Some Issues in the Mathematical and Computational Modeling of the Earth's Subsurface

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The subsurface includes

- vadose zone
- aquifers and petroleum reservoirs
- volcanism
- earthquakes and crustal dynamics
- mantle dynamics
- etc.

Importance to Society

Societal Impact

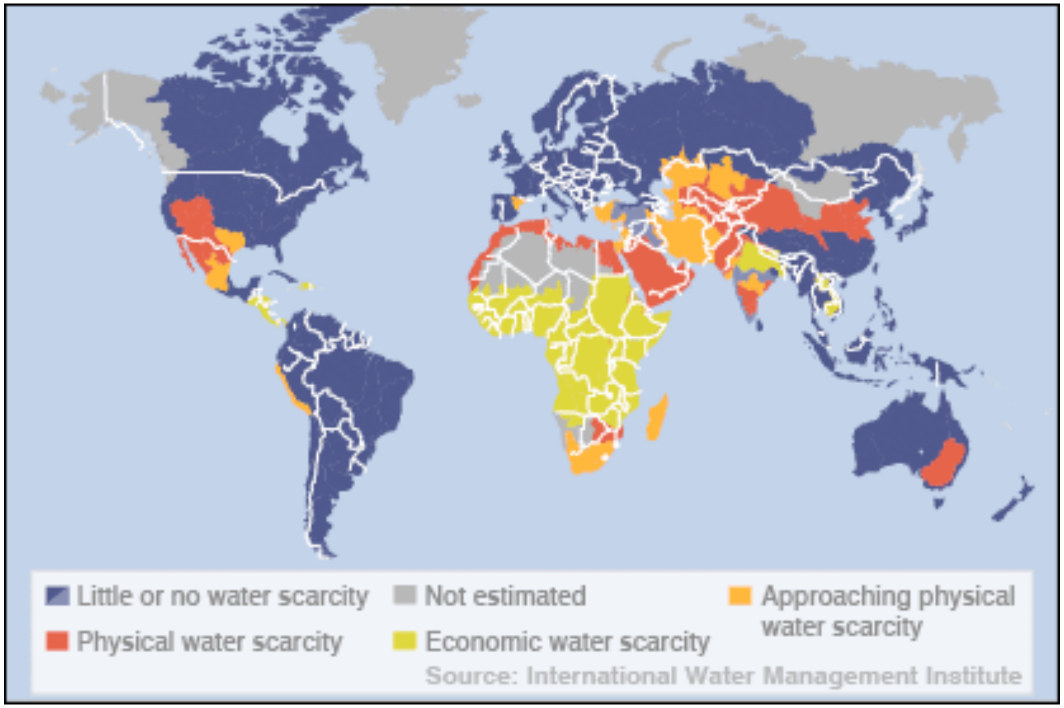
Accurate modeling of subsurface flow is important for:

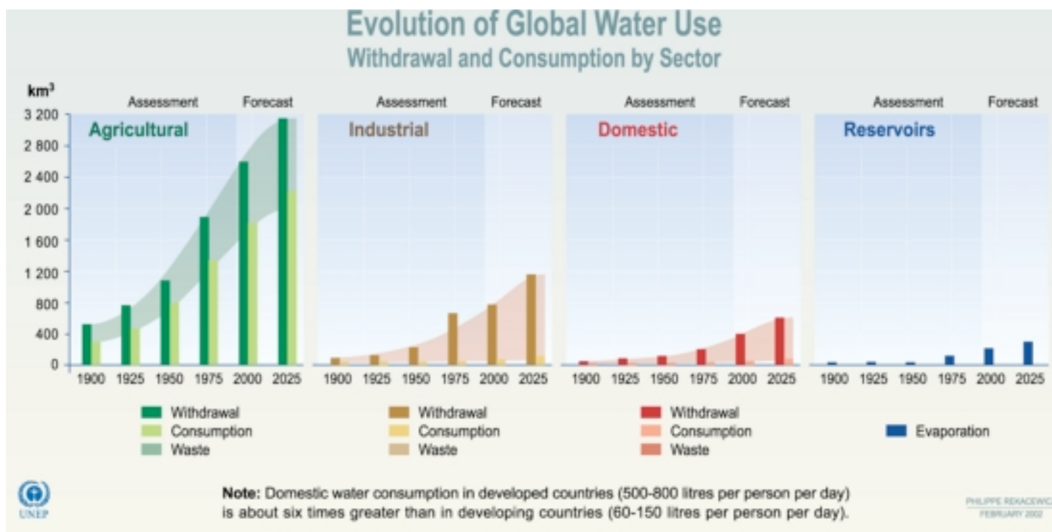
1. Groundwater management and contaminant clean-up (sustainability)
2. Energy production (petroleum and geothermal) (unsustainable)
3. Geologic carbon sequestration (bridge technology)
4. Minimizing damage from earthquakes and volcanoes
5. Spin-off technology related to porous media in general
6. Scientific understanding of the Earth's interior in general

