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Reply on RC1

Maximilian O. Kottwitz et al.

Author comment on "Investigating the effects of intersection flow localization in equivalent-continuum-based upscaling of flow in discrete fracture networks" by Maximilian O. Kottwitz et al., Solid Earth Discuss., <https://doi.org/10.5194/se-2020-208-AC1>, 2021

We sincerely thank the anonymous referee for reviewing this manuscript. The constructive comments helped us to clarify the scope of our manuscript. Please find below a point-by-point response to the referees' comments with initial comments of the reviewer in italic and our response in normal font. As an alternative, we provided a color-coded PDF as a supplement.

On behalf of all authors,
Yours sincerely,
Maximilian Oskar Kottwitz

Scope and implicationns:

The one major comment I have is about scope. The authors very clearly lay out their theoretical and numerical arguments. What I was missing is a bit more on the scope and on how useful their methodology is for characterizing natural systems. Such a discussion should include a short review of how well and on which scales fracture networks can be characterized in the first place (e.g by geophysical methods and/or imaging techniques). I am mainly thinking about scales here. My understanding is that if samples can be CT-scanned (e.g. mm to cm-scales) direct flow simulations that resolve the actual fracture geometries would be performed without simplifying the fractures as simple geometric entities. Here flow at fracture intersections would be naturally resolved. On larger scales, the apertures of fractures are very hard to determine and consequently fractures are often represented in models as reduced-order elements – the DFN approach. It remained a bit unclear to me for which input datasets and flow simulation approaches, flow localization at fracture intersection really needs to be considered in the way the authors describe. The authors address these points in the discussion and conclusion sections, where they talk about system sizes but I think it would help the reader if the authors expanded this discussion.

We fully agree on the necessity to clarify the scope of our presented ECM approach and the scale dependence of IFL effects.
Generally, the structure of fractured systems is intrinsically multi-scale and thus requires different modeling approaches, broadly separated in direct- and continuum-flow

approaches. Direct flow simulations (using Navier-Stokes or Stokes equations) require an explicit representation of a medium's void space, which is only naturally retrievable by non-destructive imaging techniques (CT-scans, for example). However, they are limited to mm- or cm-scales, as you pointed out. Above these scales, pore-spaces cannot be imaged anymore (so natural data are not available) and direct-flow simulations become computationally infeasible to conduct. To be still able to simulate flow at scales above a few cm, we thus have to either use the DFN approach (if matrix is impermeable) or continuum-flow approaches. They average the hydraulics of any rock medium to an effective permeability tensor on the local scale (computational cell, size above 1 centimeter) to simulate flow on the global scale (meters to kilometers). So the ECM method used in this study only applies to these "continuum-scales" at which no direct representation of the medium's void space is possible.

To clarify this in the paper, we extend and partly rephrased the introduction from lines 28 to 33 according to:

"Numerical modeling of fluid flow is most accurately based on the Navier-Stokes equations (Bear, 1972). For a single phase of incompressible and iso-viscous fluid in an iso-thermal system, they simplify to the Stokes equations if laminar flow conditions are considered (i.e., Reynolds numbers below 1 -10). Assuming an impermeable rock matrix, one can solve for the velocity distribution resulting from prescribed pressure boundary conditions, allowing to determine the rock's effective permeability utilizing Darcy's law for flow through porous media (e.g., Andrä et al., 2013b; Osorno et al., 2015; Eichheimer et al., 2019, 2020; Kottwitz et al., 2020). Those so-called direct-flow modeling approaches crucially rely on a digital representation of a rock that separates pore-space from the matrix, which results from high-resolution X-ray computed tomographies (Andrä et al., 2013a; Cnudde and Boone, 2013). However, they are limited in maximum scannable size and respective trade-off to numerical resolution, making them applicable to small scales only (nanometers to a couple of centimeters at most). At larger scales (above a couple of centimeters), so-called continuum-flow approaches serve to model fluid flow, usually based on the concepts for flow through porous media proposed by Darcy (Darcy, 1856). Instead of a representation of the medium's pore-space, they require an initial hydraulic representation of the medium. This is given by prescribed effective permeabilities for certain control volumes within the medium, which upscale hydraulic properties from smaller scales to observation scales. Thus, the key of this so-called upscaling problem (e.g., Zhou et al., 2010; Hauge et al., 2012; Lie, 2019) is to adequately represent the rock structure with an appropriate model of effective permeabilities, which for fractured rock masses is often cumbersome due to their structural heterogeneity (Dershowitz and Einstein, 1988; Odling et al., 1999). The main problem is that acquiring detailed natural fracture data in 3D is intricate, as seismic imaging techniques suffer from resolution limits (Cartwright and Huuse, 2005; Malehmir et al., 2017), preventing a multi-scale structural assessment of individual features in fracture formations. Hence, outcrop (2D) and borehole (1D) studies are the only possibilities to acquire detailed natural fracture data, despite their reduced dimensionality (Lei et al., 2017), and acquiring deterministic knowledge of all individual structures in a fracture formation is impossible. Due to this, the discrete fracture network (DFN) method has been extensively used as a conceptual framework to provide statistically-based approximations of real fracture networks for decades (Long et al., 1982; Cacas et al., 1990; Bogdanov et al., 2003; Darcel et al., 2003; Xu and Dowd, 2010; Davy et al., 2013; Maillot et al., 2016). In this approach, each fracture in a given network is represented with a reduced order object (lines in 2D and discs or rectangles in 3D) with a prescribed location, size, and orientation. Naturally measured structural properties like size- and orientation-distributions (Odling et al., 1999; Healy et al., 2017), as well as fracture density and spacing (Ortega et al., 2006), serve as a quantitative basis to prescribe their geometrical properties (e.g., Hyman et al., 2015; Alghalandis, 2017)."

