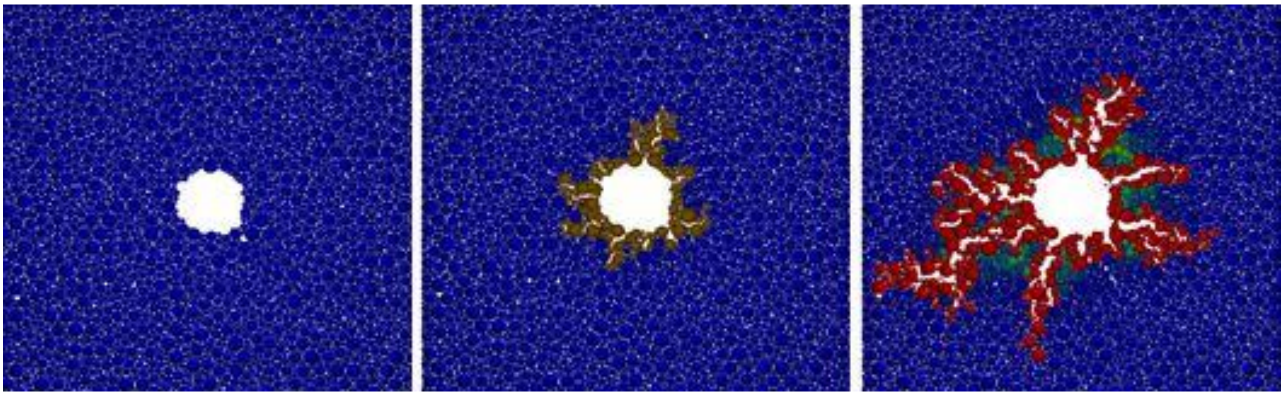
which has the same form as the heat- flow equation. Hence, Darcy flow in response for pressure gradients induced by thermal expansion of the pore fluid which can be modelled in the identical way as heat flow was modelled (see equation 5), but using different coefficients. ie. β is the compressibility of the fluid, γ is the thermal expansion coefficient of the fluid, and α_p is the Darcy diffusivity of the solid. The effective friction between fracture surfaces in contact is

$$\tau = \mu(F_n - P) \qquad (9)$$

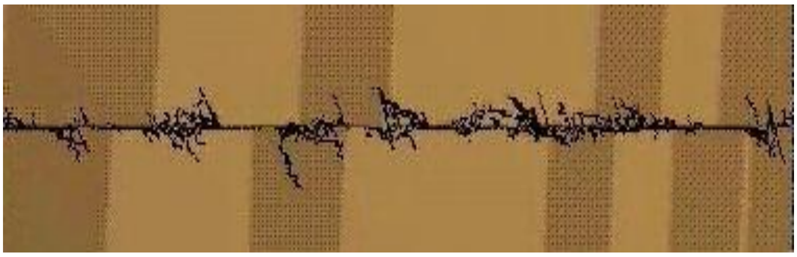
where τ is the shear stress between contacting particles, F_n is the normal force between particles, and P is the pore fluid pressure. Hence, according to equation 9, as the pore fluid is heated and becomes more pressurised, the effective friction of the fault or joint decreases, allowing further slip. In the case of a geothermal reservoir flow pathway, this additional slip would tend to increase permeability as the mismatch between joint surfaces increases. However, this increase in permeability is counter-balanced – at least to some extent – by the rubbing off of rock particles and powder which tends to fill the narrow fluid pathways along the joints, thereby decreasing the permeability. It would be the balance between these two effects that will determine whether fluid flow pathways can remain open long enough for the geothermal energy and reservoir system to be viable.

6. SIMULATION OF HYDRAULIC FRACTURING

The snapshots below (Wang, 2008) show a fluid filled void with pressure being increased and subsequent hydraulic fracturing and growth of complex fracture patterns as the pressurised fluid opens gaps and flows further into the opening fractures. This simulates the processes used in initiating flow in geothermal reservoirs except that the existing pre-stress and joint or fracture pattern has a controlling influence on the pattern of fracture growth in real cases. Nonetheless, this example illustrates the potential of the particle model to simulate the processes needed to solve the key geophysical problem that could unlock the pathway to successfully realising the potential of cheap, green ongoing energy resources through exploitation of geothermal reservoirs which requires ongoing fluid pathways to be established and maintained. Numerical experimentation using the particle model provides a means to solve this basic problem, and yield the breakthroughs required to make geothermal energy a reality.



The example to the right (Mora & Place 1997) shows the evolution of a fault gouge layer and off-branching fractures as the initial pre-existing joint surface slips. This slip is caused by the driving background shear stress field that is gradually increased to simulate the effect of increasing pore fluid pressure as water is injected into the reservoir system. This increased water pressure would push apart the joint surfaces and thus cause continued slip events leading to an increase in permeability along the fault as depicted above. However, as described previously, this increased permeability along the joints due to slip will be offset to some degree by the joint space becoming filled with fault gouge material as rock grains and powder rub off the adjacent joint surfaces during slip.



7. CONCLUSIONS

The Lattice Solid Model particle based method has the ability to provide breakthroughs in the understanding of the mechanical properties of hot rocks, their efficient fracturing, and the ability to produce sustained fluid pathways through the induced fracture network. In situ measurements to assess the fracture of rocks require theoretical interpretation of the energy budget and fracture propagation. These theories can be incorporated into a continuum model by interconnecting the length scales of fragmentation. Here particle-based models can be used to extract data of fracture creation that are subsequently passed to the continuum models (ie.

using up-scaling). This ab-initio approach has the potential to exploit a model of large-scale fragmentation based on processes at the smallest scale which represents an independent source of data more closely related to the complexity of fragmentation.

Further development and application of the thermo- and hydro-mechanically coupled ESyS_Particle simulation software system will benefit geothermal exploitation, by delivering new multi-scale, numerical capabilities to model fracturing, heat flow, and solid–fluid coupling; and hence, to model the generation and sustainability of the hot-fractured rock geothermal energy fracture systems required to exploit this new green-energy resource. This may prove to be the key to realising the vision of ongoing sustainable green geothermal energy to power the world!

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