Note the:

- Ties to Atmosphere and Ocean modeling
- Requirement for geophysical characterization

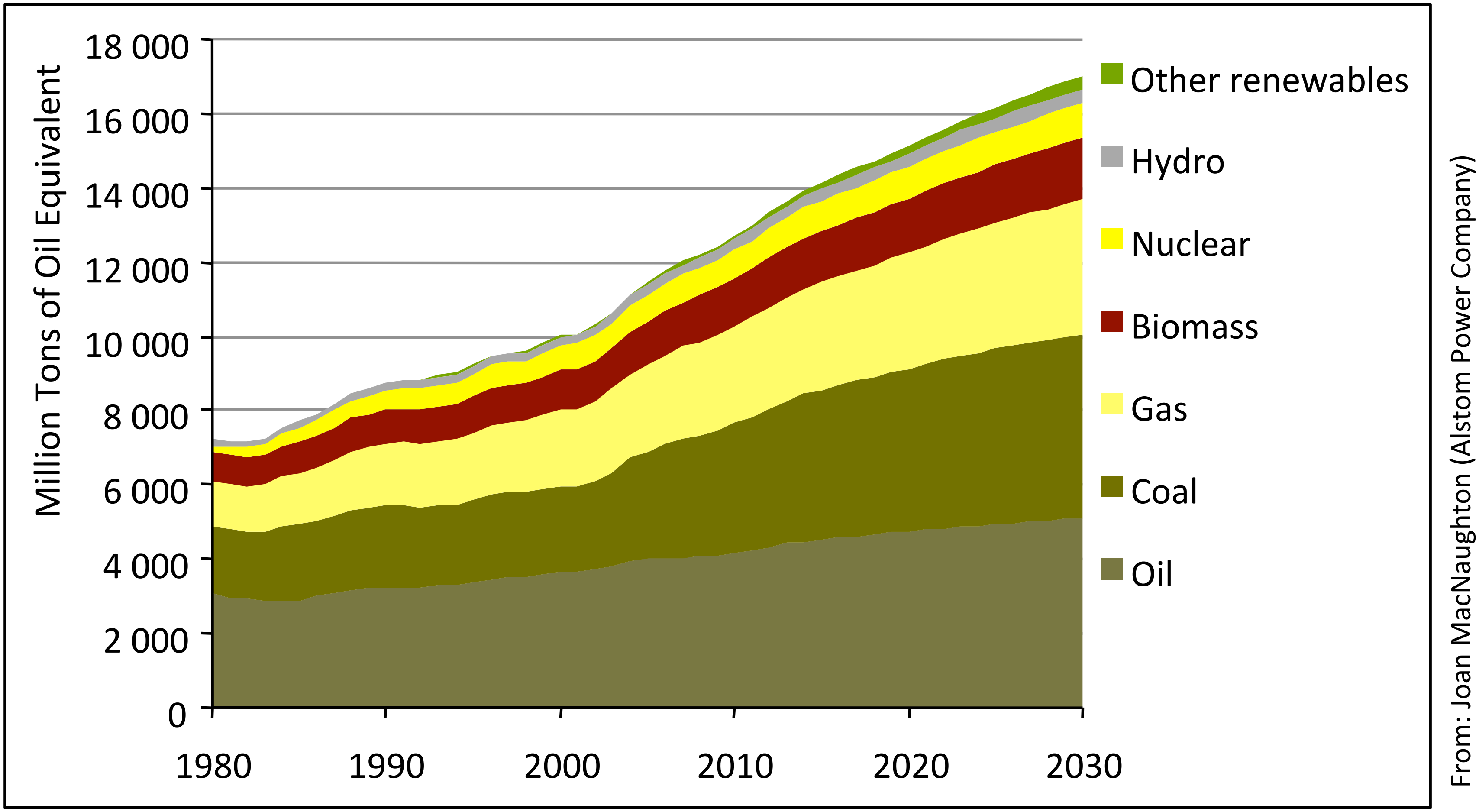
World Stress on Groundwater Resources





