High-Performance computing for reactive flow and transport

Tony Ladd
University of Florida

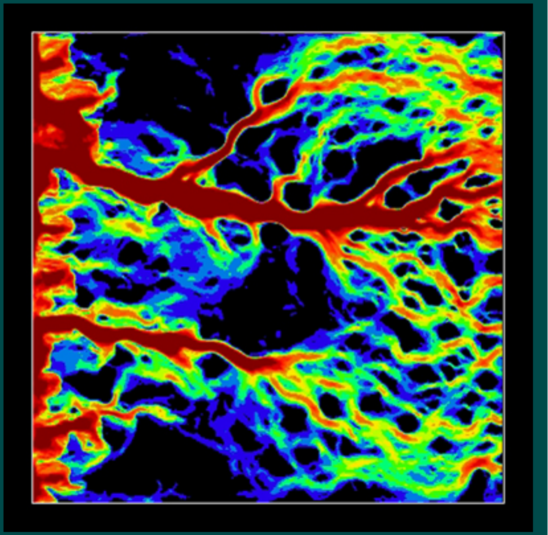
Piotr Szymczak
University of Warsaw

US DOE Geosciences (DE-FG02-98ER14853) and
Polish Ministry of Science and Higher Education

Evolution of fracture permeability

- How does fracture permeability evolve when there is dissolution – Sequestration

