High-Performance Computing in Basin Modeling: Simulating mechanical compaction through vertical effective stress using level sets

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Introduction

Basin Modeling is the application of numerical techniques to the study of the evolution of sedimentary basins. The temperature and fluid pressure in basins influences the behavior of geo-materials, e.g., how sediments lithify, how fluids flow, how stratigraphic layers deform.

The large deformation of the rock layers presents a challenge numerically, in that the geometry can become quite complex. This is often addressed by modifying the computational mesh to align with the geometry. This work explores the use of a method to *implicitly* represent interfaces on a fixed computational grid.

Objectives

In order to simulate large deformation in the stratigraphic layering of sedimentary basins, we apply an implicit interface tracking method, the level set method, to the modeling of geological processes acting over long time scales (Ma).

- The motivation for using the level set method is to implicitly capture interface dynamics without modifying the underlying computational grid.
- At layer boundaries between different lithologies, the interface is embedded in a potential function as a constant level set.
- We construct a speed function, based on sedimentation and compaction to prescribe motion normal to the layer interfaces.
- The compaction is a function of the pore fluid pressure in the basin, treated as a porous medium.

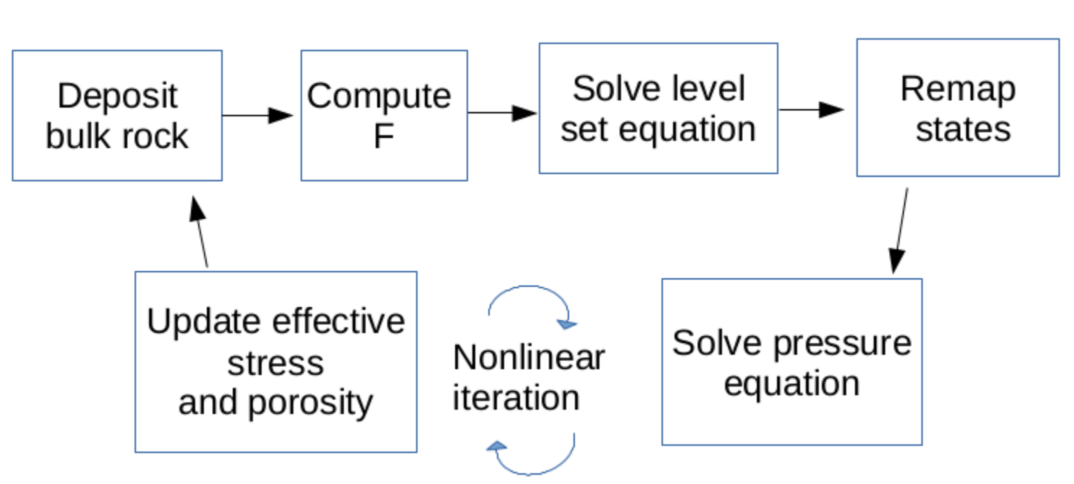

Figure 1: One time step in the simulation procedure. F is the speed function that moves the interfaces. The sequential solution steps split the operator of the mechanical deposition from the fluid flow problem. This nonlinearity is iterated over.

Porous Medium Model

The following physical assumptions form the core of the model: Conservation of rock mass, Darcy's law and vertical effective stress (VES). Furthermore, Athy's law is used as the relation between the porosity and the VES, determining the compaction. Additionally a speed function, F, is defined by the sedimentation rate, ω, and the compaction in a vertical column.

- VES: $\sigma_z' = \sigma_z - p$
- Athy: $\phi = \phi_0 \exp(-\beta\sigma_z')$
- Darcy flux: $q = -\left(\frac{k}{\mu}\nabla(p - \rho_f g z)\right)$
- Speed function: $F = \omega + \int_{z'}^{0} \frac{1}{1-\phi}\frac{\partial \phi}{\partial t}$

where σ_z is the overburden, p the pore fluid pressure, ϕ the porosity, ϕ_0 and β are material dependent coefficients. k is the permeability of the rock, μ is the viscosity of the pore fluid and $\rho_f g z$ gives the hydrostatic pressure at a point of depth z.

Figure 2: These sedimentary layers were created over 72 million years ago (Late Cretaceous), before the Laramide orogeny, when modern-day Colorado was submerged under the Western Interior Seaway. Today, they are exposed in a hogback, outside Fort Collins, CO, USA.