In this paper, we demonstrated and quantified the effects of IFL on the permeability tensor at the local scale by conducting direct-flow simulations at scales where it is possible to conduct those (1cm system size) while maintaining a sufficiently high numerical resolution to ensure the accuracy of the results. Based on these results, we demonstrated that a fracture-and-pipe parametrization as presented here results in a more accurate representation of the local scale hydraulics than a fracture-only parametrization (usually considered in comparable studies from the literature). Admittedly, we only briefly discussed the importance of IFL effects at the global scale, where we predominantly focused on the resolution dependency of current ECM methods. We thus performed a more sophisticated parameter study of IFL effects on network-scale permeability to extend the discussion part of this study. As this was also the main request of the second reviewer, we would refer to our reply to the review of the second reviewer at this stage.

Another point that the authors may want to discuss is if their effective permeability models also preserve other properties, like e.g. break-through times, spatial pressure variations, and solute transport pattern. It's a bit outside the scope of the paper, so the authors do not need to do this – I just kept thinking that break-through times would probably be affected for fracture networks where ILF matters.

This indeed represents an exciting question as solute or particle transport tend to be sensitive to local permeability variations. For example, Makedonska et al. 2016 (DOI: 10.1016/j.advwatres.2016.06.010) have shown that early breakthrough times are sensitive to local changes of permeability, induced by in-fracture aperture variability. However, addressing this issue in more detail requires the solution of the transport problem, and this is – as you already pointed out – outside the scope of this paper but could be the scope of a follow-up study. We added the following statement to the conclusion part at Line 351:

“Analyzing the effects of IFL on mass transport through fracture networks poses an interesting question for a follow-up study. For example, Makdonska et al., (2016) have shown that early breakthrough times of solute transport through kilometer-scale DFNs are sensitive to local permeability fluctuations. Thus, local permeability increases induced by IFL could potentially affect transport behavior as well.”

Minor technical points:

l. 7: It's not really a problem to include matrix properties in full Stokes simulations. All major CFD packages involve multi-physics solvers that can handle energy or mass exchange between solid and fluid regions. Maybe unnecessary to make this statement here?

In full Stokes simulations, the viscosity of the matrix is significantly larger than that of the fluid (usually water), which is why it makes sense to assume the matrix to be rigid and only simulate the motion of the fluid through the pores/cracks. However, we are aware that the major commercial CFD packages indeed have the possibility to include matrix properties (by using hybrid formulations based on the Stokes-Brinkman eq., for example). The situation is different when performing Darcy-like continuum-flow simulations in fractured reservoirs, where the matrix can indeed be incorporated in a straightforward manner. Including such matrix properties in fracture network simulations is actually one of the significant advantages of continuum flow methods (e.g., ECM method) compared to discrete flow methods in fracture networks (e.g., DFN method), which assume the matrix to be impermeable.