- Coupling between erosion and transport



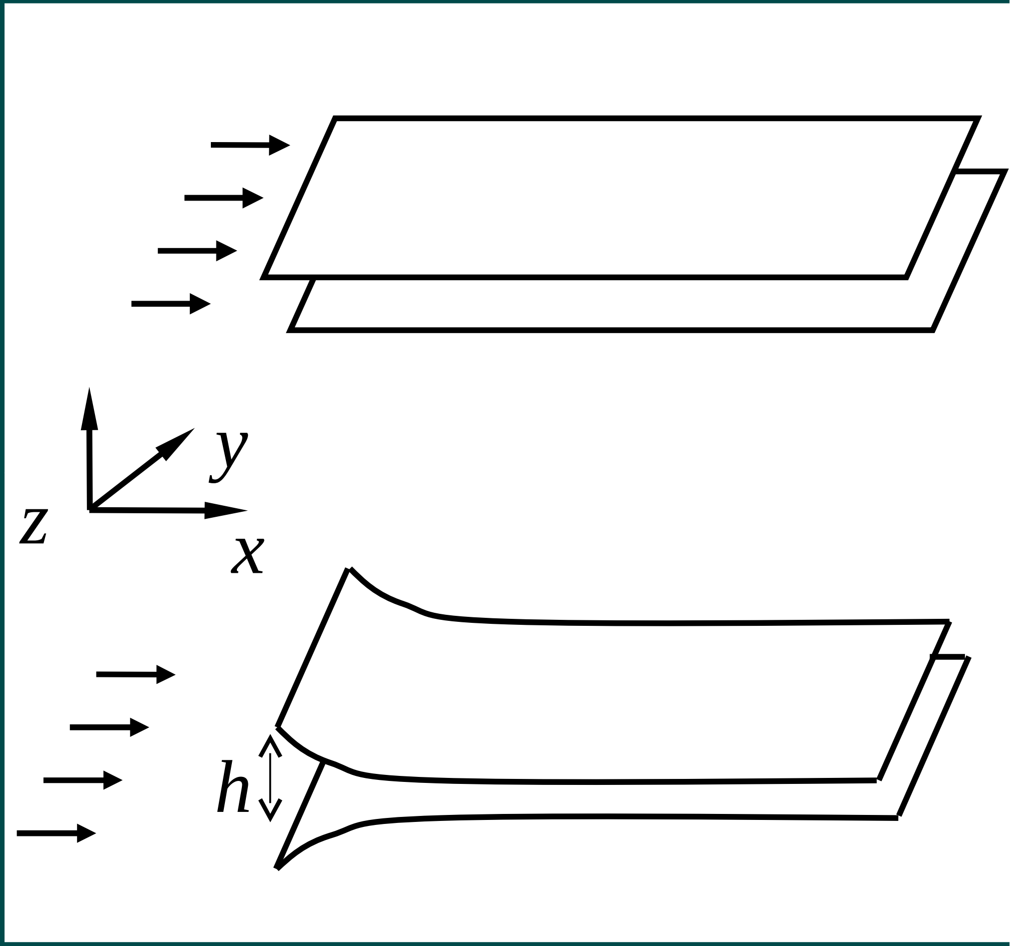
- Highly localized regions of porosity

- What is the essential physics?

- How can we make models at reservoir scale?

One-dimensional approach

- Used in fracture-network models – $Q \sim h^3$
- Uniform initial aperture
- Fracture opens uniformly

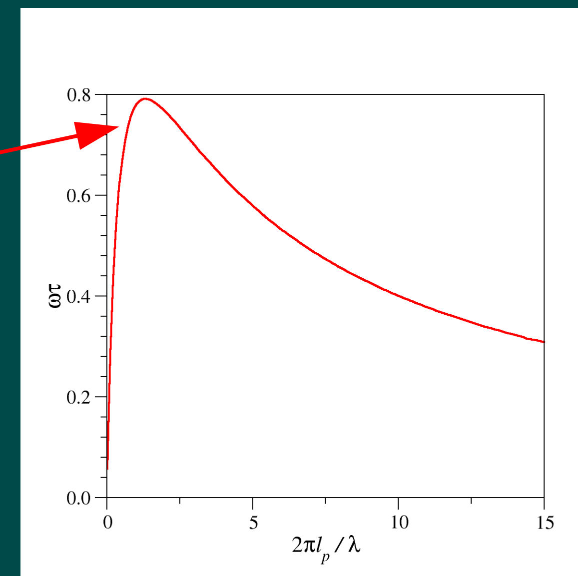


Dreybrodt, Water Resourc. Res., 98, 639, 1990, *ibid*. 32, 2923, 1996; Groves and Howard, *ibid*. 30, 607, 1994

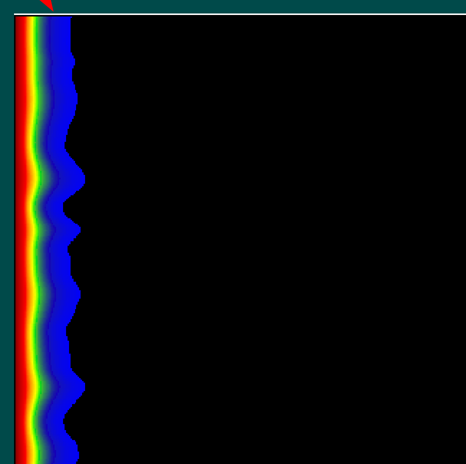
What actually happens

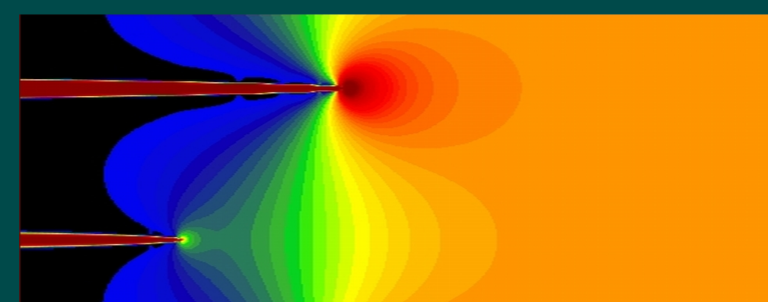
- Highly localized growth of fracture aperture
- Much more rapid penetration and breakthrough