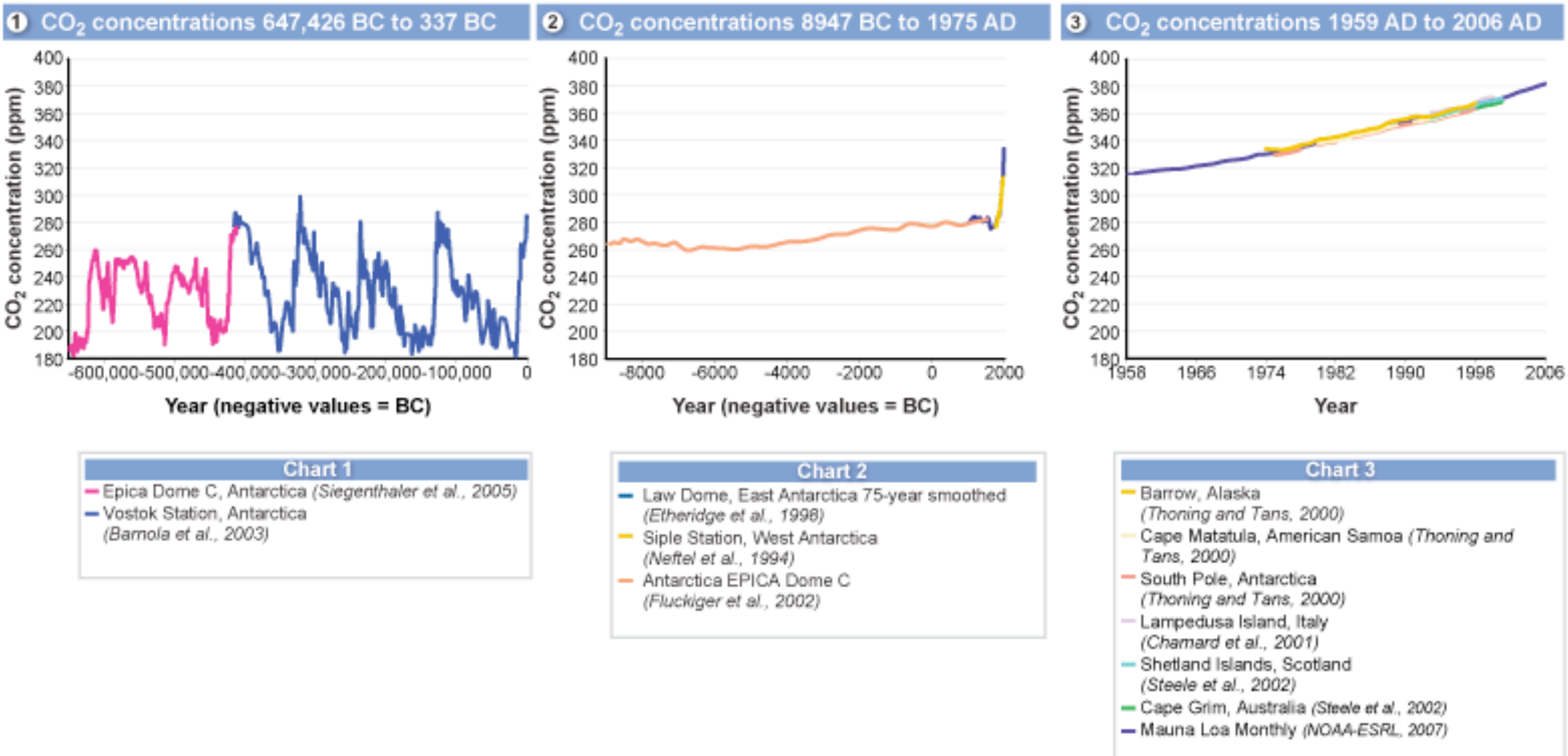
Source: Igor A. Shiklomanov, State Hydrological Institute (SHI, St. Petersburg) and United Nations Educational,Scientific and Cultural Organisation (UNESCO, Paris), 1999.