System of Equations and Solution Method

Using the generic finite element (FEM) package deal.II [Bangerth et al., 2007], the PDEs are solved sequentially. The system that is discretized in space using FEM and finite differences in time is, in domain Ω:

$$\frac{\partial u_i}{\partial t} + \vec{w} \cdot \nabla u_i = 0$$

$$-\nabla \cdot \left(\frac{k}{\mu}\nabla(p - \rho_f g z)\right) = \frac{C(\sigma_z')}{1-\phi}\frac{\partial(\sigma_z - p)}{\partial t}$$

$$\rho c \frac{\partial T}{\partial t} - \nabla \cdot \lambda \nabla T = 0$$

$$\hat{e}_z \cdot \nabla \sigma_z = \rho_b g$$

$$\hat{e}_z \cdot \nabla F = \frac{1}{1-\phi}\frac{\partial \phi}{\partial t}$$

u_i are the level set potential functions, one for each layer i, C is the rock compressibility, T temperature, c heat capacity, λ thermal conductivity, and $\vec{w}$ is the velocity field related to the speed function through the normal $\hat{n}$ by $F = \hat{n} \cdot \vec{w}$.

Level Set Methods

The design of the level set method is to *implicitly* represent an evolving interface, by embedding the interface in a higher dimensional function as a constant level set, often taken to be the 0 level set. $\frac{\partial u}{\partial t} + \vec{w} \cdot \nabla u = 0$. The time-dependent advection equation is solved with a level set solver due to de Luna [Guermond et al., 2017], leveraging an entropy viscosity stabilization along with a compression term to reduce numerical diffusion. Below is an example of an interface represented through the level set potential function. The undulation comes from the spatially varying velocity field.

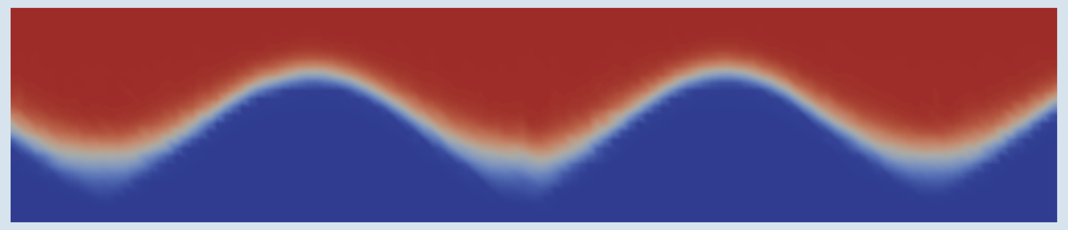

Figure 3: The level set potential function, between -1 and 1, defining an interface at 0; blue is negative and red is positive. The width of the transition zone can vary, while only the 0 level set determines the location of the interface.

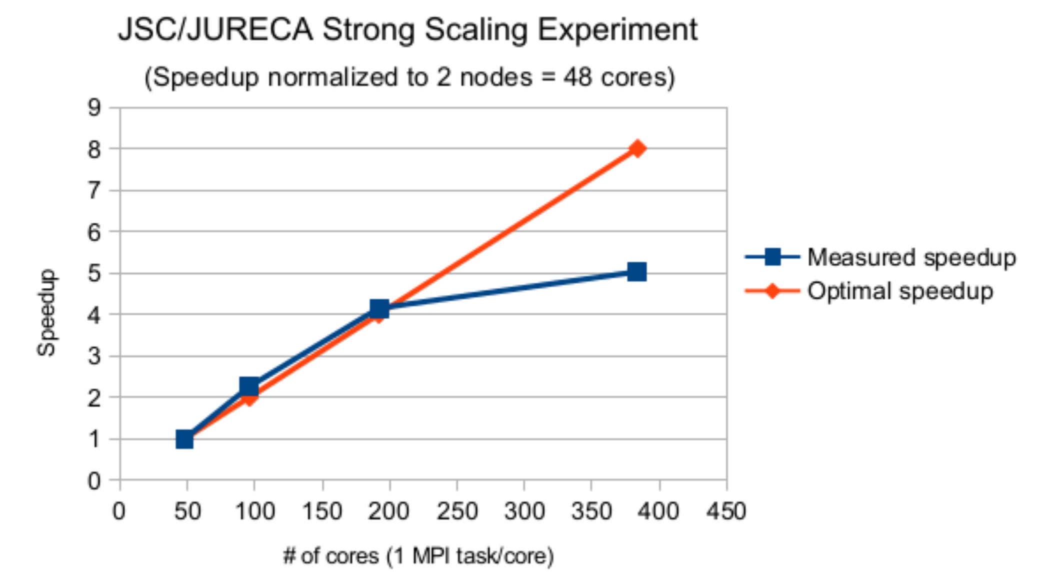

Figure 4: Strong scaling plot with around 1 million degrees of freedom in a 2-D model run. Average of three run times were used for the timing and normalized to 48 cores. Communication overhead becomes dominant in the largest core data point.

Results

We show figures of a basin simulation and some strong scaling information of the application as it runs on Forschungszentrum Jülich's Jureca supercomputer.