Towards a macroscale model of evolving fracture permeability

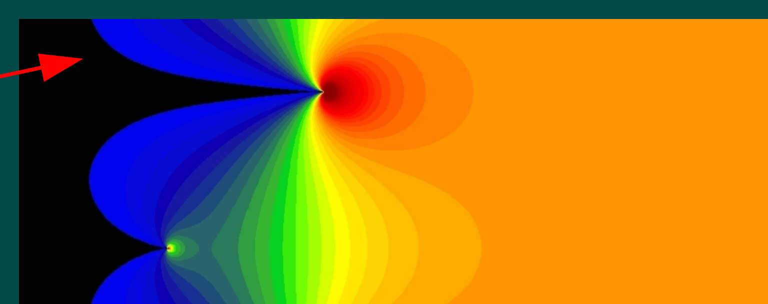


- Linear stability analysis:
- Wavelength selection!
- Initial wavelength and growth rates





- Later times
- Laplacian growth
- *p*-field from conformal map

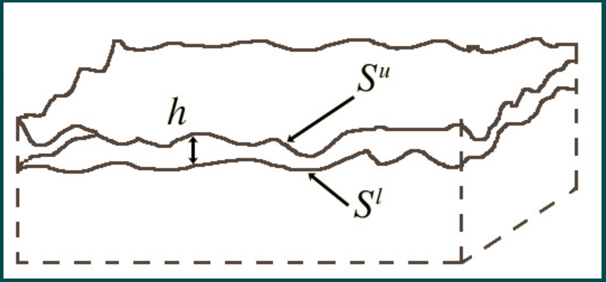


Numerical simulations

- Provide key insights – such as universal instability of fracture dissolution
- Data to verify and refine theoretical ideas
- 2D simulations – simple and relatively fast
- 3D simulations – most accurate and detailed information

2D simulations – depth-averaged fields

- Reynolds approximation for flow



$$\nabla \cdot (hu) = 0, \quad u = \frac{h^2}{12} \eta \nabla p$$

- Convection-Diffusion-Reaction for transport

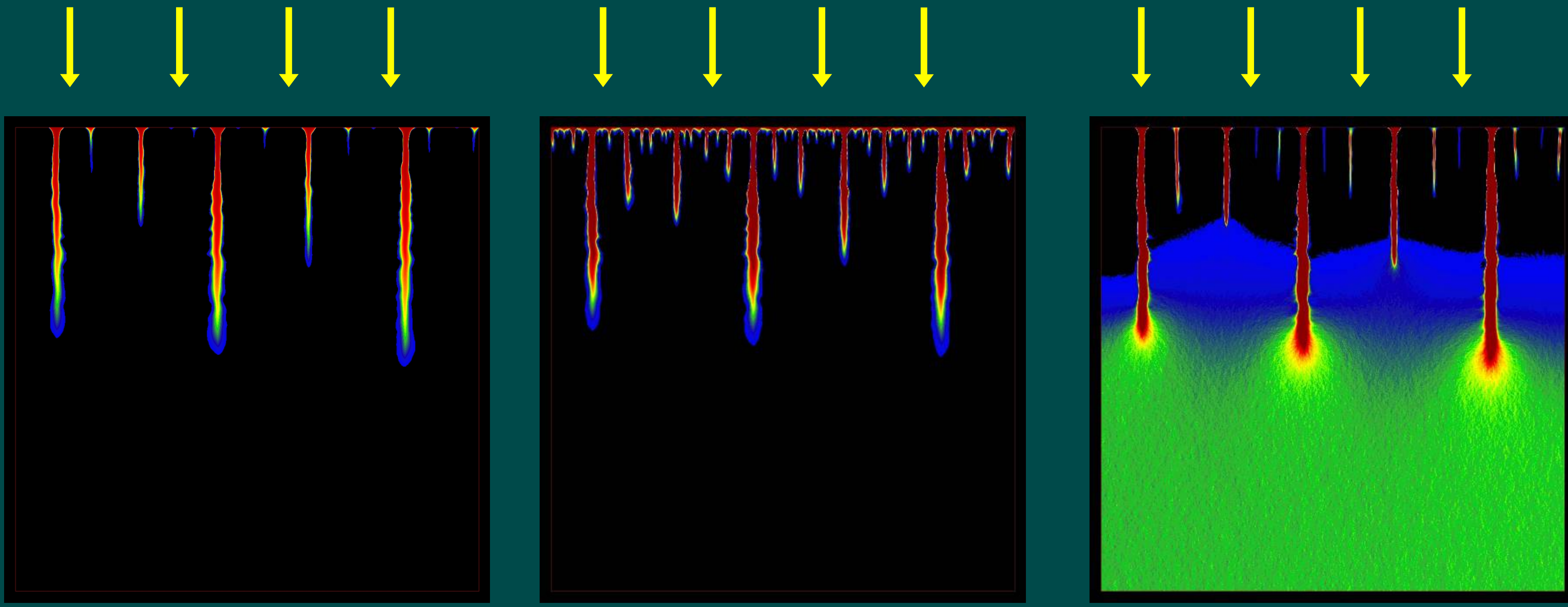
$$\nabla \cdot (huc) = \nabla (Dh) \nabla c + R(c), \quad R(c) = 2k(c_{sat} - c)$$