World Energy Demand (Fossil and Nuclear Fuels)



World energy demand is expected to expand by 45% between now and 2030 — an average rate of increase of 1.6% per year — with coal accounting for more than a third of the overall rise

Historic Atmospheric CO_2 Levels



Environmental Protection Agency

The Need for Scientific Computation

Engineering: High fidelity multiscale and multiphysics simulation of

- multiphase flow and transport;
- geochemical reactions, mineralogy, and phase behavior;
- geomechanical deformation

is a tool that has the potential to improve the design and monitoring, and reduce risks, of mankind's interaction with geological formations.

Computational simulation may be the *only* means to account for:

- the lack of characterization of the subsurface environment;
- the complexity and multiscale nature of many interacting processes;
- the large size of deep reservoirs;
- the need for long time predictions.

The ultimate goal is to achieve predictive simulations useful to decision makers, so engineers can reliably predict, control, optimize, and manage human interaction with geosystems.

Science: To test hypotheses and understand the basic behavior of complex geosystems, including those in the deep Earth.

Some Recent Advances

Categories

1. Flow
2. Transport
3. Reactions
4. Geomechanics
5. Quasi-continua
6. Mathematical analysis
7. Uncertainty
8. Education

Flow: Modeling Subsurface Heterogeneity

Problem: Accurately model the flow of fluids in highly heterogeneous rocks. Full resolution requires too fine a computational mesh to be practical.

Progress: Multiscale finite elements.
Compute over a coarse mesh using "multiscale" finite elements that approximate the solution internal to the element but relax the approximation on the interfaces.

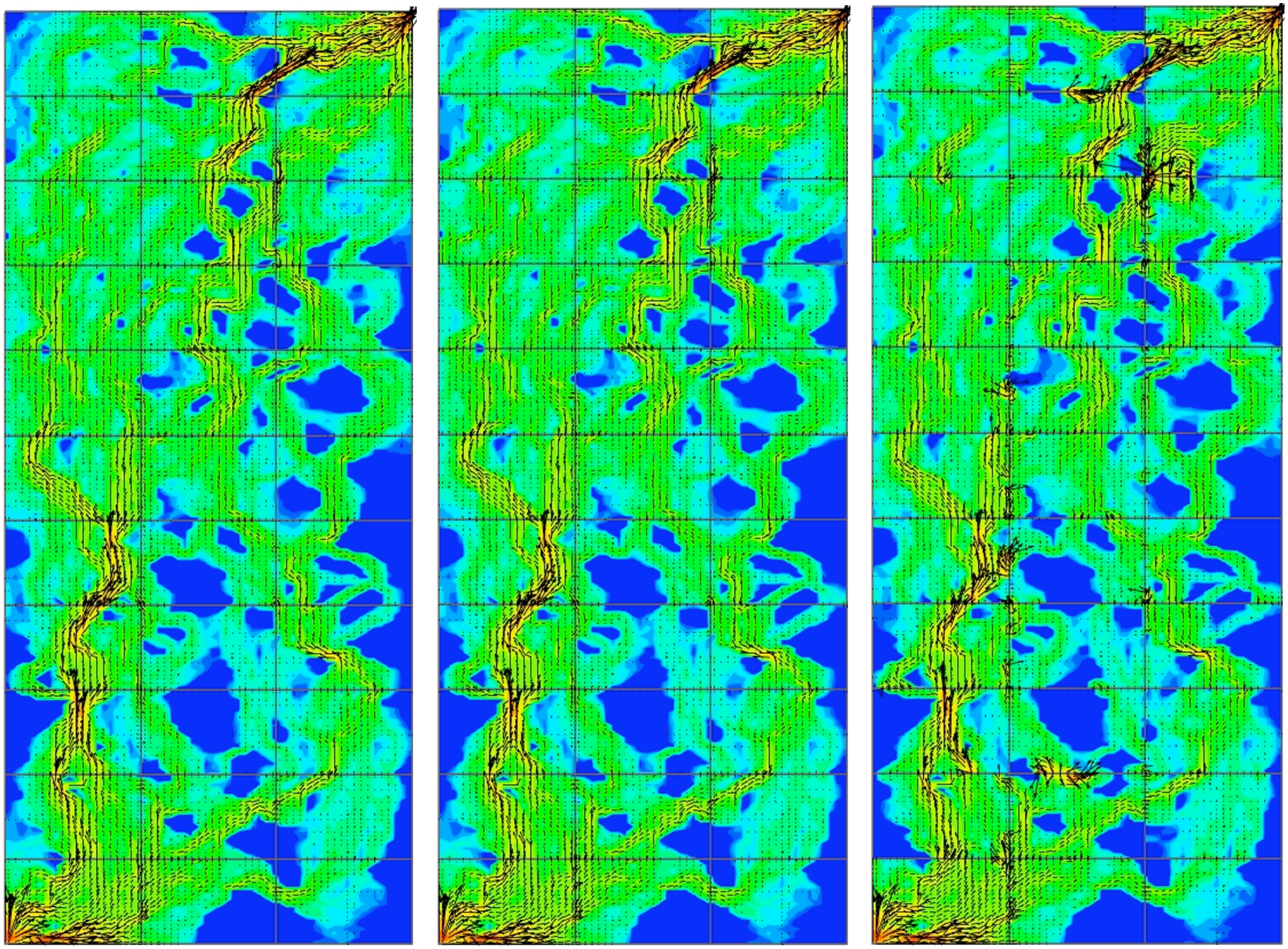
CMG: What scales can be relaxed?