We rephrased the abstract starting at line 7 to:

“While continuum methods have the advantage of lower computational costs and the possibility of including matrix properties, choosing the right cell size to discretize the

fracture network into an ECM is crucial to provide accurate flow results and conserve anisotropic flow properties.”

l. 12: I assume the authors coined the term "intersection flow localizations (IFL)" if so, please make it clear that this is your invention and not something that's established in the literature.

Yes, we haven't found it elsewhere. Thus, we changed line 12 to:

"... in a process, we term intersection flow localization (IFL)."

l. 28f: Maybe expand this, to make it clear how natural fracture networks can be characterized?

See our answer to the first comment, where we indicated an extension of the introduction regarding this and multi-scale modeling approaches.

l. 64: Are you sure pflotran and modflow have these shortcomings?

Modflow was recently extended with the "XT3D" option in their Node Property Flow Package (Modflow 6, see <https://pubs.er.usgs.gov/publication/tm6A56>). By that, they enable incorporating a full three-dimensional permeability tensor into the simulations at the cost of an increased local stencil in their staggered-grid finite-difference discretization scheme. However, up to now this still runs sequentially and not in parallel, making it difficult to conduct high-resolution simulations.

Pflotran on the other hand is massively parallelized by utilizing the PETSC interface to MPI, but until now doesn't have the possibility to include permeability tensors at the local level. Hence the flow-solver we developed combines the advantages of both codes. We rephrased line 64 accordingly:

"There, current issues in commonly used 3D flow solvers, such as PFLOTTRAN (Lichtner et al., 2016) are a lack of a fully anisotropic permeability representation at the local cell level. So-called stair-case patterns ... predicting effective permeabilities of fractured media. On the other hand, MODFLOW (McDonald and Harbaugh, 1988) introduced support for local permeability anisotropy but not within a massively parallelized framework, making it difficult to conduct large numbers of high-resolution simulations. However, assessing permeabilities in a Monte-Carlo-like framework (e.g., de Dreuzy, 2012) is necessary to explore the variance of hydraulic system properties induced by stochastically generated input data. Hence, a flow-solver that combines the advantages of local permeability anisotropy and massive parallelization should be beneficial for numerical permeability assessments of fracture networks."

Equation 4: Shouldn't there be a length scale over which the pressure drop ΔP occurs?

Correct – thanks for pointing this out. Accidentally, we confused the delta sign with the gradient operator, which intrinsically incorporates length scale measures. We added length-scale parameter (L) accordingly in equations 4,5,6 and 8.

l. 256: Maybe expand what's in this SKB 2010 reference? This is the only place where you talk about naturally systems; I think it would help to be more specific.

The two test cases we generated to demonstrate the resolution dependency of ECM upscaling methods could have been chosen completely arbitrarily, as our main intention was to put the ECM method at test and not targeted to characterize peculiar natural systems. Discussing the applicability of the DFN method to characterize natural systems is, of course, a highly relevant question (issues of fracture terminations or spatial

clustering, for example) and still an ongoing research topic, but out of the scope of this study. The accuracy of the ECM method to predict network permeabilities is strongly depending on the quality of the input DFN, which itself is always a question of available data and resources to acquire this data. To clarify this, we added the following line to the conclusion at line 356:

"It is important to note, that the accuracy of ECM methods to predict flow are always linked to the quality of the input DFN. Improving the DFN method to better characterize natural fracture systems, especially in terms of fracture termination rules and spatial clustering, is still an ongoing topic of research."

Only for the sake of comparability we have chosen to use similar input data as provided by the DFN/ECM comparison study of Hadgu et al. (2017). Their input data were based on measurements reported for the cited SKB project, but strictly speaking generic, as they slightly manipulated the data (as written in table 1 of their study). We thus rephrased line 256 to:

"For comparability reasons, we use similar input data as Hadgu et al.(2017), who separated all fractures into three orthogonal sets, based on the data reported in SKB (2010)."

l. 390: are these really nodal velocities? Or rather cell (integration point) velocities (as stated in the next line)?

You are right, these are actually velocities in the integration points. The nodal Darcy velocities are then averaged from the surrounding integration point velocities. We changed line 389 accordingly:

"Following this, we evaluate the Darcy velocities at the integration points u based on the newly solved nodal pressures by: ..."

Please also note the supplement to this comment:

<https://se.copernicus.org/preprints/se-2020-208/se-2020-208-AC1-supplement.pdf>