- Erosion (aperture opening)

$$\frac{dh}{dt} = \gamma R(c), \quad \gamma = \frac{c_{sat}}{c_{sol}}$$

Cheung and Rajaram, GRL, 22, 2075, 2002
Detwiler and Rajaram WRR., 43, W04403, 2007

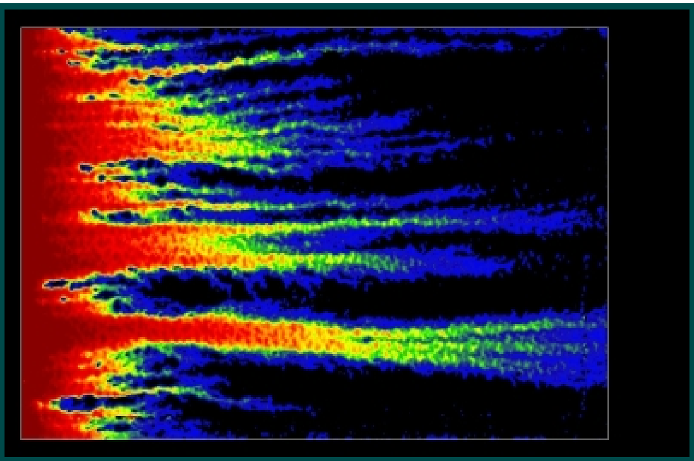
2D simulations of channel growth



concentration aperture flow

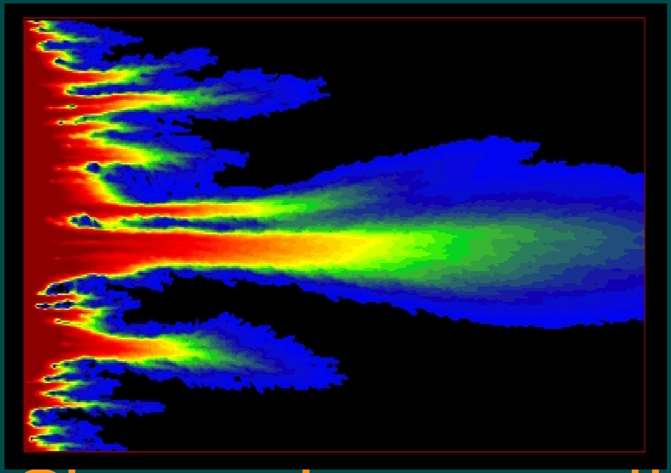
Dissolution rates in the channels are much larger than in the matrix – flow is focused in the channels