Future:

- Shale barriers and fractures
- Problems with strong nonlinearities
- Extensions to transport
- Preservation of monotonicity
- Reliability (have we *really* relaxed the weaker scales, and to an acceptable degree?)

Example: Multiscale Mortar Methods

(T. Arbogast, Hailong Xiao, and Guangri Xue)



RT0 (60×220) HMS (3×11) Error 40.6% P2 (3×11) Error 10.6%

Speed and Velocity

Flow: Unstructured Meshing

Problem: Accurately model the flow of fluids in highly distorted, anisotropic meshes.

Progress:

- Mixed and finite volume methods
- Multipoint flux methods
- Mimetic methods
- Discontinuous Galerkin (DG) methods

CMG: What kind of meshes need to be used?

Future:

- Shale barriers and fractures
- Problems with strong nonlinearities
- Preservation of monotonicity
- Fewer unknowns (higher order?)

Floe: Linear Solver Technology

Problem: Very large systems of linear equations must be solved. These must be preconditioned for efficient solution.

Progress:

- Multigrid, Krylov methods, domain decomposition methods.
- Multistage preconditioners.
- Preconditioners based on multiscale ideas, such as multiscale finite elements.

CMG: The best preconditioners are physics-based.

Future:

- Solver performance that does not degrade due to heterogeneity.
- Changing computer architectures: parallelism, GPUs, and memory hierarchy
- Better and faster.

Modeling Transport Processes

Problem: Transport is dominated by strong local effects that are controlled by large-scale conservation considerations.

- Mathematical instability results from the creation of shocks.
- Often artificial CFL constraints are imposed on the numerics.
- The maximum principle must be maintained.
- Time-stepping is essentially a serial process, not amenable to parallel processing, especially when CFL limited.

Progress:

- Discontinuous Galerkin (DG) methods often perform well.
- Eulerian-Lagrangian methods, which allow long time steps.

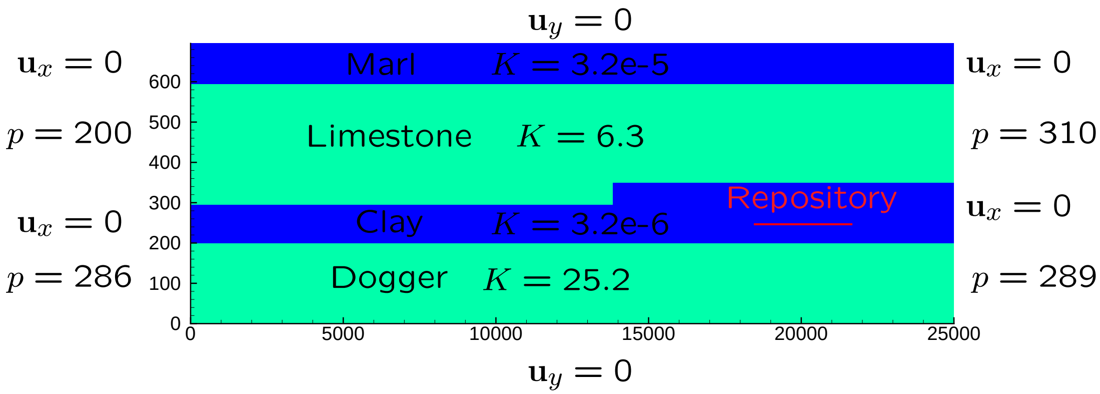
CMG: Solve the correct equations and preserve important features.