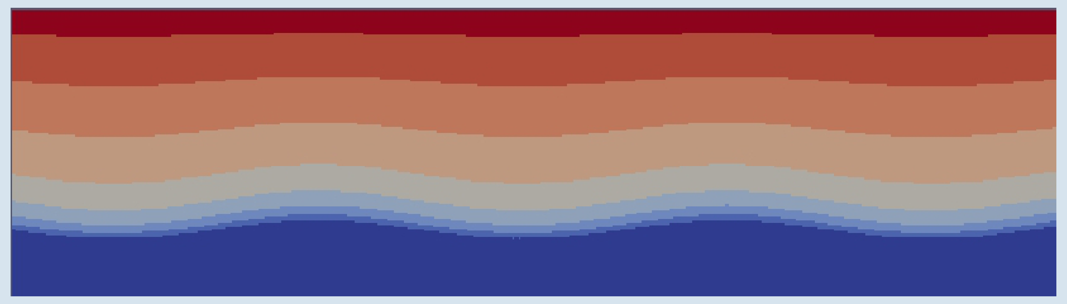

Figure 5: A sediment stack composed of 8 layers (identified by color), equally deposited in time over 1 Ma, under spatially variable deposition. The domain is 1km across and 400 m deep. The lower layers have compacted significantly on top of the basement layer in dark blue.

Results

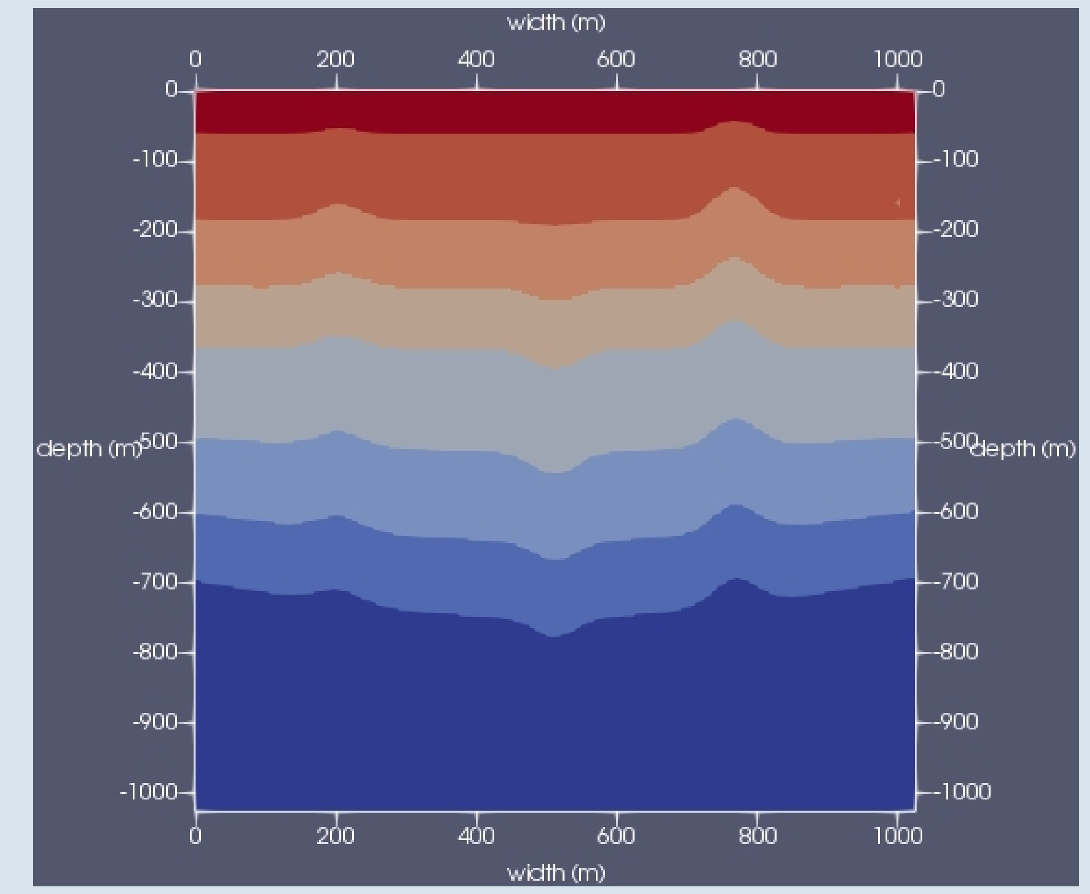

Figure 6: A sediment stack composed of 8 layers (identified by color), equally deposited in time over 1 Ma, under spatially and temporally variable deposition. In the center, the sedimentation rate was higher earlier with more compaction, and on the flanks, the sedimentation rate is low. These localized variations show themselves in the mounds and the central trough.

Conclusions

- Coupled the movement of stratigraphic layer interfaces, represented through a level set interface tracking method, to the physical processes of sedimentation and compaction.
- The speed function, the nexus of the coupling between the geometry and the physics, can be flexibly elaborated with other physical processes.
- The implicit representation of interfaces on a fixed grid avoids expensive re-gridding and lends itself to parallelization.

References

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