3D simulations – explicit fracture topography



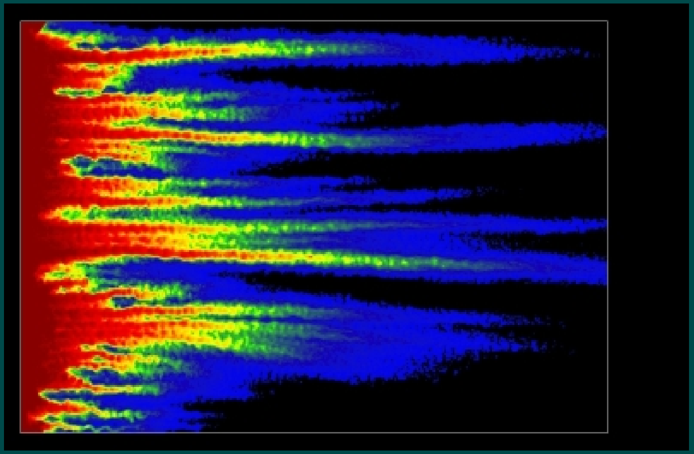
experiment

2D



Channels more diffuse, tendency to merge

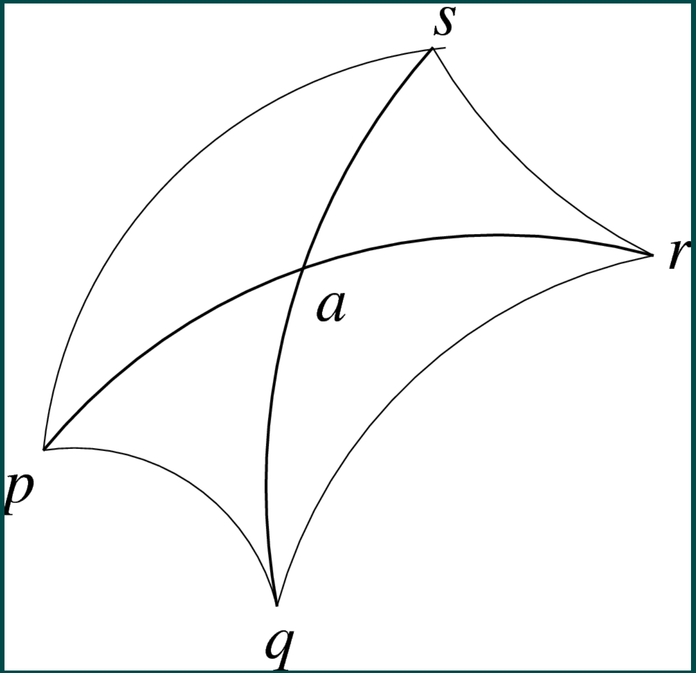
3D



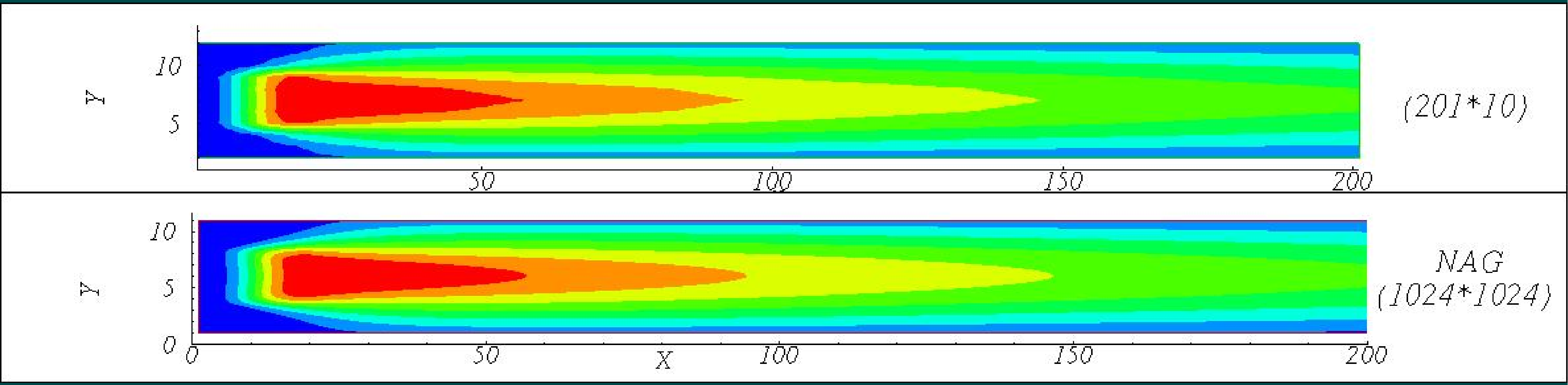
More accurate, but only feasible for laboratory scale