Future:

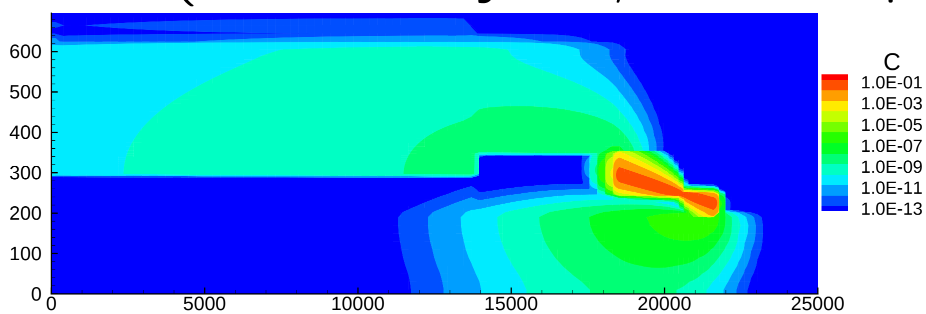
- Preconditioners for DG methods.
- Slope limiting and the maximum principle on general meshes.
- Conservative Eulerian-Lagrangian methods for nonlinear problems.
- Operator splitting between advection and other processes.

(T. Arbogast, Chieh-Sen Wang, Wenhao Wang, and Jianxian Qiu)

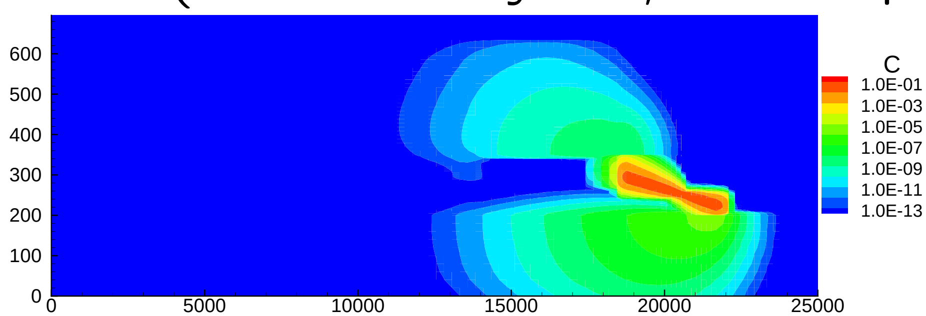
Leaking Iodine-129 at 2.5×10^5 years



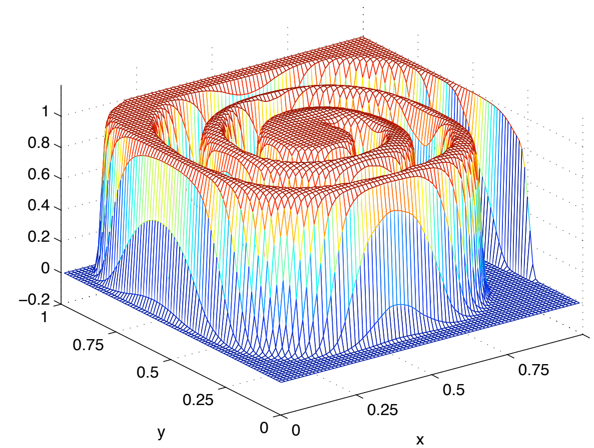
Godunov ($\Delta t = 100$ years, 2500 steps)