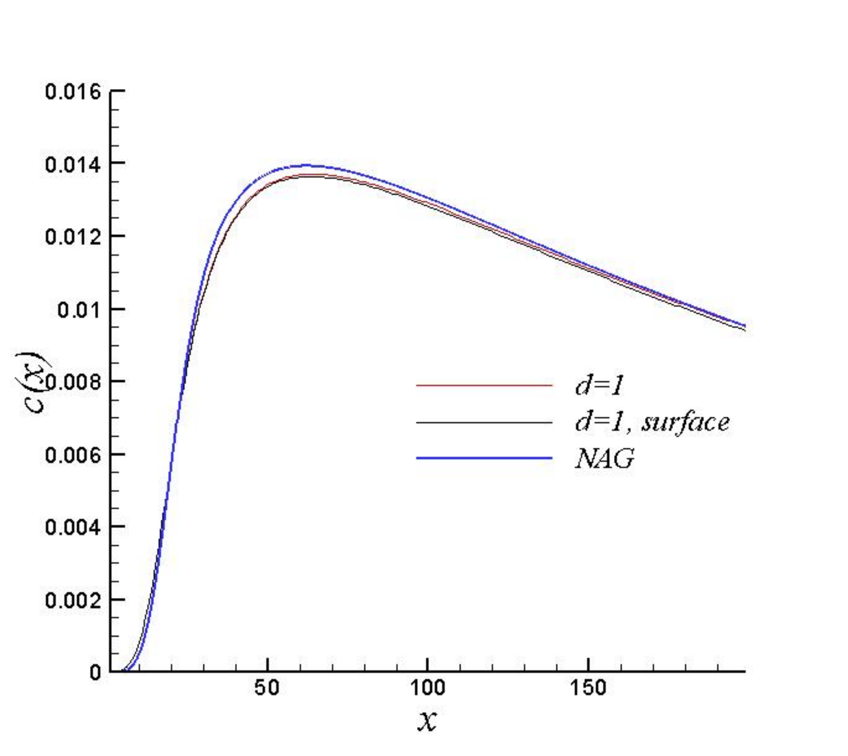
Geometry – defined by surface intersections with grid (marker positions)

- Markers moved along the normal direction
- Local Bezier surfaces around *a*
  - New positions – old normals
- Find intersection of the grid line *a* was on with Bezier surface – new position of *a*.
- Occasionally markers disappear (no intersections)
- New markers are placed by interpolation when needed