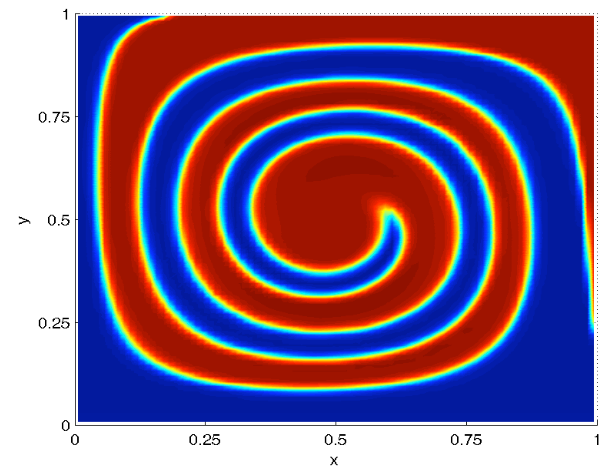


VCCMM ($\Delta t = 2500$ years, 100 steps)



Swirling flow with $\Delta t = 8h$ (CFL=8)





Problem: Reaction dynamics tend to be governed by very stiff systems which are often constrained by inequalities. They are often difficult to formulate in porous materials, because of the need to pose the dynamics in non-well-mixed coarse grid models devoid of a true pore scale.

Progress:

- Finer gridding.
- Better experimental results.

CMG: This problem has tightly coupled mathematical and chemical structure. Careful numerics and experimental validation is critical here.

Future:

- A true upscaling theory of reactive transport.
- Reactions along streamlines, even for multiple phases.

Problem: Model the movement of the earth under various loading.

Progress:

- Locking free elements
- Unstructured gridding and adaptivity

CMG: Proper physics versus numerical constraints.

Future:

- Physics-based preconditioners and better solver strategies.
- Large-scale crack formation and fault reactivation.
- Large-scale earthquake simulation and wave propagation.
- Volcano formation and eruption simulation.
- Mid-ocean ridge formation.
- Core to crust simulation of the entire Earth.

Analysis of Partial Differential Systems

Problem: The equations of subsurface processes are usually posed at a macro (i.e., Darcy) scale. Thus implicit "homogenization" of physical processes is already inherent in the equations. It is possible that this inherent process is flawed. Mathematical analysis can clarify whether the equations reflect the desired physical properties, where they fall short, and what intrinsic mathematical difficulties are present.

Progress: Many simplified equations have been analyzed, including, e.g., compositional Darcy flow. Many upscaling theories have been justified, e.g., homogenized permeabilities.

CMG: Mathematical models of physical systems should have mathematically sound equations.

Future:

- Full compositional flow with full phase behavior.
- Partially molten or melted materials (McKenzie equations, glaciers).
- Homogenization of nonlinear systems.
- Homogenization of nonstationary heterogeneous systems.
- Modeling systems with non-continuum behavior (ice sheets).

Uncertainty Quantification

Problem: Interaction with geosystems poses risks to human health and safety, and also to the environment. It can also be quite costly in economic terms. How do we know we understand these systems?

Progress:

- Karhunen-Loeve expansions of stochastic processes.
- Ensemble Kalman-Filtering
- A-posteriori numerical error estimation and mesh adaptivity

CMG: This is inherently interdisciplinary:

- Verification is largely a mathematical question of approximating the mathematical model correctly. In principle, this can be done deductively.
- Validation is largely a geoscience question that the mathematical model faithfully represents all pertinent aspects of the physical system. This is checked inductively by experimental comparisons.

Future:

- Methods not based on assumptions of Gaussian statistics.
- Adaptive model selection based on scale.

Modeling quasi-continua

Problem: Many problems exhibit behaviors associated to a moderate number of discrete entities that are neither small enough to model directly nor large enough to approximate as a homogenized macro-system. Perhaps in principle we understand how to model the system discretely, but we do not have the computational resources to solve the problem.

Progress: Progress is slow and very problem dependent.

- Discrete fractures and faults
- Ice sheets
- Volcanoes
- Partially molten or melted materials (magma and glaciers)

CMG: Collaboration is critical to overcome computational limitations.

Future:

- Validated models
- General theories

Interdisciplinary Education

Problem: A disciplinary view of mathematical modeling misses the surprisingly complex interactions between the

- Mathematical structure of the equations
- Behavior of numerical approximation algorithms
- Constraints imposed by high performance, scientific computers
- Physical complexity of the physical system

We need scientists well trained for interdisciplinary work.

Progress: Many interdisciplinary programs have been initiated, and students are being trained to recognize the broader issues. Moreover, as scientists and mathematicians work together, they have become more interdisciplinary themselves.

CMG: The CMG program helped make this happen, and it can continue to do so.

Future: Depends on NSF!