Channel flow test: *Pe* =125 *Da* = 0.08

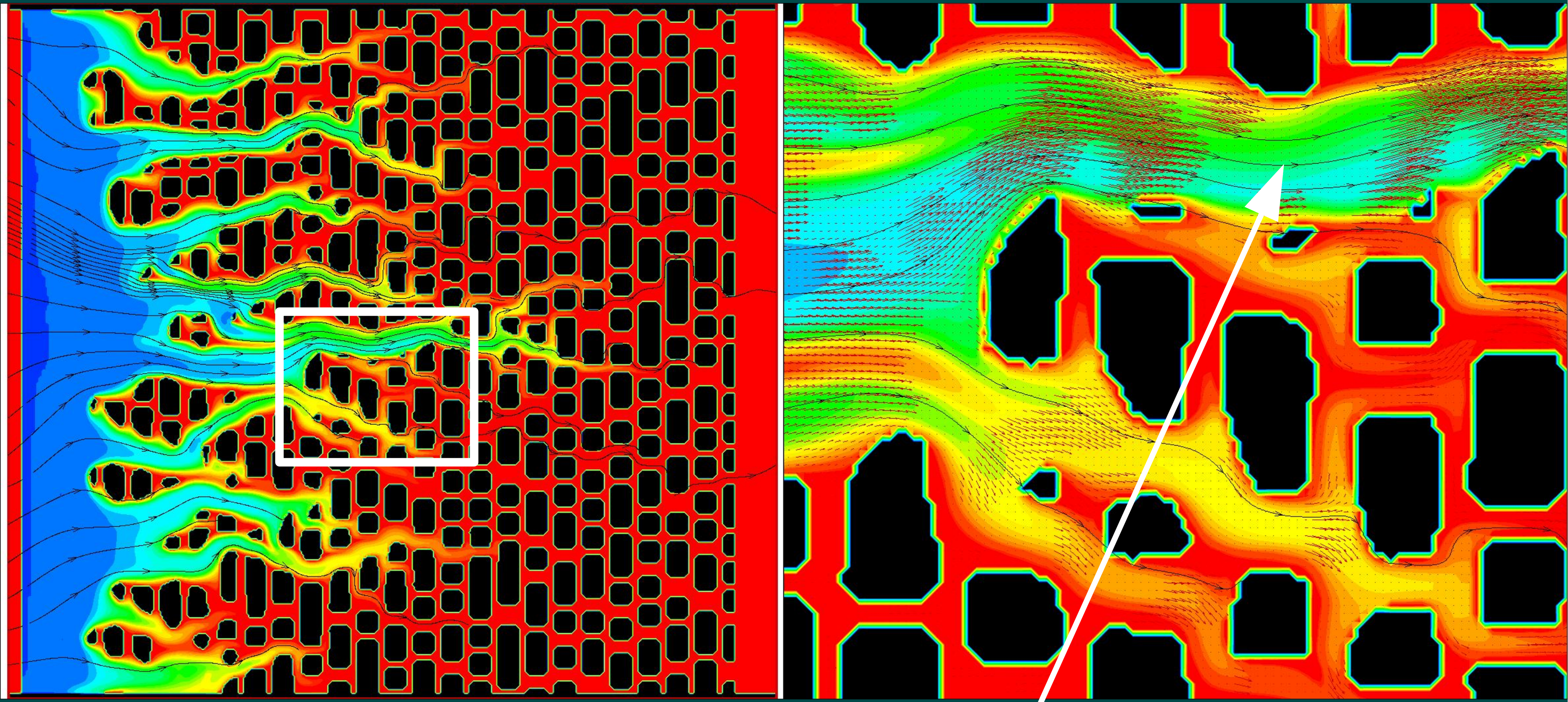




Quantitative agreement with NAG solver at different surface positions

10 grid points across channel

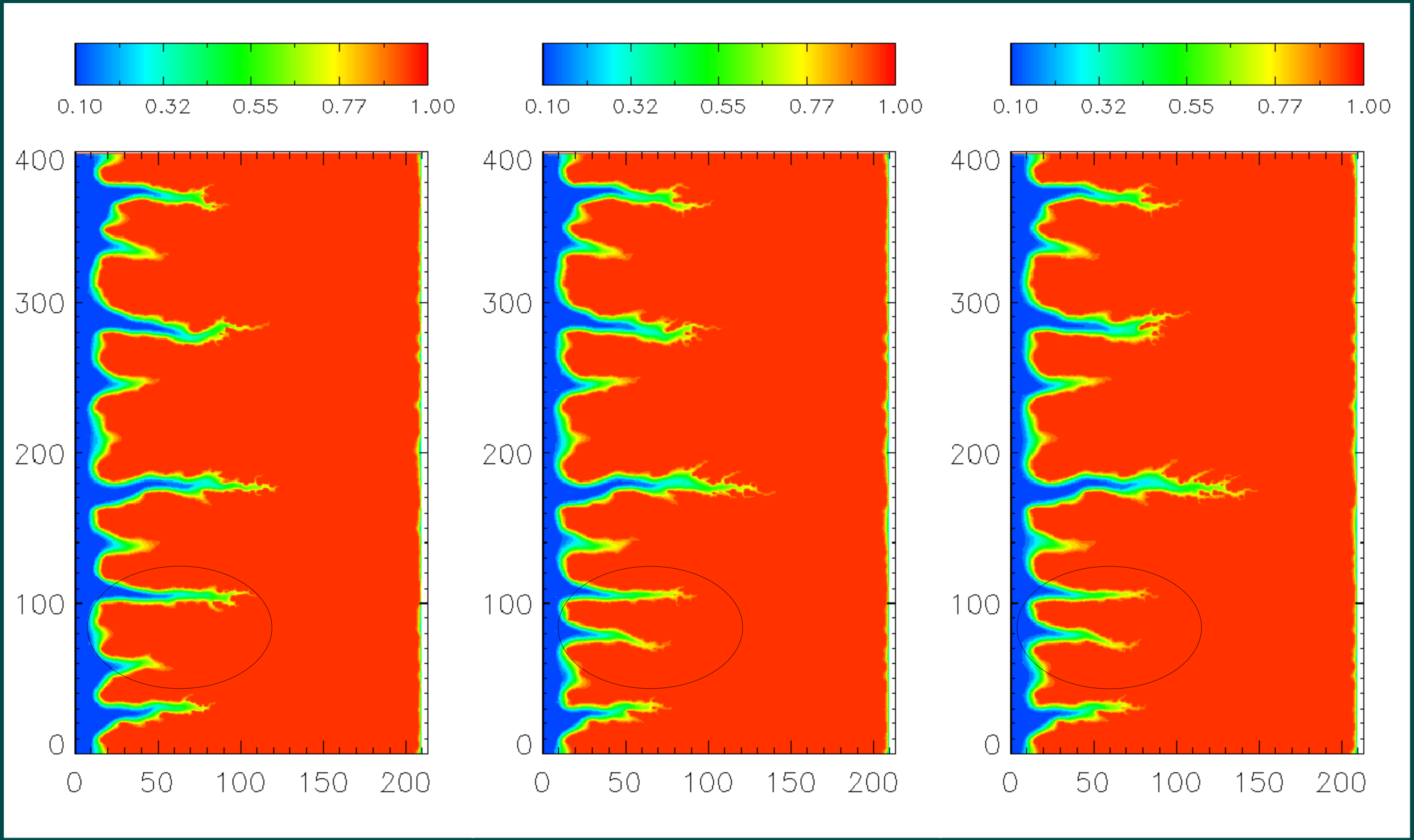
Detailed velocity and concentration fields



Velocity field is *not* 2D: strong 3D variations

(Image not accurate representation of surface position)

Convergent simulations of erosion



Conclusions

- Pursuing a theoretical and computational approach to understanding evolution of fracture permeability
- LSA suggests universal dissolutional instability
  - Peak growth rate – wavelength selection
- 2D modeling at laboratory and field scale
- 3D modeling limited to laboratory scale at present

HPC – current

- Current system – 128 cores (128GByte) Gigabit
  - Scaling up to ~ 100 cpus

- Field scale in 2D – 10^9 grid points (1km x 100m)
  - Large sparse matrix solve ($N = 10^9$)
  - 100GByte + 1-10 Pflop

- Lab scale in 3D – 10^8 grid points (10cm x 10cm)
  - 100GByte + 10-100 PFlop

HPC – future

- Future local system – 256 cores (192GByte) IB

- Lab scale in 3D – 10^9 grid points (10cm x 10cm)
    - 100GByte + 100 Pflop

- NERSC
    - Wall clock time 500 – 1000 hours per year
    - Software support – programming expertise
    - Collaborations with national labs?